# Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 08:45 AM JST

| | | |
|---|---|---|
| PDB ID | : | 4YD9 / pdb_00004yd9 |
| Title | : | Crystal structure of squid hemocyanin |
| Authors | : | Matsuno, A.; Gai, Z.; Kato, K.; Tanaka, Y.; Yao, M. |
| Deposited on | : | 2015-02-21 |
| Resolution | : | 3.00 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

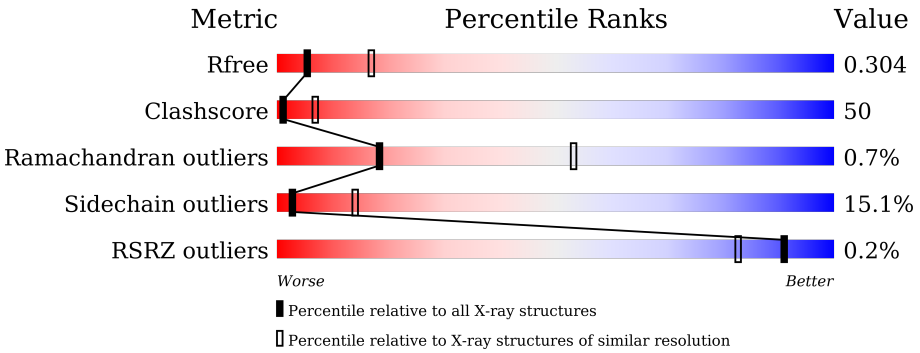
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4 | : | 9.0.015 (Gargrove) |
| Density-Fitness | : | 1.0.12 |
| 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:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



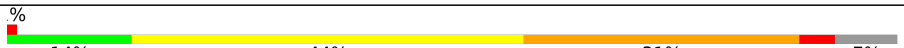
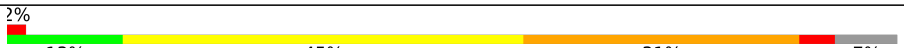
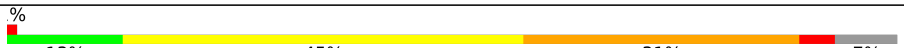
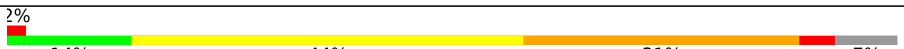
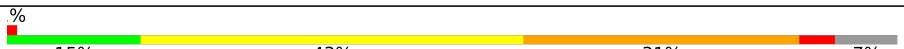
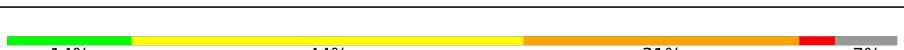
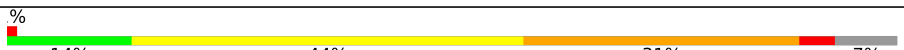
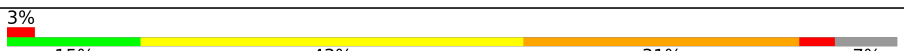
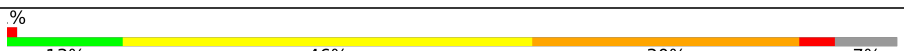
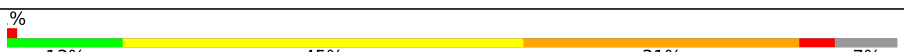

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 180053 | 2672 (3.00-3.00) |
| Clashscore | 190562 | 2977 (3.00-3.00) |
| Ramachandran outliers | 187476 | 2877 (3.00-3.00) |
| Sidechain outliers | 187428 | 2880 (3.00-3.00) |
| RSRZ outliers | 180081 | 2671 (3.00-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 2000 | 49% 28% 5% 17% |
| 1 | D | 2000 | 48% 30% 5% 17% |
| 1 | G | 2000 | 47% 30% 6% 17% |
| 1 | J | 2000 | 47% 31% 5% 17% |
| 1 | M | 2000 | 50% 27% 5% 17% |
| 1 | P | 2000 | 49% 28% 6% 17% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | S | 2000 |   |
| 1 | V | 2000 |   |
| 1 | Y | 2000 |   |
| 1 | b | 2000 |   |
| 2 | B | 920 |   |
| 2 | E | 920 |   |
| 2 | H | 920 |   |
| 2 | K | 920 |   |
| 2 | N | 920 |   |
| 2 | Q | 920 |   |
| 2 | T | 920 |   |
| 2 | W | 920 |   |
| 2 | Z | 920 |   |
| 2 | c | 920 |   |
| 3 | C | 394 |   |
| 3 | F | 394 |   |
| 3 | I | 394 |   |
| 3 | L | 394 |   |
| 3 | O | 394 |   |
| 3 | R | 394 |   |
| 3 | U | 394 |   |
| 3 | X | 394 |   |
| 3 | a | 394 |   |
| 3 | d | 394 |   |
| 4 | 1 | 2 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | 2 | 2 | 50% 50% |
| 4 | 4 | 2 | 100% |
| 4 | 6 | 2 | 50% 50% |
| 4 | 7 | 2 | 100% |
| 4 | 8 | 2 | 100% |
| 4 | 9 | 2 | 100% |
| 4 | BA | 2 | 100% |
| 4 | HA | 2 | 50% 50% |
| 4 | IA | 2 | 100% |
| 4 | JA | 2 | 50% 50% |
| 4 | MA | 2 | 100% |
| 4 | OA | 2 | 100% |
| 4 | QA | 2 | 50% 50% |
| 4 | RA | 2 | 50% 50% |
| 4 | e | 2 | 50% 50% |
| 4 | f | 2 | 50% 50% |
| 4 | i | 2 | 50% 50% |
| 4 | j | 2 | 100% |
| 4 | m | 2 | 100% |
| 4 | n | 2 | 100% |
| 4 | o | 2 | 50% 50% |
| 4 | p | 2 | 50% 50% |
| 4 | q | 2 | 100% |
| 4 | s | 2 | 50% 50% |
| 4 | t | 2 | 50% 50% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | u | 2 | 50% 50% |
| 4 | v | 2 | 100% |
| 4 | x | 2 | 50% 50% |
| 5 | AA | 4 | 25% 50% 25% |
| 5 | FA | 4 | 100% |
| 5 | KA | 4 | 75% 25% |
| 5 | PA | 4 | 50% 50% |
| 5 | g | 4 | 50% 50% |
| 5 | l | 4 | 50% 50% |
| 6 | 3 | 3 | 33% 33% 33% |
| 6 | 5 | 3 | 100% |
| 6 | CA | 3 | 33% 67% |
| 6 | DA | 3 | 33% 67% |
| 6 | EA | 3 | 33% 33% 33% |
| 6 | GA | 3 | 100% |
| 6 | LA | 3 | 100% |
| 6 | NA | 3 | 67% 33% |
| 6 | h | 3 | 67% 33% |
| 6 | k | 3 | 33% 67% |
| 6 | r | 3 | 33% 33% 33% |
| 6 | w | 3 | 67% 33% |
| 6 | y | 3 | 100% |
| 7 | z | 5 | 20% 40% 40% |
| 8 | 0 | 4 | 25% 75% |

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

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 4 | NAG | MA | 1 | - | - | X | - |
| 4 | NAG | m | 1 | - | - | X | - |
| 4 | NAG | q | 2 | - | - | X | - |
| 6 | NAG | GA | 1 | - | - | X | - |
| 6 | NAG | GA | 2 | - | - | X | - |
| 6 | NAG | r | 1 | - | - | X | - |
| 8 | NAG | 0 | 2 | - | - | X | - |
| 9 | CUO | A | 5001 | - | - | X | - |
| 9 | CUO | C | 3401[A] | - | - | X | - |
| 9 | CUO | C | 3401[B] | - | - | X | - |
| 9 | CUO | F | 3401[A] | - | - | X | - |
| 9 | CUO | F | 3401[B] | - | - | X | - |
| 9 | CUO | I | 3401[A] | - | - | X | - |
| 9 | CUO | L | 3401[A] | - | - | X | - |
| 9 | CUO | L | 3401[B] | - | - | X | - |
| 9 | CUO | M | 2105 | - | - | X | - |
| 9 | CUO | O | 3401[A] | - | - | X | - |
| 9 | CUO | O | 3401[B] | - | - | X | - |
| 9 | CUO | R | 3401[A] | - | - | X | - |
| 9 | CUO | S | 2104 | - | - | X | - |
| 9 | CUO | U | 3401[A] | - | - | X | - |
| 9 | CUO | U | 3401[B] | - | - | X | - |
| 9 | CUO | X | 3401[A] | - | - | X | - |
| 9 | CUO | X | 3401[B] | - | - | X | - |
| 9 | CUO | a | 3401[A] | - | - | X | - |
| 9 | CUO | a | 3401[B] | - | - | X | - |
| 9 | CUO | d | 3401[A] | - | - | X | - |
| 9 | CUO | d | 3401[B] | - | - | X | - |

## 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 261470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called hemocyanin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | D | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | G | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | J | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | M | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | P | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | S | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | V | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | Y | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | b | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |

- Molecule 2 is a protein called hemocyanin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | E | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | H | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | K | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | N | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | Q | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | T | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | W | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | Z | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | c | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |

- Molecule 3 is a protein called hemocyanin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | F | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | I | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | L | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | O | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | R | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | U | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | X | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | a | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | d | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |

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



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | e | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | f | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | i | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | j | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | m | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | n | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | o | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | p | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | q | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | s | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | t | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | u | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | v | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | x | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 1 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 2 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 4 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 6 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 7 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 8 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 9 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | BA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |

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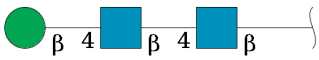
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|
| 4 | HA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 | 0 |
| 4 | IA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 | 0 |
| 4 | JA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 | 0 |
| 4 | MA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 | 0 |
| 4 | OA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 | 0 |
| 4 | QA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 | 0 |
| 4 | RA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 | 0 |

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



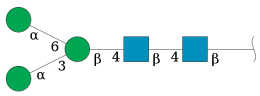

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|
| 5 | g | 4 | Total C N O<br>50 28 2 20 | 0 | 0 | 0 |
| 5 | l | 4 | Total C N O<br>50 28 2 20 | 0 | 0 | 0 |
| 5 | AA | 4 | Total C N O<br>50 28 2 20 | 0 | 0 | 0 |
| 5 | FA | 4 | Total C N O<br>50 28 2 20 | 0 | 0 | 0 |
| 5 | KA | 4 | Total C N O<br>50 28 2 20 | 0 | 0 | 0 |
| 5 | PA | 4 | Total C N O<br>50 28 2 20 | 0 | 0 | 0 |

- Molecule 6 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 | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | h | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | k | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | r | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | w | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | y | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | 3 | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | 5 | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | CA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | DA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | EA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | GA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | LA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | NA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



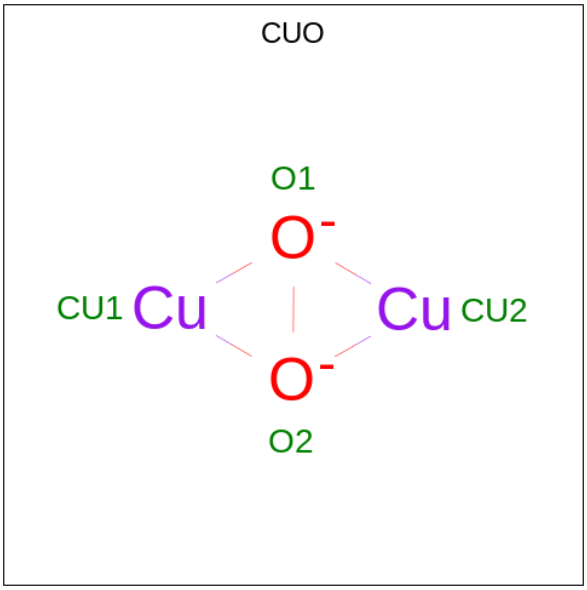

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | z | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 61 | 34 | 2 | 25 | | | |

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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 | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | 0 | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |

- Molecule 9 is CU2-O2 CLUSTER (CCD ID: CUO) (formula: $Cu_2O_2$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 9 | A | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | A | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | A | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | A | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | A | 1 | Total | Cu | O | 0 | 1 |
| | | | 8 | 4 | 4 | | |
| 9 | B | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | B | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 9 | C | 1 | Total Cu O<br>8 4 4 | 0 | 1 |
| 9 | D | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | D | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | D | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | D | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | D | 1 | Total Cu O<br>8 4 4 | 0 | 1 |
| 9 | E | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | E | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | F | 1 | Total Cu O<br>8 4 4 | 0 | 1 |
| 9 | G | 1 | Total Cu O<br>8 4 4 | 0 | 1 |
| 9 | G | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | G | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | G | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | G | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | H | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | H | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | I | 1 | Total Cu O<br>8 4 4 | 0 | 1 |
| 9 | J | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | J | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | J | 1 | Total Cu O<br>4 2 2 | 0 | 0 |
| 9 | J | 1 | Total Cu O<br>4 2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 9 | J | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | K | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | K | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | L | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | M | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | M | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | M | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | M | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | M | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | N | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | N | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | O | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | P | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | P | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | P | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | P | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | P | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | Q | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Q | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | R | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | S | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 9 | S | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | S | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | S | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | S | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | T | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | T | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | U | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | V | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | V | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | V | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | V | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | V | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | W | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | W | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | X | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | Y | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | Y | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Y | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Y | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Y | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Z | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 9 | Z | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | a | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | b | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | b | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | b | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | b | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | b | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | c | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | c | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | d | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |

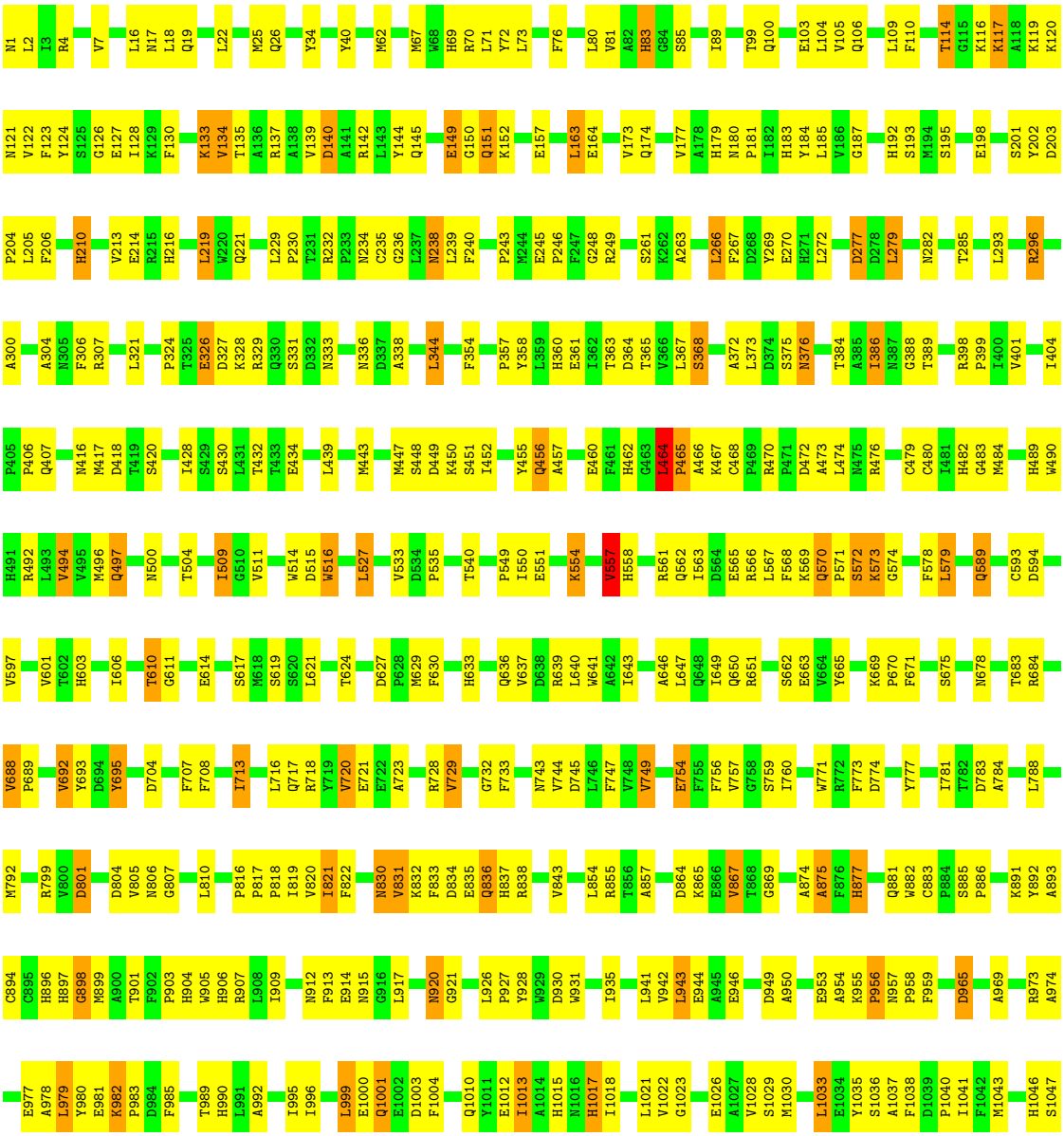
# 3 Residue-property plots (i)

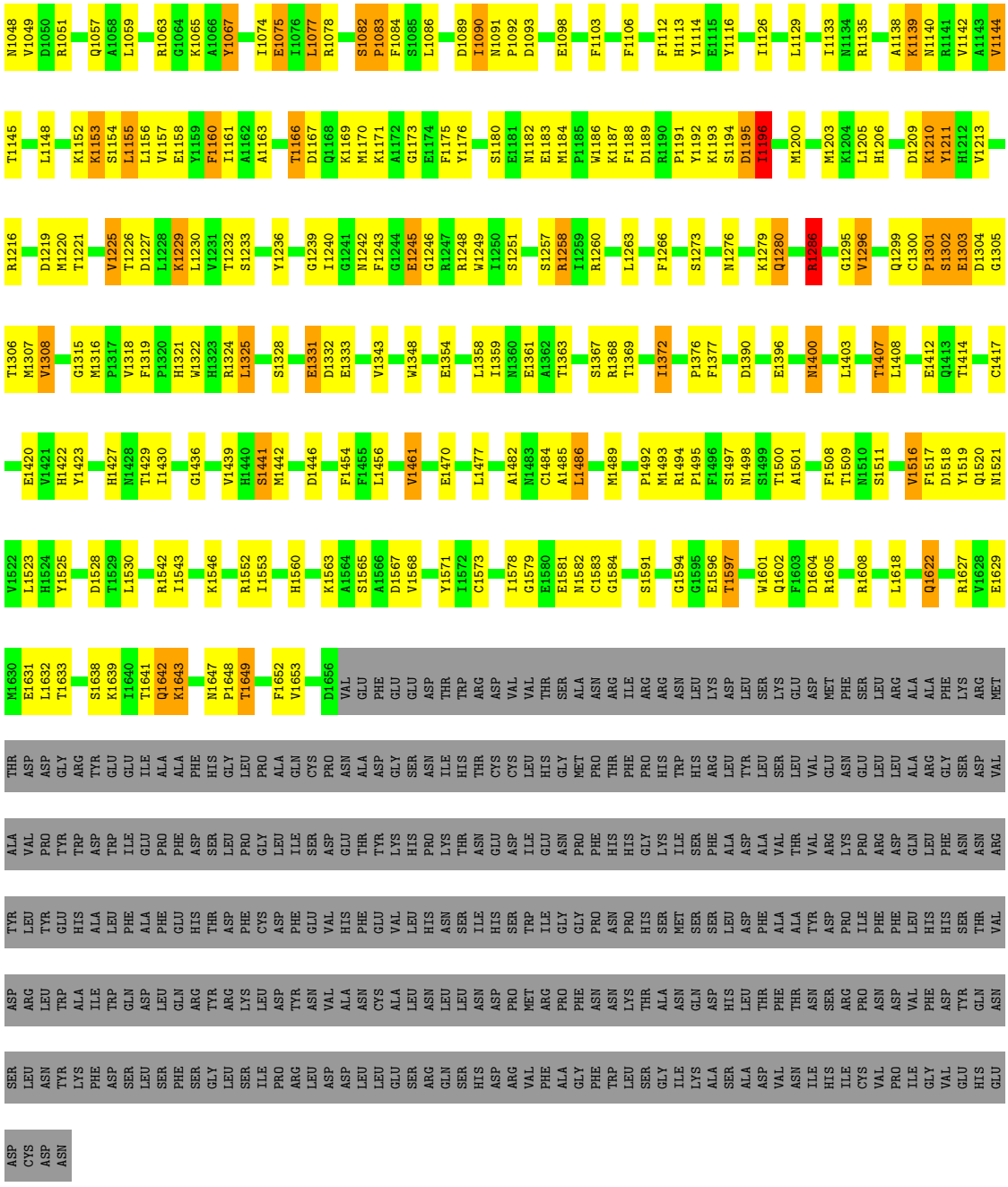
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: hemocyanin

Chain A:



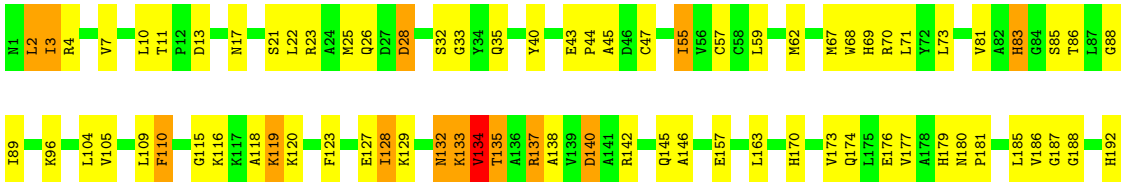



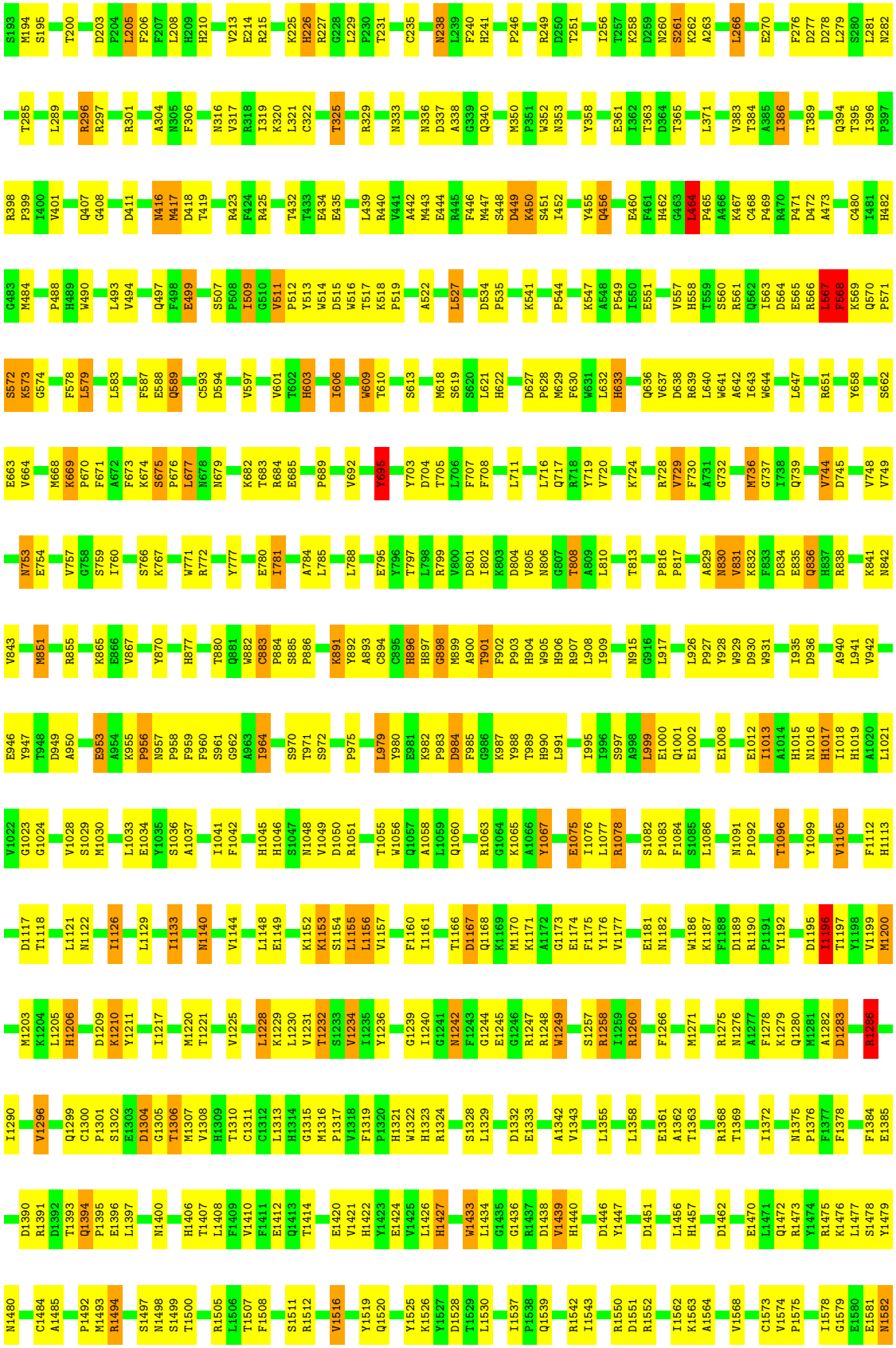


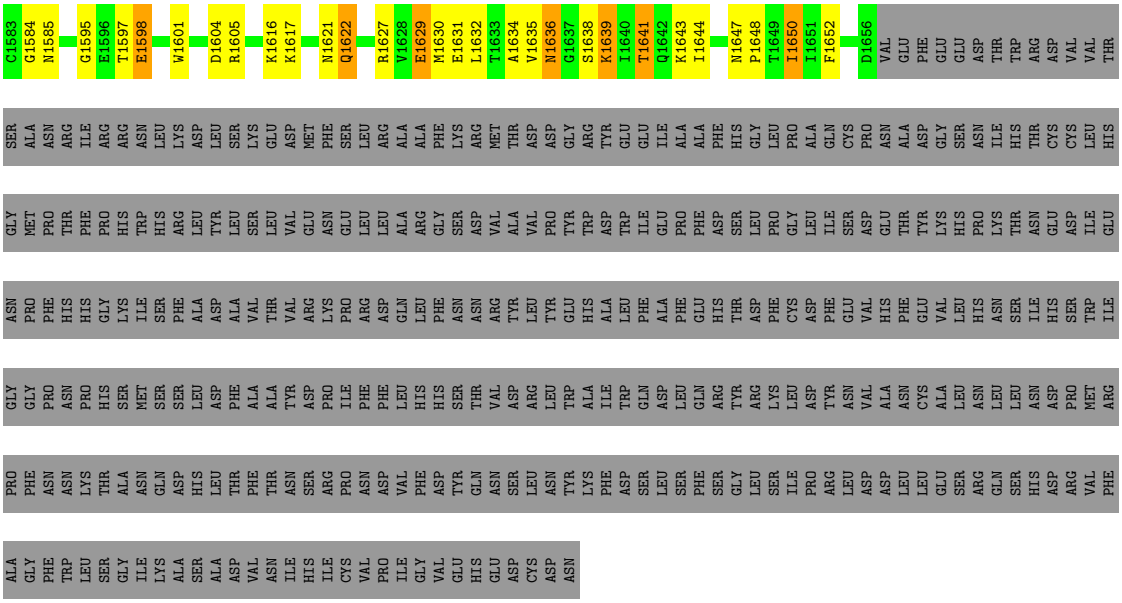
• Molecule 1: hemocyanin

Chain D:



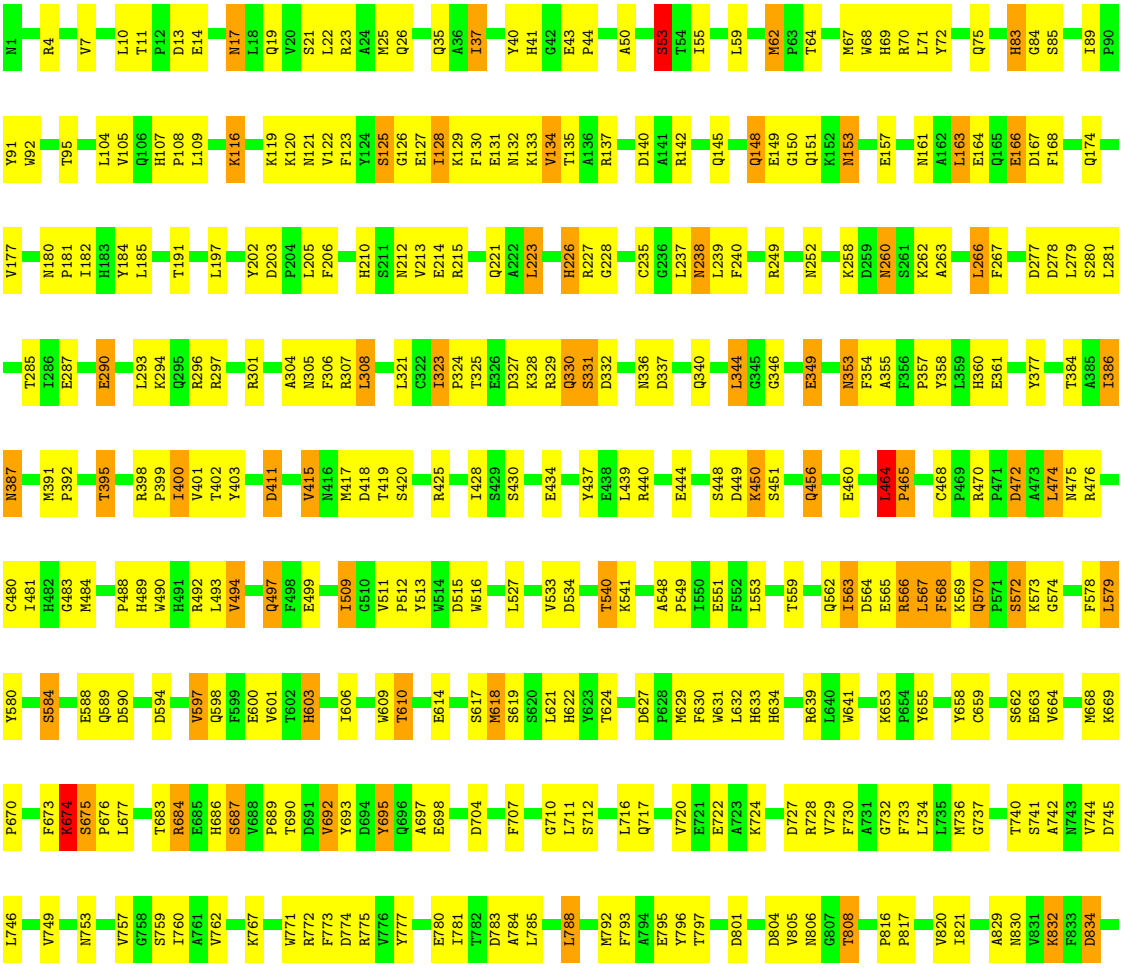

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T285 L289 R296 R297 R301 A304 N305 F306 N316 V317 R318 I319 K320 L321 C322 T325 R329 N333 N336 D337 A338 G339 Q340 M350 P351 W352 N353 Y358 E361 I362 T363 D364 T365 L371 V383 T384 A385 I386 T389 Q394 T395 I396 P397
R398 P399 I400 V401 Q407 G408 D411 N416 M417 D418 T419 R423 F424 R425 T432 T433 E434 E435 L439 R440 V441 A442 M443 E444 R445 F446 M447 S448 D449 K450 S451 I452 Y455 Q456 E460 F461 H462 G463 L464 P465 A466 K467 C468 P469 R470 P471 D472 A473 C480 I481 H482
G483 M484 P488 H489 W490 L493 V494 Q497 F498 E499 S507 P508 I509 G510 V511 P512 Y513 W514 D515 W516 T517 K518 P519 A522 L527 D534 P535 K541 P544 K547 A548 P549 I550 E551 V557 H558 T559 S560 R561 Q562 I563 D564 E565 R566 L567 F568 K569 Q570 P571
S572 K573 G574 F578 L579 L583 F587 E588 Q589 C593 D594 V597 V601 T602 H603 I606 W609 T610 S613 M618 S619 S620 L621 H622 D627 P628 M629 F630 W631 L632 H633 Q636 V637 D638 R639 L640 W641 A642 I643 W644 L647 R651 Y658 S662
E663 V664 M668 K669 P670 F671 A672 F673 K674 S675 P676 L677 N678 N679 K682 T683 R684 E685 P689 V692 V695 Y703 D704 T705 L706 F707 F708 L711 L716 Q717 R718 Y719 V720 K724 R728 V729 F730 A731 G732 M736 G737 I738 Q739 V744 D745 V748 V749
N753 E754 V757 G758 S759 I760 S766 K767 W771 R772 Y777 E780 I781 A784 L785 L788 E795 Y796 T797 L798 R799 V800 D801 I802 K803 D804 V805 N806 G807 T808 A809 L810 T813 P816 P817 A829 N830 V831 K832 F833 D834 E835 Q836 H837 R838 K841 N842
V843 M851 R855 K865 E866 V867 Y870 H877 T880 Q881 W882 C883 P884 S885 P886 K891 Y892 A893 C894 C895 H896 H897 G898 M899 A900 T901 P902 P903 H904 W905 H906 R907 L908 I909 N915 G916 L917 L926 P927 Y928 W929 D930 W931 I935 D936 A940 L941 V942
E946 Y947 T948 D949 A950 E953 A954 K955 P956 N957 P958 F959 F960 S961 G962 A963 I964 S970 T971 S972 P975 L979 Y980 E981 K982 P983 D984 F985 G986 K987 Y988 T989 H990 L991 I995 I996 S997 A998 L999 E1000 Q1001 E1002 E1008 E1012 I1013 A1014 H1015 N1016 H1017 I1018 H1019 A1020 L1021
V1022 G1023 G1024 V1028 S1029 M1030 L1033 E1034 Y1035 S1036 A1037 I1041 F1042 H1045 H1046 S1047 N1048 V1049 D1050 R1051 T1055 W1056 Q1057 A1058 L1059 Q1060 R1063 G1064 K1065 A1066 Y1067 E1075 I1076 L1077 R1078 S1082 P1083 F1084 S1085 L1086 N1091 P1092 T1096 Y1099 V1105 F1112 H1113
D1117 T1118 L1121 N1122 I1126 L1129 I1133 N1140 V1144 L1148 E1149 K1152 K1153 S1154 L1155 L1156 V1157 F1160 I1161 T1166 D1167 Q1168 K1169 M1170 K1171 A1172 G1173 E1174 F1175 Y1176 V1177 E1181 N1182 W1186 K1187 F1188 D1189 R1190 P1191 Y1192 D1195 T1196 T1197 Y1198 V1199 M1200
M1203 K1204 L1205 H1206 D1209 K1210 Y1211 I1217 M1220 T1221 V1225 L1228 K1229 L1230 V1231 T1232 S1233 V1234 I1235 Y1236 G1239 I1240 G1241 N1242 F1243 G1244 E1245 G1246 R1247 R1248 W1249 S1257 R1258 I1259 R1260 F1266 M1271 R1275 N1276 A1277 F1278 K1279 Q1280 M1281 A1282 D1283 R1286
I1290 V1296 Q1299 C1300 P1301 S1302 E1303 D1304 G1305 T1306 M1307 V1308 H1309 T1310 C1311 C1312 L1313 H1314 G1315 M1316 P1317 Y1318 F1319 P1320 H1321 W1322 H1323 R1324 S1328 L1329 D1332 E1333 A1342 V1343 L1355 L1358 E1361 A1362 T1363 R1368 T1369 I1372 N1375 P1376 F1377 F1378 F1384 E1385
D1390 R1391 D1392 T1393 Q1394 P1395 E1396 L1397 N1400 H1406 T1407 L1408 F1409 V1410 F1411 E1412 Q1413 T1414 E1420 V1421 H1422 Y1423 E1424 V1425 L1426 H1427 W1433 L1434 G1435 G1436 R1437 D1438 V1439 H1440 D1446 Y1447 D1451 L1456 H1457 D1462 E1470 L1471 Q1472 R1473 Y1474 R1475 K1476 L1477 S1478 Y1479
N1480 C1484 A1485 P1492 M1493 R1494 S1497 N1498 S1499 T1500 R1505 L1506 T1507 F1508 S1511 R1512 V1516 Y1519 Q1520 Y1525 K1526 Y1527 D1528 T1529 L1530 I1537 P1538 Q1539 R1542 I1543 R1550 D1551 R1552 I1562 K1563 A1564 V1568 C1573 V1574 P1575 I1578 G1579 E1580 E1581 N1582

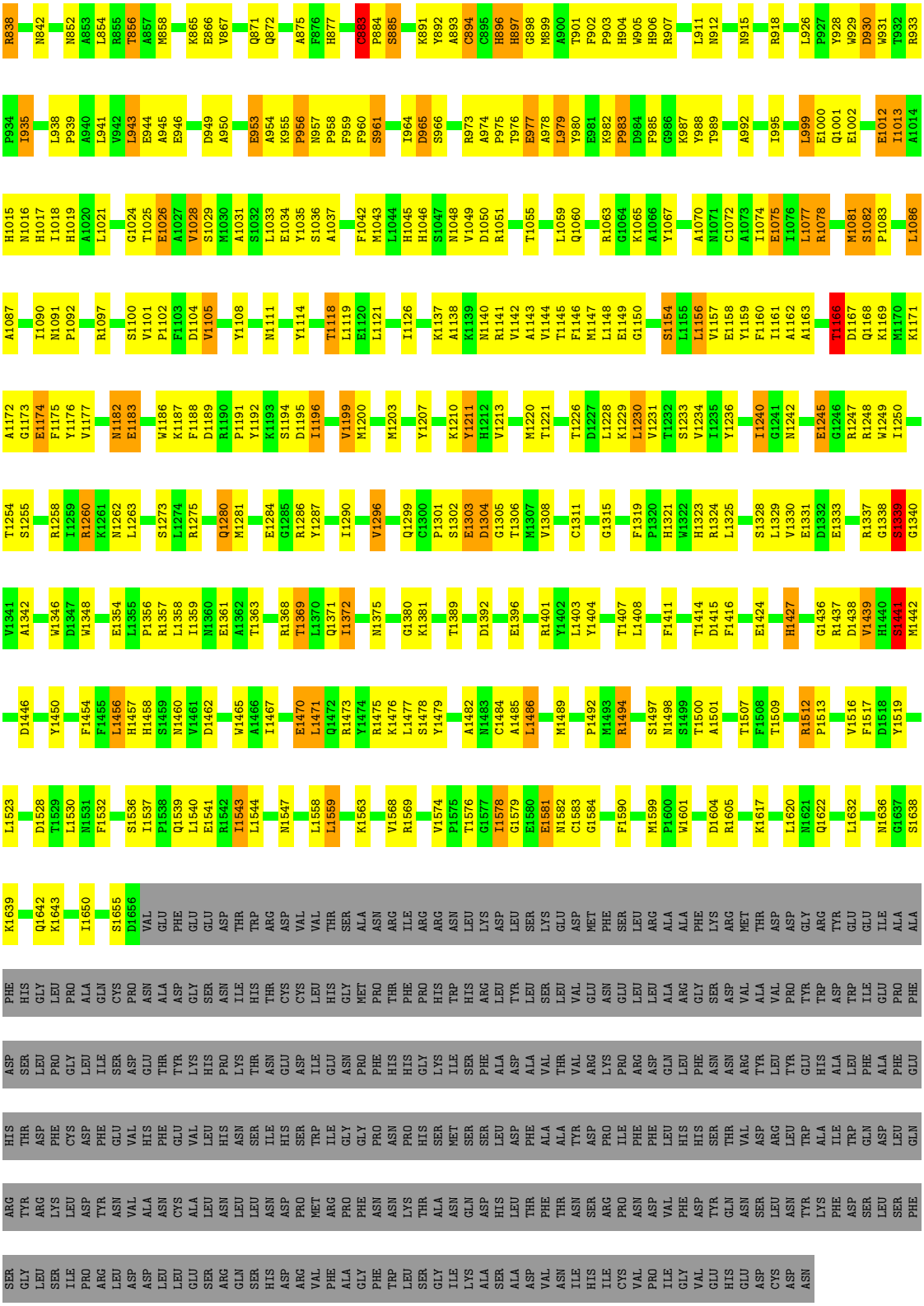



- Molecule 1: hemocyanin

Chain G:

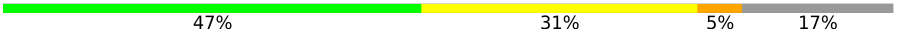


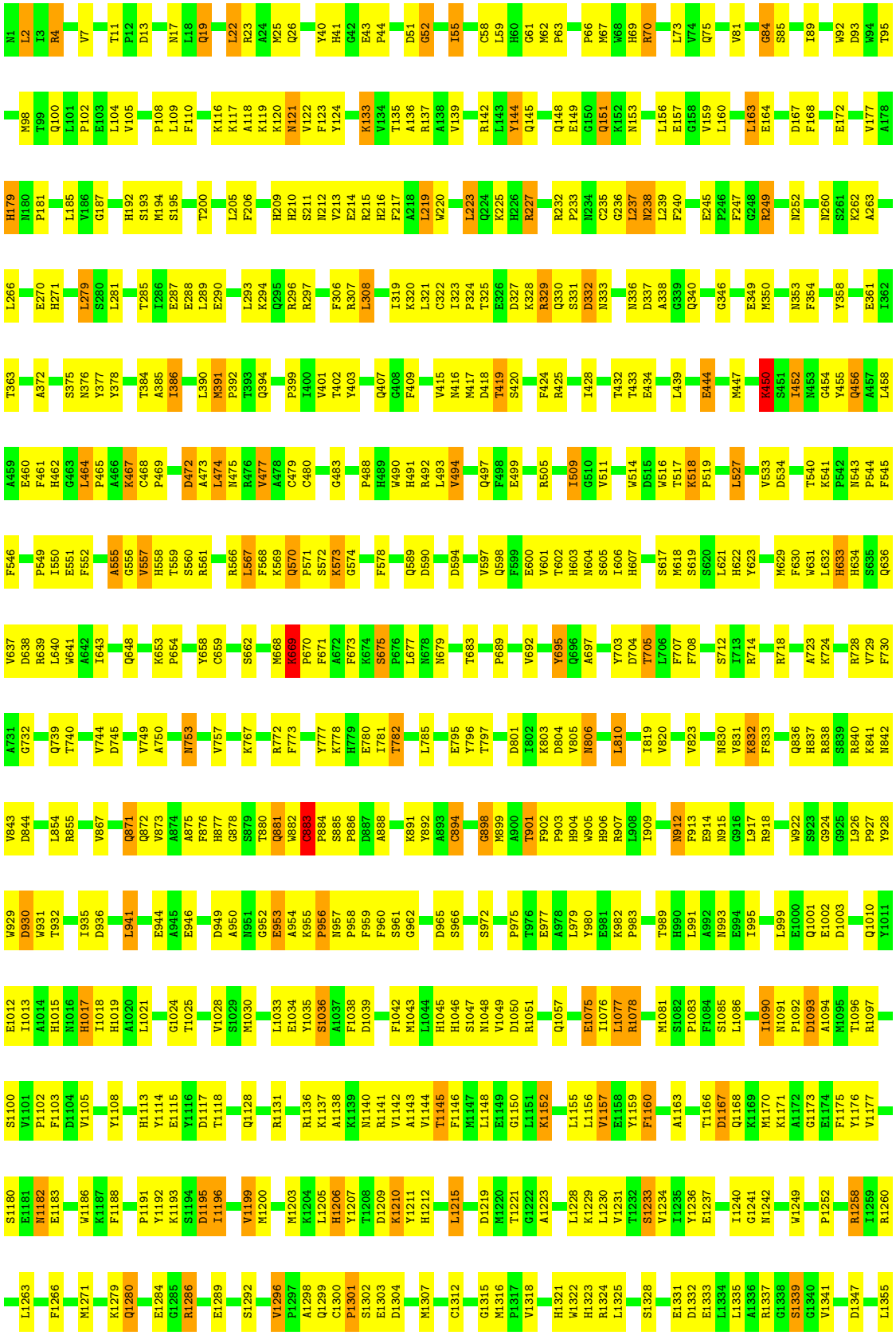



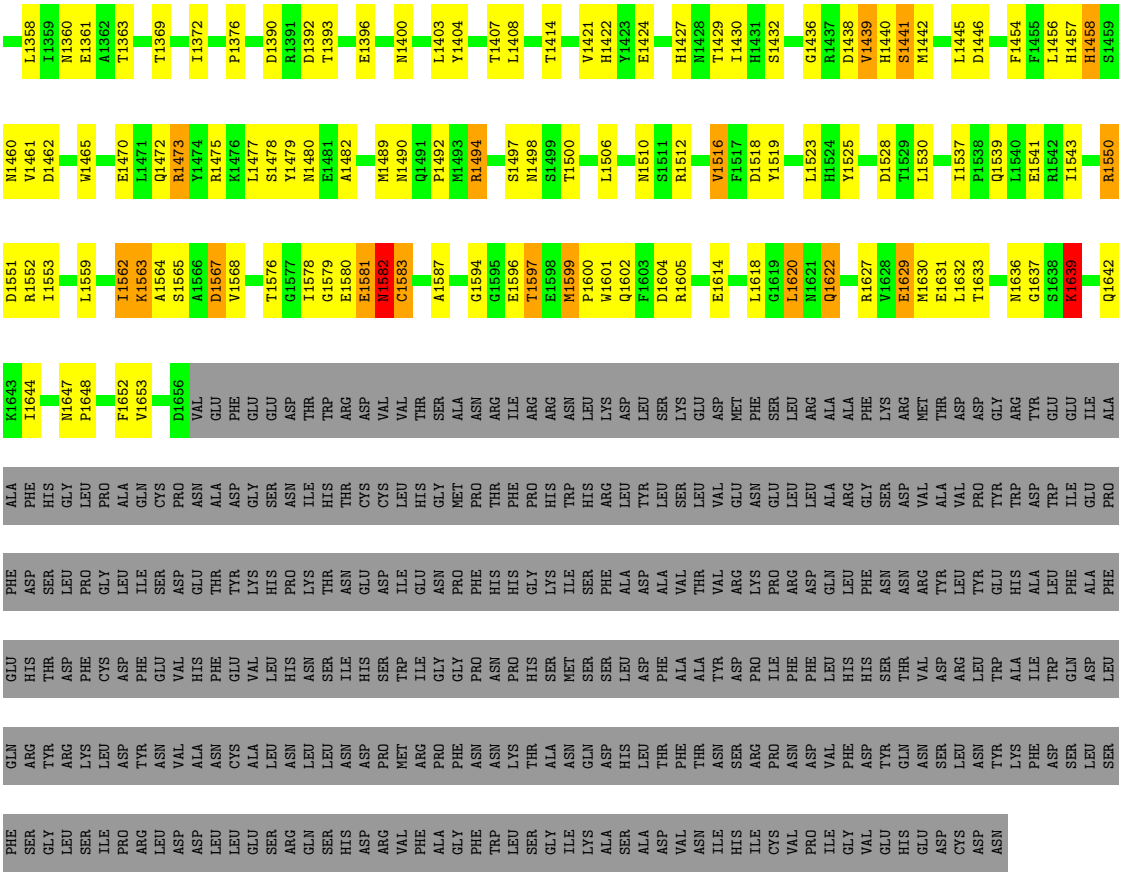


• Molecule 1: hemocyanin

Chain J:



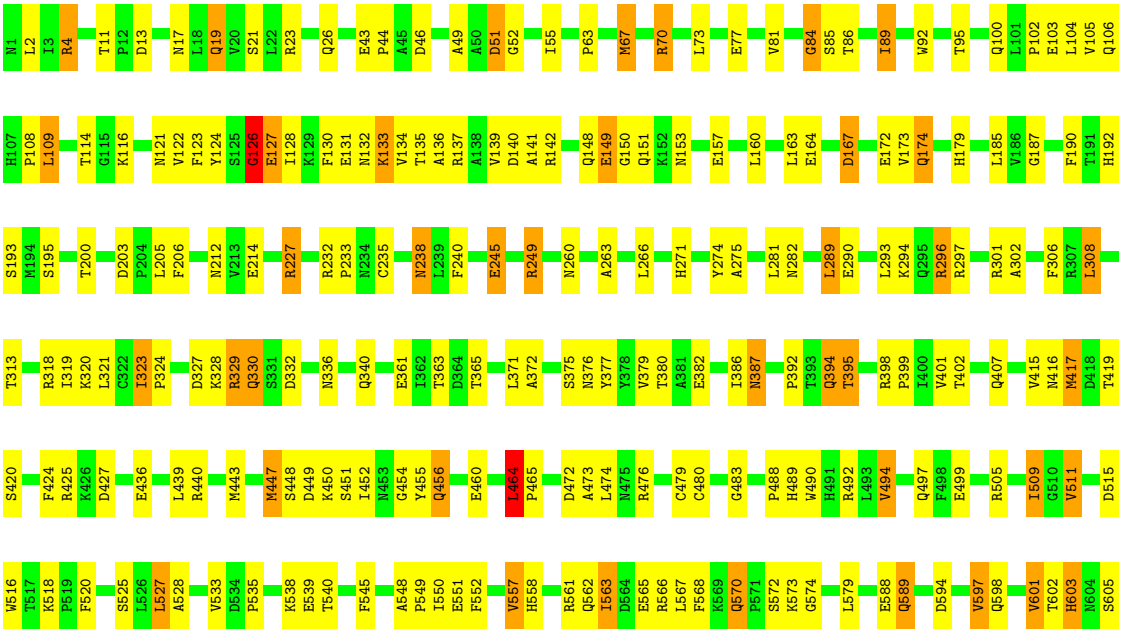

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M98 T99 Q100 L101 P102 E103 L104 V105 P108 L109 F110 K116 K117 A118 K119 K120 N121 V122 F123 Y124 K133 V134 T135 A136 R137 A138 V139 R142 L143 Y144 Q145 Q148 E149 G150 Q151 K152 N153 L156 E157 G158 V159 L160 L163 E164 D167 F168 E172 V177 A178
H179 N180 P181 L185 V186 G187 H192 S193 M194 S195 T200 L205 F206 H209 H210 S211 N212 V213 E214 R215 H216 F217 A218 L219 W220 L223 Q224 K225 H226 R227 R232 P233 N234 C235 G236 L237 N238 L239 F240 E245 P246 F247 G248 R249 N252 N260 S261 K262 A263
L266 E270 H271 L279 S280 L281 T285 I286 E287 E288 L289 E290 L293 K294 Q295 R296 R297 F306 R307 L308 I319 K320 L321 C322 I323 P324 T325 E326 D327 K328 R329 Q330 S331 D332 N333 N336 D337 A338 G339 Q340 G346 E349 M350 N353 F354 Y358 E361 I362
T363 A372 S375 N376 Y377 Y378 T384 A385 I386 L390 M391 P392 T393 Q394 P399 I400 V401 T402 Y403 Q407 G408 F409 V415 M416 M417 D418 T419 S420 F424 R425 I428 T432 T433 E434 L439 E444 M447 K450 S451 I452 M453 G454 Y455 A457 L458
A459 E460 F461 H462 G463 L464 P465 A466 K467 C468 P469 D472 A473 L474 N475 R476 V477 A478 C479 C480 G483 P488 H489 W490 H491 R492 L493 V494 Q497 F498 E499 R505 I509 G510 V511 W514 D515 W516 T517 K518 P519 L527 V533 D534 T540 K541 P542 N543 P544 F545
F546 P549 I550 E551 F552 A555 G556 V557 H558 T559 S560 R561 R566 L567 F568 K569 Q570 P571 S572 K573 G574 F578 Q589 D590 D594 V597 Q598 F599 E600 V601 T602 H603 N604 S605 I606 H607 S617 M618 S619 S620 L621 H622 Y623 M629 F630 W631 L632 H633 H634 S635 Q636
V637 D638 R639 L640 W641 A642 I643 Q648 K653 P654 Y658 C659 S662 M668 K669 P670 F671 A672 F673 K674 S675 P676 L677 N678 N679 T683 P689 V692 Y695 Q696 A697 Y703 D704 T705 L706 F707 F708 S712 I713 R714 R718 A723 K724 R728 V729 F730
A731 G732 Q739 T740 V744 D745 V749 A750 N753 V757 K767 R772 F773 Y777 K778 H779 E780 I781 T782 L785 E795 Y796 T797 D801 I802 K803 D804 V805 N806 L810 I819 V820 V823 N830 V831 K832 F833 Q836 H837 R838 S839 R840 K841 N842
V843 D844 L854 R855 V867 Q871 Q872 V873 A874 A875 F876 H877 G878 S879 T880 Q881 W882 G883 P884 S885 P886 D887 A888 K891 Y892 A893 C894 G898 M899 A900 T901 F902 P903 H904 W905 H906 R907 L908 I909 N912 F913 E914 N915 G916 L917 R918 W922 S923 G924 G925 L926 P927 Y928
W929 D930 W931 T932 I935 D936 L941 E944 A945 E946 D949 A950 N951 G952 E953 A954 K955 P956 N957 P958 F959 F960 S961 G962 D965 S966 S972 P975 T976 E977 A978 L979 Y980 E981 K982 P983 T989 H990 L991 A992 N993 E994 I995 L999 E1000 Q1001 E1002 D1003 Q1010 Y1011
E1012 I1013 A1014 H1015 N1016 H1017 I1018 H1019 A1020 L1021 G1024 T1025 V1028 S1029 M1030 L1033 E1034 Y1035 S1036 A1037 F1038 D1039 F1042 M1043 L1044 H1045 H1046 S1047 N1048 V1049 D1050 R1051 Q1057 E1075 I1076 L1077 R1078 M1081 S1082 P1083 F1084 S1085 L1086 I1090 N1091 P1092 D1093 A1094 M1095 T1096 R1097
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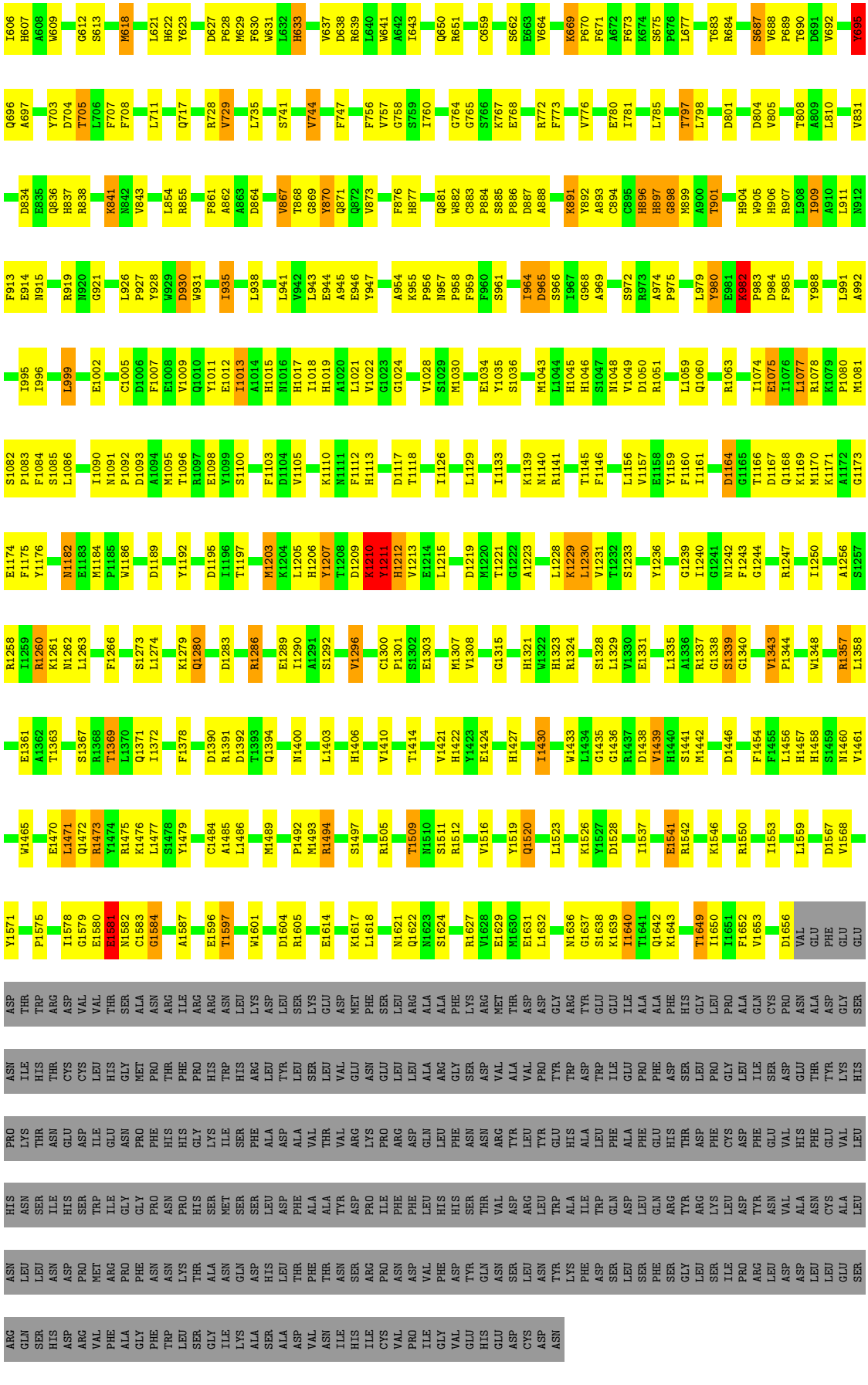


• Molecule 1: hemocyanin

Chain M:



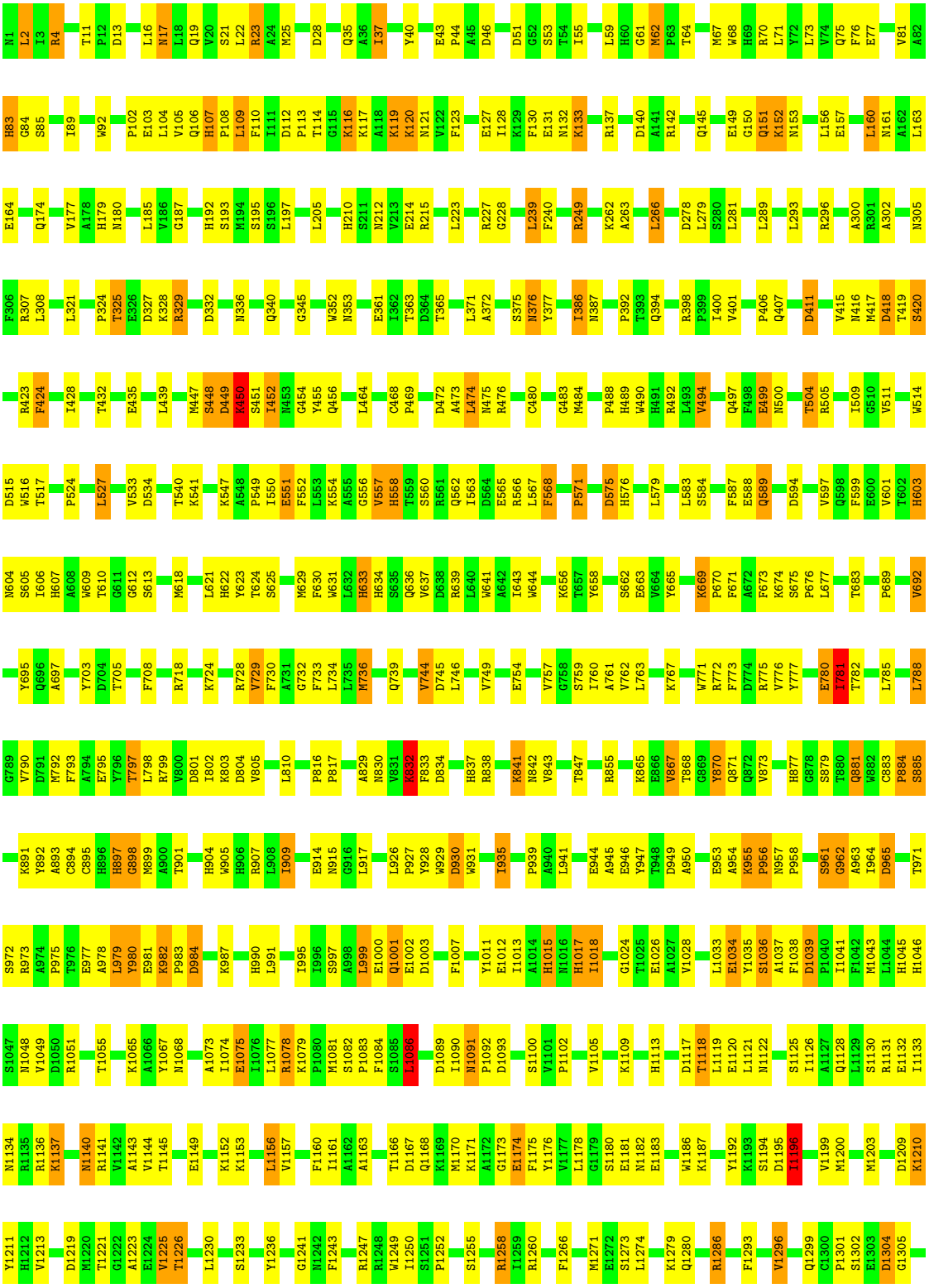



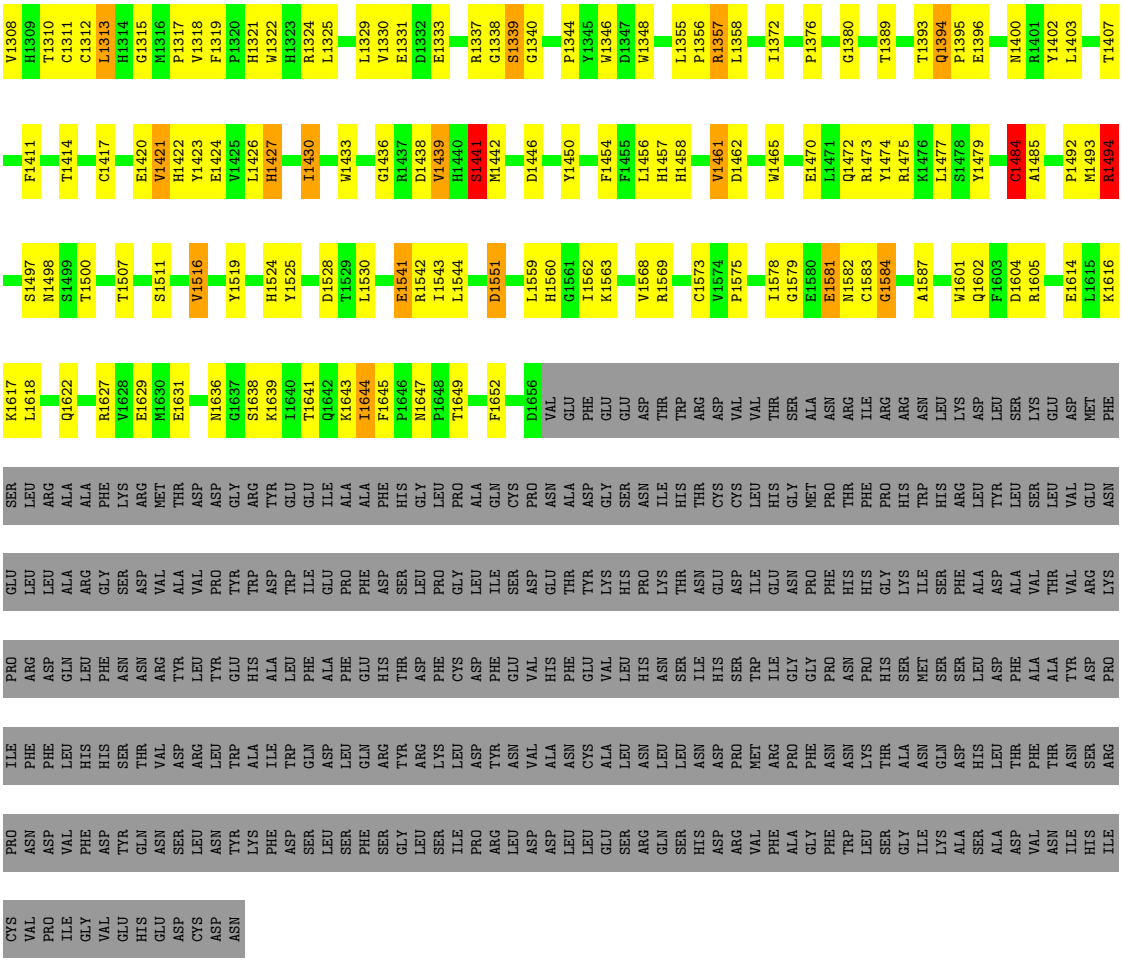

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ASP THR TRP ARG ASP VAL VAL THR SER ALA ASN ARG ILE ARG ARG ASN LEU LYS ASP LEU SER LYS GLU ASP MET PHE SER LEU ARG ALA ALA PHE LYS ARG MET THR ASP GLY ARG TYR GLU GLU ILE ALA ALA PHE HIS GLY LEU PRO ALA CYS ASP PHE ASP SER LEU PRO GLY LEU ILE SER ASP ASP GLY SER
ASN ILE HIS THR CYS CYS LEU HIS GLY MET PRO THR PHE PRO HIS TRP HIS SER ARG LEU TYR LEU SER LEU VAL GLU ASN GLU LEU LEU ALA ARG GLY SER ASP VAL PRO TYR TRP ASP TRP ILE GLU PHE ASP SER LEU PRO GLY LEU ILE SER THR HIS
PRO LYS THR ASN GLU ASP ILE GLU ASN PRO PHE HIS HIS GLY LYS ILE SER PHE ALA ASP ALA VAL THR VAL ARG LYS PRO ARG ASP GLN LEU LEU PHE HIS ASN ARG TYR LEU TYR GLU HIS ALA LEU PHE GLU HIS THR ASP PHE PHE CYS ASP PHE GLU VAL HIS PHE VAL LEU
HIS ASN SER ILE HIS SER TRP ILE GLY GLY PRO ASN PRO HIS SER THR VAL ASP ARG LEU TRP GLN ASP LEU GLN ARG TYR ARG LYS LEU ILE ASP SER LEU PHE ASP SER GLY LEU SER ASP PHE ASN VAL ALA ASN ALA CYS LEU
ASN LEU LEU ASN ASP PRO PHE ASP VAL PHE ASP ASN GLN ILE GLY VAL GLU HIS GLU ASP CYS ASP
ARG GLN SER HIS ASP ARG VAL PHE ALA GLY PHE TRP LEU SER GLY ILE LYS ALA SER ALA ASP VAL ASN ILE HIS ILE CYS VAL PRO ILE GLY VAL GLU HIS GLU ASP CYS ASP ASN

• Molecule 1: hemocyanin

Chain P:



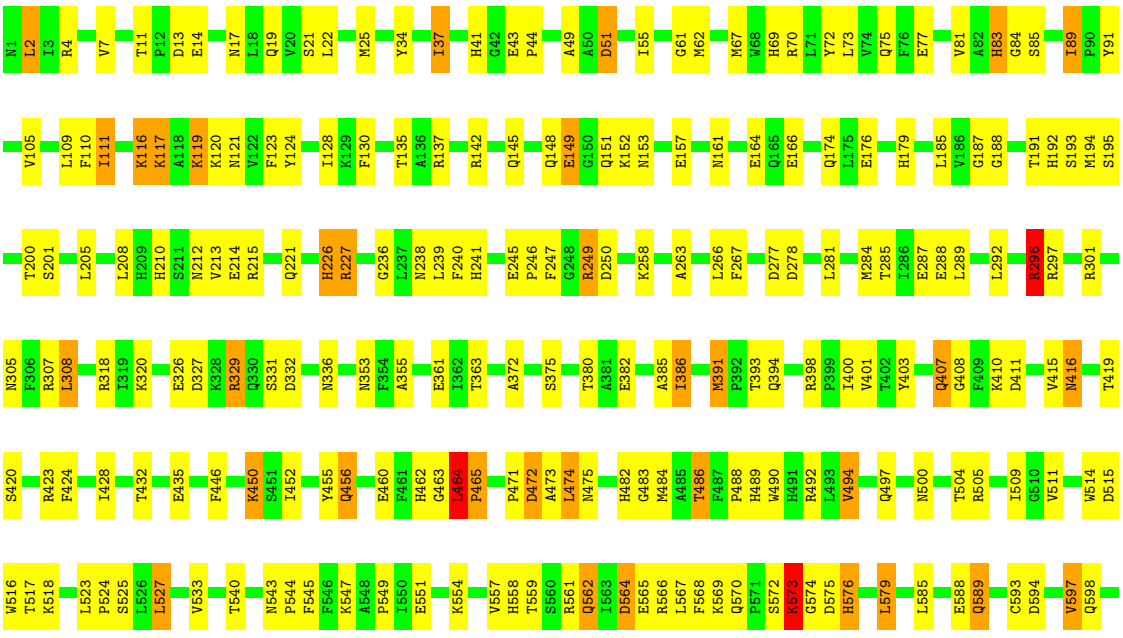



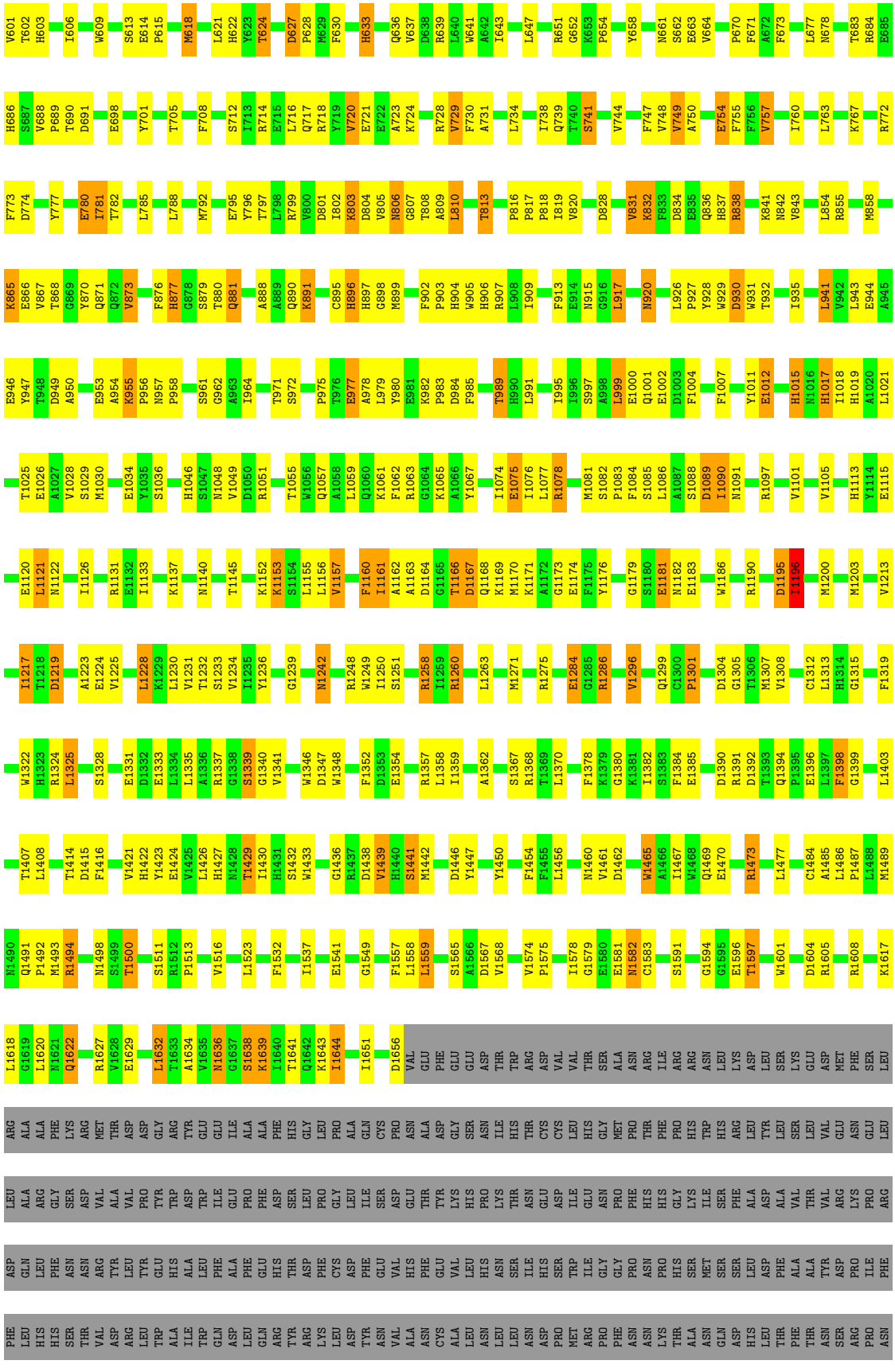


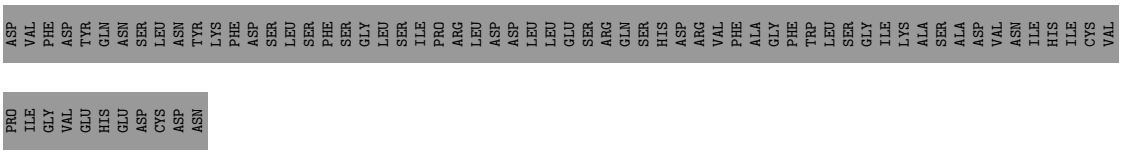
• Molecule 1: hemocyanin

Chain S:



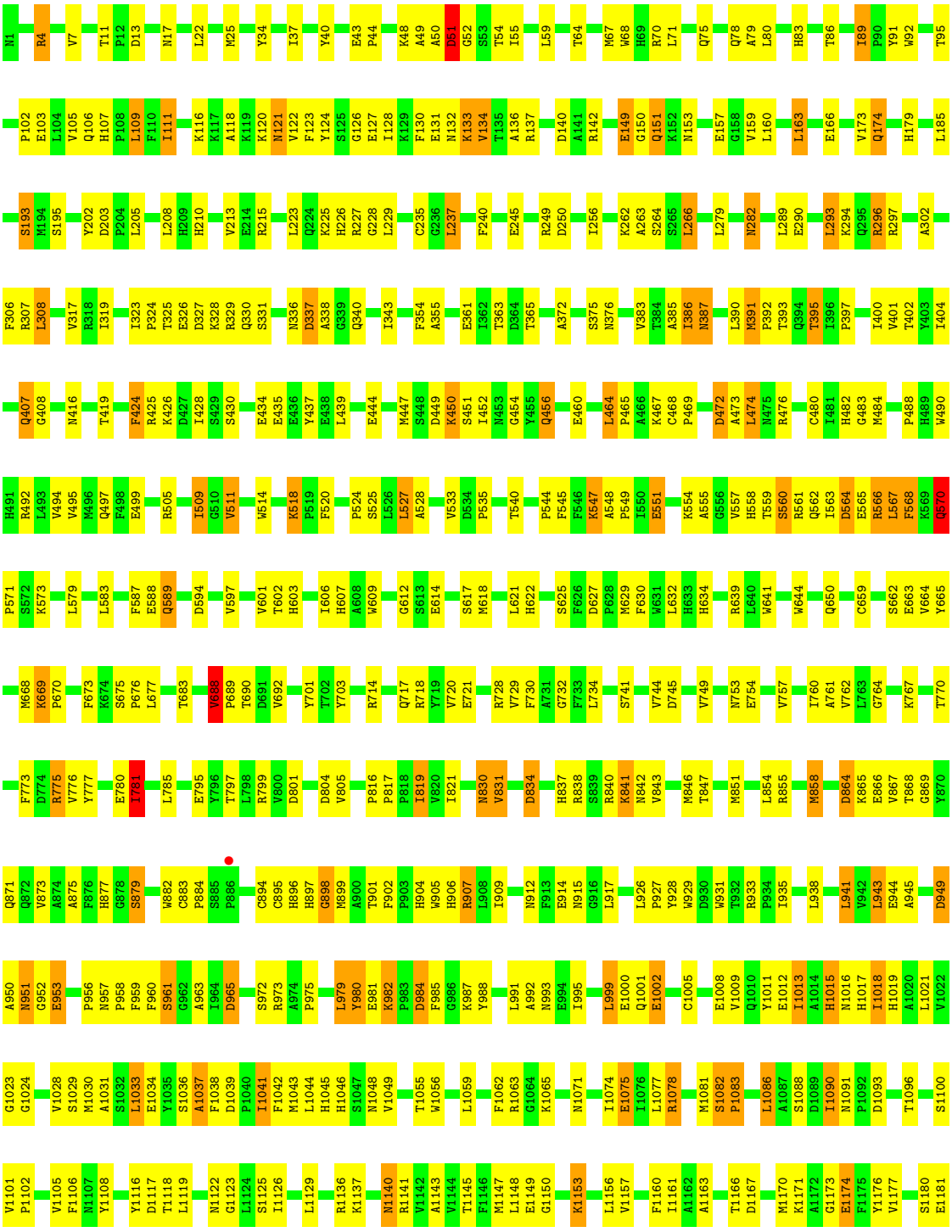



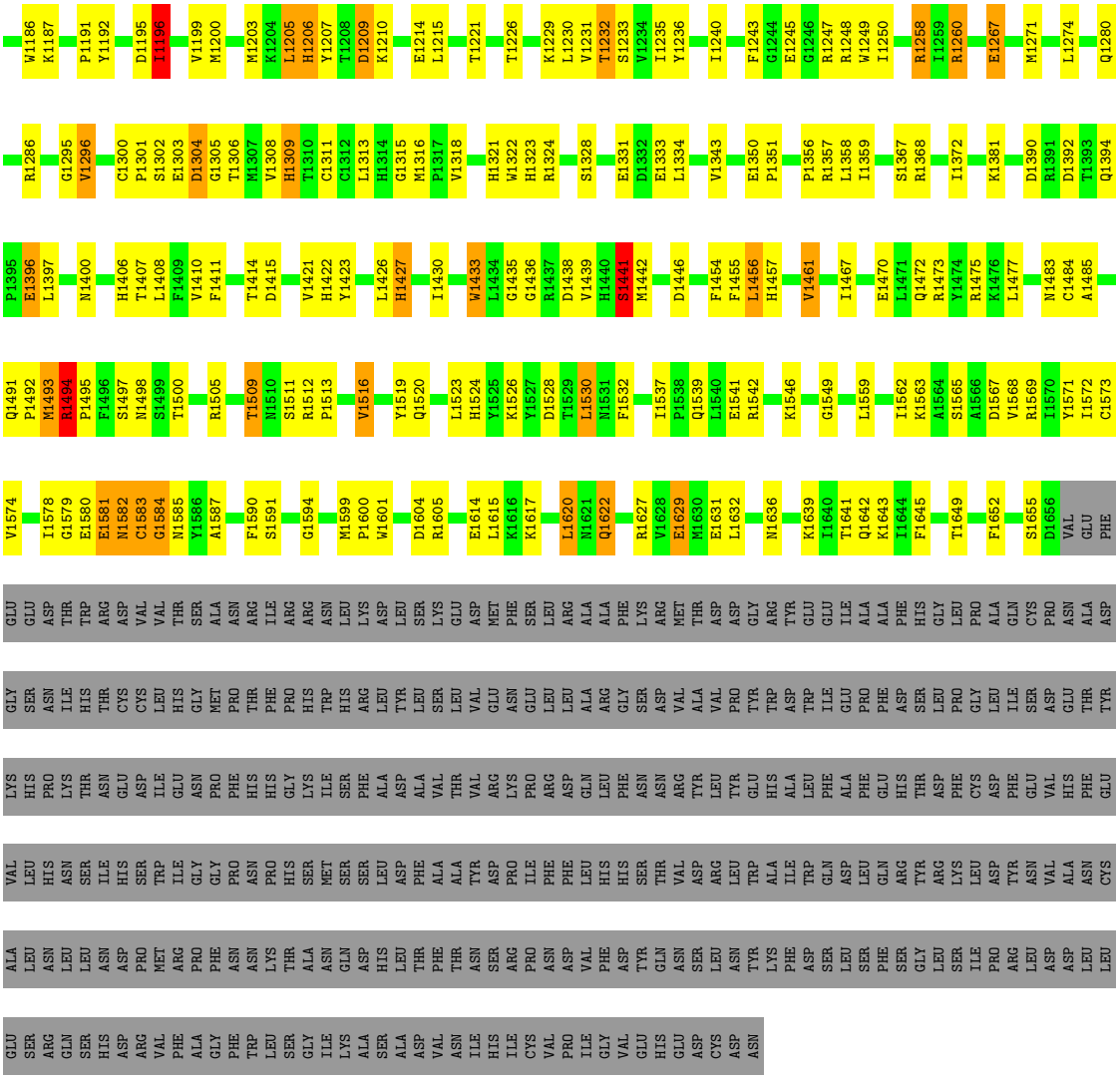

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ARG ALA ALA PHE LYS ARG MET THR ASP ASP GLY ARG TYR GLU GLU ILE ALA PHE HIS GLY LEU CYS PRO ASN ALA ASP GLY SER ASN ILE HIS THR TRP CYS LEU HIS GLY MET PRO THR PHE PRO HIS SER TRP HIS ASN LEU SER LYS ASP GLU ASP MET PHE SER LEU
LEU ALA ARG GLY SER ASP VAL ALA VAL PRO TYR TRP ASP TRP ILE GLU PRO PHE ASP SER LEU PRO GLY LEU ILE SER ASP GLU THR TYR LYS HIS PRO LYS THR ASN GLU ASP ILE GLU ASN PRO PHE HIS HIS GLY LYS ILE SER PHE ALA ASP ALA VAL THR VAL ARG LYS PRO ARG
ASP GLN LEU PHE ASN ASN ARG TYR LEU TYR GLU HIS ALA LEU PHE ALA PHE GLU HIS THR ASP PHE CYS ASP PHE GLU VAL LEU HIS PHE GLU VAL LEU HIS ASN SER ILE HIS SER TRP ILE GLY GLY PRO ASN PRO HIS SER MET SER SER LEU ASP PRO ILE PHE
PHE LEU HIS HIS SER THR ASN ARG LEU TRP ALA ILE TRP GLN ASP LEU GLN ARG TYR ARG LYS LEU ASP TYR ASN VAL ALA ASN CYS ALA LEU ASN LEU LEU ASN ASP CYS ALA GLN ASP THR ALA ASN ASN LYS THR ALA SER ASN GLN ASP HIS LEU PHE THR ASN SER ARG PRO ILE ASN




• Molecule 1: hemocyanin

Chain V: 48% 29% 5% 17%

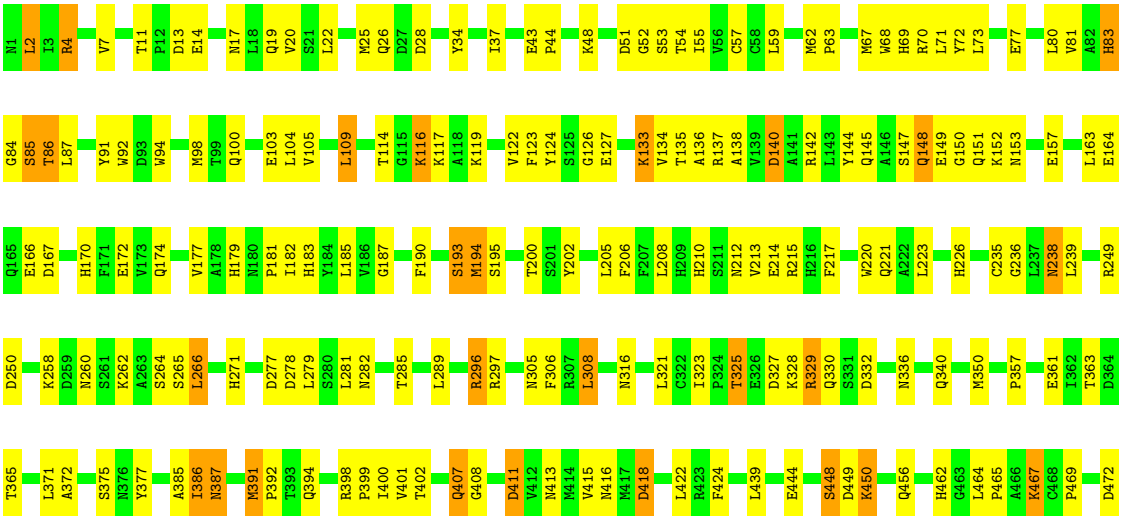


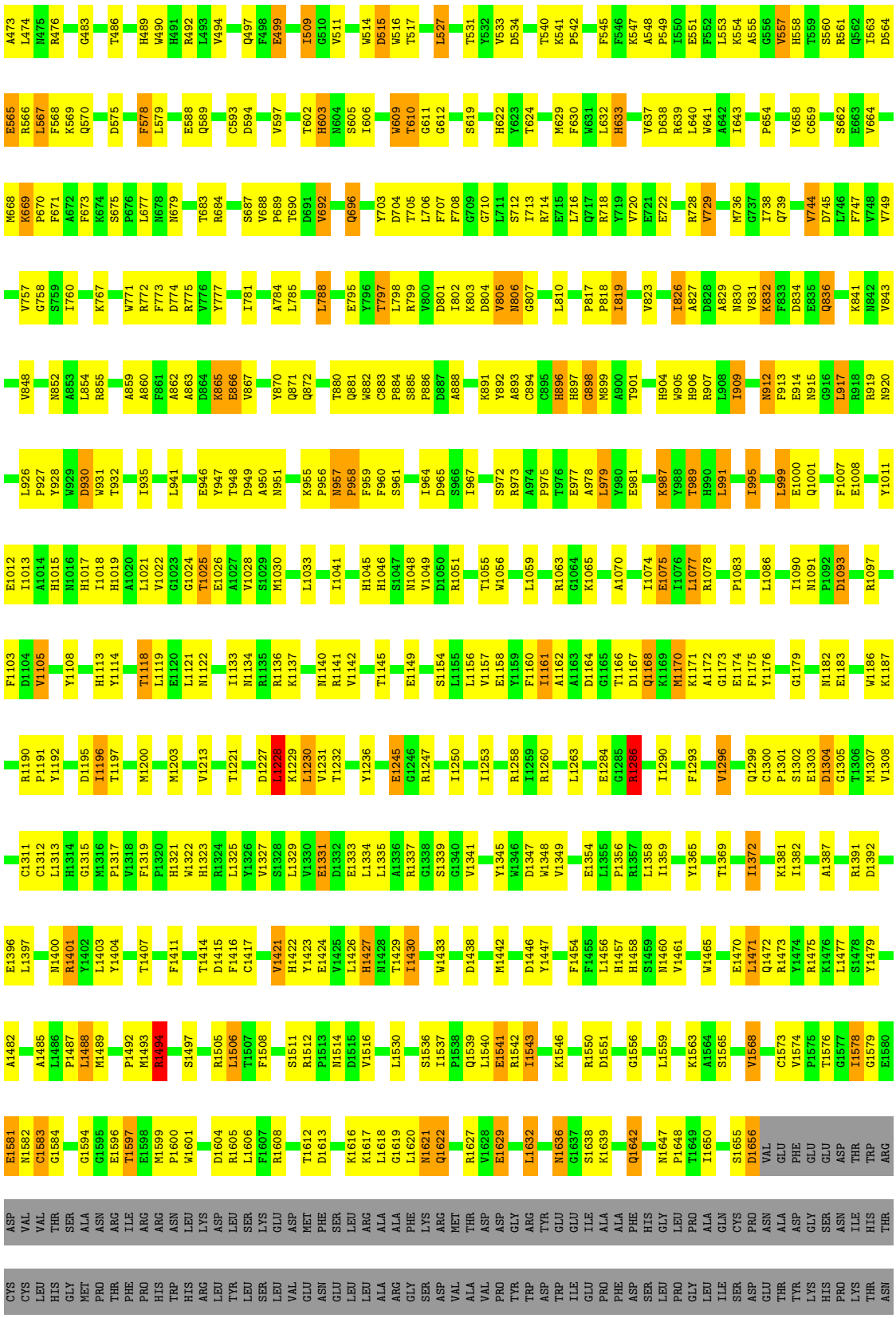


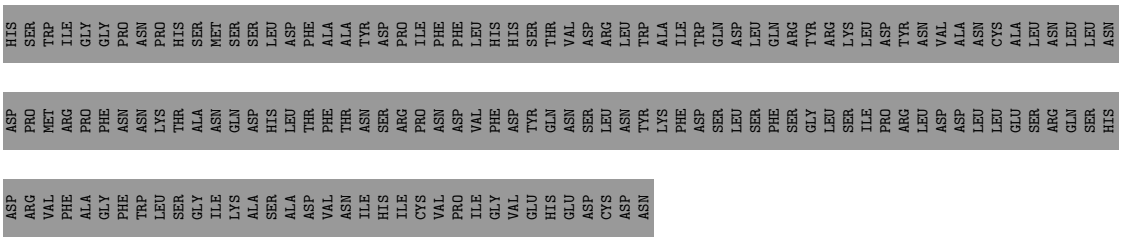
• Molecule 1: hemocyanin

Chain Y:




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ASP VAL VAL THR SER ALA ASN ARG ILE ARG ARG ASN LEU LYS ASP LEU SER LYS GLU ASP MET PHE SER LEU ARG ARG ASP GLN LEU ARG ALA ALA PHE LYS ARG ASN ARG TYR LEU TYR GLU ILE ALA ALA ALA PHE HIS SER LEU PRO GLY LEU PRO ALA GLN CYS PRO ASN ALA ASP GLY SER ASN ILE HIS THR
CYS CYS LEU HIS GLY MET PRO THR PHE PRO HIS TRP HIS ARG LEU TYR LEU SER LEU VAL GLU ASN GLU LEU ARG GLY SER ASP VAL ALA ARG GLY GLU ILE GLU PRO ALA PHE GLU GLY TRP ASP TRP ILE GLU PRO PHE ASP SER LEU PRO GLY LEU ILE SER ASP GLU THR TYR LYS HIS PRO LYS THR ASN
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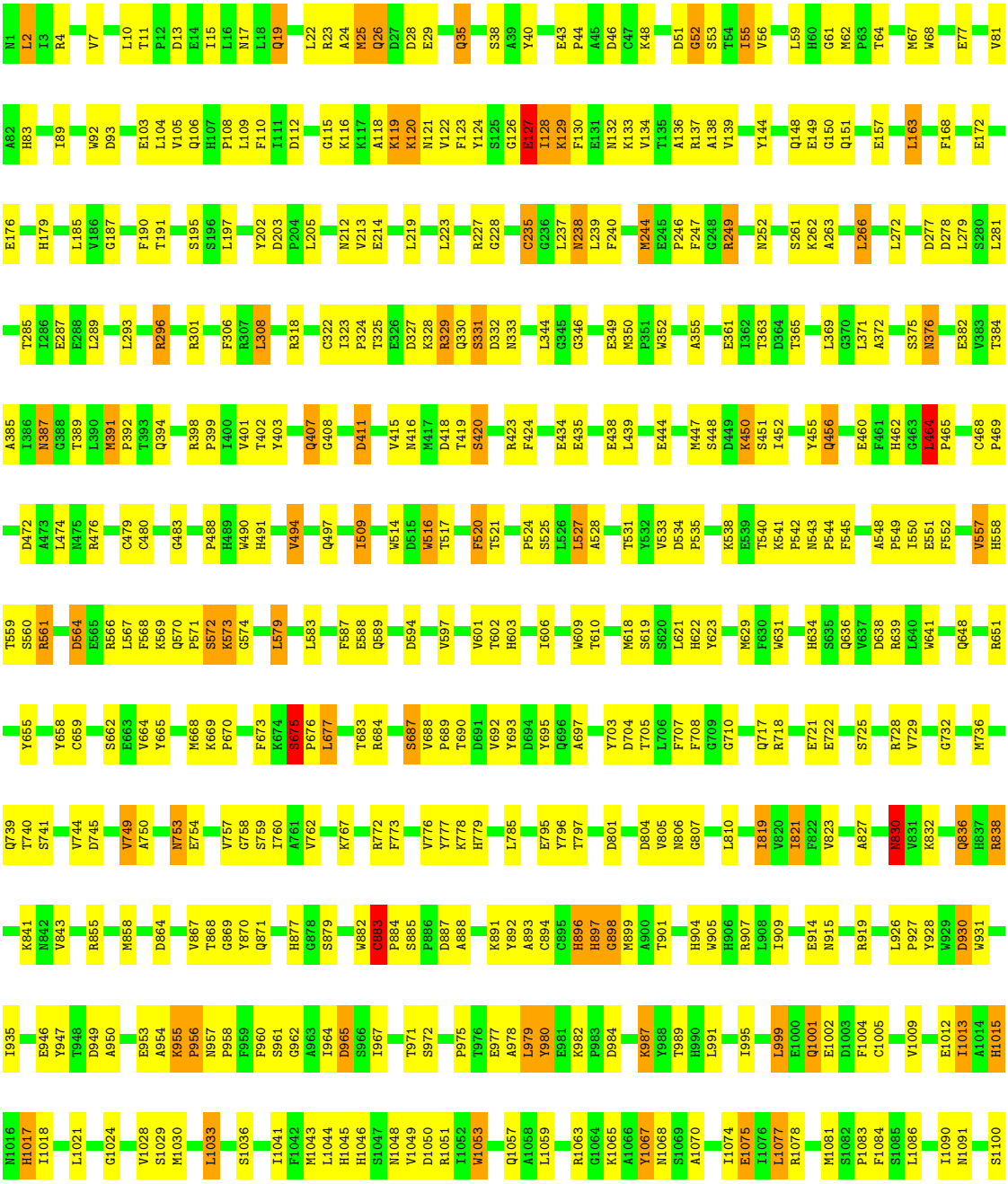


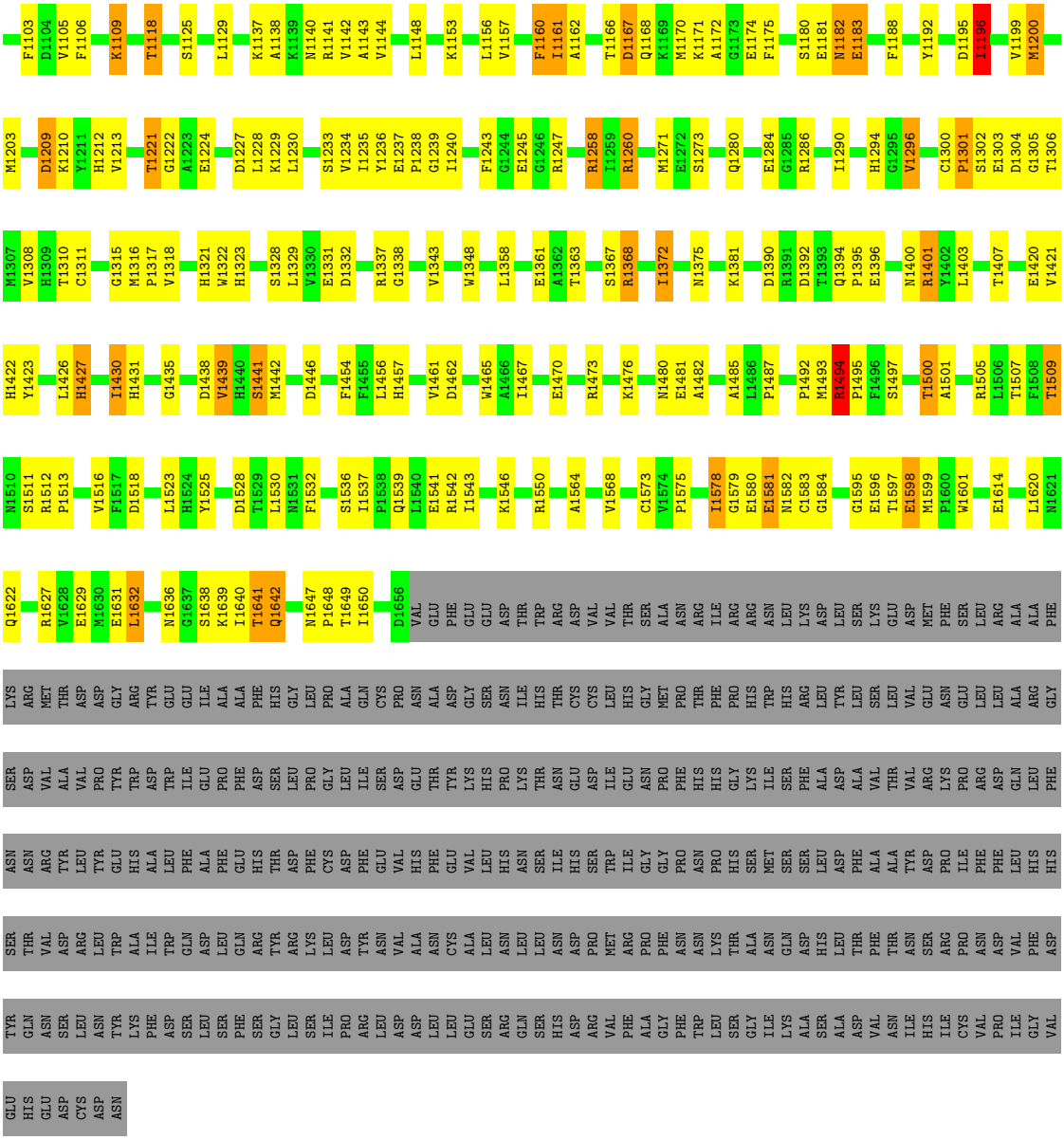


• Molecule 1: hemocyanin

Chain b:

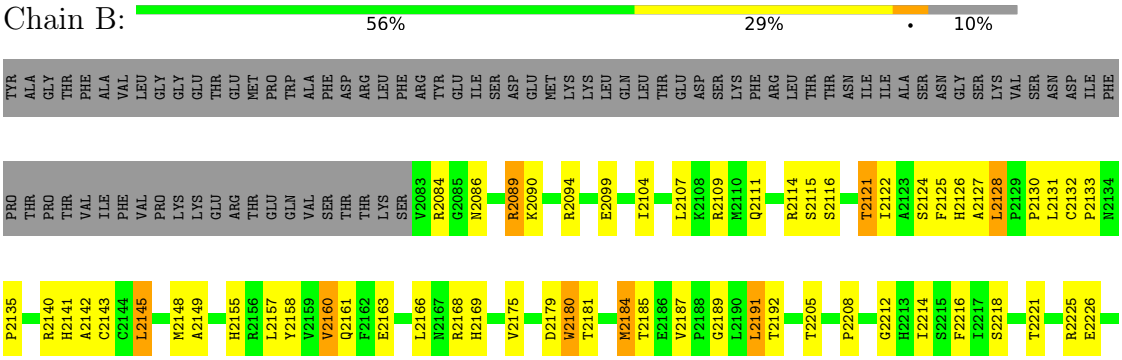


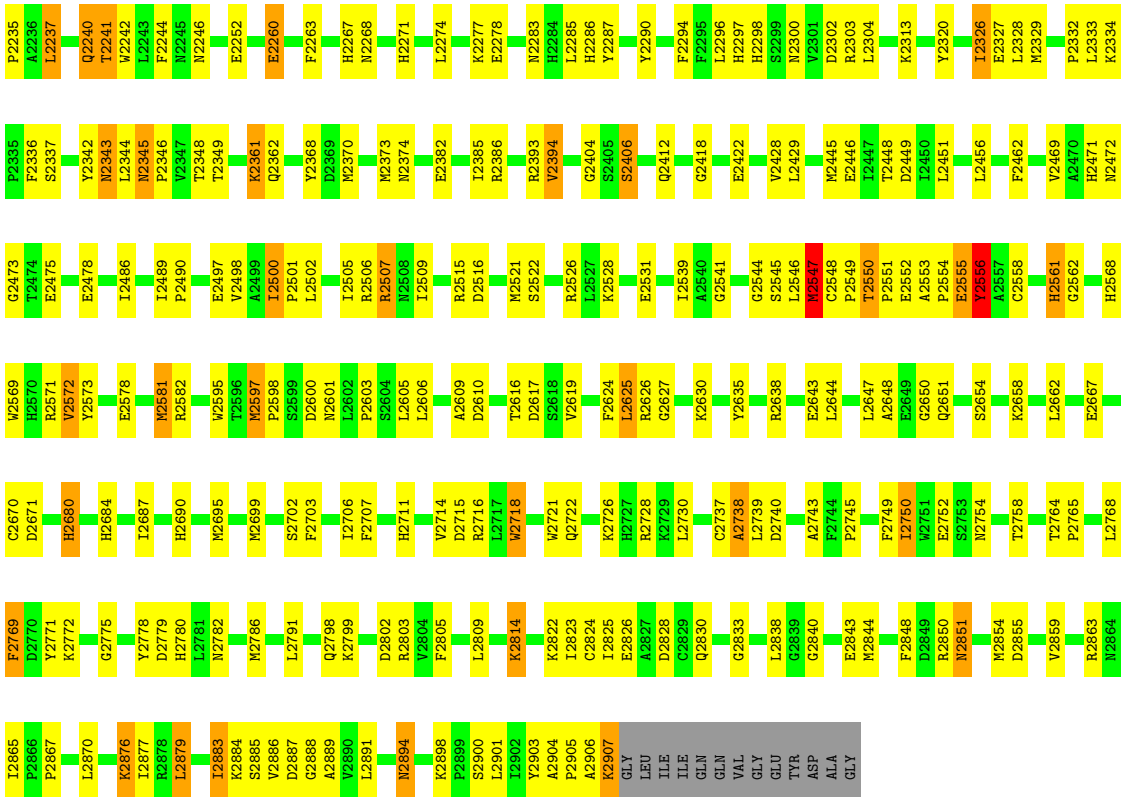





• Molecule 2: hemocyanin

Chain B:

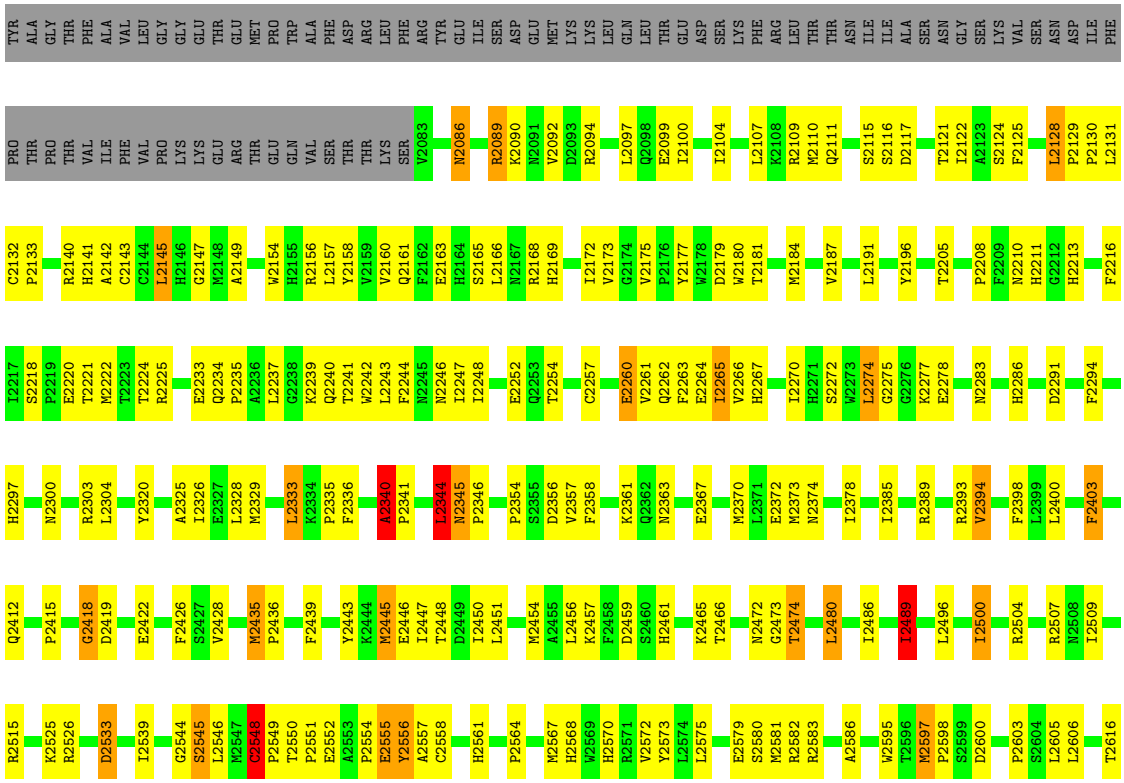


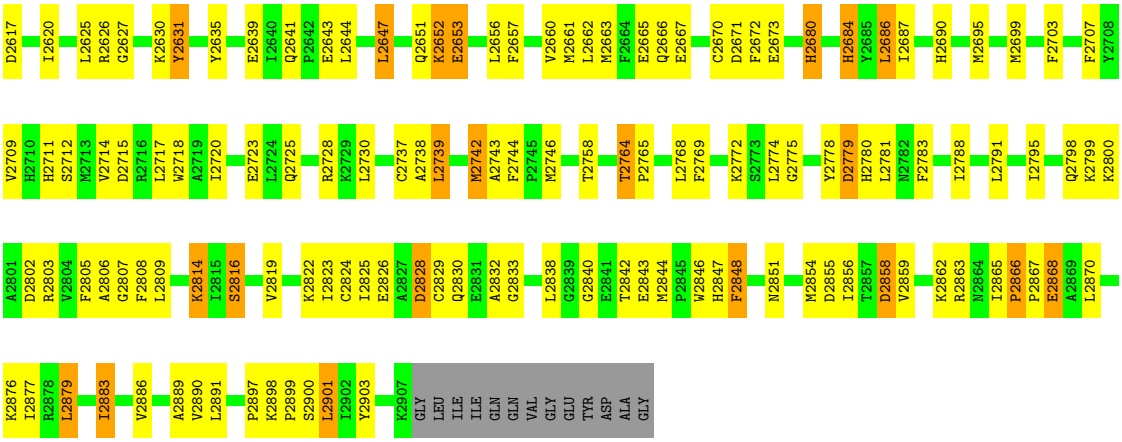


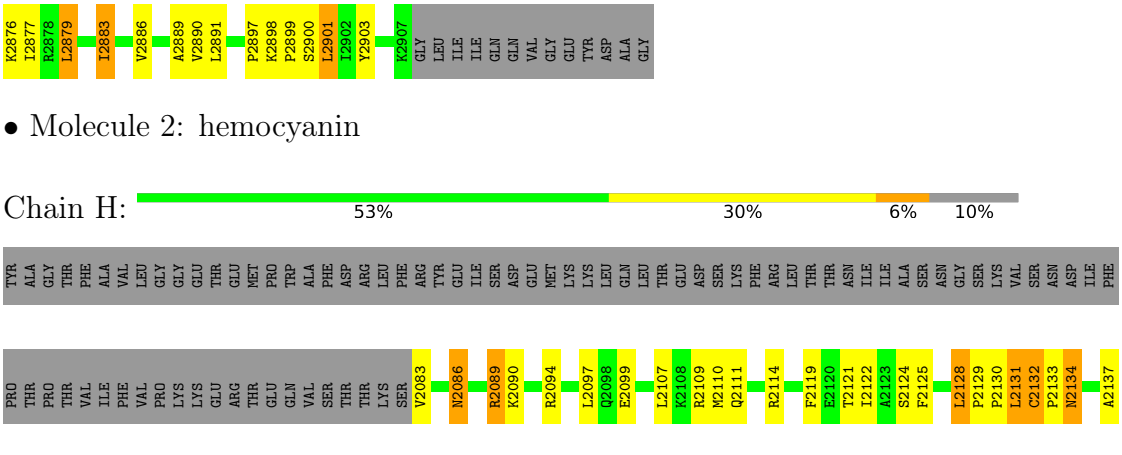
• Molecule 2: hemocyanin

Chain E:

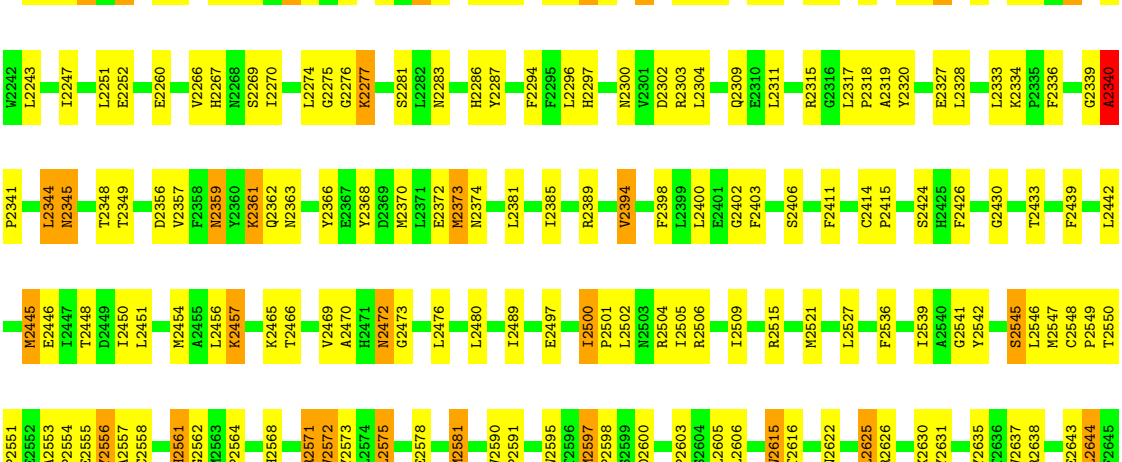


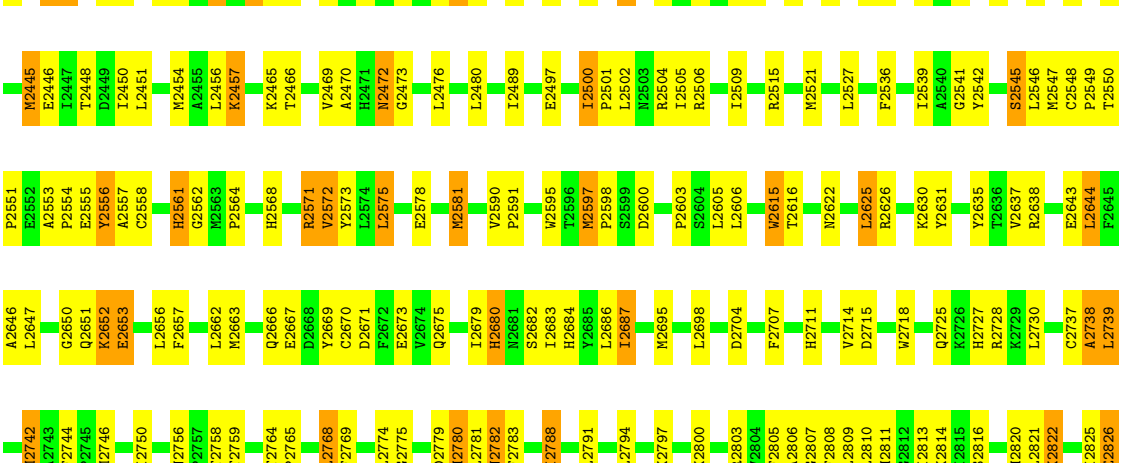



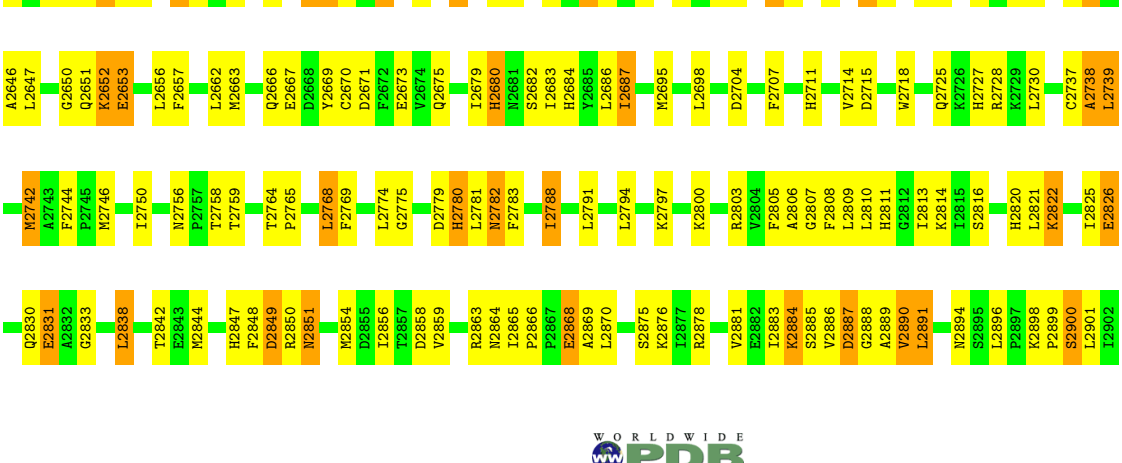








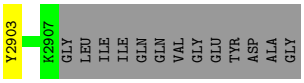






• Molecule 2: hemocyanin

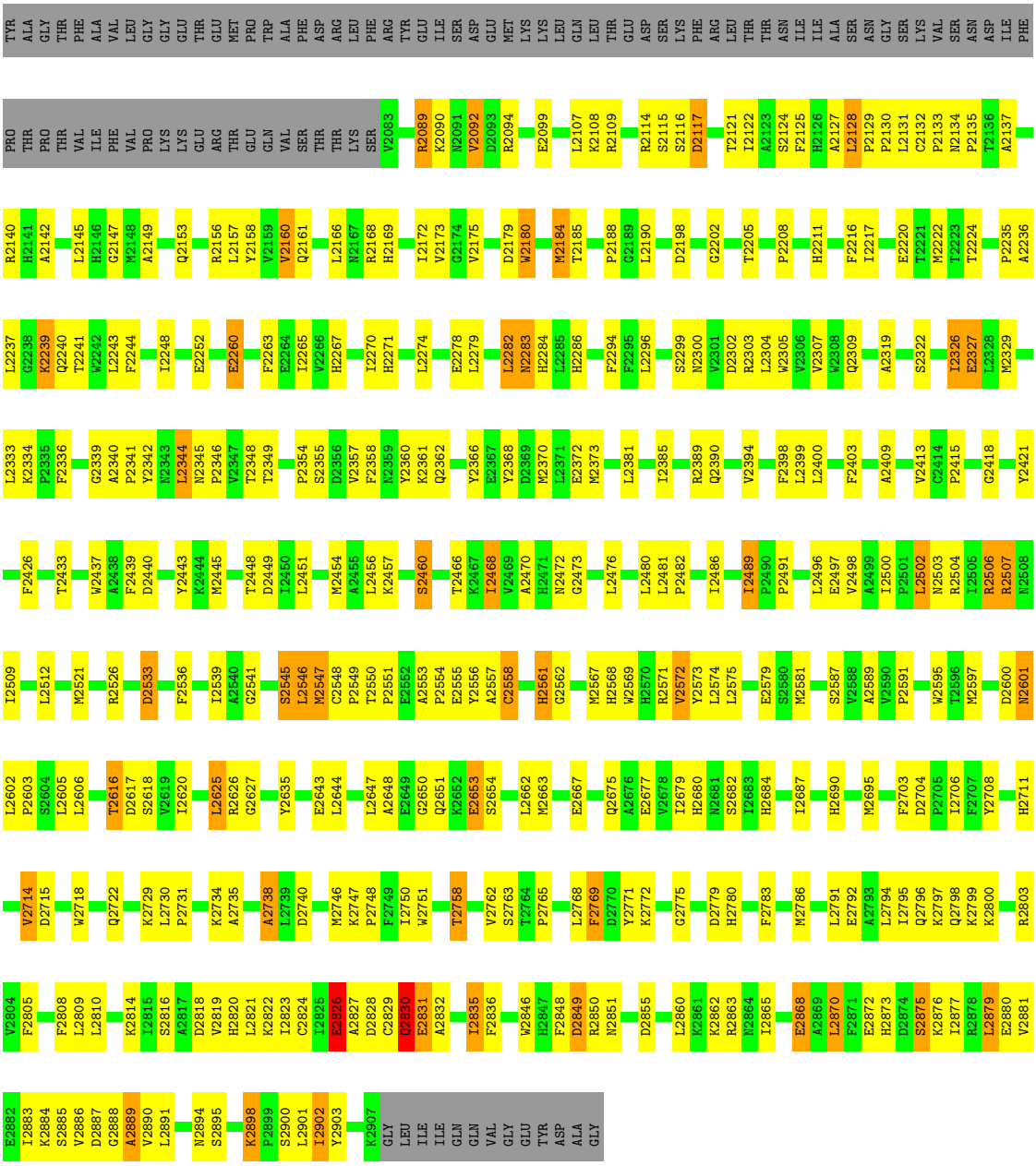
Chain H:




• Molecule 2: hemocyanin

Chain K:

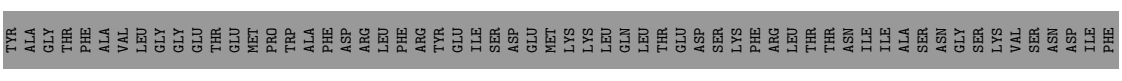


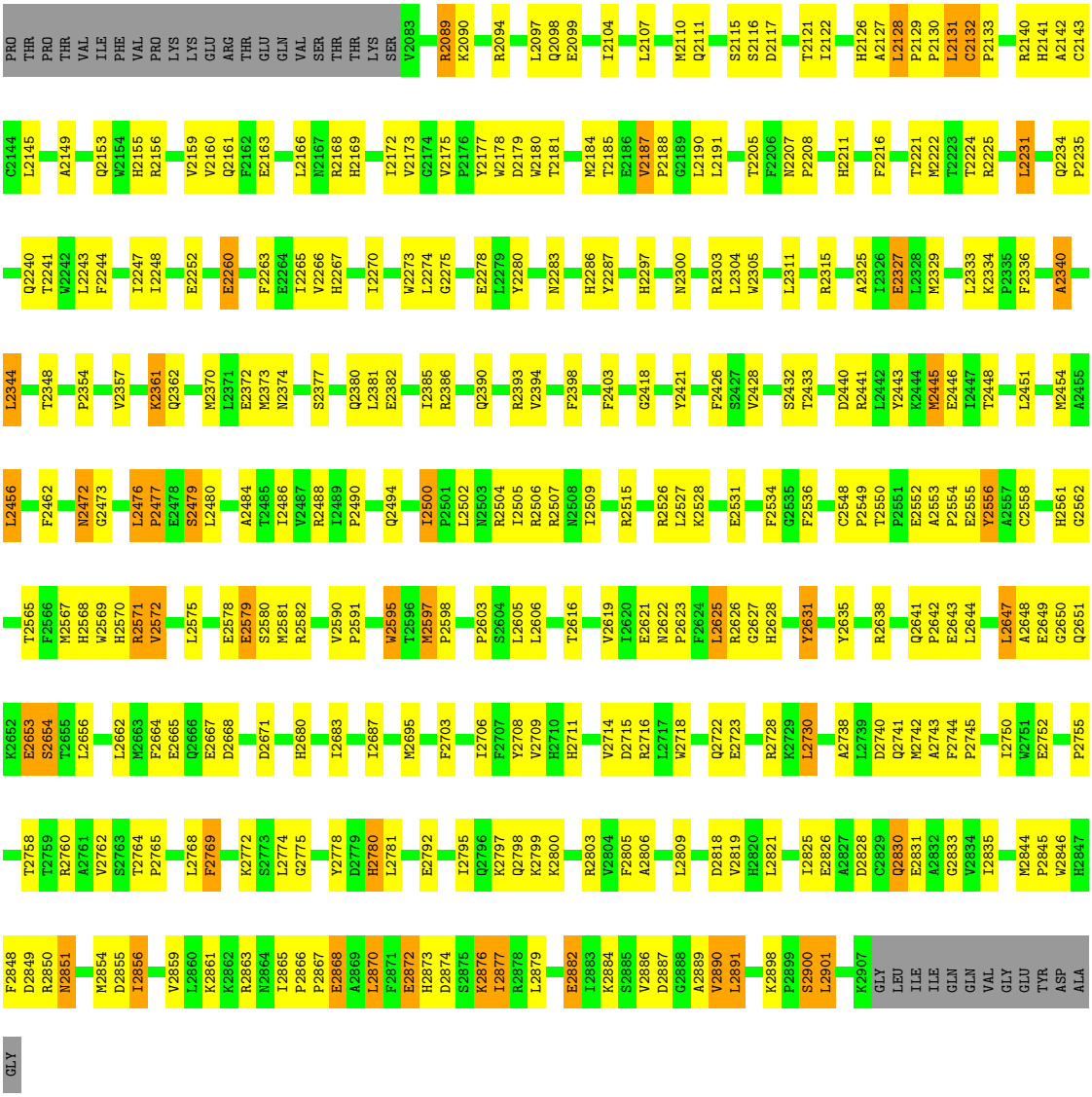




• Molecule 2: hemocyanin

Chain N:



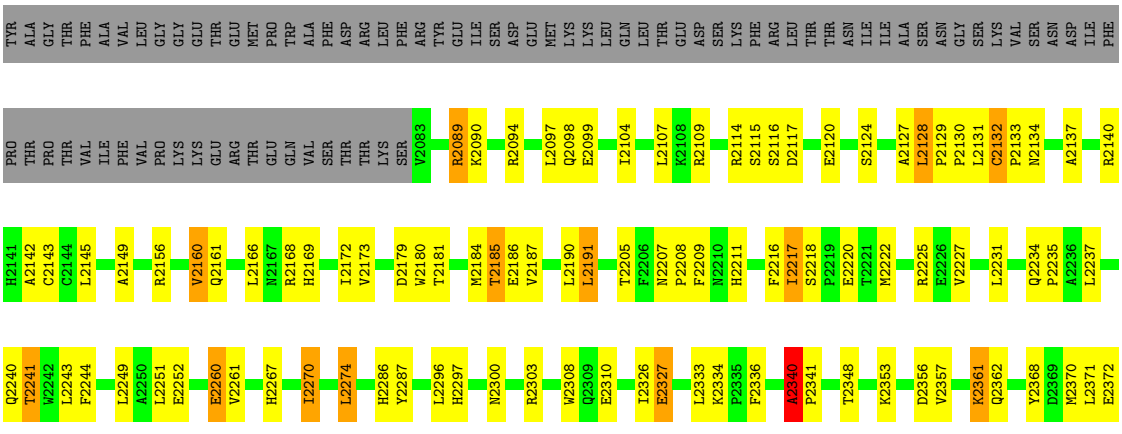



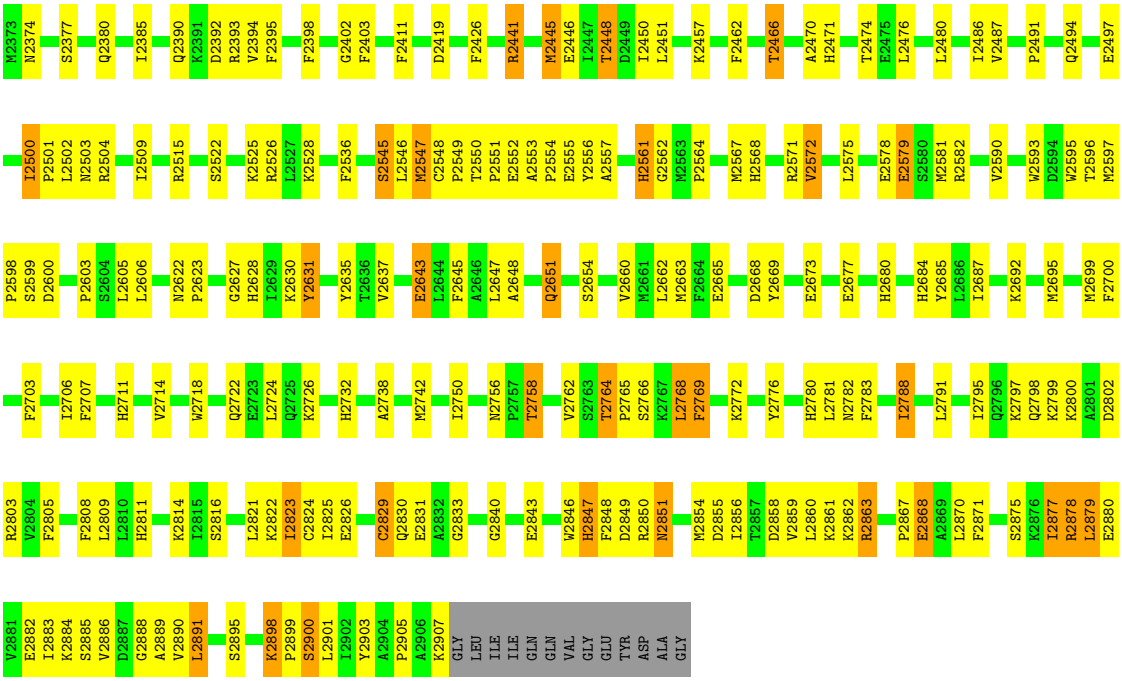


• Molecule 2: hemocyanin

Chain Q:



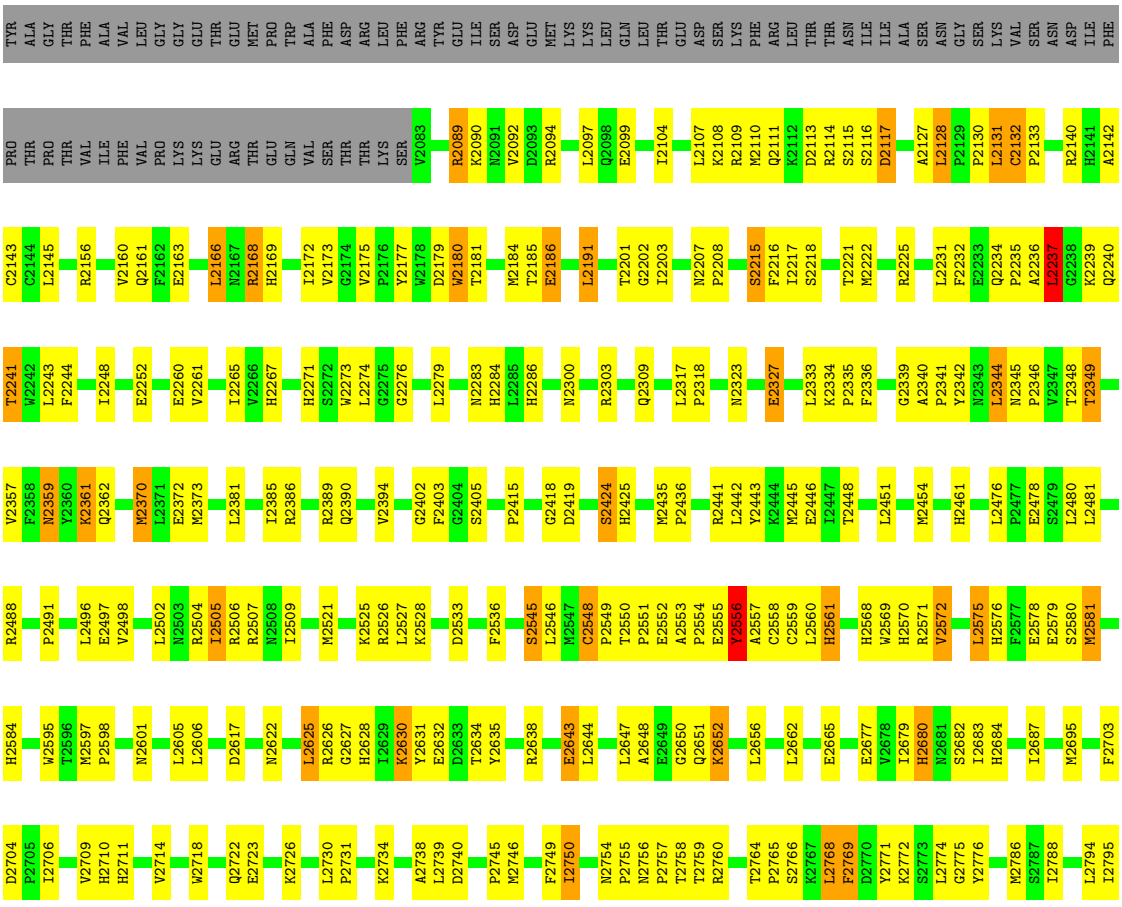



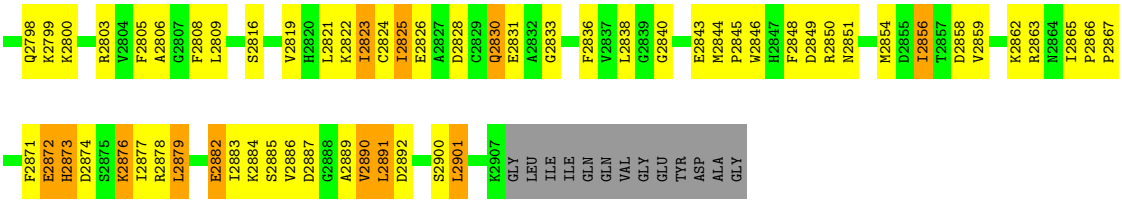


• Molecule 2: hemocyanin

Chain T:

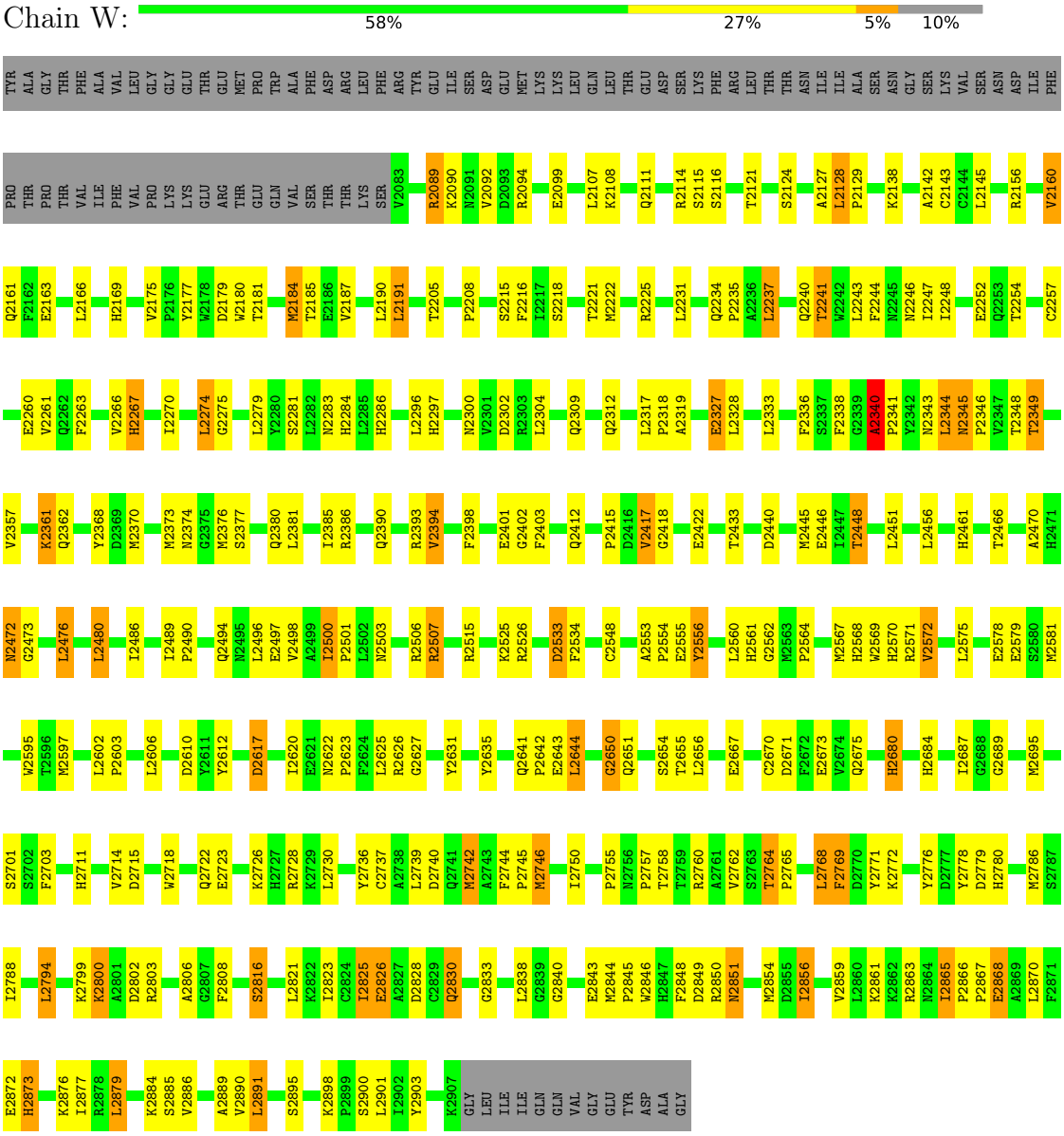




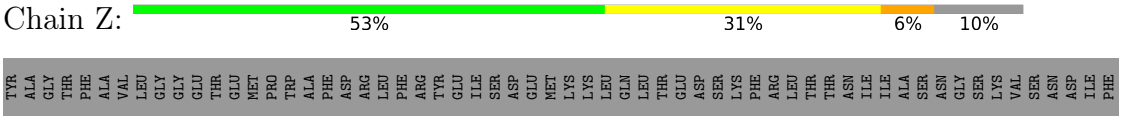
• Molecule 2: hemocyanin

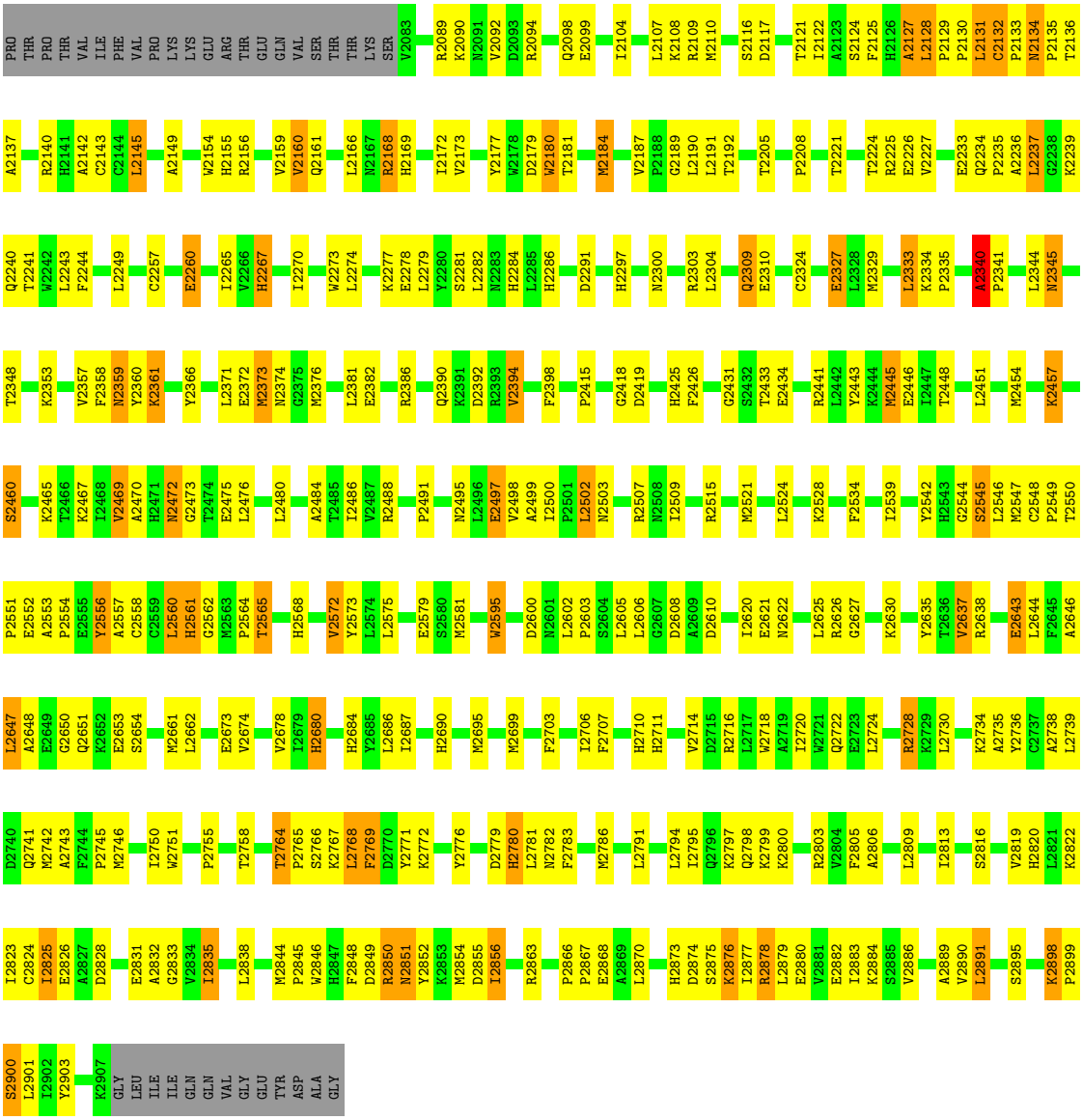
Chain W:




• Molecule 2: hemocyanin

Chain Z:

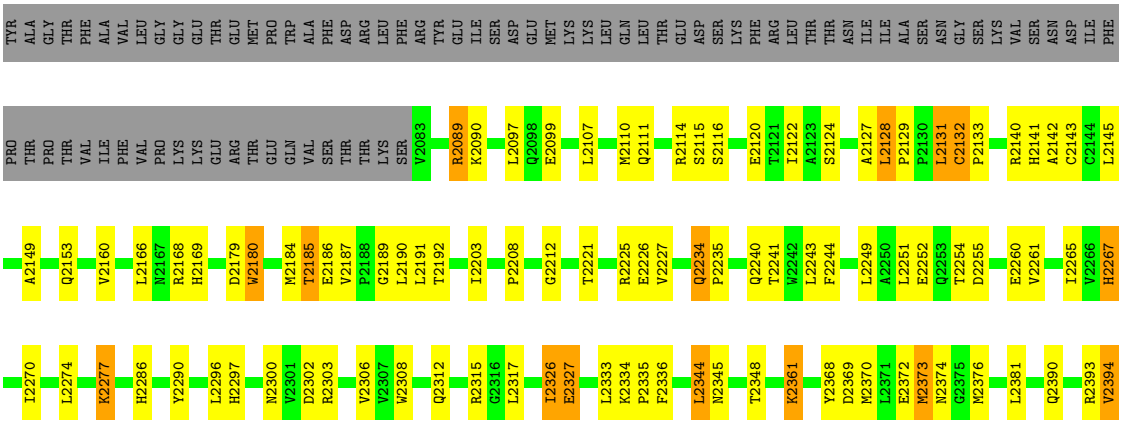


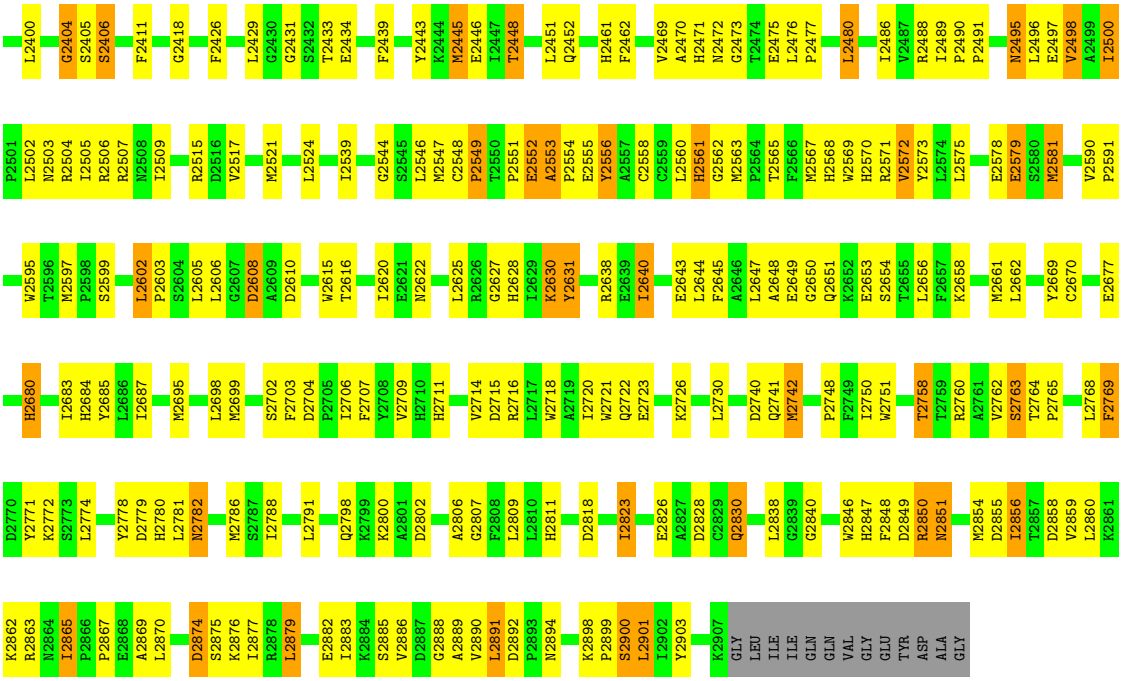


• Molecule 2: hemocyanin

Chain c:

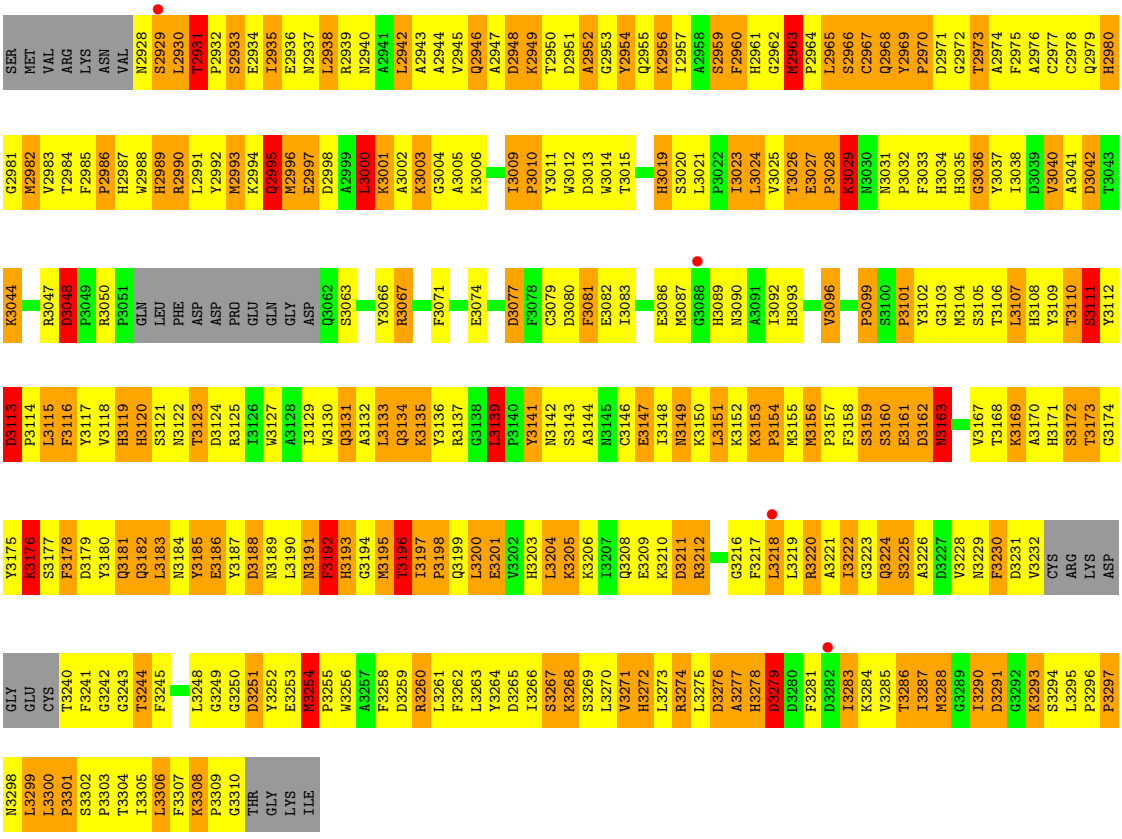




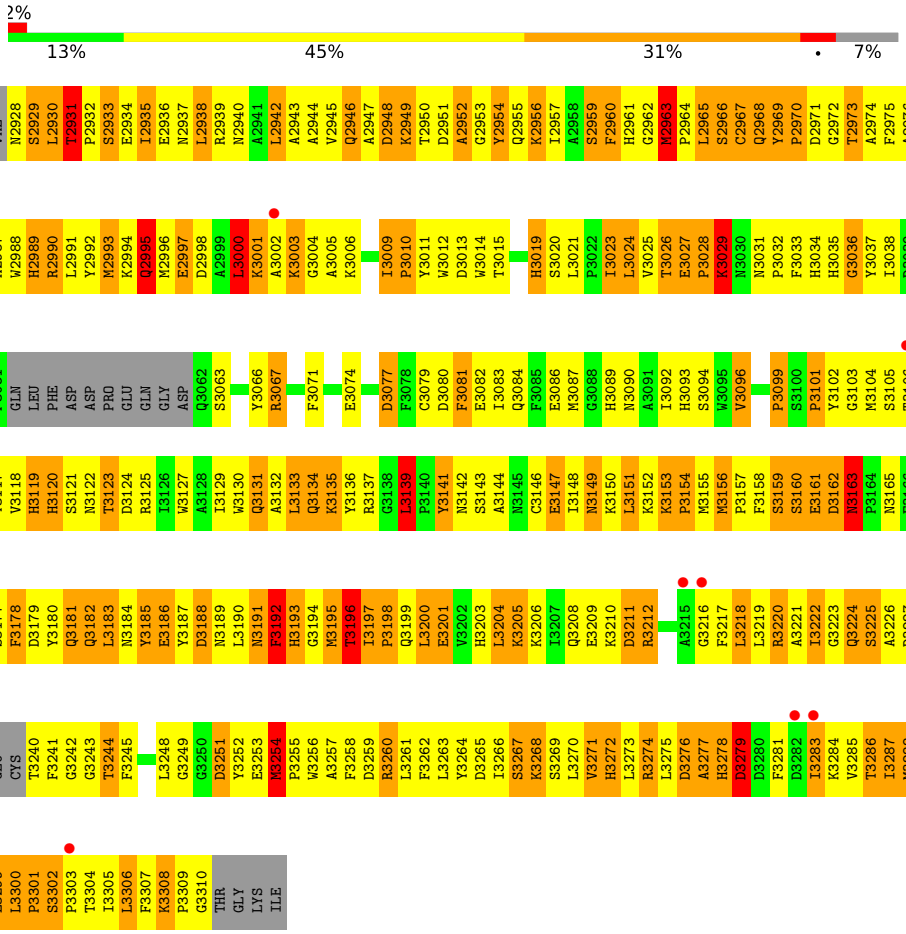
• Molecule 3: hemocyanin



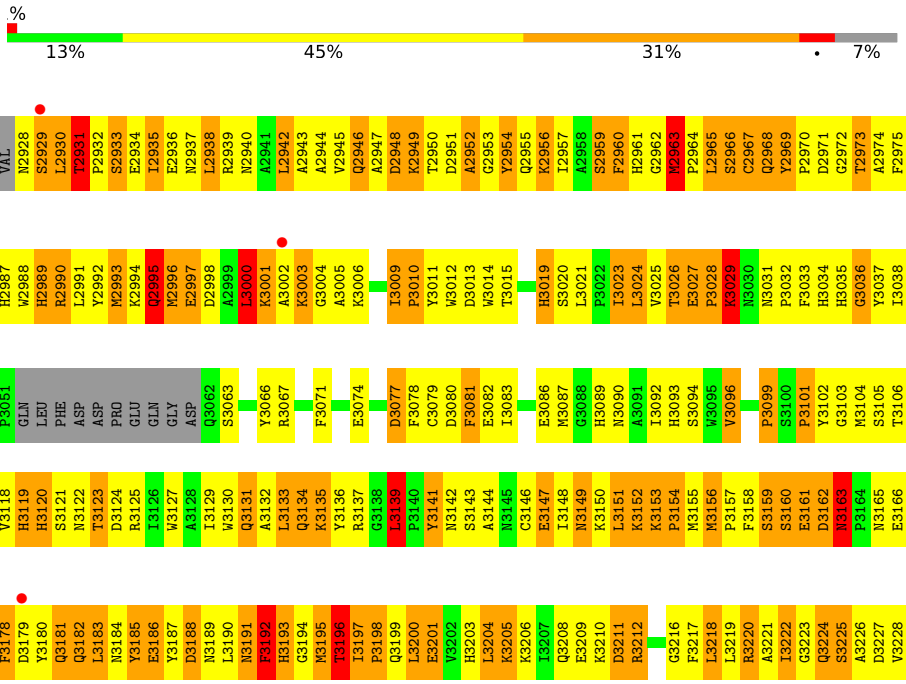
• Molecule 3: hemocyanin

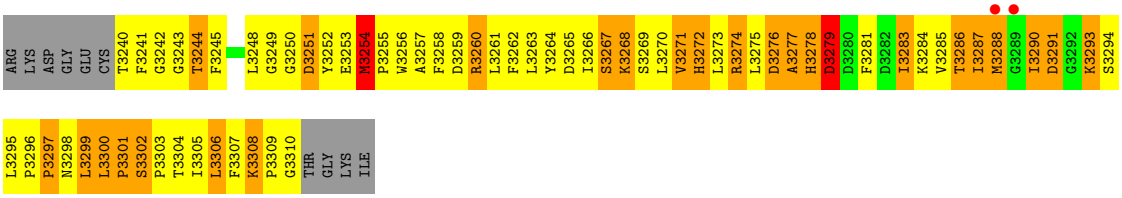
Chain F:




• Molecule 3: hemocyanin

Chain I:



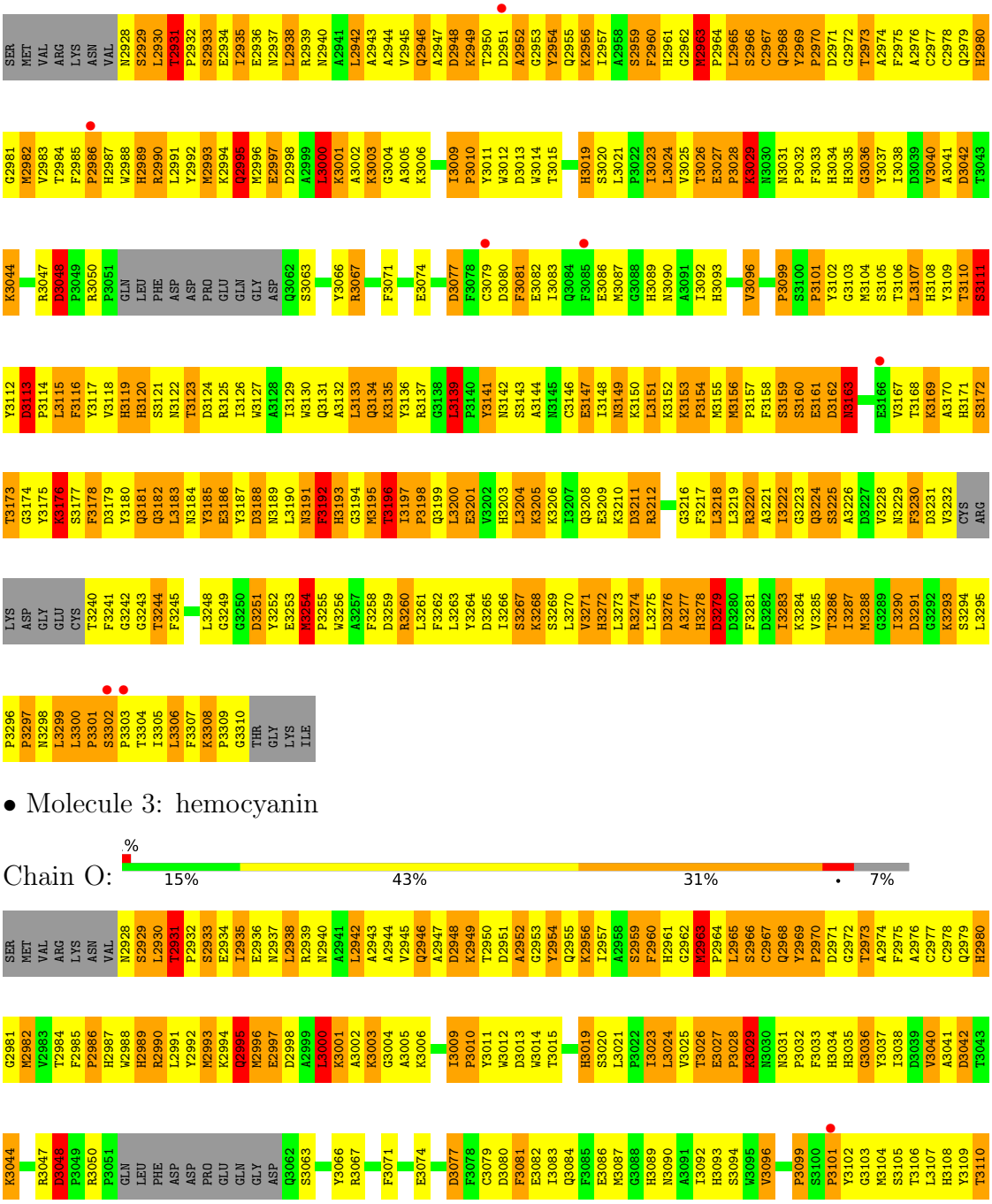




• Molecule 3: hemocyanin

Chain L:

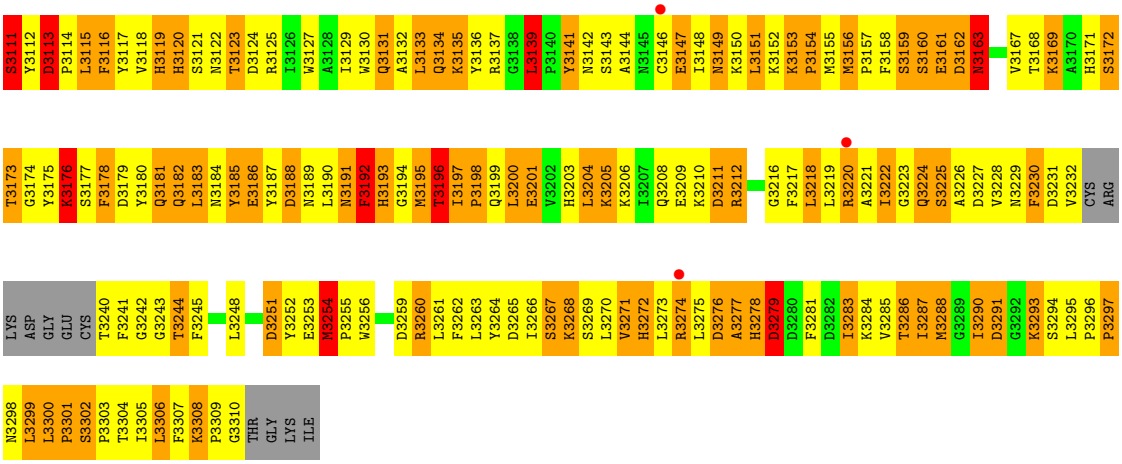


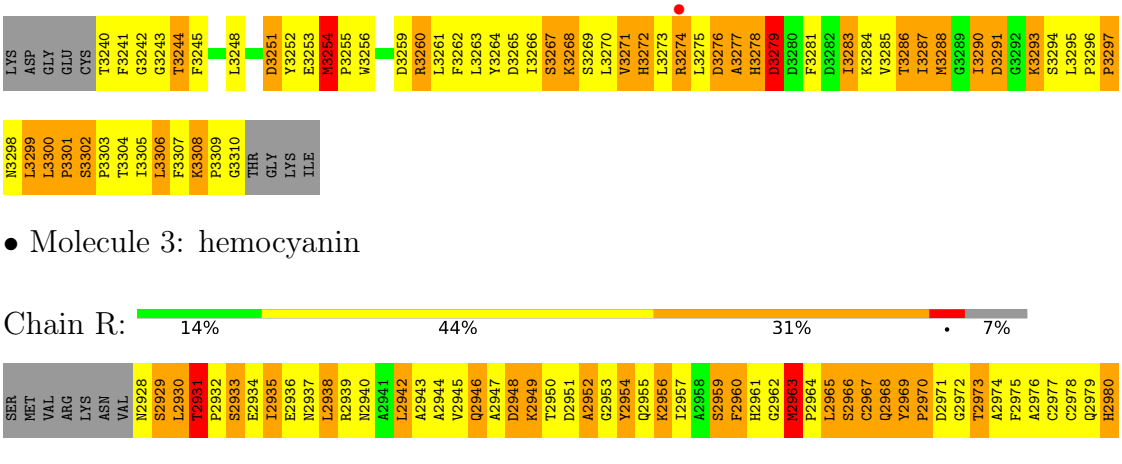



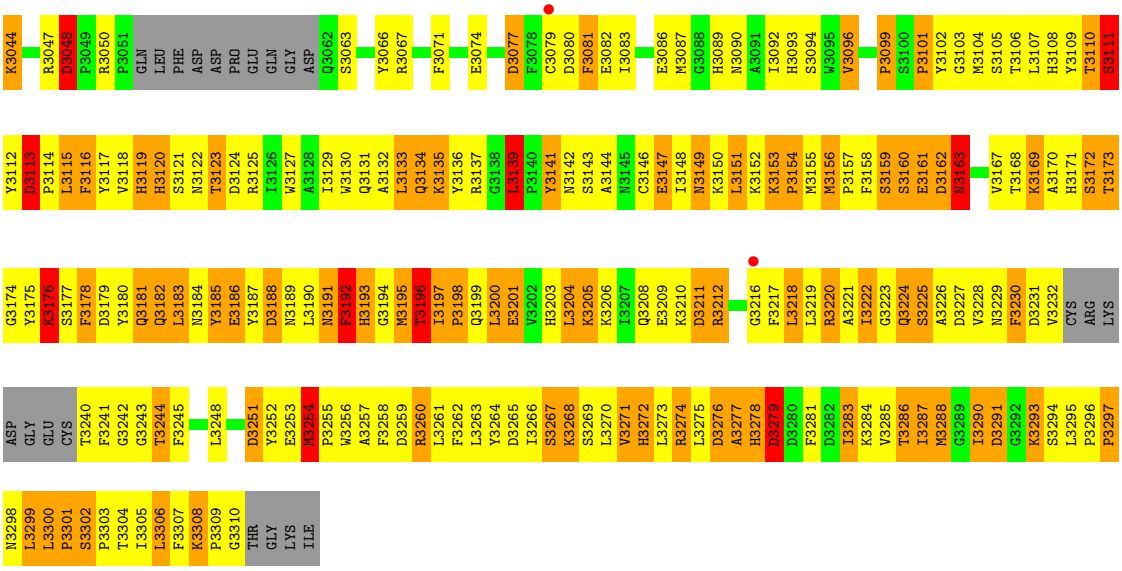


• Molecule 3: hemocyanin

Chain O:

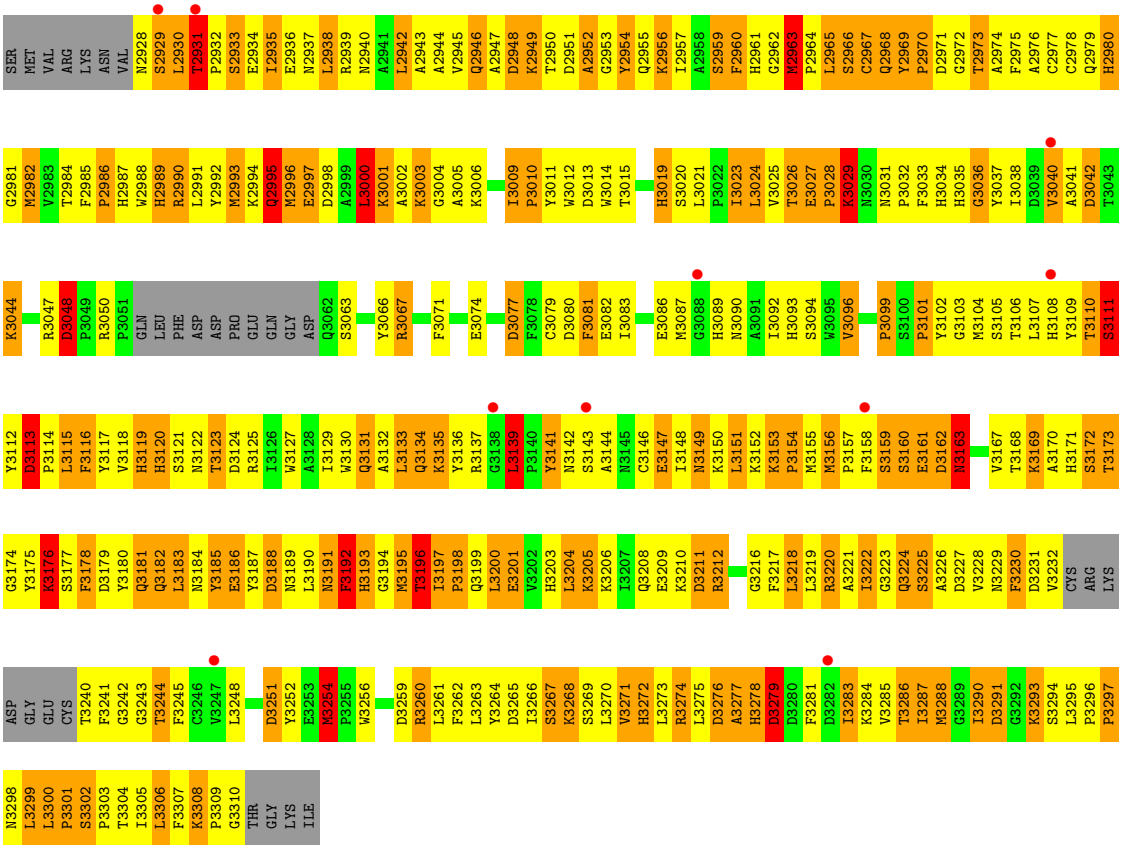






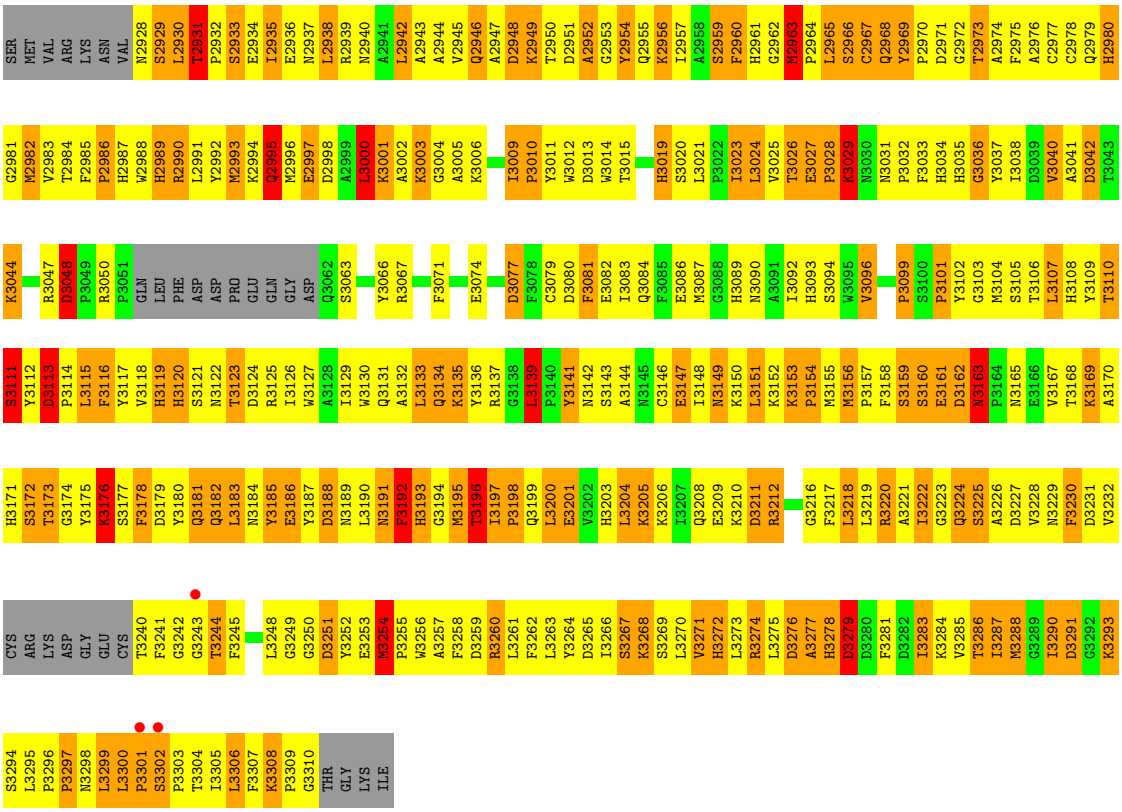
• Molecule 3: hemocyanin



• Molecule 3: hemocyanin

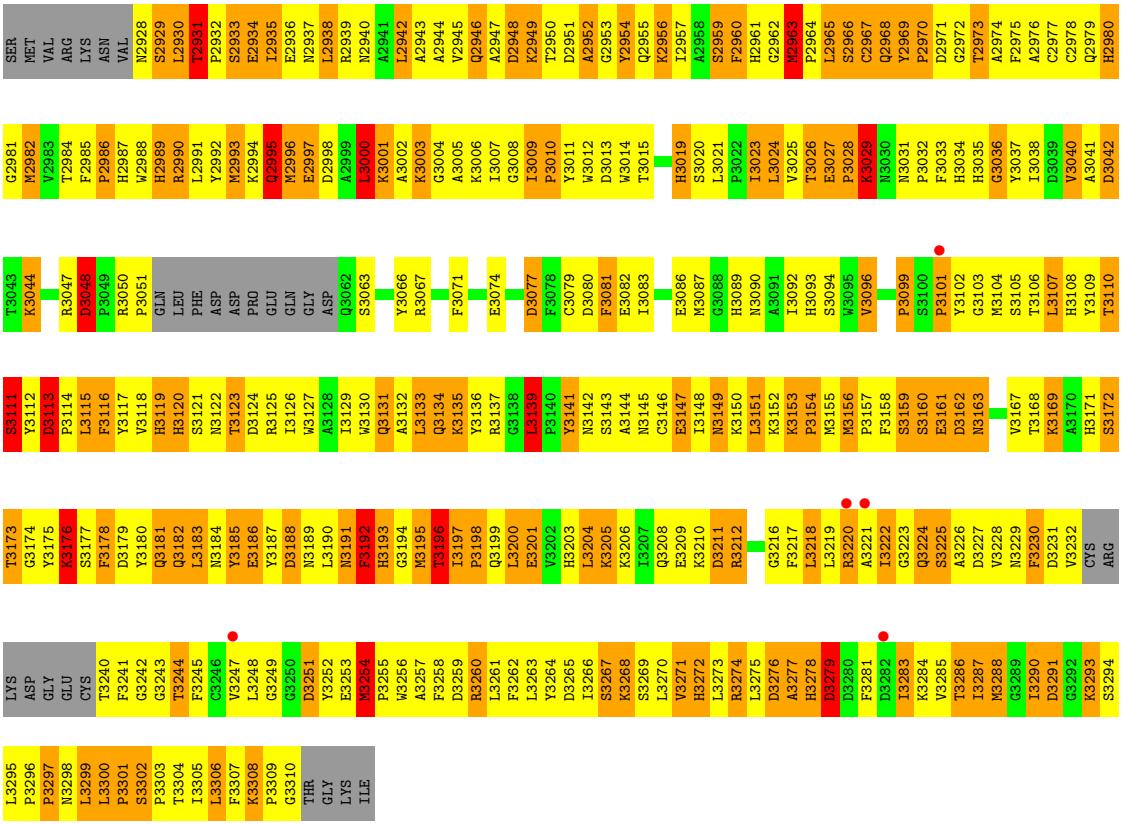




• Molecule 3: hemocyanin

Chain d:



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

Chain e:







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

Chain f:







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

Chain i:







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

Chain j:







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

Chain m:







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

Chain n:







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

Chain o:






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

Chain p:







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

Chain q:







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

Chain s:







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

Chain t:







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

Chain u:







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

Chain v:






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

Chain x:







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

Chain 1:







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

Chain 2:

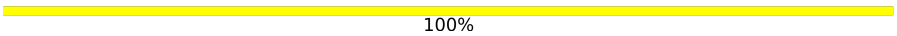






• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:







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

Chain 6:







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

Chain 7:

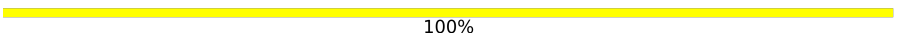






• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:






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

Chain 9:







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

Chain BA:







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

Chain HA:

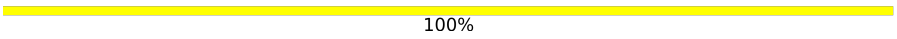






• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:







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

Chain JA:







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

Chain MA:






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

Chain OA:







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

Chain QA:







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

Chain RA:







• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:







• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

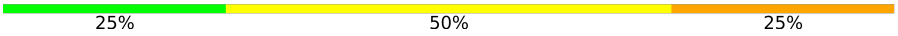






• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:







• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:







• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA:







• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PA:

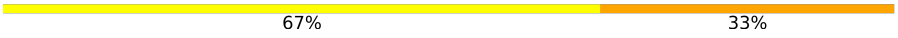






• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:







• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

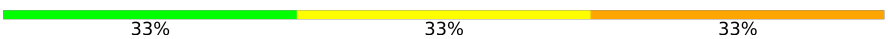






• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:







• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

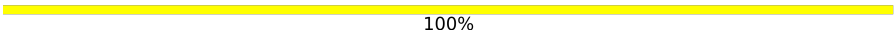
Chain w:






• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:

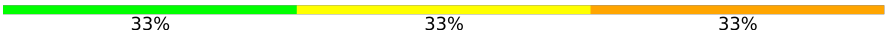






• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:







• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:







• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:







• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:

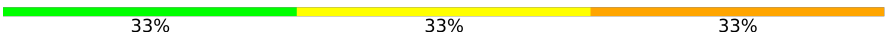






• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:







• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:






• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA:







• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:

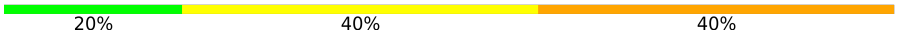






• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:







• Molecule 8: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:






# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 171.37Å 538.66Å 310.92Å<br>90.00° 104.09° 90.00° | Depositor |
| Resolution (Å) | 49.10 – 3.00<br>49.10 – 3.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.9 (49.10-3.00)<br>89.6 (49.10-3.00) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.11 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.74 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX 1.9_1692 | Depositor |
| R, $R_{free}$ | 0.274 , 0.303<br>0.275 , 0.304 | Depositor<br>DCC |
| $R_{free}$ test set | 53588 reflections (4.95%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 64.8 | Xtriage |
| Anisotropy | 0.538 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.28 , 69.7 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.42$, $< L^2 > = 0.24$ | Xtriage |
| Estimated twinning fraction | 0.055 for h,-k,-h-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 261470 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 68.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.37 | 0/13698 | 0.89 | 40/18607 (0.2%) |
| 1 | D | 0.37 | 0/13698 | 0.89 | 21/18607 (0.1%) |
| 1 | G | 0.37 | 1/13698 (0.0%) | 0.86 | 27/18607 (0.1%) |
| 1 | J | 0.37 | 0/13698 | 0.87 | 22/18607 (0.1%) |
| 1 | M | 0.35 | 0/13698 | 0.87 | 32/18607 (0.2%) |
| 1 | P | 0.36 | 1/13698 (0.0%) | 0.86 | 34/18607 (0.2%) |
| 1 | S | 0.36 | 0/13698 | 0.86 | 32/18607 (0.2%) |
| 1 | V | 0.36 | 0/13698 | 0.85 | 33/18607 (0.2%) |
| 1 | Y | 0.34 | 0/13698 | 0.84 | 21/18607 (0.1%) |
| 1 | b | 0.35 | 0/13698 | 0.87 | 26/18607 (0.1%) |
| 2 | B | 0.34 | 0/6909 | 0.85 | 12/9383 (0.1%) |
| 2 | E | 0.35 | 0/6909 | 0.87 | 17/9383 (0.2%) |
| 2 | H | 0.35 | 0/6909 | 0.84 | 14/9383 (0.1%) |
| 2 | K | 0.35 | 0/6909 | 0.85 | 13/9383 (0.1%) |
| 2 | N | 0.35 | 0/6909 | 0.84 | 9/9383 (0.1%) |
| 2 | Q | 0.34 | 0/6909 | 0.83 | 11/9383 (0.1%) |
| 2 | T | 0.34 | 0/6909 | 0.82 | 9/9383 (0.1%) |
| 2 | W | 0.33 | 0/6909 | 0.84 | 18/9383 (0.2%) |
| 2 | Z | 0.33 | 0/6909 | 0.84 | 13/9383 (0.1%) |
| 2 | c | 0.33 | 0/6909 | 0.82 | 9/9383 (0.1%) |
| 3 | C | 1.08 | 36/6100 (0.6%) | 1.39 | 120/8282 (1.4%) |
| 3 | F | 1.08 | 36/6100 (0.6%) | 1.40 | 120/8282 (1.4%) |
| 3 | I | 1.08 | 34/6100 (0.6%) | 1.40 | 120/8282 (1.4%) |
| 3 | L | 1.08 | 36/6100 (0.6%) | 1.39 | 120/8282 (1.4%) |
| 3 | O | 1.08 | 36/6100 (0.6%) | 1.39 | 120/8282 (1.4%) |
| 3 | R | 1.08 | 36/6100 (0.6%) | 1.40 | 120/8282 (1.4%) |
| 3 | U | 1.08 | 36/6100 (0.6%) | 1.40 | 122/8282 (1.5%) |
| 3 | X | 1.08 | 38/6100 (0.6%) | 1.40 | 116/8282 (1.4%) |
| 3 | a | 1.08 | 34/6100 (0.6%) | 1.39 | 120/8282 (1.4%) |
| 3 | d | 1.08 | 38/6100 (0.6%) | 1.40 | 122/8282 (1.5%) |
| All | All | 0.60 | 362/267070 (0.1%) | 1.01 | 1613/362720 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 2 |
| 1 | D | 0 | 3 |
| 1 | G | 0 | 1 |
| 1 | J | 0 | 2 |
| 1 | M | 0 | 1 |
| 1 | S | 0 | 3 |
| 1 | Y | 0 | 1 |
| 1 | b | 0 | 2 |
| 2 | B | 0 | 1 |
| 2 | K | 0 | 3 |
| 2 | N | 0 | 1 |
| 2 | Q | 0 | 1 |
| 2 | T | 0 | 2 |
| 2 | W | 0 | 1 |
| 2 | Z | 0 | 2 |
| 2 | c | 0 | 1 |
| 3 | C | 0 | 4 |
| 3 | F | 0 | 4 |
| 3 | I | 0 | 4 |
| 3 | L | 0 | 4 |
| 3 | O | 0 | 4 |
| 3 | R | 0 | 4 |
| 3 | U | 0 | 4 |
| 3 | X | 0 | 4 |
| 3 | a | 0 | 4 |
| 3 | d | 0 | 4 |
| All | All | 0 | 67 |

All (362) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | a | 3296[A] | PRO | C-N | 6.78 | 1.41 | 1.33 |
| 3 | a | 3296[B] | PRO | C-N | 6.78 | 1.41 | 1.33 |
| 3 | O | 3296[A] | PRO | C-N | 6.77 | 1.41 | 1.33 |
| 3 | O | 3296[B] | PRO | C-N | 6.77 | 1.41 | 1.33 |
| 3 | L | 3296[A] | PRO | C-N | 6.76 | 1.41 | 1.33 |
| 3 | L | 3296[B] | PRO | C-N | 6.76 | 1.41 | 1.33 |
| 3 | C | 3296[A] | PRO | C-N | 6.75 | 1.41 | 1.33 |
| 3 | C | 3296[B] | PRO | C-N | 6.75 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | X | 3296[A] | PRO | C-N | 6.75 | 1.41 | 1.33 |
| 3 | X | 3296[B] | PRO | C-N | 6.75 | 1.41 | 1.33 |
| 3 | U | 3296[A] | PRO | C-N | 6.75 | 1.41 | 1.33 |
| 3 | U | 3296[B] | PRO | C-N | 6.75 | 1.41 | 1.33 |
| 3 | d | 3296[A] | PRO | C-N | 6.74 | 1.41 | 1.33 |
| 3 | d | 3296[B] | PRO | C-N | 6.74 | 1.41 | 1.33 |
| 3 | F | 3296[A] | PRO | C-N | 6.71 | 1.41 | 1.33 |
| 3 | F | 3296[B] | PRO | C-N | 6.71 | 1.41 | 1.33 |
| 3 | R | 3296[A] | PRO | C-N | 6.71 | 1.41 | 1.33 |
| 3 | R | 3296[B] | PRO | C-N | 6.71 | 1.41 | 1.33 |
| 3 | I | 3296[A] | PRO | C-N | 6.68 | 1.41 | 1.33 |
| 3 | I | 3296[B] | PRO | C-N | 6.68 | 1.41 | 1.33 |
| 3 | U | 2989[A] | HIS | CA-C | -6.45 | 1.46 | 1.53 |
| 3 | U | 2989[B] | HIS | CA-C | -6.45 | 1.46 | 1.53 |
| 3 | I | 2989[A] | HIS | CA-C | -6.45 | 1.46 | 1.53 |
| 3 | I | 2989[B] | HIS | CA-C | -6.45 | 1.46 | 1.53 |
| 3 | L | 2989[A] | HIS | CA-C | -6.44 | 1.46 | 1.53 |
| 3 | L | 2989[B] | HIS | CA-C | -6.44 | 1.46 | 1.53 |
| 3 | C | 2989[A] | HIS | CA-C | -6.40 | 1.46 | 1.53 |
| 3 | C | 2989[B] | HIS | CA-C | -6.40 | 1.46 | 1.53 |
| 3 | d | 2989[A] | HIS | CA-C | -6.38 | 1.46 | 1.53 |
| 3 | d | 2989[B] | HIS | CA-C | -6.38 | 1.46 | 1.53 |
| 3 | F | 2989[A] | HIS | CA-C | -6.36 | 1.46 | 1.53 |
| 3 | F | 2989[B] | HIS | CA-C | -6.36 | 1.46 | 1.53 |
| 3 | F | 3308[A] | LYS | C-N | 6.36 | 1.41 | 1.33 |
| 3 | F | 3308[B] | LYS | C-N | 6.36 | 1.41 | 1.33 |
| 3 | R | 2989[A] | HIS | CA-C | -6.35 | 1.46 | 1.53 |
| 3 | R | 2989[B] | HIS | CA-C | -6.35 | 1.46 | 1.53 |
| 3 | C | 3308[A] | LYS | C-N | 6.33 | 1.41 | 1.33 |
| 3 | C | 3308[B] | LYS | C-N | 6.33 | 1.41 | 1.33 |
| 3 | U | 2963[A] | MET | C-N | 6.33 | 1.41 | 1.33 |
| 3 | U | 2963[B] | MET | C-N | 6.33 | 1.41 | 1.33 |
| 3 | X | 2989[A] | HIS | CA-C | -6.31 | 1.46 | 1.53 |
| 3 | X | 2989[B] | HIS | CA-C | -6.31 | 1.46 | 1.53 |
| 3 | d | 2963[A] | MET | C-N | 6.31 | 1.41 | 1.33 |
| 3 | d | 2963[B] | MET | C-N | 6.31 | 1.41 | 1.33 |
| 3 | d | 3308[A] | LYS | C-N | 6.31 | 1.40 | 1.33 |
| 3 | d | 3308[B] | LYS | C-N | 6.31 | 1.40 | 1.33 |
| 3 | L | 2963[A] | MET | C-N | 6.31 | 1.41 | 1.33 |
| 3 | L | 2963[B] | MET | C-N | 6.31 | 1.41 | 1.33 |
| 3 | L | 3308[A] | LYS | C-N | 6.30 | 1.40 | 1.33 |
| 3 | L | 3308[B] | LYS | C-N | 6.30 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | X | 3308[A] | LYS | C-N | 6.30 | 1.40 | 1.33 |
| 3 | X | 3308[B] | LYS | C-N | 6.30 | 1.40 | 1.33 |
| 3 | a | 2989[A] | HIS | CA-C | -6.29 | 1.46 | 1.53 |
| 3 | a | 2989[B] | HIS | CA-C | -6.29 | 1.46 | 1.53 |
| 3 | I | 2963[A] | MET | C-N | 6.29 | 1.41 | 1.33 |
| 3 | I | 2963[B] | MET | C-N | 6.29 | 1.41 | 1.33 |
| 3 | X | 2963[A] | MET | C-N | 6.29 | 1.41 | 1.33 |
| 3 | X | 2963[B] | MET | C-N | 6.29 | 1.41 | 1.33 |
| 3 | a | 3308[A] | LYS | C-N | 6.28 | 1.40 | 1.33 |
| 3 | a | 3308[B] | LYS | C-N | 6.28 | 1.40 | 1.33 |
| 3 | O | 2989[A] | HIS | CA-C | -6.28 | 1.46 | 1.53 |
| 3 | O | 2989[B] | HIS | CA-C | -6.28 | 1.46 | 1.53 |
| 3 | R | 3308[A] | LYS | C-N | 6.28 | 1.40 | 1.33 |
| 3 | R | 3308[B] | LYS | C-N | 6.28 | 1.40 | 1.33 |
| 3 | F | 2963[A] | MET | C-N | 6.27 | 1.41 | 1.33 |
| 3 | F | 2963[B] | MET | C-N | 6.27 | 1.41 | 1.33 |
| 3 | O | 2963[A] | MET | C-N | 6.27 | 1.41 | 1.33 |
| 3 | O | 2963[B] | MET | C-N | 6.27 | 1.41 | 1.33 |
| 3 | U | 3308[A] | LYS | C-N | 6.26 | 1.40 | 1.33 |
| 3 | U | 3308[B] | LYS | C-N | 6.26 | 1.40 | 1.33 |
| 3 | a | 2963[A] | MET | C-N | 6.25 | 1.41 | 1.33 |
| 3 | a | 2963[B] | MET | C-N | 6.25 | 1.41 | 1.33 |
| 3 | C | 2963[A] | MET | C-N | 6.23 | 1.41 | 1.33 |
| 3 | C | 2963[B] | MET | C-N | 6.23 | 1.41 | 1.33 |
| 3 | I | 3308[A] | LYS | C-N | 6.23 | 1.40 | 1.33 |
| 3 | I | 3308[B] | LYS | C-N | 6.23 | 1.40 | 1.33 |
| 3 | R | 2963[A] | MET | C-N | 6.22 | 1.41 | 1.33 |
| 3 | R | 2963[B] | MET | C-N | 6.22 | 1.41 | 1.33 |
| 3 | O | 3308[A] | LYS | C-N | 6.19 | 1.40 | 1.33 |
| 3 | O | 3308[B] | LYS | C-N | 6.19 | 1.40 | 1.33 |
| 3 | I | 3153[A] | LYS | C-N | 6.19 | 1.40 | 1.33 |
| 3 | I | 3153[B] | LYS | C-N | 6.19 | 1.40 | 1.33 |
| 3 | L | 3153[A] | LYS | C-N | 6.12 | 1.40 | 1.33 |
| 3 | L | 3153[B] | LYS | C-N | 6.12 | 1.40 | 1.33 |
| 3 | I | 3048[A] | ASP | C-N | 6.11 | 1.41 | 1.33 |
| 3 | I | 3048[B] | ASP | C-N | 6.11 | 1.41 | 1.33 |
| 3 | U | 3153[A] | LYS | C-N | 6.11 | 1.40 | 1.33 |
| 3 | U | 3153[B] | LYS | C-N | 6.11 | 1.40 | 1.33 |
| 3 | a | 3048[A] | ASP | C-N | 6.11 | 1.41 | 1.33 |
| 3 | a | 3048[B] | ASP | C-N | 6.11 | 1.41 | 1.33 |
| 3 | X | 3153[A] | LYS | C-N | 6.11 | 1.40 | 1.33 |
| 3 | X | 3153[B] | LYS | C-N | 6.11 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | O | 3048[A] | ASP | C-N | 6.09 | 1.41 | 1.33 |
| 3 | O | 3048[B] | ASP | C-N | 6.09 | 1.41 | 1.33 |
| 3 | R | 3048[A] | ASP | C-N | 6.08 | 1.41 | 1.33 |
| 3 | R | 3048[B] | ASP | C-N | 6.08 | 1.41 | 1.33 |
| 3 | F | 3153[A] | LYS | C-N | 6.08 | 1.40 | 1.33 |
| 3 | F | 3153[B] | LYS | C-N | 6.08 | 1.40 | 1.33 |
| 3 | U | 3048[A] | ASP | C-N | 6.07 | 1.41 | 1.33 |
| 3 | U | 3048[B] | ASP | C-N | 6.07 | 1.41 | 1.33 |
| 3 | F | 3048[A] | ASP | C-N | 6.07 | 1.41 | 1.33 |
| 3 | F | 3048[B] | ASP | C-N | 6.07 | 1.41 | 1.33 |
| 3 | R | 3153[A] | LYS | C-N | 6.06 | 1.40 | 1.33 |
| 3 | R | 3153[B] | LYS | C-N | 6.06 | 1.40 | 1.33 |
| 3 | X | 3048[A] | ASP | C-N | 6.06 | 1.41 | 1.33 |
| 3 | X | 3048[B] | ASP | C-N | 6.06 | 1.41 | 1.33 |
| 3 | a | 3153[A] | LYS | C-N | 6.06 | 1.40 | 1.33 |
| 3 | a | 3153[B] | LYS | C-N | 6.06 | 1.40 | 1.33 |
| 3 | d | 3153[A] | LYS | C-N | 6.04 | 1.40 | 1.33 |
| 3 | d | 3153[B] | LYS | C-N | 6.04 | 1.40 | 1.33 |
| 3 | C | 3153[A] | LYS | C-N | 6.04 | 1.40 | 1.33 |
| 3 | C | 3153[B] | LYS | C-N | 6.04 | 1.40 | 1.33 |
| 3 | O | 3153[A] | LYS | C-N | 6.03 | 1.40 | 1.33 |
| 3 | O | 3153[B] | LYS | C-N | 6.03 | 1.40 | 1.33 |
| 3 | L | 3048[A] | ASP | C-N | 6.02 | 1.41 | 1.33 |
| 3 | L | 3048[B] | ASP | C-N | 6.02 | 1.41 | 1.33 |
| 3 | d | 3048[A] | ASP | C-N | 6.00 | 1.41 | 1.33 |
| 3 | d | 3048[B] | ASP | C-N | 6.00 | 1.41 | 1.33 |
| 3 | C | 3048[A] | ASP | C-N | 5.97 | 1.41 | 1.33 |
| 3 | C | 3048[B] | ASP | C-N | 5.97 | 1.41 | 1.33 |
| 3 | d | 3254[A] | MET | C-N | 5.91 | 1.40 | 1.33 |
| 3 | d | 3254[B] | MET | C-N | 5.91 | 1.40 | 1.33 |
| 3 | R | 3254[A] | MET | C-N | 5.88 | 1.40 | 1.33 |
| 3 | R | 3254[B] | MET | C-N | 5.88 | 1.40 | 1.33 |
| 3 | a | 3254[A] | MET | C-N | 5.88 | 1.40 | 1.33 |
| 3 | a | 3254[B] | MET | C-N | 5.88 | 1.40 | 1.33 |
| 3 | L | 3254[A] | MET | C-N | 5.88 | 1.40 | 1.33 |
| 3 | L | 3254[B] | MET | C-N | 5.88 | 1.40 | 1.33 |
| 3 | O | 3254[A] | MET | C-N | 5.87 | 1.40 | 1.33 |
| 3 | O | 3254[B] | MET | C-N | 5.87 | 1.40 | 1.33 |
| 3 | I | 3254[A] | MET | C-N | 5.86 | 1.40 | 1.33 |
| 3 | I | 3254[B] | MET | C-N | 5.86 | 1.40 | 1.33 |
| 3 | U | 3254[A] | MET | C-N | 5.86 | 1.40 | 1.33 |
| 3 | U | 3254[B] | MET | C-N | 5.86 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | X | 3254[A] | MET | C-N | 5.85 | 1.40 | 1.33 |
| 3 | X | 3254[B] | MET | C-N | 5.85 | 1.40 | 1.33 |
| 3 | F | 3254[A] | MET | C-N | 5.85 | 1.40 | 1.33 |
| 3 | F | 3254[B] | MET | C-N | 5.85 | 1.40 | 1.33 |
| 3 | C | 3254[A] | MET | C-N | 5.76 | 1.40 | 1.33 |
| 3 | C | 3254[B] | MET | C-N | 5.76 | 1.40 | 1.33 |
| 3 | R | 2931[A] | THR | C-N | 5.66 | 1.41 | 1.33 |
| 3 | R | 2931[B] | THR | C-N | 5.66 | 1.41 | 1.33 |
| 3 | U | 2931[A] | THR | C-N | 5.60 | 1.40 | 1.33 |
| 3 | U | 2931[B] | THR | C-N | 5.60 | 1.40 | 1.33 |
| 3 | F | 2931[A] | THR | C-N | 5.59 | 1.40 | 1.33 |
| 3 | F | 2931[B] | THR | C-N | 5.59 | 1.40 | 1.33 |
| 3 | a | 2931[A] | THR | C-N | 5.59 | 1.40 | 1.33 |
| 3 | a | 2931[B] | THR | C-N | 5.59 | 1.40 | 1.33 |
| 3 | I | 2931[A] | THR | C-N | 5.58 | 1.40 | 1.33 |
| 3 | I | 2931[B] | THR | C-N | 5.58 | 1.40 | 1.33 |
| 3 | d | 2931[A] | THR | C-N | 5.57 | 1.40 | 1.33 |
| 3 | d | 2931[B] | THR | C-N | 5.57 | 1.40 | 1.33 |
| 3 | O | 2931[A] | THR | C-N | 5.56 | 1.40 | 1.33 |
| 3 | O | 2931[B] | THR | C-N | 5.56 | 1.40 | 1.33 |
| 3 | X | 2931[A] | THR | C-N | 5.56 | 1.40 | 1.33 |
| 3 | X | 2931[B] | THR | C-N | 5.56 | 1.40 | 1.33 |
| 3 | C | 2931[A] | THR | C-N | 5.55 | 1.40 | 1.33 |
| 3 | C | 2931[B] | THR | C-N | 5.55 | 1.40 | 1.33 |
| 3 | L | 2931[A] | THR | C-N | 5.54 | 1.40 | 1.33 |
| 3 | L | 2931[B] | THR | C-N | 5.54 | 1.40 | 1.33 |
| 3 | F | 3009[A] | ILE | C-N | 5.50 | 1.40 | 1.33 |
| 3 | F | 3009[B] | ILE | C-N | 5.50 | 1.40 | 1.33 |
| 3 | C | 3009[A] | ILE | C-N | 5.50 | 1.40 | 1.33 |
| 3 | C | 3009[B] | ILE | C-N | 5.50 | 1.40 | 1.33 |
| 3 | O | 3009[A] | ILE | C-N | 5.45 | 1.40 | 1.33 |
| 3 | O | 3009[B] | ILE | C-N | 5.45 | 1.40 | 1.33 |
| 3 | R | 3009[A] | ILE | C-N | 5.45 | 1.40 | 1.33 |
| 3 | R | 3009[B] | ILE | C-N | 5.45 | 1.40 | 1.33 |
| 3 | I | 3009[A] | ILE | C-N | 5.45 | 1.40 | 1.33 |
| 3 | I | 3009[B] | ILE | C-N | 5.45 | 1.40 | 1.33 |
| 3 | U | 3009[A] | ILE | C-N | 5.42 | 1.40 | 1.33 |
| 3 | U | 3009[B] | ILE | C-N | 5.42 | 1.40 | 1.33 |
| 3 | a | 3009[A] | ILE | C-N | 5.42 | 1.40 | 1.33 |
| 3 | a | 3009[B] | ILE | C-N | 5.42 | 1.40 | 1.33 |
| 3 | L | 3009[A] | ILE | C-N | 5.39 | 1.40 | 1.33 |
| 3 | L | 3009[B] | ILE | C-N | 5.39 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | d | 2969[A] | TYR | C-N | 5.39 | 1.40 | 1.33 |
| 3 | d | 2969[B] | TYR | C-N | 5.39 | 1.40 | 1.33 |
| 3 | R | 3139[A] | LEU | C-N | 5.38 | 1.40 | 1.33 |
| 3 | R | 3139[B] | LEU | C-N | 5.38 | 1.40 | 1.33 |
| 3 | a | 3139[A] | LEU | C-N | 5.38 | 1.40 | 1.33 |
| 3 | a | 3139[B] | LEU | C-N | 5.38 | 1.40 | 1.33 |
| 3 | O | 2969[A] | TYR | C-N | 5.37 | 1.40 | 1.33 |
| 3 | O | 2969[B] | TYR | C-N | 5.37 | 1.40 | 1.33 |
| 3 | U | 2969[A] | TYR | C-N | 5.37 | 1.40 | 1.33 |
| 3 | U | 2969[B] | TYR | C-N | 5.37 | 1.40 | 1.33 |
| 3 | X | 3009[A] | ILE | C-N | 5.36 | 1.40 | 1.33 |
| 3 | X | 3009[B] | ILE | C-N | 5.36 | 1.40 | 1.33 |
| 3 | a | 2969[A] | TYR | C-N | 5.36 | 1.40 | 1.33 |
| 3 | a | 2969[B] | TYR | C-N | 5.36 | 1.40 | 1.33 |
| 3 | d | 3139[A] | LEU | C-N | 5.34 | 1.40 | 1.33 |
| 3 | d | 3139[B] | LEU | C-N | 5.34 | 1.40 | 1.33 |
| 3 | d | 3009[A] | ILE | C-N | 5.33 | 1.40 | 1.33 |
| 3 | d | 3009[B] | ILE | C-N | 5.33 | 1.40 | 1.33 |
| 3 | X | 3154[A] | PRO | N-CD | 5.33 | 1.55 | 1.47 |
| 3 | X | 3154[B] | PRO | N-CD | 5.33 | 1.55 | 1.47 |
| 3 | F | 3139[A] | LEU | C-N | 5.31 | 1.40 | 1.33 |
| 3 | F | 3139[B] | LEU | C-N | 5.31 | 1.40 | 1.33 |
| 3 | L | 2969[A] | TYR | C-N | 5.31 | 1.40 | 1.33 |
| 3 | L | 2969[B] | TYR | C-N | 5.31 | 1.40 | 1.33 |
| 3 | O | 3154[A] | PRO | N-CD | 5.31 | 1.55 | 1.47 |
| 3 | O | 3154[B] | PRO | N-CD | 5.31 | 1.55 | 1.47 |
| 3 | U | 3139[A] | LEU | C-N | 5.31 | 1.40 | 1.33 |
| 3 | U | 3139[B] | LEU | C-N | 5.31 | 1.40 | 1.33 |
| 3 | C | 3154[A] | PRO | N-CD | 5.31 | 1.55 | 1.47 |
| 3 | C | 3154[B] | PRO | N-CD | 5.31 | 1.55 | 1.47 |
| 3 | C | 3139[A] | LEU | C-N | 5.31 | 1.40 | 1.33 |
| 3 | C | 3139[B] | LEU | C-N | 5.31 | 1.40 | 1.33 |
| 3 | X | 2969[A] | TYR | C-N | 5.31 | 1.40 | 1.33 |
| 3 | X | 2969[B] | TYR | C-N | 5.31 | 1.40 | 1.33 |
| 3 | R | 3154[A] | PRO | N-CD | 5.30 | 1.55 | 1.47 |
| 3 | R | 3154[B] | PRO | N-CD | 5.30 | 1.55 | 1.47 |
| 3 | X | 3139[A] | LEU | C-N | 5.30 | 1.40 | 1.33 |
| 3 | X | 3139[B] | LEU | C-N | 5.30 | 1.40 | 1.33 |
| 3 | C | 2969[A] | TYR | C-N | 5.29 | 1.40 | 1.33 |
| 3 | C | 2969[B] | TYR | C-N | 5.29 | 1.40 | 1.33 |
| 3 | F | 2969[A] | TYR | C-N | 5.29 | 1.40 | 1.33 |
| 3 | F | 2969[B] | TYR | C-N | 5.29 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | L | 3139[A] | LEU | C-N | 5.29 | 1.40 | 1.33 |
| 3 | L | 3139[B] | LEU | C-N | 5.29 | 1.40 | 1.33 |
| 3 | a | 3154[A] | PRO | N-CD | 5.29 | 1.55 | 1.47 |
| 3 | a | 3154[B] | PRO | N-CD | 5.29 | 1.55 | 1.47 |
| 3 | O | 3139[A] | LEU | C-N | 5.28 | 1.40 | 1.33 |
| 3 | O | 3139[B] | LEU | C-N | 5.28 | 1.40 | 1.33 |
| 3 | R | 2969[A] | TYR | C-N | 5.28 | 1.40 | 1.33 |
| 3 | R | 2969[B] | TYR | C-N | 5.28 | 1.40 | 1.33 |
| 3 | I | 2969[A] | TYR | C-N | 5.27 | 1.40 | 1.33 |
| 3 | I | 2969[B] | TYR | C-N | 5.27 | 1.40 | 1.33 |
| 3 | I | 3139[A] | LEU | C-N | 5.27 | 1.40 | 1.33 |
| 3 | I | 3139[B] | LEU | C-N | 5.27 | 1.40 | 1.33 |
| 3 | X | 3028[A] | PRO | N-CD | 5.25 | 1.55 | 1.47 |
| 3 | X | 3028[B] | PRO | N-CD | 5.25 | 1.55 | 1.47 |
| 3 | L | 3154[A] | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 3 | L | 3154[B] | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 1 | P | 1339 | SER | CA-C | 5.24 | 1.58 | 1.53 |
| 3 | d | 3154[A] | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 3 | d | 3154[B] | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 3 | R | 3028[A] | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 3 | R | 3028[B] | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 3 | a | 3028[A] | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 3 | a | 3028[B] | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 3 | I | 3154[A] | PRO | N-CD | 5.23 | 1.55 | 1.47 |
| 3 | I | 3154[B] | PRO | N-CD | 5.23 | 1.55 | 1.47 |
| 3 | U | 3154[A] | PRO | N-CD | 5.23 | 1.55 | 1.47 |
| 3 | U | 3154[B] | PRO | N-CD | 5.23 | 1.55 | 1.47 |
| 3 | F | 3154[A] | PRO | N-CD | 5.22 | 1.55 | 1.47 |
| 3 | F | 3154[B] | PRO | N-CD | 5.22 | 1.55 | 1.47 |
| 3 | O | 3028[A] | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 3 | O | 3028[B] | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 3 | L | 3198[A] | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 3 | L | 3198[B] | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 3 | U | 2986[A] | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 3 | U | 2986[B] | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 3 | a | 2986[A] | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 3 | a | 2986[B] | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 3 | C | 3028[A] | PRO | N-CD | 5.20 | 1.55 | 1.47 |
| 3 | C | 3028[B] | PRO | N-CD | 5.20 | 1.55 | 1.47 |
| 3 | F | 3028[A] | PRO | N-CD | 5.20 | 1.55 | 1.47 |
| 3 | F | 3028[B] | PRO | N-CD | 5.20 | 1.55 | 1.47 |
| 3 | O | 2986[A] | PRO | N-CD | 5.20 | 1.55 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | O | 2986[B] | PRO | N-CD | 5.20 | 1.55 | 1.47 |
| 3 | U | 3010[A] | PRO | N-CD | 5.19 | 1.55 | 1.47 |
| 3 | U | 3010[B] | PRO | N-CD | 5.19 | 1.55 | 1.47 |
| 3 | I | 3028[A] | PRO | N-CD | 5.19 | 1.55 | 1.47 |
| 3 | I | 3028[B] | PRO | N-CD | 5.19 | 1.55 | 1.47 |
| 3 | L | 2986[A] | PRO | N-CD | 5.19 | 1.55 | 1.47 |
| 3 | L | 2986[B] | PRO | N-CD | 5.19 | 1.55 | 1.47 |
| 3 | X | 3010[A] | PRO | N-CD | 5.18 | 1.55 | 1.47 |
| 3 | X | 3010[B] | PRO | N-CD | 5.18 | 1.55 | 1.47 |
| 3 | C | 3010[A] | PRO | N-CD | 5.18 | 1.55 | 1.47 |
| 3 | C | 3010[B] | PRO | N-CD | 5.18 | 1.55 | 1.47 |
| 3 | a | 3010[A] | PRO | N-CD | 5.18 | 1.55 | 1.47 |
| 3 | a | 3010[B] | PRO | N-CD | 5.18 | 1.55 | 1.47 |
| 3 | d | 3028[A] | PRO | N-CD | 5.18 | 1.54 | 1.47 |
| 3 | d | 3028[B] | PRO | N-CD | 5.18 | 1.54 | 1.47 |
| 3 | L | 3010[A] | PRO | N-CD | 5.17 | 1.54 | 1.47 |
| 3 | L | 3010[B] | PRO | N-CD | 5.17 | 1.54 | 1.47 |
| 3 | L | 3028[A] | PRO | N-CD | 5.17 | 1.54 | 1.47 |
| 3 | L | 3028[B] | PRO | N-CD | 5.17 | 1.54 | 1.47 |
| 3 | I | 3198[A] | PRO | N-CD | 5.17 | 1.54 | 1.47 |
| 3 | I | 3198[B] | PRO | N-CD | 5.17 | 1.54 | 1.47 |
| 3 | O | 3198[A] | PRO | N-CD | 5.16 | 1.54 | 1.47 |
| 3 | O | 3198[B] | PRO | N-CD | 5.16 | 1.54 | 1.47 |
| 3 | X | 2986[A] | PRO | N-CD | 5.16 | 1.54 | 1.47 |
| 3 | X | 2986[B] | PRO | N-CD | 5.16 | 1.54 | 1.47 |
| 3 | I | 2986[A] | PRO | N-CD | 5.16 | 1.54 | 1.47 |
| 3 | I | 2986[B] | PRO | N-CD | 5.16 | 1.54 | 1.47 |
| 3 | R | 3198[A] | PRO | N-CD | 5.16 | 1.54 | 1.47 |
| 3 | R | 3198[B] | PRO | N-CD | 5.16 | 1.54 | 1.47 |
| 3 | F | 2986[A] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | F | 2986[B] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | R | 3010[A] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | R | 3010[B] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | d | 3010[A] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | d | 3010[B] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | C | 2986[A] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | C | 2986[B] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | O | 3010[A] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | O | 3010[B] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | U | 3028[A] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | U | 3028[B] | PRO | N-CD | 5.15 | 1.54 | 1.47 |
| 3 | I | 3010[A] | PRO | N-CD | 5.13 | 1.54 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | I | 3010[B] | PRO | N-CD | 5.13 | 1.54 | 1.47 |
| 1 | G | 1339 | SER | CA-C | 5.13 | 1.58 | 1.53 |
| 3 | d | 3297[A] | PRO | N-CD | 5.13 | 1.54 | 1.47 |
| 3 | d | 3297[B] | PRO | N-CD | 5.13 | 1.54 | 1.47 |
| 3 | d | 2986[A] | PRO | N-CD | 5.12 | 1.54 | 1.47 |
| 3 | d | 2986[B] | PRO | N-CD | 5.12 | 1.54 | 1.47 |
| 3 | a | 3198[A] | PRO | N-CD | 5.12 | 1.54 | 1.47 |
| 3 | a | 3198[B] | PRO | N-CD | 5.12 | 1.54 | 1.47 |
| 3 | C | 3198[A] | PRO | N-CD | 5.12 | 1.54 | 1.47 |
| 3 | C | 3198[B] | PRO | N-CD | 5.12 | 1.54 | 1.47 |
| 3 | R | 2986[A] | PRO | N-CD | 5.12 | 1.54 | 1.47 |
| 3 | R | 2986[B] | PRO | N-CD | 5.12 | 1.54 | 1.47 |
| 3 | I | 3297[A] | PRO | N-CD | 5.11 | 1.54 | 1.47 |
| 3 | I | 3297[B] | PRO | N-CD | 5.11 | 1.54 | 1.47 |
| 3 | R | 2970[A] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | R | 2970[B] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | a | 3297[A] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | a | 3297[B] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | d | 3198[A] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | d | 3198[B] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | X | 3198[A] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | X | 3198[B] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | L | 3297[A] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | L | 3297[B] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | R | 3297[A] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | R | 3297[B] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | F | 3010[A] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | F | 3010[B] | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 3 | U | 3198[A] | PRO | N-CD | 5.09 | 1.54 | 1.47 |
| 3 | U | 3198[B] | PRO | N-CD | 5.09 | 1.54 | 1.47 |
| 3 | F | 2970[A] | PRO | N-CD | 5.09 | 1.54 | 1.47 |
| 3 | F | 2970[B] | PRO | N-CD | 5.09 | 1.54 | 1.47 |
| 3 | F | 3198[A] | PRO | N-CD | 5.08 | 1.54 | 1.47 |
| 3 | F | 3198[B] | PRO | N-CD | 5.08 | 1.54 | 1.47 |
| 3 | F | 3297[A] | PRO | N-CD | 5.07 | 1.54 | 1.47 |
| 3 | F | 3297[B] | PRO | N-CD | 5.07 | 1.54 | 1.47 |
| 3 | X | 3297[A] | PRO | N-CD | 5.06 | 1.54 | 1.47 |
| 3 | X | 3297[B] | PRO | N-CD | 5.06 | 1.54 | 1.47 |
| 3 | U | 3297[A] | PRO | N-CD | 5.06 | 1.54 | 1.47 |
| 3 | U | 3297[B] | PRO | N-CD | 5.06 | 1.54 | 1.47 |
| 3 | L | 2970[A] | PRO | N-CD | 5.06 | 1.54 | 1.47 |
| 3 | L | 2970[B] | PRO | N-CD | 5.06 | 1.54 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | d | 2970[A] | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 3 | d | 2970[B] | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 3 | C | 3297[A] | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 3 | C | 3297[B] | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 3 | O | 2970[A] | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 3 | O | 2970[B] | PRO | N-CD | 5.05 | 1.54 | 1.47 |
| 3 | O | 3297[A] | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 3 | O | 3297[B] | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 3 | C | 2970[A] | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 3 | C | 2970[B] | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 3 | d | 3051[A] | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 3 | d | 3051[B] | PRO | N-CD | 5.03 | 1.54 | 1.47 |
| 3 | X | 3027[A] | GLU | C-N | 5.02 | 1.40 | 1.34 |
| 3 | X | 3027[B] | GLU | C-N | 5.02 | 1.40 | 1.34 |
| 3 | X | 2970[A] | PRO | N-CD | 5.02 | 1.54 | 1.47 |
| 3 | X | 2970[B] | PRO | N-CD | 5.02 | 1.54 | 1.47 |
| 3 | U | 2970[A] | PRO | N-CD | 5.00 | 1.54 | 1.47 |
| 3 | U | 2970[B] | PRO | N-CD | 5.00 | 1.54 | 1.47 |

All (1613) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 464 | LEU | CA-C-N | -16.02 | 99.82 | 119.84 |
| 1 | D | 464 | LEU | C-N-CA | -16.02 | 99.82 | 119.84 |
| 1 | J | 883 | CYS | CA-C-N | -12.76 | 103.89 | 119.84 |
| 1 | J | 883 | CYS | C-N-CA | -12.76 | 103.89 | 119.84 |
| 1 | b | 464 | LEU | CA-C-N | -12.27 | 104.50 | 119.84 |
| 1 | b | 464 | LEU | C-N-CA | -12.27 | 104.50 | 119.84 |
| 2 | Z | 2128 | LEU | CA-C-N | -11.05 | 109.00 | 120.38 |
| 2 | Z | 2128 | LEU | C-N-CA | -11.05 | 109.00 | 120.38 |
| 3 | d | 3120[A] | HIS | N-CA-C | 10.77 | 122.99 | 111.03 |
| 3 | d | 3120[B] | HIS | N-CA-C | 10.77 | 122.99 | 111.03 |
| 3 | L | 3120[A] | HIS | N-CA-C | 10.76 | 122.97 | 111.03 |
| 3 | L | 3120[B] | HIS | N-CA-C | 10.76 | 122.97 | 111.03 |
| 3 | R | 3120[A] | HIS | N-CA-C | 10.73 | 122.94 | 111.03 |
| 3 | R | 3120[B] | HIS | N-CA-C | 10.73 | 122.94 | 111.03 |
| 3 | I | 3120[A] | HIS | N-CA-C | 10.72 | 122.93 | 111.03 |
| 3 | I | 3120[B] | HIS | N-CA-C | 10.72 | 122.93 | 111.03 |
| 3 | U | 3120[A] | HIS | N-CA-C | 10.72 | 122.92 | 111.03 |
| 3 | U | 3120[B] | HIS | N-CA-C | 10.72 | 122.92 | 111.03 |
| 3 | a | 3120[A] | HIS | N-CA-C | 10.70 | 122.91 | 111.03 |
| 3 | a | 3120[B] | HIS | N-CA-C | 10.70 | 122.91 | 111.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 3120[A] | HIS | N-CA-C | 10.70 | 122.91 | 111.03 |
| 3 | C | 3120[B] | HIS | N-CA-C | 10.70 | 122.91 | 111.03 |
| 3 | F | 3120[A] | HIS | N-CA-C | 10.68 | 122.89 | 111.03 |
| 3 | F | 3120[B] | HIS | N-CA-C | 10.68 | 122.89 | 111.03 |
| 3 | O | 3120[A] | HIS | N-CA-C | 10.68 | 122.89 | 111.03 |
| 3 | O | 3120[B] | HIS | N-CA-C | 10.68 | 122.89 | 111.03 |
| 3 | X | 3120[A] | HIS | N-CA-C | 10.67 | 122.87 | 111.03 |
| 3 | X | 3120[B] | HIS | N-CA-C | 10.67 | 122.87 | 111.03 |
| 1 | Y | 898 | GLY | N-CA-C | 10.57 | 127.05 | 114.48 |
| 2 | N | 2340 | ALA | CA-C-N | -10.46 | 108.99 | 119.56 |
| 2 | N | 2340 | ALA | C-N-CA | -10.46 | 108.99 | 119.56 |
| 1 | D | 898 | GLY | N-CA-C | 10.43 | 126.89 | 114.48 |
| 1 | D | 1286 | ARG | N-CA-C | 10.35 | 123.65 | 111.02 |
| 1 | V | 898 | GLY | N-CA-C | 9.98 | 126.36 | 114.48 |
| 1 | M | 464 | LEU | CA-C-N | -9.82 | 109.96 | 120.47 |
| 1 | M | 464 | LEU | C-N-CA | -9.82 | 109.96 | 120.47 |
| 3 | a | 3279[A] | ASP | N-CA-C | -9.80 | 97.02 | 110.35 |
| 3 | a | 3279[B] | ASP | N-CA-C | -9.80 | 97.02 | 110.35 |
| 3 | L | 3279[A] | ASP | N-CA-C | -9.80 | 97.02 | 110.35 |
| 3 | L | 3279[B] | ASP | N-CA-C | -9.80 | 97.02 | 110.35 |
| 3 | R | 3279[A] | ASP | N-CA-C | -9.79 | 97.03 | 110.35 |
| 3 | R | 3279[B] | ASP | N-CA-C | -9.79 | 97.03 | 110.35 |
| 3 | O | 3279[A] | ASP | N-CA-C | -9.79 | 97.04 | 110.35 |
| 3 | O | 3279[B] | ASP | N-CA-C | -9.79 | 97.04 | 110.35 |
| 1 | A | 1584 | GLY | N-CA-C | 9.78 | 124.73 | 111.03 |
| 3 | C | 3279[A] | ASP | N-CA-C | -9.78 | 97.04 | 110.35 |
| 3 | C | 3279[B] | ASP | N-CA-C | -9.78 | 97.04 | 110.35 |
| 3 | U | 3279[A] | ASP | N-CA-C | -9.78 | 97.05 | 110.35 |
| 3 | U | 3279[B] | ASP | N-CA-C | -9.78 | 97.05 | 110.35 |
| 3 | F | 3279[A] | ASP | N-CA-C | -9.77 | 97.06 | 110.35 |
| 3 | F | 3279[B] | ASP | N-CA-C | -9.77 | 97.06 | 110.35 |
| 3 | d | 3279[A] | ASP | N-CA-C | -9.76 | 97.07 | 110.35 |
| 3 | d | 3279[B] | ASP | N-CA-C | -9.76 | 97.07 | 110.35 |
| 3 | X | 3279[A] | ASP | N-CA-C | -9.75 | 97.09 | 110.35 |
| 3 | X | 3279[B] | ASP | N-CA-C | -9.75 | 97.09 | 110.35 |
| 3 | I | 3279[A] | ASP | N-CA-C | -9.74 | 97.11 | 110.35 |
| 3 | I | 3279[B] | ASP | N-CA-C | -9.74 | 97.11 | 110.35 |
| 1 | b | 883 | CYS | CA-C-N | -9.37 | 107.60 | 120.25 |
| 1 | b | 883 | CYS | C-N-CA | -9.37 | 107.60 | 120.25 |
| 1 | M | 898 | GLY | N-CA-C | 9.26 | 125.49 | 114.48 |
| 3 | I | 2948[A] | ASP | N-CA-C | -9.24 | 98.74 | 112.04 |
| 3 | I | 2948[B] | ASP | N-CA-C | -9.24 | 98.74 | 112.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | R | 2948[A] | ASP | N-CA-C | -9.23 | 98.75 | 112.04 |
| 3 | R | 2948[B] | ASP | N-CA-C | -9.23 | 98.75 | 112.04 |
| 3 | F | 2948[A] | ASP | N-CA-C | -9.22 | 98.76 | 112.04 |
| 3 | F | 2948[B] | ASP | N-CA-C | -9.22 | 98.76 | 112.04 |
| 3 | L | 2948[A] | ASP | N-CA-C | -9.22 | 98.76 | 112.04 |
| 3 | L | 2948[B] | ASP | N-CA-C | -9.22 | 98.76 | 112.04 |
| 3 | U | 2948[A] | ASP | N-CA-C | -9.21 | 98.78 | 112.04 |
| 3 | U | 2948[B] | ASP | N-CA-C | -9.21 | 98.78 | 112.04 |
| 3 | X | 2948[A] | ASP | N-CA-C | -9.21 | 98.78 | 112.04 |
| 3 | X | 2948[B] | ASP | N-CA-C | -9.21 | 98.78 | 112.04 |
| 3 | C | 2948[A] | ASP | N-CA-C | -9.19 | 98.80 | 112.04 |
| 3 | C | 2948[B] | ASP | N-CA-C | -9.19 | 98.80 | 112.04 |
| 3 | a | 2948[A] | ASP | N-CA-C | -9.19 | 98.80 | 112.04 |
| 3 | a | 2948[B] | ASP | N-CA-C | -9.19 | 98.80 | 112.04 |
| 3 | O | 2948[A] | ASP | N-CA-C | -9.19 | 98.81 | 112.04 |
| 3 | O | 2948[B] | ASP | N-CA-C | -9.19 | 98.81 | 112.04 |
| 1 | b | 675 | SER | CA-C-N | -9.19 | 109.45 | 119.19 |
| 1 | b | 675 | SER | C-N-CA | -9.19 | 109.45 | 119.19 |
| 3 | d | 2948[A] | ASP | N-CA-C | -9.19 | 98.81 | 112.04 |
| 3 | d | 2948[B] | ASP | N-CA-C | -9.19 | 98.81 | 112.04 |
| 2 | N | 2128 | LEU | CA-C-N | -9.05 | 111.06 | 120.38 |
| 2 | N | 2128 | LEU | C-N-CA | -9.05 | 111.06 | 120.38 |
| 2 | W | 2128 | LEU | CA-C-N | -8.97 | 111.14 | 120.38 |
| 2 | W | 2128 | LEU | C-N-CA | -8.97 | 111.14 | 120.38 |
| 1 | M | 982 | LYS | CA-C-N | -8.96 | 110.65 | 120.14 |
| 1 | M | 982 | LYS | C-N-CA | -8.96 | 110.65 | 120.14 |
| 2 | T | 2128 | LEU | CA-C-N | -8.76 | 111.36 | 120.38 |
| 2 | T | 2128 | LEU | C-N-CA | -8.76 | 111.36 | 120.38 |
| 1 | G | 1584 | GLY | N-CA-C | 8.71 | 123.23 | 111.03 |
| 3 | I | 3176[A] | LYS | N-CA-C | -8.63 | 99.14 | 110.53 |
| 3 | I | 3176[B] | LYS | N-CA-C | -8.63 | 99.14 | 110.53 |
| 2 | c | 2128 | LEU | CA-C-N | -8.62 | 111.51 | 120.38 |
| 2 | c | 2128 | LEU | C-N-CA | -8.62 | 111.51 | 120.38 |
| 3 | R | 3176[A] | LYS | N-CA-C | -8.61 | 99.16 | 110.53 |
| 3 | R | 3176[B] | LYS | N-CA-C | -8.61 | 99.16 | 110.53 |
| 3 | U | 3176[A] | LYS | N-CA-C | -8.61 | 99.17 | 110.53 |
| 3 | U | 3176[B] | LYS | N-CA-C | -8.61 | 99.17 | 110.53 |
| 3 | O | 3176[A] | LYS | N-CA-C | -8.60 | 99.17 | 110.53 |
| 3 | O | 3176[B] | LYS | N-CA-C | -8.60 | 99.17 | 110.53 |
| 3 | L | 3176[A] | LYS | N-CA-C | -8.59 | 99.19 | 110.53 |
| 3 | L | 3176[B] | LYS | N-CA-C | -8.59 | 99.19 | 110.53 |
| 3 | d | 3176[A] | LYS | N-CA-C | -8.59 | 99.19 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | d | 3176[B] | LYS | N-CA-C | -8.59 | 99.19 | 110.53 |
| 3 | F | 3176[A] | LYS | N-CA-C | -8.57 | 99.21 | 110.53 |
| 3 | F | 3176[B] | LYS | N-CA-C | -8.57 | 99.21 | 110.53 |
| 2 | K | 2128 | LEU | CA-C-N | -8.57 | 111.55 | 120.38 |
| 2 | K | 2128 | LEU | C-N-CA | -8.57 | 111.55 | 120.38 |
| 3 | a | 3176[A] | LYS | N-CA-C | -8.57 | 99.21 | 110.53 |
| 3 | a | 3176[B] | LYS | N-CA-C | -8.57 | 99.21 | 110.53 |
| 2 | Q | 2128 | LEU | CA-C-N | -8.55 | 111.57 | 120.38 |
| 2 | Q | 2128 | LEU | C-N-CA | -8.55 | 111.57 | 120.38 |
| 3 | X | 3176[A] | LYS | N-CA-C | -8.54 | 99.25 | 110.53 |
| 3 | X | 3176[B] | LYS | N-CA-C | -8.54 | 99.25 | 110.53 |
| 3 | C | 3176[A] | LYS | N-CA-C | -8.54 | 99.26 | 110.53 |
| 3 | C | 3176[B] | LYS | N-CA-C | -8.54 | 99.26 | 110.53 |
| 1 | D | 669 | LYS | CA-C-N | -8.50 | 110.61 | 120.89 |
| 1 | D | 669 | LYS | C-N-CA | -8.50 | 110.61 | 120.89 |
| 1 | b | 450 | LYS | N-CA-C | 8.46 | 121.20 | 109.18 |
| 1 | A | 898 | GLY | N-CA-C | 8.42 | 127.93 | 115.64 |
| 1 | J | 898 | GLY | N-CA-C | 8.42 | 126.43 | 114.64 |
| 3 | X | 2952[A] | ALA | N-CA-C | -8.31 | 100.99 | 112.12 |
| 3 | X | 2952[B] | ALA | N-CA-C | -8.31 | 100.99 | 112.12 |
| 3 | d | 2952[A] | ALA | N-CA-C | -8.29 | 101.01 | 112.12 |
| 3 | d | 2952[B] | ALA | N-CA-C | -8.29 | 101.01 | 112.12 |
| 3 | a | 2952[A] | ALA | N-CA-C | -8.29 | 101.01 | 112.12 |
| 3 | a | 2952[B] | ALA | N-CA-C | -8.29 | 101.01 | 112.12 |
| 3 | L | 2952[A] | ALA | N-CA-C | -8.27 | 101.04 | 112.12 |
| 3 | L | 2952[B] | ALA | N-CA-C | -8.27 | 101.04 | 112.12 |
| 3 | R | 2952[A] | ALA | N-CA-C | -8.26 | 101.05 | 112.12 |
| 3 | R | 2952[B] | ALA | N-CA-C | -8.26 | 101.05 | 112.12 |
| 3 | U | 2952[A] | ALA | N-CA-C | -8.26 | 101.06 | 112.12 |
| 3 | U | 2952[B] | ALA | N-CA-C | -8.26 | 101.06 | 112.12 |
| 3 | O | 2952[A] | ALA | N-CA-C | -8.24 | 101.08 | 112.12 |
| 3 | O | 2952[B] | ALA | N-CA-C | -8.24 | 101.08 | 112.12 |
| 3 | F | 2952[A] | ALA | N-CA-C | -8.23 | 101.09 | 112.12 |
| 3 | F | 2952[B] | ALA | N-CA-C | -8.23 | 101.09 | 112.12 |
| 1 | D | 1582 | ASN | N-CA-C | 8.22 | 121.01 | 108.52 |
| 3 | I | 2952[A] | ALA | N-CA-C | -8.22 | 101.11 | 112.12 |
| 3 | I | 2952[B] | ALA | N-CA-C | -8.22 | 101.11 | 112.12 |
| 3 | C | 2952[A] | ALA | N-CA-C | -8.21 | 101.12 | 112.12 |
| 3 | C | 2952[B] | ALA | N-CA-C | -8.21 | 101.12 | 112.12 |
| 1 | D | 982 | LYS | CA-C-N | -8.18 | 111.31 | 119.90 |
| 1 | D | 982 | LYS | C-N-CA | -8.18 | 111.31 | 119.90 |
| 1 | b | 898 | GLY | N-CA-C | 8.15 | 124.18 | 114.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | d | 3003[A] | LYS | N-CA-C | -8.08 | 100.48 | 111.87 |
| 3 | d | 3003[B] | LYS | N-CA-C | -8.08 | 100.48 | 111.87 |
| 3 | I | 3003[A] | LYS | N-CA-C | -8.07 | 100.49 | 111.87 |
| 3 | I | 3003[B] | LYS | N-CA-C | -8.07 | 100.49 | 111.87 |
| 3 | U | 3003[A] | LYS | N-CA-C | -8.07 | 100.49 | 111.87 |
| 3 | U | 3003[B] | LYS | N-CA-C | -8.07 | 100.49 | 111.87 |
| 3 | L | 3003[A] | LYS | N-CA-C | -8.07 | 100.50 | 111.87 |
| 3 | L | 3003[B] | LYS | N-CA-C | -8.07 | 100.50 | 111.87 |
| 3 | F | 3003[A] | LYS | N-CA-C | -8.06 | 100.50 | 111.87 |
| 3 | F | 3003[B] | LYS | N-CA-C | -8.06 | 100.50 | 111.87 |
| 3 | C | 3003[A] | LYS | N-CA-C | -8.05 | 100.51 | 111.87 |
| 3 | C | 3003[B] | LYS | N-CA-C | -8.05 | 100.51 | 111.87 |
| 3 | X | 3003[A] | LYS | N-CA-C | -8.04 | 100.53 | 111.87 |
| 3 | X | 3003[B] | LYS | N-CA-C | -8.04 | 100.53 | 111.87 |
| 3 | R | 3003[A] | LYS | N-CA-C | -8.04 | 100.53 | 111.87 |
| 3 | R | 3003[B] | LYS | N-CA-C | -8.04 | 100.53 | 111.87 |
| 2 | B | 2128 | LEU | CA-C-N | -8.04 | 112.10 | 120.38 |
| 2 | B | 2128 | LEU | C-N-CA | -8.04 | 112.10 | 120.38 |
| 3 | O | 3003[A] | LYS | N-CA-C | -8.03 | 100.55 | 111.87 |
| 3 | O | 3003[B] | LYS | N-CA-C | -8.03 | 100.55 | 111.87 |
| 3 | a | 3003[A] | LYS | N-CA-C | -8.03 | 100.55 | 111.87 |
| 3 | a | 3003[B] | LYS | N-CA-C | -8.03 | 100.55 | 111.87 |
| 2 | Q | 2340 | ALA | CA-C-N | -8.01 | 111.54 | 119.87 |
| 2 | Q | 2340 | ALA | C-N-CA | -8.01 | 111.54 | 119.87 |
| 1 | Y | 85 | SER | N-CA-C | 7.88 | 119.02 | 108.38 |
| 2 | H | 2128 | LEU | CA-C-N | -7.87 | 112.27 | 120.38 |
| 2 | H | 2128 | LEU | C-N-CA | -7.87 | 112.27 | 120.38 |
| 2 | Z | 2340 | ALA | CA-C-N | -7.82 | 111.74 | 119.87 |
| 2 | Z | 2340 | ALA | C-N-CA | -7.82 | 111.74 | 119.87 |
| 2 | E | 2548 | CYS | CA-C-N | -7.80 | 111.71 | 119.90 |
| 2 | E | 2548 | CYS | C-N-CA | -7.80 | 111.71 | 119.90 |
| 1 | A | 464 | LEU | CA-C-N | -7.78 | 111.63 | 121.04 |
| 1 | A | 464 | LEU | C-N-CA | -7.78 | 111.63 | 121.04 |
| 2 | W | 2472 | ASN | N-CA-C | 7.72 | 119.77 | 111.36 |
| 1 | M | 1082 | SER | CA-C-N | -7.69 | 110.23 | 119.84 |
| 1 | M | 1082 | SER | C-N-CA | -7.69 | 110.23 | 119.84 |
| 3 | I | 2966[A] | SER | N-CA-C | 7.66 | 119.71 | 111.36 |
| 3 | I | 2966[B] | SER | N-CA-C | 7.66 | 119.71 | 111.36 |
| 3 | a | 3192[A] | PHE | N-CA-C | -7.65 | 100.46 | 110.33 |
| 3 | a | 3192[B] | PHE | N-CA-C | -7.65 | 100.46 | 110.33 |
| 3 | R | 2966[A] | SER | N-CA-C | 7.65 | 119.69 | 111.36 |
| 3 | R | 2966[B] | SER | N-CA-C | 7.65 | 119.69 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | U | 2966[A] | SER | N-CA-C | 7.64 | 119.69 | 111.36 |
| 3 | U | 2966[B] | SER | N-CA-C | 7.64 | 119.69 | 111.36 |
| 3 | R | 3192[A] | PHE | N-CA-C | -7.64 | 100.48 | 110.33 |
| 3 | R | 3192[B] | PHE | N-CA-C | -7.64 | 100.48 | 110.33 |
| 3 | U | 3192[A] | PHE | N-CA-C | -7.64 | 100.48 | 110.33 |
| 3 | U | 3192[B] | PHE | N-CA-C | -7.64 | 100.48 | 110.33 |
| 3 | d | 2966[A] | SER | N-CA-C | 7.64 | 119.69 | 111.36 |
| 3 | d | 2966[B] | SER | N-CA-C | 7.64 | 119.69 | 111.36 |
| 3 | F | 3192[A] | PHE | N-CA-C | -7.64 | 100.48 | 110.33 |
| 3 | F | 3192[B] | PHE | N-CA-C | -7.64 | 100.48 | 110.33 |
| 3 | C | 2966[A] | SER | N-CA-C | 7.63 | 119.68 | 111.36 |
| 3 | C | 2966[B] | SER | N-CA-C | 7.63 | 119.68 | 111.36 |
| 3 | I | 3192[A] | PHE | N-CA-C | -7.62 | 100.49 | 110.33 |
| 3 | I | 3192[B] | PHE | N-CA-C | -7.62 | 100.49 | 110.33 |
| 3 | C | 3192[A] | PHE | N-CA-C | -7.62 | 100.50 | 110.33 |
| 3 | C | 3192[B] | PHE | N-CA-C | -7.62 | 100.50 | 110.33 |
| 3 | F | 2966[A] | SER | N-CA-C | 7.61 | 119.66 | 111.36 |
| 3 | F | 2966[B] | SER | N-CA-C | 7.61 | 119.66 | 111.36 |
| 3 | d | 3192[A] | PHE | N-CA-C | -7.61 | 100.51 | 110.33 |
| 3 | d | 3192[B] | PHE | N-CA-C | -7.61 | 100.51 | 110.33 |
| 3 | L | 2966[A] | SER | N-CA-C | 7.60 | 119.65 | 111.36 |
| 3 | L | 2966[B] | SER | N-CA-C | 7.60 | 119.65 | 111.36 |
| 3 | X | 3192[A] | PHE | N-CA-C | -7.60 | 100.53 | 110.33 |
| 3 | X | 3192[B] | PHE | N-CA-C | -7.60 | 100.53 | 110.33 |
| 3 | O | 3192[A] | PHE | N-CA-C | -7.60 | 100.53 | 110.33 |
| 3 | O | 3192[B] | PHE | N-CA-C | -7.60 | 100.53 | 110.33 |
| 3 | X | 2966[A] | SER | N-CA-C | 7.60 | 119.64 | 111.36 |
| 3 | X | 2966[B] | SER | N-CA-C | 7.60 | 119.64 | 111.36 |
| 3 | a | 2966[A] | SER | N-CA-C | 7.60 | 119.64 | 111.36 |
| 3 | a | 2966[B] | SER | N-CA-C | 7.60 | 119.64 | 111.36 |
| 1 | b | 830 | ASN | N-CA-C | 7.60 | 119.20 | 111.07 |
| 3 | I | 3009[A] | ILE | CA-C-N | -7.59 | 113.01 | 120.52 |
| 3 | I | 3009[A] | ILE | C-N-CA | -7.59 | 113.01 | 120.52 |
| 3 | I | 3009[B] | ILE | CA-C-N | -7.59 | 113.01 | 120.52 |
| 3 | I | 3009[B] | ILE | C-N-CA | -7.59 | 113.01 | 120.52 |
| 3 | O | 2966[A] | SER | N-CA-C | 7.58 | 119.62 | 111.36 |
| 3 | O | 2966[B] | SER | N-CA-C | 7.58 | 119.62 | 111.36 |
| 3 | L | 3192[A] | PHE | N-CA-C | -7.58 | 100.55 | 110.33 |
| 3 | L | 3192[B] | PHE | N-CA-C | -7.58 | 100.55 | 110.33 |
| 1 | P | 982 | LYS | CA-C-N | -7.57 | 112.19 | 119.76 |
| 1 | P | 982 | LYS | C-N-CA | -7.57 | 112.19 | 119.76 |
| 3 | O | 3009[A] | ILE | CA-C-N | -7.56 | 113.04 | 120.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | O | 3009[A] | ILE | C-N-CA | -7.56 | 113.04 | 120.52 |
| 3 | O | 3009[B] | ILE | CA-C-N | -7.56 | 113.04 | 120.52 |
| 3 | O | 3009[B] | ILE | C-N-CA | -7.56 | 113.04 | 120.52 |
| 3 | U | 3009[A] | ILE | CA-C-N | -7.53 | 113.06 | 120.52 |
| 3 | U | 3009[A] | ILE | C-N-CA | -7.53 | 113.06 | 120.52 |
| 3 | U | 3009[B] | ILE | CA-C-N | -7.53 | 113.06 | 120.52 |
| 3 | U | 3009[B] | ILE | C-N-CA | -7.53 | 113.06 | 120.52 |
| 3 | R | 3009[A] | ILE | CA-C-N | -7.53 | 113.07 | 120.52 |
| 3 | R | 3009[A] | ILE | C-N-CA | -7.53 | 113.07 | 120.52 |
| 3 | R | 3009[B] | ILE | CA-C-N | -7.53 | 113.07 | 120.52 |
| 3 | R | 3009[B] | ILE | C-N-CA | -7.53 | 113.07 | 120.52 |
| 3 | F | 3009[A] | ILE | CA-C-N | -7.51 | 113.08 | 120.52 |
| 3 | F | 3009[A] | ILE | C-N-CA | -7.51 | 113.08 | 120.52 |
| 3 | F | 3009[B] | ILE | CA-C-N | -7.51 | 113.08 | 120.52 |
| 3 | F | 3009[B] | ILE | C-N-CA | -7.51 | 113.08 | 120.52 |
| 3 | C | 3009[A] | ILE | CA-C-N | -7.51 | 113.08 | 120.52 |
| 3 | C | 3009[A] | ILE | C-N-CA | -7.51 | 113.08 | 120.52 |
| 3 | C | 3009[B] | ILE | CA-C-N | -7.51 | 113.08 | 120.52 |
| 3 | C | 3009[B] | ILE | C-N-CA | -7.51 | 113.08 | 120.52 |
| 3 | a | 3009[A] | ILE | CA-C-N | -7.51 | 113.09 | 120.52 |
| 3 | a | 3009[A] | ILE | C-N-CA | -7.51 | 113.09 | 120.52 |
| 3 | a | 3009[B] | ILE | CA-C-N | -7.51 | 113.09 | 120.52 |
| 3 | a | 3009[B] | ILE | C-N-CA | -7.51 | 113.09 | 120.52 |
| 3 | X | 3009[A] | ILE | CA-C-N | -7.49 | 113.10 | 120.52 |
| 3 | X | 3009[A] | ILE | C-N-CA | -7.49 | 113.10 | 120.52 |
| 3 | X | 3009[B] | ILE | CA-C-N | -7.49 | 113.10 | 120.52 |
| 3 | X | 3009[B] | ILE | C-N-CA | -7.49 | 113.10 | 120.52 |
| 3 | L | 3009[A] | ILE | CA-C-N | -7.47 | 113.12 | 120.52 |
| 3 | L | 3009[A] | ILE | C-N-CA | -7.47 | 113.12 | 120.52 |
| 3 | L | 3009[B] | ILE | CA-C-N | -7.47 | 113.12 | 120.52 |
| 3 | L | 3009[B] | ILE | C-N-CA | -7.47 | 113.12 | 120.52 |
| 3 | d | 3009[A] | ILE | CA-C-N | -7.44 | 113.15 | 120.52 |
| 3 | d | 3009[A] | ILE | C-N-CA | -7.44 | 113.15 | 120.52 |
| 3 | d | 3009[B] | ILE | CA-C-N | -7.44 | 113.15 | 120.52 |
| 3 | d | 3009[B] | ILE | C-N-CA | -7.44 | 113.15 | 120.52 |
| 1 | A | 1195 | ASP | CA-C-N | 7.44 | 135.10 | 121.70 |
| 1 | A | 1195 | ASP | C-N-CA | 7.44 | 135.10 | 121.70 |
| 1 | G | 464 | LEU | CA-C-N | -7.42 | 112.06 | 121.04 |
| 1 | G | 464 | LEU | C-N-CA | -7.42 | 112.06 | 121.04 |
| 1 | S | 464 | LEU | CA-C-N | -7.38 | 112.11 | 121.04 |
| 1 | S | 464 | LEU | C-N-CA | -7.38 | 112.11 | 121.04 |
| 1 | P | 116 | LYS | CB-CA-C | -7.34 | 108.10 | 116.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 883 | CYS | CA-C-N | -7.32 | 110.69 | 119.84 |
| 1 | G | 883 | CYS | C-N-CA | -7.32 | 110.69 | 119.84 |
| 2 | E | 2866 | PRO | CA-C-N | 7.31 | 127.32 | 119.28 |
| 2 | E | 2866 | PRO | C-N-CA | 7.31 | 127.32 | 119.28 |
| 3 | d | 3173[A] | THR | CA-C-N | 7.28 | 128.02 | 119.94 |
| 3 | d | 3173[A] | THR | C-N-CA | 7.28 | 128.02 | 119.94 |
| 3 | d | 3173[B] | THR | CA-C-N | 7.28 | 128.02 | 119.94 |
| 3 | d | 3173[B] | THR | C-N-CA | 7.28 | 128.02 | 119.94 |
| 3 | F | 3296[A] | PRO | CA-C-O | -7.26 | 115.67 | 120.90 |
| 3 | F | 3296[B] | PRO | CA-C-O | -7.26 | 115.67 | 120.90 |
| 3 | I | 3296[A] | PRO | CA-C-O | -7.26 | 115.67 | 120.90 |
| 3 | I | 3296[B] | PRO | CA-C-O | -7.26 | 115.67 | 120.90 |
| 3 | R | 3296[A] | PRO | CA-C-O | -7.26 | 115.67 | 120.90 |
| 3 | R | 3296[B] | PRO | CA-C-O | -7.26 | 115.67 | 120.90 |
| 3 | X | 3296[A] | PRO | CA-C-O | -7.26 | 115.67 | 120.90 |
| 3 | X | 3296[B] | PRO | CA-C-O | -7.26 | 115.67 | 120.90 |
| 1 | b | 228 | GLY | N-CA-C | 7.25 | 125.05 | 114.10 |
| 3 | R | 3173[A] | THR | CA-C-N | 7.24 | 127.98 | 119.94 |
| 3 | R | 3173[A] | THR | C-N-CA | 7.24 | 127.98 | 119.94 |
| 3 | R | 3173[B] | THR | CA-C-N | 7.24 | 127.98 | 119.94 |
| 3 | R | 3173[B] | THR | C-N-CA | 7.24 | 127.98 | 119.94 |
| 3 | U | 3296[A] | PRO | CA-C-O | -7.24 | 115.69 | 120.90 |
| 3 | U | 3296[B] | PRO | CA-C-O | -7.24 | 115.69 | 120.90 |
| 1 | G | 323 | ILE | CA-C-N | 7.22 | 127.26 | 119.89 |
| 1 | G | 323 | ILE | C-N-CA | 7.22 | 127.26 | 119.89 |
| 3 | L | 3173[A] | THR | CA-C-N | 7.22 | 127.95 | 119.94 |
| 3 | L | 3173[A] | THR | C-N-CA | 7.22 | 127.95 | 119.94 |
| 3 | L | 3173[B] | THR | CA-C-N | 7.22 | 127.95 | 119.94 |
| 3 | L | 3173[B] | THR | C-N-CA | 7.22 | 127.95 | 119.94 |
| 3 | L | 3296[A] | PRO | CA-C-O | -7.22 | 115.70 | 120.90 |
| 3 | L | 3296[B] | PRO | CA-C-O | -7.22 | 115.70 | 120.90 |
| 3 | a | 3296[A] | PRO | CA-C-O | -7.22 | 115.70 | 120.90 |
| 3 | a | 3296[B] | PRO | CA-C-O | -7.22 | 115.70 | 120.90 |
| 3 | O | 3173[A] | THR | CA-C-N | 7.21 | 127.94 | 119.94 |
| 3 | O | 3173[A] | THR | C-N-CA | 7.21 | 127.94 | 119.94 |
| 3 | O | 3173[B] | THR | CA-C-N | 7.21 | 127.94 | 119.94 |
| 3 | O | 3173[B] | THR | C-N-CA | 7.21 | 127.94 | 119.94 |
| 3 | C | 3173[A] | THR | CA-C-N | 7.19 | 127.92 | 119.94 |
| 3 | C | 3173[A] | THR | C-N-CA | 7.19 | 127.92 | 119.94 |
| 3 | C | 3173[B] | THR | CA-C-N | 7.19 | 127.92 | 119.94 |
| 3 | C | 3173[B] | THR | C-N-CA | 7.19 | 127.92 | 119.94 |
| 3 | C | 3296[A] | PRO | CA-C-O | -7.18 | 115.73 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 3296[B] | PRO | CA-C-O | -7.18 | 115.73 | 120.90 |
| 3 | F | 3173[A] | THR | CA-C-N | 7.18 | 127.91 | 119.94 |
| 3 | F | 3173[A] | THR | C-N-CA | 7.18 | 127.91 | 119.94 |
| 3 | F | 3173[B] | THR | CA-C-N | 7.18 | 127.91 | 119.94 |
| 3 | F | 3173[B] | THR | C-N-CA | 7.18 | 127.91 | 119.94 |
| 3 | I | 3173[A] | THR | CA-C-N | 7.18 | 127.91 | 119.94 |
| 3 | I | 3173[A] | THR | C-N-CA | 7.18 | 127.91 | 119.94 |
| 3 | I | 3173[B] | THR | CA-C-N | 7.18 | 127.91 | 119.94 |
| 3 | I | 3173[B] | THR | C-N-CA | 7.18 | 127.91 | 119.94 |
| 3 | U | 3173[A] | THR | CA-C-N | 7.17 | 127.90 | 119.94 |
| 3 | U | 3173[A] | THR | C-N-CA | 7.17 | 127.90 | 119.94 |
| 3 | U | 3173[B] | THR | CA-C-N | 7.17 | 127.90 | 119.94 |
| 3 | U | 3173[B] | THR | C-N-CA | 7.17 | 127.90 | 119.94 |
| 3 | F | 3153[A] | LYS | CA-C-N | -7.17 | 113.29 | 120.31 |
| 3 | F | 3153[A] | LYS | C-N-CA | -7.17 | 113.29 | 120.31 |
| 3 | F | 3153[B] | LYS | CA-C-N | -7.17 | 113.29 | 120.31 |
| 3 | F | 3153[B] | LYS | C-N-CA | -7.17 | 113.29 | 120.31 |
| 3 | U | 3196[A] | THR | N-CA-C | -7.17 | 100.88 | 110.55 |
| 3 | U | 3196[B] | THR | N-CA-C | -7.17 | 100.88 | 110.55 |
| 3 | a | 3173[A] | THR | CA-C-N | 7.17 | 127.89 | 119.94 |
| 3 | a | 3173[A] | THR | C-N-CA | 7.17 | 127.89 | 119.94 |
| 3 | a | 3173[B] | THR | CA-C-N | 7.17 | 127.89 | 119.94 |
| 3 | a | 3173[B] | THR | C-N-CA | 7.17 | 127.89 | 119.94 |
| 3 | X | 3173[A] | THR | CA-C-N | 7.16 | 127.89 | 119.94 |
| 3 | X | 3173[A] | THR | C-N-CA | 7.16 | 127.89 | 119.94 |
| 3 | X | 3173[B] | THR | CA-C-N | 7.16 | 127.89 | 119.94 |
| 3 | X | 3173[B] | THR | C-N-CA | 7.16 | 127.89 | 119.94 |
| 3 | d | 3153[A] | LYS | CA-C-N | -7.16 | 113.30 | 120.31 |
| 3 | d | 3153[A] | LYS | C-N-CA | -7.16 | 113.30 | 120.31 |
| 3 | d | 3153[B] | LYS | CA-C-N | -7.16 | 113.30 | 120.31 |
| 3 | d | 3153[B] | LYS | C-N-CA | -7.16 | 113.30 | 120.31 |
| 3 | U | 3153[A] | LYS | CA-C-N | -7.15 | 113.30 | 120.31 |
| 3 | U | 3153[A] | LYS | C-N-CA | -7.15 | 113.30 | 120.31 |
| 3 | U | 3153[B] | LYS | CA-C-N | -7.15 | 113.30 | 120.31 |
| 3 | U | 3153[B] | LYS | C-N-CA | -7.15 | 113.30 | 120.31 |
| 3 | R | 3153[A] | LYS | CA-C-N | -7.14 | 113.31 | 120.31 |
| 3 | R | 3153[A] | LYS | C-N-CA | -7.14 | 113.31 | 120.31 |
| 3 | R | 3153[B] | LYS | CA-C-N | -7.14 | 113.31 | 120.31 |
| 3 | R | 3153[B] | LYS | C-N-CA | -7.14 | 113.31 | 120.31 |
| 1 | S | 1195 | ASP | CA-C-N | 7.14 | 134.56 | 121.70 |
| 1 | S | 1195 | ASP | C-N-CA | 7.14 | 134.56 | 121.70 |
| 1 | M | 417 | MET | N-CA-C | 7.14 | 119.60 | 108.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | L | 3153[A] | LYS | CA-C-N | -7.13 | 113.32 | 120.31 |
| 3 | L | 3153[A] | LYS | C-N-CA | -7.13 | 113.32 | 120.31 |
| 3 | L | 3153[B] | LYS | CA-C-N | -7.13 | 113.32 | 120.31 |
| 3 | L | 3153[B] | LYS | C-N-CA | -7.13 | 113.32 | 120.31 |
| 3 | d | 3296[A] | PRO | CA-C-O | -7.13 | 115.76 | 120.90 |
| 3 | d | 3296[B] | PRO | CA-C-O | -7.13 | 115.76 | 120.90 |
| 3 | X | 3153[A] | LYS | CA-C-N | -7.13 | 113.32 | 120.31 |
| 3 | X | 3153[A] | LYS | C-N-CA | -7.13 | 113.32 | 120.31 |
| 3 | X | 3153[B] | LYS | CA-C-N | -7.13 | 113.32 | 120.31 |
| 3 | X | 3153[B] | LYS | C-N-CA | -7.13 | 113.32 | 120.31 |
| 3 | a | 3153[A] | LYS | CA-C-N | -7.13 | 113.32 | 120.31 |
| 3 | a | 3153[A] | LYS | C-N-CA | -7.13 | 113.32 | 120.31 |
| 3 | a | 3153[B] | LYS | CA-C-N | -7.13 | 113.32 | 120.31 |
| 3 | a | 3153[B] | LYS | C-N-CA | -7.13 | 113.32 | 120.31 |
| 3 | O | 3296[A] | PRO | CA-C-O | -7.13 | 115.77 | 120.90 |
| 3 | O | 3296[B] | PRO | CA-C-O | -7.13 | 115.77 | 120.90 |
| 3 | O | 3153[A] | LYS | CA-C-N | -7.13 | 113.33 | 120.31 |
| 3 | O | 3153[A] | LYS | C-N-CA | -7.13 | 113.33 | 120.31 |
| 3 | O | 3153[B] | LYS | CA-C-N | -7.13 | 113.33 | 120.31 |
| 3 | O | 3153[B] | LYS | C-N-CA | -7.13 | 113.33 | 120.31 |
| 3 | I | 3153[A] | LYS | CA-C-N | -7.12 | 113.33 | 120.31 |
| 3 | I | 3153[A] | LYS | C-N-CA | -7.12 | 113.33 | 120.31 |
| 3 | I | 3153[B] | LYS | CA-C-N | -7.12 | 113.33 | 120.31 |
| 3 | I | 3153[B] | LYS | C-N-CA | -7.12 | 113.33 | 120.31 |
| 3 | I | 3196[A] | THR | N-CA-C | -7.12 | 100.94 | 110.55 |
| 3 | I | 3196[B] | THR | N-CA-C | -7.12 | 100.94 | 110.55 |
| 3 | O | 3196[A] | THR | N-CA-C | -7.12 | 100.94 | 110.55 |
| 3 | O | 3196[B] | THR | N-CA-C | -7.12 | 100.94 | 110.55 |
| 3 | L | 3196[A] | THR | N-CA-C | -7.11 | 100.95 | 110.55 |
| 3 | L | 3196[B] | THR | N-CA-C | -7.11 | 100.95 | 110.55 |
| 3 | R | 3196[A] | THR | N-CA-C | -7.11 | 100.95 | 110.55 |
| 3 | R | 3196[B] | THR | N-CA-C | -7.11 | 100.95 | 110.55 |
| 3 | d | 3196[A] | THR | N-CA-C | -7.11 | 100.95 | 110.55 |
| 3 | d | 3196[B] | THR | N-CA-C | -7.11 | 100.95 | 110.55 |
| 3 | F | 3196[A] | THR | N-CA-C | -7.11 | 100.96 | 110.55 |
| 3 | F | 3196[B] | THR | N-CA-C | -7.11 | 100.96 | 110.55 |
| 3 | C | 3196[A] | THR | N-CA-C | -7.10 | 100.96 | 110.55 |
| 3 | C | 3196[B] | THR | N-CA-C | -7.10 | 100.96 | 110.55 |
| 2 | E | 2128 | LEU | CA-C-N | -7.10 | 113.06 | 120.38 |
| 2 | E | 2128 | LEU | C-N-CA | -7.10 | 113.06 | 120.38 |
| 3 | X | 3196[A] | THR | N-CA-C | -7.10 | 100.96 | 110.55 |
| 3 | X | 3196[B] | THR | N-CA-C | -7.10 | 100.96 | 110.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | a | 3196[A] | THR | N-CA-C | -7.08 | 100.99 | 110.55 |
| 3 | a | 3196[B] | THR | N-CA-C | -7.08 | 100.99 | 110.55 |
| 3 | C | 3153[A] | LYS | CA-C-N | -7.05 | 113.40 | 120.31 |
| 3 | C | 3153[A] | LYS | C-N-CA | -7.05 | 113.40 | 120.31 |
| 3 | C | 3153[B] | LYS | CA-C-N | -7.05 | 113.40 | 120.31 |
| 3 | C | 3153[B] | LYS | C-N-CA | -7.05 | 113.40 | 120.31 |
| 1 | M | 897 | HIS | N-CA-C | -7.00 | 99.17 | 108.34 |
| 3 | I | 3308[A] | LYS | CA-C-N | -6.98 | 113.47 | 120.31 |
| 3 | I | 3308[A] | LYS | C-N-CA | -6.98 | 113.47 | 120.31 |
| 3 | I | 3308[B] | LYS | CA-C-N | -6.98 | 113.47 | 120.31 |
| 3 | I | 3308[B] | LYS | C-N-CA | -6.98 | 113.47 | 120.31 |
| 1 | P | 418 | ASP | N-CA-C | 6.98 | 118.97 | 111.36 |
| 1 | J | 117 | LYS | N-CA-C | 6.93 | 117.64 | 108.07 |
| 3 | R | 3308[A] | LYS | CA-C-N | -6.93 | 113.52 | 120.31 |
| 3 | R | 3308[A] | LYS | C-N-CA | -6.93 | 113.52 | 120.31 |
| 3 | R | 3308[B] | LYS | CA-C-N | -6.93 | 113.52 | 120.31 |
| 3 | R | 3308[B] | LYS | C-N-CA | -6.93 | 113.52 | 120.31 |
| 3 | C | 3308[A] | LYS | CA-C-N | -6.93 | 113.52 | 120.31 |
| 3 | C | 3308[A] | LYS | C-N-CA | -6.93 | 113.52 | 120.31 |
| 3 | C | 3308[B] | LYS | CA-C-N | -6.93 | 113.52 | 120.31 |
| 3 | C | 3308[B] | LYS | C-N-CA | -6.93 | 113.52 | 120.31 |
| 1 | P | 1584 | GLY | N-CA-C | 6.93 | 123.34 | 111.15 |
| 1 | S | 1636 | ASN | N-CA-C | -6.93 | 103.74 | 111.71 |
| 3 | F | 2931[A] | THR | CA-C-N | -6.90 | 112.65 | 119.76 |
| 3 | F | 2931[A] | THR | C-N-CA | -6.90 | 112.65 | 119.76 |
| 3 | F | 2931[B] | THR | CA-C-N | -6.90 | 112.65 | 119.76 |
| 3 | F | 2931[B] | THR | C-N-CA | -6.90 | 112.65 | 119.76 |
| 3 | X | 3308[A] | LYS | CA-C-N | -6.90 | 113.55 | 120.31 |
| 3 | X | 3308[A] | LYS | C-N-CA | -6.90 | 113.55 | 120.31 |
| 3 | X | 3308[B] | LYS | CA-C-N | -6.90 | 113.55 | 120.31 |
| 3 | X | 3308[B] | LYS | C-N-CA | -6.90 | 113.55 | 120.31 |
| 3 | O | 3308[A] | LYS | CA-C-N | -6.90 | 113.55 | 120.31 |
| 3 | O | 3308[A] | LYS | C-N-CA | -6.90 | 113.55 | 120.31 |
| 3 | O | 3308[B] | LYS | CA-C-N | -6.90 | 113.55 | 120.31 |
| 3 | O | 3308[B] | LYS | C-N-CA | -6.90 | 113.55 | 120.31 |
| 3 | R | 2931[A] | THR | CA-C-N | -6.90 | 112.66 | 119.76 |
| 3 | R | 2931[A] | THR | C-N-CA | -6.90 | 112.66 | 119.76 |
| 3 | R | 2931[B] | THR | CA-C-N | -6.90 | 112.66 | 119.76 |
| 3 | R | 2931[B] | THR | C-N-CA | -6.90 | 112.66 | 119.76 |
| 3 | d | 3308[A] | LYS | CA-C-N | -6.89 | 113.55 | 120.31 |
| 3 | d | 3308[A] | LYS | C-N-CA | -6.89 | 113.55 | 120.31 |
| 3 | d | 3308[B] | LYS | CA-C-N | -6.89 | 113.55 | 120.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | d | 3308[B] | LYS | C-N-CA | -6.89 | 113.55 | 120.31 |
| 3 | F | 3308[A] | LYS | CA-C-N | -6.89 | 113.56 | 120.31 |
| 3 | F | 3308[A] | LYS | C-N-CA | -6.89 | 113.56 | 120.31 |
| 3 | F | 3308[B] | LYS | CA-C-N | -6.89 | 113.56 | 120.31 |
| 3 | F | 3308[B] | LYS | C-N-CA | -6.89 | 113.56 | 120.31 |
| 3 | L | 3308[A] | LYS | CA-C-N | -6.89 | 113.56 | 120.31 |
| 3 | L | 3308[A] | LYS | C-N-CA | -6.89 | 113.56 | 120.31 |
| 3 | L | 3308[B] | LYS | CA-C-N | -6.89 | 113.56 | 120.31 |
| 3 | L | 3308[B] | LYS | C-N-CA | -6.89 | 113.56 | 120.31 |
| 3 | O | 2931[A] | THR | CA-C-N | -6.89 | 112.67 | 119.76 |
| 3 | O | 2931[A] | THR | C-N-CA | -6.89 | 112.67 | 119.76 |
| 3 | O | 2931[B] | THR | CA-C-N | -6.89 | 112.67 | 119.76 |
| 3 | O | 2931[B] | THR | C-N-CA | -6.89 | 112.67 | 119.76 |
| 1 | Y | 957 | ASN | CA-C-N | -6.89 | 113.60 | 120.21 |
| 1 | Y | 957 | ASN | C-N-CA | -6.89 | 113.60 | 120.21 |
| 3 | U | 2931[A] | THR | CA-C-N | -6.89 | 112.67 | 119.76 |
| 3 | U | 2931[A] | THR | C-N-CA | -6.89 | 112.67 | 119.76 |
| 3 | U | 2931[B] | THR | CA-C-N | -6.89 | 112.67 | 119.76 |
| 3 | U | 2931[B] | THR | C-N-CA | -6.89 | 112.67 | 119.76 |
| 2 | W | 2650 | GLY | N-CA-C | 6.89 | 120.97 | 112.64 |
| 3 | d | 2931[A] | THR | CA-C-N | -6.89 | 112.67 | 119.76 |
| 3 | d | 2931[A] | THR | C-N-CA | -6.89 | 112.67 | 119.76 |
| 3 | d | 2931[B] | THR | CA-C-N | -6.89 | 112.67 | 119.76 |
| 3 | d | 2931[B] | THR | C-N-CA | -6.89 | 112.67 | 119.76 |
| 3 | U | 3308[A] | LYS | CA-C-N | -6.88 | 113.56 | 120.31 |
| 3 | U | 3308[A] | LYS | C-N-CA | -6.88 | 113.56 | 120.31 |
| 3 | U | 3308[B] | LYS | CA-C-N | -6.88 | 113.56 | 120.31 |
| 3 | U | 3308[B] | LYS | C-N-CA | -6.88 | 113.56 | 120.31 |
| 3 | a | 3308[A] | LYS | CA-C-N | -6.88 | 113.57 | 120.31 |
| 3 | a | 3308[A] | LYS | C-N-CA | -6.88 | 113.57 | 120.31 |
| 3 | a | 3308[B] | LYS | CA-C-N | -6.88 | 113.57 | 120.31 |
| 3 | a | 3308[B] | LYS | C-N-CA | -6.88 | 113.57 | 120.31 |
| 3 | U | 3197[A] | ILE | O-C-N | 6.87 | 124.82 | 120.42 |
| 3 | U | 3197[B] | ILE | O-C-N | 6.87 | 124.82 | 120.42 |
| 2 | E | 2340 | ALA | CA-C-N | -6.86 | 112.71 | 119.64 |
| 2 | E | 2340 | ALA | C-N-CA | -6.86 | 112.71 | 119.64 |
| 3 | a | 3197[A] | ILE | O-C-N | 6.86 | 124.81 | 120.42 |
| 3 | a | 3197[B] | ILE | O-C-N | 6.86 | 124.81 | 120.42 |
| 3 | X | 2931[A] | THR | CA-C-N | -6.85 | 112.70 | 119.76 |
| 3 | X | 2931[A] | THR | C-N-CA | -6.85 | 112.70 | 119.76 |
| 3 | X | 2931[B] | THR | CA-C-N | -6.85 | 112.70 | 119.76 |
| 3 | X | 2931[B] | THR | C-N-CA | -6.85 | 112.70 | 119.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | I | 3197[A] | ILE | O-C-N | 6.85 | 124.80 | 120.42 |
| 3 | I | 3197[B] | ILE | O-C-N | 6.85 | 124.80 | 120.42 |
| 3 | X | 3197[A] | ILE | O-C-N | 6.84 | 124.80 | 120.42 |
| 3 | X | 3197[B] | ILE | O-C-N | 6.84 | 124.80 | 120.42 |
| 1 | G | 675 | SER | CA-C-N | -6.83 | 111.30 | 119.84 |
| 1 | G | 675 | SER | C-N-CA | -6.83 | 111.30 | 119.84 |
| 3 | C | 2931[A] | THR | CA-C-N | -6.83 | 112.72 | 119.76 |
| 3 | C | 2931[A] | THR | C-N-CA | -6.83 | 112.72 | 119.76 |
| 3 | C | 2931[B] | THR | CA-C-N | -6.83 | 112.72 | 119.76 |
| 3 | C | 2931[B] | THR | C-N-CA | -6.83 | 112.72 | 119.76 |
| 3 | L | 2931[A] | THR | CA-C-N | -6.83 | 112.72 | 119.76 |
| 3 | L | 2931[A] | THR | C-N-CA | -6.83 | 112.72 | 119.76 |
| 3 | L | 2931[B] | THR | CA-C-N | -6.83 | 112.72 | 119.76 |
| 3 | L | 2931[B] | THR | C-N-CA | -6.83 | 112.72 | 119.76 |
| 3 | a | 2931[A] | THR | CA-C-N | -6.83 | 112.73 | 119.76 |
| 3 | a | 2931[A] | THR | C-N-CA | -6.83 | 112.73 | 119.76 |
| 3 | a | 2931[B] | THR | CA-C-N | -6.83 | 112.73 | 119.76 |
| 3 | a | 2931[B] | THR | C-N-CA | -6.83 | 112.73 | 119.76 |
| 3 | d | 3197[A] | ILE | O-C-N | 6.80 | 124.78 | 120.42 |
| 3 | d | 3197[B] | ILE | O-C-N | 6.80 | 124.78 | 120.42 |
| 3 | I | 2931[A] | THR | CA-C-N | -6.80 | 112.76 | 119.76 |
| 3 | I | 2931[A] | THR | C-N-CA | -6.80 | 112.76 | 119.76 |
| 3 | I | 2931[B] | THR | CA-C-N | -6.80 | 112.76 | 119.76 |
| 3 | I | 2931[B] | THR | C-N-CA | -6.80 | 112.76 | 119.76 |
| 3 | F | 3197[A] | ILE | O-C-N | 6.79 | 124.77 | 120.42 |
| 3 | F | 3197[B] | ILE | O-C-N | 6.79 | 124.77 | 120.42 |
| 3 | C | 3197[A] | ILE | O-C-N | 6.79 | 124.76 | 120.42 |
| 3 | C | 3197[B] | ILE | O-C-N | 6.79 | 124.76 | 120.42 |
| 3 | d | 3000[A] | LEU | N-CA-C | -6.77 | 96.59 | 108.23 |
| 3 | d | 3000[B] | LEU | N-CA-C | -6.77 | 96.59 | 108.23 |
| 1 | P | 228 | GLY | N-CA-C | 6.76 | 124.11 | 114.64 |
| 3 | O | 3139[A] | LEU | CA-C-N | -6.76 | 113.00 | 119.76 |
| 3 | O | 3139[A] | LEU | C-N-CA | -6.76 | 113.00 | 119.76 |
| 3 | O | 3139[B] | LEU | CA-C-N | -6.76 | 113.00 | 119.76 |
| 3 | O | 3139[B] | LEU | C-N-CA | -6.76 | 113.00 | 119.76 |
| 3 | U | 3000[A] | LEU | N-CA-C | -6.75 | 96.62 | 108.23 |
| 3 | U | 3000[B] | LEU | N-CA-C | -6.75 | 96.62 | 108.23 |
| 3 | C | 3000[A] | LEU | N-CA-C | -6.74 | 96.64 | 108.23 |
| 3 | C | 3000[B] | LEU | N-CA-C | -6.74 | 96.64 | 108.23 |
| 3 | R | 3000[A] | LEU | N-CA-C | -6.74 | 96.64 | 108.23 |
| 3 | R | 3000[B] | LEU | N-CA-C | -6.74 | 96.64 | 108.23 |
| 3 | F | 3000[A] | LEU | N-CA-C | -6.74 | 96.64 | 108.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | F | 3000[B] | LEU | N-CA-C | -6.74 | 96.64 | 108.23 |
| 3 | L | 3000[A] | LEU | N-CA-C | -6.73 | 96.65 | 108.23 |
| 3 | L | 3000[B] | LEU | N-CA-C | -6.73 | 96.65 | 108.23 |
| 3 | O | 3000[A] | LEU | N-CA-C | -6.73 | 96.65 | 108.23 |
| 3 | O | 3000[B] | LEU | N-CA-C | -6.73 | 96.65 | 108.23 |
| 1 | G | 1486 | LEU | CA-C-N | -6.73 | 112.76 | 119.56 |
| 1 | G | 1486 | LEU | C-N-CA | -6.73 | 112.76 | 119.56 |
| 1 | M | 126 | GLY | CA-C-N | 6.73 | 133.81 | 121.70 |
| 1 | M | 126 | GLY | C-N-CA | 6.73 | 133.81 | 121.70 |
| 3 | d | 3139[A] | LEU | CA-C-N | -6.73 | 113.03 | 119.76 |
| 3 | d | 3139[A] | LEU | C-N-CA | -6.73 | 113.03 | 119.76 |
| 3 | d | 3139[B] | LEU | CA-C-N | -6.73 | 113.03 | 119.76 |
| 3 | d | 3139[B] | LEU | C-N-CA | -6.73 | 113.03 | 119.76 |
| 3 | X | 3000[A] | LEU | N-CA-C | -6.73 | 96.66 | 108.23 |
| 3 | X | 3000[B] | LEU | N-CA-C | -6.73 | 96.66 | 108.23 |
| 1 | Y | 669 | LYS | CA-C-N | -6.72 | 112.75 | 120.89 |
| 1 | Y | 669 | LYS | C-N-CA | -6.72 | 112.75 | 120.89 |
| 3 | L | 3197[A] | ILE | O-C-N | 6.72 | 124.72 | 120.42 |
| 3 | L | 3197[B] | ILE | O-C-N | 6.72 | 124.72 | 120.42 |
| 1 | P | 417 | MET | N-CA-C | 6.71 | 118.60 | 111.28 |
| 3 | a | 3139[A] | LEU | CA-C-N | -6.71 | 113.05 | 119.76 |
| 3 | a | 3139[A] | LEU | C-N-CA | -6.71 | 113.05 | 119.76 |
| 3 | a | 3139[B] | LEU | CA-C-N | -6.71 | 113.05 | 119.76 |
| 3 | a | 3139[B] | LEU | C-N-CA | -6.71 | 113.05 | 119.76 |
| 3 | O | 2967[A] | CYS | N-CA-C | 6.71 | 116.91 | 108.45 |
| 3 | O | 2967[B] | CYS | N-CA-C | 6.71 | 116.91 | 108.45 |
| 3 | R | 3139[A] | LEU | CA-C-N | -6.71 | 113.05 | 119.76 |
| 3 | R | 3139[A] | LEU | C-N-CA | -6.71 | 113.05 | 119.76 |
| 3 | R | 3139[B] | LEU | CA-C-N | -6.71 | 113.05 | 119.76 |
| 3 | R | 3139[B] | LEU | C-N-CA | -6.71 | 113.05 | 119.76 |
| 3 | R | 3197[A] | ILE | O-C-N | 6.70 | 124.71 | 120.42 |
| 3 | R | 3197[B] | ILE | O-C-N | 6.70 | 124.71 | 120.42 |
| 3 | U | 3139[A] | LEU | CA-C-N | -6.70 | 113.06 | 119.76 |
| 3 | U | 3139[A] | LEU | C-N-CA | -6.70 | 113.06 | 119.76 |
| 3 | U | 3139[B] | LEU | CA-C-N | -6.70 | 113.06 | 119.76 |
| 3 | U | 3139[B] | LEU | C-N-CA | -6.70 | 113.06 | 119.76 |
| 3 | a | 3000[A] | LEU | N-CA-C | -6.70 | 96.71 | 108.23 |
| 3 | a | 3000[B] | LEU | N-CA-C | -6.70 | 96.71 | 108.23 |
| 3 | I | 3000[A] | LEU | N-CA-C | -6.70 | 96.71 | 108.23 |
| 3 | I | 3000[B] | LEU | N-CA-C | -6.70 | 96.71 | 108.23 |
| 3 | L | 3139[A] | LEU | CA-C-N | -6.69 | 113.07 | 119.76 |
| 3 | L | 3139[A] | LEU | C-N-CA | -6.69 | 113.07 | 119.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | L | 3139[B] | LEU | CA-C-N | -6.69 | 113.07 | 119.76 |
| 3 | L | 3139[B] | LEU | C-N-CA | -6.69 | 113.07 | 119.76 |
| 3 | a | 2967[A] | CYS | N-CA-C | 6.68 | 116.87 | 108.45 |
| 3 | a | 2967[B] | CYS | N-CA-C | 6.68 | 116.87 | 108.45 |
| 3 | C | 3139[A] | LEU | CA-C-N | -6.68 | 113.08 | 119.76 |
| 3 | C | 3139[A] | LEU | C-N-CA | -6.68 | 113.08 | 119.76 |
| 3 | C | 3139[B] | LEU | CA-C-N | -6.68 | 113.08 | 119.76 |
| 3 | C | 3139[B] | LEU | C-N-CA | -6.68 | 113.08 | 119.76 |
| 3 | I | 2967[A] | CYS | N-CA-C | 6.68 | 116.86 | 108.45 |
| 3 | I | 2967[B] | CYS | N-CA-C | 6.68 | 116.86 | 108.45 |
| 3 | F | 3139[A] | LEU | CA-C-N | -6.67 | 113.09 | 119.76 |
| 3 | F | 3139[A] | LEU | C-N-CA | -6.67 | 113.09 | 119.76 |
| 3 | F | 3139[B] | LEU | CA-C-N | -6.67 | 113.09 | 119.76 |
| 3 | F | 3139[B] | LEU | C-N-CA | -6.67 | 113.09 | 119.76 |
| 3 | L | 2967[A] | CYS | N-CA-C | 6.67 | 116.86 | 108.45 |
| 3 | L | 2967[B] | CYS | N-CA-C | 6.67 | 116.86 | 108.45 |
| 3 | I | 3139[A] | LEU | CA-C-N | -6.66 | 113.10 | 119.76 |
| 3 | I | 3139[A] | LEU | C-N-CA | -6.66 | 113.10 | 119.76 |
| 3 | I | 3139[B] | LEU | CA-C-N | -6.66 | 113.10 | 119.76 |
| 3 | I | 3139[B] | LEU | C-N-CA | -6.66 | 113.10 | 119.76 |
| 1 | P | 450 | LYS | N-CA-C | 6.66 | 120.00 | 109.81 |
| 3 | R | 2967[A] | CYS | N-CA-C | 6.65 | 116.83 | 108.45 |
| 3 | R | 2967[B] | CYS | N-CA-C | 6.65 | 116.83 | 108.45 |
| 1 | P | 1086 | LEU | N-CA-C | 6.64 | 119.13 | 111.02 |
| 3 | X | 2967[A] | CYS | N-CA-C | 6.64 | 116.82 | 108.45 |
| 3 | X | 2967[B] | CYS | N-CA-C | 6.64 | 116.82 | 108.45 |
| 3 | X | 3139[A] | LEU | CA-C-N | -6.64 | 113.12 | 119.76 |
| 3 | X | 3139[A] | LEU | C-N-CA | -6.64 | 113.12 | 119.76 |
| 3 | X | 3139[B] | LEU | CA-C-N | -6.64 | 113.12 | 119.76 |
| 3 | X | 3139[B] | LEU | C-N-CA | -6.64 | 113.12 | 119.76 |
| 3 | O | 3197[A] | ILE | O-C-N | 6.64 | 124.67 | 120.42 |
| 3 | O | 3197[B] | ILE | O-C-N | 6.64 | 124.67 | 120.42 |
| 3 | C | 2967[A] | CYS | N-CA-C | 6.63 | 116.81 | 108.45 |
| 3 | C | 2967[B] | CYS | N-CA-C | 6.63 | 116.81 | 108.45 |
| 3 | L | 3291[A] | ASP | N-CA-C | -6.63 | 102.25 | 110.41 |
| 3 | L | 3291[B] | ASP | N-CA-C | -6.63 | 102.25 | 110.41 |
| 3 | d | 2967[A] | CYS | N-CA-C | 6.63 | 116.81 | 108.45 |
| 3 | d | 2967[B] | CYS | N-CA-C | 6.63 | 116.81 | 108.45 |
| 3 | F | 2967[A] | CYS | N-CA-C | 6.63 | 116.80 | 108.45 |
| 3 | F | 2967[B] | CYS | N-CA-C | 6.63 | 116.80 | 108.45 |
| 3 | a | 3291[A] | ASP | N-CA-C | -6.63 | 102.26 | 110.41 |
| 3 | a | 3291[B] | ASP | N-CA-C | -6.63 | 102.26 | 110.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | R | 3291[A] | ASP | N-CA-C | -6.62 | 102.27 | 110.41 |
| 3 | R | 3291[B] | ASP | N-CA-C | -6.62 | 102.27 | 110.41 |
| 3 | F | 3291[A] | ASP | N-CA-C | -6.61 | 102.28 | 110.41 |
| 3 | F | 3291[B] | ASP | N-CA-C | -6.61 | 102.28 | 110.41 |
| 3 | U | 2967[A] | CYS | N-CA-C | 6.60 | 116.77 | 108.45 |
| 3 | U | 2967[B] | CYS | N-CA-C | 6.60 | 116.77 | 108.45 |
| 3 | C | 3291[A] | ASP | N-CA-C | -6.59 | 102.30 | 110.41 |
| 3 | C | 3291[B] | ASP | N-CA-C | -6.59 | 102.30 | 110.41 |
| 3 | L | 3254[A] | MET | CA-C-N | -6.59 | 113.50 | 120.03 |
| 3 | L | 3254[A] | MET | C-N-CA | -6.59 | 113.50 | 120.03 |
| 3 | L | 3254[B] | MET | CA-C-N | -6.59 | 113.50 | 120.03 |
| 3 | L | 3254[B] | MET | C-N-CA | -6.59 | 113.50 | 120.03 |
| 3 | O | 3291[A] | ASP | N-CA-C | -6.59 | 102.30 | 110.41 |
| 3 | O | 3291[B] | ASP | N-CA-C | -6.59 | 102.30 | 110.41 |
| 3 | X | 3291[A] | ASP | N-CA-C | -6.59 | 102.30 | 110.41 |
| 3 | X | 3291[B] | ASP | N-CA-C | -6.59 | 102.30 | 110.41 |
| 3 | d | 3291[A] | ASP | N-CA-C | -6.59 | 102.30 | 110.41 |
| 3 | d | 3291[B] | ASP | N-CA-C | -6.59 | 102.30 | 110.41 |
| 3 | U | 3291[A] | ASP | N-CA-C | -6.58 | 102.31 | 110.41 |
| 3 | U | 3291[B] | ASP | N-CA-C | -6.58 | 102.31 | 110.41 |
| 3 | I | 3291[A] | ASP | N-CA-C | -6.58 | 102.32 | 110.41 |
| 3 | I | 3291[B] | ASP | N-CA-C | -6.58 | 102.32 | 110.41 |
| 1 | G | 1296 | VAL | CA-C-N | -6.57 | 111.62 | 119.84 |
| 1 | G | 1296 | VAL | C-N-CA | -6.57 | 111.62 | 119.84 |
| 3 | I | 3254[A] | MET | CA-C-N | -6.56 | 113.54 | 120.03 |
| 3 | I | 3254[A] | MET | C-N-CA | -6.56 | 113.54 | 120.03 |
| 3 | I | 3254[B] | MET | CA-C-N | -6.56 | 113.54 | 120.03 |
| 3 | I | 3254[B] | MET | C-N-CA | -6.56 | 113.54 | 120.03 |
| 1 | J | 823 | VAL | CA-C-N | 6.55 | 126.31 | 119.76 |
| 1 | J | 823 | VAL | C-N-CA | 6.55 | 126.31 | 119.76 |
| 3 | O | 3254[A] | MET | CA-C-N | -6.55 | 113.54 | 120.03 |
| 3 | O | 3254[A] | MET | C-N-CA | -6.55 | 113.54 | 120.03 |
| 3 | O | 3254[B] | MET | CA-C-N | -6.55 | 113.54 | 120.03 |
| 3 | O | 3254[B] | MET | C-N-CA | -6.55 | 113.54 | 120.03 |
| 3 | d | 3254[A] | MET | CA-C-N | -6.53 | 113.57 | 120.03 |
| 3 | d | 3254[A] | MET | C-N-CA | -6.53 | 113.57 | 120.03 |
| 3 | d | 3254[B] | MET | CA-C-N | -6.53 | 113.57 | 120.03 |
| 3 | d | 3254[B] | MET | C-N-CA | -6.53 | 113.57 | 120.03 |
| 3 | U | 2963[A] | MET | CA-C-N | -6.52 | 112.79 | 119.83 |
| 3 | U | 2963[A] | MET | C-N-CA | -6.52 | 112.79 | 119.83 |
| 3 | U | 2963[B] | MET | CA-C-N | -6.52 | 112.79 | 119.83 |
| 3 | U | 2963[B] | MET | C-N-CA | -6.52 | 112.79 | 119.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | L | 3036[A] | GLY | N-CA-C | -6.52 | 102.16 | 111.42 |
| 3 | L | 3036[B] | GLY | N-CA-C | -6.52 | 102.16 | 111.42 |
| 3 | U | 3254[A] | MET | CA-C-N | -6.52 | 113.58 | 120.03 |
| 3 | U | 3254[A] | MET | C-N-CA | -6.52 | 113.58 | 120.03 |
| 3 | U | 3254[B] | MET | CA-C-N | -6.52 | 113.58 | 120.03 |
| 3 | U | 3254[B] | MET | C-N-CA | -6.52 | 113.58 | 120.03 |
| 3 | a | 3254[A] | MET | CA-C-N | -6.52 | 113.58 | 120.03 |
| 3 | a | 3254[A] | MET | C-N-CA | -6.52 | 113.58 | 120.03 |
| 3 | a | 3254[B] | MET | CA-C-N | -6.52 | 113.58 | 120.03 |
| 3 | a | 3254[B] | MET | C-N-CA | -6.52 | 113.58 | 120.03 |
| 3 | X | 3254[A] | MET | CA-C-N | -6.52 | 113.58 | 120.03 |
| 3 | X | 3254[A] | MET | C-N-CA | -6.52 | 113.58 | 120.03 |
| 3 | X | 3254[B] | MET | CA-C-N | -6.52 | 113.58 | 120.03 |
| 3 | X | 3254[B] | MET | C-N-CA | -6.52 | 113.58 | 120.03 |
| 3 | F | 3254[A] | MET | CA-C-N | -6.51 | 113.58 | 120.03 |
| 3 | F | 3254[A] | MET | C-N-CA | -6.51 | 113.58 | 120.03 |
| 3 | F | 3254[B] | MET | CA-C-N | -6.51 | 113.58 | 120.03 |
| 3 | F | 3254[B] | MET | C-N-CA | -6.51 | 113.58 | 120.03 |
| 3 | U | 3036[A] | GLY | N-CA-C | -6.51 | 102.17 | 111.42 |
| 3 | U | 3036[B] | GLY | N-CA-C | -6.51 | 102.17 | 111.42 |
| 3 | R | 3036[A] | GLY | N-CA-C | -6.51 | 102.18 | 111.42 |
| 3 | R | 3036[B] | GLY | N-CA-C | -6.51 | 102.18 | 111.42 |
| 3 | R | 3254[A] | MET | CA-C-N | -6.51 | 113.59 | 120.03 |
| 3 | R | 3254[A] | MET | C-N-CA | -6.51 | 113.59 | 120.03 |
| 3 | R | 3254[B] | MET | CA-C-N | -6.51 | 113.59 | 120.03 |
| 3 | R | 3254[B] | MET | C-N-CA | -6.51 | 113.59 | 120.03 |
| 3 | C | 3036[A] | GLY | N-CA-C | -6.50 | 102.19 | 111.42 |
| 3 | C | 3036[B] | GLY | N-CA-C | -6.50 | 102.19 | 111.42 |
| 1 | A | 404 | ILE | CA-C-N | 6.50 | 124.34 | 119.66 |
| 1 | A | 404 | ILE | C-N-CA | 6.50 | 124.34 | 119.66 |
| 3 | a | 3036[A] | GLY | N-CA-C | -6.50 | 102.19 | 111.42 |
| 3 | a | 3036[B] | GLY | N-CA-C | -6.50 | 102.19 | 111.42 |
| 3 | I | 3036[A] | GLY | N-CA-C | -6.50 | 102.19 | 111.42 |
| 3 | I | 3036[B] | GLY | N-CA-C | -6.50 | 102.19 | 111.42 |
| 3 | L | 2969[A] | TYR | N-CA-C | -6.49 | 99.35 | 109.87 |
| 3 | L | 2969[B] | TYR | N-CA-C | -6.49 | 99.35 | 109.87 |
| 3 | L | 2963[A] | MET | CA-C-N | -6.49 | 112.82 | 119.83 |
| 3 | L | 2963[A] | MET | C-N-CA | -6.49 | 112.82 | 119.83 |
| 3 | L | 2963[B] | MET | CA-C-N | -6.49 | 112.82 | 119.83 |
| 3 | L | 2963[B] | MET | C-N-CA | -6.49 | 112.82 | 119.83 |
| 3 | O | 3036[A] | GLY | N-CA-C | -6.49 | 102.21 | 111.42 |
| 3 | O | 3036[B] | GLY | N-CA-C | -6.49 | 102.21 | 111.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | d | 3036[A] | GLY | N-CA-C | -6.49 | 102.21 | 111.42 |
| 3 | d | 3036[B] | GLY | N-CA-C | -6.49 | 102.21 | 111.42 |
| 3 | F | 2969[A] | TYR | N-CA-C | -6.48 | 99.37 | 109.87 |
| 3 | F | 2969[B] | TYR | N-CA-C | -6.48 | 99.37 | 109.87 |
| 3 | U | 2969[A] | TYR | N-CA-C | -6.48 | 99.37 | 109.87 |
| 3 | U | 2969[B] | TYR | N-CA-C | -6.48 | 99.37 | 109.87 |
| 3 | d | 2969[A] | TYR | N-CA-C | -6.48 | 99.38 | 109.87 |
| 3 | d | 2969[B] | TYR | N-CA-C | -6.48 | 99.38 | 109.87 |
| 3 | C | 2969[A] | TYR | N-CA-C | -6.47 | 99.38 | 109.87 |
| 3 | C | 2969[B] | TYR | N-CA-C | -6.47 | 99.38 | 109.87 |
| 3 | O | 2969[A] | TYR | N-CA-C | -6.47 | 99.38 | 109.87 |
| 3 | O | 2969[B] | TYR | N-CA-C | -6.47 | 99.38 | 109.87 |
| 1 | G | 1082 | SER | CA-C-N | -6.47 | 111.75 | 119.84 |
| 1 | G | 1082 | SER | C-N-CA | -6.47 | 111.75 | 119.84 |
| 3 | a | 2969[A] | TYR | N-CA-C | -6.47 | 99.38 | 109.87 |
| 3 | a | 2969[B] | TYR | N-CA-C | -6.47 | 99.38 | 109.87 |
| 3 | F | 3036[A] | GLY | N-CA-C | -6.47 | 102.23 | 111.42 |
| 3 | F | 3036[B] | GLY | N-CA-C | -6.47 | 102.23 | 111.42 |
| 3 | X | 2969[A] | TYR | N-CA-C | -6.47 | 99.39 | 109.87 |
| 3 | X | 2969[B] | TYR | N-CA-C | -6.47 | 99.39 | 109.87 |
| 1 | V | 1581 | GLU | N-CA-C | 6.47 | 116.39 | 107.73 |
| 3 | X | 3036[A] | GLY | N-CA-C | -6.47 | 102.24 | 111.42 |
| 3 | X | 3036[B] | GLY | N-CA-C | -6.47 | 102.24 | 111.42 |
| 2 | c | 2558 | CYS | N-CA-C | 6.46 | 121.30 | 113.41 |
| 3 | C | 3254[A] | MET | CA-C-N | -6.46 | 113.63 | 120.03 |
| 3 | C | 3254[A] | MET | C-N-CA | -6.46 | 113.63 | 120.03 |
| 3 | C | 3254[B] | MET | CA-C-N | -6.46 | 113.63 | 120.03 |
| 3 | C | 3254[B] | MET | C-N-CA | -6.46 | 113.63 | 120.03 |
| 3 | R | 2969[A] | TYR | N-CA-C | -6.46 | 99.40 | 109.87 |
| 3 | R | 2969[B] | TYR | N-CA-C | -6.46 | 99.40 | 109.87 |
| 3 | I | 2969[A] | TYR | N-CA-C | -6.46 | 99.40 | 109.87 |
| 3 | I | 2969[B] | TYR | N-CA-C | -6.46 | 99.40 | 109.87 |
| 3 | O | 2963[A] | MET | CA-C-N | -6.46 | 112.85 | 119.83 |
| 3 | O | 2963[A] | MET | C-N-CA | -6.46 | 112.85 | 119.83 |
| 3 | O | 2963[B] | MET | CA-C-N | -6.46 | 112.85 | 119.83 |
| 3 | O | 2963[B] | MET | C-N-CA | -6.46 | 112.85 | 119.83 |
| 3 | a | 2963[A] | MET | CA-C-N | -6.45 | 112.86 | 119.83 |
| 3 | a | 2963[A] | MET | C-N-CA | -6.45 | 112.86 | 119.83 |
| 3 | a | 2963[B] | MET | CA-C-N | -6.45 | 112.86 | 119.83 |
| 3 | a | 2963[B] | MET | C-N-CA | -6.45 | 112.86 | 119.83 |
| 3 | X | 2963[A] | MET | CA-C-N | -6.45 | 112.87 | 119.83 |
| 3 | X | 2963[A] | MET | C-N-CA | -6.45 | 112.87 | 119.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | X | 2963[B] | MET | CA-C-N | -6.45 | 112.87 | 119.83 |
| 3 | X | 2963[B] | MET | C-N-CA | -6.45 | 112.87 | 119.83 |
| 3 | F | 2963[A] | MET | CA-C-N | -6.44 | 112.87 | 119.83 |
| 3 | F | 2963[A] | MET | C-N-CA | -6.44 | 112.87 | 119.83 |
| 3 | F | 2963[B] | MET | CA-C-N | -6.44 | 112.87 | 119.83 |
| 3 | F | 2963[B] | MET | C-N-CA | -6.44 | 112.87 | 119.83 |
| 3 | I | 2963[A] | MET | CA-C-N | -6.43 | 112.89 | 119.83 |
| 3 | I | 2963[A] | MET | C-N-CA | -6.43 | 112.89 | 119.83 |
| 3 | I | 2963[B] | MET | CA-C-N | -6.43 | 112.89 | 119.83 |
| 3 | I | 2963[B] | MET | C-N-CA | -6.43 | 112.89 | 119.83 |
| 3 | R | 2963[A] | MET | CA-C-N | -6.43 | 112.89 | 119.83 |
| 3 | R | 2963[A] | MET | C-N-CA | -6.43 | 112.89 | 119.83 |
| 3 | R | 2963[B] | MET | CA-C-N | -6.43 | 112.89 | 119.83 |
| 3 | R | 2963[B] | MET | C-N-CA | -6.43 | 112.89 | 119.83 |
| 1 | b | 758 | GLY | N-CA-C | 6.42 | 119.93 | 111.52 |
| 1 | J | 669 | LYS | CA-C-N | -6.42 | 113.08 | 119.56 |
| 1 | J | 669 | LYS | C-N-CA | -6.42 | 113.08 | 119.56 |
| 3 | d | 2963[A] | MET | CA-C-N | -6.41 | 112.91 | 119.83 |
| 3 | d | 2963[A] | MET | C-N-CA | -6.41 | 112.91 | 119.83 |
| 3 | d | 2963[B] | MET | CA-C-N | -6.41 | 112.91 | 119.83 |
| 3 | d | 2963[B] | MET | C-N-CA | -6.41 | 112.91 | 119.83 |
| 3 | C | 2963[A] | MET | CA-C-N | -6.41 | 112.91 | 119.83 |
| 3 | C | 2963[A] | MET | C-N-CA | -6.41 | 112.91 | 119.83 |
| 3 | C | 2963[B] | MET | CA-C-N | -6.41 | 112.91 | 119.83 |
| 3 | C | 2963[B] | MET | C-N-CA | -6.41 | 112.91 | 119.83 |
| 1 | V | 675 | SER | CA-C-N | -6.39 | 111.86 | 119.84 |
| 1 | V | 675 | SER | C-N-CA | -6.39 | 111.86 | 119.84 |
| 3 | L | 3178[A] | PHE | N-CA-C | -6.39 | 103.57 | 112.45 |
| 3 | L | 3178[B] | PHE | N-CA-C | -6.39 | 103.57 | 112.45 |
| 2 | Z | 2764 | THR | CA-C-N | 6.38 | 126.60 | 119.32 |
| 2 | Z | 2764 | THR | C-N-CA | 6.38 | 126.60 | 119.32 |
| 2 | T | 2340 | ALA | CA-C-N | -6.37 | 111.87 | 119.84 |
| 2 | T | 2340 | ALA | C-N-CA | -6.37 | 111.87 | 119.84 |
| 3 | U | 3178[A] | PHE | N-CA-C | -6.37 | 103.59 | 112.45 |
| 3 | U | 3178[B] | PHE | N-CA-C | -6.37 | 103.59 | 112.45 |
| 3 | O | 3178[A] | PHE | N-CA-C | -6.37 | 103.59 | 112.45 |
| 3 | O | 3178[B] | PHE | N-CA-C | -6.37 | 103.59 | 112.45 |
| 1 | M | 675 | SER | CA-C-N | -6.37 | 111.88 | 119.84 |
| 1 | M | 675 | SER | C-N-CA | -6.37 | 111.88 | 119.84 |
| 3 | a | 3178[A] | PHE | N-CA-C | -6.35 | 103.62 | 112.45 |
| 3 | a | 3178[B] | PHE | N-CA-C | -6.35 | 103.62 | 112.45 |
| 3 | X | 3178[A] | PHE | N-CA-C | -6.35 | 103.63 | 112.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | X | 3178[B] | PHE | N-CA-C | -6.35 | 103.63 | 112.45 |
| 3 | I | 3048[A] | ASP | CA-C-N | -6.34 | 113.45 | 119.85 |
| 3 | I | 3048[A] | ASP | C-N-CA | -6.34 | 113.45 | 119.85 |
| 3 | I | 3048[B] | ASP | CA-C-N | -6.34 | 113.45 | 119.85 |
| 3 | I | 3048[B] | ASP | C-N-CA | -6.34 | 113.45 | 119.85 |
| 1 | S | 1639 | LYS | N-CA-C | 6.34 | 121.83 | 111.37 |
| 3 | U | 3048[A] | ASP | CA-C-N | -6.33 | 113.46 | 119.85 |
| 3 | U | 3048[A] | ASP | C-N-CA | -6.33 | 113.46 | 119.85 |
| 3 | U | 3048[B] | ASP | CA-C-N | -6.33 | 113.46 | 119.85 |
| 3 | U | 3048[B] | ASP | C-N-CA | -6.33 | 113.46 | 119.85 |
| 3 | I | 3178[A] | PHE | N-CA-C | -6.32 | 103.66 | 112.45 |
| 3 | I | 3178[B] | PHE | N-CA-C | -6.32 | 103.66 | 112.45 |
| 3 | R | 3178[A] | PHE | N-CA-C | -6.32 | 103.66 | 112.45 |
| 3 | R | 3178[B] | PHE | N-CA-C | -6.32 | 103.66 | 112.45 |
| 3 | F | 3048[A] | ASP | CA-C-N | -6.32 | 113.47 | 119.85 |
| 3 | F | 3048[A] | ASP | C-N-CA | -6.32 | 113.47 | 119.85 |
| 3 | F | 3048[B] | ASP | CA-C-N | -6.32 | 113.47 | 119.85 |
| 3 | F | 3048[B] | ASP | C-N-CA | -6.32 | 113.47 | 119.85 |
| 3 | F | 3178[A] | PHE | N-CA-C | -6.32 | 103.67 | 112.45 |
| 3 | F | 3178[B] | PHE | N-CA-C | -6.32 | 103.67 | 112.45 |
| 3 | R | 3048[A] | ASP | CA-C-N | -6.32 | 113.47 | 119.85 |
| 3 | R | 3048[A] | ASP | C-N-CA | -6.32 | 113.47 | 119.85 |
| 3 | R | 3048[B] | ASP | CA-C-N | -6.32 | 113.47 | 119.85 |
| 3 | R | 3048[B] | ASP | C-N-CA | -6.32 | 113.47 | 119.85 |
| 3 | I | 3296[A] | PRO | CA-C-N | -6.30 | 114.04 | 120.85 |
| 3 | I | 3296[A] | PRO | C-N-CA | -6.30 | 114.04 | 120.85 |
| 3 | I | 3296[B] | PRO | CA-C-N | -6.30 | 114.04 | 120.85 |
| 3 | I | 3296[B] | PRO | C-N-CA | -6.30 | 114.04 | 120.85 |
| 3 | C | 3178[A] | PHE | N-CA-C | -6.30 | 103.69 | 112.45 |
| 3 | C | 3178[B] | PHE | N-CA-C | -6.30 | 103.69 | 112.45 |
| 3 | C | 3048[A] | ASP | CA-C-N | -6.30 | 113.49 | 119.85 |
| 3 | C | 3048[A] | ASP | C-N-CA | -6.30 | 113.49 | 119.85 |
| 3 | C | 3048[B] | ASP | CA-C-N | -6.30 | 113.49 | 119.85 |
| 3 | C | 3048[B] | ASP | C-N-CA | -6.30 | 113.49 | 119.85 |
| 3 | L | 3048[A] | ASP | CA-C-N | -6.30 | 113.49 | 119.85 |
| 3 | L | 3048[A] | ASP | C-N-CA | -6.30 | 113.49 | 119.85 |
| 3 | L | 3048[B] | ASP | CA-C-N | -6.30 | 113.49 | 119.85 |
| 3 | L | 3048[B] | ASP | C-N-CA | -6.30 | 113.49 | 119.85 |
| 3 | a | 3197[A] | ILE | N-CA-C | -6.30 | 104.79 | 112.35 |
| 3 | a | 3197[B] | ILE | N-CA-C | -6.30 | 104.79 | 112.35 |
| 3 | d | 3178[A] | PHE | N-CA-C | -6.29 | 103.70 | 112.45 |
| 3 | d | 3178[B] | PHE | N-CA-C | -6.29 | 103.70 | 112.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | X | 3048[A] | ASP | CA-C-N | -6.29 | 113.50 | 119.85 |
| 3 | X | 3048[A] | ASP | C-N-CA | -6.29 | 113.50 | 119.85 |
| 3 | X | 3048[B] | ASP | CA-C-N | -6.29 | 113.50 | 119.85 |
| 3 | X | 3048[B] | ASP | C-N-CA | -6.29 | 113.50 | 119.85 |
| 2 | Z | 2545 | SER | CA-C-N | 6.29 | 133.01 | 121.70 |
| 2 | Z | 2545 | SER | C-N-CA | 6.29 | 133.01 | 121.70 |
| 3 | d | 3048[A] | ASP | CA-C-N | -6.28 | 113.50 | 119.85 |
| 3 | d | 3048[A] | ASP | C-N-CA | -6.28 | 113.50 | 119.85 |
| 3 | d | 3048[B] | ASP | CA-C-N | -6.28 | 113.50 | 119.85 |
| 3 | d | 3048[B] | ASP | C-N-CA | -6.28 | 113.50 | 119.85 |
| 3 | L | 3116[A] | PHE | N-CA-C | 6.28 | 118.13 | 111.28 |
| 3 | L | 3116[B] | PHE | N-CA-C | 6.28 | 118.13 | 111.28 |
| 3 | a | 3296[A] | PRO | CA-C-N | -6.28 | 114.07 | 120.85 |
| 3 | a | 3296[A] | PRO | C-N-CA | -6.28 | 114.07 | 120.85 |
| 3 | a | 3296[B] | PRO | CA-C-N | -6.28 | 114.07 | 120.85 |
| 3 | a | 3296[B] | PRO | C-N-CA | -6.28 | 114.07 | 120.85 |
| 3 | C | 3296[A] | PRO | CA-C-N | -6.28 | 114.07 | 120.85 |
| 3 | C | 3296[A] | PRO | C-N-CA | -6.28 | 114.07 | 120.85 |
| 3 | C | 3296[B] | PRO | CA-C-N | -6.28 | 114.07 | 120.85 |
| 3 | C | 3296[B] | PRO | C-N-CA | -6.28 | 114.07 | 120.85 |
| 3 | L | 3197[A] | ILE | N-CA-C | -6.28 | 104.82 | 112.35 |
| 3 | L | 3197[B] | ILE | N-CA-C | -6.28 | 104.82 | 112.35 |
| 3 | X | 3296[A] | PRO | CA-C-N | -6.28 | 114.07 | 120.85 |
| 3 | X | 3296[A] | PRO | C-N-CA | -6.28 | 114.07 | 120.85 |
| 3 | X | 3296[B] | PRO | CA-C-N | -6.28 | 114.07 | 120.85 |
| 3 | X | 3296[B] | PRO | C-N-CA | -6.28 | 114.07 | 120.85 |
| 3 | I | 3197[A] | ILE | N-CA-C | -6.27 | 104.83 | 112.35 |
| 3 | I | 3197[B] | ILE | N-CA-C | -6.27 | 104.83 | 112.35 |
| 3 | L | 3296[A] | PRO | CA-C-N | -6.27 | 114.08 | 120.85 |
| 3 | L | 3296[A] | PRO | C-N-CA | -6.27 | 114.08 | 120.85 |
| 3 | L | 3296[B] | PRO | CA-C-N | -6.27 | 114.08 | 120.85 |
| 3 | L | 3296[B] | PRO | C-N-CA | -6.27 | 114.08 | 120.85 |
| 3 | R | 3197[A] | ILE | N-CA-C | -6.27 | 104.83 | 112.35 |
| 3 | R | 3197[B] | ILE | N-CA-C | -6.27 | 104.83 | 112.35 |
| 1 | V | 323 | ILE | CA-C-N | 6.26 | 126.29 | 119.90 |
| 1 | V | 323 | ILE | C-N-CA | 6.26 | 126.29 | 119.90 |
| 1 | b | 897 | HIS | N-CA-C | -6.26 | 100.11 | 108.19 |
| 3 | O | 3296[A] | PRO | CA-C-N | -6.26 | 114.09 | 120.85 |
| 3 | O | 3296[A] | PRO | C-N-CA | -6.26 | 114.09 | 120.85 |
| 3 | O | 3296[B] | PRO | CA-C-N | -6.26 | 114.09 | 120.85 |
| 3 | O | 3296[B] | PRO | C-N-CA | -6.26 | 114.09 | 120.85 |
| 3 | U | 3197[A] | ILE | N-CA-C | -6.26 | 104.84 | 112.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | U | 3197[B] | ILE | N-CA-C | -6.26 | 104.84 | 112.35 |
| 3 | U | 3296[A] | PRO | CA-C-N | -6.26 | 114.09 | 120.85 |
| 3 | U | 3296[A] | PRO | C-N-CA | -6.26 | 114.09 | 120.85 |
| 3 | U | 3296[B] | PRO | CA-C-N | -6.26 | 114.09 | 120.85 |
| 3 | U | 3296[B] | PRO | C-N-CA | -6.26 | 114.09 | 120.85 |
| 3 | a | 3048[A] | ASP | CA-C-N | -6.26 | 113.53 | 119.85 |
| 3 | a | 3048[A] | ASP | C-N-CA | -6.26 | 113.53 | 119.85 |
| 3 | a | 3048[B] | ASP | CA-C-N | -6.26 | 113.53 | 119.85 |
| 3 | a | 3048[B] | ASP | C-N-CA | -6.26 | 113.53 | 119.85 |
| 3 | O | 3048[A] | ASP | CA-C-N | -6.26 | 113.53 | 119.85 |
| 3 | O | 3048[A] | ASP | C-N-CA | -6.26 | 113.53 | 119.85 |
| 3 | O | 3048[B] | ASP | CA-C-N | -6.26 | 113.53 | 119.85 |
| 3 | O | 3048[B] | ASP | C-N-CA | -6.26 | 113.53 | 119.85 |
| 3 | R | 3296[A] | PRO | CA-C-N | -6.25 | 114.10 | 120.85 |
| 3 | R | 3296[A] | PRO | C-N-CA | -6.25 | 114.10 | 120.85 |
| 3 | R | 3296[B] | PRO | CA-C-N | -6.25 | 114.10 | 120.85 |
| 3 | R | 3296[B] | PRO | C-N-CA | -6.25 | 114.10 | 120.85 |
| 3 | a | 3116[A] | PHE | N-CA-C | 6.25 | 118.09 | 111.28 |
| 3 | a | 3116[B] | PHE | N-CA-C | 6.25 | 118.09 | 111.28 |
| 3 | X | 3197[A] | ILE | N-CA-C | -6.25 | 104.85 | 112.35 |
| 3 | X | 3197[B] | ILE | N-CA-C | -6.25 | 104.85 | 112.35 |
| 3 | O | 3197[A] | ILE | N-CA-C | -6.25 | 104.85 | 112.35 |
| 3 | O | 3197[B] | ILE | N-CA-C | -6.25 | 104.85 | 112.35 |
| 3 | R | 3116[A] | PHE | N-CA-C | 6.25 | 118.09 | 111.28 |
| 3 | R | 3116[B] | PHE | N-CA-C | 6.25 | 118.09 | 111.28 |
| 3 | d | 3296[A] | PRO | CA-C-N | -6.25 | 114.11 | 120.85 |
| 3 | d | 3296[A] | PRO | C-N-CA | -6.25 | 114.11 | 120.85 |
| 3 | d | 3296[B] | PRO | CA-C-N | -6.25 | 114.11 | 120.85 |
| 3 | d | 3296[B] | PRO | C-N-CA | -6.25 | 114.11 | 120.85 |
| 2 | B | 2345 | ASN | CA-C-N | 6.24 | 125.65 | 118.85 |
| 2 | B | 2345 | ASN | C-N-CA | 6.24 | 125.65 | 118.85 |
| 3 | d | 3197[A] | ILE | N-CA-C | -6.24 | 104.86 | 112.35 |
| 3 | d | 3197[B] | ILE | N-CA-C | -6.24 | 104.86 | 112.35 |
| 3 | C | 3197[A] | ILE | N-CA-C | -6.23 | 104.87 | 112.35 |
| 3 | C | 3197[B] | ILE | N-CA-C | -6.23 | 104.87 | 112.35 |
| 3 | C | 3116[A] | PHE | N-CA-C | 6.21 | 118.05 | 111.28 |
| 3 | C | 3116[B] | PHE | N-CA-C | 6.21 | 118.05 | 111.28 |
| 3 | F | 3116[A] | PHE | N-CA-C | 6.21 | 118.05 | 111.28 |
| 3 | F | 3116[B] | PHE | N-CA-C | 6.21 | 118.05 | 111.28 |
| 3 | F | 3197[A] | ILE | N-CA-C | -6.21 | 104.89 | 112.35 |
| 3 | F | 3197[B] | ILE | N-CA-C | -6.21 | 104.89 | 112.35 |
| 3 | F | 3296[A] | PRO | CA-C-N | -6.21 | 114.14 | 120.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | F | 3296[A] | PRO | C-N-CA | -6.21 | 114.14 | 120.85 |
| 3 | F | 3296[B] | PRO | CA-C-N | -6.21 | 114.14 | 120.85 |
| 3 | F | 3296[B] | PRO | C-N-CA | -6.21 | 114.14 | 120.85 |
| 1 | b | 296 | ARG | N-CA-C | -6.21 | 105.75 | 113.38 |
| 2 | T | 2215 | SER | N-CA-C | 6.21 | 117.71 | 111.07 |
| 1 | J | 1296 | VAL | CA-C-N | -6.20 | 112.09 | 119.84 |
| 1 | J | 1296 | VAL | C-N-CA | -6.20 | 112.09 | 119.84 |
| 3 | X | 3116[A] | PHE | N-CA-C | 6.19 | 118.03 | 111.28 |
| 3 | X | 3116[B] | PHE | N-CA-C | 6.19 | 118.03 | 111.28 |
| 3 | U | 3116[A] | PHE | N-CA-C | 6.18 | 118.02 | 111.28 |
| 3 | U | 3116[B] | PHE | N-CA-C | 6.18 | 118.02 | 111.28 |
| 3 | d | 3116[A] | PHE | N-CA-C | 6.17 | 118.01 | 111.28 |
| 3 | d | 3116[B] | PHE | N-CA-C | 6.17 | 118.01 | 111.28 |
| 3 | I | 3116[A] | PHE | N-CA-C | 6.17 | 118.00 | 111.28 |
| 3 | I | 3116[B] | PHE | N-CA-C | 6.17 | 118.00 | 111.28 |
| 1 | b | 1296 | VAL | CA-C-N | -6.17 | 112.13 | 119.84 |
| 1 | b | 1296 | VAL | C-N-CA | -6.17 | 112.13 | 119.84 |
| 2 | B | 2489 | ILE | CA-C-N | 6.16 | 124.09 | 119.66 |
| 2 | B | 2489 | ILE | C-N-CA | 6.16 | 124.09 | 119.66 |
| 2 | N | 2831 | GLU | N-CA-C | 6.16 | 119.73 | 111.24 |
| 1 | J | 1637 | GLY | N-CA-C | -6.15 | 100.49 | 110.95 |
| 2 | H | 2764 | THR | CA-C-N | 6.15 | 126.60 | 119.47 |
| 2 | H | 2764 | THR | C-N-CA | 6.15 | 126.60 | 119.47 |
| 2 | K | 2545 | SER | CA-C-N | 6.14 | 132.76 | 121.70 |
| 2 | K | 2545 | SER | C-N-CA | 6.14 | 132.76 | 121.70 |
| 1 | Y | 83 | HIS | N-CA-C | 6.13 | 121.04 | 113.50 |
| 3 | O | 3116[A] | PHE | N-CA-C | 6.13 | 117.96 | 111.28 |
| 3 | O | 3116[B] | PHE | N-CA-C | 6.13 | 117.96 | 111.28 |
| 1 | P | 669 | LYS | CA-C-N | -6.12 | 113.92 | 120.47 |
| 1 | P | 669 | LYS | C-N-CA | -6.12 | 113.92 | 120.47 |
| 1 | S | 1251 | SER | CA-C-N | 6.12 | 126.09 | 120.03 |
| 1 | S | 1251 | SER | C-N-CA | 6.12 | 126.09 | 120.03 |
| 2 | E | 2545 | SER | CA-C-N | 6.12 | 132.71 | 121.70 |
| 2 | E | 2545 | SER | C-N-CA | 6.12 | 132.71 | 121.70 |
| 2 | W | 2345 | ASN | CA-C-N | 6.11 | 127.48 | 119.84 |
| 2 | W | 2345 | ASN | C-N-CA | 6.11 | 127.48 | 119.84 |
| 1 | A | 1296 | VAL | CA-C-N | -6.11 | 112.20 | 119.84 |
| 1 | A | 1296 | VAL | C-N-CA | -6.11 | 112.20 | 119.84 |
| 1 | V | 1296 | VAL | CA-C-N | -6.10 | 112.21 | 119.84 |
| 1 | V | 1296 | VAL | C-N-CA | -6.10 | 112.21 | 119.84 |
| 2 | T | 2545 | SER | CA-C-N | 6.10 | 132.68 | 121.70 |
| 2 | T | 2545 | SER | C-N-CA | 6.10 | 132.68 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | S | 1091 | ASN | CA-C-N | 6.09 | 126.62 | 120.04 |
| 1 | S | 1091 | ASN | C-N-CA | 6.09 | 126.62 | 120.04 |
| 1 | D | 1296 | VAL | CA-C-N | -6.08 | 112.24 | 119.84 |
| 1 | D | 1296 | VAL | C-N-CA | -6.08 | 112.24 | 119.84 |
| 1 | A | 1082 | SER | CA-C-N | -6.08 | 112.25 | 119.84 |
| 1 | A | 1082 | SER | C-N-CA | -6.08 | 112.25 | 119.84 |
| 1 | D | 953 | GLU | N-CA-C | 6.08 | 117.63 | 108.46 |
| 1 | A | 570 | GLN | CA-C-N | -6.06 | 112.27 | 119.84 |
| 1 | A | 570 | GLN | C-N-CA | -6.06 | 112.27 | 119.84 |
| 1 | S | 465 | PRO | N-CA-C | -6.03 | 106.17 | 114.98 |
| 1 | Y | 323 | ILE | CA-C-N | 6.01 | 126.02 | 119.89 |
| 1 | Y | 323 | ILE | C-N-CA | 6.01 | 126.02 | 119.89 |
| 1 | J | 1237 | GLU | CA-C-N | 6.00 | 125.95 | 119.78 |
| 1 | J | 1237 | GLU | C-N-CA | 6.00 | 125.95 | 119.78 |
| 1 | A | 116 | LYS | CB-CA-C | -5.99 | 109.09 | 117.23 |
| 1 | V | 669 | LYS | CA-C-N | -5.99 | 112.36 | 119.84 |
| 1 | V | 669 | LYS | C-N-CA | -5.99 | 112.36 | 119.84 |
| 2 | c | 2553 | ALA | CA-C-N | 5.98 | 126.48 | 120.14 |
| 2 | c | 2553 | ALA | C-N-CA | 5.98 | 126.48 | 120.14 |
| 2 | N | 2472 | ASN | N-CA-C | 5.97 | 117.79 | 111.28 |
| 1 | A | 388 | GLY | N-CA-C | -5.97 | 107.59 | 114.69 |
| 1 | P | 1091 | ASN | CA-C-N | 5.97 | 126.48 | 120.04 |
| 1 | P | 1091 | ASN | C-N-CA | 5.97 | 126.48 | 120.04 |
| 1 | J | 323 | ILE | CA-C-N | 5.96 | 125.98 | 119.90 |
| 1 | J | 323 | ILE | C-N-CA | 5.96 | 125.98 | 119.90 |
| 1 | S | 296 | ARG | N-CA-C | -5.96 | 105.84 | 113.23 |
| 1 | Y | 1296 | VAL | CA-C-N | -5.95 | 112.41 | 119.84 |
| 1 | Y | 1296 | VAL | C-N-CA | -5.95 | 112.41 | 119.84 |
| 1 | G | 1441 | SER | N-CA-C | 5.95 | 116.09 | 108.24 |
| 1 | P | 1039 | ASP | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | P | 1039 | ASP | C-N-CA | 5.94 | 125.62 | 119.56 |
| 2 | W | 2340 | ALA | CA-C-N | -5.93 | 113.54 | 120.12 |
| 2 | W | 2340 | ALA | C-N-CA | -5.93 | 113.54 | 120.12 |
| 2 | H | 2472 | ASN | N-CA-C | 5.91 | 117.80 | 111.36 |
| 1 | M | 1296 | VAL | CA-C-N | -5.89 | 112.47 | 119.84 |
| 1 | M | 1296 | VAL | C-N-CA | -5.89 | 112.47 | 119.84 |
| 2 | N | 2418 | GLY | N-CA-C | 5.89 | 120.02 | 112.83 |
| 1 | J | 1039 | ASP | CA-C-N | 5.89 | 125.57 | 119.56 |
| 1 | J | 1039 | ASP | C-N-CA | 5.89 | 125.57 | 119.56 |
| 1 | V | 1209 | ASP | N-CA-C | 5.86 | 118.28 | 108.73 |
| 2 | H | 2340 | ALA | CA-C-N | -5.86 | 113.78 | 119.87 |
| 2 | H | 2340 | ALA | C-N-CA | -5.86 | 113.78 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | V | 51 | ASP | N-CA-C | 5.85 | 118.13 | 111.11 |
| 3 | O | 2993[A] | MET | N-CA-C | -5.85 | 104.81 | 111.07 |
| 3 | O | 2993[B] | MET | N-CA-C | -5.85 | 104.81 | 111.07 |
| 2 | Z | 2127 | ALA | CB-CA-C | -5.85 | 109.28 | 117.23 |
| 2 | Q | 2545 | SER | CA-C-N | 5.84 | 132.22 | 121.70 |
| 2 | Q | 2545 | SER | C-N-CA | 5.84 | 132.22 | 121.70 |
| 3 | U | 2993[A] | MET | N-CA-C | -5.82 | 104.84 | 111.07 |
| 3 | U | 2993[B] | MET | N-CA-C | -5.82 | 104.84 | 111.07 |
| 1 | A | 465 | PRO | N-CA-C | -5.82 | 106.49 | 114.98 |
| 3 | a | 2993[A] | MET | N-CA-C | -5.81 | 104.86 | 111.07 |
| 3 | a | 2993[B] | MET | N-CA-C | -5.81 | 104.86 | 111.07 |
| 2 | B | 2556 | TYR | N-CA-C | 5.81 | 115.51 | 107.73 |
| 3 | L | 2993[A] | MET | N-CA-C | -5.80 | 104.86 | 111.07 |
| 3 | L | 2993[B] | MET | N-CA-C | -5.80 | 104.86 | 111.07 |
| 1 | P | 780 | GLU | N-CA-C | 5.79 | 119.53 | 112.23 |
| 3 | d | 2993[A] | MET | N-CA-C | -5.79 | 104.87 | 111.07 |
| 3 | d | 2993[B] | MET | N-CA-C | -5.79 | 104.87 | 111.07 |
| 1 | P | 1494 | ARG | CA-C-N | -5.78 | 112.61 | 119.84 |
| 1 | P | 1494 | ARG | C-N-CA | -5.78 | 112.61 | 119.84 |
| 3 | I | 2993[A] | MET | N-CA-C | -5.78 | 104.89 | 111.07 |
| 3 | I | 2993[B] | MET | N-CA-C | -5.78 | 104.89 | 111.07 |
| 3 | R | 2993[A] | MET | N-CA-C | -5.78 | 104.89 | 111.07 |
| 3 | R | 2993[B] | MET | N-CA-C | -5.78 | 104.89 | 111.07 |
| 3 | C | 2993[A] | MET | N-CA-C | -5.77 | 104.90 | 111.07 |
| 3 | C | 2993[B] | MET | N-CA-C | -5.77 | 104.90 | 111.07 |
| 3 | U | 2969[A] | TYR | CA-C-N | -5.77 | 112.93 | 119.28 |
| 3 | U | 2969[A] | TYR | C-N-CA | -5.77 | 112.93 | 119.28 |
| 3 | U | 2969[B] | TYR | CA-C-N | -5.77 | 112.93 | 119.28 |
| 3 | U | 2969[B] | TYR | C-N-CA | -5.77 | 112.93 | 119.28 |
| 1 | A | 1229 | LYS | N-CA-C | 5.76 | 118.17 | 109.41 |
| 2 | Z | 2472 | ASN | N-CA-C | 5.76 | 117.56 | 111.28 |
| 3 | O | 2969[A] | TYR | CA-C-N | -5.76 | 112.94 | 119.28 |
| 3 | O | 2969[A] | TYR | C-N-CA | -5.76 | 112.94 | 119.28 |
| 3 | O | 2969[B] | TYR | CA-C-N | -5.76 | 112.94 | 119.28 |
| 3 | O | 2969[B] | TYR | C-N-CA | -5.76 | 112.94 | 119.28 |
| 3 | X | 2993[A] | MET | N-CA-C | -5.76 | 104.91 | 111.07 |
| 3 | X | 2993[B] | MET | N-CA-C | -5.76 | 104.91 | 111.07 |
| 3 | F | 2993[A] | MET | N-CA-C | -5.75 | 104.92 | 111.07 |
| 3 | F | 2993[B] | MET | N-CA-C | -5.75 | 104.92 | 111.07 |
| 1 | V | 982 | LYS | CA-C-N | -5.75 | 112.02 | 120.46 |
| 1 | V | 982 | LYS | C-N-CA | -5.75 | 112.02 | 120.46 |
| 1 | S | 780 | GLU | N-CA-C | 5.74 | 118.48 | 111.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 125 | SER | N-CA-C | 5.74 | 117.96 | 108.49 |
| 2 | E | 2764 | THR | CA-C-N | 5.73 | 125.85 | 119.32 |
| 2 | E | 2764 | THR | C-N-CA | 5.73 | 125.85 | 119.32 |
| 3 | a | 2969[A] | TYR | CA-C-N | -5.73 | 112.97 | 119.28 |
| 3 | a | 2969[A] | TYR | C-N-CA | -5.73 | 112.97 | 119.28 |
| 3 | a | 2969[B] | TYR | CA-C-N | -5.73 | 112.97 | 119.28 |
| 3 | a | 2969[B] | TYR | C-N-CA | -5.73 | 112.97 | 119.28 |
| 3 | d | 2969[A] | TYR | CA-C-N | -5.73 | 112.98 | 119.28 |
| 3 | d | 2969[A] | TYR | C-N-CA | -5.73 | 112.98 | 119.28 |
| 3 | d | 2969[B] | TYR | CA-C-N | -5.73 | 112.98 | 119.28 |
| 3 | d | 2969[B] | TYR | C-N-CA | -5.73 | 112.98 | 119.28 |
| 3 | C | 2969[A] | TYR | CA-C-N | -5.73 | 112.98 | 119.28 |
| 3 | C | 2969[A] | TYR | C-N-CA | -5.73 | 112.98 | 119.28 |
| 3 | C | 2969[B] | TYR | CA-C-N | -5.73 | 112.98 | 119.28 |
| 3 | C | 2969[B] | TYR | C-N-CA | -5.73 | 112.98 | 119.28 |
| 1 | Y | 1227 | ASP | N-CA-C | 5.73 | 115.67 | 108.45 |
| 3 | F | 2969[A] | TYR | CA-C-N | -5.72 | 112.99 | 119.28 |
| 3 | F | 2969[A] | TYR | C-N-CA | -5.72 | 112.99 | 119.28 |
| 3 | F | 2969[B] | TYR | CA-C-N | -5.72 | 112.99 | 119.28 |
| 3 | F | 2969[B] | TYR | C-N-CA | -5.72 | 112.99 | 119.28 |
| 3 | R | 2969[A] | TYR | CA-C-N | -5.72 | 112.99 | 119.28 |
| 3 | R | 2969[A] | TYR | C-N-CA | -5.72 | 112.99 | 119.28 |
| 3 | R | 2969[B] | TYR | CA-C-N | -5.72 | 112.99 | 119.28 |
| 3 | R | 2969[B] | TYR | C-N-CA | -5.72 | 112.99 | 119.28 |
| 2 | K | 2617 | ASP | N-CA-C | -5.72 | 105.89 | 112.92 |
| 3 | L | 2969[A] | TYR | CA-C-N | -5.71 | 112.99 | 119.28 |
| 3 | L | 2969[A] | TYR | C-N-CA | -5.71 | 112.99 | 119.28 |
| 3 | L | 2969[B] | TYR | CA-C-N | -5.71 | 112.99 | 119.28 |
| 3 | L | 2969[B] | TYR | C-N-CA | -5.71 | 112.99 | 119.28 |
| 1 | P | 1296 | VAL | CA-C-N | -5.71 | 112.70 | 119.84 |
| 1 | P | 1296 | VAL | C-N-CA | -5.71 | 112.70 | 119.84 |
| 2 | c | 2556 | TYR | N-CA-C | 5.71 | 116.92 | 107.73 |
| 3 | O | 2995[A] | GLN | N-CA-C | -5.70 | 104.06 | 111.02 |
| 3 | O | 2995[B] | GLN | N-CA-C | -5.70 | 104.06 | 111.02 |
| 1 | G | 1166 | THR | N-CA-C | 5.70 | 118.35 | 111.40 |
| 3 | X | 2969[A] | TYR | CA-C-N | -5.70 | 113.01 | 119.28 |
| 3 | X | 2969[A] | TYR | C-N-CA | -5.70 | 113.01 | 119.28 |
| 3 | X | 2969[B] | TYR | CA-C-N | -5.70 | 113.01 | 119.28 |
| 3 | X | 2969[B] | TYR | C-N-CA | -5.70 | 113.01 | 119.28 |
| 2 | W | 2865 | ILE | CA-C-N | 5.69 | 123.82 | 119.66 |
| 2 | W | 2865 | ILE | C-N-CA | 5.69 | 123.82 | 119.66 |
| 1 | V | 1494 | ARG | CA-C-N | -5.69 | 113.16 | 119.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | V | 1494 | ARG | C-N-CA | -5.69 | 113.16 | 119.19 |
| 3 | d | 2995[A] | GLN | N-CA-C | -5.68 | 104.09 | 111.02 |
| 3 | d | 2995[B] | GLN | N-CA-C | -5.68 | 104.09 | 111.02 |
| 1 | M | 323 | ILE | CA-C-N | 5.67 | 125.60 | 119.76 |
| 1 | M | 323 | ILE | C-N-CA | 5.67 | 125.60 | 119.76 |
| 1 | M | 1210 | LYS | CA-C-N | 5.67 | 131.91 | 121.70 |
| 1 | M | 1210 | LYS | C-N-CA | 5.67 | 131.91 | 121.70 |
| 3 | C | 2995[A] | GLN | N-CA-C | -5.67 | 104.10 | 111.02 |
| 3 | C | 2995[B] | GLN | N-CA-C | -5.67 | 104.10 | 111.02 |
| 3 | I | 2969[A] | TYR | CA-C-N | -5.67 | 113.05 | 119.28 |
| 3 | I | 2969[A] | TYR | C-N-CA | -5.67 | 113.05 | 119.28 |
| 3 | I | 2969[B] | TYR | CA-C-N | -5.67 | 113.05 | 119.28 |
| 3 | I | 2969[B] | TYR | C-N-CA | -5.67 | 113.05 | 119.28 |
| 3 | R | 2995[A] | GLN | N-CA-C | -5.66 | 104.11 | 111.02 |
| 3 | R | 2995[B] | GLN | N-CA-C | -5.66 | 104.11 | 111.02 |
| 3 | L | 2995[A] | GLN | N-CA-C | -5.65 | 104.13 | 111.02 |
| 3 | L | 2995[B] | GLN | N-CA-C | -5.65 | 104.13 | 111.02 |
| 3 | a | 2995[A] | GLN | N-CA-C | -5.65 | 104.13 | 111.02 |
| 3 | a | 2995[B] | GLN | N-CA-C | -5.65 | 104.13 | 111.02 |
| 1 | S | 1339 | SER | CA-C-N | 5.65 | 131.86 | 121.70 |
| 1 | S | 1339 | SER | C-N-CA | 5.65 | 131.86 | 121.70 |
| 2 | H | 2134 | ASN | N-CA-C | -5.64 | 103.14 | 108.22 |
| 1 | V | 1582 | ASN | CA-C-N | 5.64 | 131.85 | 121.70 |
| 1 | V | 1582 | ASN | C-N-CA | 5.64 | 131.85 | 121.70 |
| 1 | M | 758 | GLY | N-CA-C | 5.64 | 119.22 | 110.88 |
| 3 | I | 2995[A] | GLN | N-CA-C | -5.63 | 104.15 | 111.02 |
| 3 | I | 2995[B] | GLN | N-CA-C | -5.63 | 104.15 | 111.02 |
| 2 | W | 2689 | GLY | N-CA-C | 5.63 | 118.41 | 111.93 |
| 1 | Y | 823 | VAL | CA-C-N | 5.63 | 125.39 | 119.76 |
| 1 | Y | 823 | VAL | C-N-CA | 5.63 | 125.39 | 119.76 |
| 3 | U | 2995[A] | GLN | N-CA-C | -5.62 | 104.16 | 111.02 |
| 3 | U | 2995[B] | GLN | N-CA-C | -5.62 | 104.16 | 111.02 |
| 1 | A | 1251 | SER | CA-C-N | 5.62 | 125.56 | 119.78 |
| 1 | A | 1251 | SER | C-N-CA | 5.62 | 125.56 | 119.78 |
| 1 | S | 867 | VAL | N-CA-C | 5.61 | 118.92 | 111.17 |
| 3 | F | 2995[A] | GLN | N-CA-C | -5.61 | 104.17 | 111.02 |
| 3 | F | 2995[B] | GLN | N-CA-C | -5.61 | 104.17 | 111.02 |
| 3 | U | 3167[A] | VAL | N-CA-C | 5.61 | 115.81 | 110.42 |
| 3 | U | 3167[B] | VAL | N-CA-C | 5.61 | 115.81 | 110.42 |
| 1 | P | 1079 | LYS | CA-C-N | 5.61 | 125.54 | 119.76 |
| 1 | P | 1079 | LYS | C-N-CA | 5.61 | 125.54 | 119.76 |
| 3 | X | 2995[A] | GLN | N-CA-C | -5.60 | 104.19 | 111.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | X | 2995[B] | GLN | N-CA-C | -5.60 | 104.19 | 111.02 |
| 1 | A | 557 | VAL | N-CA-C | 5.60 | 117.00 | 110.62 |
| 1 | S | 1296 | VAL | CA-C-N | -5.60 | 112.84 | 119.84 |
| 1 | S | 1296 | VAL | C-N-CA | -5.60 | 112.84 | 119.84 |
| 3 | d | 3167[A] | VAL | N-CA-C | 5.59 | 115.79 | 110.42 |
| 3 | d | 3167[B] | VAL | N-CA-C | 5.59 | 115.79 | 110.42 |
| 3 | I | 3167[A] | VAL | N-CA-C | 5.57 | 115.77 | 110.42 |
| 3 | I | 3167[B] | VAL | N-CA-C | 5.57 | 115.77 | 110.42 |
| 3 | R | 3167[A] | VAL | N-CA-C | 5.57 | 115.76 | 110.42 |
| 3 | R | 3167[B] | VAL | N-CA-C | 5.57 | 115.76 | 110.42 |
| 3 | L | 3167[A] | VAL | N-CA-C | 5.56 | 115.76 | 110.42 |
| 3 | L | 3167[B] | VAL | N-CA-C | 5.56 | 115.76 | 110.42 |
| 3 | a | 3167[A] | VAL | N-CA-C | 5.56 | 115.75 | 110.42 |
| 3 | a | 3167[B] | VAL | N-CA-C | 5.56 | 115.75 | 110.42 |
| 3 | C | 3167[A] | VAL | N-CA-C | 5.55 | 115.75 | 110.42 |
| 3 | C | 3167[B] | VAL | N-CA-C | 5.55 | 115.75 | 110.42 |
| 3 | F | 3167[A] | VAL | N-CA-C | 5.54 | 115.74 | 110.42 |
| 3 | F | 3167[B] | VAL | N-CA-C | 5.54 | 115.74 | 110.42 |
| 2 | W | 2764 | THR | CA-C-N | 5.54 | 125.64 | 119.32 |
| 2 | W | 2764 | THR | C-N-CA | 5.54 | 125.64 | 119.32 |
| 3 | X | 3167[A] | VAL | N-CA-C | 5.54 | 115.74 | 110.42 |
| 3 | X | 3167[B] | VAL | N-CA-C | 5.54 | 115.74 | 110.42 |
| 1 | A | 1286 | ARG | N-CA-C | 5.54 | 117.18 | 111.03 |
| 1 | P | 107 | HIS | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | P | 107 | HIS | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | M | 296 | ARG | N-CA-C | -5.54 | 106.57 | 113.38 |
| 3 | O | 3167[A] | VAL | N-CA-C | 5.53 | 115.73 | 110.42 |
| 3 | O | 3167[B] | VAL | N-CA-C | 5.53 | 115.73 | 110.42 |
| 1 | P | 832 | LYS | N-CA-C | 5.53 | 115.58 | 108.34 |
| 2 | E | 2345 | ASN | CA-C-N | 5.52 | 124.87 | 118.85 |
| 2 | E | 2345 | ASN | C-N-CA | 5.52 | 124.87 | 118.85 |
| 2 | Q | 2207 | ASN | CA-C-N | 5.52 | 125.19 | 119.56 |
| 2 | Q | 2207 | ASN | C-N-CA | 5.52 | 125.19 | 119.56 |
| 1 | G | 465 | PRO | N-CA-C | -5.52 | 106.92 | 114.98 |
| 1 | M | 669 | LYS | CA-C-N | -5.52 | 114.07 | 119.64 |
| 1 | M | 669 | LYS | C-N-CA | -5.52 | 114.07 | 119.64 |
| 1 | D | 229 | LEU | CA-C-N | 5.50 | 125.42 | 119.76 |
| 1 | D | 229 | LEU | C-N-CA | 5.50 | 125.42 | 119.76 |
| 2 | K | 2217 | ILE | N-CA-C | -5.50 | 104.00 | 110.21 |
| 1 | S | 1494 | ARG | CA-C-N | -5.50 | 112.97 | 119.84 |
| 1 | S | 1494 | ARG | C-N-CA | -5.50 | 112.97 | 119.84 |
| 1 | G | 133 | LYS | N-CA-C | 5.50 | 117.54 | 109.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | b | 1091 | ASN | CA-C-N | 5.50 | 125.19 | 119.64 |
| 1 | b | 1091 | ASN | C-N-CA | 5.50 | 125.19 | 119.64 |
| 2 | N | 2490 | PRO | O-C-N | 5.48 | 123.73 | 121.15 |
| 2 | W | 2489 | ILE | CA-C-N | 5.48 | 123.61 | 119.66 |
| 2 | W | 2489 | ILE | C-N-CA | 5.48 | 123.61 | 119.66 |
| 1 | A | 830 | ASN | CA-C-N | 5.47 | 131.55 | 121.70 |
| 1 | A | 830 | ASN | C-N-CA | 5.47 | 131.55 | 121.70 |
| 1 | P | 1339 | SER | CA-C-N | 5.47 | 131.54 | 121.70 |
| 1 | P | 1339 | SER | C-N-CA | 5.47 | 131.54 | 121.70 |
| 1 | S | 416 | ASN | N-CA-C | 5.46 | 117.66 | 111.11 |
| 2 | Q | 2237 | LEU | CB-CA-C | -5.44 | 109.83 | 117.23 |
| 3 | U | 3005[A] | ALA | N-CA-C | -5.43 | 100.75 | 109.39 |
| 3 | U | 3005[B] | ALA | N-CA-C | -5.43 | 100.75 | 109.39 |
| 3 | O | 3101[A] | PRO | O-C-N | 5.43 | 128.74 | 122.23 |
| 3 | O | 3101[B] | PRO | O-C-N | 5.43 | 128.74 | 122.23 |
| 1 | A | 114 | THR | CB-CA-C | -5.42 | 110.30 | 116.54 |
| 3 | R | 3005[A] | ALA | N-CA-C | -5.42 | 100.77 | 109.39 |
| 3 | R | 3005[B] | ALA | N-CA-C | -5.42 | 100.77 | 109.39 |
| 3 | d | 3119[A] | HIS | N-CA-C | -5.42 | 105.37 | 111.28 |
| 3 | d | 3119[B] | HIS | N-CA-C | -5.42 | 105.37 | 111.28 |
| 3 | R | 3119[A] | HIS | N-CA-C | -5.42 | 105.37 | 111.28 |
| 3 | R | 3119[B] | HIS | N-CA-C | -5.42 | 105.37 | 111.28 |
| 1 | M | 1339 | SER | CA-C-N | 5.42 | 131.46 | 121.70 |
| 1 | M | 1339 | SER | C-N-CA | 5.42 | 131.46 | 121.70 |
| 1 | P | 675 | SER | CA-C-N | -5.42 | 113.07 | 119.84 |
| 1 | P | 675 | SER | C-N-CA | -5.42 | 113.07 | 119.84 |
| 1 | V | 296 | ARG | N-CA-C | -5.42 | 106.83 | 113.50 |
| 3 | I | 3005[A] | ALA | N-CA-C | -5.42 | 100.78 | 109.39 |
| 3 | I | 3005[B] | ALA | N-CA-C | -5.42 | 100.78 | 109.39 |
| 3 | O | 3005[A] | ALA | N-CA-C | -5.42 | 100.78 | 109.39 |
| 3 | O | 3005[B] | ALA | N-CA-C | -5.42 | 100.78 | 109.39 |
| 3 | F | 3005[A] | ALA | N-CA-C | -5.41 | 100.79 | 109.39 |
| 3 | F | 3005[B] | ALA | N-CA-C | -5.41 | 100.79 | 109.39 |
| 3 | X | 3101[A] | PRO | O-C-N | 5.41 | 128.72 | 122.23 |
| 3 | X | 3101[B] | PRO | O-C-N | 5.41 | 128.72 | 122.23 |
| 3 | C | 3101[A] | PRO | O-C-N | 5.40 | 128.72 | 122.23 |
| 3 | C | 3101[B] | PRO | O-C-N | 5.40 | 128.72 | 122.23 |
| 3 | I | 3101[A] | PRO | O-C-N | 5.40 | 128.71 | 122.23 |
| 3 | I | 3101[B] | PRO | O-C-N | 5.40 | 128.71 | 122.23 |
| 3 | U | 3119[A] | HIS | N-CA-C | -5.40 | 105.39 | 111.28 |
| 3 | U | 3119[B] | HIS | N-CA-C | -5.40 | 105.39 | 111.28 |
| 3 | a | 3101[A] | PRO | O-C-N | 5.40 | 128.71 | 122.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | a | 3101[B] | PRO | O-C-N | 5.40 | 128.71 | 122.23 |
| 3 | a | 3113[A] | ASP | N-CA-C | 5.40 | 116.47 | 109.72 |
| 3 | a | 3113[B] | ASP | N-CA-C | 5.40 | 116.47 | 109.72 |
| 2 | B | 2764 | THR | CA-C-N | 5.40 | 125.48 | 119.32 |
| 2 | B | 2764 | THR | C-N-CA | 5.40 | 125.48 | 119.32 |
| 2 | N | 2553 | ALA | N-CA-C | 5.40 | 119.58 | 112.35 |
| 3 | O | 3119[A] | HIS | N-CA-C | -5.40 | 105.39 | 111.28 |
| 3 | O | 3119[B] | HIS | N-CA-C | -5.40 | 105.39 | 111.28 |
| 3 | X | 3005[A] | ALA | N-CA-C | -5.40 | 100.80 | 109.39 |
| 3 | X | 3005[B] | ALA | N-CA-C | -5.40 | 100.80 | 109.39 |
| 3 | a | 3119[A] | HIS | N-CA-C | -5.40 | 105.39 | 111.28 |
| 3 | a | 3119[B] | HIS | N-CA-C | -5.40 | 105.39 | 111.28 |
| 3 | C | 3005[A] | ALA | N-CA-C | -5.40 | 100.81 | 109.39 |
| 3 | C | 3005[B] | ALA | N-CA-C | -5.40 | 100.81 | 109.39 |
| 1 | b | 1494 | ARG | CA-C-N | -5.40 | 113.09 | 119.84 |
| 1 | b | 1494 | ARG | C-N-CA | -5.40 | 113.09 | 119.84 |
| 2 | Q | 2764 | THR | CA-C-N | 5.39 | 125.73 | 119.47 |
| 2 | Q | 2764 | THR | C-N-CA | 5.39 | 125.73 | 119.47 |
| 3 | d | 3005[A] | ALA | N-CA-C | -5.39 | 100.81 | 109.39 |
| 3 | d | 3005[B] | ALA | N-CA-C | -5.39 | 100.81 | 109.39 |
| 3 | U | 3101[A] | PRO | O-C-N | 5.39 | 128.70 | 122.23 |
| 3 | U | 3101[B] | PRO | O-C-N | 5.39 | 128.70 | 122.23 |
| 1 | V | 1082 | SER | CA-C-N | -5.39 | 113.10 | 119.84 |
| 1 | V | 1082 | SER | C-N-CA | -5.39 | 113.10 | 119.84 |
| 1 | V | 688 | VAL | CA-C-N | 5.39 | 126.58 | 119.84 |
| 1 | V | 688 | VAL | C-N-CA | 5.39 | 126.58 | 119.84 |
| 2 | B | 2490 | PRO | O-C-N | 5.39 | 123.68 | 121.15 |
| 3 | C | 3119[A] | HIS | N-CA-C | -5.39 | 105.41 | 111.28 |
| 3 | C | 3119[B] | HIS | N-CA-C | -5.39 | 105.41 | 111.28 |
| 2 | B | 2418 | GLY | N-CA-C | 5.38 | 119.19 | 112.73 |
| 3 | R | 3101[A] | PRO | O-C-N | 5.38 | 128.69 | 122.23 |
| 3 | R | 3101[B] | PRO | O-C-N | 5.38 | 128.69 | 122.23 |
| 3 | R | 3113[A] | ASP | N-CA-C | 5.38 | 116.45 | 109.72 |
| 3 | R | 3113[B] | ASP | N-CA-C | 5.38 | 116.45 | 109.72 |
| 3 | U | 3113[A] | ASP | N-CA-C | 5.38 | 116.45 | 109.72 |
| 3 | U | 3113[B] | ASP | N-CA-C | 5.38 | 116.45 | 109.72 |
| 1 | V | 551 | GLU | N-CA-C | 5.38 | 117.15 | 111.28 |
| 3 | C | 3113[A] | ASP | N-CA-C | 5.38 | 116.44 | 109.72 |
| 3 | C | 3113[B] | ASP | N-CA-C | 5.38 | 116.44 | 109.72 |
| 2 | K | 2418 | GLY | N-CA-C | 5.38 | 119.39 | 112.83 |
| 1 | M | 1286 | ARG | N-CA-C | 5.38 | 117.00 | 111.03 |
| 3 | X | 3113[A] | ASP | N-CA-C | 5.37 | 116.44 | 109.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | X | 3113[B] | ASP | N-CA-C | 5.37 | 116.44 | 109.72 |
| 3 | a | 3005[A] | ALA | N-CA-C | -5.37 | 100.85 | 109.39 |
| 3 | a | 3005[B] | ALA | N-CA-C | -5.37 | 100.85 | 109.39 |
| 3 | L | 3101[A] | PRO | O-C-N | 5.37 | 128.68 | 122.23 |
| 3 | L | 3101[B] | PRO | O-C-N | 5.37 | 128.68 | 122.23 |
| 3 | F | 3119[A] | HIS | N-CA-C | -5.37 | 105.43 | 111.28 |
| 3 | F | 3119[B] | HIS | N-CA-C | -5.37 | 105.43 | 111.28 |
| 3 | C | 3300[A] | LEU | CA-C-N | -5.37 | 113.13 | 119.84 |
| 3 | C | 3300[A] | LEU | C-N-CA | -5.37 | 113.13 | 119.84 |
| 3 | C | 3300[B] | LEU | CA-C-N | -5.37 | 113.13 | 119.84 |
| 3 | C | 3300[B] | LEU | C-N-CA | -5.37 | 113.13 | 119.84 |
| 3 | O | 3113[A] | ASP | N-CA-C | 5.37 | 116.43 | 109.72 |
| 3 | O | 3113[B] | ASP | N-CA-C | 5.37 | 116.43 | 109.72 |
| 3 | L | 3005[A] | ALA | N-CA-C | -5.36 | 100.86 | 109.39 |
| 3 | L | 3005[B] | ALA | N-CA-C | -5.36 | 100.86 | 109.39 |
| 3 | L | 3119[A] | HIS | N-CA-C | -5.36 | 105.43 | 111.28 |
| 3 | L | 3119[B] | HIS | N-CA-C | -5.36 | 105.43 | 111.28 |
| 3 | X | 3119[A] | HIS | N-CA-C | -5.36 | 105.43 | 111.28 |
| 3 | X | 3119[B] | HIS | N-CA-C | -5.36 | 105.43 | 111.28 |
| 1 | D | 1512 | ARG | CA-C-N | 5.36 | 124.81 | 119.24 |
| 1 | D | 1512 | ARG | C-N-CA | 5.36 | 124.81 | 119.24 |
| 2 | E | 2558 | CYS | N-CA-C | 5.36 | 120.69 | 113.72 |
| 3 | U | 3300[A] | LEU | CA-C-N | -5.36 | 113.14 | 119.84 |
| 3 | U | 3300[A] | LEU | C-N-CA | -5.36 | 113.14 | 119.84 |
| 3 | U | 3300[B] | LEU | CA-C-N | -5.36 | 113.14 | 119.84 |
| 3 | U | 3300[B] | LEU | C-N-CA | -5.36 | 113.14 | 119.84 |
| 3 | F | 3113[A] | ASP | N-CA-C | 5.36 | 116.42 | 109.72 |
| 3 | F | 3113[B] | ASP | N-CA-C | 5.36 | 116.42 | 109.72 |
| 3 | d | 3300[A] | LEU | CA-C-N | -5.36 | 113.14 | 119.84 |
| 3 | d | 3300[A] | LEU | C-N-CA | -5.36 | 113.14 | 119.84 |
| 3 | d | 3300[B] | LEU | CA-C-N | -5.36 | 113.14 | 119.84 |
| 3 | d | 3300[B] | LEU | C-N-CA | -5.36 | 113.14 | 119.84 |
| 3 | C | 3277[A] | ALA | N-CA-C | -5.35 | 106.33 | 112.86 |
| 3 | C | 3277[B] | ALA | N-CA-C | -5.35 | 106.33 | 112.86 |
| 1 | M | 232 | ARG | CA-C-N | 5.35 | 125.61 | 119.83 |
| 1 | M | 232 | ARG | C-N-CA | 5.35 | 125.61 | 119.83 |
| 3 | I | 3119[A] | HIS | N-CA-C | -5.35 | 105.45 | 111.28 |
| 3 | I | 3119[B] | HIS | N-CA-C | -5.35 | 105.45 | 111.28 |
| 1 | V | 404 | ILE | CA-C-N | 5.35 | 123.56 | 119.66 |
| 1 | V | 404 | ILE | C-N-CA | 5.35 | 123.56 | 119.66 |
| 3 | d | 3113[A] | ASP | N-CA-C | 5.35 | 116.40 | 109.72 |
| 3 | d | 3113[B] | ASP | N-CA-C | 5.35 | 116.40 | 109.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | R | 3300[A] | LEU | CA-C-N | -5.34 | 113.16 | 119.84 |
| 3 | R | 3300[A] | LEU | C-N-CA | -5.34 | 113.16 | 119.84 |
| 3 | R | 3300[B] | LEU | CA-C-N | -5.34 | 113.16 | 119.84 |
| 3 | R | 3300[B] | LEU | C-N-CA | -5.34 | 113.16 | 119.84 |
| 1 | Y | 1494 | ARG | CA-C-N | -5.34 | 113.16 | 119.84 |
| 1 | Y | 1494 | ARG | C-N-CA | -5.34 | 113.16 | 119.84 |
| 3 | I | 3113[A] | ASP | N-CA-C | 5.34 | 116.40 | 109.72 |
| 3 | I | 3113[B] | ASP | N-CA-C | 5.34 | 116.40 | 109.72 |
| 3 | O | 3277[A] | ALA | N-CA-C | -5.34 | 106.34 | 112.86 |
| 3 | O | 3277[B] | ALA | N-CA-C | -5.34 | 106.34 | 112.86 |
| 3 | a | 3277[A] | ALA | N-CA-C | -5.34 | 106.34 | 112.86 |
| 3 | a | 3277[B] | ALA | N-CA-C | -5.34 | 106.34 | 112.86 |
| 3 | F | 3101[A] | PRO | O-C-N | 5.34 | 128.64 | 122.23 |
| 3 | F | 3101[B] | PRO | O-C-N | 5.34 | 128.64 | 122.23 |
| 3 | L | 3300[A] | LEU | CA-C-N | -5.34 | 113.17 | 119.84 |
| 3 | L | 3300[A] | LEU | C-N-CA | -5.34 | 113.17 | 119.84 |
| 3 | L | 3300[B] | LEU | CA-C-N | -5.34 | 113.17 | 119.84 |
| 3 | L | 3300[B] | LEU | C-N-CA | -5.34 | 113.17 | 119.84 |
| 3 | d | 3101[A] | PRO | O-C-N | 5.34 | 128.64 | 122.23 |
| 3 | d | 3101[B] | PRO | O-C-N | 5.34 | 128.64 | 122.23 |
| 3 | X | 3277[A] | ALA | N-CA-C | -5.34 | 106.35 | 112.86 |
| 3 | X | 3277[B] | ALA | N-CA-C | -5.34 | 106.35 | 112.86 |
| 3 | U | 3027[A] | GLU | CA-C-N | -5.33 | 113.13 | 119.05 |
| 3 | U | 3027[A] | GLU | C-N-CA | -5.33 | 113.13 | 119.05 |
| 3 | U | 3027[B] | GLU | CA-C-N | -5.33 | 113.13 | 119.05 |
| 3 | U | 3027[B] | GLU | C-N-CA | -5.33 | 113.13 | 119.05 |
| 3 | F | 3277[A] | ALA | N-CA-C | -5.33 | 106.36 | 112.86 |
| 3 | F | 3277[B] | ALA | N-CA-C | -5.33 | 106.36 | 112.86 |
| 1 | M | 921 | GLY | N-CA-C | 5.33 | 121.26 | 113.48 |
| 3 | L | 3113[A] | ASP | N-CA-C | 5.33 | 116.38 | 109.72 |
| 3 | L | 3113[B] | ASP | N-CA-C | 5.33 | 116.38 | 109.72 |
| 1 | S | 463 | GLY | N-CA-C | 5.32 | 119.07 | 110.87 |
| 1 | b | 127 | GLU | CA-CB-CG | 5.32 | 124.75 | 114.10 |
| 3 | O | 3300[A] | LEU | CA-C-N | -5.32 | 113.19 | 119.84 |
| 3 | O | 3300[A] | LEU | C-N-CA | -5.32 | 113.19 | 119.84 |
| 3 | O | 3300[B] | LEU | CA-C-N | -5.32 | 113.19 | 119.84 |
| 3 | O | 3300[B] | LEU | C-N-CA | -5.32 | 113.19 | 119.84 |
| 3 | R | 3163[A] | ASN | CA-C-N | -5.32 | 113.19 | 119.84 |
| 3 | R | 3163[A] | ASN | C-N-CA | -5.32 | 113.19 | 119.84 |
| 3 | R | 3163[B] | ASN | CA-C-N | -5.32 | 113.19 | 119.84 |
| 3 | R | 3163[B] | ASN | C-N-CA | -5.32 | 113.19 | 119.84 |
| 2 | E | 2489 | ILE | CA-C-N | 5.32 | 125.86 | 120.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | E | 2489 | ILE | C-N-CA | 5.32 | 125.86 | 120.38 |
| 3 | a | 3300[A] | LEU | CA-C-N | -5.32 | 113.19 | 119.84 |
| 3 | a | 3300[A] | LEU | C-N-CA | -5.32 | 113.19 | 119.84 |
| 3 | a | 3300[B] | LEU | CA-C-N | -5.32 | 113.19 | 119.84 |
| 3 | a | 3300[B] | LEU | C-N-CA | -5.32 | 113.19 | 119.84 |
| 2 | H | 2558 | CYS | N-CA-C | 5.32 | 119.86 | 112.90 |
| 3 | L | 3163[A] | ASN | CA-C-N | -5.32 | 113.20 | 119.84 |
| 3 | L | 3163[A] | ASN | C-N-CA | -5.32 | 113.20 | 119.84 |
| 3 | L | 3163[B] | ASN | CA-C-N | -5.32 | 113.20 | 119.84 |
| 3 | L | 3163[B] | ASN | C-N-CA | -5.32 | 113.20 | 119.84 |
| 3 | R | 3277[A] | ALA | N-CA-C | -5.32 | 106.37 | 112.86 |
| 3 | R | 3277[B] | ALA | N-CA-C | -5.32 | 106.37 | 112.86 |
| 1 | S | 1582 | ASN | CA-C-N | 5.32 | 131.27 | 121.70 |
| 1 | S | 1582 | ASN | C-N-CA | 5.32 | 131.27 | 121.70 |
| 3 | I | 3027[A] | GLU | CA-C-N | -5.31 | 113.16 | 119.05 |
| 3 | I | 3027[A] | GLU | C-N-CA | -5.31 | 113.16 | 119.05 |
| 3 | I | 3027[B] | GLU | CA-C-N | -5.31 | 113.16 | 119.05 |
| 3 | I | 3027[B] | GLU | C-N-CA | -5.31 | 113.16 | 119.05 |
| 2 | K | 2489 | ILE | CA-C-N | 5.31 | 125.85 | 120.38 |
| 2 | K | 2489 | ILE | C-N-CA | 5.31 | 125.85 | 120.38 |
| 3 | I | 3277[A] | ALA | N-CA-C | -5.31 | 106.39 | 112.86 |
| 3 | I | 3277[B] | ALA | N-CA-C | -5.31 | 106.39 | 112.86 |
| 3 | X | 3300[A] | LEU | CA-C-N | -5.30 | 113.21 | 119.84 |
| 3 | X | 3300[A] | LEU | C-N-CA | -5.30 | 113.21 | 119.84 |
| 3 | X | 3300[B] | LEU | CA-C-N | -5.30 | 113.21 | 119.84 |
| 3 | X | 3300[B] | LEU | C-N-CA | -5.30 | 113.21 | 119.84 |
| 1 | Y | 1286 | ARG | N-CA-C | 5.30 | 116.75 | 110.97 |
| 3 | F | 3163[A] | ASN | CA-C-N | -5.30 | 113.21 | 119.84 |
| 3 | F | 3163[A] | ASN | C-N-CA | -5.30 | 113.21 | 119.84 |
| 3 | F | 3163[B] | ASN | CA-C-N | -5.30 | 113.21 | 119.84 |
| 3 | F | 3163[B] | ASN | C-N-CA | -5.30 | 113.21 | 119.84 |
| 3 | U | 3277[A] | ALA | N-CA-C | -5.30 | 106.39 | 112.86 |
| 3 | U | 3277[B] | ALA | N-CA-C | -5.30 | 106.39 | 112.86 |
| 3 | F | 3300[A] | LEU | CA-C-N | -5.30 | 113.22 | 119.84 |
| 3 | F | 3300[A] | LEU | C-N-CA | -5.30 | 113.22 | 119.84 |
| 3 | F | 3300[B] | LEU | CA-C-N | -5.30 | 113.22 | 119.84 |
| 3 | F | 3300[B] | LEU | C-N-CA | -5.30 | 113.22 | 119.84 |
| 2 | c | 2418 | GLY | N-CA-C | 5.30 | 120.18 | 113.24 |
| 1 | J | 450 | LYS | N-CA-C | 5.30 | 116.33 | 108.86 |
| 3 | L | 3027[A] | GLU | CA-C-N | -5.29 | 113.17 | 119.05 |
| 3 | L | 3027[A] | GLU | C-N-CA | -5.29 | 113.17 | 119.05 |
| 3 | L | 3027[B] | GLU | CA-C-N | -5.29 | 113.17 | 119.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | L | 3027[B] | GLU | C-N-CA | -5.29 | 113.17 | 119.05 |
| 1 | b | 1286 | ARG | N-CA-C | 5.29 | 116.74 | 110.97 |
| 1 | G | 1512 | ARG | CA-C-N | 5.29 | 124.47 | 118.97 |
| 1 | G | 1512 | ARG | C-N-CA | 5.29 | 124.47 | 118.97 |
| 3 | L | 3277[A] | ALA | N-CA-C | -5.29 | 106.41 | 112.86 |
| 3 | L | 3277[B] | ALA | N-CA-C | -5.29 | 106.41 | 112.86 |
| 3 | X | 3027[A] | GLU | CA-C-N | -5.29 | 113.18 | 119.05 |
| 3 | X | 3027[A] | GLU | C-N-CA | -5.29 | 113.18 | 119.05 |
| 3 | X | 3027[B] | GLU | CA-C-N | -5.29 | 113.18 | 119.05 |
| 3 | X | 3027[B] | GLU | C-N-CA | -5.29 | 113.18 | 119.05 |
| 3 | d | 3027[A] | GLU | CA-C-N | -5.28 | 113.19 | 119.05 |
| 3 | d | 3027[A] | GLU | C-N-CA | -5.28 | 113.19 | 119.05 |
| 3 | d | 3027[B] | GLU | CA-C-N | -5.28 | 113.19 | 119.05 |
| 3 | d | 3027[B] | GLU | C-N-CA | -5.28 | 113.19 | 119.05 |
| 1 | G | 897 | HIS | N-CA-C | -5.28 | 101.80 | 108.45 |
| 3 | I | 3163[A] | ASN | CA-C-N | -5.28 | 113.25 | 119.84 |
| 3 | I | 3163[A] | ASN | C-N-CA | -5.28 | 113.25 | 119.84 |
| 3 | I | 3163[B] | ASN | CA-C-N | -5.28 | 113.25 | 119.84 |
| 3 | I | 3163[B] | ASN | C-N-CA | -5.28 | 113.25 | 119.84 |
| 3 | F | 3027[A] | GLU | CA-C-N | -5.27 | 113.20 | 119.05 |
| 3 | F | 3027[A] | GLU | C-N-CA | -5.27 | 113.20 | 119.05 |
| 3 | F | 3027[B] | GLU | CA-C-N | -5.27 | 113.20 | 119.05 |
| 3 | F | 3027[B] | GLU | C-N-CA | -5.27 | 113.20 | 119.05 |
| 1 | M | 1637 | GLY | N-CA-C | -5.27 | 100.68 | 113.18 |
| 3 | d | 3277[A] | ALA | N-CA-C | -5.27 | 106.43 | 112.86 |
| 3 | d | 3277[B] | ALA | N-CA-C | -5.27 | 106.43 | 112.86 |
| 3 | I | 3300[A] | LEU | CA-C-N | -5.27 | 113.25 | 119.84 |
| 3 | I | 3300[A] | LEU | C-N-CA | -5.27 | 113.25 | 119.84 |
| 3 | I | 3300[B] | LEU | CA-C-N | -5.27 | 113.25 | 119.84 |
| 3 | I | 3300[B] | LEU | C-N-CA | -5.27 | 113.25 | 119.84 |
| 3 | X | 3163[A] | ASN | CA-C-N | -5.27 | 113.25 | 119.84 |
| 3 | X | 3163[A] | ASN | C-N-CA | -5.27 | 113.25 | 119.84 |
| 3 | X | 3163[B] | ASN | CA-C-N | -5.27 | 113.25 | 119.84 |
| 3 | X | 3163[B] | ASN | C-N-CA | -5.27 | 113.25 | 119.84 |
| 3 | O | 3027[A] | GLU | CA-C-N | -5.26 | 113.21 | 119.05 |
| 3 | O | 3027[A] | GLU | C-N-CA | -5.26 | 113.21 | 119.05 |
| 3 | O | 3027[B] | GLU | CA-C-N | -5.26 | 113.21 | 119.05 |
| 3 | O | 3027[B] | GLU | C-N-CA | -5.26 | 113.21 | 119.05 |
| 3 | C | 3163[A] | ASN | CA-C-N | -5.26 | 113.26 | 119.84 |
| 3 | C | 3163[A] | ASN | C-N-CA | -5.26 | 113.26 | 119.84 |
| 3 | C | 3163[B] | ASN | CA-C-N | -5.26 | 113.26 | 119.84 |
| 3 | C | 3163[B] | ASN | C-N-CA | -5.26 | 113.26 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | O | 3163[A] | ASN | CA-C-N | -5.26 | 113.27 | 119.84 |
| 3 | O | 3163[A] | ASN | C-N-CA | -5.26 | 113.27 | 119.84 |
| 3 | O | 3163[B] | ASN | CA-C-N | -5.26 | 113.27 | 119.84 |
| 3 | O | 3163[B] | ASN | C-N-CA | -5.26 | 113.27 | 119.84 |
| 3 | U | 3163[A] | ASN | CA-C-N | -5.26 | 113.27 | 119.84 |
| 3 | U | 3163[A] | ASN | C-N-CA | -5.26 | 113.27 | 119.84 |
| 3 | U | 3163[B] | ASN | CA-C-N | -5.26 | 113.27 | 119.84 |
| 3 | U | 3163[B] | ASN | C-N-CA | -5.26 | 113.27 | 119.84 |
| 3 | a | 3027[A] | GLU | CA-C-N | -5.26 | 113.21 | 119.05 |
| 3 | a | 3027[A] | GLU | C-N-CA | -5.26 | 113.21 | 119.05 |
| 3 | a | 3027[B] | GLU | CA-C-N | -5.26 | 113.21 | 119.05 |
| 3 | a | 3027[B] | GLU | C-N-CA | -5.26 | 113.21 | 119.05 |
| 3 | a | 3163[A] | ASN | CA-C-N | -5.26 | 113.27 | 119.84 |
| 3 | a | 3163[A] | ASN | C-N-CA | -5.26 | 113.27 | 119.84 |
| 3 | a | 3163[B] | ASN | CA-C-N | -5.26 | 113.27 | 119.84 |
| 3 | a | 3163[B] | ASN | C-N-CA | -5.26 | 113.27 | 119.84 |
| 1 | J | 1036 | SER | N-CA-C | 5.25 | 117.42 | 111.11 |
| 3 | R | 3027[A] | GLU | CA-C-N | -5.25 | 113.22 | 119.05 |
| 3 | R | 3027[A] | GLU | C-N-CA | -5.25 | 113.22 | 119.05 |
| 3 | R | 3027[B] | GLU | CA-C-N | -5.25 | 113.22 | 119.05 |
| 3 | R | 3027[B] | GLU | C-N-CA | -5.25 | 113.22 | 119.05 |
| 1 | A | 877 | HIS | N-CA-C | -5.25 | 106.46 | 112.92 |
| 1 | S | 573 | LYS | CA-C-N | 5.25 | 131.15 | 121.70 |
| 1 | S | 573 | LYS | C-N-CA | 5.25 | 131.15 | 121.70 |
| 1 | V | 1584 | GLY | N-CA-C | 5.25 | 125.62 | 113.18 |
| 3 | C | 3027[A] | GLU | CA-C-N | -5.25 | 113.23 | 119.05 |
| 3 | C | 3027[A] | GLU | C-N-CA | -5.25 | 113.23 | 119.05 |
| 3 | C | 3027[B] | GLU | CA-C-N | -5.25 | 113.23 | 119.05 |
| 3 | C | 3027[B] | GLU | C-N-CA | -5.25 | 113.23 | 119.05 |
| 3 | d | 3163[A] | ASN | CA-C-N | -5.25 | 113.28 | 119.84 |
| 3 | d | 3163[A] | ASN | C-N-CA | -5.25 | 113.28 | 119.84 |
| 3 | d | 3163[B] | ASN | CA-C-N | -5.25 | 113.28 | 119.84 |
| 3 | d | 3163[B] | ASN | C-N-CA | -5.25 | 113.28 | 119.84 |
| 1 | V | 131 | GLU | CB-CA-C | -5.24 | 110.52 | 116.54 |
| 3 | F | 3197[A] | ILE | CA-C-N | -5.24 | 113.24 | 119.05 |
| 3 | F | 3197[A] | ILE | C-N-CA | -5.24 | 113.24 | 119.05 |
| 3 | F | 3197[B] | ILE | CA-C-N | -5.24 | 113.24 | 119.05 |
| 3 | F | 3197[B] | ILE | C-N-CA | -5.24 | 113.24 | 119.05 |
| 1 | G | 50 | ALA | CB-CA-C | -5.24 | 110.52 | 116.54 |
| 2 | Z | 2418 | GLY | N-CA-C | 5.23 | 120.09 | 113.24 |
| 1 | P | 1647 | ASN | CA-C-N | 5.23 | 125.53 | 119.93 |
| 1 | P | 1647 | ASN | C-N-CA | 5.23 | 125.53 | 119.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | M | 1581 | GLU | N-CA-C | 5.23 | 115.25 | 107.88 |
| 1 | A | 565 | GLU | N-CA-C | 5.22 | 116.22 | 108.86 |
| 3 | L | 3029[A] | LYS | N-CA-C | 5.22 | 117.48 | 109.07 |
| 3 | L | 3029[B] | LYS | N-CA-C | 5.22 | 117.48 | 109.07 |
| 3 | U | 3197[A] | ILE | CA-C-N | -5.22 | 113.25 | 119.05 |
| 3 | U | 3197[A] | ILE | C-N-CA | -5.22 | 113.25 | 119.05 |
| 3 | U | 3197[B] | ILE | CA-C-N | -5.22 | 113.25 | 119.05 |
| 3 | U | 3197[B] | ILE | C-N-CA | -5.22 | 113.25 | 119.05 |
| 3 | a | 3197[A] | ILE | CA-C-N | -5.22 | 113.26 | 119.05 |
| 3 | a | 3197[A] | ILE | C-N-CA | -5.22 | 113.26 | 119.05 |
| 3 | a | 3197[B] | ILE | CA-C-N | -5.22 | 113.26 | 119.05 |
| 3 | a | 3197[B] | ILE | C-N-CA | -5.22 | 113.26 | 119.05 |
| 3 | I | 3197[A] | ILE | CA-C-N | -5.21 | 113.27 | 119.05 |
| 3 | I | 3197[A] | ILE | C-N-CA | -5.21 | 113.27 | 119.05 |
| 3 | I | 3197[B] | ILE | CA-C-N | -5.21 | 113.27 | 119.05 |
| 3 | I | 3197[B] | ILE | C-N-CA | -5.21 | 113.27 | 119.05 |
| 1 | S | 627 | ASP | CA-C-N | 5.21 | 124.87 | 119.56 |
| 1 | S | 627 | ASP | C-N-CA | 5.21 | 124.87 | 119.56 |
| 1 | D | 1316 | MET | CA-C-N | 5.21 | 124.82 | 119.56 |
| 1 | D | 1316 | MET | C-N-CA | 5.21 | 124.82 | 119.56 |
| 3 | X | 3197[A] | ILE | CA-C-N | -5.20 | 113.27 | 119.05 |
| 3 | X | 3197[A] | ILE | C-N-CA | -5.20 | 113.27 | 119.05 |
| 3 | X | 3197[B] | ILE | CA-C-N | -5.20 | 113.27 | 119.05 |
| 3 | X | 3197[B] | ILE | C-N-CA | -5.20 | 113.27 | 119.05 |
| 1 | V | 50 | ALA | CB-CA-C | -5.20 | 110.16 | 117.23 |
| 1 | b | 465 | PRO | N-CA-C | -5.20 | 101.76 | 112.47 |
| 3 | C | 3197[A] | ILE | CA-C-N | -5.20 | 113.28 | 119.05 |
| 3 | C | 3197[A] | ILE | C-N-CA | -5.20 | 113.28 | 119.05 |
| 3 | C | 3197[B] | ILE | CA-C-N | -5.20 | 113.28 | 119.05 |
| 3 | C | 3197[B] | ILE | C-N-CA | -5.20 | 113.28 | 119.05 |
| 1 | V | 985 | PHE | CB-CA-C | -5.20 | 110.56 | 116.54 |
| 3 | R | 3197[A] | ILE | CA-C-N | -5.19 | 113.29 | 119.05 |
| 3 | R | 3197[A] | ILE | C-N-CA | -5.19 | 113.29 | 119.05 |
| 3 | R | 3197[B] | ILE | CA-C-N | -5.19 | 113.29 | 119.05 |
| 3 | R | 3197[B] | ILE | C-N-CA | -5.19 | 113.29 | 119.05 |
| 2 | W | 2490 | PRO | O-C-N | 5.19 | 123.59 | 121.15 |
| 3 | X | 3029[A] | LYS | N-CA-C | 5.19 | 117.42 | 109.07 |
| 3 | X | 3029[B] | LYS | N-CA-C | 5.19 | 117.42 | 109.07 |
| 3 | a | 3029[A] | LYS | N-CA-C | 5.19 | 117.42 | 109.07 |
| 3 | a | 3029[B] | LYS | N-CA-C | 5.19 | 117.42 | 109.07 |
| 1 | P | 897 | HIS | N-CA-C | -5.19 | 101.58 | 108.74 |
| 2 | Z | 2728 | ARG | N-CA-C | -5.19 | 104.03 | 110.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 3029[A] | LYS | N-CA-C | 5.18 | 117.42 | 109.07 |
| 3 | C | 3029[B] | LYS | N-CA-C | 5.18 | 117.42 | 109.07 |
| 1 | G | 1339 | SER | CA-C-N | 5.18 | 131.02 | 121.70 |
| 1 | G | 1339 | SER | C-N-CA | 5.18 | 131.02 | 121.70 |
| 2 | H | 2237 | LEU | CB-CA-C | -5.18 | 110.62 | 116.63 |
| 2 | H | 2489 | ILE | CA-C-N | 5.18 | 125.72 | 120.38 |
| 2 | H | 2489 | ILE | C-N-CA | 5.18 | 125.72 | 120.38 |
| 1 | Y | 758 | GLY | N-CA-C | 5.18 | 118.04 | 110.63 |
| 3 | O | 3029[A] | LYS | N-CA-C | 5.18 | 117.41 | 109.07 |
| 3 | O | 3029[B] | LYS | N-CA-C | 5.18 | 117.41 | 109.07 |
| 1 | Y | 1636 | ASN | N-CA-C | -5.18 | 102.39 | 110.10 |
| 3 | d | 3029[A] | LYS | N-CA-C | 5.17 | 117.40 | 109.07 |
| 3 | d | 3029[B] | LYS | N-CA-C | 5.17 | 117.40 | 109.07 |
| 2 | H | 2132 | CYS | CA-C-N | -5.17 | 113.38 | 119.84 |
| 2 | H | 2132 | CYS | C-N-CA | -5.17 | 113.38 | 119.84 |
| 3 | R | 3029[A] | LYS | N-CA-C | 5.17 | 117.39 | 109.07 |
| 3 | R | 3029[B] | LYS | N-CA-C | 5.17 | 117.39 | 109.07 |
| 1 | P | 1441 | SER | N-CA-C | 5.16 | 115.06 | 108.24 |
| 3 | U | 3029[A] | LYS | N-CA-C | 5.16 | 117.38 | 109.07 |
| 3 | U | 3029[B] | LYS | N-CA-C | 5.16 | 117.38 | 109.07 |
| 2 | T | 2556 | TYR | N-CA-C | 5.16 | 115.15 | 107.88 |
| 1 | M | 1584 | GLY | N-CA-C | 5.15 | 125.40 | 113.18 |
| 3 | d | 3197[A] | ILE | CA-C-N | -5.15 | 113.33 | 119.05 |
| 3 | d | 3197[A] | ILE | C-N-CA | -5.15 | 113.33 | 119.05 |
| 3 | d | 3197[B] | ILE | CA-C-N | -5.15 | 113.33 | 119.05 |
| 3 | d | 3197[B] | ILE | C-N-CA | -5.15 | 113.33 | 119.05 |
| 3 | F | 3029[A] | LYS | N-CA-C | 5.15 | 117.36 | 109.07 |
| 3 | F | 3029[B] | LYS | N-CA-C | 5.15 | 117.36 | 109.07 |
| 1 | S | 562 | GLN | N-CA-C | 5.14 | 117.55 | 111.33 |
| 1 | Y | 296 | ARG | N-CA-C | -5.14 | 106.85 | 113.23 |
| 1 | D | 675 | SER | CA-C-N | -5.14 | 113.41 | 119.84 |
| 1 | D | 675 | SER | C-N-CA | -5.14 | 113.41 | 119.84 |
| 3 | I | 3029[A] | LYS | N-CA-C | 5.14 | 117.34 | 109.07 |
| 3 | I | 3029[B] | LYS | N-CA-C | 5.14 | 117.34 | 109.07 |
| 3 | L | 3197[A] | ILE | CA-C-N | -5.13 | 113.35 | 119.05 |
| 3 | L | 3197[A] | ILE | C-N-CA | -5.13 | 113.35 | 119.05 |
| 3 | L | 3197[B] | ILE | CA-C-N | -5.13 | 113.35 | 119.05 |
| 3 | L | 3197[B] | ILE | C-N-CA | -5.13 | 113.35 | 119.05 |
| 1 | A | 99 | THR | N-CA-C | -5.13 | 107.68 | 114.04 |
| 1 | S | 1486 | LEU | CA-C-N | -5.13 | 114.50 | 120.04 |
| 1 | S | 1486 | LEU | C-N-CA | -5.13 | 114.50 | 120.04 |
| 3 | O | 3197[A] | ILE | CA-C-N | -5.13 | 113.36 | 119.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | O | 3197[A] | ILE | C-N-CA | -5.13 | 113.36 | 119.05 |
| 3 | O | 3197[B] | ILE | CA-C-N | -5.13 | 113.36 | 119.05 |
| 3 | O | 3197[B] | ILE | C-N-CA | -5.13 | 113.36 | 119.05 |
| 1 | J | 1582 | ASN | CA-C-N | 5.12 | 130.92 | 121.70 |
| 1 | J | 1582 | ASN | C-N-CA | 5.12 | 130.92 | 121.70 |
| 1 | P | 898 | GLY | N-CA-C | 5.12 | 125.31 | 113.18 |
| 1 | J | 1195 | ASP | N-CA-C | 5.11 | 116.93 | 111.36 |
| 3 | F | 3120[A] | HIS | CA-C-N | -5.09 | 111.83 | 121.54 |
| 3 | F | 3120[A] | HIS | C-N-CA | -5.09 | 111.83 | 121.54 |
| 3 | F | 3120[B] | HIS | CA-C-N | -5.09 | 111.83 | 121.54 |
| 3 | F | 3120[B] | HIS | C-N-CA | -5.09 | 111.83 | 121.54 |
| 2 | B | 2237 | LEU | CB-CA-C | -5.08 | 110.32 | 117.23 |
| 3 | L | 3120[A] | HIS | CA-C-N | -5.07 | 111.85 | 121.54 |
| 3 | L | 3120[A] | HIS | C-N-CA | -5.07 | 111.85 | 121.54 |
| 3 | L | 3120[B] | HIS | CA-C-N | -5.07 | 111.85 | 121.54 |
| 3 | L | 3120[B] | HIS | C-N-CA | -5.07 | 111.85 | 121.54 |
| 2 | c | 2764 | THR | CA-C-N | 5.07 | 125.10 | 119.32 |
| 2 | c | 2764 | THR | C-N-CA | 5.07 | 125.10 | 119.32 |
| 3 | I | 3120[A] | HIS | CA-C-N | -5.07 | 111.86 | 121.54 |
| 3 | I | 3120[A] | HIS | C-N-CA | -5.07 | 111.86 | 121.54 |
| 3 | I | 3120[B] | HIS | CA-C-N | -5.07 | 111.86 | 121.54 |
| 3 | I | 3120[B] | HIS | C-N-CA | -5.07 | 111.86 | 121.54 |
| 2 | K | 2826 | GLU | CB-CA-C | -5.07 | 110.75 | 116.63 |
| 1 | Y | 958 | PRO | CA-C-O | -5.07 | 115.17 | 122.31 |
| 1 | A | 627 | ASP | CA-C-N | 5.06 | 125.09 | 119.32 |
| 1 | A | 627 | ASP | C-N-CA | 5.06 | 125.09 | 119.32 |
| 1 | G | 1581 | GLU | N-CA-C | 5.06 | 116.94 | 108.99 |
| 3 | C | 3120[A] | HIS | CA-C-N | -5.06 | 111.88 | 121.54 |
| 3 | C | 3120[A] | HIS | C-N-CA | -5.06 | 111.88 | 121.54 |
| 3 | C | 3120[B] | HIS | CA-C-N | -5.06 | 111.88 | 121.54 |
| 3 | C | 3120[B] | HIS | C-N-CA | -5.06 | 111.88 | 121.54 |
| 2 | T | 2418 | GLY | N-CA-C | 5.06 | 120.00 | 113.27 |
| 1 | A | 688 | VAL | CA-C-N | 5.06 | 126.16 | 119.84 |
| 1 | A | 688 | VAL | C-N-CA | 5.06 | 126.16 | 119.84 |
| 1 | A | 1295 | GLY | N-CA-C | 5.06 | 120.22 | 111.98 |
| 3 | U | 3120[A] | HIS | CA-C-N | -5.06 | 111.88 | 121.54 |
| 3 | U | 3120[A] | HIS | C-N-CA | -5.06 | 111.88 | 121.54 |
| 3 | U | 3120[B] | HIS | CA-C-N | -5.06 | 111.88 | 121.54 |
| 3 | U | 3120[B] | HIS | C-N-CA | -5.06 | 111.88 | 121.54 |
| 2 | K | 2558 | CYS | N-CA-C | 5.05 | 119.72 | 113.50 |
| 3 | O | 3120[A] | HIS | CA-C-N | -5.05 | 111.89 | 121.54 |
| 3 | O | 3120[A] | HIS | C-N-CA | -5.05 | 111.89 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | O | 3120[B] | HIS | CA-C-N | -5.05 | 111.89 | 121.54 |
| 3 | O | 3120[B] | HIS | C-N-CA | -5.05 | 111.89 | 121.54 |
| 1 | V | 1295 | GLY | N-CA-C | 5.04 | 120.20 | 111.98 |
| 3 | d | 3120[A] | HIS | CA-C-N | -5.04 | 111.91 | 121.54 |
| 3 | d | 3120[A] | HIS | C-N-CA | -5.04 | 111.91 | 121.54 |
| 3 | d | 3120[B] | HIS | CA-C-N | -5.04 | 111.91 | 121.54 |
| 3 | d | 3120[B] | HIS | C-N-CA | -5.04 | 111.91 | 121.54 |
| 1 | D | 568 | PHE | N-CA-C | 5.04 | 117.43 | 111.33 |
| 1 | V | 566 | ARG | CB-CA-C | -5.04 | 110.38 | 117.23 |
| 1 | A | 1486 | LEU | CA-C-N | -5.03 | 114.64 | 119.87 |
| 1 | A | 1486 | LEU | C-N-CA | -5.03 | 114.64 | 119.87 |
| 3 | R | 3120[A] | HIS | CA-C-N | -5.03 | 111.93 | 121.54 |
| 3 | R | 3120[A] | HIS | C-N-CA | -5.03 | 111.93 | 121.54 |
| 3 | R | 3120[B] | HIS | CA-C-N | -5.03 | 111.93 | 121.54 |
| 3 | R | 3120[B] | HIS | C-N-CA | -5.03 | 111.93 | 121.54 |
| 1 | S | 1537 | ILE | CB-CA-C | -5.03 | 109.02 | 114.35 |
| 1 | A | 1300 | CYS | CA-C-N | 5.03 | 126.12 | 119.84 |
| 1 | A | 1300 | CYS | C-N-CA | 5.03 | 126.12 | 119.84 |
| 2 | K | 2704 | ASP | CA-C-N | 5.02 | 125.05 | 119.32 |
| 2 | K | 2704 | ASP | C-N-CA | 5.02 | 125.05 | 119.32 |
| 1 | V | 1441 | SER | N-CA-C | 5.02 | 114.78 | 108.45 |
| 3 | a | 3120[A] | HIS | CA-C-N | -5.02 | 111.95 | 121.54 |
| 3 | a | 3120[A] | HIS | C-N-CA | -5.02 | 111.95 | 121.54 |
| 3 | a | 3120[B] | HIS | CA-C-N | -5.02 | 111.95 | 121.54 |
| 3 | a | 3120[B] | HIS | C-N-CA | -5.02 | 111.95 | 121.54 |
| 1 | A | 675 | SER | CA-C-N | -5.02 | 113.57 | 119.84 |
| 1 | A | 675 | SER | C-N-CA | -5.02 | 113.57 | 119.84 |
| 1 | b | 823 | VAL | CA-C-N | 5.02 | 125.17 | 119.90 |
| 1 | b | 823 | VAL | C-N-CA | 5.02 | 125.17 | 119.90 |
| 1 | A | 296 | ARG | N-CA-C | -5.01 | 107.17 | 113.28 |
| 1 | b | 323 | ILE | CA-C-N | 5.01 | 125.00 | 119.89 |
| 1 | b | 323 | ILE | C-N-CA | 5.01 | 125.00 | 119.89 |
| 3 | U | 2934[A] | GLU | N-CA-C | -5.01 | 105.82 | 111.28 |
| 3 | U | 2934[B] | GLU | N-CA-C | -5.01 | 105.82 | 111.28 |
| 3 | d | 2934[A] | GLU | N-CA-C | -5.01 | 105.82 | 111.28 |
| 3 | d | 2934[B] | GLU | N-CA-C | -5.01 | 105.82 | 111.28 |
| 2 | Z | 2128 | LEU | N-CA-C | 5.01 | 120.27 | 113.16 |
| 2 | W | 2476 | LEU | CA-C-N | 5.00 | 124.93 | 119.78 |
| 2 | W | 2476 | LEU | C-N-CA | 5.00 | 124.93 | 119.78 |

There are no chirality outliers.

All (67) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 464 | LEU | Peptide |
| 1 | A | 982 | LYS | Peptide |
| 2 | B | 2127 | ALA | Peptide |
| 3 | C | 3113[A] | ASP | Mainchain |
| 3 | C | 3113[B] | ASP | Mainchain |
| 3 | C | 3149[A] | ASN | Peptide |
| 3 | C | 3149[B] | ASN | Peptide |
| 1 | D | 464 | LEU | Peptide |
| 1 | D | 567 | LEU | Peptide |
| 1 | D | 883 | CYS | Peptide |
| 3 | F | 3113[A] | ASP | Mainchain |
| 3 | F | 3113[B] | ASP | Mainchain |
| 3 | F | 3149[A] | ASN | Peptide |
| 3 | F | 3149[B] | ASN | Peptide |
| 1 | G | 464 | LEU | Peptide |
| 3 | I | 3113[A] | ASP | Mainchain |
| 3 | I | 3113[B] | ASP | Mainchain |
| 3 | I | 3149[A] | ASN | Peptide |
| 3 | I | 3149[B] | ASN | Peptide |
| 1 | J | 1639 | LYS | Peptide |
| 1 | J | 464 | LEU | Peptide |
| 2 | K | 2127 | ALA | Peptide |
| 2 | K | 2830 | GLN | Peptide |
| 2 | K | 2889 | ALA | Peptide |
| 3 | L | 3113[A] | ASP | Mainchain |
| 3 | L | 3113[B] | ASP | Mainchain |
| 3 | L | 3149[A] | ASN | Peptide |
| 3 | L | 3149[B] | ASN | Peptide |
| 1 | M | 464 | LEU | Peptide |
| 2 | N | 2127 | ALA | Peptide |
| 3 | O | 3113[A] | ASP | Mainchain |
| 3 | O | 3113[B] | ASP | Mainchain |
| 3 | O | 3149[A] | ASN | Peptide |
| 3 | O | 3149[B] | ASN | Peptide |
| 2 | Q | 2127 | ALA | Peptide |
| 3 | R | 3113[A] | ASP | Mainchain |
| 3 | R | 3113[B] | ASP | Mainchain |
| 3 | R | 3149[A] | ASN | Peptide |
| 3 | R | 3149[B] | ASN | Peptide |
| 1 | S | 1638 | SER | Peptide |
| 1 | S | 464 | LEU | Peptide |
| 1 | S | 866 | GLU | Peptide |
| 2 | T | 2127 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | T | 2548 | CYS | Peptide |
| 3 | U | 3113[A] | ASP | Mainchain |
| 3 | U | 3113[B] | ASP | Mainchain |
| 3 | U | 3149[A] | ASN | Peptide |
| 3 | U | 3149[B] | ASN | Peptide |
| 2 | W | 2127 | ALA | Peptide |
| 3 | X | 3113[A] | ASP | Mainchain |
| 3 | X | 3113[B] | ASP | Mainchain |
| 3 | X | 3149[A] | ASN | Peptide |
| 3 | X | 3149[B] | ASN | Peptide |
| 1 | Y | 464 | LEU | Peptide |
| 2 | Z | 2127 | ALA | Peptide |
| 2 | Z | 2497 | GLU | Peptide |
| 3 | a | 3113[A] | ASP | Mainchain |
| 3 | a | 3113[B] | ASP | Mainchain |
| 3 | a | 3149[A] | ASN | Peptide |
| 3 | a | 3149[B] | ASN | Peptide |
| 1 | b | 127 | GLU | Peptide |
| 1 | b | 464 | LEU | Peptide |
| 2 | c | 2127 | ALA | Peptide |
| 3 | d | 3113[A] | ASP | Mainchain |
| 3 | d | 3113[B] | ASP | Mainchain |
| 3 | d | 3149[A] | ASN | Peptide |
| 3 | d | 3149[B] | ASN | Peptide |

## 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 | 13318 | 0 | 12755 | 476 | 1 |
| 1 | D | 13318 | 0 | 12755 | 482 | 0 |
| 1 | G | 13318 | 0 | 12754 | 503 | 0 |
| 1 | J | 13318 | 0 | 12755 | 508 | 0 |
| 1 | M | 13318 | 0 | 12755 | 448 | 0 |
| 1 | P | 13318 | 0 | 12755 | 450 | 0 |
| 1 | S | 13318 | 0 | 12755 | 451 | 0 |
| 1 | V | 13318 | 0 | 12755 | 448 | 0 |
| 1 | Y | 13318 | 0 | 12744 | 528 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | b | 13318 | 0 | 12754 | 452 | 1 |
| 2 | B | 6704 | 0 | 6445 | 213 | 0 |
| 2 | E | 6704 | 0 | 6445 | 245 | 0 |
| 2 | H | 6704 | 0 | 6445 | 243 | 0 |
| 2 | K | 6704 | 0 | 6445 | 218 | 0 |
| 2 | N | 6704 | 0 | 6445 | 203 | 0 |
| 2 | Q | 6704 | 0 | 6445 | 218 | 0 |
| 2 | T | 6704 | 0 | 6445 | 221 | 0 |
| 2 | W | 6704 | 0 | 6445 | 226 | 0 |
| 2 | Z | 6704 | 0 | 6444 | 238 | 0 |
| 2 | c | 6704 | 0 | 6445 | 224 | 0 |
| 3 | C | 5912 | 0 | 5607 | 2341 | 0 |
| 3 | F | 5912 | 0 | 5599 | 2386 | 0 |
| 3 | I | 5912 | 0 | 5601 | 2460 | 0 |
| 3 | L | 5912 | 0 | 5604 | 2354 | 0 |
| 3 | O | 5912 | 0 | 5604 | 2061 | 0 |
| 3 | R | 5912 | 0 | 5598 | 2438 | 0 |
| 3 | U | 5912 | 0 | 5612 | 2074 | 0 |
| 3 | X | 5912 | 0 | 5598 | 2059 | 0 |
| 3 | a | 5912 | 0 | 5594 | 2398 | 0 |
| 3 | d | 5912 | 0 | 5608 | 2177 | 0 |
| 4 | 1 | 28 | 0 | 25 | 1 | 0 |
| 4 | 2 | 28 | 0 | 25 | 1 | 0 |
| 4 | 4 | 28 | 0 | 25 | 0 | 0 |
| 4 | 6 | 28 | 0 | 25 | 2 | 0 |
| 4 | 7 | 28 | 0 | 25 | 6 | 0 |
| 4 | 8 | 28 | 0 | 25 | 0 | 0 |
| 4 | 9 | 28 | 0 | 25 | 2 | 0 |
| 4 | BA | 28 | 0 | 25 | 5 | 0 |
| 4 | HA | 28 | 0 | 25 | 6 | 0 |
| 4 | IA | 28 | 0 | 25 | 0 | 0 |
| 4 | JA | 28 | 0 | 25 | 2 | 0 |
| 4 | MA | 28 | 0 | 25 | 9 | 0 |
| 4 | OA | 28 | 0 | 25 | 2 | 0 |
| 4 | QA | 28 | 0 | 25 | 4 | 0 |
| 4 | RA | 28 | 0 | 25 | 1 | 0 |
| 4 | e | 28 | 0 | 25 | 0 | 0 |
| 4 | f | 28 | 0 | 25 | 2 | 0 |
| 4 | i | 28 | 0 | 25 | 3 | 0 |
| 4 | j | 28 | 0 | 25 | 4 | 0 |
| 4 | m | 28 | 0 | 25 | 9 | 0 |
| 4 | n | 28 | 0 | 25 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | o | 28 | 0 | 25 | 3 | 0 |
| 4 | p | 28 | 0 | 25 | 0 | 0 |
| 4 | q | 28 | 0 | 25 | 7 | 0 |
| 4 | s | 28 | 0 | 25 | 2 | 0 |
| 4 | t | 28 | 0 | 25 | 1 | 0 |
| 4 | u | 28 | 0 | 25 | 6 | 0 |
| 4 | v | 28 | 0 | 25 | 2 | 0 |
| 4 | x | 28 | 0 | 25 | 0 | 0 |
| 5 | AA | 50 | 0 | 43 | 1 | 0 |
| 5 | FA | 50 | 0 | 43 | 2 | 0 |
| 5 | KA | 50 | 0 | 43 | 1 | 0 |
| 5 | PA | 50 | 0 | 43 | 1 | 0 |
| 5 | g | 50 | 0 | 43 | 0 | 0 |
| 5 | l | 50 | 0 | 43 | 2 | 0 |
| 6 | 3 | 39 | 0 | 34 | 3 | 0 |
| 6 | 5 | 39 | 0 | 34 | 2 | 0 |
| 6 | CA | 39 | 0 | 34 | 3 | 0 |
| 6 | DA | 39 | 0 | 34 | 2 | 0 |
| 6 | EA | 39 | 0 | 34 | 1 | 0 |
| 6 | GA | 39 | 0 | 34 | 9 | 0 |
| 6 | LA | 39 | 0 | 34 | 5 | 0 |
| 6 | NA | 39 | 0 | 34 | 3 | 0 |
| 6 | h | 39 | 0 | 34 | 1 | 0 |
| 6 | k | 39 | 0 | 34 | 4 | 0 |
| 6 | r | 39 | 0 | 34 | 8 | 0 |
| 6 | w | 39 | 0 | 34 | 2 | 0 |
| 6 | y | 39 | 0 | 34 | 0 | 0 |
| 7 | z | 61 | 0 | 52 | 2 | 0 |
| 8 | 0 | 50 | 0 | 43 | 8 | 0 |
| 9 | A | 24 | 0 | 0 | 2 | 0 |
| 9 | B | 8 | 0 | 0 | 0 | 0 |
| 9 | C | 8 | 0 | 0 | 7 | 0 |
| 9 | D | 24 | 0 | 0 | 2 | 0 |
| 9 | E | 8 | 0 | 0 | 0 | 0 |
| 9 | F | 8 | 0 | 0 | 7 | 0 |
| 9 | G | 24 | 0 | 0 | 1 | 0 |
| 9 | H | 8 | 0 | 0 | 0 | 0 |
| 9 | I | 8 | 0 | 0 | 6 | 0 |
| 9 | J | 24 | 0 | 0 | 2 | 0 |
| 9 | K | 8 | 0 | 0 | 0 | 0 |
| 9 | L | 8 | 0 | 0 | 7 | 0 |
| 9 | M | 24 | 0 | 0 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 9 | N | 8 | 0 | 0 | 0 | 0 |
| 9 | O | 8 | 0 | 0 | 10 | 0 |
| 9 | P | 24 | 0 | 0 | 0 | 0 |
| 9 | Q | 8 | 0 | 0 | 0 | 0 |
| 9 | R | 8 | 0 | 0 | 6 | 0 |
| 9 | S | 24 | 0 | 0 | 3 | 0 |
| 9 | T | 8 | 0 | 0 | 1 | 0 |
| 9 | U | 8 | 0 | 0 | 10 | 0 |
| 9 | V | 24 | 0 | 0 | 2 | 0 |
| 9 | W | 8 | 0 | 0 | 1 | 0 |
| 9 | X | 8 | 0 | 0 | 10 | 0 |
| 9 | Y | 24 | 0 | 0 | 3 | 0 |
| 9 | Z | 8 | 0 | 0 | 0 | 0 |
| 9 | a | 8 | 0 | 0 | 7 | 0 |
| 9 | b | 24 | 0 | 0 | 1 | 0 |
| 9 | c | 8 | 0 | 0 | 0 | 0 |
| 9 | d | 8 | 0 | 0 | 10 | 0 |
| All | All | 261470 | 0 | 249531 | 25303 | 1 |

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 50.

All (25303) 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) |
|---|---|---|---|
| 3:F:2975[B]:PHE:CD1 | 3:a:3107[B]:LEU:HD11 | 1.20 | 1.69 |
| 3:F:2969[B]:TYR:HD1 | 3:a:2961[B]:HIS:CG | 1.09 | 1.68 |
| 3:C:3079[B]:CYS:CB | 3:L:3161[B]:GLU:HG2 | 1.22 | 1.65 |
| 3:C:2982[B]:MET:SD | 3:L:3156[B]:MET:HB2 | 1.37 | 1.64 |
| 3:F:2970[B]:PRO:HD3 | 3:a:2989[B]:HIS:CD2 | 1.23 | 1.64 |
| 3:U:3256[B]:TRP:CG | 3:d:2969[B]:TYR:HB2 | 1.33 | 1.63 |
| 3:U:3254[B]:MET:HE1 | 3:d:3254[B]:MET:CE | 1.27 | 1.63 |
| 3:C:2975[B]:PHE:CD1 | 3:L:3107[B]:LEU:HD11 | 1.28 | 1.63 |
| 3:I:3174[B]:GLY:CA | 3:R:3154[B]:PRO:HB3 | 1.17 | 1.62 |
| 3:U:2969[B]:TYR:CE1 | 3:d:3107[B]:LEU:CD1 | 1.82 | 1.61 |
| 2:Z:2867:PRO:CG | 3:a:2932[A]:PRO:HG2 | 1.28 | 1.60 |
| 3:O:3153[B]:LYS:CD | 3:X:3176[B]:LYS:HD3 | 1.31 | 1.60 |
| 3:F:3157[B]:PRO:HA | 3:a:2982[B]:MET:SD | 1.41 | 1.59 |
| 3:C:3156[B]:MET:CE | 3:L:2979[B]:GLN:HG3 | 1.25 | 1.59 |
| 3:O:2963[B]:MET:HE1 | 3:X:2975[B]:PHE:CG | 1.08 | 1.58 |
| 3:F:3155[B]:MET:CB | 3:a:3153[B]:LYS:HD2 | 1.33 | 1.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3196[A]:THR:CG2 | 1:J:416:ASN:HD22 | 0.95 | 1.57 |
| 3:U:3256[B]:TRP:CB | 3:d:2969[B]:TYR:HB2 | 1.22 | 1.57 |
| 3:O:2968[B]:GLN:NE2 | 3:X:2985[B]:PHE:CA | 1.68 | 1.56 |
| 3:C:3156[B]:MET:HE2 | 3:L:2979[B]:GLN:CG | 1.15 | 1.56 |
| 3:F:3153[B]:LYS:CG | 3:a:3155[B]:MET:HB2 | 1.08 | 1.56 |
| 3:O:2968[B]:GLN:CB | 3:X:2988[B]:TRP:HB2 | 1.29 | 1.56 |
| 3:C:2985[B]:PHE:CZ | 3:L:2970[B]:PRO:HA | 1.07 | 1.56 |
| 3:F:2975[B]:PHE:HD1 | 3:a:3107[B]:LEU:CD1 | 1.19 | 1.56 |
| 3:F:3155[B]:MET:HB2 | 3:a:3153[B]:LYS:CG | 1.33 | 1.56 |
| 3:I:2989[B]:HIS:CG | 3:R:2970[B]:PRO:HD3 | 1.37 | 1.55 |
| 3:I:3163[B]:ASN:CB | 3:R:3150[B]:LYS:HE3 | 1.28 | 1.55 |
| 3:C:2985[B]:PHE:HZ | 3:L:2970[B]:PRO:CA | 0.91 | 1.55 |
| 3:F:2984[B]:THR:HG21 | 3:a:3159[B]:SER:CB | 1.14 | 1.55 |
| 3:O:2970[B]:PRO:CD | 3:X:2991[B]:LEU:HB2 | 1.37 | 1.54 |
| 3:O:2970[B]:PRO:HG2 | 3:X:2991[B]:LEU:CA | 1.12 | 1.54 |
| 3:C:2965[B]:LEU:CD2 | 3:L:3253[B]:GLU:CD | 1.79 | 1.54 |
| 3:C:3158[B]:PHE:CD2 | 3:L:3153[B]:LYS:CE | 1.89 | 1.54 |
| 3:I:2975[B]:PHE:CD1 | 3:R:3107[B]:LEU:HD11 | 1.42 | 1.53 |
| 3:F:3149[B]:ASN:CB | 3:a:3163[B]:ASN:ND2 | 1.68 | 1.53 |
| 3:C:2974[B]:ALA:CB | 3:L:3249[B]:GLY:CA | 1.83 | 1.53 |
| 3:F:2983[B]:VAL:CG2 | 3:a:3161[B]:GLU:N | 1.70 | 1.53 |
| 3:F:3155[B]:MET:HB2 | 3:a:3153[B]:LYS:CD | 1.06 | 1.53 |
| 3:U:3255[B]:PRO:HG2 | 3:d:3252[B]:TYR:C | 1.29 | 1.53 |
| 1:Y:1546:LYS:CG | 3:d:3001[B]:LYS:HE3 | 1.35 | 1.52 |
| 3:F:2970[B]:PRO:CD | 3:a:2989[B]:HIS:CD2 | 1.91 | 1.52 |
| 3:O:2965[B]:LEU:HD12 | 3:X:2979[B]:GLN:CD | 1.15 | 1.52 |
| 3:I:3150[B]:LYS:C | 3:R:3159[B]:SER:HA | 1.18 | 1.52 |
| 3:O:2970[B]:PRO:CG | 3:X:2991[B]:LEU:N | 1.69 | 1.52 |
| 3:C:2982[B]:MET:CG | 3:L:3156[B]:MET:HB2 | 1.38 | 1.51 |
| 3:I:3159[B]:SER:C | 3:R:3150[B]:LYS:HB3 | 1.31 | 1.51 |
| 3:O:3153[B]:LYS:HD3 | 3:X:3176[B]:LYS:CD | 1.35 | 1.51 |
| 3:F:3154[B]:PRO:N | 3:a:3155[B]:MET:CG | 1.73 | 1.51 |
| 3:F:3159[B]:SER:HB3 | 3:a:2984[B]:THR:CG2 | 1.38 | 1.50 |
| 3:I:3251[B]:ASP:CB | 3:R:3251[B]:ASP:HB3 | 1.07 | 1.50 |
| 3:I:3150[B]:LYS:HB3 | 3:R:3159[B]:SER:C | 1.11 | 1.50 |
| 3:F:2966[B]:SER:C | 3:a:3256[B]:TRP:CD1 | 1.87 | 1.49 |
| 3:O:2963[B]:MET:CE | 3:X:2975[B]:PHE:CG | 1.92 | 1.49 |
| 3:C:3150[B]:LYS:HZ3 | 3:L:3160[B]:SER:CB | 1.22 | 1.49 |
| 3:I:2989[B]:HIS:CD2 | 3:R:2970[B]:PRO:HD3 | 1.48 | 1.49 |
| 1:Y:1546:LYS:HB2 | 3:d:3001[B]:LYS:NZ | 1.21 | 1.49 |
| 3:O:3169[B]:LYS:CG | 3:X:3148[B]:ILE:CG2 | 1.81 | 1.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3220[B]:ARG:HA | 3:d:2973[B]:THR:CA | 1.28 | 1.48 |
| 3:R:2956[A]:LYS:O | 3:R:2960[A]:PHE:CE1 | 1.67 | 1.48 |
| 3:I:3149[B]:ASN:CB | 3:R:3163[B]:ASN:ND2 | 1.74 | 1.48 |
| 3:L:2956[A]:LYS:O | 3:L:2960[A]:PHE:CE1 | 1.67 | 1.48 |
| 3:U:3256[B]:TRP:HB2 | 3:d:2969[B]:TYR:CB | 1.42 | 1.48 |
| 3:C:3090[B]:ASN:HD22 | 3:L:2972[B]:GLY:C | 1.20 | 1.47 |
| 3:I:2956[B]:LYS:O | 3:I:2960[B]:PHE:CE1 | 1.67 | 1.47 |
| 3:L:3089[B]:HIS:CE1 | 3:L:3119[B]:HIS:NE2 | 1.83 | 1.47 |
| 3:U:3089[B]:HIS:CE1 | 3:U:3119[B]:HIS:NE2 | 1.83 | 1.47 |
| 3:a:2956[B]:LYS:O | 3:a:2960[B]:PHE:CE1 | 1.67 | 1.47 |
| 3:d:2956[A]:LYS:O | 3:d:2960[A]:PHE:CE1 | 1.67 | 1.47 |
| 3:d:3089[A]:HIS:CE1 | 3:d:3119[A]:HIS:NE2 | 1.83 | 1.47 |
| 3:C:3160[B]:SER:CB | 3:L:3150[B]:LYS:NZ | 1.75 | 1.47 |
| 3:F:3150[B]:LYS:NZ | 3:a:3160[B]:SER:HB3 | 1.26 | 1.47 |
| 3:I:3089[A]:HIS:CE1 | 3:I:3119[A]:HIS:NE2 | 1.83 | 1.47 |
| 3:U:3254[B]:MET:CE | 3:d:3254[B]:MET:HE3 | 0.99 | 1.47 |
| 3:L:3089[A]:HIS:CE1 | 3:L:3119[A]:HIS:NE2 | 1.82 | 1.47 |
| 3:U:3089[A]:HIS:CE1 | 3:U:3119[A]:HIS:NE2 | 1.83 | 1.47 |
| 3:F:3160[B]:SER:HB3 | 3:a:3150[B]:LYS:NZ | 1.21 | 1.47 |
| 3:L:2956[B]:LYS:O | 3:L:2960[B]:PHE:CE1 | 1.67 | 1.47 |
| 3:O:2968[B]:GLN:NE2 | 3:X:2985[B]:PHE:N | 1.63 | 1.47 |
| 3:U:2969[B]:TYR:CE1 | 3:d:3107[B]:LEU:HD11 | 1.44 | 1.47 |
| 3:X:3089[B]:HIS:CE1 | 3:X:3119[B]:HIS:NE2 | 1.82 | 1.47 |
| 3:C:3089[A]:HIS:CE1 | 3:C:3119[A]:HIS:NE2 | 1.83 | 1.46 |
| 3:X:3089[A]:HIS:CE1 | 3:X:3119[A]:HIS:NE2 | 1.83 | 1.46 |
| 3:C:2956[B]:LYS:O | 3:C:2960[B]:PHE:CE1 | 1.67 | 1.46 |
| 3:C:3089[B]:HIS:CE1 | 3:C:3119[B]:HIS:NE2 | 1.83 | 1.46 |
| 3:O:3089[B]:HIS:CE1 | 3:O:3119[B]:HIS:NE2 | 1.83 | 1.46 |
| 3:d:3089[B]:HIS:CE1 | 3:d:3119[B]:HIS:NE2 | 1.82 | 1.46 |
| 3:F:2956[A]:LYS:O | 3:F:2960[A]:PHE:CE1 | 1.67 | 1.46 |
| 1:S:416:ASN:CG | 3:X:3196[A]:THR:HG21 | 1.41 | 1.46 |
| 3:a:3089[A]:HIS:CE1 | 3:a:3119[A]:HIS:NE2 | 1.83 | 1.46 |
| 3:F:2970[B]:PRO:HD3 | 3:a:2989[B]:HIS:CG | 1.45 | 1.46 |
| 3:O:2956[A]:LYS:O | 3:O:2960[A]:PHE:CE1 | 1.67 | 1.46 |
| 3:O:3153[B]:LYS:HG2 | 3:X:3176[B]:LYS:CE | 1.41 | 1.46 |
| 3:d:2956[B]:LYS:O | 3:d:2960[B]:PHE:CE1 | 1.67 | 1.46 |
| 3:F:2984[B]:THR:CG2 | 3:a:3159[B]:SER:HB3 | 0.98 | 1.45 |
| 3:I:3154[B]:PRO:HB3 | 3:R:3174[B]:GLY:CA | 1.43 | 1.45 |
| 1:S:416:ASN:OD1 | 3:X:3196[A]:THR:CG2 | 1.64 | 1.45 |
| 3:a:2956[A]:LYS:O | 3:a:2960[A]:PHE:CE1 | 1.67 | 1.45 |
| 3:F:3089[A]:HIS:CE1 | 3:F:3119[A]:HIS:NE2 | 1.83 | 1.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2956[A]:LYS:O | 3:I:2960[A]:PHE:CE1 | 1.67 | 1.45 |
| 3:U:2956[B]:LYS:O | 3:U:2960[B]:PHE:CE1 | 1.67 | 1.45 |
| 3:C:2956[A]:LYS:O | 3:C:2960[A]:PHE:CE1 | 1.67 | 1.45 |
| 3:F:2982[B]:MET:CG | 3:a:2967[B]:CYS:SG | 2.05 | 1.45 |
| 3:O:3108[B]:HIS:HB3 | 3:X:2969[B]:TYR:C | 1.05 | 1.45 |
| 3:F:3089[B]:HIS:CE1 | 3:F:3119[B]:HIS:NE2 | 1.83 | 1.45 |
| 3:F:3174[B]:GLY:N | 3:a:3154[B]:PRO:HB3 | 1.19 | 1.44 |
| 3:I:2975[B]:PHE:HD1 | 3:R:3107[B]:LEU:CD1 | 1.28 | 1.44 |
| 3:O:2965[B]:LEU:CD1 | 3:X:2979[B]:GLN:NE2 | 1.75 | 1.44 |
| 3:U:2956[A]:LYS:O | 3:U:2960[A]:PHE:CE1 | 1.67 | 1.44 |
| 3:U:3155[B]:MET:CA | 3:d:3150[B]:LYS:HG2 | 1.45 | 1.44 |
| 3:C:3163[B]:ASN:ND2 | 3:L:3149[B]:ASN:CB | 1.78 | 1.44 |
| 3:I:3089[B]:HIS:CE1 | 3:I:3119[B]:HIS:NE2 | 1.82 | 1.44 |
| 1:Y:1616:LYS:HD3 | 3:d:3187[B]:TYR:C | 1.23 | 1.44 |
| 3:C:3079[B]:CYS:SG | 3:L:3161[B]:GLU:CB | 2.03 | 1.44 |
| 3:F:3155[B]:MET:CB | 3:a:3153[B]:LYS:CD | 1.84 | 1.44 |
| 3:F:3252[B]:TYR:N | 3:a:3108[B]:HIS:NE2 | 1.63 | 1.44 |
| 3:I:3251[B]:ASP:HB3 | 3:R:3251[B]:ASP:CB | 0.98 | 1.44 |
| 3:X:2956[B]:LYS:O | 3:X:2960[B]:PHE:CE1 | 1.68 | 1.44 |
| 3:I:2959[B]:SER:CB | 3:R:3255[B]:PRO:HB2 | 1.46 | 1.44 |
| 3:I:3150[B]:LYS:HE3 | 3:R:3163[B]:ASN:CB | 1.46 | 1.44 |
| 3:O:2956[B]:LYS:O | 3:O:2960[B]:PHE:CE1 | 1.67 | 1.44 |
| 3:R:3089[A]:HIS:CE1 | 3:R:3119[A]:HIS:NE2 | 1.83 | 1.44 |
| 3:C:3153[B]:LYS:CE | 3:L:3158[B]:PHE:CD2 | 1.99 | 1.43 |
| 3:C:3154[B]:PRO:CD | 3:L:3174[B]:GLY:HA2 | 1.46 | 1.43 |
| 3:O:3089[A]:HIS:CE1 | 3:O:3119[A]:HIS:NE2 | 1.83 | 1.43 |
| 3:R:2956[B]:LYS:O | 3:R:2960[B]:PHE:CE1 | 1.67 | 1.43 |
| 3:F:2956[B]:LYS:O | 3:F:2960[B]:PHE:CE1 | 1.67 | 1.43 |
| 3:F:2965[B]:LEU:N | 3:a:3221[B]:ALA:CB | 1.78 | 1.43 |
| 3:a:3089[B]:HIS:CE1 | 3:a:3119[B]:HIS:NE2 | 1.82 | 1.43 |
| 3:I:2969[B]:TYR:HD1 | 3:R:2961[B]:HIS:CG | 1.35 | 1.43 |
| 3:I:3196[A]:THR:HG21 | 1:J:416:ASN:ND2 | 1.14 | 1.43 |
| 3:R:3089[B]:HIS:CE1 | 3:R:3119[B]:HIS:NE2 | 1.83 | 1.43 |
| 3:X:2956[A]:LYS:O | 3:X:2960[A]:PHE:CE1 | 1.67 | 1.43 |
| 2:E:2868:GLU:CG | 3:F:2932[A]:PRO:O | 1.65 | 1.42 |
| 3:O:3108[B]:HIS:CB | 3:X:2969[B]:TYR:C | 1.92 | 1.42 |
| 3:U:3254[B]:MET:CB | 3:d:3254[B]:MET:HA | 1.45 | 1.42 |
| 3:U:2975[B]:PHE:CG | 3:d:3256[B]:TRP:CD1 | 2.06 | 1.42 |
| 3:F:3251[B]:ASP:CB | 3:a:3251[B]:ASP:HB3 | 0.96 | 1.42 |
| 3:U:2965[B]:LEU:N | 3:d:3220[B]:ARG:NH1 | 1.66 | 1.42 |
| 3:F:3157[B]:PRO:O | 3:a:3150[B]:LYS:CD | 1.66 | 1.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3174[B]:GLY:CA | 3:R:3154[B]:PRO:CB | 1.94 | 1.41 |
| 3:I:3149[B]:ASN:HB2 | 3:R:3163[B]:ASN:ND2 | 1.09 | 1.41 |
| 3:U:3169[B]:LYS:C | 3:d:3148[B]:ILE:HB | 1.45 | 1.41 |
| 3:F:3153[B]:LYS:C | 3:a:3155[B]:MET:HG3 | 1.45 | 1.41 |
| 3:C:2984[B]:THR:CG2 | 3:L:3159[B]:SER:OG | 1.68 | 1.41 |
| 3:C:2988[B]:TRP:NE1 | 3:L:3153[B]:LYS:HZ3 | 1.19 | 1.41 |
| 3:F:2983[B]:VAL:HG21 | 3:a:3161[B]:GLU:N | 1.08 | 1.41 |
| 3:I:2989[B]:HIS:CD2 | 3:R:2970[B]:PRO:CD | 2.00 | 1.41 |
| 3:C:2972[B]:GLY:C | 3:L:3090[B]:ASN:HD22 | 1.25 | 1.40 |
| 3:C:3158[B]:PHE:CD2 | 3:L:3153[B]:LYS:HE2 | 1.44 | 1.40 |
| 3:U:3254[B]:MET:HE3 | 3:d:3254[B]:MET:CB | 1.50 | 1.40 |
| 3:F:2984[B]:THR:CG2 | 3:a:3159[B]:SER:CB | 1.76 | 1.40 |
| 3:F:3161[B]:GLU:CG | 3:a:3079[B]:CYS:SG | 2.08 | 1.40 |
| 3:O:2968[B]:GLN:NE2 | 3:X:2985[B]:PHE:HA | 1.22 | 1.40 |
| 3:U:2969[B]:TYR:CZ | 3:d:3107[B]:LEU:HD12 | 1.53 | 1.40 |
| 3:C:2983[B]:VAL:CG2 | 3:L:3160[B]:SER:HA | 1.50 | 1.40 |
| 3:C:2984[B]:THR:HG23 | 3:L:3159[B]:SER:CB | 1.50 | 1.40 |
| 3:C:3150[B]:LYS:NZ | 3:L:3160[B]:SER:CB | 1.80 | 1.40 |
| 3:F:2966[B]:SER:CA | 3:a:3256[B]:TRP:CD1 | 2.02 | 1.40 |
| 3:I:3169[B]:LYS:O | 3:R:3152[B]:LYS:CG | 1.68 | 1.40 |
| 3:U:3256[B]:TRP:CE3 | 3:d:2969[B]:TYR:HB3 | 1.56 | 1.40 |
| 3:C:2969[B]:TYR:CE2 | 3:L:3120[B]:HIS:NE2 | 1.82 | 1.40 |
| 3:C:3172[B]:SER:N | 3:L:3152[B]:LYS:HB2 | 1.27 | 1.40 |
| 3:U:2965[B]:LEU:CA | 3:d:3220[B]:ARG:NH1 | 1.85 | 1.40 |
| 3:C:2983[B]:VAL:HG21 | 3:L:3161[B]:GLU:N | 1.15 | 1.40 |
| 3:C:3256[B]:TRP:CD2 | 3:L:2965[B]:LEU:O | 1.72 | 1.39 |
| 3:C:2983[B]:VAL:HG23 | 3:L:3160[B]:SER:CA | 1.49 | 1.39 |
| 3:F:3153[B]:LYS:CG | 3:a:3155[B]:MET:CB | 2.00 | 1.39 |
| 3:O:3038[B]:ILE:CG1 | 3:X:2969[B]:TYR:OH | 1.69 | 1.39 |
| 3:F:2969[B]:TYR:HD1 | 3:a:2961[B]:HIS:CD2 | 1.08 | 1.39 |
| 3:O:3169[B]:LYS:CB | 3:X:3148[B]:ILE:HG21 | 1.52 | 1.39 |
| 3:F:3153[B]:LYS:CD | 3:a:3155[B]:MET:HB2 | 1.51 | 1.39 |
| 3:F:3174[B]:GLY:CA | 3:a:3154[B]:PRO:HB3 | 1.53 | 1.39 |
| 3:I:2964[B]:PRO:C | 3:R:3221[B]:ALA:HB1 | 1.45 | 1.38 |
| 3:U:3169[B]:LYS:HG2 | 3:d:3148[B]:ILE:N | 1.10 | 1.38 |
| 3:C:2975[B]:PHE:CE1 | 3:L:3107[B]:LEU:HD11 | 1.57 | 1.38 |
| 3:O:3038[B]:ILE:HD13 | 3:X:2969[B]:TYR:CE2 | 1.59 | 1.38 |
| 3:C:2969[B]:TYR:C | 3:L:2985[B]:PHE:CE2 | 1.80 | 1.37 |
| 3:C:2974[B]:ALA:HB3 | 3:L:3249[B]:GLY:CA | 0.91 | 1.37 |
| 3:F:3152[B]:LYS:HB2 | 3:a:3172[B]:SER:N | 1.30 | 1.37 |
| 3:U:2965[B]:LEU:N | 3:d:3220[B]:ARG:HH12 | 1.19 | 1.37 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3169[B]:LYS:CG | 3:d:3148[B]:ILE:H | 1.36 | 1.37 |
| 3:U:2965[B]:LEU:HD11 | 3:d:3221[B]:ALA:N | 1.39 | 1.37 |
| 3:C:2982[B]:MET:CB | 3:L:3156[B]:MET:CB | 2.02 | 1.37 |
| 3:C:3156[B]:MET:SD | 3:L:2982[B]:MET:HB2 | 1.64 | 1.37 |
| 3:O:3169[B]:LYS:HG3 | 3:X:3148[B]:ILE:CG2 | 0.91 | 1.37 |
| 3:C:3155[B]:MET:CG | 3:L:3153[B]:LYS:C | 1.96 | 1.36 |
| 3:I:3154[B]:PRO:HG2 | 3:R:3155[B]:MET:SD | 1.65 | 1.36 |
| 2:Z:2867:PRO:CG | 3:a:2932[A]:PRO:CG | 2.02 | 1.36 |
| 3:I:3174[B]:GLY:N | 3:R:3154[B]:PRO:HB3 | 1.04 | 1.36 |
| 3:U:2970[B]:PRO:HA | 3:d:3086[B]:GLU:CD | 1.47 | 1.36 |
| 3:U:3155[B]:MET:C | 3:d:3150[B]:LYS:CG | 1.84 | 1.36 |
| 3:C:3154[B]:PRO:HD3 | 3:L:3174[B]:GLY:CA | 1.53 | 1.36 |
| 3:O:2976[B]:ALA:HB2 | 3:X:3156[B]:MET:SD | 1.63 | 1.36 |
| 3:F:3152[B]:LYS:CD | 3:a:3170[B]:ALA:O | 1.70 | 1.36 |
| 3:O:2976[B]:ALA:N | 3:X:3156[B]:MET:HG2 | 1.07 | 1.36 |
| 3:F:3170[B]:ALA:C | 3:a:3152[B]:LYS:HD2 | 1.36 | 1.36 |
| 3:U:2975[B]:PHE:CD1 | 3:d:3256[B]:TRP:CD1 | 2.12 | 1.36 |
| 3:U:3154[B]:PRO:HG3 | 3:d:2984[B]:THR:CG2 | 1.56 | 1.36 |
| 3:F:2975[B]:PHE:C | 3:a:3253[B]:GLU:HB2 | 1.16 | 1.35 |
| 3:I:3221[B]:ALA:CB | 3:R:2965[B]:LEU:N | 1.86 | 1.35 |
| 3:O:2965[B]:LEU:CD1 | 3:X:2979[B]:GLN:HE22 | 1.30 | 1.35 |
| 3:C:2975[B]:PHE:CD1 | 3:L:3107[B]:LEU:CD1 | 2.09 | 1.35 |
| 3:F:2982[B]:MET:CE | 3:a:2967[B]:CYS:SG | 2.12 | 1.35 |
| 3:I:3155[B]:MET:HB2 | 3:R:3153[B]:LYS:CD | 1.55 | 1.35 |
| 3:F:3173[B]:THR:C | 3:a:3154[B]:PRO:HD3 | 1.50 | 1.35 |
| 3:I:2961[B]:HIS:CD2 | 3:R:2969[B]:TYR:HD1 | 1.35 | 1.35 |
| 3:X:2952[B]:ALA:HB3 | 3:X:2953[B]:GLY:C | 1.52 | 1.35 |
| 3:I:3152[B]:LYS:CB | 3:R:3172[B]:SER:H | 1.18 | 1.35 |
| 3:O:2952[A]:ALA:HB3 | 3:O:2953[A]:GLY:C | 1.52 | 1.35 |
| 3:O:2970[B]:PRO:HD2 | 3:X:2991[B]:LEU:CB | 1.54 | 1.35 |
| 3:I:3154[B]:PRO:HB3 | 3:R:3174[B]:GLY:N | 1.38 | 1.35 |
| 3:U:3255[B]:PRO:CG | 3:d:3252[B]:TYR:C | 1.98 | 1.35 |
| 3:U:3256[B]:TRP:CG | 3:d:2969[B]:TYR:CB | 2.08 | 1.35 |
| 3:F:2967[B]:CYS:SG | 3:a:2982[B]:MET:CE | 2.15 | 1.34 |
| 3:F:2984[B]:THR:HG21 | 3:a:3159[B]:SER:OG | 1.19 | 1.34 |
| 3:I:2968[B]:GLN:HE21 | 3:R:3086[B]:GLU:CG | 1.31 | 1.34 |
| 3:I:3107[B]:LEU:HD11 | 3:R:2975[B]:PHE:CD1 | 1.61 | 1.34 |
| 3:I:3159[B]:SER:HA | 3:R:3150[B]:LYS:C | 1.50 | 1.34 |
| 3:U:2952[A]:ALA:HB3 | 3:U:2953[A]:GLY:C | 1.52 | 1.34 |
| 1:Y:1550:ARG:NH2 | 3:d:3008[B]:GLY:O | 1.59 | 1.34 |
| 3:F:3161[B]:GLU:HG2 | 3:a:3079[B]:CYS:SG | 1.67 | 1.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3221[B]:ALA:HB1 | 3:R:2965[B]:LEU:N | 1.03 | 1.34 |
| 3:C:3147[B]:GLU:CG | 3:L:3160[B]:SER:O | 1.75 | 1.34 |
| 3:F:3159[B]:SER:CB | 3:a:2984[B]:THR:CG2 | 2.02 | 1.34 |
| 3:U:3220[B]:ARG:CA | 3:d:2973[B]:THR:HA | 1.48 | 1.34 |
| 1:Y:1616:LYS:CD | 3:d:3187[B]:TYR:C | 1.94 | 1.34 |
| 3:F:3107[B]:LEU:HD11 | 3:a:2975[B]:PHE:CD1 | 1.62 | 1.34 |
| 3:U:2965[B]:LEU:HD12 | 3:d:3220[B]:ARG:CA | 1.55 | 1.34 |
| 3:d:2952[B]:ALA:HB3 | 3:d:2953[B]:GLY:C | 1.52 | 1.34 |
| 3:C:2979[B]:GLN:HG3 | 3:L:3156[B]:MET:CE | 1.56 | 1.34 |
| 3:O:2952[B]:ALA:HB3 | 3:O:2953[B]:GLY:C | 1.52 | 1.34 |
| 3:C:3150[B]:LYS:CA | 3:L:3172[B]:SER:HB3 | 1.58 | 1.33 |
| 3:F:3147[B]:GLU:OE1 | 3:a:3163[B]:ASN:N | 1.61 | 1.33 |
| 3:I:2965[B]:LEU:N | 3:R:3221[B]:ALA:HB1 | 1.01 | 1.33 |
| 3:I:3174[B]:GLY:N | 3:R:3154[B]:PRO:CB | 1.89 | 1.33 |
| 3:U:3156[B]:MET:CE | 3:d:2982[B]:MET:CG | 2.06 | 1.33 |
| 2:W:2868:GLU:OE1 | 3:X:2933[A]:SER:N | 1.60 | 1.33 |
| 3:C:3253[B]:GLU:HB2 | 3:L:2975[B]:PHE:C | 1.51 | 1.33 |
| 3:I:3173[B]:THR:OG1 | 3:R:3173[B]:THR:CG2 | 1.75 | 1.33 |
| 3:R:2952[B]:ALA:HB3 | 3:R:2953[B]:GLY:C | 1.52 | 1.33 |
| 3:U:3152[B]:LYS:CG | 3:d:3154[B]:PRO:HB3 | 1.56 | 1.33 |
| 3:F:3153[B]:LYS:CB | 3:a:3155[B]:MET:HB2 | 1.58 | 1.33 |
| 3:F:3253[B]:GLU:OE1 | 3:a:2974[B]:ALA:HB1 | 1.24 | 1.33 |
| 3:O:2963[B]:MET:CE | 3:X:2975[B]:PHE:CD1 | 2.10 | 1.33 |
| 3:a:3089[B]:HIS:HE1 | 3:a:3119[B]:HIS:NE2 | 1.20 | 1.33 |
| 3:F:3157[B]:PRO:CA | 3:a:2982[B]:MET:SD | 2.14 | 1.33 |
| 3:F:3159[B]:SER:HA | 3:a:3150[B]:LYS:C | 1.30 | 1.33 |
| 3:I:2952[B]:ALA:HB3 | 3:I:2953[B]:GLY:C | 1.52 | 1.33 |
| 3:I:2982[B]:MET:SD | 3:R:3157[B]:PRO:CA | 2.15 | 1.33 |
| 3:O:3108[B]:HIS:C | 3:X:2970[B]:PRO:CD | 1.86 | 1.33 |
| 3:a:3196[A]:THR:HG21 | 1:b:416:ASN:CG | 1.53 | 1.33 |
| 3:C:2968[B]:GLN:NE2 | 3:L:3258[B]:PHE:HZ | 1.27 | 1.33 |
| 3:O:2963[B]:MET:HE1 | 3:X:2975[B]:PHE:CD1 | 1.64 | 1.33 |
| 3:U:3252[B]:TYR:HE2 | 3:d:3222[B]:ILE:CD1 | 1.41 | 1.33 |
| 3:a:2952[A]:ALA:HB3 | 3:a:2953[A]:GLY:C | 1.52 | 1.33 |
| 3:C:2952[B]:ALA:HB3 | 3:C:2953[B]:GLY:C | 1.52 | 1.32 |
| 3:F:2952[B]:ALA:HB3 | 3:F:2953[B]:GLY:C | 1.52 | 1.32 |
| 3:F:3159[B]:SER:CB | 3:a:2984[B]:THR:HG21 | 1.56 | 1.32 |
| 3:F:3255[B]:PRO:HD3 | 3:a:2962[B]:GLY:O | 1.29 | 1.32 |
| 3:I:2952[A]:ALA:HB3 | 3:I:2953[A]:GLY:C | 1.52 | 1.32 |
| 3:L:2952[B]:ALA:HB3 | 3:L:2953[B]:GLY:C | 1.52 | 1.32 |
| 3:O:2970[B]:PRO:HD2 | 3:X:2991[B]:LEU:CG | 1.57 | 1.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3086[B]:GLU:OE2 | 3:d:2970[B]:PRO:HG3 | 1.15 | 1.32 |
| 3:d:2952[A]:ALA:HB3 | 3:d:2953[A]:GLY:C | 1.52 | 1.32 |
| 3:I:2975[B]:PHE:C | 3:R:3253[B]:GLU:HB2 | 1.51 | 1.32 |
| 3:I:3150[B]:LYS:CB | 3:R:3159[B]:SER:C | 2.00 | 1.32 |
| 3:L:2952[A]:ALA:HB3 | 3:L:2953[A]:GLY:C | 1.52 | 1.32 |
| 3:O:3157[B]:PRO:O | 3:X:3149[B]:ASN:C | 1.71 | 1.32 |
| 3:a:2952[B]:ALA:HB3 | 3:a:2953[B]:GLY:C | 1.52 | 1.32 |
| 3:F:3153[B]:LYS:CD | 3:a:3155[B]:MET:CB | 2.05 | 1.32 |
| 3:R:2952[A]:ALA:HB3 | 3:R:2953[A]:GLY:C | 1.52 | 1.32 |
| 3:U:2979[B]:GLN:NE2 | 3:d:3153[B]:LYS:HZ1 | 1.27 | 1.32 |
| 3:F:2952[A]:ALA:HB3 | 3:F:2953[A]:GLY:C | 1.52 | 1.32 |
| 3:U:2952[B]:ALA:HB3 | 3:U:2953[B]:GLY:C | 1.52 | 1.32 |
| 3:C:2982[B]:MET:CB | 3:L:3156[B]:MET:HB3 | 1.59 | 1.32 |
| 3:I:3163[B]:ASN:ND2 | 3:R:3150[B]:LYS:HG3 | 1.43 | 1.32 |
| 3:I:3255[B]:PRO:HB2 | 3:R:2959[B]:SER:CB | 1.58 | 1.32 |
| 3:X:2952[A]:ALA:HB3 | 3:X:2953[A]:GLY:C | 1.52 | 1.32 |
| 3:a:3196[A]:THR:HG21 | 1:b:416:ASN:OD1 | 1.30 | 1.32 |
| 3:C:2952[A]:ALA:HB3 | 3:C:2953[A]:GLY:C | 1.52 | 1.31 |
| 3:I:2970[B]:PRO:HD3 | 3:R:2989[B]:HIS:CD2 | 1.64 | 1.31 |
| 3:U:2970[B]:PRO:CA | 3:d:3086[B]:GLU:OE1 | 1.78 | 1.31 |
| 3:U:3154[B]:PRO:CG | 3:d:2984[B]:THR:HG21 | 1.57 | 1.31 |
| 1:Y:1616:LYS:HD3 | 3:d:3188[B]:ASP:N | 1.03 | 1.31 |
| 3:C:3159[B]:SER:CB | 3:L:2984[B]:THR:HG23 | 1.58 | 1.31 |
| 3:I:3153[B]:LYS:O | 3:R:3155[B]:MET:N | 1.64 | 1.31 |
| 3:I:3169[B]:LYS:CE | 3:R:3149[B]:ASN:OD1 | 1.76 | 1.31 |
| 3:C:3148[B]:ILE:O | 3:L:3169[B]:LYS:C | 1.71 | 1.31 |
| 3:C:3169[B]:LYS:C | 3:L:3148[B]:ILE:O | 1.63 | 1.31 |
| 3:F:3259[B]:ASP:CB | 3:a:3162[B]:ASP:HB3 | 1.58 | 1.31 |
| 3:O:2963[B]:MET:SD | 3:X:2975[B]:PHE:CD2 | 2.24 | 1.31 |
| 3:C:3160[B]:SER:OG | 3:L:2983[B]:VAL:HG23 | 1.23 | 1.31 |
| 3:C:3162[B]:ASP:C | 3:L:3147[B]:GLU:OE1 | 1.73 | 1.31 |
| 3:I:2982[B]:MET:SD | 3:R:3157[B]:PRO:HA | 1.70 | 1.31 |
| 3:I:3150[B]:LYS:O | 3:R:3159[B]:SER:CA | 1.78 | 1.31 |
| 3:O:2965[B]:LEU:CD1 | 3:X:2979[B]:GLN:OE1 | 1.72 | 1.31 |
| 3:L:3089[A]:HIS:HE1 | 3:L:3119[A]:HIS:NE2 | 1.20 | 1.30 |
| 3:O:2970[B]:PRO:CG | 3:X:2991[B]:LEU:CA | 2.02 | 1.30 |
| 3:C:2979[B]:GLN:CG | 3:L:3156[B]:MET:HE2 | 1.30 | 1.30 |
| 3:F:3170[B]:ALA:O | 3:a:3152[B]:LYS:CD | 1.77 | 1.30 |
| 3:U:2969[B]:TYR:CZ | 3:d:3107[B]:LEU:CD1 | 2.07 | 1.30 |
| 3:U:3089[A]:HIS:HE1 | 3:U:3119[A]:HIS:NE2 | 1.21 | 1.30 |
| 3:C:3160[B]:SER:HB2 | 3:L:3150[B]:LYS:NZ | 1.33 | 1.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:1546:LYS:HB2 | 3:d:3001[B]:LYS:CE | 1.59 | 1.30 |
| 3:C:3160[B]:SER:CB | 3:L:3150[B]:LYS:HZ3 | 1.32 | 1.30 |
| 3:C:3163[B]:ASN:N | 3:L:3147[B]:GLU:OE1 | 1.62 | 1.30 |
| 3:I:2961[B]:HIS:HA | 3:R:2975[B]:PHE:CZ | 1.65 | 1.30 |
| 3:I:3150[B]:LYS:O | 3:R:3159[B]:SER:HA | 1.28 | 1.30 |
| 3:d:3089[B]:HIS:HE1 | 3:d:3119[B]:HIS:NE2 | 1.20 | 1.30 |
| 3:I:3150[B]:LYS:C | 3:R:3159[B]:SER:CA | 2.01 | 1.30 |
| 3:I:3161[B]:GLU:CG | 3:R:3079[B]:CYS:SG | 2.20 | 1.30 |
| 3:O:3169[B]:LYS:CG | 3:X:3148[B]:ILE:HG21 | 1.41 | 1.30 |
| 3:U:3254[B]:MET:HB3 | 3:d:3254[B]:MET:CA | 1.60 | 1.30 |
| 3:C:3153[B]:LYS:O | 3:L:3154[B]:PRO:HA | 1.31 | 1.29 |
| 3:F:2970[B]:PRO:CD | 3:a:2989[B]:HIS:NE2 | 1.92 | 1.29 |
| 3:F:2975[B]:PHE:C | 3:a:3253[B]:GLU:CB | 1.93 | 1.29 |
| 3:F:3149[B]:ASN:HB2 | 3:a:3163[B]:ASN:ND2 | 0.98 | 1.29 |
| 3:I:3159[B]:SER:CA | 3:R:3150[B]:LYS:HB3 | 1.55 | 1.29 |
| 3:O:2970[B]:PRO:HG2 | 3:X:2991[B]:LEU:N | 0.98 | 1.29 |
| 3:O:3153[B]:LYS:CG | 3:X:3176[B]:LYS:HD3 | 1.62 | 1.29 |
| 3:R:3089[A]:HIS:HE1 | 3:R:3119[A]:HIS:NE2 | 1.21 | 1.29 |
| 3:U:2971[B]:ASP:CA | 3:d:3090[B]:ASN:HD22 | 1.45 | 1.29 |
| 3:U:2975[B]:PHE:CE2 | 3:d:3254[B]:MET:HG3 | 1.66 | 1.29 |
| 3:U:3256[B]:TRP:HB2 | 3:d:2969[B]:TYR:CA | 1.60 | 1.29 |
| 3:F:3256[B]:TRP:HE1 | 3:a:2965[B]:LEU:CD1 | 1.45 | 1.29 |
| 3:I:2965[B]:LEU:N | 3:R:3221[B]:ALA:CB | 1.95 | 1.29 |
| 2:Z:2800:LYS:O | 3:a:3023[A]:ILE:CD1 | 1.80 | 1.29 |
| 3:C:3156[B]:MET:HB2 | 3:L:2982[B]:MET:SD | 1.70 | 1.29 |
| 3:F:3159[B]:SER:OG | 3:a:2984[B]:THR:HG21 | 1.19 | 1.29 |
| 3:U:3254[B]:MET:CA | 3:d:3254[B]:MET:HA | 1.60 | 1.29 |
| 3:F:3173[B]:THR:O | 3:a:3154[B]:PRO:HD3 | 1.30 | 1.29 |
| 3:F:3174[B]:GLY:N | 3:a:3154[B]:PRO:CB | 1.95 | 1.29 |
| 3:C:3161[B]:GLU:N | 3:L:2983[B]:VAL:HG21 | 1.45 | 1.29 |
| 3:U:3255[B]:PRO:HG2 | 3:d:3252[B]:TYR:CA | 1.62 | 1.29 |
| 3:X:3089[B]:HIS:HE1 | 3:X:3119[B]:HIS:NE2 | 1.20 | 1.29 |
| 3:C:2965[B]:LEU:CD2 | 3:L:3253[B]:GLU:OE1 | 1.74 | 1.28 |
| 3:I:2989[B]:HIS:CD2 | 3:R:2970[B]:PRO:N | 2.00 | 1.28 |
| 3:O:3101[B]:PRO:CB | 3:X:2971[B]:ASP:O | 1.77 | 1.28 |
| 3:C:3147[B]:GLU:HG2 | 3:L:3161[B]:GLU:CA | 1.52 | 1.28 |
| 3:C:3159[B]:SER:CB | 3:L:2984[B]:THR:CG2 | 2.12 | 1.28 |
| 3:F:2969[B]:TYR:CD1 | 3:a:2961[B]:HIS:CG | 1.98 | 1.28 |
| 3:F:2970[B]:PRO:N | 3:a:2989[B]:HIS:NE2 | 1.82 | 1.28 |
| 2:W:2868:GLU:HG2 | 3:X:2932[A]:PRO:O | 1.22 | 1.28 |
| 3:O:3141[A]:TYR:HD2 | 3:O:3142[A]:ASN:N | 1.32 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3257[B]:ALA:H | 3:d:2968[B]:GLN:CA | 1.44 | 1.28 |
| 3:F:3153[B]:LYS:HD2 | 3:a:3155[B]:MET:CB | 1.63 | 1.28 |
| 3:I:3196[A]:THR:CB | 1:J:416:ASN:HD22 | 1.46 | 1.28 |
| 3:R:3141[B]:TYR:HD2 | 3:R:3142[B]:ASN:N | 1.32 | 1.28 |
| 3:C:2982[B]:MET:CG | 3:L:3156[B]:MET:CB | 2.06 | 1.28 |
| 3:I:3221[B]:ALA:HB1 | 3:R:2964[B]:PRO:C | 1.56 | 1.28 |
| 3:O:3038[B]:ILE:HG12 | 3:X:2969[B]:TYR:OH | 1.22 | 1.28 |
| 3:U:3141[B]:TYR:HD2 | 3:U:3142[B]:ASN:N | 1.32 | 1.28 |
| 3:F:3159[B]:SER:HA | 3:a:3150[B]:LYS:O | 1.34 | 1.27 |
| 3:I:3173[B]:THR:OG1 | 3:R:3173[B]:THR:HG23 | 1.16 | 1.27 |
| 3:U:3152[B]:LYS:HB2 | 3:d:3154[B]:PRO:CA | 1.63 | 1.27 |
| 3:U:3152[B]:LYS:HA | 3:d:3152[B]:LYS:O | 1.21 | 1.27 |
| 3:X:3141[B]:TYR:HD2 | 3:X:3142[B]:ASN:N | 1.32 | 1.27 |
| 3:C:2983[B]:VAL:CG2 | 3:L:3161[B]:GLU:H | 1.46 | 1.27 |
| 3:C:3154[B]:PRO:CD | 3:L:3174[B]:GLY:CA | 2.10 | 1.27 |
| 3:I:2975[B]:PHE:O | 3:R:3253[B]:GLU:HB2 | 1.13 | 1.27 |
| 3:I:3149[B]:ASN:OD1 | 3:R:3169[B]:LYS:CE | 1.83 | 1.27 |
| 3:I:3173[B]:THR:CG2 | 3:R:3173[B]:THR:OG1 | 1.80 | 1.27 |
| 3:I:3248[B]:LEU:CB | 3:R:2972[B]:GLY:O | 1.81 | 1.27 |
| 3:O:3163[B]:ASN:HB2 | 3:X:3149[B]:ASN:CA | 1.62 | 1.27 |
| 3:C:3154[B]:PRO:CG | 3:L:3174[B]:GLY:HA2 | 1.64 | 1.27 |
| 3:F:3251[B]:ASP:HB3 | 3:a:3251[B]:ASP:CB | 0.80 | 1.27 |
| 3:I:3150[B]:LYS:HB3 | 3:R:3159[B]:SER:CA | 1.48 | 1.27 |
| 3:L:3141[B]:TYR:HD2 | 3:L:3142[B]:ASN:N | 1.32 | 1.27 |
| 3:O:3141[B]:TYR:HD2 | 3:O:3142[B]:ASN:N | 1.32 | 1.27 |
| 3:R:3141[A]:TYR:HD2 | 3:R:3142[A]:ASN:N | 1.32 | 1.27 |
| 3:C:2972[B]:GLY:O | 3:L:3090[B]:ASN:ND2 | 1.67 | 1.27 |
| 3:C:3089[A]:HIS:HE1 | 3:C:3119[A]:HIS:NE2 | 1.21 | 1.27 |
| 3:O:2967[B]:CYS:SG | 3:X:3153[B]:LYS:HB3 | 1.74 | 1.27 |
| 3:I:3141[A]:TYR:HD2 | 3:I:3142[A]:ASN:N | 1.32 | 1.27 |
| 3:U:2965[B]:LEU:CD1 | 3:d:3221[B]:ALA:H | 1.47 | 1.27 |
| 3:U:3169[B]:LYS:CE | 3:d:3147[B]:GLU:HA | 1.64 | 1.27 |
| 3:U:3254[B]:MET:CE | 3:d:3254[B]:MET:CE | 1.92 | 1.27 |
| 3:F:3256[B]:TRP:CB | 3:a:2966[B]:SER:HA | 1.63 | 1.26 |
| 3:O:3158[B]:PHE:O | 3:X:3148[B]:ILE:HG22 | 1.22 | 1.26 |
| 3:C:3154[B]:PRO:CB | 3:L:3174[B]:GLY:HA3 | 1.65 | 1.26 |
| 3:L:3141[A]:TYR:HD2 | 3:L:3142[A]:ASN:N | 1.32 | 1.26 |
| 1:S:416:ASN:OD1 | 3:X:3196[A]:THR:HG21 | 1.18 | 1.26 |
| 3:U:3082[B]:GLU:OE1 | 3:d:2970[B]:PRO:HB3 | 1.29 | 1.26 |
| 3:C:3141[A]:TYR:HD2 | 3:C:3142[A]:ASN:N | 1.32 | 1.26 |
| 3:C:3149[B]:ASN:HD22 | 3:L:3163[B]:ASN:ND2 | 1.34 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3163[B]:ASN:ND2 | 3:R:3149[B]:ASN:HB2 | 1.50 | 1.26 |
| 3:O:3040[B]:VAL:HG21 | 3:X:2969[B]:TYR:CD1 | 1.68 | 1.26 |
| 3:U:3141[A]:TYR:HD2 | 3:U:3142[A]:ASN:N | 1.32 | 1.26 |
| 3:a:3141[A]:TYR:HD2 | 3:a:3142[A]:ASN:N | 1.32 | 1.26 |
| 3:C:2982[B]:MET:HG3 | 3:L:3156[B]:MET:SD | 1.75 | 1.26 |
| 3:C:3090[B]:ASN:ND2 | 3:L:2972[B]:GLY:HA3 | 1.46 | 1.26 |
| 3:C:3147[B]:GLU:OE1 | 3:L:3163[B]:ASN:N | 1.67 | 1.26 |
| 3:I:3153[B]:LYS:CG | 3:R:3155[B]:MET:HB2 | 1.64 | 1.26 |
| 3:O:2976[B]:ALA:O | 3:X:3154[B]:PRO:CG | 1.83 | 1.26 |
| 3:O:3272[A]:HIS:NE2 | 1:P:1542:ARG:NH2 | 1.84 | 1.26 |
| 3:C:2978[B]:CYS:N | 3:L:3254[B]:MET:CB | 1.95 | 1.26 |
| 3:C:3024[A]:LEU:HD12 | 3:C:3025[A]:VAL:N | 1.51 | 1.26 |
| 3:C:3159[B]:SER:OG | 3:L:2984[B]:THR:CG2 | 1.83 | 1.26 |
| 3:I:2975[B]:PHE:CZ | 3:R:2961[B]:HIS:HA | 1.69 | 1.26 |
| 3:I:3221[B]:ALA:CB | 3:R:2964[B]:PRO:C | 2.08 | 1.26 |
| 3:O:2965[B]:LEU:CB | 3:X:3254[B]:MET:HE1 | 1.65 | 1.26 |
| 3:O:2969[B]:TYR:CG | 3:X:3158[B]:PHE:CE1 | 2.24 | 1.26 |
| 3:O:3109[B]:TYR:CD1 | 3:X:2970[B]:PRO:N | 2.03 | 1.26 |
| 3:a:3024[B]:LEU:HD12 | 3:a:3025[B]:VAL:N | 1.51 | 1.26 |
| 3:d:3141[A]:TYR:HD2 | 3:d:3142[A]:ASN:N | 1.32 | 1.26 |
| 3:d:3141[B]:TYR:HD2 | 3:d:3142[B]:ASN:N | 1.32 | 1.26 |
| 3:F:3120[B]:HIS:NE2 | 3:a:2969[B]:TYR:CE2 | 2.04 | 1.25 |
| 3:I:2961[B]:HIS:CG | 3:R:2969[B]:TYR:HD1 | 1.52 | 1.25 |
| 3:I:2982[B]:MET:SD | 3:R:3157[B]:PRO:HB3 | 1.75 | 1.25 |
| 3:O:3163[B]:ASN:HB3 | 3:X:3149[B]:ASN:N | 1.51 | 1.25 |
| 3:C:3152[B]:LYS:HB2 | 3:L:3172[B]:SER:N | 1.49 | 1.25 |
| 3:C:3153[B]:LYS:HZ3 | 3:L:2988[B]:TRP:CD1 | 1.53 | 1.25 |
| 3:F:2965[B]:LEU:CD1 | 3:a:3256[B]:TRP:HE1 | 1.48 | 1.25 |
| 3:F:3141[B]:TYR:HD2 | 3:F:3142[B]:ASN:N | 1.32 | 1.25 |
| 3:I:3024[A]:LEU:HD12 | 3:I:3025[A]:VAL:N | 1.51 | 1.25 |
| 3:O:3024[A]:LEU:HD12 | 3:O:3025[A]:VAL:N | 1.51 | 1.25 |
| 3:X:3141[A]:TYR:HD2 | 3:X:3142[A]:ASN:N | 1.32 | 1.25 |
| 3:a:3024[A]:LEU:HD12 | 3:a:3025[A]:VAL:N | 1.51 | 1.25 |
| 3:F:3169[B]:LYS:O | 3:a:3152[B]:LYS:HG3 | 1.35 | 1.25 |
| 3:L:3089[B]:HIS:HE1 | 3:L:3119[B]:HIS:NE2 | 1.21 | 1.25 |
| 3:O:3024[B]:LEU:HD12 | 3:O:3025[B]:VAL:N | 1.51 | 1.25 |
| 3:C:3255[B]:PRO:HB2 | 3:L:2959[B]:SER:O | 1.19 | 1.25 |
| 3:F:3174[B]:GLY:HA2 | 3:a:3154[B]:PRO:CG | 1.65 | 1.25 |
| 3:F:3256[B]:TRP:CE2 | 3:a:2965[B]:LEU:HB3 | 1.70 | 1.25 |
| 3:I:3172[B]:SER:N | 3:R:3152[B]:LYS:HB2 | 1.41 | 1.25 |
| 3:O:2963[B]:MET:HE1 | 3:X:2975[B]:PHE:CB | 1.65 | 1.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2965[B]:LEU:O | 3:L:3256[B]:TRP:O | 1.55 | 1.25 |
| 3:C:3169[B]:LYS:O | 3:L:3152[B]:LYS:HG3 | 1.37 | 1.25 |
| 3:F:3113[A]:ASP:OD2 | 3:F:3114[A]:PRO:HD2 | 1.07 | 1.25 |
| 3:F:3113[B]:ASP:OD2 | 3:F:3114[B]:PRO:HD2 | 1.07 | 1.25 |
| 3:F:3259[B]:ASP:HB3 | 3:a:3162[B]:ASP:CB | 1.65 | 1.25 |
| 3:I:3108[B]:HIS:CE1 | 3:R:3251[B]:ASP:OD1 | 1.88 | 1.25 |
| 3:I:3174[B]:GLY:HA2 | 3:R:3154[B]:PRO:CG | 1.67 | 1.25 |
| 3:O:2970[B]:PRO:CD | 3:X:2991[B]:LEU:CB | 2.07 | 1.25 |
| 3:O:3038[B]:ILE:HG21 | 3:X:2969[B]:TYR:CZ | 1.72 | 1.25 |
| 3:O:3101[B]:PRO:HB2 | 3:X:2971[B]:ASP:C | 1.60 | 1.25 |
| 3:O:3102[B]:TYR:N | 3:X:2971[B]:ASP:HA | 1.51 | 1.25 |
| 3:R:3113[A]:ASP:OD2 | 3:R:3114[A]:PRO:HD2 | 1.07 | 1.25 |
| 3:R:3113[B]:ASP:OD2 | 3:R:3114[B]:PRO:HD2 | 1.07 | 1.25 |
| 3:U:3160[B]:SER:OG | 3:d:3259[B]:ASP:HB3 | 1.24 | 1.25 |
| 3:a:3089[A]:HIS:HE1 | 3:a:3119[A]:HIS:NE2 | 1.21 | 1.25 |
| 3:a:3113[A]:ASP:OD2 | 3:a:3114[A]:PRO:HD2 | 1.07 | 1.25 |
| 3:d:3089[A]:HIS:HE1 | 3:d:3119[A]:HIS:NE2 | 1.21 | 1.25 |
| 3:C:2988[B]:TRP:CD1 | 3:L:3153[B]:LYS:HZ3 | 1.54 | 1.25 |
| 3:C:3159[B]:SER:OG | 3:L:2984[B]:THR:HG21 | 1.14 | 1.25 |
| 3:F:3141[A]:TYR:HD2 | 3:F:3142[A]:ASN:N | 1.32 | 1.25 |
| 3:O:2965[B]:LEU:CD1 | 3:X:2979[B]:GLN:CD | 1.92 | 1.25 |
| 3:U:3113[A]:ASP:OD2 | 3:U:3114[A]:PRO:HD2 | 1.07 | 1.25 |
| 3:U:3155[B]:MET:C | 3:d:3150[B]:LYS:HG3 | 1.42 | 1.25 |
| 3:U:3252[B]:TYR:CE2 | 3:d:3222[B]:ILE:HD13 | 1.71 | 1.25 |
| 1:Y:1616:LYS:CD | 3:d:3187[B]:TYR:CA | 2.15 | 1.25 |
| 3:C:3113[B]:ASP:OD2 | 3:C:3114[B]:PRO:HD2 | 1.07 | 1.24 |
| 3:I:3135[A]:LYS:CG | 3:I:3141[A]:TYR:HE1 | 1.50 | 1.24 |
| 3:I:3135[B]:LYS:CG | 3:I:3141[B]:TYR:HE1 | 1.51 | 1.24 |
| 3:I:3141[B]:TYR:HD2 | 3:I:3142[B]:ASN:N | 1.32 | 1.24 |
| 3:L:3113[A]:ASP:OD2 | 3:L:3114[A]:PRO:HD2 | 1.07 | 1.24 |
| 3:O:2970[B]:PRO:HD2 | 3:X:2991[B]:LEU:CD1 | 1.66 | 1.24 |
| 3:O:3158[B]:PHE:O | 3:X:3148[B]:ILE:CG2 | 1.85 | 1.24 |
| 3:C:3162[B]:ASP:OD2 | 3:L:3259[B]:ASP:N | 1.68 | 1.24 |
| 3:F:2967[B]:CYS:SG | 3:a:2982[B]:MET:HE2 | 1.71 | 1.24 |
| 3:I:3113[B]:ASP:OD2 | 3:I:3114[B]:PRO:HD2 | 1.07 | 1.24 |
| 3:I:3169[B]:LYS:CD | 3:R:3149[B]:ASN:OD1 | 1.85 | 1.24 |
| 3:I:3196[A]:THR:CB | 1:J:416:ASN:ND2 | 1.98 | 1.24 |
| 3:O:3135[B]:LYS:CG | 3:O:3141[B]:TYR:HE1 | 1.50 | 1.24 |
| 3:R:3024[B]:LEU:HD12 | 3:R:3025[B]:VAL:N | 1.51 | 1.24 |
| 1:Y:1546:LYS:CB | 3:d:3001[B]:LYS:HE3 | 1.66 | 1.24 |
| 3:F:2966[B]:SER:O | 3:a:3256[B]:TRP:HB3 | 1.25 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3154[B]:PRO:HG2 | 3:a:3155[B]:MET:SD | 1.78 | 1.24 |
| 3:L:3135[B]:LYS:CG | 3:L:3141[B]:TYR:HE1 | 1.51 | 1.24 |
| 3:U:3153[B]:LYS:CE | 3:d:2979[B]:GLN:HE22 | 1.48 | 1.24 |
| 3:U:3230[B]:PHE:HB2 | 3:U:3243[B]:GLY:CA | 1.68 | 1.24 |
| 3:X:3089[A]:HIS:HE1 | 3:X:3119[A]:HIS:NE2 | 1.21 | 1.24 |
| 3:C:3153[B]:LYS:HE2 | 3:L:3158[B]:PHE:CD2 | 1.66 | 1.24 |
| 3:I:2964[B]:PRO:C | 3:R:3221[B]:ALA:CB | 2.08 | 1.24 |
| 3:I:3089[B]:HIS:HE1 | 3:I:3119[B]:HIS:NE2 | 1.20 | 1.24 |
| 3:I:3230[A]:PHE:HB2 | 3:I:3243[A]:GLY:CA | 1.68 | 1.24 |
| 2:Q:2868:GLU:OE2 | 3:R:2932[A]:PRO:C | 1.80 | 1.24 |
| 3:R:3135[A]:LYS:CG | 3:R:3141[A]:TYR:HE1 | 1.50 | 1.24 |
| 3:X:3230[B]:PHE:HB2 | 3:X:3243[B]:GLY:CA | 1.68 | 1.24 |
| 3:a:3135[B]:LYS:CG | 3:a:3141[B]:TYR:HE1 | 1.51 | 1.24 |
| 3:C:3024[B]:LEU:HD12 | 3:C:3025[B]:VAL:N | 1.51 | 1.24 |
| 3:C:3160[B]:SER:HA | 3:L:2983[B]:VAL:CG2 | 1.67 | 1.24 |
| 3:F:3024[B]:LEU:HD12 | 3:F:3025[B]:VAL:N | 1.51 | 1.24 |
| 3:F:3157[B]:PRO:O | 3:a:3150[B]:LYS:HD3 | 1.14 | 1.24 |
| 3:I:3163[B]:ASN:CB | 3:R:3150[B]:LYS:CE | 2.14 | 1.24 |
| 3:L:3135[A]:LYS:CG | 3:L:3141[A]:TYR:HE1 | 1.50 | 1.24 |
| 3:U:2971[B]:ASP:HA | 3:d:3090[B]:ASN:ND2 | 1.52 | 1.24 |
| 1:Y:1616:LYS:CD | 3:d:3188[B]:ASP:N | 1.97 | 1.24 |
| 3:C:3090[B]:ASN:ND2 | 3:L:2972[B]:GLY:CA | 2.01 | 1.23 |
| 3:F:3174[B]:GLY:CA | 3:a:3154[B]:PRO:CB | 2.15 | 1.23 |
| 3:I:3161[B]:GLU:HB3 | 3:R:3079[B]:CYS:SG | 1.79 | 1.23 |
| 3:U:2965[B]:LEU:CB | 3:d:3220[B]:ARG:NH1 | 2.00 | 1.23 |
| 3:U:3135[A]:LYS:CG | 3:U:3141[A]:TYR:HE1 | 1.50 | 1.23 |
| 3:C:3135[B]:LYS:CG | 3:C:3141[B]:TYR:HE1 | 1.50 | 1.23 |
| 3:C:3248[B]:LEU:HD22 | 3:L:2971[B]:ASP:OD1 | 1.38 | 1.23 |
| 3:F:3089[A]:HIS:HE1 | 3:F:3119[A]:HIS:NE2 | 1.21 | 1.23 |
| 3:F:3256[B]:TRP:NE1 | 3:a:2965[B]:LEU:CB | 1.90 | 1.23 |
| 3:I:2961[B]:HIS:CG | 3:R:2975[B]:PHE:CZ | 2.26 | 1.23 |
| 3:I:3155[B]:MET:CB | 3:R:3153[B]:LYS:HD2 | 1.66 | 1.23 |
| 3:I:3160[B]:SER:OG | 3:R:2983[B]:VAL:N | 1.71 | 1.23 |
| 3:O:2969[B]:TYR:CD1 | 3:X:3158[B]:PHE:CD1 | 2.25 | 1.23 |
| 3:O:3113[B]:ASP:OD2 | 3:O:3114[B]:PRO:HD2 | 1.07 | 1.23 |
| 3:X:3113[B]:ASP:OD2 | 3:X:3114[B]:PRO:HD2 | 1.07 | 1.23 |
| 3:a:3141[B]:TYR:HD2 | 3:a:3142[B]:ASN:N | 1.32 | 1.23 |
| 3:d:3024[B]:LEU:HD12 | 3:d:3025[B]:VAL:N | 1.51 | 1.23 |
| 3:F:3298[A]:ASN:CB | 3:F:3300[A]:LEU:HD23 | 1.69 | 1.23 |
| 3:I:2982[B]:MET:CG | 3:R:2967[B]:CYS:SG | 2.27 | 1.23 |
| 3:I:3113[A]:ASP:OD2 | 3:I:3114[A]:PRO:HD2 | 1.07 | 1.23 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3173[B]:THR:O | 3:R:3154[B]:PRO:HD3 | 1.34 | 1.23 |
| 3:L:3024[A]:LEU:HD12 | 3:L:3025[A]:VAL:N | 1.51 | 1.23 |
| 3:L:3024[B]:LEU:HD12 | 3:L:3025[B]:VAL:N | 1.51 | 1.23 |
| 3:L:3217[A]:PHE:HE1 | 3:L:3230[A]:PHE:CZ | 1.57 | 1.23 |
| 3:X:3024[A]:LEU:HD12 | 3:X:3025[A]:VAL:N | 1.51 | 1.23 |
| 3:X:3298[A]:ASN:CB | 3:X:3300[A]:LEU:HD23 | 1.69 | 1.23 |
| 3:d:3230[B]:PHE:HB2 | 3:d:3243[B]:GLY:CA | 1.68 | 1.23 |
| 3:C:2969[B]:TYR:OH | 3:L:3120[B]:HIS:CD2 | 1.91 | 1.23 |
| 3:C:3141[B]:TYR:HD2 | 3:C:3142[B]:ASN:N | 1.32 | 1.23 |
| 3:F:2966[B]:SER:O | 3:a:3256[B]:TRP:CB | 1.84 | 1.23 |
| 3:F:3256[B]:TRP:HE1 | 3:a:2965[B]:LEU:CB | 1.49 | 1.23 |
| 3:F:3256[B]:TRP:HB3 | 3:a:2966[B]:SER:CA | 1.69 | 1.23 |
| 3:I:2969[B]:TYR:HD1 | 3:R:2961[B]:HIS:CD2 | 1.50 | 1.23 |
| 3:I:2970[B]:PRO:HD3 | 3:R:2989[B]:HIS:CG | 1.71 | 1.23 |
| 3:I:3107[B]:LEU:CD1 | 3:R:2975[B]:PHE:HD1 | 1.50 | 1.23 |
| 3:I:3163[B]:ASN:HB2 | 3:R:3150[B]:LYS:CE | 1.67 | 1.23 |
| 3:O:3135[A]:LYS:CG | 3:O:3141[A]:TYR:HE1 | 1.51 | 1.23 |
| 3:O:3298[B]:ASN:CB | 3:O:3300[B]:LEU:HD23 | 1.69 | 1.23 |
| 3:R:3217[A]:PHE:HE1 | 3:R:3230[A]:PHE:CZ | 1.57 | 1.23 |
| 3:R:3217[B]:PHE:HE1 | 3:R:3230[B]:PHE:CZ | 1.57 | 1.23 |
| 3:U:3298[B]:ASN:CB | 3:U:3300[B]:LEU:HD23 | 1.69 | 1.23 |
| 3:X:3024[B]:LEU:HD12 | 3:X:3025[B]:VAL:N | 1.51 | 1.23 |
| 3:X:3135[A]:LYS:CG | 3:X:3141[A]:TYR:HE1 | 1.51 | 1.23 |
| 3:C:2965[B]:LEU:HD21 | 3:L:3253[B]:GLU:CD | 1.41 | 1.23 |
| 3:C:2970[B]:PRO:HD2 | 9:C:3401[B]:CUO:O1 | 1.36 | 1.23 |
| 3:C:3113[A]:ASP:OD2 | 3:C:3114[A]:PRO:HD2 | 1.07 | 1.23 |
| 3:F:2975[B]:PHE:CD1 | 3:a:3107[B]:LEU:CD1 | 2.02 | 1.23 |
| 3:F:3157[B]:PRO:O | 3:a:3150[B]:LYS:CE | 1.87 | 1.23 |
| 3:L:3113[B]:ASP:OD2 | 3:L:3114[B]:PRO:HD2 | 1.07 | 1.23 |
| 3:O:3113[A]:ASP:OD2 | 3:O:3114[A]:PRO:HD2 | 1.07 | 1.23 |
| 3:R:3298[B]:ASN:CB | 3:R:3300[B]:LEU:HD23 | 1.69 | 1.23 |
| 3:d:3135[B]:LYS:CG | 3:d:3141[B]:TYR:HE1 | 1.50 | 1.23 |
| 3:C:2982[B]:MET:HB2 | 3:L:3156[B]:MET:SD | 1.79 | 1.22 |
| 3:F:2966[B]:SER:C | 3:a:3256[B]:TRP:CG | 2.17 | 1.22 |
| 3:O:3108[B]:HIS:C | 3:X:2970[B]:PRO:HD3 | 1.32 | 1.22 |
| 3:R:2979[B]:GLN:HG2 | 3:R:3155[B]:MET:CE | 1.69 | 1.22 |
| 3:a:2979[A]:GLN:HG2 | 3:a:3155[A]:MET:CE | 1.69 | 1.22 |
| 3:d:3135[A]:LYS:CG | 3:d:3141[A]:TYR:HE1 | 1.50 | 1.22 |
| 3:C:3154[B]:PRO:HB3 | 3:L:3174[B]:GLY:CA | 1.69 | 1.22 |
| 3:C:3156[B]:MET:HE2 | 3:L:2979[B]:GLN:CB | 1.64 | 1.22 |
| 3:F:3024[A]:LEU:HD12 | 3:F:3025[A]:VAL:N | 1.51 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3230[A]:PHE:HB2 | 3:F:3243[A]:GLY:CA | 1.68 | 1.22 |
| 3:I:2979[A]:GLN:HG2 | 3:I:3155[A]:MET:CE | 1.69 | 1.22 |
| 3:I:3163[B]:ASN:N | 3:R:3147[B]:GLU:OE1 | 1.69 | 1.22 |
| 3:L:3298[B]:ASN:CB | 3:L:3300[B]:LEU:HD23 | 1.69 | 1.22 |
| 3:O:3135[B]:LYS:CG | 3:O:3141[B]:TYR:CE1 | 2.23 | 1.22 |
| 3:O:3217[B]:PHE:HE1 | 3:O:3230[B]:PHE:CZ | 1.57 | 1.22 |
| 3:R:3135[B]:LYS:CG | 3:R:3141[B]:TYR:HE1 | 1.50 | 1.22 |
| 3:U:3024[A]:LEU:HD12 | 3:U:3025[A]:VAL:N | 1.51 | 1.22 |
| 3:a:2979[B]:GLN:HG2 | 3:a:3155[B]:MET:CE | 1.69 | 1.22 |
| 3:a:3217[B]:PHE:HE1 | 3:a:3230[B]:PHE:CZ | 1.57 | 1.22 |
| 3:d:3113[B]:ASP:OD2 | 3:d:3114[B]:PRO:HD2 | 1.07 | 1.22 |
| 3:d:3230[A]:PHE:HB2 | 3:d:3243[A]:GLY:CA | 1.68 | 1.22 |
| 3:d:3298[A]:ASN:CB | 3:d:3300[A]:LEU:HD23 | 1.69 | 1.22 |
| 3:C:2979[A]:GLN:HG2 | 3:C:3155[A]:MET:CE | 1.69 | 1.22 |
| 3:C:3153[B]:LYS:NZ | 3:L:3158[B]:PHE:CD2 | 2.07 | 1.22 |
| 3:F:2979[A]:GLN:HG2 | 3:F:3155[A]:MET:CE | 1.69 | 1.22 |
| 3:I:2969[B]:TYR:CD1 | 3:R:2961[B]:HIS:CG | 2.27 | 1.22 |
| 3:I:3024[B]:LEU:HD12 | 3:I:3025[B]:VAL:N | 1.51 | 1.22 |
| 3:I:3149[B]:ASN:CB | 3:R:3163[B]:ASN:HD21 | 1.41 | 1.22 |
| 3:I:3259[B]:ASP:CB | 3:R:3162[B]:ASP:HB3 | 1.70 | 1.22 |
| 3:I:3298[B]:ASN:CB | 3:I:3300[B]:LEU:HD23 | 1.69 | 1.22 |
| 3:L:2979[B]:GLN:HG2 | 3:L:3155[B]:MET:CE | 1.69 | 1.22 |
| 3:L:3230[B]:PHE:HB2 | 3:L:3243[B]:GLY:CA | 1.68 | 1.22 |
| 3:O:3160[B]:SER:HB3 | 3:X:3149[B]:ASN:OD1 | 1.31 | 1.22 |
| 3:O:3217[A]:PHE:HE1 | 3:O:3230[A]:PHE:CZ | 1.57 | 1.22 |
| 3:O:3230[A]:PHE:HB2 | 3:O:3243[A]:GLY:CA | 1.68 | 1.22 |
| 3:O:3230[B]:PHE:HB2 | 3:O:3243[B]:GLY:CA | 1.68 | 1.22 |
| 3:U:2979[B]:GLN:HG2 | 3:U:3155[B]:MET:CE | 1.69 | 1.22 |
| 3:U:3135[A]:LYS:CG | 3:U:3141[A]:TYR:CE1 | 2.23 | 1.22 |
| 3:X:3217[B]:PHE:HE1 | 3:X:3230[B]:PHE:CZ | 1.57 | 1.22 |
| 3:a:3135[A]:LYS:CG | 3:a:3141[A]:TYR:HE1 | 1.50 | 1.22 |
| 3:d:3024[A]:LEU:HD12 | 3:d:3025[A]:VAL:N | 1.51 | 1.22 |
| 3:C:2972[B]:GLY:C | 3:L:3090[B]:ASN:ND2 | 1.96 | 1.22 |
| 3:C:3298[A]:ASN:CB | 3:C:3300[A]:LEU:HD23 | 1.69 | 1.22 |
| 3:F:3230[B]:PHE:HB2 | 3:F:3243[B]:GLY:CA | 1.68 | 1.22 |
| 3:I:3135[A]:LYS:CG | 3:I:3141[A]:TYR:CE1 | 2.23 | 1.22 |
| 3:O:3298[A]:ASN:CB | 3:O:3300[A]:LEU:HD23 | 1.69 | 1.22 |
| 3:U:3135[B]:LYS:CG | 3:U:3141[B]:TYR:HE1 | 1.51 | 1.22 |
| 3:U:3173[B]:THR:HG23 | 3:d:3152[B]:LYS:C | 1.56 | 1.22 |
| 3:X:3135[B]:LYS:CG | 3:X:3141[B]:TYR:HE1 | 1.50 | 1.22 |
| 3:C:2974[B]:ALA:CB | 3:L:3249[B]:GLY:HA2 | 1.52 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3090[B]:ASN:CG | 3:L:2972[B]:GLY:HA3 | 1.61 | 1.22 |
| 3:C:3135[A]:LYS:CG | 3:C:3141[A]:TYR:HE1 | 1.50 | 1.22 |
| 3:C:3135[B]:LYS:CG | 3:C:3141[B]:TYR:CE1 | 2.23 | 1.22 |
| 3:F:3160[B]:SER:CB | 3:a:3150[B]:LYS:NZ | 2.03 | 1.22 |
| 3:F:3217[A]:PHE:HE1 | 3:F:3230[A]:PHE:CZ | 1.57 | 1.22 |
| 3:I:3169[B]:LYS:CG | 3:R:3149[B]:ASN:OD1 | 1.87 | 1.22 |
| 3:L:3217[B]:PHE:HE1 | 3:L:3230[B]:PHE:CZ | 1.57 | 1.22 |
| 3:O:2976[B]:ALA:N | 3:X:3156[B]:MET:CG | 2.00 | 1.22 |
| 2:Q:2868:GLU:OE2 | 3:R:2932[A]:PRO:O | 1.58 | 1.22 |
| 3:R:2979[A]:GLN:HG2 | 3:R:3155[A]:MET:CE | 1.69 | 1.22 |
| 3:R:3135[A]:LYS:CG | 3:R:3141[A]:TYR:CE1 | 2.23 | 1.22 |
| 3:U:2979[A]:GLN:HG2 | 3:U:3155[A]:MET:CE | 1.69 | 1.22 |
| 3:a:3113[B]:ASP:OD2 | 3:a:3114[B]:PRO:HD2 | 1.07 | 1.22 |
| 3:a:3230[A]:PHE:HB2 | 3:a:3243[A]:GLY:CA | 1.68 | 1.22 |
| 3:a:3298[A]:ASN:CB | 3:a:3300[A]:LEU:HD23 | 1.69 | 1.22 |
| 3:C:2964[B]:PRO:O | 3:L:3255[B]:PRO:CB | 1.86 | 1.21 |
| 3:C:3135[A]:LYS:CG | 3:C:3141[A]:TYR:CE1 | 2.23 | 1.21 |
| 3:F:3135[A]:LYS:CG | 3:F:3141[A]:TYR:HE1 | 1.51 | 1.21 |
| 3:I:2982[B]:MET:SD | 3:R:3157[B]:PRO:CB | 2.28 | 1.21 |
| 3:I:3217[B]:PHE:HE1 | 3:I:3230[B]:PHE:CZ | 1.57 | 1.21 |
| 3:I:3230[B]:PHE:HB2 | 3:I:3243[B]:GLY:CA | 1.68 | 1.21 |
| 3:O:3163[B]:ASN:CB | 3:X:3149[B]:ASN:CA | 2.18 | 1.21 |
| 3:R:3024[A]:LEU:HD12 | 3:R:3025[A]:VAL:N | 1.51 | 1.21 |
| 3:U:3113[B]:ASP:OD2 | 3:U:3114[B]:PRO:HD2 | 1.07 | 1.21 |
| 3:U:3176[B]:LYS:CD | 3:d:3152[B]:LYS:HD2 | 1.68 | 1.21 |
| 3:U:3217[A]:PHE:HE1 | 3:U:3230[A]:PHE:CZ | 1.57 | 1.21 |
| 3:U:3230[A]:PHE:HB2 | 3:U:3243[A]:GLY:CA | 1.68 | 1.21 |
| 3:X:3230[A]:PHE:HB2 | 3:X:3243[A]:GLY:CA | 1.68 | 1.21 |
| 3:a:3230[B]:PHE:HB2 | 3:a:3243[B]:GLY:CA | 1.68 | 1.21 |
| 3:d:3217[B]:PHE:HE1 | 3:d:3230[B]:PHE:CZ | 1.57 | 1.21 |
| 3:I:2961[B]:HIS:CD2 | 3:R:2969[B]:TYR:CD1 | 2.13 | 1.21 |
| 3:L:3135[B]:LYS:CG | 3:L:3141[B]:TYR:CE1 | 2.23 | 1.21 |
| 3:R:3230[A]:PHE:HB2 | 3:R:3243[A]:GLY:CA | 1.68 | 1.21 |
| 3:U:3024[B]:LEU:HD12 | 3:U:3025[B]:VAL:N | 1.51 | 1.21 |
| 3:U:3155[B]:MET:N | 3:d:3150[B]:LYS:HG2 | 1.55 | 1.21 |
| 3:a:3135[B]:LYS:CG | 3:a:3141[B]:TYR:CE1 | 2.23 | 1.21 |
| 3:a:3217[A]:PHE:HE1 | 3:a:3230[A]:PHE:CZ | 1.57 | 1.21 |
| 3:F:2982[B]:MET:HE3 | 3:a:2977[B]:CYS:CB | 1.69 | 1.21 |
| 3:F:3089[B]:HIS:HE1 | 3:F:3119[B]:HIS:NE2 | 1.21 | 1.21 |
| 3:F:3135[B]:LYS:CG | 3:F:3141[B]:TYR:CE1 | 2.23 | 1.21 |
| 3:F:3298[B]:ASN:CB | 3:F:3300[B]:LEU:HD23 | 1.69 | 1.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3150[B]:LYS:HG2 | 3:R:3158[B]:PHE:CA | 1.45 | 1.21 |
| 3:L:3298[A]:ASN:CB | 3:L:3300[A]:LEU:HD23 | 1.69 | 1.21 |
| 3:R:3230[B]:PHE:HB2 | 3:R:3243[B]:GLY:CA | 1.68 | 1.21 |
| 3:X:3135[B]:LYS:CG | 3:X:3141[B]:TYR:CE1 | 2.23 | 1.21 |
| 3:d:3217[A]:PHE:HE1 | 3:d:3230[A]:PHE:CZ | 1.57 | 1.21 |
| 3:d:3298[B]:ASN:CB | 3:d:3300[B]:LEU:HD23 | 1.69 | 1.21 |
| 3:F:3135[A]:LYS:CG | 3:F:3141[A]:TYR:CE1 | 2.23 | 1.21 |
| 3:F:3135[B]:LYS:CG | 3:F:3141[B]:TYR:HE1 | 1.51 | 1.21 |
| 3:I:2975[B]:PHE:CZ | 3:R:2961[B]:HIS:CG | 2.29 | 1.21 |
| 3:I:2989[B]:HIS:CE1 | 3:R:2969[B]:TYR:HA | 1.74 | 1.21 |
| 3:O:3089[B]:HIS:HE1 | 3:O:3119[B]:HIS:NE2 | 1.21 | 1.21 |
| 3:U:3298[A]:ASN:CB | 3:U:3300[A]:LEU:HD23 | 1.69 | 1.21 |
| 3:X:2979[A]:GLN:HG2 | 3:X:3155[A]:MET:CE | 1.69 | 1.21 |
| 3:a:3293[B]:LYS:CB | 3:a:3294[B]:SER:HB2 | 1.71 | 1.21 |
| 3:a:3298[B]:ASN:CB | 3:a:3300[B]:LEU:HD23 | 1.69 | 1.21 |
| 3:C:2969[B]:TYR:CZ | 3:L:3120[B]:HIS:NE2 | 1.92 | 1.21 |
| 3:C:2979[B]:GLN:HG2 | 3:C:3155[B]:MET:CE | 1.69 | 1.21 |
| 3:C:2984[B]:THR:CG2 | 3:L:3159[B]:SER:CB | 2.15 | 1.21 |
| 3:C:3150[B]:LYS:CA | 3:L:3172[B]:SER:CB | 2.18 | 1.21 |
| 3:C:3217[B]:PHE:HE1 | 3:C:3230[B]:PHE:CZ | 1.57 | 1.21 |
| 3:C:3252[B]:TYR:CZ | 3:L:3223[B]:GLY:O | 1.94 | 1.21 |
| 3:C:3293[A]:LYS:CB | 3:C:3294[A]:SER:HB2 | 1.71 | 1.21 |
| 3:F:3108[B]:HIS:CE1 | 3:a:3251[B]:ASP:OD1 | 1.94 | 1.21 |
| 3:I:2982[B]:MET:CE | 3:R:2966[B]:SER:HB3 | 1.68 | 1.21 |
| 3:I:3217[A]:PHE:HE1 | 3:I:3230[A]:PHE:CZ | 1.57 | 1.21 |
| 3:L:3230[A]:PHE:HB2 | 3:L:3243[A]:GLY:CA | 1.68 | 1.21 |
| 3:O:2979[A]:GLN:HG2 | 3:O:3155[A]:MET:CE | 1.69 | 1.21 |
| 3:O:3135[A]:LYS:CG | 3:O:3141[A]:TYR:CE1 | 2.23 | 1.21 |
| 1:S:1617:LYS:HE2 | 3:X:3135[B]:LYS:NZ | 1.56 | 1.21 |
| 3:X:3113[A]:ASP:OD2 | 3:X:3114[A]:PRO:HD2 | 1.07 | 1.21 |
| 3:d:2979[B]:GLN:HG2 | 3:d:3155[B]:MET:CE | 1.69 | 1.21 |
| 3:d:3113[A]:ASP:OD2 | 3:d:3114[A]:PRO:HD2 | 1.07 | 1.21 |
| 3:d:3135[A]:LYS:CG | 3:d:3141[A]:TYR:CE1 | 2.23 | 1.21 |
| 3:C:3230[B]:PHE:HB2 | 3:C:3243[B]:GLY:CA | 1.68 | 1.20 |
| 3:C:3293[B]:LYS:CB | 3:C:3294[B]:SER:HB2 | 1.71 | 1.20 |
| 3:F:3147[B]:GLU:OE1 | 3:a:3162[B]:ASP:CA | 1.85 | 1.20 |
| 3:F:3217[B]:PHE:HE1 | 3:F:3230[B]:PHE:CZ | 1.57 | 1.20 |
| 3:F:3293[A]:LYS:CB | 3:F:3294[A]:SER:HB2 | 1.71 | 1.20 |
| 3:I:2979[B]:GLN:HG2 | 3:I:3155[B]:MET:CE | 1.69 | 1.20 |
| 3:O:2970[B]:PRO:CD | 3:X:2991[B]:LEU:HD13 | 1.69 | 1.20 |
| 3:O:3160[B]:SER:HA | 3:X:3151[B]:LEU:CD1 | 1.70 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3217[B]:PHE:HE1 | 3:U:3230[B]:PHE:CZ | 1.57 | 1.20 |
| 3:U:3255[B]:PRO:CG | 3:d:3252[B]:TYR:CA | 2.20 | 1.20 |
| 3:d:2979[A]:GLN:HG2 | 3:d:3155[A]:MET:CE | 1.69 | 1.20 |
| 3:C:3217[A]:PHE:HE1 | 3:C:3230[A]:PHE:CZ | 1.57 | 1.20 |
| 3:C:3256[B]:TRP:CZ2 | 3:L:2965[B]:LEU:HB3 | 1.75 | 1.20 |
| 3:C:3298[B]:ASN:CB | 3:C:3300[B]:LEU:HD23 | 1.69 | 1.20 |
| 3:F:2979[B]:GLN:HG2 | 3:F:3155[B]:MET:CE | 1.69 | 1.20 |
| 3:I:3293[B]:LYS:CB | 3:I:3294[B]:SER:HB2 | 1.71 | 1.20 |
| 3:I:3298[A]:ASN:CB | 3:I:3300[A]:LEU:HD23 | 1.69 | 1.20 |
| 3:O:2979[B]:GLN:HG2 | 3:O:3155[B]:MET:CE | 1.69 | 1.20 |
| 3:R:3089[B]:HIS:HE1 | 3:R:3119[B]:HIS:NE2 | 1.20 | 1.20 |
| 3:U:3104[B]:MET:HA | 3:U:3110[B]:THR:HG23 | 1.23 | 1.20 |
| 3:U:3293[B]:LYS:CB | 3:U:3294[B]:SER:HB2 | 1.71 | 1.20 |
| 1:Y:1616:LYS:O | 3:d:3187[B]:TYR:HB2 | 1.03 | 1.20 |
| 3:C:2982[B]:MET:SD | 3:L:3156[B]:MET:CB | 2.29 | 1.20 |
| 3:C:3230[A]:PHE:HB2 | 3:C:3243[A]:GLY:CA | 1.68 | 1.20 |
| 3:I:3135[B]:LYS:CG | 3:I:3141[B]:TYR:CE1 | 2.23 | 1.20 |
| 3:I:3293[A]:LYS:CB | 3:I:3294[A]:SER:HB2 | 1.71 | 1.20 |
| 3:L:3135[A]:LYS:CG | 3:L:3141[A]:TYR:CE1 | 2.23 | 1.20 |
| 3:O:3163[B]:ASN:CB | 3:X:3149[B]:ASN:HA | 1.71 | 1.20 |
| 3:O:3293[B]:LYS:CB | 3:O:3294[B]:SER:HB2 | 1.71 | 1.20 |
| 3:R:3135[B]:LYS:CG | 3:R:3141[B]:TYR:CE1 | 2.23 | 1.20 |
| 3:U:3089[B]:HIS:HE1 | 3:U:3119[B]:HIS:NE2 | 1.21 | 1.20 |
| 3:U:3135[B]:LYS:CG | 3:U:3141[B]:TYR:CE1 | 2.23 | 1.20 |
| 3:U:3253[B]:GLU:CA | 3:d:3255[B]:PRO:HG2 | 1.69 | 1.20 |
| 3:X:3217[A]:PHE:HE1 | 3:X:3230[A]:PHE:CZ | 1.57 | 1.20 |
| 2:Z:2800:LYS:O | 3:a:3023[A]:ILE:HD11 | 1.33 | 1.20 |
| 3:a:3135[A]:LYS:CG | 3:a:3141[A]:TYR:CE1 | 2.23 | 1.20 |
| 3:C:3169[B]:LYS:HG3 | 3:L:3149[B]:ASN:OD1 | 1.04 | 1.20 |
| 3:I:3120[B]:HIS:NE2 | 3:R:2969[B]:TYR:CE2 | 2.10 | 1.20 |
| 3:I:3155[B]:MET:HG3 | 3:R:3153[B]:LYS:C | 1.67 | 1.20 |
| 3:I:3160[B]:SER:CA | 3:R:2983[B]:VAL:H | 1.52 | 1.20 |
| 3:L:2979[A]:GLN:HG2 | 3:L:3155[A]:MET:CE | 1.69 | 1.20 |
| 3:O:3293[A]:LYS:CB | 3:O:3294[A]:SER:HB2 | 1.71 | 1.20 |
| 2:E:2868:GLU:HG3 | 3:F:2932[A]:PRO:O | 1.15 | 1.20 |
| 1:G:1636:ASN:OD1 | 6:r:1:NAG:H82 | 1.42 | 1.20 |
| 3:I:3150[B]:LYS:HD2 | 3:R:3160[B]:SER:N | 1.53 | 1.20 |
| 3:I:3163[B]:ASN:HD22 | 3:R:3150[B]:LYS:CG | 1.55 | 1.20 |
| 3:I:3255[B]:PRO:HD3 | 3:R:2962[B]:GLY:O | 1.41 | 1.20 |
| 3:R:3298[A]:ASN:CB | 3:R:3300[A]:LEU:HD23 | 1.69 | 1.20 |
| 3:X:3135[A]:LYS:CG | 3:X:3141[A]:TYR:CE1 | 2.23 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3293[B]:LYS:CB | 3:X:3294[B]:SER:HB2 | 1.71 | 1.20 |
| 3:X:3298[B]:ASN:CB | 3:X:3300[B]:LEU:HD23 | 1.69 | 1.20 |
| 3:d:3135[B]:LYS:CG | 3:d:3141[B]:TYR:CE1 | 2.23 | 1.20 |
| 3:F:3163[B]:ASN:CB | 3:a:3150[B]:LYS:HE3 | 1.70 | 1.19 |
| 3:F:3293[B]:LYS:HB2 | 3:F:3294[B]:SER:CB | 1.72 | 1.19 |
| 3:I:3293[B]:LYS:HB2 | 3:I:3294[B]:SER:CB | 1.72 | 1.19 |
| 3:L:3293[A]:LYS:CB | 3:L:3294[A]:SER:HB2 | 1.71 | 1.19 |
| 3:O:3293[A]:LYS:HB2 | 3:O:3294[A]:SER:CB | 1.72 | 1.19 |
| 3:U:3257[B]:ALA:N | 3:d:2968[B]:GLN:HA | 1.37 | 1.19 |
| 3:U:3293[A]:LYS:CB | 3:U:3294[A]:SER:HB2 | 1.71 | 1.19 |
| 3:d:3293[A]:LYS:HB2 | 3:d:3294[A]:SER:CB | 1.72 | 1.19 |
| 3:O:2968[B]:GLN:HB2 | 3:X:2988[B]:TRP:CB | 1.71 | 1.19 |
| 3:O:3161[B]:GLU:OE2 | 3:X:3151[B]:LEU:CD1 | 1.88 | 1.19 |
| 3:O:3255[B]:PRO:HG2 | 3:X:3163[B]:ASN:HB3 | 1.22 | 1.19 |
| 3:R:3293[A]:LYS:CB | 3:R:3294[A]:SER:HB2 | 1.71 | 1.19 |
| 3:C:3090[B]:ASN:ND2 | 3:L:2972[B]:GLY:C | 1.99 | 1.19 |
| 3:O:3109[B]:TYR:CD1 | 3:X:2970[B]:PRO:CD | 2.08 | 1.19 |
| 3:R:3293[B]:LYS:CB | 3:R:3294[B]:SER:HB2 | 1.71 | 1.19 |
| 3:U:3255[B]:PRO:HG2 | 3:d:3252[B]:TYR:O | 1.37 | 1.19 |
| 3:d:3293[B]:LYS:CB | 3:d:3294[B]:SER:HB2 | 1.71 | 1.19 |
| 3:C:3217[B]:PHE:CZ | 3:C:3230[B]:PHE:HE1 | 1.61 | 1.19 |
| 3:F:3293[B]:LYS:CB | 3:F:3294[B]:SER:HB2 | 1.71 | 1.19 |
| 3:I:3150[B]:LYS:CD | 3:R:3160[B]:SER:N | 2.05 | 1.19 |
| 3:R:3104[A]:MET:HA | 3:R:3110[A]:THR:HG23 | 1.23 | 1.19 |
| 3:d:3293[A]:LYS:CB | 3:d:3294[A]:SER:HB2 | 1.71 | 1.19 |
| 3:C:3174[B]:GLY:HA2 | 3:L:3154[B]:PRO:HD3 | 1.20 | 1.19 |
| 3:L:3217[A]:PHE:CZ | 3:L:3230[A]:PHE:HE1 | 1.61 | 1.19 |
| 3:O:3159[B]:SER:O | 3:X:3148[B]:ILE:HA | 1.39 | 1.19 |
| 3:U:3153[B]:LYS:HE2 | 3:d:2979[B]:GLN:NE2 | 1.58 | 1.19 |
| 3:U:3256[B]:TRP:CD2 | 3:d:2969[B]:TYR:CB | 2.25 | 1.19 |
| 3:X:3293[A]:LYS:HB2 | 3:X:3294[A]:SER:CB | 1.72 | 1.19 |
| 1:Y:1546:LYS:CB | 3:d:3001[B]:LYS:NZ | 2.06 | 1.19 |
| 3:a:3217[B]:PHE:CZ | 3:a:3230[B]:PHE:HE1 | 1.61 | 1.19 |
| 3:a:3293[B]:LYS:HB2 | 3:a:3294[B]:SER:CB | 1.72 | 1.19 |
| 3:d:3217[B]:PHE:CZ | 3:d:3230[B]:PHE:HE1 | 1.61 | 1.19 |
| 3:C:3251[B]:ASP:OD1 | 3:L:3108[B]:HIS:HE1 | 1.26 | 1.18 |
| 3:F:3163[B]:ASN:ND2 | 3:a:3149[B]:ASN:HB2 | 1.57 | 1.18 |
| 3:F:3217[A]:PHE:CZ | 3:F:3230[A]:PHE:HE1 | 1.61 | 1.18 |
| 3:I:3160[B]:SER:N | 3:R:3150[B]:LYS:CD | 2.04 | 1.18 |
| 3:L:3217[B]:PHE:CZ | 3:L:3230[B]:PHE:HE1 | 1.61 | 1.18 |
| 3:U:3153[B]:LYS:HB2 | 3:d:3154[B]:PRO:O | 1.39 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3169[B]:LYS:O | 3:d:3148[B]:ILE:CB | 1.91 | 1.18 |
| 3:U:3255[B]:PRO:HG3 | 3:d:3252[B]:TYR:HA | 1.22 | 1.18 |
| 3:a:3293[A]:LYS:CB | 3:a:3294[A]:SER:HB2 | 1.71 | 1.18 |
| 3:C:2985[B]:PHE:CZ | 3:L:2970[B]:PRO:CA | 1.80 | 1.18 |
| 3:C:3104[B]:MET:HA | 3:C:3110[B]:THR:HG23 | 1.23 | 1.18 |
| 3:C:3156[B]:MET:HB2 | 3:L:2982[B]:MET:CG | 1.73 | 1.18 |
| 3:C:3293[A]:LYS:HB2 | 3:C:3294[A]:SER:CB | 1.72 | 1.18 |
| 3:L:3293[B]:LYS:CB | 3:L:3294[B]:SER:HB2 | 1.71 | 1.18 |
| 3:O:2969[B]:TYR:OH | 3:X:2994[B]:LYS:CB | 1.92 | 1.18 |
| 3:O:3104[B]:MET:HA | 3:O:3110[B]:THR:HG23 | 1.23 | 1.18 |
| 3:R:3217[A]:PHE:CZ | 3:R:3230[A]:PHE:HE1 | 1.61 | 1.18 |
| 3:X:3293[A]:LYS:CB | 3:X:3294[A]:SER:HB2 | 1.71 | 1.18 |
| 3:F:2965[B]:LEU:N | 3:a:3221[B]:ALA:HB1 | 0.86 | 1.18 |
| 3:F:2982[B]:MET:CE | 3:a:2966[B]:SER:HB3 | 1.73 | 1.18 |
| 3:I:3159[B]:SER:HA | 3:R:3150[B]:LYS:O | 1.38 | 1.18 |
| 3:R:3293[A]:LYS:HB2 | 3:R:3294[A]:SER:CB | 1.72 | 1.18 |
| 1:S:416:ASN:OD1 | 3:X:3196[A]:THR:CB | 1.90 | 1.18 |
| 3:U:3156[B]:MET:HE1 | 3:d:2982[B]:MET:CG | 1.71 | 1.18 |
| 3:U:3217[A]:PHE:CZ | 3:U:3230[A]:PHE:HE1 | 1.61 | 1.18 |
| 3:a:3104[B]:MET:HA | 3:a:3110[B]:THR:HG23 | 1.24 | 1.18 |
| 3:C:3255[B]:PRO:HB3 | 3:L:2964[B]:PRO:O | 1.40 | 1.18 |
| 3:C:3255[B]:PRO:CB | 3:L:2959[B]:SER:O | 1.90 | 1.18 |
| 3:C:3293[B]:LYS:HB2 | 3:C:3294[B]:SER:CB | 1.72 | 1.18 |
| 3:F:3152[B]:LYS:CB | 3:a:3172[B]:SER:H | 1.57 | 1.18 |
| 3:F:3217[B]:PHE:CZ | 3:F:3230[B]:PHE:HE1 | 1.61 | 1.18 |
| 3:I:3256[B]:TRP:HE1 | 3:R:2965[B]:LEU:CB | 1.44 | 1.18 |
| 3:O:3153[B]:LYS:HG2 | 3:X:3176[B]:LYS:HE3 | 1.20 | 1.18 |
| 3:O:3154[B]:PRO:CG | 3:X:3175[B]:TYR:HB3 | 1.74 | 1.18 |
| 3:R:3293[B]:LYS:HB2 | 3:R:3294[B]:SER:CB | 1.72 | 1.18 |
| 3:d:3293[B]:LYS:HB2 | 3:d:3294[B]:SER:CB | 1.73 | 1.18 |
| 3:C:3160[B]:SER:OG | 3:L:2983[B]:VAL:CG2 | 1.92 | 1.18 |
| 3:F:2968[B]:GLN:HE21 | 3:a:3086[B]:GLU:CG | 1.51 | 1.18 |
| 3:F:3160[B]:SER:CB | 3:a:3150[B]:LYS:HZ3 | 1.54 | 1.18 |
| 3:I:3163[B]:ASN:HB3 | 3:R:3150[B]:LYS:HE3 | 1.24 | 1.18 |
| 3:L:3293[A]:LYS:HB2 | 3:L:3294[A]:SER:CB | 1.72 | 1.18 |
| 2:Z:2867:PRO:HG3 | 3:a:2932[A]:PRO:CG | 1.66 | 1.18 |
| 3:d:3217[A]:PHE:CZ | 3:d:3230[A]:PHE:HE1 | 1.61 | 1.18 |
| 3:C:3135[B]:LYS:HG3 | 3:C:3141[B]:TYR:CE1 | 1.80 | 1.17 |
| 3:C:3217[A]:PHE:CZ | 3:C:3230[A]:PHE:HE1 | 1.61 | 1.17 |
| 3:F:2982[B]:MET:HE3 | 3:a:2977[B]:CYS:SG | 1.84 | 1.17 |
| 3:I:2989[B]:HIS:NE2 | 3:R:2969[B]:TYR:C | 2.01 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3135[B]:LYS:HG3 | 3:I:3141[B]:TYR:CE1 | 1.80 | 1.17 |
| 3:I:3221[B]:ALA:HB3 | 3:R:2964[B]:PRO:CB | 1.74 | 1.17 |
| 3:I:3248[B]:LEU:HB3 | 3:R:2972[B]:GLY:O | 1.38 | 1.17 |
| 3:O:3217[A]:PHE:CZ | 3:O:3230[A]:PHE:HE1 | 1.61 | 1.17 |
| 3:O:3217[B]:PHE:CZ | 3:O:3230[B]:PHE:HE1 | 1.61 | 1.17 |
| 3:O:3293[B]:LYS:HB2 | 3:O:3294[B]:SER:CB | 1.72 | 1.17 |
| 3:U:3293[A]:LYS:HB2 | 3:U:3294[A]:SER:CB | 1.72 | 1.17 |
| 3:U:3293[B]:LYS:HB2 | 3:U:3294[B]:SER:CB | 1.72 | 1.17 |
| 3:d:3217[B]:PHE:CE1 | 3:d:3230[B]:PHE:CZ | 2.32 | 1.17 |
| 3:C:2974[B]:ALA:O | 3:L:3107[B]:LEU:HD13 | 1.42 | 1.17 |
| 3:I:3293[A]:LYS:HB2 | 3:I:3294[A]:SER:CB | 1.72 | 1.17 |
| 3:R:3217[B]:PHE:CZ | 3:R:3230[B]:PHE:HE1 | 1.61 | 1.17 |
| 3:U:3217[B]:PHE:CZ | 3:U:3230[B]:PHE:HE1 | 1.61 | 1.17 |
| 3:X:3217[B]:PHE:CE1 | 3:X:3230[B]:PHE:CZ | 2.32 | 1.17 |
| 1:Y:1546:LYS:CB | 3:d:3001[B]:LYS:CE | 2.19 | 1.17 |
| 3:a:3293[A]:LYS:HB2 | 3:a:3294[A]:SER:CB | 1.73 | 1.17 |
| 3:C:3154[B]:PRO:CG | 3:L:3174[B]:GLY:CA | 2.23 | 1.17 |
| 3:C:3160[B]:SER:CB | 3:L:2983[B]:VAL:HG23 | 1.72 | 1.17 |
| 3:C:3253[B]:GLU:HB2 | 3:L:2976[B]:ALA:N | 1.22 | 1.17 |
| 3:F:2970[B]:PRO:HA | 3:a:2985[B]:PHE:CZ | 1.79 | 1.17 |
| 3:F:2989[B]:HIS:CE1 | 3:a:2969[B]:TYR:HA | 1.59 | 1.17 |
| 3:F:3253[B]:GLU:HB2 | 3:a:2975[B]:PHE:C | 1.68 | 1.17 |
| 3:I:3153[B]:LYS:C | 3:R:3155[B]:MET:HG3 | 1.37 | 1.17 |
| 3:I:3217[B]:PHE:CZ | 3:I:3230[B]:PHE:HE1 | 1.61 | 1.17 |
| 3:L:2970[B]:PRO:HD2 | 9:L:3401[B]:CUO:O1 | 1.02 | 1.17 |
| 3:L:3217[B]:PHE:CE1 | 3:L:3230[B]:PHE:CZ | 2.32 | 1.17 |
| 3:O:3038[B]:ILE:HD13 | 3:X:2969[B]:TYR:CZ | 1.79 | 1.17 |
| 3:O:3158[B]:PHE:N | 3:X:3152[B]:LYS:HB2 | 1.60 | 1.17 |
| 3:R:3217[A]:PHE:CE1 | 3:R:3230[A]:PHE:CZ | 2.32 | 1.17 |
| 3:U:2970[B]:PRO:HA | 3:d:3086[B]:GLU:OE1 | 1.00 | 1.17 |
| 3:X:3104[A]:MET:HA | 3:X:3110[A]:THR:HG23 | 1.23 | 1.17 |
| 3:a:3217[A]:PHE:CZ | 3:a:3230[A]:PHE:HE1 | 1.61 | 1.17 |
| 3:a:3217[B]:PHE:CE1 | 3:a:3230[B]:PHE:CZ | 2.32 | 1.17 |
| 3:C:3159[B]:SER:OG | 3:L:3150[B]:LYS:O | 1.61 | 1.17 |
| 3:C:3163[B]:ASN:HB3 | 3:L:3149[B]:ASN:ND2 | 1.59 | 1.17 |
| 3:C:3217[B]:PHE:CE1 | 3:C:3230[B]:PHE:CZ | 2.32 | 1.17 |
| 3:F:3217[B]:PHE:CE1 | 3:F:3230[B]:PHE:CZ | 2.32 | 1.17 |
| 3:I:3089[A]:HIS:HE1 | 3:I:3119[A]:HIS:NE2 | 1.21 | 1.17 |
| 3:I:3160[B]:SER:N | 3:R:3150[B]:LYS:HD2 | 1.58 | 1.17 |
| 3:I:3160[B]:SER:HA | 3:R:2983[B]:VAL:H | 1.03 | 1.17 |
| 3:O:3255[B]:PRO:CG | 3:X:3163[B]:ASN:HB3 | 1.73 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3253[B]:GLU:CA | 3:d:3255[B]:PRO:CG | 2.20 | 1.17 |
| 3:X:3217[B]:PHE:CZ | 3:X:3230[B]:PHE:HE1 | 1.61 | 1.17 |
| 3:a:3135[A]:LYS:HG3 | 3:a:3141[A]:TYR:CE1 | 1.80 | 1.17 |
| 3:F:3135[B]:LYS:HG3 | 3:F:3141[B]:TYR:CE1 | 1.79 | 1.17 |
| 3:I:2966[B]:SER:CB | 3:R:3254[B]:MET:HG3 | 1.73 | 1.17 |
| 3:O:2970[B]:PRO:N | 3:X:2991[B]:LEU:HB2 | 1.59 | 1.17 |
| 3:O:3135[B]:LYS:HG3 | 3:O:3141[B]:TYR:CE1 | 1.80 | 1.17 |
| 3:X:3293[B]:LYS:HB2 | 3:X:3294[B]:SER:CB | 1.72 | 1.17 |
| 3:C:3090[B]:ASN:ND2 | 3:L:2972[B]:GLY:O | 1.75 | 1.16 |
| 3:C:3217[A]:PHE:CE1 | 3:C:3230[A]:PHE:CZ | 2.32 | 1.16 |
| 3:F:2961[B]:HIS:HA | 3:a:2975[B]:PHE:HZ | 1.10 | 1.16 |
| 3:F:3293[A]:LYS:HB2 | 3:F:3294[A]:SER:CB | 1.72 | 1.16 |
| 3:I:2969[B]:TYR:CD1 | 3:R:2961[B]:HIS:CD2 | 2.20 | 1.16 |
| 3:L:3217[A]:PHE:CE1 | 3:L:3230[A]:PHE:CZ | 2.32 | 1.16 |
| 3:O:2968[B]:GLN:CB | 3:X:2988[B]:TRP:CB | 2.22 | 1.16 |
| 3:O:3217[B]:PHE:CE1 | 3:O:3230[B]:PHE:CZ | 2.32 | 1.16 |
| 3:U:3135[A]:LYS:HG3 | 3:U:3141[A]:TYR:CE1 | 1.79 | 1.16 |
| 3:U:3135[B]:LYS:HG3 | 3:U:3141[B]:TYR:CE1 | 1.80 | 1.16 |
| 3:U:3153[B]:LYS:HB3 | 3:d:3153[B]:LYS:CD | 1.73 | 1.16 |
| 3:X:3217[A]:PHE:CE1 | 3:X:3230[A]:PHE:CZ | 2.33 | 1.16 |
| 3:X:3217[A]:PHE:CZ | 3:X:3230[A]:PHE:HE1 | 1.61 | 1.16 |
| 2:Z:2472:ASN:HB3 | 4:MA:1:NAG:H82 | 1.27 | 1.16 |
| 3:d:3217[A]:PHE:CE1 | 3:d:3230[A]:PHE:CZ | 2.32 | 1.16 |
| 3:C:2982[B]:MET:HG3 | 3:L:3156[B]:MET:CG | 1.75 | 1.16 |
| 3:F:3173[B]:THR:C | 3:a:3154[B]:PRO:CD | 2.17 | 1.16 |
| 2:H:2800:LYS:O | 3:I:3023[A]:ILE:HD11 | 1.42 | 1.16 |
| 3:I:3152[B]:LYS:HB2 | 3:R:3172[B]:SER:N | 1.15 | 1.16 |
| 3:O:3217[A]:PHE:CE1 | 3:O:3230[A]:PHE:CZ | 2.32 | 1.16 |
| 3:R:3217[B]:PHE:CE1 | 3:R:3230[B]:PHE:CZ | 2.32 | 1.16 |
| 3:U:3152[B]:LYS:CA | 3:d:3152[B]:LYS:O | 1.92 | 1.16 |
| 3:U:3170[B]:ALA:HA | 3:d:3148[B]:ILE:CG2 | 1.74 | 1.16 |
| 3:U:3217[A]:PHE:CE1 | 3:U:3230[A]:PHE:CZ | 2.32 | 1.16 |
| 3:U:3219[B]:LEU:O | 3:d:2971[B]:ASP:O | 1.62 | 1.16 |
| 3:U:3254[B]:MET:CB | 3:d:3254[B]:MET:CA | 2.18 | 1.16 |
| 3:C:2984[B]:THR:HG21 | 3:L:3159[B]:SER:OG | 1.01 | 1.16 |
| 3:C:3169[B]:LYS:CG | 3:L:3149[B]:ASN:OD1 | 1.94 | 1.16 |
| 3:F:2975[B]:PHE:O | 3:a:3253[B]:GLU:HB2 | 1.01 | 1.16 |
| 3:F:2983[B]:VAL:HG21 | 3:a:3161[B]:GLU:CA | 1.73 | 1.16 |
| 3:F:3196[B]:THR:N | 3:F:3199[B]:GLN:OE1 | 1.79 | 1.16 |
| 3:I:3169[B]:LYS:O | 3:R:3152[B]:LYS:HG3 | 1.01 | 1.16 |
| 3:I:3217[A]:PHE:CE1 | 3:I:3230[A]:PHE:CZ | 2.32 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3293[B]:LYS:HB2 | 3:L:3294[B]:SER:CB | 1.72 | 1.16 |
| 3:O:2969[B]:TYR:OH | 3:X:2994[B]:LYS:HB3 | 0.99 | 1.16 |
| 3:O:2970[B]:PRO:CB | 3:X:2991[B]:LEU:N | 2.09 | 1.16 |
| 3:O:3101[B]:PRO:C | 3:X:2971[B]:ASP:HA | 1.68 | 1.16 |
| 3:R:2960[B]:PHE:HD2 | 3:R:3157[B]:PRO:HG3 | 1.10 | 1.16 |
| 3:U:3170[B]:ALA:CA | 3:d:3148[B]:ILE:HG21 | 1.75 | 1.16 |
| 3:a:3135[B]:LYS:HG3 | 3:a:3141[B]:TYR:CE1 | 1.80 | 1.16 |
| 3:a:3217[A]:PHE:CE1 | 3:a:3230[A]:PHE:CZ | 2.32 | 1.16 |
| 3:C:2985[B]:PHE:CE2 | 3:L:2969[B]:TYR:C | 2.23 | 1.16 |
| 3:F:3255[B]:PRO:CD | 3:a:2962[B]:GLY:O | 1.94 | 1.16 |
| 3:I:3149[B]:ASN:CG | 3:R:3163[B]:ASN:ND2 | 2.04 | 1.16 |
| 3:R:2937[A]:ASN:HB2 | 3:R:3006[A]:LYS:HE2 | 1.28 | 1.16 |
| 3:U:2937[B]:ASN:HB2 | 3:U:3006[B]:LYS:HE2 | 1.28 | 1.16 |
| 3:a:3196[B]:THR:N | 3:a:3199[B]:GLN:OE1 | 1.79 | 1.16 |
| 3:C:2968[B]:GLN:O | 3:L:2985[B]:PHE:CD2 | 1.98 | 1.16 |
| 3:F:3154[B]:PRO:HA | 3:a:3153[B]:LYS:O | 1.46 | 1.16 |
| 3:F:3196[A]:THR:N | 3:F:3199[A]:GLN:OE1 | 1.79 | 1.16 |
| 3:I:3155[B]:MET:HG3 | 3:R:3154[B]:PRO:N | 1.38 | 1.16 |
| 3:O:3153[B]:LYS:CG | 3:X:3176[B]:LYS:CD | 2.22 | 1.16 |
| 3:R:3196[A]:THR:N | 3:R:3199[A]:GLN:OE1 | 1.79 | 1.16 |
| 3:R:3196[B]:THR:N | 3:R:3199[B]:GLN:OE1 | 1.79 | 1.16 |
| 3:U:3196[A]:THR:N | 3:U:3199[A]:GLN:OE1 | 1.79 | 1.16 |
| 3:U:3217[B]:PHE:CE1 | 3:U:3230[B]:PHE:CZ | 2.32 | 1.16 |
| 3:d:2937[A]:ASN:HB2 | 3:d:3006[A]:LYS:HE2 | 1.28 | 1.16 |
| 3:C:3079[B]:CYS:SG | 3:L:3161[B]:GLU:CD | 2.27 | 1.15 |
| 3:C:3104[A]:MET:HA | 3:C:3110[A]:THR:HG23 | 1.23 | 1.15 |
| 3:F:3135[A]:LYS:HG3 | 3:F:3141[A]:TYR:CE1 | 1.80 | 1.15 |
| 3:F:3154[B]:PRO:CD | 3:a:3155[B]:MET:SD | 2.34 | 1.15 |
| 3:F:3217[A]:PHE:CE1 | 3:F:3230[A]:PHE:CZ | 2.32 | 1.15 |
| 3:I:3104[B]:MET:HA | 3:I:3110[B]:THR:HG23 | 1.23 | 1.15 |
| 3:I:3217[A]:PHE:CZ | 3:I:3230[A]:PHE:HE1 | 1.61 | 1.15 |
| 3:O:3135[A]:LYS:HG3 | 3:O:3141[A]:TYR:CE1 | 1.80 | 1.15 |
| 3:R:3217[A]:PHE:CZ | 3:R:3230[A]:PHE:CE1 | 2.35 | 1.15 |
| 3:U:2960[A]:PHE:HD2 | 3:U:3157[A]:PRO:HG3 | 1.10 | 1.15 |
| 3:U:3162[B]:ASP:N | 3:d:3260[B]:ARG:NH1 | 1.93 | 1.15 |
| 3:d:3196[B]:THR:N | 3:d:3199[B]:GLN:OE1 | 1.79 | 1.15 |
| 3:d:3217[B]:PHE:CZ | 3:d:3230[B]:PHE:CE1 | 2.35 | 1.15 |
| 6:GA:1:NAG:H4 | 6:GA:2:NAG:O7 | 1.46 | 1.15 |
| 3:C:3253[B]:GLU:CB | 3:L:2976[B]:ALA:N | 1.95 | 1.15 |
| 3:C:3256[B]:TRP:CE2 | 3:L:2965[B]:LEU:HB3 | 1.77 | 1.15 |
| 3:I:3135[A]:LYS:HG3 | 3:I:3141[A]:TYR:CE1 | 1.79 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3196[B]:THR:N | 3:L:3199[B]:GLN:OE1 | 1.79 | 1.15 |
| 3:O:3089[A]:HIS:HE1 | 3:O:3119[A]:HIS:NE2 | 1.21 | 1.15 |
| 2:Q:2868:GLU:OE2 | 3:R:2933[A]:SER:N | 1.77 | 1.15 |
| 3:R:3135[B]:LYS:HG3 | 3:R:3141[B]:TYR:CE1 | 1.80 | 1.15 |
| 3:U:3217[A]:PHE:CZ | 3:U:3230[A]:PHE:CE1 | 2.35 | 1.15 |
| 3:X:2937[A]:ASN:HB2 | 3:X:3006[A]:LYS:HE2 | 1.28 | 1.15 |
| 3:X:3196[A]:THR:N | 3:X:3199[A]:GLN:OE1 | 1.79 | 1.15 |
| 1:Y:1616:LYS:O | 3:d:3187[B]:TYR:CB | 1.93 | 1.15 |
| 3:I:3150[B]:LYS:HG3 | 3:R:3163[B]:ASN:ND2 | 1.61 | 1.15 |
| 3:I:3154[B]:PRO:CG | 3:R:3155[B]:MET:SD | 2.34 | 1.15 |
| 3:L:3217[A]:PHE:CZ | 3:L:3230[A]:PHE:CE1 | 2.35 | 1.15 |
| 3:L:3217[B]:PHE:CZ | 3:L:3230[B]:PHE:CE1 | 2.35 | 1.15 |
| 3:U:3160[B]:SER:OG | 3:d:3259[B]:ASP:CB | 1.93 | 1.15 |
| 3:C:2937[B]:ASN:HB2 | 3:C:3006[B]:LYS:HE2 | 1.28 | 1.15 |
| 3:C:3196[A]:THR:N | 3:C:3199[A]:GLN:OE1 | 1.79 | 1.15 |
| 3:C:3222[B]:ILE:HD12 | 3:L:2963[B]:MET:HE1 | 1.27 | 1.15 |
| 3:F:3217[A]:PHE:CZ | 3:F:3230[A]:PHE:CE1 | 2.35 | 1.15 |
| 3:I:3161[B]:GLU:CB | 3:R:3079[B]:CYS:SG | 2.35 | 1.15 |
| 3:I:3217[B]:PHE:CZ | 3:I:3230[B]:PHE:CE1 | 2.35 | 1.15 |
| 3:L:3135[B]:LYS:HG3 | 3:L:3141[B]:TYR:CE1 | 1.80 | 1.15 |
| 3:L:3196[A]:THR:N | 3:L:3199[A]:GLN:OE1 | 1.79 | 1.15 |
| 3:R:3135[A]:LYS:HG3 | 3:R:3141[A]:TYR:CE1 | 1.80 | 1.15 |
| 3:R:3217[B]:PHE:CZ | 3:R:3230[B]:PHE:CE1 | 2.35 | 1.15 |
| 3:U:3086[B]:GLU:OE2 | 3:d:2970[B]:PRO:CG | 1.95 | 1.15 |
| 3:F:2961[B]:HIS:HA | 3:a:2975[B]:PHE:CZ | 1.82 | 1.15 |
| 3:F:3217[B]:PHE:CZ | 3:F:3230[B]:PHE:CE1 | 2.35 | 1.15 |
| 3:O:2976[B]:ALA:C | 3:X:3154[B]:PRO:HG2 | 1.64 | 1.15 |
| 3:O:3253[B]:GLU:OE1 | 3:X:3161[B]:GLU:OE1 | 1.62 | 1.15 |
| 3:X:3217[B]:PHE:CZ | 3:X:3230[B]:PHE:CE1 | 2.35 | 1.15 |
| 3:a:3217[B]:PHE:CZ | 3:a:3230[B]:PHE:CE1 | 2.35 | 1.15 |
| 3:d:2937[B]:ASN:HB2 | 3:d:3006[B]:LYS:HE2 | 1.28 | 1.15 |
| 3:d:3135[B]:LYS:HG3 | 3:d:3141[B]:TYR:CE1 | 1.79 | 1.15 |
| 3:C:2983[B]:VAL:HG23 | 3:L:3160[B]:SER:CB | 1.78 | 1.14 |
| 3:F:2937[A]:ASN:HB2 | 3:F:3006[A]:LYS:HE2 | 1.28 | 1.14 |
| 3:F:2960[B]:PHE:HD2 | 3:F:3157[B]:PRO:HG3 | 1.10 | 1.14 |
| 3:I:3256[B]:TRP:CE2 | 3:R:2965[B]:LEU:HB3 | 1.81 | 1.14 |
| 3:L:3135[A]:LYS:HG3 | 3:L:3141[A]:TYR:CE1 | 1.79 | 1.14 |
| 3:O:2973[B]:THR:HB | 3:X:3158[B]:PHE:HE2 | 1.11 | 1.14 |
| 3:U:2979[B]:GLN:NE2 | 3:d:3153[B]:LYS:NZ | 1.95 | 1.14 |
| 3:d:3196[A]:THR:N | 3:d:3199[A]:GLN:OE1 | 1.79 | 1.14 |
| 3:C:2959[B]:SER:O | 3:L:3255[B]:PRO:HB2 | 1.43 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3093[B]:HIS:CE1 | 3:L:2971[B]:ASP:HB3 | 1.42 | 1.14 |
| 3:F:3108[B]:HIS:NE2 | 3:a:3252[B]:TYR:N | 1.93 | 1.14 |
| 3:F:3155[B]:MET:HG3 | 3:a:3154[B]:PRO:N | 1.53 | 1.14 |
| 3:I:3150[B]:LYS:CE | 3:R:3163[B]:ASN:HB2 | 1.77 | 1.14 |
| 3:I:3173[B]:THR:HG23 | 3:R:3173[B]:THR:OG1 | 1.42 | 1.14 |
| 3:I:3217[B]:PHE:CE1 | 3:I:3230[B]:PHE:CZ | 2.32 | 1.14 |
| 3:O:3154[B]:PRO:HD2 | 3:X:3176[B]:LYS:CE | 1.77 | 1.14 |
| 3:O:3196[B]:THR:N | 3:O:3199[B]:GLN:OE1 | 1.79 | 1.14 |
| 3:U:2965[B]:LEU:CD1 | 3:d:3220[B]:ARG:CA | 2.26 | 1.14 |
| 3:U:3149[B]:ASN:C | 3:d:3154[B]:PRO:HB2 | 1.70 | 1.14 |
| 3:U:3217[B]:PHE:CZ | 3:U:3230[B]:PHE:CE1 | 2.35 | 1.14 |
| 3:C:2976[B]:ALA:N | 3:L:3253[B]:GLU:HB2 | 1.62 | 1.14 |
| 3:C:2979[B]:GLN:CG | 3:L:3156[B]:MET:CE | 2.14 | 1.14 |
| 3:C:3135[A]:LYS:HG3 | 3:C:3141[A]:TYR:CE1 | 1.79 | 1.14 |
| 3:C:3149[B]:ASN:O | 3:L:3168[B]:THR:O | 1.62 | 1.14 |
| 2:E:2868:GLU:OE2 | 3:F:2932[A]:PRO:C | 1.89 | 1.14 |
| 3:F:3256[B]:TRP:HE1 | 3:a:2965[B]:LEU:CG | 1.60 | 1.14 |
| 3:O:3217[B]:PHE:CZ | 3:O:3230[B]:PHE:CE1 | 2.35 | 1.14 |
| 3:R:2937[B]:ASN:HB2 | 3:R:3006[B]:LYS:HE2 | 1.28 | 1.14 |
| 3:U:3196[B]:THR:N | 3:U:3199[B]:GLN:OE1 | 1.79 | 1.14 |
| 3:a:3104[A]:MET:HA | 3:a:3110[A]:THR:HG23 | 1.23 | 1.14 |
| 3:d:3217[A]:PHE:CZ | 3:d:3230[A]:PHE:CE1 | 2.35 | 1.14 |
| 3:C:3217[A]:PHE:CZ | 3:C:3230[A]:PHE:CE1 | 2.35 | 1.14 |
| 3:C:3217[B]:PHE:CZ | 3:C:3230[B]:PHE:CE1 | 2.35 | 1.14 |
| 3:F:3152[B]:LYS:CB | 3:a:3172[B]:SER:N | 2.07 | 1.14 |
| 3:I:2966[B]:SER:HA | 3:R:3256[B]:TRP:CB | 1.74 | 1.14 |
| 3:I:2970[B]:PRO:CD | 3:R:2989[B]:HIS:CD2 | 2.29 | 1.14 |
| 3:L:3230[B]:PHE:HB2 | 3:L:3243[B]:GLY:HA2 | 1.14 | 1.14 |
| 3:O:2965[B]:LEU:CB | 3:X:3254[B]:MET:CE | 2.25 | 1.14 |
| 3:O:2968[B]:GLN:NE2 | 3:X:2984[B]:THR:C | 2.00 | 1.14 |
| 3:U:2975[B]:PHE:HE2 | 3:d:3254[B]:MET:CG | 1.58 | 1.14 |
| 3:U:3159[B]:SER:HB2 | 3:d:3150[B]:LYS:CD | 1.73 | 1.14 |
| 3:X:3135[B]:LYS:HG3 | 3:X:3141[B]:TYR:CE1 | 1.79 | 1.14 |
| 3:X:3196[B]:THR:N | 3:X:3199[B]:GLN:OE1 | 1.79 | 1.14 |
| 3:C:3149[B]:ASN:ND2 | 3:L:3163[B]:ASN:ND2 | 1.94 | 1.14 |
| 3:C:3154[B]:PRO:HA | 3:L:3153[B]:LYS:O | 1.48 | 1.14 |
| 3:I:3159[B]:SER:C | 3:R:3150[B]:LYS:CB | 2.20 | 1.14 |
| 3:I:3254[B]:MET:HG3 | 3:R:2966[B]:SER:CB | 1.76 | 1.14 |
| 3:O:3196[A]:THR:N | 3:O:3199[A]:GLN:OE1 | 1.79 | 1.14 |
| 3:O:3217[A]:PHE:CZ | 3:O:3230[A]:PHE:CE1 | 2.35 | 1.14 |
| 3:U:3155[B]:MET:O | 3:d:3150[B]:LYS:HG3 | 1.47 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3169[B]:LYS:CD | 3:d:3147[B]:GLU:HA | 1.76 | 1.14 |
| 3:a:3217[A]:PHE:CZ | 3:a:3230[A]:PHE:CE1 | 2.35 | 1.14 |
| 3:C:3156[B]:MET:CB | 3:L:2982[B]:MET:CB | 2.24 | 1.13 |
| 3:C:3196[B]:THR:N | 3:C:3199[B]:GLN:OE1 | 1.79 | 1.13 |
| 3:F:2959[B]:SER:HB2 | 3:a:3255[B]:PRO:HB2 | 1.17 | 1.13 |
| 3:F:2966[B]:SER:CA | 3:a:3256[B]:TRP:HD1 | 1.33 | 1.13 |
| 3:F:2985[B]:PHE:CZ | 3:a:2970[B]:PRO:HA | 1.80 | 1.13 |
| 2:H:2797:LYS:NZ | 3:I:3028[A]:PRO:HD3 | 1.60 | 1.13 |
| 3:I:3156[B]:MET:HB2 | 3:R:2982[B]:MET:HG3 | 1.14 | 1.13 |
| 3:O:2960[B]:PHE:HD2 | 3:O:3157[B]:PRO:HG3 | 1.10 | 1.13 |
| 3:O:3108[B]:HIS:O | 3:X:2970[B]:PRO:CD | 1.88 | 1.13 |
| 3:O:3153[B]:LYS:CD | 3:X:3176[B]:LYS:CD | 2.04 | 1.13 |
| 3:R:3293[B]:LYS:HD3 | 3:R:3294[B]:SER:HB3 | 1.14 | 1.13 |
| 3:U:3256[B]:TRP:HB2 | 3:d:2969[B]:TYR:N | 1.62 | 1.13 |
| 3:X:3217[A]:PHE:CZ | 3:X:3230[A]:PHE:CE1 | 2.35 | 1.13 |
| 3:X:3230[B]:PHE:HB2 | 3:X:3243[B]:GLY:HA2 | 1.14 | 1.13 |
| 2:Z:2867:PRO:HG3 | 3:a:2932[A]:PRO:HG3 | 1.26 | 1.13 |
| 3:a:3196[A]:THR:N | 3:a:3199[A]:GLN:OE1 | 1.79 | 1.13 |
| 3:a:3293[B]:LYS:HD3 | 3:a:3294[B]:SER:HB3 | 1.14 | 1.13 |
| 3:d:3230[B]:PHE:HB2 | 3:d:3243[B]:GLY:HA2 | 1.14 | 1.13 |
| 3:C:2983[B]:VAL:CG2 | 3:L:3160[B]:SER:CA | 2.14 | 1.13 |
| 3:F:3154[B]:PRO:HD2 | 3:a:3155[B]:MET:SD | 1.86 | 1.13 |
| 3:F:3293[B]:LYS:HD3 | 3:F:3294[B]:SER:HB3 | 1.13 | 1.13 |
| 3:I:2982[B]:MET:HE3 | 3:R:2977[B]:CYS:CB | 1.78 | 1.13 |
| 3:I:3217[A]:PHE:CZ | 3:I:3230[A]:PHE:CE1 | 2.35 | 1.13 |
| 3:U:3293[A]:LYS:HD3 | 3:U:3294[A]:SER:HB3 | 1.13 | 1.13 |
| 3:X:2979[B]:GLN:HG2 | 3:X:3155[B]:MET:CE | 1.69 | 1.13 |
| 3:X:3135[A]:LYS:HG3 | 3:X:3141[A]:TYR:CE1 | 1.80 | 1.13 |
| 3:d:3135[A]:LYS:HG3 | 3:d:3141[A]:TYR:CE1 | 1.79 | 1.13 |
| 3:C:2965[B]:LEU:HD23 | 3:L:3253[B]:GLU:OE2 | 1.44 | 1.13 |
| 3:C:2975[B]:PHE:HD1 | 3:L:3107[B]:LEU:CD1 | 1.52 | 1.13 |
| 3:C:3230[B]:PHE:HB2 | 3:C:3243[B]:GLY:HA2 | 1.14 | 1.13 |
| 3:I:2966[B]:SER:HB2 | 3:R:3254[B]:MET:CG | 1.79 | 1.13 |
| 3:I:3155[B]:MET:HB2 | 3:R:3153[B]:LYS:CG | 1.76 | 1.13 |
| 3:U:3256[B]:TRP:CD2 | 3:d:2969[B]:TYR:HB3 | 1.80 | 1.13 |
| 3:F:2965[B]:LEU:CA | 3:a:3221[B]:ALA:HB1 | 1.77 | 1.13 |
| 3:F:2981[B]:GLY:HA2 | 3:a:2968[B]:GLN:OE1 | 1.45 | 1.13 |
| 3:F:3169[B]:LYS:O | 3:a:3152[B]:LYS:CG | 1.97 | 1.13 |
| 3:I:2972[B]:GLY:CA | 3:R:3090[B]:ASN:HB3 | 1.77 | 1.13 |
| 3:I:3160[B]:SER:OG | 3:R:2982[B]:MET:CA | 1.96 | 1.13 |
| 3:I:3196[A]:THR:N | 3:I:3199[A]:GLN:OE1 | 1.79 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:2937[A]:ASN:HB2 | 3:L:3006[A]:LYS:HE2 | 1.28 | 1.13 |
| 3:O:3108[B]:HIS:HB3 | 3:X:2970[B]:PRO:N | 1.63 | 1.13 |
| 3:O:3153[B]:LYS:CG | 3:X:3176[B]:LYS:CE | 2.27 | 1.13 |
| 3:U:3154[B]:PRO:CD | 3:d:2984[B]:THR:HG21 | 1.78 | 1.13 |
| 3:U:3170[B]:ALA:O | 3:d:3152[B]:LYS:NZ | 1.80 | 1.13 |
| 3:U:3253[B]:GLU:HA | 3:d:3255[B]:PRO:CG | 1.77 | 1.13 |
| 3:C:2968[B]:GLN:NE2 | 3:L:3258[B]:PHE:CZ | 2.17 | 1.13 |
| 3:C:3284[B]:LYS:HD3 | 3:C:3285[B]:VAL:N | 1.64 | 1.13 |
| 3:C:3149[B]:ASN:CB | 3:L:3163[B]:ASN:ND2 | 2.12 | 1.12 |
| 3:C:3163[B]:ASN:HD22 | 3:L:3149[B]:ASN:CG | 1.56 | 1.12 |
| 3:C:3169[B]:LYS:O | 3:L:3148[B]:ILE:O | 1.65 | 1.13 |
| 2:E:2800:LYS:O | 3:F:3023[A]:ILE:CD1 | 1.97 | 1.12 |
| 3:F:3153[B]:LYS:HG2 | 3:a:3155[B]:MET:HB2 | 1.23 | 1.13 |
| 3:F:3284[B]:LYS:HD3 | 3:F:3285[B]:VAL:N | 1.64 | 1.13 |
| 3:I:3174[B]:GLY:HA2 | 3:R:3154[B]:PRO:HG3 | 1.29 | 1.13 |
| 3:C:3252[B]:TYR:CE1 | 3:L:3223[B]:GLY:O | 2.01 | 1.12 |
| 2:E:2868:GLU:OE2 | 3:F:2933[A]:SER:N | 1.80 | 1.12 |
| 3:F:3154[B]:PRO:CD | 3:a:3155[B]:MET:HG3 | 1.79 | 1.12 |
| 3:I:2982[B]:MET:HE2 | 3:R:2966[B]:SER:HB3 | 1.15 | 1.12 |
| 3:I:3196[B]:THR:N | 3:I:3199[B]:GLN:OE1 | 1.79 | 1.12 |
| 3:I:3254[B]:MET:C | 3:R:2966[B]:SER:OG | 1.92 | 1.12 |
| 3:R:3284[A]:LYS:HD3 | 3:R:3285[A]:VAL:N | 1.64 | 1.12 |
| 3:U:3152[B]:LYS:O | 3:d:3152[B]:LYS:C | 1.92 | 1.12 |
| 3:a:3135[A]:LYS:HG2 | 3:a:3141[A]:TYR:HE1 | 1.14 | 1.12 |
| 3:a:3284[B]:LYS:HD3 | 3:a:3285[B]:VAL:N | 1.64 | 1.12 |
| 3:d:2960[B]:PHE:HD2 | 3:d:3157[B]:PRO:HG3 | 1.10 | 1.12 |
| 3:C:3174[B]:GLY:HA2 | 3:L:3154[B]:PRO:CD | 1.79 | 1.12 |
| 3:F:3256[B]:TRP:HB3 | 3:a:2966[B]:SER:C | 1.73 | 1.12 |
| 3:I:3153[B]:LYS:CD | 3:R:3155[B]:MET:HB2 | 1.79 | 1.12 |
| 3:O:2973[B]:THR:HB | 3:X:3158[B]:PHE:CE2 | 1.84 | 1.12 |
| 3:O:2975[B]:PHE:HE2 | 3:X:3172[B]:SER:CB | 1.61 | 1.12 |
| 3:R:2960[A]:PHE:HD2 | 3:R:3157[A]:PRO:HG3 | 1.10 | 1.12 |
| 3:U:2969[B]:TYR:CE1 | 3:d:3107[B]:LEU:HD13 | 1.84 | 1.12 |
| 3:d:3293[B]:LYS:HD3 | 3:d:3294[B]:SER:HB3 | 1.13 | 1.12 |
| 3:C:2982[B]:MET:CG | 3:L:3156[B]:MET:SD | 2.36 | 1.12 |
| 3:F:2974[B]:ALA:HB1 | 3:a:3253[B]:GLU:OE1 | 1.48 | 1.12 |
| 3:F:2977[B]:CYS:O | 3:a:3254[B]:MET:CE | 1.81 | 1.12 |
| 3:F:3150[B]:LYS:NZ | 3:a:3160[B]:SER:CB | 2.11 | 1.12 |
| 3:I:2975[B]:PHE:HZ | 3:R:2961[B]:HIS:CA | 1.60 | 1.12 |
| 3:L:2937[B]:ASN:HB2 | 3:L:3006[B]:LYS:HE2 | 1.28 | 1.12 |
| 3:O:2963[B]:MET:SD | 3:X:2975[B]:PHE:CE2 | 2.43 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3230[B]:PHE:HB2 | 3:O:3243[B]:GLY:HA2 | 1.14 | 1.12 |
| 3:O:3284[B]:LYS:HD3 | 3:O:3285[B]:VAL:N | 1.64 | 1.12 |
| 3:U:3252[B]:TYR:HE2 | 3:d:3222[B]:ILE:HD13 | 1.00 | 1.12 |
| 4:j:1:NAG:H61 | 4:j:2:NAG:HN2 | 1.08 | 1.12 |
| 3:C:2964[B]:PRO:O | 3:L:3255[B]:PRO:HB3 | 1.43 | 1.12 |
| 3:C:3154[B]:PRO:HB3 | 3:L:3151[B]:LEU:O | 1.47 | 1.12 |
| 3:C:3156[B]:MET:SD | 3:L:2982[B]:MET:CB | 2.38 | 1.12 |
| 3:C:3254[B]:MET:O | 3:L:2976[B]:ALA:CA | 1.91 | 1.12 |
| 3:F:3153[B]:LYS:NZ | 3:a:3157[B]:PRO:HD2 | 1.64 | 1.12 |
| 3:I:2963[B]:MET:HE1 | 3:R:3223[B]:GLY:HA3 | 1.29 | 1.12 |
| 3:I:3153[B]:LYS:HB2 | 3:R:3158[B]:PHE:HB2 | 1.29 | 1.12 |
| 3:I:3165[B]:ASN:O | 3:R:3149[B]:ASN:HB3 | 1.49 | 1.12 |
| 3:U:3155[B]:MET:N | 3:d:3150[B]:LYS:CA | 2.13 | 1.12 |
| 3:a:2960[B]:PHE:HD2 | 3:a:3157[B]:PRO:HG3 | 1.10 | 1.12 |
| 3:d:3293[A]:LYS:HD3 | 3:d:3294[A]:SER:HB3 | 1.14 | 1.12 |
| 3:C:3089[B]:HIS:HE1 | 3:C:3119[B]:HIS:NE2 | 1.21 | 1.12 |
| 3:C:3173[B]:THR:OG1 | 3:L:3152[B]:LYS:HA | 1.42 | 1.12 |
| 3:F:2960[A]:PHE:HD2 | 3:F:3157[A]:PRO:HG3 | 1.10 | 1.12 |
| 3:F:3154[B]:PRO:CG | 3:a:3155[B]:MET:SD | 2.38 | 1.12 |
| 3:I:2977[B]:CYS:SG | 3:R:2978[B]:CYS:O | 2.08 | 1.12 |
| 3:L:3293[A]:LYS:HD3 | 3:L:3294[A]:SER:HB3 | 1.14 | 1.12 |
| 3:L:3293[B]:LYS:HD3 | 3:L:3294[B]:SER:HB3 | 1.13 | 1.12 |
| 3:O:3040[B]:VAL:CG2 | 3:X:2969[B]:TYR:CD1 | 2.31 | 1.12 |
| 3:R:3104[B]:MET:HA | 3:R:3110[B]:THR:HG23 | 1.23 | 1.12 |
| 3:U:3254[B]:MET:HE3 | 3:d:3254[B]:MET:HB2 | 1.22 | 1.12 |
| 3:U:3255[B]:PRO:HD3 | 3:d:3253[B]:GLU:C | 1.73 | 1.12 |
| 3:a:3230[B]:PHE:HB2 | 3:a:3243[B]:GLY:HA2 | 1.14 | 1.12 |
| 3:C:3284[A]:LYS:HD3 | 3:C:3285[A]:VAL:N | 1.64 | 1.11 |
| 3:F:3230[B]:PHE:HB2 | 3:F:3243[B]:GLY:HA2 | 1.14 | 1.11 |
| 3:L:3104[A]:MET:HA | 3:L:3110[A]:THR:HG23 | 1.23 | 1.11 |
| 3:L:3104[B]:MET:HA | 3:L:3110[B]:THR:HG23 | 1.24 | 1.11 |
| 3:O:3153[B]:LYS:HD3 | 3:X:3176[B]:LYS:HD2 | 1.28 | 1.11 |
| 3:O:3251[B]:ASP:HB2 | 3:X:2968[B]:GLN:OE1 | 1.47 | 1.11 |
| 3:U:2965[B]:LEU:CB | 3:d:3220[B]:ARG:HH11 | 1.61 | 1.11 |
| 3:X:2960[A]:PHE:HD2 | 3:X:3157[A]:PRO:HG3 | 1.10 | 1.11 |
| 3:X:3284[A]:LYS:HD3 | 3:X:3285[A]:VAL:N | 1.64 | 1.11 |
| 3:X:3284[B]:LYS:HD3 | 3:X:3285[B]:VAL:N | 1.64 | 1.11 |
| 3:d:3284[B]:LYS:HD3 | 3:d:3285[B]:VAL:N | 1.64 | 1.11 |
| 3:C:3147[B]:GLU:CG | 3:L:3161[B]:GLU:HA | 1.78 | 1.11 |
| 3:C:3256[B]:TRP:O | 3:L:2965[B]:LEU:O | 1.68 | 1.11 |
| 3:I:3284[A]:LYS:HD3 | 3:I:3285[A]:VAL:N | 1.64 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3284[A]:LYS:HD3 | 3:L:3285[A]:VAL:N | 1.64 | 1.11 |
| 3:U:3284[A]:LYS:HD3 | 3:U:3285[A]:VAL:N | 1.64 | 1.11 |
| 3:d:3104[B]:MET:HA | 3:d:3110[B]:THR:HG23 | 1.23 | 1.11 |
| 3:C:2969[B]:TYR:C | 3:L:2985[B]:PHE:HE2 | 1.23 | 1.11 |
| 3:C:3158[B]:PHE:HD2 | 3:L:3153[B]:LYS:CE | 1.39 | 1.11 |
| 3:C:3163[B]:ASN:CG | 3:L:3149[B]:ASN:HD22 | 1.56 | 1.11 |
| 3:C:3163[B]:ASN:CB | 3:L:3149[B]:ASN:HD22 | 1.63 | 1.11 |
| 3:F:3154[B]:PRO:HB3 | 3:a:3174[B]:GLY:N | 1.65 | 1.11 |
| 3:F:3284[A]:LYS:HD3 | 3:F:3285[A]:VAL:N | 1.64 | 1.11 |
| 3:I:2937[A]:ASN:HB2 | 3:I:3006[A]:LYS:HE2 | 1.28 | 1.11 |
| 3:I:3174[B]:GLY:HA2 | 3:R:3154[B]:PRO:CB | 1.71 | 1.11 |
| 3:O:3253[B]:GLU:HG3 | 3:X:3160[B]:SER:HA | 1.20 | 1.11 |
| 1:Y:1616:LYS:HD2 | 3:d:3187[B]:TYR:HA | 1.17 | 1.11 |
| 3:a:3284[A]:LYS:HD3 | 3:a:3285[A]:VAL:N | 1.64 | 1.11 |
| 3:a:3293[A]:LYS:HD3 | 3:a:3294[A]:SER:HB3 | 1.13 | 1.11 |
| 3:d:3284[A]:LYS:HD3 | 3:d:3285[A]:VAL:N | 1.64 | 1.11 |
| 3:C:2968[B]:GLN:CD | 3:L:3258[B]:PHE:HZ | 1.56 | 1.11 |
| 3:C:3256[B]:TRP:CD2 | 3:L:2965[B]:LEU:C | 2.22 | 1.11 |
| 3:F:3254[B]:MET:HG3 | 3:a:2966[B]:SER:HB2 | 1.19 | 1.11 |
| 3:I:2989[B]:HIS:NE2 | 3:R:2970[B]:PRO:N | 1.96 | 1.11 |
| 3:I:3160[B]:SER:HB3 | 3:R:3150[B]:LYS:HZ3 | 1.12 | 1.11 |
| 3:I:3223[B]:GLY:HA3 | 3:R:2963[B]:MET:HE1 | 1.23 | 1.11 |
| 3:I:3293[B]:LYS:HD3 | 3:I:3294[B]:SER:HB3 | 1.13 | 1.11 |
| 3:O:3104[A]:MET:HA | 3:O:3110[A]:THR:HG23 | 1.23 | 1.11 |
| 3:R:3284[B]:LYS:HD3 | 3:R:3285[B]:VAL:N | 1.64 | 1.11 |
| 3:U:3293[B]:LYS:HD3 | 3:U:3294[B]:SER:HB3 | 1.13 | 1.11 |
| 3:C:3160[B]:SER:CA | 3:L:2983[B]:VAL:HG23 | 1.79 | 1.11 |
| 3:C:3163[B]:ASN:ND2 | 3:L:3149[B]:ASN:HD22 | 1.48 | 1.11 |
| 3:C:3293[B]:LYS:HD3 | 3:C:3294[B]:SER:HB3 | 1.13 | 1.11 |
| 3:F:2937[B]:ASN:HB2 | 3:F:3006[B]:LYS:HE2 | 1.28 | 1.11 |
| 3:F:2964[B]:PRO:C | 3:a:3221[B]:ALA:HB1 | 1.75 | 1.11 |
| 3:I:3104[A]:MET:HA | 3:I:3110[A]:THR:HG23 | 1.24 | 1.11 |
| 3:I:3252[B]:TYR:HB2 | 3:R:3251[B]:ASP:O | 1.34 | 1.11 |
| 3:I:3252[B]:TYR:CB | 3:R:3251[B]:ASP:O | 1.74 | 1.11 |
| 3:L:3135[A]:LYS:HG2 | 3:L:3141[A]:TYR:HE1 | 1.14 | 1.11 |
| 3:U:3153[B]:LYS:HB3 | 3:d:3153[B]:LYS:HD2 | 1.18 | 1.11 |
| 3:U:3230[A]:PHE:HB2 | 3:U:3243[A]:GLY:HA2 | 1.14 | 1.11 |
| 3:U:3230[B]:PHE:HB2 | 3:U:3243[B]:GLY:HA2 | 1.14 | 1.11 |
| 3:U:3284[B]:LYS:HD3 | 3:U:3285[B]:VAL:N | 1.64 | 1.11 |
| 3:F:2981[B]:GLY:H | 3:a:2968[B]:GLN:HG2 | 1.12 | 1.10 |
| 3:F:2982[B]:MET:HG3 | 3:a:2967[B]:CYS:SG | 1.79 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:2800:LYS:O | 3:I:3023[A]:ILE:CD1 | 1.97 | 1.10 |
| 3:I:2937[B]:ASN:HB2 | 3:I:3006[B]:LYS:HE2 | 1.28 | 1.10 |
| 3:I:3153[B]:LYS:NZ | 3:R:3157[B]:PRO:HD2 | 1.65 | 1.10 |
| 3:O:2965[B]:LEU:HB2 | 3:X:3254[B]:MET:SD | 1.90 | 1.10 |
| 3:O:3038[B]:ILE:CG2 | 3:X:2969[B]:TYR:CZ | 2.33 | 1.10 |
| 3:O:3161[B]:GLU:OE2 | 3:X:3151[B]:LEU:HD11 | 0.95 | 1.10 |
| 3:U:3220[B]:ARG:CB | 3:d:2973[B]:THR:HA | 1.81 | 1.10 |
| 3:C:2974[B]:ALA:CB | 3:L:3249[B]:GLY:HA3 | 1.53 | 1.10 |
| 3:C:3150[B]:LYS:C | 3:L:3172[B]:SER:HB2 | 1.74 | 1.10 |
| 3:F:2964[B]:PRO:C | 3:a:3221[B]:ALA:CB | 2.23 | 1.10 |
| 3:I:2961[B]:HIS:CG | 3:R:2975[B]:PHE:HZ | 1.64 | 1.10 |
| 3:I:3090[B]:ASN:HA | 3:R:2971[B]:ASP:O | 1.48 | 1.10 |
| 3:I:3251[B]:ASP:HB3 | 3:R:3251[B]:ASP:HB2 | 1.16 | 1.10 |
| 3:I:3284[B]:LYS:HD3 | 3:I:3285[B]:VAL:N | 1.64 | 1.10 |
| 3:O:3293[A]:LYS:HD3 | 3:O:3294[A]:SER:HB3 | 1.13 | 1.10 |
| 3:U:2971[B]:ASP:O | 3:d:3247[B]:VAL:HA | 1.49 | 1.10 |
| 3:a:2960[A]:PHE:HD2 | 3:a:3157[A]:PRO:HG3 | 1.10 | 1.10 |
| 3:C:3163[B]:ASN:ND2 | 3:L:3149[B]:ASN:HB3 | 1.52 | 1.10 |
| 3:F:3150[B]:LYS:HE3 | 3:a:3163[B]:ASN:HB2 | 1.32 | 1.10 |
| 3:F:3153[B]:LYS:HB3 | 3:a:3155[B]:MET:O | 1.52 | 1.10 |
| 3:F:3154[B]:PRO:N | 3:a:3155[B]:MET:HG3 | 1.00 | 1.10 |
| 3:I:3256[B]:TRP:CB | 3:R:2966[B]:SER:HA | 1.65 | 1.10 |
| 3:L:2960[A]:PHE:HD2 | 3:L:3157[A]:PRO:HG3 | 1.10 | 1.10 |
| 3:L:3284[B]:LYS:HD3 | 3:L:3285[B]:VAL:N | 1.64 | 1.10 |
| 3:R:3230[B]:PHE:HB2 | 3:R:3243[B]:GLY:HA2 | 1.14 | 1.10 |
| 3:U:3162[B]:ASP:CG | 3:d:3259[B]:ASP:HB2 | 1.51 | 1.10 |
| 3:F:3251[B]:ASP:CA | 3:a:3251[B]:ASP:HB3 | 1.81 | 1.10 |
| 3:I:3120[B]:HIS:CD2 | 3:R:2969[B]:TYR:CE2 | 2.40 | 1.10 |
| 3:I:3253[B]:GLU:HB2 | 3:R:2975[B]:PHE:O | 1.47 | 1.10 |
| 3:R:3230[A]:PHE:HB2 | 3:R:3243[A]:GLY:HA2 | 1.14 | 1.10 |
| 3:U:2960[B]:PHE:HD2 | 3:U:3157[B]:PRO:HG3 | 1.10 | 1.10 |
| 3:U:3169[B]:LYS:O | 3:d:3148[B]:ILE:C | 1.93 | 1.10 |
| 3:U:3169[B]:LYS:HE2 | 3:d:3146[B]:CYS:HA | 1.16 | 1.10 |
| 3:U:3254[B]:MET:HE3 | 3:d:3254[B]:MET:HB3 | 1.23 | 1.10 |
| 3:d:3135[A]:LYS:HG2 | 3:d:3141[A]:TYR:HE1 | 1.14 | 1.10 |
| 3:C:2988[B]:TRP:NE1 | 3:L:3153[B]:LYS:NZ | 1.99 | 1.10 |
| 3:F:3107[B]:LEU:CD1 | 3:a:2975[B]:PHE:HD1 | 1.62 | 1.10 |
| 3:I:2975[B]:PHE:C | 3:R:3253[B]:GLU:CB | 2.25 | 1.10 |
| 3:I:3160[B]:SER:OG | 3:R:2982[B]:MET:C | 1.95 | 1.10 |
| 3:I:3169[B]:LYS:O | 3:R:3152[B]:LYS:CB | 2.00 | 1.10 |
| 3:I:3254[B]:MET:CG | 3:R:2966[B]:SER:HB2 | 1.82 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2960[A]:PHE:HD2 | 3:O:3157[A]:PRO:HG3 | 1.10 | 1.10 |
| 3:R:3135[A]:LYS:HG2 | 3:R:3141[A]:TYR:HE1 | 1.14 | 1.10 |
| 3:C:3107[B]:LEU:HD13 | 3:L:2974[B]:ALA:O | 1.50 | 1.09 |
| 3:C:3149[B]:ASN:ND2 | 3:L:3163[B]:ASN:HD22 | 1.49 | 1.09 |
| 3:C:3174[B]:GLY:CA | 3:L:3154[B]:PRO:HB3 | 1.82 | 1.09 |
| 3:I:2959[B]:SER:CB | 3:R:3255[B]:PRO:CB | 2.29 | 1.09 |
| 3:I:2975[B]:PHE:CD1 | 3:R:3107[B]:LEU:CD1 | 2.14 | 1.09 |
| 3:I:3149[B]:ASN:OD1 | 3:R:3169[B]:LYS:HE3 | 1.48 | 1.09 |
| 3:I:3160[B]:SER:HA | 3:R:2983[B]:VAL:N | 1.65 | 1.09 |
| 3:O:2967[B]:CYS:HB2 | 3:X:3155[B]:MET:HG2 | 1.10 | 1.09 |
| 3:O:3109[B]:TYR:CD1 | 3:X:2970[B]:PRO:HD2 | 1.80 | 1.09 |
| 3:O:3154[B]:PRO:HG2 | 3:X:3175[B]:TYR:CB | 1.81 | 1.09 |
| 3:O:3284[A]:LYS:HD3 | 3:O:3285[A]:VAL:N | 1.64 | 1.09 |
| 3:U:2937[A]:ASN:HB2 | 3:U:3006[A]:LYS:HE2 | 1.28 | 1.09 |
| 2:c:2867:PRO:HG3 | 3:d:2932[A]:PRO:HG2 | 1.22 | 1.09 |
| 3:C:2937[A]:ASN:HB2 | 3:C:3006[A]:LYS:HE2 | 1.28 | 1.09 |
| 3:C:2975[B]:PHE:CE1 | 3:L:3107[B]:LEU:CD1 | 2.33 | 1.09 |
| 3:F:2968[B]:GLN:HG2 | 3:a:2981[B]:GLY:H | 1.16 | 1.09 |
| 3:F:3104[A]:MET:HA | 3:F:3110[A]:THR:HG23 | 1.23 | 1.09 |
| 3:F:3104[B]:MET:HA | 3:F:3110[B]:THR:HG23 | 1.23 | 1.09 |
| 3:F:3154[B]:PRO:HB3 | 3:a:3174[B]:GLY:CA | 1.83 | 1.09 |
| 3:F:3248[B]:LEU:HB3 | 3:a:2972[B]:GLY:O | 1.50 | 1.09 |
| 3:I:2975[B]:PHE:HD1 | 3:R:3107[B]:LEU:CG | 1.65 | 1.09 |
| 3:I:3252[B]:TYR:HB2 | 3:R:3251[B]:ASP:C | 1.73 | 1.09 |
| 3:I:3293[A]:LYS:HD3 | 3:I:3294[A]:SER:HB3 | 1.14 | 1.09 |
| 3:O:3230[A]:PHE:HB2 | 3:O:3243[A]:GLY:HA2 | 1.14 | 1.09 |
| 3:R:3293[A]:LYS:HD3 | 3:R:3294[A]:SER:HB3 | 1.14 | 1.09 |
| 3:U:3155[B]:MET:N | 3:d:3150[B]:LYS:HA | 1.31 | 1.09 |
| 3:U:3162[B]:ASP:CA | 3:d:3260[B]:ARG:HH12 | 1.65 | 1.09 |
| 3:X:3135[A]:LYS:HG2 | 3:X:3141[A]:TYR:HE1 | 1.14 | 1.09 |
| 3:F:2982[B]:MET:HE3 | 3:a:2967[B]:CYS:SG | 1.86 | 1.09 |
| 3:F:2982[B]:MET:HG2 | 3:a:2967[B]:CYS:SG | 1.79 | 1.09 |
| 3:I:3163[B]:ASN:ND2 | 3:R:3149[B]:ASN:CB | 2.14 | 1.09 |
| 3:L:3135[B]:LYS:HG2 | 3:L:3141[B]:TYR:HE1 | 1.14 | 1.09 |
| 3:O:3154[B]:PRO:CG | 3:X:3175[B]:TYR:CB | 2.28 | 1.09 |
| 3:O:3255[B]:PRO:HD2 | 3:X:3169[B]:LYS:HG3 | 1.33 | 1.09 |
| 2:W:2800:LYS:O | 3:X:3023[A]:ILE:CD1 | 2.01 | 1.09 |
| 3:X:3293[A]:LYS:HD3 | 3:X:3294[A]:SER:HB3 | 1.13 | 1.09 |
| 2:E:2868:GLU:CD | 3:F:2932[A]:PRO:O | 1.95 | 1.09 |
| 3:F:3172[B]:SER:H | 3:a:3152[B]:LYS:HB2 | 1.05 | 1.09 |
| 3:L:3230[A]:PHE:HB2 | 3:L:3243[A]:GLY:HA2 | 1.14 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3038[B]:ILE:CD1 | 3:X:2969[B]:TYR:OH | 2.01 | 1.09 |
| 3:O:3108[B]:HIS:O | 3:X:2970[B]:PRO:HD3 | 0.92 | 1.09 |
| 3:O:3251[B]:ASP:HB3 | 3:X:2967[B]:CYS:CA | 1.83 | 1.09 |
| 3:U:2930[B]:LEU:H | 3:U:2930[B]:LEU:HD22 | 1.18 | 1.09 |
| 1:Y:1546:LYS:HG3 | 3:d:3001[B]:LYS:HE3 | 1.20 | 1.09 |
| 3:C:3163[B]:ASN:ND2 | 3:L:3149[B]:ASN:ND2 | 2.01 | 1.09 |
| 3:C:3174[B]:GLY:HA3 | 3:L:3154[B]:PRO:HB3 | 1.14 | 1.09 |
| 3:C:3258[B]:PHE:HZ | 3:L:2968[B]:GLN:NE2 | 1.49 | 1.09 |
| 3:C:3293[A]:LYS:HD3 | 3:C:3294[A]:SER:HB3 | 1.13 | 1.09 |
| 3:F:2967[B]:CYS:HA | 3:a:2981[B]:GLY:HA3 | 1.27 | 1.09 |
| 3:F:2982[B]:MET:CE | 3:a:2977[B]:CYS:CB | 2.31 | 1.09 |
| 3:I:3135[A]:LYS:HG2 | 3:I:3141[A]:TYR:HE1 | 1.14 | 1.09 |
| 3:I:3154[B]:PRO:CB | 3:R:3174[B]:GLY:CA | 2.29 | 1.09 |
| 3:O:2930[B]:LEU:HD22 | 3:O:2930[B]:LEU:H | 1.18 | 1.09 |
| 3:O:2937[A]:ASN:HB2 | 3:O:3006[A]:LYS:HE2 | 1.28 | 1.09 |
| 3:X:3104[B]:MET:HA | 3:X:3110[B]:THR:HG23 | 1.23 | 1.09 |
| 3:X:3135[B]:LYS:HG2 | 3:X:3141[B]:TYR:HE1 | 1.14 | 1.09 |
| 3:X:3217[B]:PHE:CE1 | 3:X:3230[B]:PHE:HZ | 1.71 | 1.09 |
| 3:d:2960[A]:PHE:HD2 | 3:d:3157[A]:PRO:HG3 | 1.10 | 1.09 |
| 3:C:2971[B]:ASP:HB3 | 3:L:3093[B]:HIS:CE1 | 1.64 | 1.08 |
| 3:C:2982[B]:MET:HB3 | 3:L:3156[B]:MET:HB3 | 1.10 | 1.08 |
| 3:C:2983[B]:VAL:CG2 | 3:L:3161[B]:GLU:OE2 | 1.68 | 1.08 |
| 3:F:3162[B]:ASP:HB3 | 3:a:3259[B]:ASP:HB3 | 1.21 | 1.08 |
| 3:F:3256[B]:TRP:NE1 | 3:a:2965[B]:LEU:CD1 | 2.16 | 1.08 |
| 3:I:2960[B]:PHE:HD2 | 3:I:3157[B]:PRO:HG3 | 1.10 | 1.08 |
| 3:O:2965[B]:LEU:CB | 3:X:3254[B]:MET:SD | 2.41 | 1.08 |
| 3:O:2965[B]:LEU:CA | 3:X:3254[B]:MET:HE1 | 1.80 | 1.08 |
| 3:O:3196[A]:THR:HG21 | 1:P:416:ASN:ND2 | 1.68 | 1.08 |
| 3:R:2930[B]:LEU:HD22 | 3:R:2930[B]:LEU:H | 1.18 | 1.08 |
| 3:U:3252[B]:TYR:CE2 | 3:d:3222[B]:ILE:CD1 | 2.33 | 1.08 |
| 3:U:3254[B]:MET:HB3 | 3:d:3254[B]:MET:CB | 1.80 | 1.08 |
| 3:U:3255[B]:PRO:CG | 3:d:3252[B]:TYR:HA | 1.79 | 1.08 |
| 3:X:2930[A]:LEU:HD22 | 3:X:2930[A]:LEU:H | 1.18 | 1.08 |
| 3:a:2937[B]:ASN:HB2 | 3:a:3006[B]:LYS:HE2 | 1.28 | 1.08 |
| 3:d:3104[A]:MET:HA | 3:d:3110[A]:THR:HG23 | 1.23 | 1.08 |
| 3:C:3160[B]:SER:CA | 3:L:2983[B]:VAL:CG2 | 2.29 | 1.08 |
| 3:C:3161[B]:GLU:OE2 | 3:L:2983[B]:VAL:HG21 | 1.53 | 1.08 |
| 3:F:3154[B]:PRO:CD | 3:a:3155[B]:MET:CG | 2.32 | 1.08 |
| 3:I:3255[B]:PRO:HB2 | 3:R:2959[B]:SER:HB2 | 1.26 | 1.08 |
| 3:O:3160[B]:SER:HA | 3:X:3151[B]:LEU:CG | 1.82 | 1.08 |
| 3:O:3162[B]:ASP:OD2 | 3:X:3150[B]:LYS:HD2 | 1.51 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3217[A]:PHE:CE1 | 3:O:3230[A]:PHE:HZ | 1.71 | 1.08 |
| 3:O:3293[B]:LYS:HD3 | 3:O:3294[B]:SER:HB3 | 1.13 | 1.08 |
| 3:U:2930[A]:LEU:HD22 | 3:U:2930[A]:LEU:H | 1.18 | 1.08 |
| 3:U:3104[A]:MET:HA | 3:U:3110[A]:THR:HG23 | 1.23 | 1.08 |
| 3:X:2937[B]:ASN:HB2 | 3:X:3006[B]:LYS:HE2 | 1.28 | 1.08 |
| 3:a:2937[A]:ASN:HB2 | 3:a:3006[A]:LYS:HE2 | 1.28 | 1.08 |
| 3:a:3217[B]:PHE:CE1 | 3:a:3230[B]:PHE:HZ | 1.71 | 1.08 |
| 3:C:2982[B]:MET:CB | 3:L:3156[B]:MET:SD | 2.41 | 1.08 |
| 3:C:2985[B]:PHE:CE1 | 3:L:2970[B]:PRO:HA | 1.88 | 1.08 |
| 3:C:3152[B]:LYS:CA | 3:L:3173[B]:THR:OG1 | 1.98 | 1.08 |
| 3:C:3217[A]:PHE:CE1 | 3:C:3230[A]:PHE:HZ | 1.71 | 1.08 |
| 3:F:2982[B]:MET:SD | 3:a:3157[B]:PRO:HA | 1.92 | 1.08 |
| 3:F:3155[B]:MET:CA | 3:a:3153[B]:LYS:HD2 | 1.82 | 1.08 |
| 3:F:3163[B]:ASN:HB3 | 3:a:3150[B]:LYS:HE3 | 1.25 | 1.08 |
| 3:O:2930[A]:LEU:H | 3:O:2930[A]:LEU:HD22 | 1.18 | 1.08 |
| 3:O:2937[B]:ASN:HB2 | 3:O:3006[B]:LYS:HE2 | 1.28 | 1.08 |
| 3:O:2969[B]:TYR:CD1 | 3:X:3158[B]:PHE:CE1 | 2.40 | 1.08 |
| 3:U:3156[B]:MET:HE2 | 3:d:2982[B]:MET:CG | 1.74 | 1.08 |
| 3:a:3230[A]:PHE:HB2 | 3:a:3243[A]:GLY:HA2 | 1.14 | 1.08 |
| 3:C:2960[A]:PHE:HD2 | 3:C:3157[A]:PRO:HG3 | 1.10 | 1.08 |
| 3:C:3120[B]:HIS:NE2 | 3:L:2969[B]:TYR:CE2 | 2.15 | 1.08 |
| 3:F:2966[B]:SER:C | 3:a:3256[B]:TRP:HB3 | 1.77 | 1.08 |
| 3:I:3253[B]:GLU:HB2 | 3:R:2975[B]:PHE:C | 1.79 | 1.08 |
| 3:O:2970[B]:PRO:CD | 3:X:2991[B]:LEU:CD1 | 2.29 | 1.08 |
| 3:O:3025[B]:VAL:HG22 | 3:O:3047[B]:ARG:HH12 | 1.19 | 1.08 |
| 3:O:3135[A]:LYS:HG2 | 3:O:3141[A]:TYR:HE1 | 1.14 | 1.08 |
| 3:O:3154[B]:PRO:HG2 | 3:X:3175[B]:TYR:HB2 | 1.30 | 1.08 |
| 3:R:2930[A]:LEU:H | 3:R:2930[A]:LEU:HD22 | 1.18 | 1.08 |
| 3:U:3113[B]:ASP:OD2 | 3:U:3114[B]:PRO:CD | 2.02 | 1.08 |
| 3:a:2930[A]:LEU:H | 3:a:2930[A]:LEU:HD22 | 1.18 | 1.08 |
| 2:c:2867:PRO:CG | 3:d:2932[A]:PRO:HG2 | 1.81 | 1.08 |
| 3:C:3152[B]:LYS:HG3 | 3:L:3169[B]:LYS:O | 1.53 | 1.08 |
| 3:F:3155[B]:MET:C | 3:a:3153[B]:LYS:HD2 | 1.79 | 1.08 |
| 3:F:3174[B]:GLY:CA | 3:a:3154[B]:PRO:CG | 2.30 | 1.08 |
| 3:F:3251[B]:ASP:HB3 | 3:a:3251[B]:ASP:HB2 | 1.29 | 1.08 |
| 3:O:3113[A]:ASP:OD2 | 3:O:3114[A]:PRO:CD | 2.02 | 1.08 |
| 3:O:3135[B]:LYS:HG2 | 3:O:3141[B]:TYR:HE1 | 1.14 | 1.08 |
| 3:X:3113[B]:ASP:OD2 | 3:X:3114[B]:PRO:CD | 2.02 | 1.08 |
| 3:X:3185[A]:TYR:O | 3:X:3186[A]:GLU:OE2 | 1.72 | 1.08 |
| 3:X:3230[A]:PHE:HB2 | 3:X:3243[A]:GLY:HA2 | 1.14 | 1.08 |
| 3:C:2960[B]:PHE:HD2 | 3:C:3157[B]:PRO:HG3 | 1.10 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2985[B]:PHE:CZ | 3:L:2970[B]:PRO:N | 2.22 | 1.07 |
| 3:C:3148[B]:ILE:O | 3:L:3169[B]:LYS:O | 1.71 | 1.07 |
| 3:C:3156[B]:MET:CB | 3:L:2982[B]:MET:HB3 | 1.84 | 1.07 |
| 3:F:2930[A]:LEU:H | 3:F:2930[A]:LEU:HD22 | 1.18 | 1.07 |
| 3:F:2966[B]:SER:HA | 3:a:3256[B]:TRP:CB | 1.83 | 1.07 |
| 3:F:3230[A]:PHE:HB2 | 3:F:3243[A]:GLY:HA2 | 1.14 | 1.07 |
| 3:I:3169[B]:LYS:C | 3:R:3152[B]:LYS:HG3 | 1.65 | 1.07 |
| 3:L:3025[B]:VAL:HG22 | 3:L:3047[B]:ARG:HH12 | 1.19 | 1.07 |
| 3:O:3113[B]:ASP:OD2 | 3:O:3114[B]:PRO:CD | 2.02 | 1.07 |
| 3:O:3154[B]:PRO:HG3 | 3:X:3175[B]:TYR:HB3 | 1.17 | 1.07 |
| 3:U:3113[A]:ASP:OD2 | 3:U:3114[A]:PRO:CD | 2.02 | 1.07 |
| 3:U:3254[B]:MET:HA | 3:d:3254[B]:MET:HA | 1.27 | 1.07 |
| 3:a:3217[A]:PHE:CE1 | 3:a:3230[A]:PHE:HZ | 1.71 | 1.07 |
| 3:d:3113[B]:ASP:OD2 | 3:d:3114[B]:PRO:CD | 2.02 | 1.07 |
| 3:C:2930[B]:LEU:HD22 | 3:C:2930[B]:LEU:H | 1.18 | 1.07 |
| 3:C:3113[B]:ASP:OD2 | 3:C:3114[B]:PRO:CD | 2.02 | 1.07 |
| 3:C:3150[B]:LYS:NZ | 3:L:3160[B]:SER:HB3 | 1.56 | 1.07 |
| 3:C:3163[B]:ASN:HD22 | 3:L:3149[B]:ASN:ND2 | 1.51 | 1.07 |
| 3:C:3256[B]:TRP:CG | 3:L:2965[B]:LEU:O | 2.01 | 1.07 |
| 3:F:2972[B]:GLY:HA3 | 3:a:3090[B]:ASN:HB3 | 1.27 | 1.07 |
| 3:F:3113[A]:ASP:OD2 | 3:F:3114[A]:PRO:CD | 2.02 | 1.07 |
| 3:F:3159[B]:SER:CA | 3:a:3150[B]:LYS:C | 2.27 | 1.07 |
| 3:F:3293[A]:LYS:HD3 | 3:F:3294[A]:SER:HB3 | 1.13 | 1.07 |
| 3:I:2971[B]:ASP:O | 3:R:3090[B]:ASN:HA | 1.54 | 1.07 |
| 3:I:3113[B]:ASP:OD2 | 3:I:3114[B]:PRO:CD | 2.02 | 1.07 |
| 3:I:3256[B]:TRP:HB3 | 3:R:2966[B]:SER:HA | 1.10 | 1.07 |
| 3:L:3025[A]:VAL:HG22 | 3:L:3047[A]:ARG:HH12 | 1.19 | 1.07 |
| 3:O:2968[B]:GLN:CA | 3:X:2988[B]:TRP:HB2 | 1.82 | 1.07 |
| 3:O:3161[B]:GLU:OE2 | 3:O:3161[B]:GLU:N | 1.88 | 1.07 |
| 3:O:3185[B]:TYR:O | 3:O:3186[B]:GLU:OE2 | 1.72 | 1.07 |
| 3:R:3025[A]:VAL:HG22 | 3:R:3047[A]:ARG:HH12 | 1.19 | 1.07 |
| 3:U:2965[B]:LEU:HB2 | 3:d:3220[B]:ARG:NH1 | 1.66 | 1.07 |
| 3:U:3025[B]:VAL:HG22 | 3:U:3047[B]:ARG:HH12 | 1.19 | 1.07 |
| 3:U:3154[B]:PRO:CG | 3:d:2984[B]:THR:CG2 | 2.25 | 1.07 |
| 3:U:3162[B]:ASP:CG | 3:d:3259[B]:ASP:CB | 2.17 | 1.07 |
| 3:U:3185[A]:TYR:O | 3:U:3186[A]:GLU:OE2 | 1.72 | 1.07 |
| 3:X:3293[B]:LYS:HD3 | 3:X:3294[B]:SER:HB3 | 1.13 | 1.07 |
| 3:C:2965[B]:LEU:O | 3:L:3256[B]:TRP:C | 1.97 | 1.07 |
| 3:C:3113[A]:ASP:OD2 | 3:C:3114[A]:PRO:CD | 2.02 | 1.07 |
| 3:C:3150[B]:LYS:NZ | 3:L:3160[B]:SER:HB2 | 1.49 | 1.07 |
| 3:C:3172[B]:SER:HB3 | 3:L:3150[B]:LYS:CA | 1.84 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3230[A]:PHE:HB2 | 3:C:3243[A]:GLY:HA2 | 1.14 | 1.07 |
| 3:C:3255[B]:PRO:CB | 3:L:2964[B]:PRO:O | 2.02 | 1.07 |
| 3:F:2946[B]:GLN:OE1 | 3:F:2947[B]:ALA:N | 1.88 | 1.07 |
| 3:F:3159[B]:SER:CA | 3:a:3150[B]:LYS:O | 2.02 | 1.07 |
| 3:F:3185[A]:TYR:O | 3:F:3186[A]:GLU:OE2 | 1.72 | 1.07 |
| 2:H:2868:GLU:HG2 | 3:I:2932[A]:PRO:O | 1.54 | 1.07 |
| 3:I:3113[A]:ASP:OD2 | 3:I:3114[A]:PRO:CD | 2.02 | 1.07 |
| 3:I:3161[A]:GLU:N | 3:I:3161[A]:GLU:OE2 | 1.88 | 1.07 |
| 3:L:2960[B]:PHE:HD2 | 3:L:3157[B]:PRO:HG3 | 1.10 | 1.07 |
| 3:L:3113[A]:ASP:OD2 | 3:L:3114[A]:PRO:CD | 2.02 | 1.07 |
| 3:L:3161[B]:GLU:N | 3:L:3161[B]:GLU:OE2 | 1.88 | 1.07 |
| 3:O:2946[B]:GLN:OE1 | 3:O:2947[B]:ALA:N | 1.88 | 1.07 |
| 3:O:3161[A]:GLU:OE2 | 3:O:3161[A]:GLU:N | 1.88 | 1.07 |
| 3:R:3025[B]:VAL:HG22 | 3:R:3047[B]:ARG:HH12 | 1.19 | 1.07 |
| 3:R:3113[B]:ASP:OD2 | 3:R:3114[B]:PRO:CD | 2.02 | 1.07 |
| 3:R:3185[B]:TYR:O | 3:R:3186[B]:GLU:OE2 | 1.72 | 1.07 |
| 3:U:3152[B]:LYS:HG3 | 3:d:3154[B]:PRO:CB | 1.82 | 1.07 |
| 3:d:2930[B]:LEU:H | 3:d:2930[B]:LEU:HD22 | 1.18 | 1.07 |
| 3:d:3113[A]:ASP:OD2 | 3:d:3114[A]:PRO:CD | 2.02 | 1.07 |
| 3:C:2988[B]:TRP:HD1 | 3:L:3153[B]:LYS:HD3 | 1.18 | 1.07 |
| 3:C:3093[B]:HIS:CE1 | 3:L:2971[B]:ASP:CB | 2.33 | 1.07 |
| 3:C:3154[B]:PRO:HD3 | 3:L:3174[B]:GLY:N | 1.69 | 1.07 |
| 3:C:3154[B]:PRO:CB | 3:L:3174[B]:GLY:CA | 2.25 | 1.07 |
| 3:I:2961[B]:HIS:CG | 3:R:2969[B]:TYR:CD1 | 2.40 | 1.07 |
| 3:I:3025[B]:VAL:HG22 | 3:I:3047[B]:ARG:HH12 | 1.19 | 1.07 |
| 3:I:3160[B]:SER:H | 3:R:3150[B]:LYS:HD3 | 1.19 | 1.07 |
| 3:I:3172[B]:SER:H | 3:R:3152[B]:LYS:CB | 1.51 | 1.07 |
| 3:I:3230[A]:PHE:HB2 | 3:I:3243[A]:GLY:HA2 | 1.14 | 1.07 |
| 3:L:3113[B]:ASP:OD2 | 3:L:3114[B]:PRO:CD | 2.02 | 1.07 |
| 3:L:3185[A]:TYR:O | 3:L:3186[A]:GLU:OE2 | 1.72 | 1.07 |
| 3:L:3185[B]:TYR:O | 3:L:3186[B]:GLU:OE2 | 1.72 | 1.07 |
| 3:O:2976[B]:ALA:O | 3:X:3154[B]:PRO:HG2 | 0.90 | 1.07 |
| 3:O:3160[B]:SER:N | 3:X:3148[B]:ILE:O | 1.88 | 1.07 |
| 1:Y:1546:LYS:CG | 3:d:3001[B]:LYS:CE | 2.31 | 1.07 |
| 3:a:3025[A]:VAL:HG22 | 3:a:3047[A]:ARG:HH12 | 1.19 | 1.07 |
| 3:a:3113[A]:ASP:OD2 | 3:a:3114[A]:PRO:CD | 2.02 | 1.07 |
| 3:a:3185[A]:TYR:O | 3:a:3186[A]:GLU:OE2 | 1.72 | 1.07 |
| 3:F:2946[A]:GLN:OE1 | 3:F:2947[A]:ALA:N | 1.88 | 1.07 |
| 3:F:3135[B]:LYS:HG2 | 3:F:3141[B]:TYR:HE1 | 1.14 | 1.07 |
| 3:I:2956[B]:LYS:HD2 | 3:R:3257[B]:ALA:HB3 | 1.32 | 1.07 |
| 3:I:2982[B]:MET:HG2 | 3:R:2967[B]:CYS:SG | 1.91 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3160[B]:SER:CB | 3:R:2983[B]:VAL:H | 1.66 | 1.07 |
| 3:I:3217[B]:PHE:CE1 | 3:I:3230[B]:PHE:HZ | 1.71 | 1.07 |
| 3:I:3230[B]:PHE:HB2 | 3:I:3243[B]:GLY:HA2 | 1.14 | 1.07 |
| 3:L:3135[B]:LYS:HG2 | 3:L:3141[B]:TYR:CE1 | 1.89 | 1.07 |
| 3:L:3161[A]:GLU:N | 3:L:3161[A]:GLU:OE2 | 1.88 | 1.07 |
| 3:O:2975[B]:PHE:C | 3:X:3156[B]:MET:HG2 | 1.78 | 1.07 |
| 3:O:3185[A]:TYR:O | 3:O:3186[A]:GLU:OE2 | 1.72 | 1.07 |
| 3:U:2965[B]:LEU:HB2 | 3:d:3220[B]:ARG:CZ | 1.69 | 1.07 |
| 3:U:3161[A]:GLU:N | 3:U:3161[A]:GLU:OE2 | 1.88 | 1.07 |
| 3:U:3185[B]:TYR:O | 3:U:3186[B]:GLU:OE2 | 1.72 | 1.07 |
| 3:U:3256[B]:TRP:CB | 3:d:2969[B]:TYR:CB | 2.00 | 1.07 |
| 3:X:2946[B]:GLN:OE1 | 3:X:2947[B]:ALA:N | 1.88 | 1.07 |
| 3:X:3025[A]:VAL:HG22 | 3:X:3047[A]:ARG:HH12 | 1.19 | 1.07 |
| 3:X:3217[A]:PHE:CE1 | 3:X:3230[A]:PHE:HZ | 1.71 | 1.07 |
| 3:a:3113[B]:ASP:OD2 | 3:a:3114[B]:PRO:CD | 2.02 | 1.07 |
| 3:d:3230[A]:PHE:HB2 | 3:d:3243[A]:GLY:HA2 | 1.14 | 1.07 |
| 3:C:3185[B]:TYR:O | 3:C:3186[B]:GLU:OE2 | 1.72 | 1.06 |
| 3:F:3162[B]:ASP:HB3 | 3:a:3259[B]:ASP:CB | 1.85 | 1.06 |
| 3:I:3135[B]:LYS:HG2 | 3:I:3141[B]:TYR:HE1 | 1.14 | 1.06 |
| 3:I:3152[B]:LYS:CB | 3:R:3172[B]:SER:N | 1.77 | 1.06 |
| 3:L:2946[B]:GLN:OE1 | 3:L:2947[B]:ALA:N | 1.88 | 1.06 |
| 3:O:3251[B]:ASP:CB | 3:X:2967[B]:CYS:HA | 1.83 | 1.06 |
| 3:R:3113[A]:ASP:OD2 | 3:R:3114[A]:PRO:CD | 2.02 | 1.06 |
| 3:U:2946[A]:GLN:OE1 | 3:U:2947[A]:ALA:N | 1.88 | 1.06 |
| 3:X:3113[A]:ASP:OD2 | 3:X:3114[A]:PRO:CD | 2.02 | 1.06 |
| 3:X:3161[A]:GLU:N | 3:X:3161[A]:GLU:OE2 | 1.88 | 1.06 |
| 3:C:2983[B]:VAL:CG2 | 3:L:3161[B]:GLU:N | 2.08 | 1.06 |
| 3:C:3149[B]:ASN:HD22 | 3:L:3163[B]:ASN:CG | 1.63 | 1.06 |
| 3:C:3150[B]:LYS:HA | 3:L:3172[B]:SER:HB3 | 1.10 | 1.06 |
| 3:C:3153[B]:LYS:HZ3 | 3:L:2988[B]:TRP:NE1 | 1.53 | 1.06 |
| 3:C:3161[A]:GLU:OE2 | 3:C:3161[A]:GLU:N | 1.88 | 1.06 |
| 3:F:3135[A]:LYS:HG2 | 3:F:3141[A]:TYR:HE1 | 1.14 | 1.06 |
| 3:I:2946[B]:GLN:OE1 | 3:I:2947[B]:ALA:N | 1.88 | 1.06 |
| 3:I:3153[B]:LYS:C | 3:R:3155[B]:MET:CG | 2.22 | 1.06 |
| 3:I:3153[B]:LYS:CB | 3:R:3155[B]:MET:HB2 | 1.84 | 1.06 |
| 3:I:3259[B]:ASP:HB3 | 3:R:3162[B]:ASP:CB | 1.84 | 1.06 |
| 3:R:2946[B]:GLN:OE1 | 3:R:2947[B]:ALA:N | 1.88 | 1.06 |
| 3:R:3135[B]:LYS:HG2 | 3:R:3141[B]:TYR:CE1 | 1.89 | 1.06 |
| 3:R:3185[A]:TYR:O | 3:R:3186[A]:GLU:OE2 | 1.72 | 1.06 |
| 3:U:3217[A]:PHE:CE1 | 3:U:3230[A]:PHE:HZ | 1.71 | 1.06 |
| 3:X:3135[B]:LYS:HG2 | 3:X:3141[B]:TYR:CE1 | 1.89 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2930[B]:LEU:H | 3:a:2930[B]:LEU:HD22 | 1.18 | 1.06 |
| 3:d:2946[B]:GLN:OE1 | 3:d:2947[B]:ALA:N | 1.88 | 1.06 |
| 3:C:2985[B]:PHE:HE2 | 3:L:2969[B]:TYR:C | 1.60 | 1.06 |
| 3:C:3135[A]:LYS:HG2 | 3:C:3141[A]:TYR:HE1 | 1.14 | 1.06 |
| 3:F:2966[B]:SER:HB2 | 3:a:3254[B]:MET:HG3 | 1.09 | 1.06 |
| 3:F:3150[B]:LYS:HE3 | 3:a:3163[B]:ASN:CB | 1.84 | 1.06 |
| 3:F:3157[B]:PRO:O | 3:a:3150[B]:LYS:HE2 | 1.49 | 1.06 |
| 3:I:2956[B]:LYS:C | 3:I:2960[B]:PHE:HE1 | 1.63 | 1.06 |
| 3:I:2975[B]:PHE:HZ | 3:R:2961[B]:HIS:CG | 1.66 | 1.06 |
| 3:I:3150[B]:LYS:NZ | 3:R:3160[B]:SER:HB3 | 1.70 | 1.06 |
| 3:I:3160[B]:SER:OG | 3:R:2982[B]:MET:HA | 1.52 | 1.06 |
| 3:I:3185[B]:TYR:O | 3:I:3186[B]:GLU:OE2 | 1.72 | 1.06 |
| 3:I:3251[B]:ASP:O | 3:R:3252[B]:TYR:CB | 1.88 | 1.06 |
| 3:O:2969[B]:TYR:CB | 3:X:3158[B]:PHE:CE1 | 2.39 | 1.06 |
| 3:R:3217[A]:PHE:CE1 | 3:R:3230[A]:PHE:HZ | 1.71 | 1.06 |
| 3:U:3025[A]:VAL:HG22 | 3:U:3047[A]:ARG:HH12 | 1.19 | 1.06 |
| 3:a:2956[A]:LYS:C | 3:a:2960[A]:PHE:HE1 | 1.64 | 1.06 |
| 2:c:2867:PRO:HG3 | 3:d:2932[A]:PRO:CG | 1.85 | 1.06 |
| 3:d:2961[A]:HIS:NE2 | 3:d:2980[A]:HIS:NE2 | 2.04 | 1.06 |
| 3:d:2961[B]:HIS:NE2 | 3:d:2980[B]:HIS:NE2 | 2.04 | 1.06 |
| 3:C:3024[B]:LEU:HD12 | 3:C:3025[B]:VAL:H | 0.89 | 1.06 |
| 3:C:3154[B]:PRO:CA | 3:L:3153[B]:LYS:O | 2.04 | 1.06 |
| 3:C:3172[B]:SER:CB | 3:L:3152[B]:LYS:H | 1.68 | 1.06 |
| 3:F:2967[B]:CYS:N | 3:a:3256[B]:TRP:CD1 | 2.21 | 1.06 |
| 3:F:2970[B]:PRO:HD3 | 3:a:2989[B]:HIS:NE2 | 1.59 | 1.06 |
| 3:F:3222[B]:ILE:HD12 | 3:F:3223[B]:GLY:H | 1.20 | 1.06 |
| 3:I:3155[B]:MET:SD | 3:R:3154[B]:PRO:HG2 | 1.96 | 1.06 |
| 3:I:3162[B]:ASP:HB3 | 3:R:3259[B]:ASP:CB | 1.86 | 1.06 |
| 3:O:2970[B]:PRO:C | 3:X:2989[B]:HIS:N | 1.96 | 1.06 |
| 3:O:3108[B]:HIS:CB | 3:X:2969[B]:TYR:O | 2.00 | 1.06 |
| 3:U:2956[A]:LYS:C | 3:U:2960[A]:PHE:HE1 | 1.64 | 1.06 |
| 3:U:2961[A]:HIS:NE2 | 3:U:2980[A]:HIS:NE2 | 2.04 | 1.06 |
| 3:U:2961[B]:HIS:NE2 | 3:U:2980[B]:HIS:NE2 | 2.03 | 1.06 |
| 3:U:3161[B]:GLU:OE2 | 3:U:3161[B]:GLU:N | 1.88 | 1.06 |
| 3:X:2946[A]:GLN:OE1 | 3:X:2947[A]:ALA:N | 1.88 | 1.06 |
| 3:X:3185[B]:TYR:O | 3:X:3186[B]:GLU:OE2 | 1.72 | 1.06 |
| 3:d:3161[A]:GLU:N | 3:d:3161[A]:GLU:OE2 | 1.88 | 1.06 |
| 3:C:2946[B]:GLN:OE1 | 3:C:2947[B]:ALA:N | 1.88 | 1.06 |
| 3:C:2963[B]:MET:HE1 | 3:L:3223[B]:GLY:H | 1.21 | 1.06 |
| 3:C:3135[B]:LYS:HG2 | 3:C:3141[B]:TYR:HE1 | 1.14 | 1.06 |
| 3:F:2975[B]:PHE:O | 3:a:3253[B]:GLU:CB | 1.94 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3113[B]:ASP:OD2 | 3:F:3114[B]:PRO:CD | 2.02 | 1.06 |
| 3:I:2961[A]:HIS:NE2 | 3:I:2980[A]:HIS:NE2 | 2.03 | 1.06 |
| 3:I:2975[B]:PHE:CZ | 3:R:2961[B]:HIS:CA | 2.37 | 1.06 |
| 3:I:3135[A]:LYS:HG2 | 3:I:3141[A]:TYR:CE1 | 1.89 | 1.06 |
| 3:L:2930[A]:LEU:HD22 | 3:L:2930[A]:LEU:H | 1.18 | 1.06 |
| 3:O:2961[A]:HIS:NE2 | 3:O:2980[A]:HIS:NE2 | 2.04 | 1.06 |
| 3:O:3135[A]:LYS:HG2 | 3:O:3141[A]:TYR:CE1 | 1.89 | 1.06 |
| 3:O:3252[B]:TYR:HB3 | 3:X:3156[B]:MET:HB2 | 1.31 | 1.06 |
| 3:R:3161[A]:GLU:OE2 | 3:R:3161[A]:GLU:N | 1.88 | 1.06 |
| 3:U:3217[B]:PHE:CE1 | 3:U:3230[B]:PHE:HZ | 1.71 | 1.06 |
| 3:C:2946[A]:GLN:OE1 | 3:C:2947[A]:ALA:N | 1.88 | 1.05 |
| 3:C:2956[A]:LYS:C | 3:C:2960[A]:PHE:HE1 | 1.64 | 1.05 |
| 3:C:2983[B]:VAL:HG21 | 3:L:3161[B]:GLU:OE2 | 1.26 | 1.05 |
| 3:C:3024[A]:LEU:HD12 | 3:C:3025[A]:VAL:H | 0.89 | 1.05 |
| 3:C:3222[B]:ILE:HD12 | 3:C:3223[B]:GLY:H | 1.20 | 1.05 |
| 3:F:2956[B]:LYS:C | 3:F:2960[B]:PHE:HE1 | 1.64 | 1.05 |
| 3:F:3024[B]:LEU:HD12 | 3:F:3025[B]:VAL:H | 0.89 | 1.05 |
| 3:F:3153[B]:LYS:HZ1 | 3:a:3157[B]:PRO:CD | 1.68 | 1.05 |
| 3:I:2961[B]:HIS:CA | 3:R:2975[B]:PHE:HZ | 1.69 | 1.05 |
| 3:I:3256[B]:TRP:HB3 | 3:R:2966[B]:SER:CA | 1.86 | 1.05 |
| 3:R:2956[A]:LYS:C | 3:R:2960[A]:PHE:HE1 | 1.63 | 1.05 |
| 3:R:3024[A]:LEU:HD12 | 3:R:3025[A]:VAL:H | 0.89 | 1.05 |
| 3:R:3222[A]:ILE:HD12 | 3:R:3223[A]:GLY:H | 1.20 | 1.05 |
| 3:U:2975[B]:PHE:CD2 | 3:d:3256[B]:TRP:HD1 | 1.72 | 1.05 |
| 3:U:3024[A]:LEU:HD12 | 3:U:3025[A]:VAL:H | 0.89 | 1.05 |
| 3:X:3222[A]:ILE:HD12 | 3:X:3223[A]:GLY:H | 1.20 | 1.05 |
| 3:a:2956[B]:LYS:C | 3:a:2960[B]:PHE:HE1 | 1.64 | 1.05 |
| 3:a:3135[A]:LYS:HG2 | 3:a:3141[A]:TYR:CE1 | 1.89 | 1.05 |
| 3:d:3161[B]:GLU:OE2 | 3:d:3161[B]:GLU:N | 1.88 | 1.05 |
| 3:d:3185[A]:TYR:O | 3:d:3186[A]:GLU:OE2 | 1.72 | 1.05 |
| 3:C:3155[B]:MET:SD | 3:L:3154[B]:PRO:HD2 | 1.96 | 1.05 |
| 3:C:3156[B]:MET:SD | 3:L:2982[B]:MET:HG3 | 1.96 | 1.05 |
| 3:C:3161[B]:GLU:N | 3:C:3161[B]:GLU:OE2 | 1.88 | 1.05 |
| 3:C:3185[A]:TYR:O | 3:C:3186[A]:GLU:OE2 | 1.72 | 1.05 |
| 3:F:3217[A]:PHE:CE1 | 3:F:3230[A]:PHE:HZ | 1.71 | 1.05 |
| 3:I:2960[A]:PHE:HD2 | 3:I:3157[A]:PRO:HG3 | 1.10 | 1.05 |
| 3:I:2989[B]:HIS:NE2 | 3:R:2969[B]:TYR:CA | 2.20 | 1.05 |
| 3:I:3150[B]:LYS:HG2 | 3:R:3158[B]:PHE:HA | 1.29 | 1.05 |
| 3:L:2930[B]:LEU:H | 3:L:2930[B]:LEU:HD22 | 1.18 | 1.05 |
| 3:O:3160[B]:SER:CB | 3:X:3151[B]:LEU:H | 1.67 | 1.05 |
| 3:R:3222[B]:ILE:HD12 | 3:R:3223[B]:GLY:H | 1.20 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2956[B]:LYS:C | 3:U:2960[B]:PHE:HE1 | 1.64 | 1.05 |
| 3:U:3135[B]:LYS:HG2 | 3:U:3141[B]:TYR:HE1 | 1.14 | 1.05 |
| 3:X:2960[B]:PHE:HD2 | 3:X:3157[B]:PRO:HG3 | 1.10 | 1.05 |
| 3:a:2946[A]:GLN:OE1 | 3:a:2947[A]:ALA:N | 1.88 | 1.05 |
| 1:A:416:ASN:CG | 3:F:3196[A]:THR:HG21 | 1.81 | 1.05 |
| 3:C:2930[A]:LEU:H | 3:C:2930[A]:LEU:HD22 | 1.18 | 1.05 |
| 3:C:2961[A]:HIS:NE2 | 3:C:2980[A]:HIS:NE2 | 2.04 | 1.05 |
| 3:C:3174[B]:GLY:CA | 3:L:3154[B]:PRO:HD3 | 1.86 | 1.05 |
| 3:C:3222[A]:ILE:HD12 | 3:C:3223[A]:GLY:H | 1.20 | 1.05 |
| 3:F:2982[B]:MET:CE | 3:a:2977[B]:CYS:HB2 | 1.85 | 1.05 |
| 3:I:2969[B]:TYR:OH | 3:R:3116[B]:PHE:CD1 | 0.78 | 1.05 |
| 3:I:3149[B]:ASN:ND2 | 3:R:3163[B]:ASN:CG | 2.14 | 1.05 |
| 3:I:3156[B]:MET:HB2 | 3:R:2982[B]:MET:CG | 1.86 | 1.05 |
| 3:I:3251[B]:ASP:HB2 | 3:R:3251[B]:ASP:HB3 | 1.36 | 1.05 |
| 3:O:2946[A]:GLN:OE1 | 3:O:2947[A]:ALA:N | 1.88 | 1.05 |
| 3:O:3156[B]:MET:CG | 3:X:3173[B]:THR:HG23 | 1.86 | 1.05 |
| 3:O:3160[B]:SER:HA | 3:X:3151[B]:LEU:HD12 | 1.34 | 1.05 |
| 3:R:2961[A]:HIS:NE2 | 3:R:2980[A]:HIS:NE2 | 2.04 | 1.05 |
| 3:U:3135[A]:LYS:HG2 | 3:U:3141[A]:TYR:CE1 | 1.89 | 1.05 |
| 3:U:3169[B]:LYS:HE2 | 3:d:3146[B]:CYS:CA | 1.84 | 1.05 |
| 3:U:3220[B]:ARG:HG2 | 3:d:2973[B]:THR:HG22 | 1.36 | 1.05 |
| 3:X:2948[A]:ASP:HB3 | 3:X:2953[A]:GLY:HA3 | 1.39 | 1.05 |
| 3:X:2961[B]:HIS:NE2 | 3:X:2980[B]:HIS:NE2 | 2.04 | 1.05 |
| 3:X:3161[B]:GLU:N | 3:X:3161[B]:GLU:OE2 | 1.88 | 1.05 |
| 3:a:2946[B]:GLN:OE1 | 3:a:2947[B]:ALA:N | 1.88 | 1.05 |
| 3:a:3161[B]:GLU:N | 3:a:3161[B]:GLU:OE2 | 1.88 | 1.05 |
| 3:C:2988[B]:TRP:HE1 | 3:L:3153[B]:LYS:NZ | 1.55 | 1.05 |
| 3:C:3135[A]:LYS:HG2 | 3:C:3141[A]:TYR:CE1 | 1.89 | 1.05 |
| 3:C:3150[B]:LYS:C | 3:L:3172[B]:SER:CB | 2.29 | 1.05 |
| 3:C:3153[B]:LYS:O | 3:L:3154[B]:PRO:CA | 2.05 | 1.05 |
| 3:C:3160[B]:SER:HB3 | 3:L:3150[B]:LYS:NZ | 1.53 | 1.05 |
| 3:F:3185[B]:TYR:O | 3:F:3186[B]:GLU:OE2 | 1.72 | 1.05 |
| 3:F:3251[B]:ASP:CB | 3:a:3251[B]:ASP:CB | 1.76 | 1.05 |
| 3:I:2956[A]:LYS:C | 3:I:2960[A]:PHE:HE1 | 1.64 | 1.05 |
| 3:I:3024[A]:LEU:HD12 | 3:I:3025[A]:VAL:H | 0.89 | 1.05 |
| 3:I:3135[B]:LYS:HG2 | 3:I:3141[B]:TYR:CE1 | 1.89 | 1.05 |
| 3:I:3259[B]:ASP:HB3 | 3:R:3162[B]:ASP:HB3 | 1.07 | 1.05 |
| 3:O:2961[B]:HIS:NE2 | 3:O:2980[B]:HIS:NE2 | 2.03 | 1.05 |
| 3:O:2963[B]:MET:HE3 | 3:X:2975[B]:PHE:CD1 | 1.86 | 1.05 |
| 3:O:3158[B]:PHE:N | 3:X:3152[B]:LYS:CB | 2.19 | 1.05 |
| 3:O:3163[B]:ASN:CA | 3:X:3149[B]:ASN:HB3 | 1.84 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3135[A]:LYS:HG2 | 3:U:3141[A]:TYR:HE1 | 1.14 | 1.05 |
| 3:a:3161[A]:GLU:N | 3:a:3161[A]:GLU:OE2 | 1.88 | 1.05 |
| 3:a:3185[B]:TYR:O | 3:a:3186[B]:GLU:OE2 | 1.72 | 1.05 |
| 3:d:3025[A]:VAL:HG22 | 3:d:3047[A]:ARG:HH12 | 1.19 | 1.05 |
| 3:d:3141[B]:TYR:CD2 | 3:d:3142[B]:ASN:N | 2.24 | 1.05 |
| 3:d:3217[A]:PHE:CE1 | 3:d:3230[A]:PHE:HZ | 1.71 | 1.05 |
| 3:C:2948[B]:ASP:HB3 | 3:C:2953[B]:GLY:HA3 | 1.39 | 1.05 |
| 3:F:2959[B]:SER:CB | 3:a:3255[B]:PRO:HB2 | 1.87 | 1.05 |
| 3:F:2961[A]:HIS:NE2 | 3:F:2980[A]:HIS:NE2 | 2.03 | 1.05 |
| 3:F:2981[B]:GLY:CA | 3:a:2968[B]:GLN:OE1 | 2.05 | 1.05 |
| 3:F:3170[B]:ALA:O | 3:a:3152[B]:LYS:HD2 | 0.89 | 1.05 |
| 3:F:3256[B]:TRP:HB3 | 3:a:2966[B]:SER:HA | 1.09 | 1.05 |
| 3:I:2959[B]:SER:CA | 3:R:3255[B]:PRO:HB2 | 1.80 | 1.05 |
| 3:I:2964[B]:PRO:CB | 3:R:3221[B]:ALA:HB3 | 1.86 | 1.05 |
| 3:I:2971[B]:ASP:OD2 | 3:R:3110[B]:THR:HG21 | 1.56 | 1.05 |
| 3:I:3141[B]:TYR:CD2 | 3:I:3142[B]:ASN:N | 2.24 | 1.05 |
| 3:L:2956[B]:LYS:C | 3:L:2960[B]:PHE:HE1 | 1.64 | 1.05 |
| 3:L:3024[B]:LEU:HD12 | 3:L:3025[B]:VAL:H | 0.89 | 1.05 |
| 3:O:3101[B]:PRO:HB2 | 3:X:2971[B]:ASP:O | 0.87 | 1.05 |
| 3:O:3141[A]:TYR:CD2 | 3:O:3142[A]:ASN:N | 2.23 | 1.05 |
| 3:O:3253[B]:GLU:CD | 3:X:3161[B]:GLU:OE1 | 1.99 | 1.05 |
| 3:R:2948[A]:ASP:HB3 | 3:R:2953[A]:GLY:HA3 | 1.39 | 1.05 |
| 3:d:2946[A]:GLN:OE1 | 3:d:2947[A]:ALA:N | 1.88 | 1.05 |
| 3:d:3025[B]:VAL:HG22 | 3:d:3047[B]:ARG:HH12 | 1.19 | 1.05 |
| 3:d:3135[A]:LYS:HG2 | 3:d:3141[A]:TYR:CE1 | 1.89 | 1.05 |
| 3:d:3185[B]:TYR:O | 3:d:3186[B]:GLU:OE2 | 1.72 | 1.05 |
| 3:C:2978[B]:CYS:N | 3:L:3254[B]:MET:HB3 | 1.19 | 1.04 |
| 3:C:3147[B]:GLU:CG | 3:L:3161[B]:GLU:CA | 2.29 | 1.04 |
| 3:C:3154[B]:PRO:C | 3:L:3153[B]:LYS:O | 2.00 | 1.04 |
| 3:C:3163[B]:ASN:ND2 | 3:L:3149[B]:ASN:HB2 | 1.68 | 1.04 |
| 3:C:3163[B]:ASN:HD21 | 3:L:3149[B]:ASN:HB3 | 1.09 | 1.04 |
| 3:C:3169[B]:LYS:HE3 | 3:L:3149[B]:ASN:OD1 | 1.51 | 1.04 |
| 3:C:3172[B]:SER:OG | 3:L:3152[B]:LYS:HG3 | 1.57 | 1.04 |
| 3:F:2930[B]:LEU:H | 3:F:2930[B]:LEU:HD22 | 1.18 | 1.04 |
| 3:F:2948[B]:ASP:HB3 | 3:F:2953[B]:GLY:HA3 | 1.39 | 1.04 |
| 3:F:2956[A]:LYS:C | 3:F:2960[A]:PHE:HE1 | 1.64 | 1.04 |
| 3:F:3150[B]:LYS:HZ3 | 3:a:3160[B]:SER:CB | 1.66 | 1.04 |
| 3:I:2946[A]:GLN:OE1 | 3:I:2947[A]:ALA:N | 1.88 | 1.04 |
| 3:I:3090[B]:ASN:HB3 | 3:R:2972[B]:GLY:HA3 | 1.37 | 1.04 |
| 3:I:3141[A]:TYR:CD2 | 3:I:3142[A]:ASN:N | 2.24 | 1.04 |
| 3:L:2946[A]:GLN:OE1 | 3:L:2947[A]:ALA:N | 1.88 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:2956[A]:LYS:C | 3:L:2960[A]:PHE:HE1 | 1.64 | 1.04 |
| 3:L:2961[A]:HIS:NE2 | 3:L:2980[A]:HIS:NE2 | 2.04 | 1.04 |
| 3:L:2966[B]:SER:HB2 | 3:L:2977[B]:CYS:HB2 | 1.39 | 1.04 |
| 3:L:3135[A]:LYS:HG2 | 3:L:3141[A]:TYR:CE1 | 1.89 | 1.04 |
| 3:O:2948[A]:ASP:HB3 | 3:O:2953[A]:GLY:HA3 | 1.39 | 1.04 |
| 3:O:2956[A]:LYS:C | 3:O:2960[A]:PHE:HE1 | 1.64 | 1.04 |
| 3:O:2970[B]:PRO:HG2 | 3:X:2991[B]:LEU:HA | 1.32 | 1.04 |
| 3:R:2956[B]:LYS:C | 3:R:2960[B]:PHE:HE1 | 1.64 | 1.04 |
| 3:R:2966[A]:SER:HB2 | 3:R:2977[A]:CYS:HB2 | 1.39 | 1.04 |
| 3:R:3135[B]:LYS:HG2 | 3:R:3141[B]:TYR:HE1 | 1.14 | 1.04 |
| 3:U:2946[B]:GLN:OE1 | 3:U:2947[B]:ALA:N | 1.88 | 1.04 |
| 3:U:3176[B]:LYS:HD2 | 3:d:3152[B]:LYS:HD2 | 1.07 | 1.04 |
| 3:a:3025[B]:VAL:HG22 | 3:a:3047[B]:ARG:HH12 | 1.19 | 1.04 |
| 3:C:2956[B]:LYS:C | 3:C:2960[B]:PHE:HE1 | 1.64 | 1.04 |
| 3:F:3155[B]:MET:CB | 3:a:3153[B]:LYS:CG | 2.21 | 1.04 |
| 3:F:3161[A]:GLU:N | 3:F:3161[A]:GLU:OE2 | 1.88 | 1.04 |
| 3:I:3025[A]:VAL:HG22 | 3:I:3047[A]:ARG:HH12 | 1.19 | 1.04 |
| 3:I:3038[B]:ILE:HG12 | 3:I:3112[B]:TYR:CD2 | 1.93 | 1.04 |
| 3:I:3196[A]:THR:HG21 | 1:J:416:ASN:CG | 1.81 | 1.04 |
| 3:U:3255[B]:PRO:HB2 | 3:d:2975[B]:PHE:HA | 1.37 | 1.04 |
| 3:X:2948[B]:ASP:HB3 | 3:X:2953[B]:GLY:HA3 | 1.39 | 1.04 |
| 3:X:2961[A]:HIS:NE2 | 3:X:2980[A]:HIS:NE2 | 2.04 | 1.04 |
| 3:X:3024[A]:LEU:HD12 | 3:X:3025[A]:VAL:H | 0.89 | 1.04 |
| 1:Y:1616:LYS:CD | 3:d:3187[B]:TYR:HA | 1.79 | 1.04 |
| 3:a:2948[A]:ASP:HB3 | 3:a:2953[A]:GLY:HA3 | 1.39 | 1.04 |
| 3:C:2985[B]:PHE:CE2 | 3:L:2970[B]:PRO:N | 2.26 | 1.04 |
| 3:C:3147[B]:GLU:HG3 | 3:L:3160[B]:SER:O | 0.87 | 1.04 |
| 3:C:3160[B]:SER:HB3 | 3:L:3150[B]:LYS:HZ2 | 1.00 | 1.04 |
| 3:C:3169[B]:LYS:HG3 | 3:L:3149[B]:ASN:CG | 1.67 | 1.04 |
| 3:C:3259[B]:ASP:CG | 3:L:3162[B]:ASP:OD1 | 1.98 | 1.04 |
| 3:F:3147[B]:GLU:OE1 | 3:a:3162[B]:ASP:C | 1.99 | 1.04 |
| 3:I:3153[B]:LYS:HD2 | 3:R:3155[B]:MET:CB | 1.86 | 1.04 |
| 3:I:3185[A]:TYR:O | 3:I:3186[A]:GLU:OE2 | 1.72 | 1.04 |
| 3:I:3256[B]:TRP:NE1 | 3:R:2965[B]:LEU:HB3 | 1.41 | 1.04 |
| 3:R:2946[A]:GLN:OE1 | 3:R:2947[A]:ALA:N | 1.88 | 1.04 |
| 3:R:2966[B]:SER:HB2 | 3:R:2977[B]:CYS:HB2 | 1.39 | 1.04 |
| 3:R:3038[A]:ILE:HG12 | 3:R:3112[A]:TYR:CD2 | 1.93 | 1.04 |
| 3:R:3135[A]:LYS:HG2 | 3:R:3141[A]:TYR:CE1 | 1.89 | 1.04 |
| 3:R:3141[A]:TYR:CD2 | 3:R:3142[A]:ASN:N | 2.24 | 1.04 |
| 3:U:2965[B]:LEU:CD1 | 3:d:3256[B]:TRP:O | 2.06 | 1.04 |
| 3:U:2969[B]:TYR:N | 3:d:3256[B]:TRP:CE2 | 2.02 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2956[A]:LYS:C | 3:d:2960[A]:PHE:HE1 | 1.64 | 1.04 |
| 3:C:3038[B]:ILE:HG12 | 3:C:3112[B]:TYR:CD2 | 1.93 | 1.04 |
| 3:C:3153[B]:LYS:NZ | 3:L:3158[B]:PHE:HD2 | 1.49 | 1.04 |
| 3:C:3156[B]:MET:CE | 3:L:2979[B]:GLN:CG | 1.93 | 1.04 |
| 3:F:2966[B]:SER:HA | 3:a:3255[B]:PRO:C | 1.82 | 1.04 |
| 3:F:3038[B]:ILE:HG12 | 3:F:3112[B]:TYR:CD2 | 1.93 | 1.04 |
| 3:F:3161[B]:GLU:HA | 3:a:3147[B]:GLU:CG | 1.87 | 1.04 |
| 3:F:3163[B]:ASN:HD22 | 3:a:3150[B]:LYS:HG3 | 1.17 | 1.04 |
| 2:H:2868:GLU:OE2 | 3:I:2932[A]:PRO:O | 1.75 | 1.04 |
| 3:I:2930[B]:LEU:H | 3:I:2930[B]:LEU:HD22 | 1.18 | 1.04 |
| 3:I:3024[B]:LEU:HD12 | 3:I:3025[B]:VAL:H | 0.89 | 1.04 |
| 3:I:3149[B]:ASN:HD22 | 3:R:3163[B]:ASN:CG | 1.65 | 1.04 |
| 3:L:2948[B]:ASP:HB3 | 3:L:2953[B]:GLY:HA3 | 1.39 | 1.04 |
| 3:O:2956[B]:LYS:C | 3:O:2960[B]:PHE:HE1 | 1.64 | 1.04 |
| 3:O:3106[B]:THR:HG21 | 3:X:2970[B]:PRO:O | 1.57 | 1.04 |
| 3:U:2973[B]:THR:HG22 | 3:d:3222[B]:ILE:CG2 | 1.87 | 1.04 |
| 3:U:3169[B]:LYS:CG | 3:d:3148[B]:ILE:N | 2.05 | 1.04 |
| 3:X:2956[A]:LYS:C | 3:X:2960[A]:PHE:HE1 | 1.64 | 1.04 |
| 3:a:2961[A]:HIS:NE2 | 3:a:2980[A]:HIS:NE2 | 2.04 | 1.04 |
| 3:a:3024[B]:LEU:HD12 | 3:a:3025[B]:VAL:H | 0.89 | 1.04 |
| 3:d:2930[A]:LEU:HD22 | 3:d:2930[A]:LEU:H | 1.18 | 1.04 |
| 3:d:3024[B]:LEU:HD12 | 3:d:3025[B]:VAL:H | 0.89 | 1.04 |
| 3:d:3038[A]:ILE:HG12 | 3:d:3112[A]:TYR:CD2 | 1.93 | 1.04 |
| 3:d:3141[A]:TYR:CD2 | 3:d:3142[A]:ASN:N | 2.24 | 1.04 |
| 3:C:2963[B]:MET:HE1 | 3:L:3222[B]:ILE:HD12 | 1.38 | 1.04 |
| 3:C:3038[A]:ILE:HG12 | 3:C:3112[A]:TYR:CD2 | 1.93 | 1.04 |
| 3:C:3141[A]:TYR:CD2 | 3:C:3142[A]:ASN:N | 2.24 | 1.04 |
| 3:F:3153[B]:LYS:HB2 | 3:a:3158[B]:PHE:HB2 | 1.38 | 1.04 |
| 3:I:2968[B]:GLN:NE2 | 3:R:3086[B]:GLU:HG2 | 1.21 | 1.04 |
| 3:I:3156[B]:MET:CB | 3:R:2982[B]:MET:HG3 | 1.87 | 1.04 |
| 3:L:3038[A]:ILE:HG12 | 3:L:3112[A]:TYR:CD2 | 1.93 | 1.04 |
| 3:L:3307[A]:PHE:HE1 | 3:L:3309[A]:PRO:HG3 | 1.23 | 1.04 |
| 3:O:3025[A]:VAL:HG22 | 3:O:3047[A]:ARG:HH12 | 1.19 | 1.04 |
| 3:O:3135[B]:LYS:HG2 | 3:O:3141[B]:TYR:CE1 | 1.89 | 1.04 |
| 3:U:2971[B]:ASP:O | 3:d:3247[B]:VAL:CA | 2.05 | 1.04 |
| 3:U:3307[B]:PHE:HE1 | 3:U:3309[B]:PRO:HG3 | 1.23 | 1.04 |
| 3:X:2930[B]:LEU:H | 3:X:2930[B]:LEU:HD22 | 1.18 | 1.04 |
| 3:a:3038[A]:ILE:HG12 | 3:a:3112[A]:TYR:CD2 | 1.93 | 1.04 |
| 3:d:3024[A]:LEU:HD12 | 3:d:3025[A]:VAL:H | 0.89 | 1.04 |
| 3:C:2961[B]:HIS:NE2 | 3:C:2980[B]:HIS:NE2 | 2.03 | 1.03 |
| 3:C:2966[A]:SER:HB2 | 3:C:2977[A]:CYS:HB2 | 1.39 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3141[B]:TYR:CD2 | 3:C:3142[B]:ASN:N | 2.24 | 1.03 |
| 3:C:3158[B]:PHE:CE2 | 3:L:3153[B]:LYS:HE2 | 1.92 | 1.03 |
| 3:F:3024[A]:LEU:HD12 | 3:F:3025[A]:VAL:H | 0.89 | 1.03 |
| 3:F:3253[B]:GLU:HB2 | 3:a:2975[B]:PHE:O | 1.55 | 1.03 |
| 1:G:1636:ASN:OD1 | 6:r:1:NAG:C8 | 2.05 | 1.03 |
| 2:H:2868:GLU:CD | 3:I:2932[A]:PRO:O | 2.01 | 1.03 |
| 3:I:2959[B]:SER:HB2 | 3:R:3255[B]:PRO:CB | 1.86 | 1.03 |
| 3:I:3038[A]:ILE:HG12 | 3:I:3112[A]:TYR:CD2 | 1.93 | 1.03 |
| 3:L:3307[B]:PHE:HE1 | 3:L:3309[B]:PRO:HG3 | 1.23 | 1.03 |
| 3:O:2969[B]:TYR:CB | 3:X:3158[B]:PHE:CZ | 2.40 | 1.03 |
| 3:O:2975[B]:PHE:HE2 | 3:X:3172[B]:SER:CA | 1.71 | 1.03 |
| 1:S:416:ASN:OD1 | 3:X:3196[A]:THR:OG1 | 1.74 | 1.03 |
| 3:X:3025[B]:VAL:HG22 | 3:X:3047[B]:ARG:HH12 | 1.19 | 1.03 |
| 3:a:2966[A]:SER:HB2 | 3:a:2977[A]:CYS:HB2 | 1.39 | 1.03 |
| 3:a:3038[B]:ILE:HG12 | 3:a:3112[B]:TYR:CD2 | 1.93 | 1.03 |
| 3:a:3135[B]:LYS:HG2 | 3:a:3141[B]:TYR:CE1 | 1.89 | 1.03 |
| 3:a:3135[B]:LYS:HG2 | 3:a:3141[B]:TYR:HE1 | 1.14 | 1.03 |
| 3:a:3307[A]:PHE:HE1 | 3:a:3309[A]:PRO:HG3 | 1.23 | 1.03 |
| 3:d:3222[A]:ILE:HD12 | 3:d:3223[A]:GLY:H | 1.20 | 1.03 |
| 3:C:3154[B]:PRO:CD | 3:L:3174[B]:GLY:N | 2.21 | 1.03 |
| 3:C:3161[B]:GLU:OE2 | 3:L:2983[B]:VAL:CG2 | 2.07 | 1.03 |
| 3:F:2948[B]:ASP:H | 3:F:2949[B]:LYS:HA | 1.23 | 1.03 |
| 3:F:3153[B]:LYS:CD | 3:a:3155[B]:MET:HB3 | 1.88 | 1.03 |
| 3:F:3161[B]:GLU:HG3 | 3:a:3079[B]:CYS:SG | 1.93 | 1.03 |
| 3:I:2948[A]:ASP:H | 3:I:2949[A]:LYS:HA | 1.23 | 1.03 |
| 3:I:3159[B]:SER:CA | 3:R:3150[B]:LYS:O | 2.05 | 1.03 |
| 3:I:3162[B]:ASP:HB3 | 3:R:3259[B]:ASP:HB3 | 1.37 | 1.03 |
| 3:I:3251[B]:ASP:O | 3:R:3252[B]:TYR:HB2 | 1.54 | 1.03 |
| 3:L:3217[A]:PHE:CE1 | 3:L:3230[A]:PHE:HZ | 1.71 | 1.03 |
| 3:O:2965[B]:LEU:HD12 | 3:X:2979[B]:GLN:OE1 | 0.86 | 1.03 |
| 3:R:3307[B]:PHE:HE1 | 3:R:3309[B]:PRO:HG3 | 1.23 | 1.03 |
| 3:U:2965[B]:LEU:O | 3:d:3257[B]:ALA:HB1 | 1.56 | 1.03 |
| 3:U:3024[B]:LEU:HD12 | 3:U:3025[B]:VAL:H | 0.89 | 1.03 |
| 3:X:2956[B]:LYS:C | 3:X:2960[B]:PHE:HE1 | 1.64 | 1.03 |
| 3:X:3038[A]:ILE:HG12 | 3:X:3112[A]:TYR:CD2 | 1.93 | 1.03 |
| 1:Y:1656:ASP:O | 3:d:2937[B]:ASN:ND2 | 1.91 | 1.03 |
| 3:C:2975[B]:PHE:C | 3:L:3253[B]:GLU:HB2 | 1.84 | 1.03 |
| 3:C:3025[B]:VAL:HG22 | 3:C:3047[B]:ARG:HH12 | 1.19 | 1.03 |
| 3:C:3163[B]:ASN:H | 3:L:3147[B]:GLU:CD | 1.66 | 1.03 |
| 3:F:2968[B]:GLN:HG2 | 3:a:2981[B]:GLY:N | 1.72 | 1.03 |
| 3:I:2982[B]:MET:HG3 | 3:R:2967[B]:CYS:SG | 1.94 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3150[B]:LYS:HD3 | 3:R:3160[B]:SER:H | 1.20 | 1.03 |
| 3:I:3154[B]:PRO:HB3 | 3:R:3174[B]:GLY:HA2 | 1.40 | 1.03 |
| 3:I:3222[A]:ILE:HD12 | 3:I:3223[A]:GLY:H | 1.20 | 1.03 |
| 3:L:2948[A]:ASP:HB3 | 3:L:2953[A]:GLY:HA3 | 1.39 | 1.03 |
| 3:L:3222[B]:ILE:HD12 | 3:L:3223[B]:GLY:H | 1.20 | 1.03 |
| 3:O:2975[B]:PHE:C | 3:X:3156[B]:MET:CG | 2.31 | 1.03 |
| 3:O:3040[B]:VAL:CG2 | 3:X:2969[B]:TYR:CE1 | 2.42 | 1.03 |
| 3:O:3222[A]:ILE:HD12 | 3:O:3223[A]:GLY:H | 1.20 | 1.03 |
| 3:R:2951[B]:ASP:O | 3:R:2956[B]:LYS:NZ | 1.92 | 1.03 |
| 3:R:3038[B]:ILE:HG12 | 3:R:3112[B]:TYR:CD2 | 1.93 | 1.03 |
| 3:U:2966[B]:SER:HB2 | 3:U:2977[B]:CYS:HB2 | 1.39 | 1.03 |
| 3:U:3154[B]:PRO:HG3 | 3:d:2984[B]:THR:HG21 | 1.20 | 1.03 |
| 3:a:3024[A]:LEU:HD12 | 3:a:3025[A]:VAL:H | 0.89 | 1.03 |
| 3:a:3307[B]:PHE:HE1 | 3:a:3309[B]:PRO:HG3 | 1.23 | 1.03 |
| 3:d:2956[B]:LYS:C | 3:d:2960[B]:PHE:HE1 | 1.64 | 1.03 |
| 3:d:3298[B]:ASN:ND2 | 3:d:3301[B]:PRO:HA | 1.74 | 1.03 |
| 3:C:2951[B]:ASP:O | 3:C:2956[B]:LYS:NZ | 1.92 | 1.03 |
| 3:C:2969[B]:TYR:CA | 3:L:2985[B]:PHE:HE2 | 1.71 | 1.03 |
| 3:F:3025[A]:VAL:HG22 | 3:F:3047[A]:ARG:HH12 | 1.19 | 1.03 |
| 3:F:3162[B]:ASP:CB | 3:a:3259[B]:ASP:HB3 | 1.88 | 1.03 |
| 3:F:3217[B]:PHE:CE1 | 3:F:3230[B]:PHE:HZ | 1.71 | 1.03 |
| 3:F:3298[B]:ASN:ND2 | 3:F:3301[B]:PRO:HA | 1.74 | 1.03 |
| 3:I:2951[B]:ASP:O | 3:I:2956[B]:LYS:NZ | 1.92 | 1.03 |
| 3:L:3298[A]:ASN:ND2 | 3:L:3301[A]:PRO:HA | 1.74 | 1.03 |
| 3:O:3038[B]:ILE:HG12 | 3:O:3112[B]:TYR:CD2 | 1.93 | 1.03 |
| 3:O:3217[B]:PHE:CE1 | 3:O:3230[B]:PHE:HZ | 1.71 | 1.03 |
| 3:R:2948[B]:ASP:HB3 | 3:R:2953[B]:GLY:HA3 | 1.39 | 1.03 |
| 3:U:2948[A]:ASP:HB3 | 3:U:2953[A]:GLY:HA3 | 1.39 | 1.03 |
| 3:U:2965[B]:LEU:HD12 | 3:d:3220[B]:ARG:HA | 1.04 | 1.03 |
| 3:U:2969[B]:TYR:OH | 3:d:3107[B]:LEU:HD12 | 1.58 | 1.03 |
| 3:U:3038[A]:ILE:HG12 | 3:U:3112[A]:TYR:CD2 | 1.93 | 1.03 |
| 3:U:3169[B]:LYS:C | 3:d:3148[B]:ILE:CB | 2.30 | 1.03 |
| 3:X:3135[A]:LYS:HG2 | 3:X:3141[A]:TYR:CE1 | 1.89 | 1.03 |
| 3:d:2951[A]:ASP:O | 3:d:2956[A]:LYS:NZ | 1.92 | 1.03 |
| 3:C:2961[B]:HIS:CE1 | 3:C:2980[B]:HIS:HE2 | 1.77 | 1.03 |
| 3:C:2982[B]:MET:HB3 | 3:L:3156[B]:MET:CB | 1.74 | 1.03 |
| 3:C:2983[B]:VAL:HG21 | 3:L:3160[B]:SER:C | 1.83 | 1.03 |
| 3:C:3156[B]:MET:HB3 | 3:L:2982[B]:MET:HB3 | 1.39 | 1.03 |
| 3:F:2948[A]:ASP:H | 3:F:2949[A]:LYS:HA | 1.23 | 1.03 |
| 3:F:2966[B]:SER:HB2 | 3:a:3254[B]:MET:CG | 1.87 | 1.03 |
| 3:F:2982[B]:MET:HE2 | 3:a:2967[B]:CYS:SG | 1.91 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3141[B]:TYR:CD2 | 3:F:3142[B]:ASN:N | 2.23 | 1.03 |
| 3:F:3172[B]:SER:N | 3:a:3152[B]:LYS:HB2 | 1.72 | 1.03 |
| 3:I:2930[A]:LEU:HD22 | 3:I:2930[A]:LEU:H | 1.18 | 1.03 |
| 3:I:2975[B]:PHE:HA | 3:R:3107[B]:LEU:CD2 | 1.88 | 1.03 |
| 3:I:2979[B]:GLN:HA | 3:R:2977[B]:CYS:SG | 1.98 | 1.03 |
| 3:I:3155[B]:MET:HB2 | 3:R:3153[B]:LYS:HD2 | 1.07 | 1.03 |
| 3:L:3151[A]:LEU:HB2 | 3:L:3175[A]:TYR:CE2 | 1.94 | 1.03 |
| 3:L:3298[B]:ASN:ND2 | 3:L:3301[B]:PRO:HA | 1.74 | 1.03 |
| 3:O:2948[A]:ASP:H | 3:O:2949[A]:LYS:HA | 1.23 | 1.03 |
| 3:O:3024[B]:LEU:HD12 | 3:O:3025[B]:VAL:H | 0.89 | 1.03 |
| 3:R:3217[B]:PHE:CE1 | 3:R:3230[B]:PHE:HZ | 1.71 | 1.03 |
| 3:U:3151[A]:LEU:HB2 | 3:U:3175[A]:TYR:CE2 | 1.94 | 1.03 |
| 3:X:2948[A]:ASP:H | 3:X:2949[A]:LYS:HA | 1.24 | 1.03 |
| 3:X:2951[B]:ASP:O | 3:X:2956[B]:LYS:NZ | 1.92 | 1.03 |
| 3:X:2966[A]:SER:HB2 | 3:X:2977[A]:CYS:HB2 | 1.39 | 1.03 |
| 3:X:3298[A]:ASN:ND2 | 3:X:3301[A]:PRO:HA | 1.74 | 1.03 |
| 1:Y:1401:ARG:CD | 3:d:3182[B]:GLN:OE1 | 2.07 | 1.03 |
| 3:a:3151[A]:LEU:HB2 | 3:a:3175[A]:TYR:CE2 | 1.94 | 1.03 |
| 3:a:3298[B]:ASN:ND2 | 3:a:3301[B]:PRO:HA | 1.74 | 1.03 |
| 3:C:3147[B]:GLU:HG3 | 3:L:3160[B]:SER:C | 1.82 | 1.02 |
| 3:C:3153[B]:LYS:HB3 | 3:L:3155[B]:MET:N | 1.71 | 1.02 |
| 3:C:3298[B]:ASN:HB3 | 3:C:3300[B]:LEU:HD23 | 1.41 | 1.02 |
| 3:F:2974[B]:ALA:H | 3:a:3249[B]:GLY:N | 1.46 | 1.02 |
| 3:F:3038[A]:ILE:HG12 | 3:F:3112[A]:TYR:CD2 | 1.93 | 1.02 |
| 3:F:3151[A]:LEU:HB2 | 3:F:3175[A]:TYR:CE2 | 1.94 | 1.02 |
| 3:I:2948[B]:ASP:H | 3:I:2949[B]:LYS:HA | 1.23 | 1.02 |
| 3:I:2961[B]:HIS:NE2 | 3:I:2980[B]:HIS:NE2 | 2.04 | 1.02 |
| 3:I:3222[B]:ILE:HD12 | 3:I:3223[B]:GLY:H | 1.20 | 1.02 |
| 3:I:3255[B]:PRO:CD | 3:R:2962[B]:GLY:O | 2.07 | 1.02 |
| 3:L:3038[B]:ILE:HG12 | 3:L:3112[B]:TYR:CD2 | 1.93 | 1.02 |
| 3:O:2961[A]:HIS:CE1 | 3:O:2980[A]:HIS:HE2 | 1.77 | 1.02 |
| 3:O:2969[B]:TYR:HB3 | 3:X:3158[B]:PHE:CZ | 1.95 | 1.02 |
| 3:O:3038[A]:ILE:HG12 | 3:O:3112[A]:TYR:CD2 | 1.93 | 1.02 |
| 3:O:3038[B]:ILE:CG2 | 3:X:2969[B]:TYR:CE1 | 2.42 | 1.02 |
| 3:O:3151[A]:LEU:HB2 | 3:O:3175[A]:TYR:CE2 | 1.94 | 1.02 |
| 3:O:3160[B]:SER:N | 3:X:3148[B]:ILE:C | 2.16 | 1.02 |
| 3:U:2968[B]:GLN:N | 3:d:3256[B]:TRP:HB2 | 1.70 | 1.02 |
| 3:U:3220[B]:ARG:CA | 3:d:2973[B]:THR:CA | 2.12 | 1.02 |
| 3:X:2948[B]:ASP:H | 3:X:2949[B]:LYS:HA | 1.23 | 1.02 |
| 3:X:3222[B]:ILE:HD12 | 3:X:3223[B]:GLY:H | 1.20 | 1.02 |
| 3:d:2948[A]:ASP:H | 3:d:2949[A]:LYS:HA | 1.24 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2951[B]:ASP:O | 3:F:2956[B]:LYS:NZ | 1.92 | 1.02 |
| 3:F:2975[B]:PHE:HD1 | 3:a:3107[B]:LEU:CG | 1.71 | 1.02 |
| 3:F:2982[B]:MET:HE2 | 3:a:2966[B]:SER:HB3 | 1.39 | 1.02 |
| 3:F:3293[B]:LYS:HD3 | 3:F:3294[B]:SER:CB | 1.90 | 1.02 |
| 3:I:2961[B]:HIS:CA | 3:R:2975[B]:PHE:CZ | 2.41 | 1.02 |
| 3:I:3151[B]:LEU:HB2 | 3:I:3175[B]:TYR:CE2 | 1.94 | 1.02 |
| 3:I:3153[B]:LYS:CB | 3:R:3158[B]:PHE:HB2 | 1.89 | 1.02 |
| 3:L:2961[A]:HIS:CE1 | 3:L:2980[A]:HIS:HE2 | 1.77 | 1.02 |
| 3:L:2961[B]:HIS:CE1 | 3:L:2980[B]:HIS:HE2 | 1.77 | 1.02 |
| 3:O:2968[B]:GLN:HB3 | 3:X:2988[B]:TRP:HB2 | 1.41 | 1.02 |
| 3:O:3253[B]:GLU:CD | 3:X:3161[B]:GLU:CD | 2.26 | 1.02 |
| 3:O:3293[B]:LYS:HD3 | 3:O:3294[B]:SER:CB | 1.90 | 1.02 |
| 3:R:3024[B]:LEU:HD12 | 3:R:3025[B]:VAL:H | 0.89 | 1.02 |
| 3:R:3151[A]:LEU:HB2 | 3:R:3175[A]:TYR:CE2 | 1.94 | 1.02 |
| 3:U:3159[B]:SER:CB | 3:d:3150[B]:LYS:HD2 | 1.87 | 1.02 |
| 1:Y:1546:LYS:HE3 | 3:d:3001[B]:LYS:O | 1.27 | 1.02 |
| 3:d:2948[A]:ASP:HB3 | 3:d:2953[A]:GLY:HA3 | 1.39 | 1.02 |
| 3:d:3038[B]:ILE:HG12 | 3:d:3112[B]:TYR:CD2 | 1.93 | 1.02 |
| 3:d:3135[B]:LYS:HG2 | 3:d:3141[B]:TYR:HE1 | 1.14 | 1.02 |
| 3:C:2966[B]:SER:HB2 | 3:C:2977[B]:CYS:HB2 | 1.39 | 1.02 |
| 3:C:3135[B]:LYS:HG2 | 3:C:3141[B]:TYR:CE1 | 1.89 | 1.02 |
| 3:C:3158[B]:PHE:HD2 | 3:L:3153[B]:LYS:HE3 | 1.22 | 1.02 |
| 3:F:2961[A]:HIS:CE1 | 3:F:2980[A]:HIS:HE2 | 1.77 | 1.02 |
| 3:F:2971[B]:ASP:O | 3:a:3090[B]:ASN:HA | 1.58 | 1.02 |
| 3:F:3161[B]:GLU:HA | 3:a:3147[B]:GLU:HG2 | 1.41 | 1.02 |
| 3:I:2948[B]:ASP:HB3 | 3:I:2953[B]:GLY:HA3 | 1.39 | 1.02 |
| 3:I:3173[B]:THR:HG21 | 3:R:3173[B]:THR:OG1 | 1.55 | 1.02 |
| 3:I:3217[A]:PHE:CE1 | 3:I:3230[A]:PHE:HZ | 1.71 | 1.02 |
| 3:I:3298[A]:ASN:ND2 | 3:I:3301[A]:PRO:HA | 1.74 | 1.02 |
| 3:L:3024[A]:LEU:HD12 | 3:L:3025[A]:VAL:H | 0.89 | 1.02 |
| 3:L:3141[A]:TYR:CD2 | 3:L:3142[A]:ASN:N | 2.24 | 1.02 |
| 3:O:2951[B]:ASP:O | 3:O:2956[B]:LYS:NZ | 1.92 | 1.02 |
| 3:O:2970[B]:PRO:O | 3:X:2990[B]:ARG:N | 1.63 | 1.02 |
| 3:O:3254[B]:MET:HE3 | 3:X:3172[B]:SER:OG | 1.58 | 1.02 |
| 3:R:3298[B]:ASN:HB3 | 3:R:3300[B]:LEU:HD23 | 1.41 | 1.02 |
| 3:U:3038[B]:ILE:HG12 | 3:U:3112[B]:TYR:CD2 | 1.93 | 1.02 |
| 3:U:3151[B]:LEU:HB2 | 3:U:3175[B]:TYR:CE2 | 1.94 | 1.02 |
| 3:U:3153[B]:LYS:HD2 | 3:d:3153[B]:LYS:HD2 | 1.39 | 1.02 |
| 3:X:3038[B]:ILE:HG12 | 3:X:3112[B]:TYR:CD2 | 1.93 | 1.02 |
| 3:X:3307[A]:PHE:HE1 | 3:X:3309[A]:PRO:HG3 | 1.23 | 1.02 |
| 3:a:2961[A]:HIS:CE1 | 3:a:2980[A]:HIS:HE2 | 1.78 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3293[A]:LYS:HD3 | 3:d:3294[A]:SER:CB | 1.90 | 1.02 |
| 3:d:3293[B]:LYS:HD3 | 3:d:3294[B]:SER:CB | 1.90 | 1.02 |
| 3:C:2951[A]:ASP:O | 3:C:2956[A]:LYS:NZ | 1.92 | 1.02 |
| 3:C:2972[B]:GLY:CA | 3:L:3090[B]:ASN:ND2 | 2.22 | 1.02 |
| 3:C:3151[B]:LEU:HB2 | 3:C:3175[B]:TYR:CE2 | 1.94 | 1.02 |
| 3:F:2966[B]:SER:HB2 | 3:F:2977[B]:CYS:HB2 | 1.39 | 1.02 |
| 3:F:2967[B]:CYS:SG | 3:a:2982[B]:MET:HE3 | 1.98 | 1.02 |
| 3:F:3298[A]:ASN:HB3 | 3:F:3300[A]:LEU:HD23 | 1.42 | 1.02 |
| 3:I:2961[A]:HIS:CE1 | 3:I:2980[A]:HIS:HE2 | 1.77 | 1.02 |
| 3:L:2966[A]:SER:HB2 | 3:L:2977[A]:CYS:HB2 | 1.39 | 1.02 |
| 3:L:3217[B]:PHE:CE1 | 3:L:3230[B]:PHE:HZ | 1.71 | 1.02 |
| 3:O:2948[B]:ASP:H | 3:O:2949[B]:LYS:HA | 1.23 | 1.02 |
| 3:O:2966[A]:SER:CB | 3:O:2977[A]:CYS:HB2 | 1.90 | 1.02 |
| 3:O:3228[A]:VAL:HG21 | 3:O:3245[A]:PHE:CZ | 1.95 | 1.02 |
| 3:R:2961[A]:HIS:CE1 | 3:R:2980[A]:HIS:HE2 | 1.77 | 1.02 |
| 3:R:2966[A]:SER:CB | 3:R:2977[A]:CYS:HB2 | 1.90 | 1.02 |
| 3:U:2961[A]:HIS:CE1 | 3:U:2980[A]:HIS:HE2 | 1.78 | 1.02 |
| 3:U:3293[A]:LYS:HD3 | 3:U:3294[A]:SER:CB | 1.90 | 1.02 |
| 1:V:1582:ASN:HB3 | 1:V:1583:CYS:HB2 | 1.41 | 1.02 |
| 3:X:2961[B]:HIS:CE1 | 3:X:2980[B]:HIS:HE2 | 1.77 | 1.02 |
| 3:X:2966[B]:SER:HB2 | 3:X:2977[B]:CYS:HB2 | 1.39 | 1.02 |
| 3:X:3024[B]:LEU:HD12 | 3:X:3025[B]:VAL:H | 0.89 | 1.02 |
| 3:X:3141[B]:TYR:CD2 | 3:X:3142[B]:ASN:N | 2.24 | 1.02 |
| 4:BA:1:NAG:O3 | 4:BA:2:NAG:N2 | 1.92 | 1.02 |
| 3:C:2983[B]:VAL:HG23 | 3:L:3160[B]:SER:OG | 1.57 | 1.02 |
| 3:C:3079[B]:CYS:SG | 3:L:3161[B]:GLU:CG | 0.92 | 1.02 |
| 3:C:3159[B]:SER:HB3 | 3:L:2984[B]:THR:HG23 | 1.03 | 1.02 |
| 3:F:3155[B]:MET:N | 3:a:3153[B]:LYS:O | 1.91 | 1.02 |
| 3:I:2948[A]:ASP:HB3 | 3:I:2953[A]:GLY:HA3 | 1.39 | 1.02 |
| 3:I:3169[B]:LYS:HE3 | 3:R:3149[B]:ASN:OD1 | 1.60 | 1.02 |
| 3:I:3248[B]:LEU:HB2 | 3:R:2972[B]:GLY:O | 1.53 | 1.02 |
| 3:L:2966[A]:SER:CB | 3:L:2977[A]:CYS:HB2 | 1.90 | 1.02 |
| 3:L:3228[B]:VAL:HG21 | 3:L:3245[B]:PHE:CZ | 1.95 | 1.02 |
| 3:L:3293[A]:LYS:HD3 | 3:L:3294[A]:SER:CB | 1.90 | 1.02 |
| 3:L:3293[B]:LYS:HD3 | 3:L:3294[B]:SER:CB | 1.90 | 1.02 |
| 3:O:2951[A]:ASP:O | 3:O:2956[A]:LYS:NZ | 1.92 | 1.02 |
| 3:O:2961[B]:HIS:CE1 | 3:O:2980[B]:HIS:HE2 | 1.77 | 1.02 |
| 3:O:2968[B]:GLN:HB2 | 3:X:2988[B]:TRP:HB2 | 1.04 | 1.02 |
| 3:O:2973[B]:THR:OG1 | 3:X:3158[B]:PHE:HZ | 1.41 | 1.02 |
| 3:O:2974[B]:ALA:CB | 3:X:2977[B]:CYS:C | 2.33 | 1.02 |
| 3:O:3024[A]:LEU:HD12 | 3:O:3025[A]:VAL:H | 0.89 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3141[B]:TYR:CD2 | 3:R:3142[B]:ASN:N | 2.23 | 1.02 |
| 3:R:3151[B]:LEU:HB2 | 3:R:3175[B]:TYR:CE2 | 1.94 | 1.02 |
| 3:U:2951[B]:ASP:O | 3:U:2956[B]:LYS:NZ | 1.92 | 1.02 |
| 3:U:2966[B]:SER:CB | 3:U:2977[B]:CYS:HB2 | 1.90 | 1.02 |
| 3:U:2970[B]:PRO:HB3 | 3:d:2985[B]:PHE:CE2 | 1.93 | 1.02 |
| 3:U:3222[A]:ILE:HD12 | 3:U:3223[A]:GLY:H | 1.20 | 1.02 |
| 3:U:3298[A]:ASN:ND2 | 3:U:3301[A]:PRO:HA | 1.74 | 1.02 |
| 3:U:3298[B]:ASN:ND2 | 3:U:3301[B]:PRO:HA | 1.74 | 1.02 |
| 2:W:2868:GLU:CG | 3:X:2932[A]:PRO:O | 2.07 | 1.02 |
| 3:X:2966[A]:SER:CB | 3:X:2977[A]:CYS:HB2 | 1.90 | 1.02 |
| 3:X:3151[A]:LEU:HB2 | 3:X:3175[A]:TYR:CE2 | 1.94 | 1.02 |
| 3:X:3307[B]:PHE:HE1 | 3:X:3309[B]:PRO:HG3 | 1.23 | 1.02 |
| 1:Y:1546:LYS:CE | 3:d:3001[B]:LYS:O | 2.02 | 1.02 |
| 3:a:2966[A]:SER:CB | 3:a:2977[A]:CYS:HB2 | 1.90 | 1.02 |
| 3:a:3141[A]:TYR:CD2 | 3:a:3142[A]:ASN:N | 2.24 | 1.02 |
| 3:d:2966[A]:SER:CB | 3:d:2977[A]:CYS:HB2 | 1.90 | 1.02 |
| 3:d:3151[A]:LEU:HB2 | 3:d:3175[A]:TYR:CE2 | 1.94 | 1.02 |
| 3:d:3151[B]:LEU:HB2 | 3:d:3175[B]:TYR:CE2 | 1.94 | 1.02 |
| 3:d:3222[B]:ILE:HD12 | 3:d:3223[B]:GLY:H | 1.20 | 1.02 |
| 3:C:3151[A]:LEU:HB2 | 3:C:3175[A]:TYR:CE2 | 1.94 | 1.01 |
| 3:C:3172[B]:SER:N | 3:L:3152[B]:LYS:CB | 2.22 | 1.01 |
| 3:F:2989[B]:HIS:CE1 | 3:a:2969[B]:TYR:CA | 2.38 | 1.01 |
| 3:F:3151[B]:LEU:HB2 | 3:F:3175[B]:TYR:CE2 | 1.94 | 1.01 |
| 3:F:3153[B]:LYS:HE3 | 3:a:3158[B]:PHE:H | 1.23 | 1.01 |
| 3:F:3222[A]:ILE:HD12 | 3:F:3223[A]:GLY:H | 1.20 | 1.01 |
| 3:F:3256[B]:TRP:HB3 | 3:a:2966[B]:SER:O | 1.59 | 1.01 |
| 3:I:2951[A]:ASP:O | 3:I:2956[A]:LYS:NZ | 1.92 | 1.01 |
| 3:O:2970[B]:PRO:CG | 3:X:2991[B]:LEU:CB | 2.36 | 1.01 |
| 3:O:2971[B]:ASP:N | 3:X:2988[B]:TRP:C | 1.93 | 1.01 |
| 3:O:3151[B]:LEU:HB2 | 3:O:3175[B]:TYR:CE2 | 1.94 | 1.01 |
| 3:O:3157[B]:PRO:C | 3:X:3152[B]:LYS:HG3 | 1.84 | 1.01 |
| 3:O:3253[B]:GLU:CG | 3:X:3160[B]:SER:HA | 1.90 | 1.01 |
| 3:R:2951[A]:ASP:O | 3:R:2956[A]:LYS:NZ | 1.92 | 1.01 |
| 3:R:3293[A]:LYS:HD3 | 3:R:3294[A]:SER:CB | 1.90 | 1.01 |
| 3:U:2951[A]:ASP:O | 3:U:2956[A]:LYS:NZ | 1.92 | 1.01 |
| 3:U:2961[B]:HIS:CE1 | 3:U:2980[B]:HIS:HE2 | 1.77 | 1.01 |
| 3:U:2966[A]:SER:HB2 | 3:U:2977[A]:CYS:HB2 | 1.39 | 1.01 |
| 3:X:3151[B]:LEU:HB2 | 3:X:3175[B]:TYR:CE2 | 1.94 | 1.01 |
| 3:X:3293[A]:LYS:HD3 | 3:X:3294[A]:SER:CB | 1.90 | 1.01 |
| 3:a:2951[A]:ASP:O | 3:a:2956[A]:LYS:NZ | 1.92 | 1.01 |
| 3:a:3151[B]:LEU:HB2 | 3:a:3175[B]:TYR:CE2 | 1.94 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3228[B]:VAL:HG21 | 3:a:3245[B]:PHE:CZ | 1.95 | 1.01 |
| 3:a:3298[A]:ASN:ND2 | 3:a:3301[A]:PRO:HA | 1.74 | 1.01 |
| 3:d:3228[B]:VAL:HG21 | 3:d:3245[B]:PHE:CZ | 1.95 | 1.01 |
| 3:d:3307[A]:PHE:HE1 | 3:d:3309[A]:PRO:HG3 | 1.23 | 1.01 |
| 3:C:3155[B]:MET:HE3 | 3:L:3154[B]:PRO:O | 1.59 | 1.01 |
| 3:C:3228[A]:VAL:HG21 | 3:C:3245[A]:PHE:CZ | 1.95 | 1.01 |
| 3:C:3248[B]:LEU:HD22 | 3:L:2971[B]:ASP:CG | 1.83 | 1.01 |
| 3:C:3259[B]:ASP:OD2 | 3:L:3162[B]:ASP:OD1 | 1.78 | 1.01 |
| 3:C:3307[A]:PHE:HE1 | 3:C:3309[A]:PRO:HG3 | 1.23 | 1.01 |
| 3:F:2966[A]:SER:CB | 3:F:2977[A]:CYS:HB2 | 1.90 | 1.01 |
| 3:F:3025[B]:VAL:HG22 | 3:F:3047[B]:ARG:HH12 | 1.19 | 1.01 |
| 3:F:3153[B]:LYS:HB3 | 3:a:3155[B]:MET:C | 1.86 | 1.01 |
| 3:F:3256[B]:TRP:NE1 | 3:a:2965[B]:LEU:HB3 | 1.29 | 1.01 |
| 3:I:2966[B]:SER:CB | 3:I:2977[B]:CYS:HB2 | 1.90 | 1.01 |
| 3:I:3150[B]:LYS:HD2 | 3:R:3160[B]:SER:CA | 1.90 | 1.01 |
| 3:I:3228[B]:VAL:HG21 | 3:I:3245[B]:PHE:CZ | 1.95 | 1.01 |
| 3:I:3256[B]:TRP:NE1 | 3:R:2965[B]:LEU:CB | 1.99 | 1.01 |
| 3:O:2948[B]:ASP:HB3 | 3:O:2953[B]:GLY:HA3 | 1.39 | 1.01 |
| 3:R:3298[B]:ASN:ND2 | 3:R:3301[B]:PRO:HA | 1.74 | 1.01 |
| 3:U:3189[A]:ASN:OD1 | 3:U:3191[A]:ASN:ND2 | 1.94 | 1.01 |
| 3:U:3293[B]:LYS:HD3 | 3:U:3294[B]:SER:CB | 1.90 | 1.01 |
| 3:a:2966[B]:SER:CB | 3:a:2977[B]:CYS:HB2 | 1.90 | 1.01 |
| 3:d:3298[A]:ASN:ND2 | 3:d:3301[A]:PRO:HA | 1.74 | 1.01 |
| 3:d:3307[B]:PHE:HE1 | 3:d:3309[B]:PRO:HG3 | 1.23 | 1.01 |
| 3:C:2961[A]:HIS:CE1 | 3:C:2980[A]:HIS:HE2 | 1.77 | 1.01 |
| 3:C:3248[B]:LEU:CD2 | 3:L:2971[B]:ASP:OD1 | 2.08 | 1.01 |
| 3:C:3293[B]:LYS:HD3 | 3:C:3294[B]:SER:CB | 1.90 | 1.01 |
| 3:F:2951[A]:ASP:O | 3:F:2956[A]:LYS:NZ | 1.92 | 1.01 |
| 3:F:2966[A]:SER:HB2 | 3:F:2977[A]:CYS:HB2 | 1.40 | 1.01 |
| 3:F:2966[B]:SER:CB | 3:F:2977[B]:CYS:HB2 | 1.90 | 1.01 |
| 3:F:2983[B]:VAL:N | 3:a:3160[B]:SER:OG | 1.91 | 1.01 |
| 3:F:3228[B]:VAL:HG21 | 3:F:3245[B]:PHE:CZ | 1.95 | 1.01 |
| 3:F:3251[B]:ASP:HB3 | 3:a:3251[B]:ASP:CG | 1.85 | 1.01 |
| 3:F:3293[A]:LYS:HD3 | 3:F:3294[A]:SER:CB | 1.90 | 1.01 |
| 3:I:2961[B]:HIS:CD2 | 3:R:2975[B]:PHE:CZ | 2.48 | 1.01 |
| 3:I:2982[B]:MET:HE2 | 3:R:2966[B]:SER:CB | 1.89 | 1.01 |
| 3:I:3150[B]:LYS:HG3 | 3:R:3163[B]:ASN:HD22 | 0.85 | 1.01 |
| 3:I:3293[B]:LYS:HD3 | 3:I:3294[B]:SER:CB | 1.90 | 1.01 |
| 3:I:3298[B]:ASN:ND2 | 3:I:3301[B]:PRO:HA | 1.74 | 1.01 |
| 3:L:2951[A]:ASP:O | 3:L:2956[A]:LYS:NZ | 1.92 | 1.01 |
| 3:L:3151[B]:LEU:HB2 | 3:L:3175[B]:TYR:CE2 | 1.94 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3228[A]:VAL:HG21 | 3:L:3245[A]:PHE:CZ | 1.95 | 1.01 |
| 3:O:2975[B]:PHE:CE2 | 3:X:3172[B]:SER:CB | 2.43 | 1.01 |
| 3:O:3293[A]:LYS:HD3 | 3:O:3294[A]:SER:CB | 1.90 | 1.01 |
| 3:R:2948[B]:ASP:H | 3:R:2949[B]:LYS:HA | 1.24 | 1.01 |
| 3:R:3189[B]:ASN:OD1 | 3:R:3191[B]:ASN:ND2 | 1.94 | 1.01 |
| 3:U:2948[B]:ASP:H | 3:U:2949[B]:LYS:HA | 1.23 | 1.01 |
| 3:U:2965[B]:LEU:H | 3:d:3220[B]:ARG:NH1 | 1.54 | 1.01 |
| 3:U:2967[B]:CYS:O | 3:d:3256[B]:TRP:CE3 | 1.88 | 1.01 |
| 3:U:2970[B]:PRO:O | 3:d:3090[B]:ASN:ND2 | 1.92 | 1.01 |
| 3:U:3222[B]:ILE:HD12 | 3:U:3223[B]:GLY:H | 1.20 | 1.01 |
| 3:U:3228[B]:VAL:HG21 | 3:U:3245[B]:PHE:CZ | 1.95 | 1.01 |
| 3:X:2951[A]:ASP:O | 3:X:2956[A]:LYS:NZ | 1.92 | 1.01 |
| 3:a:2948[B]:ASP:HB3 | 3:a:2953[B]:GLY:HA3 | 1.39 | 1.01 |
| 3:a:3293[B]:LYS:HD3 | 3:a:3294[B]:SER:CB | 1.90 | 1.01 |
| 3:C:3155[B]:MET:HG2 | 3:L:3153[B]:LYS:C | 1.81 | 1.01 |
| 3:F:3248[B]:LEU:CB | 3:a:2972[B]:GLY:O | 2.07 | 1.01 |
| 3:I:2966[B]:SER:HB2 | 3:I:2977[B]:CYS:HB2 | 1.39 | 1.01 |
| 3:I:3154[B]:PRO:CD | 3:R:3155[B]:MET:SD | 2.49 | 1.01 |
| 3:I:3162[B]:ASP:HB3 | 3:R:3259[B]:ASP:N | 1.75 | 1.01 |
| 3:L:2951[B]:ASP:O | 3:L:2956[B]:LYS:NZ | 1.92 | 1.01 |
| 3:L:3222[A]:ILE:HD12 | 3:L:3223[A]:GLY:H | 1.20 | 1.01 |
| 3:O:3189[B]:ASN:OD1 | 3:O:3191[B]:ASN:ND2 | 1.94 | 1.01 |
| 3:O:3298[A]:ASN:ND2 | 3:O:3301[A]:PRO:HA | 1.74 | 1.01 |
| 2:Q:2867:PRO:CG | 3:R:2932[A]:PRO:HG2 | 1.90 | 1.01 |
| 3:R:2952[B]:ALA:H | 3:R:2953[B]:GLY:HA2 | 1.26 | 1.01 |
| 3:R:3228[B]:VAL:HG21 | 3:R:3245[B]:PHE:CZ | 1.95 | 1.01 |
| 3:R:3298[A]:ASN:ND2 | 3:R:3301[A]:PRO:HA | 1.74 | 1.01 |
| 1:S:1617:LYS:HE2 | 3:X:3135[B]:LYS:HZ1 | 1.21 | 1.01 |
| 3:U:2952[B]:ALA:H | 3:U:2953[B]:GLY:HA2 | 1.26 | 1.01 |
| 3:U:3228[A]:VAL:HG21 | 3:U:3245[A]:PHE:CZ | 1.95 | 1.01 |
| 3:X:2966[B]:SER:CB | 3:X:2977[B]:CYS:HB2 | 1.90 | 1.01 |
| 3:X:2969[A]:TYR:HD2 | 3:X:2971[A]:ASP:H | 1.02 | 1.01 |
| 3:X:2979[A]:GLN:HG2 | 3:X:3155[A]:MET:HE1 | 1.01 | 1.01 |
| 3:X:3228[A]:VAL:HG21 | 3:X:3245[A]:PHE:CZ | 1.95 | 1.01 |
| 3:X:3228[B]:VAL:HG21 | 3:X:3245[B]:PHE:CZ | 1.95 | 1.01 |
| 3:X:3293[B]:LYS:HD3 | 3:X:3294[B]:SER:CB | 1.90 | 1.01 |
| 3:a:2951[B]:ASP:O | 3:a:2956[B]:LYS:NZ | 1.92 | 1.01 |
| 3:a:3222[A]:ILE:HD12 | 3:a:3223[A]:GLY:H | 1.20 | 1.01 |
| 3:a:3293[A]:LYS:HD3 | 3:a:3294[A]:SER:CB | 1.90 | 1.01 |
| 3:d:2948[B]:ASP:HB3 | 3:d:2953[B]:GLY:HA3 | 1.39 | 1.01 |
| 3:d:2951[B]:ASP:O | 3:d:2956[B]:LYS:NZ | 1.92 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2961[A]:HIS:CE1 | 3:d:2980[A]:HIS:HE2 | 1.77 | 1.01 |
| 3:d:2979[B]:GLN:HG2 | 3:d:3155[B]:MET:HE1 | 1.01 | 1.01 |
| 3:d:3298[B]:ASN:HB3 | 3:d:3300[B]:LEU:HD23 | 1.41 | 1.01 |
| 3:C:2948[A]:ASP:H | 3:C:2949[A]:LYS:HA | 1.24 | 1.01 |
| 3:C:2966[A]:SER:CB | 3:C:2977[A]:CYS:HB2 | 1.90 | 1.01 |
| 3:C:3158[B]:PHE:CD2 | 3:L:3153[B]:LYS:NZ | 2.27 | 1.01 |
| 3:C:3217[B]:PHE:CE1 | 3:C:3230[B]:PHE:HZ | 1.71 | 1.01 |
| 3:C:3298[A]:ASN:ND2 | 3:C:3301[A]:PRO:HA | 1.74 | 1.01 |
| 3:F:3174[B]:GLY:CA | 3:a:3154[B]:PRO:HG3 | 1.91 | 1.01 |
| 3:F:3298[A]:ASN:ND2 | 3:F:3301[A]:PRO:HA | 1.74 | 1.01 |
| 3:I:3228[A]:VAL:HG21 | 3:I:3245[A]:PHE:CZ | 1.95 | 1.01 |
| 3:I:3293[A]:LYS:HD3 | 3:I:3294[A]:SER:CB | 1.90 | 1.01 |
| 3:L:3298[A]:ASN:HB3 | 3:L:3300[A]:LEU:HD23 | 1.41 | 1.01 |
| 3:O:3228[B]:VAL:HG21 | 3:O:3245[B]:PHE:CZ | 1.95 | 1.01 |
| 3:R:2969[A]:TYR:HD2 | 3:R:2971[A]:ASP:H | 1.02 | 1.01 |
| 3:R:2979[B]:GLN:HG2 | 3:R:3155[B]:MET:HE1 | 1.01 | 1.01 |
| 3:R:3189[A]:ASN:OD1 | 3:R:3191[A]:ASN:ND2 | 1.94 | 1.01 |
| 3:U:2979[A]:GLN:HG2 | 3:U:3155[A]:MET:HE1 | 1.01 | 1.01 |
| 3:U:3189[B]:ASN:OD1 | 3:U:3191[B]:ASN:ND2 | 1.94 | 1.01 |
| 3:X:2961[A]:HIS:CE1 | 3:X:2980[A]:HIS:HE2 | 1.77 | 1.01 |
| 3:a:3222[B]:ILE:HD12 | 3:a:3223[B]:GLY:H | 1.20 | 1.01 |
| 3:F:2948[A]:ASP:HB3 | 3:F:2953[A]:GLY:HA3 | 1.39 | 1.00 |
| 3:F:2968[B]:GLN:HE21 | 3:a:3086[B]:GLU:HG2 | 0.87 | 1.00 |
| 3:F:2970[B]:PRO:HD3 | 3:a:2989[B]:HIS:CE1 | 1.95 | 1.00 |
| 3:F:2979[B]:GLN:HG2 | 3:F:3155[B]:MET:HE1 | 1.01 | 1.00 |
| 3:F:3149[B]:ASN:ND2 | 3:a:3163[B]:ASN:HB3 | 1.74 | 1.00 |
| 3:F:3253[B]:GLU:HA | 3:a:2976[B]:ALA:N | 1.75 | 1.00 |
| 3:I:2983[B]:VAL:HG23 | 3:R:3160[B]:SER:CB | 1.90 | 1.00 |
| 3:I:3151[A]:LEU:HB2 | 3:I:3175[A]:TYR:CE2 | 1.94 | 1.00 |
| 3:L:2979[A]:GLN:HG2 | 3:L:3155[A]:MET:HE1 | 1.01 | 1.00 |
| 3:O:2968[B]:GLN:OE1 | 3:X:2984[B]:THR:OG1 | 1.78 | 1.00 |
| 3:O:3109[B]:TYR:CZ | 3:X:2969[B]:TYR:C | 2.30 | 1.00 |
| 3:O:3298[B]:ASN:ND2 | 3:O:3301[B]:PRO:HA | 1.74 | 1.00 |
| 2:Q:2800:LYS:O | 3:R:3023[A]:ILE:CD1 | 2.08 | 1.00 |
| 3:R:3228[A]:VAL:HG21 | 3:R:3245[A]:PHE:CZ | 1.95 | 1.00 |
| 3:U:2952[A]:ALA:H | 3:U:2953[A]:GLY:HA2 | 1.26 | 1.00 |
| 3:U:3149[B]:ASN:O | 3:d:3154[B]:PRO:HB2 | 1.61 | 1.00 |
| 3:U:3152[B]:LYS:CB | 3:d:3154[B]:PRO:HA | 1.79 | 1.00 |
| 3:U:3155[B]:MET:HE3 | 3:d:3153[B]:LYS:HE2 | 1.43 | 1.00 |
| 3:U:3298[A]:ASN:HB3 | 3:U:3300[A]:LEU:HD23 | 1.42 | 1.00 |
| 3:X:2979[A]:GLN:HE21 | 3:X:3155[A]:MET:CE | 1.74 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3298[B]:ASN:ND2 | 3:X:3301[B]:PRO:HA | 1.74 | 1.00 |
| 3:d:2961[B]:HIS:CE1 | 3:d:2980[B]:HIS:HE2 | 1.77 | 1.00 |
| 3:d:2979[A]:GLN:HE21 | 3:d:3155[A]:MET:CE | 1.74 | 1.00 |
| 3:C:2966[B]:SER:CB | 3:C:2977[B]:CYS:HB2 | 1.90 | 1.00 |
| 3:C:2968[B]:GLN:CD | 3:L:3258[B]:PHE:CZ | 2.38 | 1.00 |
| 3:C:2979[B]:GLN:HG2 | 3:C:3155[B]:MET:HE1 | 1.01 | 1.00 |
| 3:C:3152[B]:LYS:HA | 3:L:3173[B]:THR:OG1 | 1.20 | 1.00 |
| 3:C:3189[B]:ASN:OD1 | 3:C:3191[B]:ASN:ND2 | 1.94 | 1.00 |
| 3:C:3298[B]:ASN:ND2 | 3:C:3301[B]:PRO:HA | 1.74 | 1.00 |
| 2:E:2868:GLU:OE2 | 3:F:2932[A]:PRO:O | 1.79 | 1.00 |
| 3:F:2979[B]:GLN:HE21 | 3:F:3155[B]:MET:CE | 1.74 | 1.00 |
| 3:F:3135[B]:LYS:HG2 | 3:F:3141[B]:TYR:CE1 | 1.89 | 1.00 |
| 3:F:3307[A]:PHE:HE1 | 3:F:3309[A]:PRO:HG3 | 1.23 | 1.00 |
| 3:I:2979[A]:GLN:HG2 | 3:I:3155[A]:MET:HE1 | 1.01 | 1.00 |
| 3:I:3149[B]:ASN:ND2 | 3:R:3163[B]:ASN:O | 1.94 | 1.00 |
| 3:I:3150[B]:LYS:CE | 3:R:3163[B]:ASN:CB | 2.35 | 1.00 |
| 3:I:3163[B]:ASN:HD21 | 3:R:3149[B]:ASN:CB | 1.71 | 1.00 |
| 3:L:3298[B]:ASN:HB3 | 3:L:3300[B]:LEU:HD23 | 1.42 | 1.00 |
| 3:O:3222[B]:ILE:HD12 | 3:O:3223[B]:GLY:H | 1.20 | 1.00 |
| 3:O:3307[A]:PHE:HE1 | 3:O:3309[A]:PRO:HG3 | 1.23 | 1.00 |
| 3:R:2979[A]:GLN:HG2 | 3:R:3155[A]:MET:HE1 | 1.01 | 1.00 |
| 3:R:3293[B]:LYS:HD3 | 3:R:3294[B]:SER:CB | 1.90 | 1.00 |
| 2:T:2800:LYS:O | 3:U:3023[A]:ILE:HD11 | 1.60 | 1.00 |
| 3:U:2973[B]:THR:OG1 | 3:d:3248[B]:LEU:O | 1.79 | 1.00 |
| 3:U:3169[B]:LYS:HG2 | 3:d:3147[B]:GLU:C | 1.87 | 1.00 |
| 3:X:2952[A]:ALA:H | 3:X:2953[A]:GLY:HA2 | 1.26 | 1.00 |
| 3:a:3228[A]:VAL:HG21 | 3:a:3245[A]:PHE:CZ | 1.95 | 1.00 |
| 3:a:3298[A]:ASN:HB3 | 3:a:3300[A]:LEU:HD23 | 1.41 | 1.00 |
| 3:d:2948[B]:ASP:H | 3:d:2949[B]:LYS:HA | 1.24 | 1.00 |
| 3:d:2966[B]:SER:CB | 3:d:2977[B]:CYS:HB2 | 1.90 | 1.00 |
| 3:C:2948[A]:ASP:HB3 | 3:C:2953[A]:GLY:HA3 | 1.39 | 1.00 |
| 3:C:2979[A]:GLN:HG2 | 3:C:3155[A]:MET:HE1 | 1.01 | 1.00 |
| 3:C:3113[B]:ASP:CG | 3:C:3114[B]:PRO:HD2 | 1.87 | 1.00 |
| 3:C:3256[B]:TRP:CE2 | 3:L:2965[B]:LEU:CB | 2.31 | 1.00 |
| 3:C:3293[A]:LYS:HD3 | 3:C:3294[A]:SER:CB | 1.90 | 1.00 |
| 3:I:2966[B]:SER:HA | 3:R:3256[B]:TRP:HB3 | 1.39 | 1.00 |
| 3:I:3154[B]:PRO:CB | 3:R:3174[B]:GLY:HA2 | 1.92 | 1.00 |
| 3:I:3189[A]:ASN:OD1 | 3:I:3191[A]:ASN:ND2 | 1.94 | 1.00 |
| 3:I:3254[B]:MET:HB2 | 3:R:2966[B]:SER:OG | 1.60 | 1.00 |
| 3:I:3255[B]:PRO:HB2 | 3:R:2959[B]:SER:CA | 1.90 | 1.00 |
| 3:I:3307[A]:PHE:HE1 | 3:I:3309[A]:PRO:HG3 | 1.23 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:2948[A]:ASP:H | 3:L:2949[A]:LYS:HA | 1.23 | 1.00 |
| 3:L:2960[A]:PHE:CD2 | 3:L:3157[A]:PRO:HG3 | 1.97 | 1.00 |
| 3:L:2966[B]:SER:CB | 3:L:2977[B]:CYS:HB2 | 1.90 | 1.00 |
| 3:L:2979[B]:GLN:HG2 | 3:L:3155[B]:MET:HE1 | 1.01 | 1.00 |
| 3:O:2965[B]:LEU:HD13 | 3:X:2979[B]:GLN:HE22 | 0.84 | 1.00 |
| 3:O:2972[B]:GLY:O | 3:X:2979[B]:GLN:HB3 | 1.62 | 1.00 |
| 3:O:2979[B]:GLN:HE21 | 3:O:3155[B]:MET:CE | 1.74 | 1.00 |
| 3:R:3307[A]:PHE:HE1 | 3:R:3309[A]:PRO:HG3 | 1.23 | 1.00 |
| 3:U:2948[A]:ASP:H | 3:U:2949[A]:LYS:HA | 1.24 | 1.00 |
| 3:U:2979[A]:GLN:HE21 | 3:U:3155[A]:MET:CE | 1.74 | 1.00 |
| 3:U:3159[B]:SER:CB | 3:d:3150[B]:LYS:CD | 2.35 | 1.00 |
| 3:U:3257[B]:ALA:N | 3:d:2969[B]:TYR:H | 1.60 | 1.00 |
| 3:X:3113[B]:ASP:CG | 3:X:3114[B]:PRO:HD2 | 1.87 | 1.00 |
| 3:X:3298[A]:ASN:HB3 | 3:X:3300[A]:LEU:HD23 | 1.42 | 1.00 |
| 3:a:3113[A]:ASP:CG | 3:a:3114[A]:PRO:HD2 | 1.87 | 1.00 |
| 3:a:3113[B]:ASP:CG | 3:a:3114[B]:PRO:HD2 | 1.87 | 1.00 |
| 3:C:3113[A]:ASP:CG | 3:C:3114[A]:PRO:HD2 | 1.87 | 1.00 |
| 3:C:3228[B]:VAL:HG21 | 3:C:3245[B]:PHE:CZ | 1.95 | 1.00 |
| 3:C:3248[B]:LEU:HB2 | 3:L:2973[B]:THR:N | 1.50 | 1.00 |
| 3:F:2983[B]:VAL:HG23 | 3:a:3160[B]:SER:OG | 1.59 | 1.00 |
| 3:I:2966[A]:SER:CB | 3:I:2977[A]:CYS:HB2 | 1.90 | 1.00 |
| 3:O:3255[B]:PRO:HG2 | 3:X:3163[B]:ASN:CB | 1.90 | 1.00 |
| 3:R:2966[B]:SER:CB | 3:R:2977[B]:CYS:HB2 | 1.90 | 1.00 |
| 3:R:2979[B]:GLN:HE21 | 3:R:3155[B]:MET:CE | 1.74 | 1.00 |
| 3:U:2966[A]:SER:CB | 3:U:2977[A]:CYS:HB2 | 1.90 | 1.00 |
| 3:a:2979[A]:GLN:HE21 | 3:a:3155[A]:MET:CE | 1.74 | 1.00 |
| 3:d:2966[A]:SER:HB2 | 3:d:2977[A]:CYS:HB2 | 1.39 | 1.00 |
| 3:d:3113[B]:ASP:CG | 3:d:3114[B]:PRO:HD2 | 1.87 | 1.00 |
| 3:d:3189[B]:ASN:OD1 | 3:d:3191[B]:ASN:ND2 | 1.94 | 1.00 |
| 3:F:2952[B]:ALA:H | 3:F:2953[B]:GLY:HA2 | 1.26 | 1.00 |
| 3:F:3174[B]:GLY:HA2 | 3:a:3154[B]:PRO:HG3 | 1.02 | 1.00 |
| 3:F:3228[A]:VAL:HG21 | 3:F:3245[A]:PHE:CZ | 1.95 | 1.00 |
| 3:I:3113[A]:ASP:CG | 3:I:3114[A]:PRO:HD2 | 1.87 | 1.00 |
| 3:I:3150[B]:LYS:CG | 3:R:3163[B]:ASN:HD22 | 1.74 | 1.00 |
| 3:I:3255[B]:PRO:HB3 | 3:R:2964[B]:PRO:HB2 | 1.42 | 1.00 |
| 3:I:3307[B]:PHE:HE1 | 3:I:3309[B]:PRO:HG3 | 1.23 | 1.00 |
| 3:L:2948[B]:ASP:H | 3:L:2949[B]:LYS:HA | 1.23 | 1.00 |
| 3:O:3141[B]:TYR:CD2 | 3:O:3142[B]:ASN:N | 2.23 | 1.00 |
| 3:O:3307[B]:PHE:HE1 | 3:O:3309[B]:PRO:HG3 | 1.23 | 1.00 |
| 3:R:3298[A]:ASN:HB3 | 3:R:3300[A]:LEU:HD23 | 1.41 | 1.00 |
| 3:U:3298[B]:ASN:HB3 | 3:U:3300[B]:LEU:HD23 | 1.42 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3135[B]:LYS:HG2 | 3:d:3141[B]:TYR:CE1 | 1.89 | 1.00 |
| 3:C:3025[A]:VAL:HG22 | 3:C:3047[A]:ARG:HH12 | 1.19 | 1.00 |
| 3:F:2981[B]:GLY:H | 3:a:2968[B]:GLN:CG | 1.74 | 1.00 |
| 3:F:3113[B]:ASP:CG | 3:F:3114[B]:PRO:HD2 | 1.87 | 1.00 |
| 3:I:2960[A]:PHE:CD2 | 3:I:3157[A]:PRO:HG3 | 1.97 | 1.00 |
| 3:I:3150[B]:LYS:O | 3:R:3159[B]:SER:N | 1.94 | 1.00 |
| 3:R:2948[A]:ASP:H | 3:R:2949[A]:LYS:HA | 1.23 | 1.00 |
| 3:X:3189[B]:ASN:OD1 | 3:X:3191[B]:ASN:ND2 | 1.94 | 1.00 |
| 3:d:2952[A]:ALA:H | 3:d:2953[A]:GLY:HA2 | 1.26 | 1.00 |
| 3:C:2952[A]:ALA:H | 3:C:2953[A]:GLY:HA2 | 1.26 | 1.00 |
| 3:C:3189[A]:ASN:OD1 | 3:C:3191[A]:ASN:ND2 | 1.94 | 1.00 |
| 3:F:3307[B]:PHE:HE1 | 3:F:3309[B]:PRO:HG3 | 1.23 | 1.00 |
| 3:I:2979[B]:GLN:HE21 | 3:I:3155[B]:MET:CE | 1.74 | 1.00 |
| 3:O:3298[B]:ASN:HB3 | 3:O:3300[B]:LEU:HD23 | 1.41 | 1.00 |
| 3:U:2948[B]:ASP:HB3 | 3:U:2953[B]:GLY:HA3 | 1.39 | 1.00 |
| 3:U:3141[B]:TYR:CD2 | 3:U:3142[B]:ASN:N | 2.24 | 1.00 |
| 3:C:3120[B]:HIS:NE2 | 3:L:2969[B]:TYR:CZ | 2.27 | 0.99 |
| 3:C:3159[B]:SER:HB3 | 3:L:2984[B]:THR:CG2 | 1.83 | 0.99 |
| 3:C:3307[B]:PHE:HE1 | 3:C:3309[B]:PRO:HG3 | 1.23 | 0.99 |
| 3:F:3113[A]:ASP:CG | 3:F:3114[A]:PRO:HD2 | 1.87 | 0.99 |
| 3:L:3189[A]:ASN:OD1 | 3:L:3191[A]:ASN:ND2 | 1.94 | 0.99 |
| 3:U:3135[B]:LYS:HG2 | 3:U:3141[B]:TYR:CE1 | 1.89 | 0.99 |
| 3:X:2960[B]:PHE:CD2 | 3:X:3157[B]:PRO:HG3 | 1.97 | 0.99 |
| 3:a:2952[B]:ALA:H | 3:a:2953[B]:GLY:HA2 | 1.26 | 0.99 |
| 3:a:3013[B]:ASP:HA | 3:a:3122[B]:ASN:HD21 | 1.27 | 0.99 |
| 3:a:3189[B]:ASN:OD1 | 3:a:3191[B]:ASN:ND2 | 1.94 | 0.99 |
| 3:d:2960[A]:PHE:CD2 | 3:d:3157[A]:PRO:HG3 | 1.97 | 0.99 |
| 3:C:2979[B]:GLN:HE21 | 3:C:3155[B]:MET:CE | 1.74 | 0.99 |
| 3:F:3189[A]:ASN:OD1 | 3:F:3191[A]:ASN:ND2 | 1.94 | 0.99 |
| 2:H:2868:GLU:CG | 3:I:2932[A]:PRO:O | 2.09 | 0.99 |
| 3:I:2975[B]:PHE:O | 3:R:3253[B]:GLU:CB | 2.10 | 0.99 |
| 3:I:3149[B]:ASN:HB3 | 3:R:3165[B]:ASN:O | 1.62 | 0.99 |
| 3:L:2952[B]:ALA:H | 3:L:2953[B]:GLY:HA2 | 1.26 | 0.99 |
| 3:L:3013[A]:ASP:HA | 3:L:3122[A]:ASN:HD21 | 1.27 | 0.99 |
| 3:L:3113[A]:ASP:CG | 3:L:3114[A]:PRO:HD2 | 1.87 | 0.99 |
| 3:O:2952[B]:ALA:H | 3:O:2953[B]:GLY:HA2 | 1.26 | 0.99 |
| 3:O:3169[B]:LYS:HG3 | 3:X:3148[B]:ILE:HG23 | 1.01 | 0.99 |
| 1:S:1582:ASN:HB3 | 1:S:1583:CYS:HB2 | 1.44 | 0.99 |
| 3:U:3113[A]:ASP:CG | 3:U:3114[A]:PRO:HD2 | 1.87 | 0.99 |
| 3:U:3256[B]:TRP:CD1 | 3:d:2975[B]:PHE:HE1 | 1.79 | 0.99 |
| 3:d:2966[B]:SER:HB2 | 3:d:2977[B]:CYS:HB2 | 1.39 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3013[A]:ASP:HA | 3:d:3122[A]:ASN:HD21 | 1.27 | 0.99 |
| 3:d:3228[A]:VAL:HG21 | 3:d:3245[A]:PHE:CZ | 1.95 | 0.99 |
| 3:L:3013[B]:ASP:HA | 3:L:3122[B]:ASN:HD21 | 1.27 | 0.99 |
| 3:U:3307[A]:PHE:HE1 | 3:U:3309[A]:PRO:HG3 | 1.23 | 0.99 |
| 3:C:2967[B]:CYS:HB3 | 3:L:2982[B]:MET:N | 1.72 | 0.99 |
| 3:C:2972[B]:GLY:HA3 | 3:L:3090[B]:ASN:ND2 | 1.74 | 0.99 |
| 3:F:2970[B]:PRO:CD | 3:a:2989[B]:HIS:CE1 | 2.45 | 0.99 |
| 3:F:2972[B]:GLY:CA | 3:a:3090[B]:ASN:HB3 | 1.92 | 0.99 |
| 3:I:2960[B]:PHE:CD2 | 3:I:3157[B]:PRO:HG3 | 1.97 | 0.99 |
| 3:I:3149[B]:ASN:ND2 | 3:R:3163[B]:ASN:CB | 2.24 | 0.99 |
| 3:O:2960[A]:PHE:CD2 | 3:O:3157[A]:PRO:HG3 | 1.97 | 0.99 |
| 3:O:2966[A]:SER:HB2 | 3:O:2977[A]:CYS:HB2 | 1.39 | 0.99 |
| 3:X:2960[A]:PHE:CD2 | 3:X:3157[A]:PRO:HG3 | 1.97 | 0.99 |
| 3:X:3113[A]:ASP:CG | 3:X:3114[A]:PRO:HD2 | 1.87 | 0.99 |
| 3:X:3141[A]:TYR:CD2 | 3:X:3142[A]:ASN:N | 2.24 | 0.99 |
| 3:X:3189[A]:ASN:OD1 | 3:X:3191[A]:ASN:ND2 | 1.94 | 0.99 |
| 3:d:2979[B]:GLN:HE21 | 3:d:3155[B]:MET:CE | 1.74 | 0.99 |
| 3:d:3013[B]:ASP:HA | 3:d:3122[B]:ASN:HD21 | 1.28 | 0.99 |
| 3:C:2960[A]:PHE:CD2 | 3:C:3157[A]:PRO:HG3 | 1.97 | 0.99 |
| 3:F:3135[A]:LYS:HG2 | 3:F:3141[A]:TYR:CE1 | 1.89 | 0.99 |
| 3:I:2959[B]:SER:HB2 | 3:R:3255[B]:PRO:HB2 | 1.01 | 0.99 |
| 3:I:2972[B]:GLY:HA3 | 3:R:3090[B]:ASN:HB3 | 1.01 | 0.99 |
| 3:L:2960[B]:PHE:CD2 | 3:L:3157[B]:PRO:HG3 | 1.97 | 0.99 |
| 3:L:3141[B]:TYR:CD2 | 3:L:3142[B]:ASN:N | 2.24 | 0.99 |
| 3:O:3252[B]:TYR:CB | 3:X:3156[B]:MET:HB2 | 1.88 | 0.99 |
| 3:R:3113[B]:ASP:CG | 3:R:3114[B]:PRO:HD2 | 1.87 | 0.99 |
| 3:U:2965[B]:LEU:HD12 | 3:d:3220[B]:ARG:CB | 1.87 | 0.99 |
| 3:U:2975[B]:PHE:CG | 3:d:3256[B]:TRP:HD1 | 1.61 | 0.99 |
| 3:U:3113[B]:ASP:CG | 3:U:3114[B]:PRO:HD2 | 1.87 | 0.99 |
| 3:U:3256[B]:TRP:CD1 | 3:d:2975[B]:PHE:CE1 | 2.51 | 0.99 |
| 3:d:3217[B]:PHE:CE1 | 3:d:3230[B]:PHE:HZ | 1.71 | 0.99 |
| 3:C:3013[A]:ASP:HA | 3:C:3122[A]:ASN:HD21 | 1.28 | 0.99 |
| 3:C:3162[B]:ASP:OD1 | 3:L:3259[B]:ASP:CG | 1.96 | 0.99 |
| 3:F:2960[A]:PHE:CD2 | 3:F:3157[A]:PRO:HG3 | 1.97 | 0.99 |
| 3:U:2960[A]:PHE:CD2 | 3:U:3157[A]:PRO:HG3 | 1.97 | 0.99 |
| 3:U:2979[B]:GLN:HE21 | 3:U:3155[B]:MET:CE | 1.74 | 0.99 |
| 3:U:3013[B]:ASP:HA | 3:U:3122[B]:ASN:HD21 | 1.27 | 0.99 |
| 3:d:3038[B]:ILE:CG2 | 3:d:3040[B]:VAL:HG22 | 1.93 | 0.99 |
| 3:d:3113[A]:ASP:CG | 3:d:3114[A]:PRO:HD2 | 1.87 | 0.99 |
| 3:C:3255[B]:PRO:HD2 | 3:L:2960[B]:PHE:O | 1.60 | 0.99 |
| 3:F:2979[A]:GLN:HG2 | 3:F:3155[A]:MET:HE1 | 1.01 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3038[A]:ILE:CG2 | 3:F:3040[A]:VAL:HG22 | 1.93 | 0.99 |
| 3:F:3153[B]:LYS:HG2 | 3:a:3155[B]:MET:CB | 1.78 | 0.99 |
| 3:I:2982[B]:MET:HG3 | 3:R:3156[B]:MET:HB2 | 1.41 | 0.99 |
| 3:L:3038[B]:ILE:CG2 | 3:L:3040[B]:VAL:HG22 | 1.93 | 0.99 |
| 3:L:3189[B]:ASN:OD1 | 3:L:3191[B]:ASN:ND2 | 1.94 | 0.99 |
| 3:R:2969[B]:TYR:HD2 | 3:R:2971[B]:ASP:H | 1.02 | 0.99 |
| 3:U:2969[B]:TYR:HD2 | 3:U:2971[B]:ASP:H | 1.02 | 0.99 |
| 3:U:2971[B]:ASP:HA | 3:d:3090[B]:ASN:HD22 | 0.83 | 0.99 |
| 3:a:2948[A]:ASP:H | 3:a:2949[A]:LYS:HA | 1.24 | 0.99 |
| 3:a:2960[B]:PHE:CD2 | 3:a:3157[B]:PRO:HG3 | 1.97 | 0.99 |
| 3:a:3189[A]:ASN:OD1 | 3:a:3191[A]:ASN:ND2 | 1.94 | 0.99 |
| 3:a:3298[B]:ASN:HB3 | 3:a:3300[B]:LEU:HD23 | 1.42 | 0.99 |
| 3:C:3160[B]:SER:HA | 3:L:2983[B]:VAL:HG23 | 1.35 | 0.99 |
| 3:C:3298[A]:ASN:HB3 | 3:C:3300[A]:LEU:HD23 | 1.41 | 0.99 |
| 3:F:2975[B]:PHE:HZ | 3:a:2961[B]:HIS:HA | 1.25 | 0.99 |
| 3:F:2979[A]:GLN:HE21 | 3:F:3155[A]:MET:CE | 1.74 | 0.99 |
| 3:F:3141[A]:TYR:CD2 | 3:F:3142[A]:ASN:N | 2.24 | 0.99 |
| 3:I:2966[A]:SER:HB2 | 3:I:2977[A]:CYS:HB2 | 1.39 | 0.99 |
| 3:I:2972[B]:GLY:HA3 | 3:R:3090[B]:ASN:CB | 1.91 | 0.99 |
| 3:I:3298[B]:ASN:HB3 | 3:I:3300[B]:LEU:HD23 | 1.41 | 0.99 |
| 3:L:2979[A]:GLN:HE21 | 3:L:3155[A]:MET:CE | 1.74 | 0.99 |
| 3:O:2963[B]:MET:HG2 | 3:X:2968[B]:GLN:O | 1.20 | 0.99 |
| 3:R:2960[B]:PHE:CD2 | 3:R:3157[B]:PRO:HG3 | 1.97 | 0.99 |
| 3:R:3038[A]:ILE:CG2 | 3:R:3040[A]:VAL:HG22 | 1.93 | 0.99 |
| 3:U:3169[B]:LYS:O | 3:d:3148[B]:ILE:HB | 1.55 | 0.99 |
| 3:X:3217[A]:PHE:CE1 | 3:X:3230[A]:PHE:CE1 | 2.51 | 0.99 |
| 3:a:3038[A]:ILE:CG2 | 3:a:3040[A]:VAL:HG22 | 1.93 | 0.99 |
| 3:d:2960[B]:PHE:CD2 | 3:d:3157[B]:PRO:HG3 | 1.97 | 0.99 |
| 3:d:2969[A]:TYR:HD2 | 3:d:2971[A]:ASP:H | 1.02 | 0.99 |
| 3:d:3189[A]:ASN:OD1 | 3:d:3191[A]:ASN:ND2 | 1.94 | 0.99 |
| 3:F:2960[B]:PHE:CD2 | 3:F:3157[B]:PRO:HG3 | 1.97 | 0.99 |
| 3:I:3173[B]:THR:HG1 | 3:R:3173[B]:THR:CG2 | 1.62 | 0.99 |
| 3:O:3113[A]:ASP:CG | 3:O:3114[A]:PRO:HD2 | 1.87 | 0.99 |
| 3:O:3189[A]:ASN:OD1 | 3:O:3191[A]:ASN:ND2 | 1.94 | 0.99 |
| 3:a:2979[B]:GLN:HG2 | 3:a:3155[B]:MET:HE1 | 1.01 | 0.99 |
| 3:C:3038[A]:ILE:CG2 | 3:C:3040[A]:VAL:HG22 | 1.93 | 0.99 |
| 3:F:2968[B]:GLN:NE2 | 3:a:3086[B]:GLU:HG2 | 1.72 | 0.99 |
| 3:F:2977[B]:CYS:SG | 3:a:2982[B]:MET:HE3 | 2.03 | 0.99 |
| 3:I:2979[A]:GLN:HE21 | 3:I:3155[A]:MET:CE | 1.74 | 0.99 |
| 3:L:3113[B]:ASP:CG | 3:L:3114[B]:PRO:HD2 | 1.87 | 0.99 |
| 3:O:3013[A]:ASP:HA | 3:O:3122[A]:ASN:HD21 | 1.27 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2979[A]:GLN:HE21 | 3:R:3155[A]:MET:CE | 1.74 | 0.99 |
| 3:R:3013[B]:ASP:HA | 3:R:3122[B]:ASN:HD21 | 1.27 | 0.99 |
| 3:X:3298[B]:ASN:HB3 | 3:X:3300[B]:LEU:HD23 | 1.42 | 0.99 |
| 3:a:2979[B]:GLN:HE21 | 3:a:3155[B]:MET:CE | 1.75 | 0.99 |
| 3:d:3038[A]:ILE:CG2 | 3:d:3040[A]:VAL:HG22 | 1.93 | 0.99 |
| 3:C:2960[B]:PHE:CD2 | 3:C:3157[B]:PRO:HG3 | 1.97 | 0.98 |
| 3:C:2965[B]:LEU:HD21 | 3:L:3253[B]:GLU:OE1 | 0.81 | 0.98 |
| 3:C:3156[B]:MET:HB2 | 3:L:2982[B]:MET:CB | 1.91 | 0.98 |
| 3:I:2952[A]:ALA:H | 3:I:2953[A]:GLY:HA2 | 1.26 | 0.98 |
| 3:I:2975[B]:PHE:CG | 3:R:3107[B]:LEU:HD11 | 1.97 | 0.98 |
| 3:I:3251[B]:ASP:CB | 3:R:3251[B]:ASP:CB | 1.86 | 0.98 |
| 3:L:2979[B]:GLN:HE21 | 3:L:3155[B]:MET:CE | 1.74 | 0.98 |
| 3:O:2969[A]:TYR:HD2 | 3:O:2971[A]:ASP:H | 1.02 | 0.98 |
| 3:R:2960[A]:PHE:CD2 | 3:R:3157[A]:PRO:HG3 | 1.97 | 0.98 |
| 3:R:3113[A]:ASP:CG | 3:R:3114[A]:PRO:HD2 | 1.87 | 0.98 |
| 3:U:2960[B]:PHE:CD2 | 3:U:3157[B]:PRO:HG3 | 1.97 | 0.98 |
| 3:U:3038[A]:ILE:CG2 | 3:U:3040[A]:VAL:HG22 | 1.93 | 0.98 |
| 3:U:3153[B]:LYS:CB | 3:d:3153[B]:LYS:HD2 | 1.91 | 0.98 |
| 3:d:2990[B]:ARG:NH2 | 3:d:3180[B]:TYR:HB3 | 1.79 | 0.98 |
| 3:d:3298[A]:ASN:HB3 | 3:d:3300[A]:LEU:HD23 | 1.42 | 0.98 |
| 3:C:2948[B]:ASP:H | 3:C:2949[B]:LYS:HA | 1.24 | 0.98 |
| 3:C:2979[A]:GLN:HE21 | 3:C:3155[A]:MET:CE | 1.74 | 0.98 |
| 3:C:3154[B]:PRO:HB2 | 3:L:3151[B]:LEU:HA | 1.44 | 0.98 |
| 3:C:3158[B]:PHE:CD2 | 3:L:3153[B]:LYS:HE3 | 1.94 | 0.98 |
| 3:C:3223[B]:GLY:H | 3:L:2963[B]:MET:HE1 | 1.27 | 0.98 |
| 3:F:3038[B]:ILE:CG2 | 3:F:3040[B]:VAL:HG22 | 1.93 | 0.98 |
| 3:F:3156[B]:MET:HB2 | 3:a:2982[B]:MET:CG | 1.91 | 0.98 |
| 3:L:2969[A]:TYR:HD2 | 3:L:2971[A]:ASP:H | 1.02 | 0.98 |
| 3:O:3298[A]:ASN:HB3 | 3:O:3300[A]:LEU:HD23 | 1.42 | 0.98 |
| 3:U:3155[B]:MET:N | 3:d:3150[B]:LYS:CG | 2.26 | 0.98 |
| 3:d:3217[A]:PHE:CE1 | 3:d:3230[A]:PHE:CE1 | 2.51 | 0.98 |
| 3:C:3258[B]:PHE:HZ | 3:L:2968[B]:GLN:CD | 1.71 | 0.98 |
| 3:F:2966[B]:SER:CA | 3:a:3255[B]:PRO:C | 2.36 | 0.98 |
| 3:F:3170[B]:ALA:C | 3:a:3152[B]:LYS:CD | 2.15 | 0.98 |
| 3:I:2952[B]:ALA:H | 3:I:2953[B]:GLY:HA2 | 1.26 | 0.98 |
| 3:I:2979[B]:GLN:HG2 | 3:I:3155[B]:MET:HE1 | 1.01 | 0.98 |
| 3:I:3038[A]:ILE:CG2 | 3:I:3040[A]:VAL:HG22 | 1.93 | 0.98 |
| 3:I:3169[B]:LYS:HG3 | 3:R:3149[B]:ASN:OD1 | 1.59 | 0.98 |
| 3:O:2960[B]:PHE:CD2 | 3:O:3157[B]:PRO:HG3 | 1.97 | 0.98 |
| 3:O:3113[B]:ASP:CG | 3:O:3114[B]:PRO:HD2 | 1.87 | 0.98 |
| 3:U:2990[A]:ARG:NH2 | 3:U:3180[A]:TYR:HB3 | 1.79 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3169[B]:LYS:HG3 | 3:d:3147[B]:GLU:HB3 | 1.41 | 0.98 |
| 3:X:3013[A]:ASP:HA | 3:X:3122[A]:ASN:HD21 | 1.27 | 0.98 |
| 3:a:2960[A]:PHE:CD2 | 3:a:3157[A]:PRO:HG3 | 1.97 | 0.98 |
| 3:a:2979[A]:GLN:HG2 | 3:a:3155[A]:MET:HE1 | 1.01 | 0.98 |
| 3:d:3034[B]:HIS:HB3 | 3:d:3035[B]:HIS:ND1 | 1.79 | 0.98 |
| 3:C:2965[B]:LEU:HD23 | 3:L:3253[B]:GLU:CD | 1.69 | 0.98 |
| 3:C:2990[A]:ARG:NH2 | 3:C:3180[A]:TYR:HB3 | 1.79 | 0.98 |
| 3:C:3159[B]:SER:CA | 3:L:3150[B]:LYS:C | 2.17 | 0.98 |
| 3:C:3160[B]:SER:CB | 3:L:3150[B]:LYS:HZ2 | 1.55 | 0.98 |
| 3:F:2982[B]:MET:HE2 | 3:a:2966[B]:SER:CB | 1.92 | 0.98 |
| 3:F:3149[B]:ASN:ND2 | 3:a:3163[B]:ASN:CB | 2.26 | 0.98 |
| 3:I:3113[B]:ASP:CG | 3:I:3114[B]:PRO:HD2 | 1.87 | 0.98 |
| 3:I:3174[B]:GLY:HA3 | 3:R:3154[B]:PRO:HB3 | 1.44 | 0.98 |
| 3:O:3034[A]:HIS:HB3 | 3:O:3035[A]:HIS:ND1 | 1.78 | 0.98 |
| 3:C:3153[B]:LYS:C | 3:L:3155[B]:MET:CG | 2.36 | 0.98 |
| 3:C:3254[B]:MET:O | 3:L:2976[B]:ALA:HA | 1.16 | 0.98 |
| 3:F:3066[A]:TYR:OH | 3:F:3203[A]:HIS:NE2 | 1.97 | 0.98 |
| 3:F:3156[B]:MET:HB2 | 3:a:2982[B]:MET:SD | 2.04 | 0.98 |
| 3:I:2990[B]:ARG:NH2 | 3:I:3180[B]:TYR:HB3 | 1.79 | 0.98 |
| 3:O:2979[A]:GLN:HE21 | 3:O:3155[A]:MET:CE | 1.74 | 0.98 |
| 3:O:2979[B]:GLN:HG2 | 3:O:3155[B]:MET:HE1 | 1.01 | 0.98 |
| 3:O:3038[B]:ILE:HG21 | 3:X:2969[B]:TYR:CE1 | 1.97 | 0.98 |
| 3:a:2966[B]:SER:HB2 | 3:a:2977[B]:CYS:HB2 | 1.39 | 0.98 |
| 3:C:3159[B]:SER:OG | 3:L:3150[B]:LYS:C | 2.07 | 0.98 |
| 3:F:3027[A]:GLU:OE1 | 3:F:3029[A]:LYS:N | 1.97 | 0.98 |
| 3:F:3153[B]:LYS:C | 3:a:3155[B]:MET:CG | 2.16 | 0.98 |
| 3:F:3153[B]:LYS:HB3 | 3:a:3155[B]:MET:CA | 1.94 | 0.98 |
| 3:F:3189[B]:ASN:OD1 | 3:F:3191[B]:ASN:ND2 | 1.94 | 0.98 |
| 3:I:3189[B]:ASN:OD1 | 3:I:3191[B]:ASN:ND2 | 1.94 | 0.98 |
| 3:I:3298[A]:ASN:HB3 | 3:I:3300[A]:LEU:HD23 | 1.42 | 0.98 |
| 3:R:2990[A]:ARG:NH2 | 3:R:3180[A]:TYR:HB3 | 1.79 | 0.98 |
| 3:X:2990[B]:ARG:NH2 | 3:X:3180[B]:TYR:HB3 | 1.79 | 0.98 |
| 3:a:3034[A]:HIS:HB3 | 3:a:3035[A]:HIS:ND1 | 1.78 | 0.98 |
| 3:a:3141[B]:TYR:CD2 | 3:a:3142[B]:ASN:N | 2.23 | 0.98 |
| 3:d:2952[B]:ALA:H | 3:d:2953[B]:GLY:HA2 | 1.26 | 0.98 |
| 3:C:2968[B]:GLN:OE1 | 3:L:3258[B]:PHE:CZ | 2.17 | 0.98 |
| 3:C:3150[B]:LYS:O | 3:L:3159[B]:SER:OG | 1.82 | 0.98 |
| 3:C:3217[B]:PHE:CE1 | 3:C:3230[B]:PHE:CE1 | 2.51 | 0.98 |
| 3:F:2982[B]:MET:HE1 | 3:a:2966[B]:SER:HB3 | 1.44 | 0.98 |
| 3:F:3013[A]:ASP:HA | 3:F:3122[A]:ASN:HD21 | 1.28 | 0.98 |
| 3:F:3027[B]:GLU:OE1 | 3:F:3029[B]:LYS:N | 1.97 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3038[B]:ILE:CG2 | 3:I:3040[B]:VAL:HG22 | 1.93 | 0.98 |
| 3:I:3161[B]:GLU:HG3 | 3:R:3079[B]:CYS:SG | 1.99 | 0.98 |
| 3:L:3034[B]:HIS:HB3 | 3:L:3035[B]:HIS:ND1 | 1.79 | 0.98 |
| 3:O:2990[A]:ARG:NH2 | 3:O:3180[A]:TYR:HB3 | 1.79 | 0.98 |
| 3:O:2990[B]:ARG:NH2 | 3:O:3180[B]:TYR:HB3 | 1.79 | 0.98 |
| 3:O:3217[B]:PHE:CE1 | 3:O:3230[B]:PHE:CE1 | 2.51 | 0.98 |
| 3:C:3155[B]:MET:N | 3:L:3153[B]:LYS:O | 1.96 | 0.98 |
| 3:F:2982[B]:MET:SD | 3:a:3157[B]:PRO:CA | 2.50 | 0.98 |
| 3:F:2990[B]:ARG:NH2 | 3:F:3180[B]:TYR:HB3 | 1.79 | 0.98 |
| 3:F:3147[B]:GLU:OE1 | 3:a:3162[B]:ASP:HA | 1.63 | 0.98 |
| 3:F:3169[B]:LYS:O | 3:a:3152[B]:LYS:CB | 2.12 | 0.98 |
| 3:I:2991[A]:LEU:HD23 | 3:I:3158[A]:PHE:CD1 | 1.99 | 0.98 |
| 3:O:2979[A]:GLN:HG2 | 3:O:3155[A]:MET:HE1 | 1.01 | 0.98 |
| 3:O:3038[B]:ILE:CG2 | 3:O:3040[B]:VAL:HG22 | 1.93 | 0.98 |
| 3:O:3255[B]:PRO:HA | 3:X:3161[B]:GLU:HA | 1.42 | 0.98 |
| 3:R:2952[A]:ALA:H | 3:R:2953[A]:GLY:HA2 | 1.26 | 0.98 |
| 3:U:2973[B]:THR:HG22 | 3:d:3222[B]:ILE:HG22 | 1.44 | 0.98 |
| 3:U:3141[A]:TYR:CD2 | 3:U:3142[A]:ASN:N | 2.24 | 0.98 |
| 3:X:2979[B]:GLN:HG2 | 3:X:3155[B]:MET:HE1 | 1.01 | 0.98 |
| 1:Y:1620:LEU:HD12 | 3:d:3189[B]:ASN:HB2 | 1.45 | 0.98 |
| 3:d:3066[B]:TYR:OH | 3:d:3203[B]:HIS:NE2 | 1.97 | 0.98 |
| 3:C:3173[A]:THR:HB | 3:C:3176[A]:LYS:HD2 | 1.46 | 0.98 |
| 3:F:3173[A]:THR:HB | 3:F:3176[A]:LYS:HD2 | 1.46 | 0.98 |
| 3:I:2968[B]:GLN:HG3 | 3:R:3086[B]:GLU:CG | 1.89 | 0.98 |
| 3:I:3160[B]:SER:HB2 | 3:R:2982[B]:MET:HB3 | 1.46 | 0.98 |
| 3:I:3163[B]:ASN:HB3 | 3:R:3150[B]:LYS:CE | 1.83 | 0.98 |
| 3:I:3217[B]:PHE:CE1 | 3:I:3230[B]:PHE:CE1 | 2.51 | 0.98 |
| 3:I:3253[B]:GLU:OE1 | 3:R:2974[B]:ALA:HB1 | 1.64 | 0.98 |
| 1:J:806:ASN:CG | 4:u:1:NAG:H82 | 1.89 | 0.98 |
| 3:L:2961[B]:HIS:NE2 | 3:L:2980[B]:HIS:NE2 | 2.04 | 0.98 |
| 3:L:3298[A]:ASN:HB2 | 3:L:3300[A]:LEU:N | 1.78 | 0.98 |
| 3:O:3160[B]:SER:HA | 3:X:3151[B]:LEU:HG | 1.44 | 0.98 |
| 3:R:3038[B]:ILE:CG2 | 3:R:3040[B]:VAL:HG22 | 1.93 | 0.98 |
| 3:R:3217[A]:PHE:CE1 | 3:R:3230[A]:PHE:CE1 | 2.51 | 0.98 |
| 3:U:2979[B]:GLN:HG2 | 3:U:3155[B]:MET:HE1 | 1.01 | 0.98 |
| 3:U:3256[B]:TRP:CE3 | 3:d:2969[B]:TYR:CB | 2.45 | 0.98 |
| 1:Y:416:ASN:CG | 3:d:3196[A]:THR:HG21 | 1.88 | 0.98 |
| 3:a:2990[A]:ARG:NH2 | 3:a:3180[A]:TYR:HB3 | 1.79 | 0.98 |
| 3:a:3066[A]:TYR:OH | 3:a:3203[A]:HIS:NE2 | 1.97 | 0.98 |
| 3:C:3034[A]:HIS:HB3 | 3:C:3035[A]:HIS:ND1 | 1.79 | 0.98 |
| 3:C:3163[B]:ASN:N | 3:L:3147[B]:GLU:CD | 2.20 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3163[B]:ASN:HD21 | 3:R:3149[B]:ASN:HB2 | 0.83 | 0.98 |
| 3:L:2990[A]:ARG:NH2 | 3:L:3180[A]:TYR:HB3 | 1.79 | 0.98 |
| 3:R:2991[B]:LEU:HD23 | 3:R:3158[B]:PHE:CD1 | 1.99 | 0.98 |
| 3:R:3217[B]:PHE:CE1 | 3:R:3230[B]:PHE:CE1 | 2.51 | 0.98 |
| 3:X:2952[B]:ALA:H | 3:X:2953[B]:GLY:HA2 | 1.26 | 0.98 |
| 3:X:3173[A]:THR:HB | 3:X:3176[A]:LYS:HD2 | 1.46 | 0.98 |
| 3:a:2990[B]:ARG:NH2 | 3:a:3180[B]:TYR:HB3 | 1.79 | 0.98 |
| 3:d:2991[A]:LEU:HD23 | 3:d:3158[A]:PHE:CD1 | 1.99 | 0.98 |
| 3:F:2991[A]:LEU:HD23 | 3:F:3158[A]:PHE:CD1 | 1.99 | 0.97 |
| 3:F:3217[A]:PHE:CE1 | 3:F:3230[A]:PHE:CE1 | 2.51 | 0.97 |
| 3:F:3217[B]:PHE:CE1 | 3:F:3230[B]:PHE:CE1 | 2.51 | 0.97 |
| 3:F:3298[B]:ASN:HB3 | 3:F:3300[B]:LEU:HD23 | 1.41 | 0.97 |
| 3:I:3066[B]:TYR:OH | 3:I:3203[B]:HIS:NE2 | 1.97 | 0.97 |
| 3:L:3038[A]:ILE:CG2 | 3:L:3040[A]:VAL:HG22 | 1.93 | 0.97 |
| 3:O:2952[A]:ALA:H | 3:O:2953[A]:GLY:HA2 | 1.26 | 0.97 |
| 3:O:3027[A]:GLU:OE1 | 3:O:3029[A]:LYS:N | 1.97 | 0.97 |
| 3:U:3169[B]:LYS:CE | 3:d:3146[B]:CYS:HA | 1.94 | 0.97 |
| 3:X:2991[B]:LEU:HD23 | 3:X:3158[B]:PHE:CD1 | 1.99 | 0.97 |
| 1:Y:1576:THR:HG22 | 3:d:3196[B]:THR:HG21 | 1.44 | 0.97 |
| 3:a:2948[B]:ASP:H | 3:a:2949[B]:LYS:HA | 1.24 | 0.97 |
| 3:C:3034[B]:HIS:HB3 | 3:C:3035[B]:HIS:ND1 | 1.79 | 0.97 |
| 3:C:3038[B]:ILE:CG2 | 3:C:3040[B]:VAL:HG22 | 1.93 | 0.97 |
| 3:C:3147[B]:GLU:OE1 | 3:L:3162[B]:ASP:C | 2.07 | 0.97 |
| 3:C:3161[B]:GLU:H | 3:L:2983[B]:VAL:CG2 | 1.76 | 0.97 |
| 3:C:3231[B]:ASP:O | 3:C:3284[B]:LYS:N | 1.98 | 0.97 |
| 3:C:3256[B]:TRP:CE3 | 3:L:2965[B]:LEU:O | 2.17 | 0.97 |
| 3:F:2975[B]:PHE:CZ | 3:a:2961[B]:HIS:HA | 1.98 | 0.97 |
| 3:F:3154[B]:PRO:CA | 3:a:3153[B]:LYS:O | 2.11 | 0.97 |
| 3:F:3155[B]:MET:HG3 | 3:a:3153[B]:LYS:C | 1.89 | 0.97 |
| 3:F:3156[B]:MET:HB2 | 3:a:2982[B]:MET:HG3 | 1.42 | 0.97 |
| 3:O:3027[B]:GLU:OE1 | 3:O:3029[B]:LYS:N | 1.97 | 0.97 |
| 3:O:3038[A]:ILE:CG2 | 3:O:3040[A]:VAL:HG22 | 1.93 | 0.97 |
| 3:U:3156[B]:MET:SD | 3:d:2982[B]:MET:SD | 2.61 | 0.97 |
| 3:X:3038[B]:ILE:CG2 | 3:X:3040[B]:VAL:HG22 | 1.93 | 0.97 |
| 3:C:2968[B]:GLN:OE1 | 3:L:2981[B]:GLY:HA2 | 1.64 | 0.97 |
| 3:F:2968[B]:GLN:NE2 | 3:a:3086[B]:GLU:CG | 2.22 | 0.97 |
| 3:F:2970[B]:PRO:N | 3:a:2989[B]:HIS:CD2 | 2.25 | 0.97 |
| 3:F:3254[B]:MET:CG | 3:a:2966[B]:SER:HB2 | 1.94 | 0.97 |
| 3:F:3255[B]:PRO:CG | 3:a:2962[B]:GLY:C | 2.37 | 0.97 |
| 3:I:3013[A]:ASP:HA | 3:I:3122[A]:ASN:HD21 | 1.28 | 0.97 |
| 3:L:3027[A]:GLU:OE1 | 3:L:3029[A]:LYS:N | 1.97 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2965[B]:LEU:HB2 | 3:X:3254[B]:MET:CE | 1.89 | 0.97 |
| 3:R:2991[A]:LEU:HD23 | 3:R:3158[A]:PHE:CD1 | 1.99 | 0.97 |
| 3:U:2979[B]:GLN:HE22 | 3:d:3153[B]:LYS:NZ | 1.55 | 0.97 |
| 3:U:3217[B]:PHE:CE1 | 3:U:3230[B]:PHE:CE1 | 2.51 | 0.97 |
| 3:a:3034[B]:HIS:HB3 | 3:a:3035[B]:HIS:ND1 | 1.79 | 0.97 |
| 3:a:3196[A]:THR:CG2 | 1:b:416:ASN:OD1 | 2.12 | 0.97 |
| 3:d:2979[A]:GLN:HG2 | 3:d:3155[A]:MET:HE1 | 1.01 | 0.97 |
| 3:d:3034[A]:HIS:HB3 | 3:d:3035[A]:HIS:ND1 | 1.79 | 0.97 |
| 3:C:2964[B]:PRO:O | 3:L:3255[B]:PRO:CA | 2.10 | 0.97 |
| 3:C:2991[A]:LEU:HD23 | 3:C:3158[A]:PHE:CD1 | 1.99 | 0.97 |
| 3:C:3066[A]:TYR:OH | 3:C:3203[A]:HIS:NE2 | 1.97 | 0.97 |
| 3:C:3066[B]:TYR:OH | 3:C:3203[B]:HIS:NE2 | 1.97 | 0.97 |
| 3:F:2990[A]:ARG:NH2 | 3:F:3180[A]:TYR:HB3 | 1.78 | 0.97 |
| 3:F:3169[B]:LYS:NZ | 3:a:3149[B]:ASN:ND2 | 2.12 | 0.97 |
| 3:I:2990[A]:ARG:NH2 | 3:I:3180[A]:TYR:HB3 | 1.79 | 0.97 |
| 3:I:3034[A]:HIS:HB3 | 3:I:3035[A]:HIS:ND1 | 1.79 | 0.97 |
| 3:O:2965[B]:LEU:C | 3:X:3153[B]:LYS:NZ | 2.22 | 0.97 |
| 3:O:3013[B]:ASP:HA | 3:O:3122[B]:ASN:HD21 | 1.28 | 0.97 |
| 3:O:3109[B]:TYR:HD1 | 3:X:2970[B]:PRO:HD2 | 1.24 | 0.97 |
| 3:O:3109[B]:TYR:OH | 3:X:2973[B]:THR:N | 1.97 | 0.97 |
| 3:U:3027[A]:GLU:OE1 | 3:U:3029[A]:LYS:N | 1.97 | 0.97 |
| 3:a:3027[A]:GLU:OE1 | 3:a:3029[A]:LYS:N | 1.97 | 0.97 |
| 3:I:3223[B]:GLY:CA | 3:R:2963[B]:MET:HE1 | 1.94 | 0.97 |
| 3:O:3154[B]:PRO:HD2 | 3:X:3176[B]:LYS:NZ | 1.77 | 0.97 |
| 3:O:3158[B]:PHE:H | 3:X:3152[B]:LYS:HB2 | 1.26 | 0.97 |
| 3:U:2990[B]:ARG:NH2 | 3:U:3180[B]:TYR:HB3 | 1.79 | 0.97 |
| 1:Y:806:ASN:O | 1:Y:806:ASN:ND2 | 1.96 | 0.97 |
| 3:a:2991[A]:LEU:HD23 | 3:a:3158[A]:PHE:CD1 | 1.99 | 0.97 |
| 3:d:3066[A]:TYR:OH | 3:d:3203[A]:HIS:NE2 | 1.97 | 0.97 |
| 3:C:2983[B]:VAL:HG23 | 3:L:3160[B]:SER:HA | 0.98 | 0.97 |
| 3:C:2990[B]:ARG:NH2 | 3:C:3180[B]:TYR:HB3 | 1.78 | 0.97 |
| 3:C:3027[B]:GLU:OE1 | 3:C:3029[B]:LYS:N | 1.97 | 0.97 |
| 3:F:2966[B]:SER:HA | 3:a:3256[B]:TRP:N | 1.78 | 0.97 |
| 3:F:2970[B]:PRO:HA | 3:a:2985[B]:PHE:HZ | 1.15 | 0.97 |
| 3:F:3034[A]:HIS:HB3 | 3:F:3035[A]:HIS:ND1 | 1.79 | 0.97 |
| 3:F:3156[B]:MET:CB | 3:a:2982[B]:MET:HG3 | 1.95 | 0.97 |
| 3:I:2968[B]:GLN:HB2 | 3:I:2972[B]:GLY:HA2 | 1.47 | 0.97 |
| 3:O:3173[B]:THR:HB | 3:O:3176[B]:LYS:HD2 | 1.46 | 0.97 |
| 3:R:2990[B]:ARG:NH2 | 3:R:3180[B]:TYR:HB3 | 1.78 | 0.97 |
| 3:R:3173[A]:THR:HB | 3:R:3176[A]:LYS:HD2 | 1.46 | 0.97 |
| 3:U:2965[B]:LEU:CD1 | 3:d:3221[B]:ALA:N | 2.14 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2968[A]:GLN:HB2 | 3:X:2972[A]:GLY:HA2 | 1.47 | 0.97 |
| 3:X:3013[B]:ASP:HA | 3:X:3122[B]:ASN:HD21 | 1.28 | 0.97 |
| 3:X:3298[A]:ASN:HB2 | 3:X:3300[A]:LEU:N | 1.78 | 0.97 |
| 3:a:3027[B]:GLU:OE1 | 3:a:3029[B]:LYS:N | 1.97 | 0.97 |
| 3:a:3038[B]:ILE:CG2 | 3:a:3040[B]:VAL:HG22 | 1.93 | 0.97 |
| 3:d:3027[B]:GLU:OE1 | 3:d:3029[B]:LYS:N | 1.97 | 0.97 |
| 3:C:3156[B]:MET:SD | 3:L:2982[B]:MET:CG | 2.53 | 0.97 |
| 3:C:3162[B]:ASP:CG | 3:L:3259[B]:ASP:H | 1.70 | 0.97 |
| 3:F:2991[B]:LEU:HD23 | 3:F:3158[B]:PHE:CD1 | 1.99 | 0.97 |
| 3:I:3221[B]:ALA:HB3 | 3:R:2964[B]:PRO:HB3 | 1.42 | 0.97 |
| 3:L:3066[A]:TYR:OH | 3:L:3203[A]:HIS:NE2 | 1.97 | 0.97 |
| 2:N:2868:GLU:OE2 | 3:O:2933[A]:SER:N | 1.97 | 0.97 |
| 3:O:3066[B]:TYR:OH | 3:O:3203[B]:HIS:NE2 | 1.97 | 0.97 |
| 3:R:3013[A]:ASP:HA | 3:R:3122[A]:ASN:HD21 | 1.27 | 0.97 |
| 3:R:3034[B]:HIS:HB3 | 3:R:3035[B]:HIS:ND1 | 1.79 | 0.97 |
| 3:X:3038[A]:ILE:CG2 | 3:X:3040[A]:VAL:HG22 | 1.93 | 0.97 |
| 3:a:3173[A]:THR:HB | 3:a:3176[A]:LYS:HD2 | 1.46 | 0.97 |
| 3:C:3168[B]:THR:O | 3:L:3149[B]:ASN:O | 1.83 | 0.97 |
| 3:C:3172[B]:SER:CA | 3:L:3152[B]:LYS:HB2 | 1.91 | 0.97 |
| 3:C:3173[B]:THR:HB | 3:C:3176[B]:LYS:HD2 | 1.46 | 0.97 |
| 3:C:3217[A]:PHE:CE1 | 3:C:3230[A]:PHE:CE1 | 2.51 | 0.97 |
| 3:I:2991[B]:LEU:HD23 | 3:I:3158[B]:PHE:CD1 | 1.99 | 0.97 |
| 3:I:3027[B]:GLU:OE1 | 3:I:3029[B]:LYS:N | 1.97 | 0.97 |
| 3:I:3161[B]:GLU:HG2 | 3:R:3079[B]:CYS:SG | 2.05 | 0.97 |
| 3:L:2952[A]:ALA:H | 3:L:2953[A]:GLY:HA2 | 1.26 | 0.97 |
| 3:R:3066[B]:TYR:OH | 3:R:3203[B]:HIS:NE2 | 1.97 | 0.97 |
| 3:U:3231[B]:ASP:O | 3:U:3284[B]:LYS:N | 1.98 | 0.97 |
| 3:d:2991[B]:LEU:HD23 | 3:d:3158[B]:PHE:CD1 | 1.99 | 0.97 |
| 3:C:2984[B]:THR:CG2 | 3:L:3159[B]:SER:HB3 | 1.88 | 0.97 |
| 3:F:2981[B]:GLY:N | 3:a:2968[B]:GLN:HG2 | 1.78 | 0.97 |
| 3:F:3066[B]:TYR:OH | 3:F:3203[B]:HIS:NE2 | 1.97 | 0.97 |
| 3:I:3107[B]:LEU:HD11 | 3:R:2975[B]:PHE:HD1 | 0.82 | 0.97 |
| 3:I:3173[B]:THR:HB | 3:I:3176[B]:LYS:HD2 | 1.46 | 0.97 |
| 3:I:3217[A]:PHE:CE1 | 3:I:3230[A]:PHE:CE1 | 2.51 | 0.97 |
| 3:L:3027[B]:GLU:OE1 | 3:L:3029[B]:LYS:N | 1.97 | 0.97 |
| 3:L:3217[A]:PHE:CE1 | 3:L:3230[A]:PHE:CE1 | 2.51 | 0.97 |
| 3:O:2965[B]:LEU:HB3 | 3:X:3254[B]:MET:HE1 | 1.46 | 0.97 |
| 3:R:3231[A]:ASP:O | 3:R:3284[A]:LYS:N | 1.97 | 0.97 |
| 1:S:1636:ASN:HD22 | 1:S:1639:LYS:HD2 | 1.29 | 0.97 |
| 3:U:3027[B]:GLU:OE1 | 3:U:3029[B]:LYS:N | 1.97 | 0.97 |
| 3:U:3034[A]:HIS:HB3 | 3:U:3035[A]:HIS:ND1 | 1.79 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3034[B]:HIS:HB3 | 3:U:3035[B]:HIS:ND1 | 1.79 | 0.97 |
| 3:U:3066[B]:TYR:OH | 3:U:3203[B]:HIS:NE2 | 1.97 | 0.97 |
| 3:X:2990[A]:ARG:NH2 | 3:X:3180[A]:TYR:HB3 | 1.79 | 0.97 |
| 3:a:2952[A]:ALA:H | 3:a:2953[A]:GLY:HA2 | 1.26 | 0.97 |
| 3:a:2968[B]:GLN:HB2 | 3:a:2972[B]:GLY:HA2 | 1.47 | 0.97 |
| 3:a:3173[B]:THR:HB | 3:a:3176[B]:LYS:HD2 | 1.46 | 0.97 |
| 3:C:2991[B]:LEU:HD23 | 3:C:3158[B]:PHE:CD1 | 1.99 | 0.97 |
| 3:F:3153[B]:LYS:CB | 3:a:3155[B]:MET:CB | 2.34 | 0.97 |
| 2:H:2472:ASN:HD21 | 4:s:1:NAG:H61 | 1.25 | 0.97 |
| 3:I:2975[B]:PHE:HA | 3:R:3107[B]:LEU:HD21 | 1.47 | 0.97 |
| 3:I:3013[B]:ASP:HA | 3:I:3122[B]:ASN:HD21 | 1.27 | 0.97 |
| 3:I:3150[B]:LYS:CD | 3:R:3160[B]:SER:H | 1.73 | 0.97 |
| 3:I:3231[B]:ASP:O | 3:I:3284[B]:LYS:N | 1.97 | 0.97 |
| 3:O:2991[A]:LEU:HD23 | 3:O:3158[A]:PHE:CD1 | 1.99 | 0.97 |
| 3:U:2991[B]:LEU:HD23 | 3:U:3158[B]:PHE:CD1 | 1.99 | 0.97 |
| 3:U:3038[B]:ILE:CG2 | 3:U:3040[B]:VAL:HG22 | 1.93 | 0.97 |
| 3:U:3152[B]:LYS:CB | 3:d:3154[B]:PRO:CA | 2.26 | 0.97 |
| 3:X:3231[A]:ASP:O | 3:X:3284[A]:LYS:N | 1.98 | 0.97 |
| 3:d:3231[B]:ASP:O | 3:d:3284[B]:LYS:N | 1.98 | 0.97 |
| 3:F:3034[B]:HIS:HB3 | 3:F:3035[B]:HIS:ND1 | 1.79 | 0.96 |
| 3:I:3159[B]:SER:CA | 3:R:3150[B]:LYS:CB | 2.42 | 0.96 |
| 3:I:3169[B]:LYS:HG2 | 3:R:3151[B]:LEU:H | 1.29 | 0.96 |
| 3:L:2990[B]:ARG:NH2 | 3:L:3180[B]:TYR:HB3 | 1.79 | 0.96 |
| 3:L:2991[A]:LEU:HD23 | 3:L:3158[A]:PHE:CD1 | 1.99 | 0.96 |
| 3:O:3034[B]:HIS:HB3 | 3:O:3035[B]:HIS:ND1 | 1.79 | 0.96 |
| 3:O:3231[A]:ASP:O | 3:O:3284[A]:LYS:N | 1.98 | 0.96 |
| 3:R:2961[B]:HIS:NE2 | 3:R:2980[B]:HIS:NE2 | 2.04 | 0.96 |
| 3:R:2968[A]:GLN:HB2 | 3:R:2972[A]:GLY:HA2 | 1.47 | 0.96 |
| 3:R:3066[A]:TYR:OH | 3:R:3203[A]:HIS:NE2 | 1.97 | 0.96 |
| 2:T:2800:LYS:O | 3:U:3023[A]:ILE:CD1 | 2.13 | 0.96 |
| 3:C:2969[B]:TYR:OH | 3:L:3120[B]:HIS:NE2 | 1.91 | 0.96 |
| 3:C:2971[B]:ASP:CB | 3:L:3093[B]:HIS:CE1 | 2.46 | 0.96 |
| 3:C:3013[B]:ASP:HA | 3:C:3122[B]:ASN:HD21 | 1.28 | 0.96 |
| 3:C:3159[B]:SER:HA | 3:L:3150[B]:LYS:C | 1.53 | 0.96 |
| 3:I:3231[A]:ASP:O | 3:I:3284[A]:LYS:N | 1.97 | 0.96 |
| 3:L:3034[A]:HIS:HB3 | 3:L:3035[A]:HIS:ND1 | 1.79 | 0.96 |
| 3:U:3013[A]:ASP:HA | 3:U:3122[A]:ASN:HD21 | 1.27 | 0.96 |
| 3:a:2991[B]:LEU:HD23 | 3:a:3158[B]:PHE:CD1 | 1.99 | 0.96 |
| 3:d:3027[A]:GLU:OE1 | 3:d:3029[A]:LYS:N | 1.97 | 0.96 |
| 3:C:3231[A]:ASP:O | 3:C:3284[A]:LYS:N | 1.97 | 0.96 |
| 3:F:2967[B]:CYS:SG | 3:a:2982[B]:MET:CG | 2.53 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3120[B]:HIS:CD2 | 3:R:2969[B]:TYR:HE2 | 1.83 | 0.96 |
| 3:I:3256[B]:TRP:HE1 | 3:R:2965[B]:LEU:CD1 | 1.79 | 0.96 |
| 3:L:2991[B]:LEU:HD23 | 3:L:3158[B]:PHE:CD1 | 1.99 | 0.96 |
| 3:R:3034[A]:HIS:HB3 | 3:R:3035[A]:HIS:ND1 | 1.79 | 0.96 |
| 2:T:2800:LYS:HB3 | 3:U:3023[A]:ILE:CD1 | 1.96 | 0.96 |
| 3:U:2969[A]:TYR:HD2 | 3:U:2971[A]:ASP:H | 1.02 | 0.96 |
| 3:X:2968[B]:GLN:HB2 | 3:X:2972[B]:GLY:HA2 | 1.47 | 0.96 |
| 3:X:2991[A]:LEU:HD23 | 3:X:3158[A]:PHE:CD1 | 1.99 | 0.96 |
| 3:a:2969[A]:TYR:HD2 | 3:a:2971[A]:ASP:H | 1.02 | 0.96 |
| 6:GA:2:NAG:H62 | 6:GA:3:BMA:C1 | 1.95 | 0.96 |
| 3:C:2952[B]:ALA:H | 3:C:2953[B]:GLY:HA2 | 1.26 | 0.96 |
| 3:C:3172[B]:SER:HB3 | 3:L:3149[B]:ASN:C | 1.88 | 0.96 |
| 3:C:3172[B]:SER:HB3 | 3:L:3149[B]:ASN:O | 1.65 | 0.96 |
| 3:I:3172[B]:SER:CB | 3:R:3150[B]:LYS:C | 2.39 | 0.96 |
| 3:O:3108[B]:HIS:HB3 | 3:X:2969[B]:TYR:CA | 1.95 | 0.96 |
| 2:Q:2868:GLU:CG | 3:R:2932[A]:PRO:O | 2.14 | 0.96 |
| 3:U:3173[A]:THR:HB | 3:U:3176[A]:LYS:HD2 | 1.46 | 0.96 |
| 3:U:3231[A]:ASP:O | 3:U:3284[A]:LYS:N | 1.98 | 0.96 |
| 3:X:3027[A]:GLU:OE1 | 3:X:3029[A]:LYS:N | 1.97 | 0.96 |
| 3:X:3231[B]:ASP:O | 3:X:3284[B]:LYS:N | 1.98 | 0.96 |
| 3:C:2965[B]:LEU:CB | 3:L:3256[B]:TRP:CZ2 | 2.35 | 0.96 |
| 3:F:3013[B]:ASP:HA | 3:F:3122[B]:ASN:HD21 | 1.27 | 0.96 |
| 3:I:3160[B]:SER:HB3 | 3:R:3150[B]:LYS:NZ | 1.80 | 0.96 |
| 3:O:2968[A]:GLN:HB2 | 3:O:2972[A]:GLY:HA2 | 1.47 | 0.96 |
| 3:O:2991[B]:LEU:HD23 | 3:O:3158[B]:PHE:CD1 | 1.99 | 0.96 |
| 3:R:3027[B]:GLU:OE1 | 3:R:3029[B]:LYS:N | 1.97 | 0.96 |
| 3:X:3034[B]:HIS:HB3 | 3:X:3035[B]:HIS:ND1 | 1.79 | 0.96 |
| 3:X:3066[B]:TYR:OH | 3:X:3203[B]:HIS:NE2 | 1.97 | 0.96 |
| 3:X:3293[A]:LYS:HD2 | 3:X:3294[A]:SER:N | 1.81 | 0.96 |
| 7:z:3:BMA:H2 | 7:z:4:MAN:H3 | 1.48 | 0.96 |
| 3:I:3034[B]:HIS:HB3 | 3:I:3035[B]:HIS:ND1 | 1.79 | 0.96 |
| 3:I:3153[B]:LYS:HD2 | 3:R:3155[B]:MET:HB2 | 1.42 | 0.96 |
| 3:L:3173[B]:THR:HB | 3:L:3176[B]:LYS:HD2 | 1.46 | 0.96 |
| 3:L:3231[A]:ASP:O | 3:L:3284[A]:LYS:N | 1.98 | 0.96 |
| 3:O:3293[B]:LYS:CD | 3:O:3294[B]:SER:HB3 | 1.95 | 0.96 |
| 3:R:3027[A]:GLU:OE1 | 3:R:3029[A]:LYS:N | 1.97 | 0.96 |
| 3:R:3231[B]:ASP:O | 3:R:3284[B]:LYS:N | 1.98 | 0.96 |
| 3:U:3152[B]:LYS:HB2 | 3:d:3154[B]:PRO:HA | 0.98 | 0.96 |
| 3:U:3156[B]:MET:HE2 | 3:d:2982[B]:MET:SD | 0.43 | 0.96 |
| 3:U:3161[B]:GLU:HA | 3:d:3146[B]:CYS:HB2 | 1.47 | 0.96 |
| 3:X:3066[A]:TYR:OH | 3:X:3203[A]:HIS:NE2 | 1.97 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2988[A]:TRP:HE3 | 3:d:2989[A]:HIS:HD1 | 1.14 | 0.96 |
| 3:C:3155[B]:MET:CG | 3:L:3154[B]:PRO:N | 2.27 | 0.96 |
| 3:I:3154[B]:PRO:CB | 3:R:3174[B]:GLY:N | 2.28 | 0.96 |
| 3:I:3162[B]:ASP:HB3 | 3:R:3259[B]:ASP:H | 1.28 | 0.96 |
| 3:L:2968[B]:GLN:HB2 | 3:L:2972[B]:GLY:HA2 | 1.47 | 0.96 |
| 2:Q:2868:GLU:CD | 3:R:2932[A]:PRO:O | 2.09 | 0.96 |
| 3:U:3066[A]:TYR:OH | 3:U:3203[A]:HIS:NE2 | 1.97 | 0.96 |
| 3:U:3169[B]:LYS:O | 3:d:3148[B]:ILE:CG2 | 2.13 | 0.96 |
| 3:a:3231[B]:ASP:O | 3:a:3284[B]:LYS:N | 1.97 | 0.96 |
| 3:C:2979[B]:GLN:HG3 | 3:L:3156[B]:MET:HE2 | 0.99 | 0.96 |
| 3:C:3027[A]:GLU:OE1 | 3:C:3029[A]:LYS:N | 1.97 | 0.96 |
| 3:F:3150[B]:LYS:HG3 | 3:a:3163[B]:ASN:HD22 | 1.29 | 0.96 |
| 3:L:3066[B]:TYR:OH | 3:L:3203[B]:HIS:NE2 | 1.97 | 0.96 |
| 3:O:2973[B]:THR:OG1 | 3:X:3158[B]:PHE:CZ | 2.17 | 0.96 |
| 3:O:3173[A]:THR:HB | 3:O:3176[A]:LYS:HD2 | 1.46 | 0.96 |
| 3:U:3196[A]:THR:N | 3:U:3199[A]:GLN:HB2 | 1.81 | 0.96 |
| 3:X:3293[A]:LYS:CD | 3:X:3294[A]:SER:HB3 | 1.95 | 0.96 |
| 3:C:3161[B]:GLU:H | 3:L:2983[B]:VAL:HG21 | 0.81 | 0.96 |
| 3:F:3155[B]:MET:HB3 | 3:a:3153[B]:LYS:CD | 1.96 | 0.96 |
| 3:R:3293[A]:LYS:HD2 | 3:R:3294[A]:SER:N | 1.81 | 0.96 |
| 3:U:2970[B]:PRO:HA | 3:d:3086[B]:GLU:CG | 1.96 | 0.96 |
| 3:U:3293[B]:LYS:CD | 3:U:3294[B]:SER:HB3 | 1.95 | 0.96 |
| 3:X:3293[B]:LYS:CD | 3:X:3294[B]:SER:HB3 | 1.95 | 0.96 |
| 4:j:1:NAG:H61 | 4:j:2:NAG:N2 | 1.81 | 0.96 |
| 3:C:3284[B]:LYS:HE2 | 3:C:3284[B]:LYS:HA | 1.48 | 0.96 |
| 3:F:3120[B]:HIS:NE2 | 3:a:2969[B]:TYR:HE2 | 1.60 | 0.96 |
| 3:F:3146[B]:CYS:O | 3:a:3161[B]:GLU:HG3 | 1.65 | 0.96 |
| 3:F:3196[A]:THR:N | 3:F:3199[A]:GLN:HB2 | 1.81 | 0.96 |
| 3:F:3231[B]:ASP:O | 3:F:3284[B]:LYS:N | 1.98 | 0.96 |
| 3:F:3293[B]:LYS:HD2 | 3:F:3294[B]:SER:N | 1.81 | 0.96 |
| 3:I:3293[A]:LYS:HD2 | 3:I:3294[A]:SER:N | 1.81 | 0.96 |
| 3:L:2968[A]:GLN:HB2 | 3:L:2972[A]:GLY:HA2 | 1.47 | 0.96 |
| 3:L:3173[A]:THR:HB | 3:L:3176[A]:LYS:HD2 | 1.46 | 0.96 |
| 3:L:3293[A]:LYS:CD | 3:L:3294[A]:SER:HB3 | 1.95 | 0.96 |
| 3:X:2988[A]:TRP:HE3 | 3:X:2989[A]:HIS:HD1 | 1.14 | 0.96 |
| 3:X:3027[B]:GLU:OE1 | 3:X:3029[B]:LYS:N | 1.97 | 0.96 |
| 3:X:3034[A]:HIS:HB3 | 3:X:3035[A]:HIS:ND1 | 1.79 | 0.96 |
| 3:a:3217[A]:PHE:CE1 | 3:a:3230[A]:PHE:CE1 | 2.51 | 0.96 |
| 3:d:3293[A]:LYS:HD2 | 3:d:3294[A]:SER:N | 1.81 | 0.96 |
| 3:F:3160[B]:SER:HB3 | 3:a:3150[B]:LYS:HZ2 | 1.24 | 0.95 |
| 3:F:3231[A]:ASP:O | 3:F:3284[A]:LYS:N | 1.98 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2968[A]:GLN:HB2 | 3:I:2972[A]:GLY:HA2 | 1.47 | 0.95 |
| 3:O:3024[B]:LEU:CD1 | 3:O:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:O:3066[A]:TYR:OH | 3:O:3203[A]:HIS:NE2 | 1.97 | 0.95 |
| 3:O:3293[A]:LYS:CD | 3:O:3294[A]:SER:HB3 | 1.95 | 0.95 |
| 3:a:3293[A]:LYS:CD | 3:a:3294[A]:SER:HB3 | 1.95 | 0.95 |
| 3:d:3173[B]:THR:HB | 3:d:3176[B]:LYS:HD2 | 1.46 | 0.95 |
| 3:d:3231[A]:ASP:O | 3:d:3284[A]:LYS:N | 1.98 | 0.95 |
| 3:C:3149[B]:ASN:CB | 3:L:3163[B]:ASN:HD21 | 1.77 | 0.95 |
| 3:F:3256[B]:TRP:CD1 | 3:a:2966[B]:SER:C | 2.44 | 0.95 |
| 3:I:3149[B]:ASN:OD1 | 3:R:3169[B]:LYS:CG | 2.14 | 0.95 |
| 3:L:3293[B]:LYS:HD2 | 3:L:3294[B]:SER:N | 1.81 | 0.95 |
| 3:O:2976[B]:ALA:CB | 3:X:3156[B]:MET:SD | 2.53 | 0.95 |
| 3:U:2991[A]:LEU:HD23 | 3:U:3158[A]:PHE:CD1 | 1.99 | 0.95 |
| 3:U:3173[B]:THR:HB | 3:U:3176[B]:LYS:HD2 | 1.46 | 0.95 |
| 3:U:3259[B]:ASP:HA | 3:d:2968[B]:GLN:NE2 | 1.80 | 0.95 |
| 3:X:3196[B]:THR:N | 3:X:3199[B]:GLN:HB2 | 1.81 | 0.95 |
| 3:a:3217[B]:PHE:CE1 | 3:a:3230[B]:PHE:CE1 | 2.51 | 0.95 |
| 3:a:3293[B]:LYS:HD2 | 3:a:3294[B]:SER:N | 1.81 | 0.95 |
| 3:d:3024[A]:LEU:CD1 | 3:d:3025[A]:VAL:N | 2.29 | 0.95 |
| 3:d:3293[B]:LYS:HD2 | 3:d:3294[B]:SER:N | 1.81 | 0.95 |
| 3:d:3293[B]:LYS:CD | 3:d:3294[B]:SER:HB3 | 1.95 | 0.95 |
| 3:C:3251[B]:ASP:OD1 | 3:L:3108[B]:HIS:CE1 | 2.19 | 0.95 |
| 1:D:2:LEU:HD21 | 1:D:81:VAL:HG21 | 1.47 | 0.95 |
| 3:F:2968[B]:GLN:HB2 | 3:F:2972[B]:GLY:HA2 | 1.47 | 0.95 |
| 3:I:3027[A]:GLU:OE1 | 3:I:3029[A]:LYS:N | 1.97 | 0.95 |
| 3:O:3040[B]:VAL:HG22 | 3:X:2969[B]:TYR:CE1 | 2.01 | 0.95 |
| 3:R:3284[A]:LYS:HE2 | 3:R:3284[A]:LYS:HA | 1.48 | 0.95 |
| 3:U:3152[B]:LYS:CB | 3:d:3154[B]:PRO:HB3 | 1.96 | 0.95 |
| 3:X:3024[A]:LEU:CD1 | 3:X:3025[A]:VAL:N | 2.29 | 0.95 |
| 3:X:3217[B]:PHE:CE1 | 3:X:3230[B]:PHE:CE1 | 2.51 | 0.95 |
| 3:X:3293[B]:LYS:HD2 | 3:X:3294[B]:SER:N | 1.81 | 0.95 |
| 3:a:3066[B]:TYR:OH | 3:a:3203[B]:HIS:NE2 | 1.97 | 0.95 |
| 3:a:3231[A]:ASP:O | 3:a:3284[A]:LYS:N | 1.97 | 0.95 |
| 3:a:3293[B]:LYS:CD | 3:a:3294[B]:SER:HB3 | 1.96 | 0.95 |
| 3:d:2987[B]:HIS:NE2 | 3:d:3178[B]:PHE:CE1 | 2.35 | 0.95 |
| 3:C:3163[B]:ASN:HD22 | 3:L:3149[B]:ASN:CB | 1.59 | 0.95 |
| 3:C:3293[A]:LYS:HD2 | 3:C:3294[A]:SER:N | 1.81 | 0.95 |
| 3:C:3293[B]:LYS:HD2 | 3:C:3294[B]:SER:N | 1.81 | 0.95 |
| 3:F:2952[A]:ALA:H | 3:F:2953[A]:GLY:HA2 | 1.26 | 0.95 |
| 3:F:3160[B]:SER:HA | 3:a:2983[B]:VAL:H | 1.30 | 0.95 |
| 3:F:3254[B]:MET:HB2 | 3:a:2966[B]:SER:OG | 1.64 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2965[A]:LEU:HD11 | 3:I:2975[A]:PHE:H | 1.31 | 0.95 |
| 3:I:3173[A]:THR:HB | 3:I:3176[A]:LYS:HD2 | 1.46 | 0.95 |
| 3:I:3293[A]:LYS:CD | 3:I:3294[A]:SER:HB3 | 1.95 | 0.95 |
| 3:L:2988[B]:TRP:HE3 | 3:L:2989[B]:HIS:HD1 | 1.14 | 0.95 |
| 3:L:3284[A]:LYS:HE2 | 3:L:3284[A]:LYS:HA | 1.48 | 0.95 |
| 3:O:3153[B]:LYS:HG2 | 3:X:3176[B]:LYS:NZ | 1.80 | 0.95 |
| 3:R:2988[B]:TRP:HE3 | 3:R:2989[B]:HIS:HD1 | 1.14 | 0.95 |
| 3:R:3196[B]:THR:N | 3:R:3199[B]:GLN:HB2 | 1.81 | 0.95 |
| 3:R:3293[A]:LYS:CD | 3:R:3294[A]:SER:HB3 | 1.95 | 0.95 |
| 3:U:2968[A]:GLN:HB2 | 3:U:2972[A]:GLY:HA2 | 1.47 | 0.95 |
| 3:U:2968[B]:GLN:CG | 3:d:3258[B]:PHE:CE1 | 2.28 | 0.95 |
| 3:a:3024[B]:LEU:CD1 | 3:a:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:d:3293[A]:LYS:CD | 3:d:3294[A]:SER:HB3 | 1.96 | 0.95 |
| 3:C:3024[A]:LEU:CD1 | 3:C:3025[A]:VAL:N | 2.29 | 0.95 |
| 3:C:3196[A]:THR:N | 3:C:3199[A]:GLN:HB2 | 1.81 | 0.95 |
| 3:C:3196[B]:THR:N | 3:C:3199[B]:GLN:HB2 | 1.81 | 0.95 |
| 3:C:3293[A]:LYS:CD | 3:C:3294[A]:SER:HB3 | 1.95 | 0.95 |
| 3:F:2965[B]:LEU:HD11 | 3:F:2975[B]:PHE:H | 1.32 | 0.95 |
| 3:F:2987[A]:HIS:NE2 | 3:F:3178[A]:PHE:CE1 | 2.35 | 0.95 |
| 3:I:3024[B]:LEU:CD1 | 3:I:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:I:3284[B]:LYS:HE2 | 3:I:3284[B]:LYS:HA | 1.48 | 0.95 |
| 3:L:2965[B]:LEU:HD11 | 3:L:2975[B]:PHE:H | 1.31 | 0.95 |
| 3:O:3153[B]:LYS:HG2 | 3:X:3176[B]:LYS:CD | 1.90 | 0.95 |
| 3:O:3254[B]:MET:CE | 3:X:3172[B]:SER:OG | 2.15 | 0.95 |
| 3:U:2948[B]:ASP:OD1 | 3:U:2950[B]:THR:OG1 | 1.85 | 0.95 |
| 3:U:2988[B]:TRP:HE3 | 3:U:2989[B]:HIS:HD1 | 1.14 | 0.95 |
| 3:C:2968[A]:GLN:HB2 | 3:C:2972[A]:GLY:HA2 | 1.47 | 0.95 |
| 3:C:2987[B]:HIS:NE2 | 3:C:3178[B]:PHE:CE1 | 2.35 | 0.95 |
| 3:C:3256[B]:TRP:CZ2 | 3:L:2965[B]:LEU:CB | 2.45 | 0.95 |
| 3:C:3293[B]:LYS:CD | 3:C:3294[B]:SER:HB3 | 1.95 | 0.95 |
| 3:F:3255[B]:PRO:HB2 | 3:a:2959[B]:SER:CB | 1.97 | 0.95 |
| 3:I:3155[B]:MET:CG | 3:R:3154[B]:PRO:N | 2.26 | 0.95 |
| 3:L:2948[A]:ASP:OD1 | 3:L:2950[A]:THR:OG1 | 1.85 | 0.95 |
| 3:L:3196[B]:THR:N | 3:L:3199[B]:GLN:HB2 | 1.81 | 0.95 |
| 3:O:3231[B]:ASP:O | 3:O:3284[B]:LYS:N | 1.98 | 0.95 |
| 3:O:3293[A]:LYS:HD2 | 3:O:3294[A]:SER:N | 1.81 | 0.95 |
| 3:U:3024[B]:LEU:CD1 | 3:U:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:U:3217[A]:PHE:CE1 | 3:U:3230[A]:PHE:CE1 | 2.51 | 0.95 |
| 3:a:2946[A]:GLN:O | 3:a:3037[A]:TYR:OH | 1.85 | 0.95 |
| 3:d:2990[A]:ARG:NH2 | 3:d:3180[A]:TYR:HB3 | 1.79 | 0.95 |
| 3:d:3284[A]:LYS:HE2 | 3:d:3284[A]:LYS:HA | 1.48 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3163[B]:ASN:HD21 | 3:L:3149[B]:ASN:CB | 1.56 | 0.95 |
| 3:F:3024[B]:LEU:CD1 | 3:F:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:F:3255[B]:PRO:HG3 | 3:a:2963[B]:MET:C | 1.92 | 0.95 |
| 3:I:3024[A]:LEU:CD1 | 3:I:3025[A]:VAL:N | 2.29 | 0.95 |
| 3:I:3066[A]:TYR:OH | 3:I:3203[A]:HIS:NE2 | 1.97 | 0.95 |
| 3:L:3293[B]:LYS:CD | 3:L:3294[B]:SER:HB3 | 1.95 | 0.95 |
| 3:O:2948[B]:ASP:OD1 | 3:O:2950[B]:THR:OG1 | 1.85 | 0.95 |
| 3:R:2946[A]:GLN:O | 3:R:3037[A]:TYR:OH | 1.85 | 0.95 |
| 3:R:3173[B]:THR:HB | 3:R:3176[B]:LYS:HD2 | 1.46 | 0.95 |
| 3:U:3156[B]:MET:CE | 3:d:2982[B]:MET:CE | 2.45 | 0.95 |
| 3:a:3013[A]:ASP:HA | 3:a:3122[A]:ASN:HD21 | 1.27 | 0.95 |
| 3:a:3196[A]:THR:N | 3:a:3199[A]:GLN:HB2 | 1.81 | 0.95 |
| 3:d:3196[B]:THR:N | 3:d:3199[B]:GLN:HB2 | 1.81 | 0.95 |
| 3:d:3284[B]:LYS:HE2 | 3:d:3284[B]:LYS:HA | 1.48 | 0.95 |
| 3:C:3024[B]:LEU:CD1 | 3:C:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:F:3149[B]:ASN:CG | 3:a:3163[B]:ASN:ND2 | 2.25 | 0.95 |
| 3:F:3160[B]:SER:OG | 3:a:2982[B]:MET:HA | 1.66 | 0.95 |
| 3:F:3255[B]:PRO:CG | 3:a:2962[B]:GLY:O | 2.15 | 0.95 |
| 3:L:2987[A]:HIS:NE2 | 3:L:3178[A]:PHE:CE1 | 2.35 | 0.95 |
| 3:O:2970[B]:PRO:HG2 | 3:X:2991[B]:LEU:CB | 1.94 | 0.95 |
| 3:O:3196[B]:THR:N | 3:O:3199[B]:GLN:HB2 | 1.81 | 0.95 |
| 3:R:3024[B]:LEU:CD1 | 3:R:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:U:3259[B]:ASP:HA | 3:d:2968[B]:GLN:HE21 | 1.28 | 0.95 |
| 3:X:2987[B]:HIS:NE2 | 3:X:3178[B]:PHE:CE1 | 2.35 | 0.95 |
| 3:a:2948[B]:ASP:OD1 | 3:a:2950[B]:THR:OG1 | 1.85 | 0.95 |
| 3:a:2987[A]:HIS:NE2 | 3:a:3178[A]:PHE:CE1 | 2.35 | 0.95 |
| 3:a:3293[A]:LYS:HD2 | 3:a:3294[A]:SER:N | 1.81 | 0.95 |
| 3:d:2946[A]:GLN:O | 3:d:3037[A]:TYR:OH | 1.85 | 0.95 |
| 3:C:2988[B]:TRP:HE1 | 3:L:3153[B]:LYS:HZ3 | 1.01 | 0.95 |
| 3:F:3293[B]:LYS:CD | 3:F:3294[B]:SER:HB3 | 1.95 | 0.95 |
| 3:L:3196[A]:THR:N | 3:L:3199[A]:GLN:HB2 | 1.81 | 0.95 |
| 3:U:2987[B]:HIS:NE2 | 3:U:3178[B]:PHE:CE1 | 2.34 | 0.95 |
| 3:U:3293[A]:LYS:HD2 | 3:U:3294[A]:SER:N | 1.81 | 0.95 |
| 3:a:2987[B]:HIS:NE2 | 3:a:3178[B]:PHE:CE1 | 2.35 | 0.95 |
| 3:a:3169[B]:LYS:O | 3:a:3172[B]:SER:OG | 1.85 | 0.95 |
| 3:C:2987[A]:HIS:NE2 | 3:C:3178[A]:PHE:CE1 | 2.34 | 0.95 |
| 3:F:2948[B]:ASP:OD1 | 3:F:2950[B]:THR:OG1 | 1.85 | 0.95 |
| 3:F:2989[B]:HIS:HE1 | 3:a:2969[B]:TYR:HA | 1.24 | 0.95 |
| 3:F:3153[B]:LYS:NZ | 3:a:3157[B]:PRO:CD | 2.27 | 0.95 |
| 3:F:3254[B]:MET:C | 3:a:2966[B]:SER:OG | 2.09 | 0.95 |
| 3:I:3196[A]:THR:N | 3:I:3199[A]:GLN:HB2 | 1.81 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3196[B]:THR:N | 3:I:3199[B]:GLN:HB2 | 1.81 | 0.95 |
| 3:L:2987[B]:HIS:NE2 | 3:L:3178[B]:PHE:CE1 | 2.35 | 0.95 |
| 3:L:3024[B]:LEU:CD1 | 3:L:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:O:2987[A]:HIS:NE2 | 3:O:3178[A]:PHE:CE1 | 2.35 | 0.95 |
| 3:O:2988[B]:TRP:HE3 | 3:O:2989[B]:HIS:HD1 | 1.14 | 0.95 |
| 3:O:3158[B]:PHE:C | 3:X:3148[B]:ILE:O | 2.10 | 0.95 |
| 3:U:3149[B]:ASN:C | 3:d:3154[B]:PRO:CB | 2.40 | 0.95 |
| 3:d:2965[B]:LEU:HD11 | 3:d:2975[B]:PHE:H | 1.31 | 0.95 |
| 3:d:3024[B]:LEU:CD1 | 3:d:3025[B]:VAL:N | 2.29 | 0.95 |
| 3:F:2965[A]:LEU:HD11 | 3:F:2975[A]:PHE:H | 1.31 | 0.94 |
| 3:I:2931[A]:THR:OG1 | 3:I:2934[A]:GLU:OE2 | 1.85 | 0.94 |
| 3:I:2965[B]:LEU:H | 3:R:3221[B]:ALA:HB1 | 1.15 | 0.94 |
| 3:I:3174[B]:GLY:H | 3:R:3154[B]:PRO:HB3 | 1.28 | 0.94 |
| 3:L:3231[B]:ASP:O | 3:L:3284[B]:LYS:N | 1.97 | 0.94 |
| 3:O:2946[A]:GLN:O | 3:O:3037[A]:TYR:OH | 1.85 | 0.94 |
| 3:O:2968[B]:GLN:HB2 | 3:O:2972[B]:GLY:HA2 | 1.47 | 0.94 |
| 3:O:2974[B]:ALA:HB3 | 3:X:2977[B]:CYS:CB | 1.97 | 0.94 |
| 3:R:2948[A]:ASP:OD1 | 3:R:2950[A]:THR:OG1 | 1.85 | 0.94 |
| 3:R:3024[A]:LEU:CD1 | 3:R:3025[A]:VAL:N | 2.29 | 0.94 |
| 3:R:3196[A]:THR:N | 3:R:3199[A]:GLN:HB2 | 1.81 | 0.94 |
| 3:R:3298[A]:ASN:HB2 | 3:R:3300[A]:LEU:N | 1.78 | 0.94 |
| 3:d:3173[A]:THR:HB | 3:d:3176[A]:LYS:HD2 | 1.46 | 0.94 |
| 3:F:2931[B]:THR:OG1 | 3:F:2934[B]:GLU:OE2 | 1.85 | 0.94 |
| 3:F:2975[B]:PHE:CD1 | 3:a:3107[B]:LEU:CG | 2.47 | 0.94 |
| 3:I:2946[A]:GLN:O | 3:I:3037[A]:TYR:OH | 1.85 | 0.94 |
| 3:I:2946[B]:GLN:O | 3:I:3037[B]:TYR:OH | 1.85 | 0.94 |
| 3:L:2931[B]:THR:OG1 | 3:L:2934[B]:GLU:OE2 | 1.85 | 0.94 |
| 3:L:2965[A]:LEU:HD11 | 3:L:2975[A]:PHE:H | 1.31 | 0.94 |
| 3:O:2931[A]:THR:OG1 | 3:O:2934[A]:GLU:OE2 | 1.85 | 0.94 |
| 3:O:3106[A]:THR:O | 3:O:3110[A]:THR:OG1 | 1.85 | 0.94 |
| 3:O:3169[B]:LYS:O | 3:O:3172[B]:SER:OG | 1.85 | 0.94 |
| 3:O:3217[A]:PHE:CE1 | 3:O:3230[A]:PHE:CE1 | 2.51 | 0.94 |
| 3:U:2946[A]:GLN:O | 3:U:3037[A]:TYR:OH | 1.85 | 0.94 |
| 3:U:3155[B]:MET:CA | 3:d:3150[B]:LYS:CG | 2.28 | 0.94 |
| 3:U:3298[B]:ASN:HB2 | 3:U:3300[B]:LEU:N | 1.78 | 0.94 |
| 3:C:2984[B]:THR:HG23 | 3:L:3159[B]:SER:HB3 | 0.97 | 0.94 |
| 3:F:3150[B]:LYS:HG2 | 3:a:3158[B]:PHE:CA | 1.54 | 0.94 |
| 3:F:3161[B]:GLU:CA | 3:a:3147[B]:GLU:CG | 2.45 | 0.94 |
| 3:I:2987[B]:HIS:NE2 | 3:I:3178[B]:PHE:CE1 | 2.35 | 0.94 |
| 3:I:3169[A]:LYS:O | 3:I:3172[A]:SER:OG | 1.85 | 0.94 |
| 3:I:3293[B]:LYS:HD2 | 3:I:3294[B]:SER:N | 1.81 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2946[B]:GLN:O | 3:O:3037[B]:TYR:OH | 1.85 | 0.94 |
| 3:O:2963[B]:MET:CE | 3:X:2975[B]:PHE:CD2 | 2.48 | 0.94 |
| 3:O:3284[B]:LYS:HE2 | 3:O:3284[B]:LYS:HA | 1.48 | 0.94 |
| 3:O:3293[B]:LYS:HD2 | 3:O:3294[B]:SER:N | 1.81 | 0.94 |
| 3:U:3159[B]:SER:HB2 | 3:d:3150[B]:LYS:CE | 1.97 | 0.94 |
| 3:U:3293[A]:LYS:CD | 3:U:3294[A]:SER:HB3 | 1.95 | 0.94 |
| 3:X:2946[A]:GLN:O | 3:X:3037[A]:TYR:OH | 1.85 | 0.94 |
| 3:X:3024[B]:LEU:CD1 | 3:X:3025[B]:VAL:N | 2.29 | 0.94 |
| 1:Y:1550:ARG:CZ | 3:d:3008[B]:GLY:O | 2.14 | 0.94 |
| 3:a:2931[A]:THR:OG1 | 3:a:2934[A]:GLU:OE2 | 1.85 | 0.94 |
| 3:a:2965[B]:LEU:HD11 | 3:a:2975[B]:PHE:H | 1.31 | 0.94 |
| 3:F:2974[B]:ALA:N | 3:a:3248[B]:LEU:C | 2.26 | 0.94 |
| 3:F:3163[B]:ASN:ND2 | 3:a:3149[B]:ASN:CB | 2.30 | 0.94 |
| 3:F:3169[B]:LYS:O | 3:F:3172[B]:SER:OG | 1.85 | 0.94 |
| 3:F:3251[B]:ASP:C | 3:a:3252[B]:TYR:HB2 | 1.91 | 0.94 |
| 3:F:3293[A]:LYS:HD2 | 3:F:3294[A]:SER:N | 1.81 | 0.94 |
| 3:I:3106[A]:THR:O | 3:I:3110[A]:THR:OG1 | 1.86 | 0.94 |
| 3:I:3159[B]:SER:CA | 3:R:3150[B]:LYS:C | 2.39 | 0.94 |
| 3:L:3024[A]:LEU:CD1 | 3:L:3025[A]:VAL:N | 2.29 | 0.94 |
| 3:O:2965[B]:LEU:HD11 | 3:O:2975[B]:PHE:H | 1.31 | 0.94 |
| 3:O:3024[A]:LEU:CD1 | 3:O:3025[A]:VAL:N | 2.29 | 0.94 |
| 3:R:3106[B]:THR:O | 3:R:3110[B]:THR:OG1 | 1.85 | 0.94 |
| 3:R:3169[B]:LYS:O | 3:R:3172[B]:SER:OG | 1.85 | 0.94 |
| 3:R:3293[B]:LYS:CD | 3:R:3294[B]:SER:HB3 | 1.95 | 0.94 |
| 3:R:3293[B]:LYS:HD2 | 3:R:3294[B]:SER:N | 1.81 | 0.94 |
| 3:U:2931[A]:THR:OG1 | 3:U:2934[A]:GLU:OE2 | 1.85 | 0.94 |
| 3:U:3284[A]:LYS:HA | 3:U:3284[A]:LYS:HE2 | 1.48 | 0.94 |
| 3:X:2987[A]:HIS:NE2 | 3:X:3178[A]:PHE:CE1 | 2.35 | 0.94 |
| 3:a:2968[A]:GLN:HB2 | 3:a:2972[A]:GLY:HA2 | 1.47 | 0.94 |
| 3:a:3196[B]:THR:N | 3:a:3199[B]:GLN:HB2 | 1.81 | 0.94 |
| 3:a:3298[A]:ASN:HB2 | 3:a:3300[A]:LEU:N | 1.78 | 0.94 |
| 3:d:3217[B]:PHE:CE1 | 3:d:3230[B]:PHE:CE1 | 2.51 | 0.94 |
| 1:D:1494:ARG:HH11 | 1:D:1494:ARG:HG3 | 1.29 | 0.94 |
| 3:F:2988[B]:TRP:HE3 | 3:F:2989[B]:HIS:HD1 | 1.14 | 0.94 |
| 3:F:3149[B]:ASN:HB2 | 3:a:3163[B]:ASN:HD22 | 1.22 | 0.94 |
| 3:F:3173[B]:THR:HB | 3:F:3176[B]:LYS:HD2 | 1.46 | 0.94 |
| 3:I:3163[B]:ASN:ND2 | 3:R:3149[B]:ASN:CG | 2.26 | 0.94 |
| 3:L:3217[B]:PHE:CE1 | 3:L:3230[B]:PHE:CE1 | 2.51 | 0.94 |
| 2:N:2800:LYS:O | 3:O:3023[A]:ILE:CD1 | 2.14 | 0.94 |
| 3:O:3284[A]:LYS:HE2 | 3:O:3284[A]:LYS:HA | 1.48 | 0.94 |
| 3:U:2931[B]:THR:OG1 | 3:U:2934[B]:GLU:OE2 | 1.85 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2965[B]:LEU:H | 3:d:3220[B]:ARG:CZ | 1.79 | 0.94 |
| 3:U:3196[B]:THR:N | 3:U:3199[B]:GLN:HB2 | 1.81 | 0.94 |
| 3:a:3106[A]:THR:O | 3:a:3110[A]:THR:OG1 | 1.85 | 0.94 |
| 3:F:3024[A]:LEU:CD1 | 3:F:3025[A]:VAL:N | 2.29 | 0.94 |
| 3:F:3106[B]:THR:O | 3:F:3110[B]:THR:OG1 | 1.85 | 0.94 |
| 3:F:3196[B]:THR:N | 3:F:3199[B]:GLN:HB2 | 1.81 | 0.94 |
| 3:I:2987[A]:HIS:NE2 | 3:I:3178[A]:PHE:CE1 | 2.35 | 0.94 |
| 3:I:2988[A]:TRP:HE3 | 3:I:2989[A]:HIS:HD1 | 1.13 | 0.94 |
| 3:L:2948[B]:ASP:OD1 | 3:L:2950[B]:THR:OG1 | 1.85 | 0.94 |
| 3:L:3293[A]:LYS:HD2 | 3:L:3294[A]:SER:N | 1.81 | 0.94 |
| 3:O:2970[B]:PRO:O | 3:X:2989[B]:HIS:N | 1.99 | 0.94 |
| 3:O:3157[B]:PRO:C | 3:X:3149[B]:ASN:C | 2.33 | 0.94 |
| 3:U:2975[B]:PHE:HB2 | 3:d:3256[B]:TRP:CG | 2.03 | 0.94 |
| 3:U:3024[A]:LEU:CD1 | 3:U:3025[A]:VAL:N | 2.29 | 0.94 |
| 3:U:3156[B]:MET:CE | 3:d:2982[B]:MET:SD | 1.04 | 0.94 |
| 3:U:3254[B]:MET:CB | 3:d:3254[B]:MET:CB | 2.42 | 0.94 |
| 3:U:3293[B]:LYS:HD2 | 3:U:3294[B]:SER:N | 1.81 | 0.94 |
| 3:X:3284[B]:LYS:HE2 | 3:X:3284[B]:LYS:HA | 1.48 | 0.94 |
| 3:a:3024[A]:LEU:CD1 | 3:a:3025[A]:VAL:N | 2.29 | 0.94 |
| 3:d:2946[B]:GLN:O | 3:d:3037[B]:TYR:OH | 1.85 | 0.94 |
| 3:d:3169[A]:LYS:O | 3:d:3172[A]:SER:OG | 1.85 | 0.94 |
| 3:d:3196[A]:THR:N | 3:d:3199[A]:GLN:HB2 | 1.81 | 0.94 |
| 3:C:2965[B]:LEU:HD11 | 3:C:2975[B]:PHE:H | 1.31 | 0.94 |
| 3:C:3079[B]:CYS:SG | 3:L:3161[B]:GLU:HG3 | 0.93 | 0.94 |
| 3:F:2979[A]:GLN:CG | 3:F:3155[A]:MET:HE1 | 1.97 | 0.94 |
| 3:I:2969[A]:TYR:HD2 | 3:I:2971[A]:ASP:H | 1.02 | 0.94 |
| 3:I:3251[B]:ASP:OD1 | 3:R:3108[B]:HIS:CE1 | 2.20 | 0.94 |
| 3:O:2931[B]:THR:OG1 | 3:O:2934[B]:GLU:OE2 | 1.85 | 0.94 |
| 3:O:2987[B]:HIS:NE2 | 3:O:3178[B]:PHE:CE1 | 2.35 | 0.94 |
| 3:R:2948[B]:ASP:OD1 | 3:R:2950[B]:THR:OG1 | 1.85 | 0.94 |
| 3:U:2974[B]:ALA:HB1 | 3:d:3220[B]:ARG:HG2 | 1.47 | 0.94 |
| 3:U:3176[B]:LYS:HD2 | 3:d:3152[B]:LYS:CD | 1.96 | 0.94 |
| 3:U:3284[B]:LYS:HE2 | 3:U:3284[B]:LYS:HA | 1.48 | 0.94 |
| 3:X:2931[A]:THR:OG1 | 3:X:2934[A]:GLU:OE2 | 1.85 | 0.94 |
| 3:C:2931[A]:THR:OG1 | 3:C:2934[A]:GLU:OE2 | 1.85 | 0.94 |
| 3:C:2968[B]:GLN:HB2 | 3:C:2972[B]:GLY:HA2 | 1.47 | 0.94 |
| 3:C:3150[B]:LYS:HA | 3:L:3172[B]:SER:CB | 1.89 | 0.94 |
| 3:C:3197[B]:ILE:HD12 | 1:D:1617:LYS:O | 1.67 | 0.94 |
| 3:F:2987[B]:HIS:NE2 | 3:F:3178[B]:PHE:CE1 | 2.35 | 0.94 |
| 3:F:3120[B]:HIS:CD2 | 3:a:2969[B]:TYR:HE2 | 1.86 | 0.94 |
| 3:F:3159[B]:SER:HB3 | 3:a:2984[B]:THR:HG23 | 0.96 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3284[B]:LYS:HE2 | 3:F:3284[B]:LYS:HA | 1.48 | 0.94 |
| 3:I:2948[A]:ASP:OD1 | 3:I:2950[A]:THR:OG1 | 1.85 | 0.94 |
| 3:I:2969[B]:TYR:HD2 | 3:I:2971[B]:ASP:H | 1.02 | 0.94 |
| 3:I:2976[B]:ALA:O | 3:R:2976[B]:ALA:O | 1.84 | 0.94 |
| 3:I:2989[B]:HIS:CG | 3:R:2970[B]:PRO:CD | 2.31 | 0.94 |
| 3:I:3255[B]:PRO:HB3 | 3:R:2964[B]:PRO:CB | 1.96 | 0.94 |
| 3:I:3293[B]:LYS:CD | 3:I:3294[B]:SER:HB3 | 1.95 | 0.94 |
| 3:L:2931[A]:THR:OG1 | 3:L:2934[A]:GLU:OE2 | 1.85 | 0.94 |
| 3:L:2946[B]:GLN:O | 3:L:3037[B]:TYR:OH | 1.85 | 0.94 |
| 3:L:3298[B]:ASN:HB2 | 3:L:3300[B]:LEU:N | 1.78 | 0.94 |
| 3:O:2965[B]:LEU:C | 3:X:3153[B]:LYS:HZ2 | 1.67 | 0.94 |
| 3:O:2988[A]:TRP:HE3 | 3:O:2989[A]:HIS:HD1 | 1.13 | 0.94 |
| 3:O:3160[B]:SER:OG | 3:X:3150[B]:LYS:HB2 | 1.67 | 0.94 |
| 3:O:3163[B]:ASN:HB2 | 3:X:3149[B]:ASN:HA | 0.94 | 0.94 |
| 3:R:2987[B]:HIS:NE2 | 3:R:3178[B]:PHE:CE1 | 2.35 | 0.94 |
| 3:U:2975[B]:PHE:CE2 | 3:d:3254[B]:MET:CG | 2.40 | 0.94 |
| 3:U:2980[B]:HIS:HB2 | 3:d:2969[B]:TYR:CE1 | 2.03 | 0.94 |
| 3:U:2987[A]:HIS:NE2 | 3:U:3178[A]:PHE:CE1 | 2.35 | 0.94 |
| 3:X:2931[B]:THR:OG1 | 3:X:2934[B]:GLU:OE2 | 1.85 | 0.94 |
| 3:X:3169[B]:LYS:O | 3:X:3172[B]:SER:OG | 1.85 | 0.94 |
| 3:a:2948[A]:ASP:OD1 | 3:a:2950[A]:THR:OG1 | 1.85 | 0.94 |
| 3:d:2931[B]:THR:OG1 | 3:d:2934[B]:GLU:OE2 | 1.85 | 0.94 |
| 3:d:2979[A]:GLN:CG | 3:d:3155[A]:MET:HE1 | 1.97 | 0.94 |
| 3:C:2946[A]:GLN:O | 3:C:3037[A]:TYR:OH | 1.85 | 0.94 |
| 3:C:3154[B]:PRO:HG3 | 3:L:3174[B]:GLY:HA2 | 1.50 | 0.94 |
| 3:C:3174[B]:GLY:HA2 | 3:L:3154[B]:PRO:CG | 1.98 | 0.94 |
| 3:F:2966[B]:SER:CA | 3:a:3256[B]:TRP:CG | 2.50 | 0.94 |
| 3:F:2969[B]:TYR:HD2 | 3:F:2971[B]:ASP:H | 1.02 | 0.94 |
| 3:F:3158[B]:PHE:H | 3:a:3153[B]:LYS:NZ | 1.65 | 0.94 |
| 3:O:3196[A]:THR:N | 3:O:3199[A]:GLN:HB2 | 1.81 | 0.94 |
| 3:U:2979[B]:GLN:CG | 3:U:3155[B]:MET:HE1 | 1.97 | 0.94 |
| 3:U:3170[B]:ALA:CA | 3:d:3148[B]:ILE:CG2 | 2.40 | 0.94 |
| 3:U:3253[B]:GLU:HA | 3:d:3255[B]:PRO:HG2 | 0.94 | 0.94 |
| 1:Y:1401:ARG:HD3 | 3:d:3182[B]:GLN:OE1 | 1.68 | 0.94 |
| 3:d:3169[B]:LYS:O | 3:d:3172[B]:SER:OG | 1.85 | 0.94 |
| 3:C:3153[B]:LYS:NZ | 3:L:3158[B]:PHE:CE2 | 2.32 | 0.94 |
| 3:I:3150[B]:LYS:CB | 3:R:3159[B]:SER:CA | 2.30 | 0.94 |
| 3:I:3169[B]:LYS:O | 3:I:3172[B]:SER:OG | 1.85 | 0.94 |
| 3:L:3106[A]:THR:O | 3:L:3110[A]:THR:OG1 | 1.85 | 0.94 |
| 3:U:2968[B]:GLN:HB2 | 3:U:2972[B]:GLY:HA2 | 1.47 | 0.94 |
| 3:X:2965[A]:LEU:HD11 | 3:X:2975[A]:PHE:H | 1.31 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3173[B]:THR:HB | 3:X:3176[B]:LYS:HD2 | 1.46 | 0.94 |
| 3:C:2948[A]:ASP:OD1 | 3:C:2950[A]:THR:OG1 | 1.85 | 0.93 |
| 3:C:2979[A]:GLN:CG | 3:C:3155[A]:MET:HE1 | 1.97 | 0.93 |
| 3:C:3106[A]:THR:O | 3:C:3110[A]:THR:OG1 | 1.85 | 0.93 |
| 3:C:3169[B]:LYS:O | 3:C:3172[B]:SER:OG | 1.85 | 0.93 |
| 3:I:2948[B]:ASP:OD1 | 3:I:2950[B]:THR:OG1 | 1.85 | 0.93 |
| 3:R:2946[B]:GLN:O | 3:R:3037[B]:TYR:OH | 1.85 | 0.93 |
| 3:R:2965[A]:LEU:HD11 | 3:R:2975[A]:PHE:H | 1.31 | 0.93 |
| 3:R:2987[A]:HIS:NE2 | 3:R:3178[A]:PHE:CE1 | 2.35 | 0.93 |
| 3:R:3298[B]:ASN:HB2 | 3:R:3300[B]:LEU:N | 1.78 | 0.93 |
| 2:W:2472:ASN:HD21 | 4:HA:1:NAG:H61 | 1.31 | 0.93 |
| 3:X:2946[B]:GLN:O | 3:X:3037[B]:TYR:OH | 1.85 | 0.93 |
| 3:X:3196[A]:THR:N | 3:X:3199[A]:GLN:HB2 | 1.81 | 0.93 |
| 3:X:3284[A]:LYS:HE2 | 3:X:3284[A]:LYS:HA | 1.48 | 0.93 |
| 3:a:2931[B]:THR:OG1 | 3:a:2934[B]:GLU:OE2 | 1.85 | 0.93 |
| 3:a:3284[B]:LYS:HE2 | 3:a:3284[B]:LYS:HA | 1.48 | 0.93 |
| 3:C:2948[B]:ASP:OD1 | 3:C:2950[B]:THR:OG1 | 1.85 | 0.93 |
| 3:F:2968[A]:GLN:HB2 | 3:F:2972[A]:GLY:HA2 | 1.47 | 0.93 |
| 3:F:3293[A]:LYS:CD | 3:F:3294[A]:SER:HB3 | 1.95 | 0.93 |
| 3:L:2946[A]:GLN:O | 3:L:3037[A]:TYR:OH | 1.85 | 0.93 |
| 3:L:3134[A]:GLN:O | 3:L:3137[A]:ARG:N | 2.02 | 0.93 |
| 3:O:2969[B]:TYR:HH | 3:X:2994[B]:LYS:HB3 | 1.21 | 0.93 |
| 3:R:2968[B]:GLN:HB2 | 3:R:2972[B]:GLY:HA2 | 1.47 | 0.93 |
| 3:d:3106[A]:THR:O | 3:d:3110[A]:THR:OG1 | 1.85 | 0.93 |
| 3:d:3106[B]:THR:O | 3:d:3110[B]:THR:OG1 | 1.85 | 0.93 |
| 3:F:3155[B]:MET:HB2 | 3:a:3153[B]:LYS:HG2 | 1.50 | 0.93 |
| 3:F:3169[A]:LYS:O | 3:F:3172[A]:SER:OG | 1.85 | 0.93 |
| 3:F:3284[A]:LYS:HE2 | 3:F:3284[A]:LYS:HA | 1.48 | 0.93 |
| 3:I:3172[B]:SER:N | 3:R:3152[B]:LYS:CB | 2.07 | 0.93 |
| 3:L:2960[A]:PHE:HD2 | 3:L:3157[A]:PRO:CG | 1.82 | 0.93 |
| 3:L:2979[A]:GLN:CG | 3:L:3155[A]:MET:HE1 | 1.97 | 0.93 |
| 3:L:3106[B]:THR:O | 3:L:3110[B]:THR:OG1 | 1.85 | 0.93 |
| 3:O:2973[B]:THR:HG1 | 3:X:3158[B]:PHE:HZ | 0.94 | 0.93 |
| 3:U:2965[A]:LEU:HD11 | 3:U:2975[A]:PHE:H | 1.31 | 0.93 |
| 3:U:3255[B]:PRO:HD3 | 3:d:3253[B]:GLU:O | 1.67 | 0.93 |
| 3:U:3298[A]:ASN:HB2 | 3:U:3300[A]:LEU:N | 1.78 | 0.93 |
| 3:X:2963[B]:MET:HG2 | 3:X:3108[B]:HIS:CD2 | 2.04 | 0.93 |
| 3:a:3106[B]:THR:O | 3:a:3110[B]:THR:OG1 | 1.85 | 0.93 |
| 3:d:2932[A]:PRO:HA | 3:d:2935[A]:ILE:CD1 | 1.99 | 0.93 |
| 3:d:2932[B]:PRO:HA | 3:d:2935[B]:ILE:CD1 | 1.99 | 0.93 |
| 3:F:3153[B]:LYS:HG2 | 3:a:3155[B]:MET:CG | 1.99 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3196[A]:THR:CG2 | 1:J:416:ASN:ND2 | 1.75 | 0.93 |
| 3:L:2932[A]:PRO:HA | 3:L:2935[A]:ILE:CD1 | 1.99 | 0.93 |
| 3:O:2963[B]:MET:CG | 3:X:2968[B]:GLN:O | 2.12 | 0.93 |
| 3:O:2967[B]:CYS:HB2 | 3:X:3155[B]:MET:CG | 1.97 | 0.93 |
| 3:R:2931[B]:THR:OG1 | 3:R:2934[B]:GLU:OE2 | 1.85 | 0.93 |
| 3:U:2932[A]:PRO:HA | 3:U:2935[A]:ILE:CD1 | 1.99 | 0.93 |
| 3:U:2948[A]:ASP:OD1 | 3:U:2950[A]:THR:OG1 | 1.85 | 0.93 |
| 3:U:3169[B]:LYS:O | 3:U:3172[B]:SER:OG | 1.85 | 0.93 |
| 3:a:2932[B]:PRO:HA | 3:a:2935[B]:ILE:CD1 | 1.99 | 0.93 |
| 3:a:2963[A]:MET:HG2 | 3:a:3108[A]:HIS:CD2 | 2.04 | 0.93 |
| 3:d:2987[A]:HIS:NE2 | 3:d:3178[A]:PHE:CE1 | 2.35 | 0.93 |
| 3:C:2969[A]:TYR:HD2 | 3:C:2971[A]:ASP:H | 1.02 | 0.93 |
| 3:C:3161[B]:GLU:HG3 | 3:L:3146[B]:CYS:O | 1.69 | 0.93 |
| 3:C:3172[B]:SER:HB3 | 3:L:3150[B]:LYS:N | 1.82 | 0.93 |
| 3:F:2946[B]:GLN:O | 3:F:3037[B]:TYR:OH | 1.85 | 0.93 |
| 3:F:2963[B]:MET:HG2 | 3:F:3108[B]:HIS:CD2 | 2.04 | 0.93 |
| 3:F:2988[A]:TRP:HE3 | 3:F:2989[A]:HIS:HD1 | 1.14 | 0.93 |
| 3:F:3163[B]:ASN:HD21 | 3:a:3149[B]:ASN:HB2 | 1.20 | 0.93 |
| 3:I:2932[B]:PRO:HA | 3:I:2935[B]:ILE:HD12 | 1.51 | 0.93 |
| 3:O:2948[A]:ASP:OD1 | 3:O:2950[A]:THR:OG1 | 1.85 | 0.93 |
| 3:O:2960[B]:PHE:HD2 | 3:O:3157[B]:PRO:CG | 1.82 | 0.93 |
| 3:O:2965[A]:LEU:HD11 | 3:O:2975[A]:PHE:H | 1.31 | 0.93 |
| 3:O:3040[B]:VAL:HG21 | 3:X:2969[B]:TYR:HD1 | 1.21 | 0.93 |
| 3:R:2931[A]:THR:OG1 | 3:R:2934[A]:GLU:OE2 | 1.85 | 0.93 |
| 3:U:3106[B]:THR:O | 3:U:3110[B]:THR:OG1 | 1.86 | 0.93 |
| 3:U:3162[B]:ASP:N | 3:d:3260[B]:ARG:HH12 | 1.57 | 0.93 |
| 3:X:2948[B]:ASP:OD1 | 3:X:2950[B]:THR:OG1 | 1.85 | 0.93 |
| 2:Z:2867:PRO:HG2 | 3:a:2932[A]:PRO:CG | 1.78 | 0.93 |
| 3:a:2946[B]:GLN:O | 3:a:3037[B]:TYR:OH | 1.85 | 0.93 |
| 3:d:2963[B]:MET:HG2 | 3:d:3108[B]:HIS:CD2 | 2.04 | 0.93 |
| 3:F:2931[A]:THR:OG1 | 3:F:2934[A]:GLU:OE2 | 1.85 | 0.93 |
| 3:F:2965[B]:LEU:CD1 | 3:a:3256[B]:TRP:NE1 | 2.30 | 0.93 |
| 3:I:2932[A]:PRO:HA | 3:I:2935[A]:ILE:HD12 | 1.51 | 0.93 |
| 3:I:2966[B]:SER:HB3 | 3:R:2982[B]:MET:HE2 | 1.46 | 0.93 |
| 3:I:3106[B]:THR:O | 3:I:3110[B]:THR:OG1 | 1.85 | 0.93 |
| 3:I:3254[B]:MET:CB | 3:R:2966[B]:SER:OG | 2.16 | 0.93 |
| 3:L:3284[B]:LYS:HE2 | 3:L:3284[B]:LYS:HA | 1.48 | 0.93 |
| 3:O:3106[B]:THR:O | 3:O:3110[B]:THR:OG1 | 1.85 | 0.93 |
| 3:R:3106[A]:THR:O | 3:R:3110[A]:THR:OG1 | 1.85 | 0.93 |
| 3:R:3169[A]:LYS:O | 3:R:3172[A]:SER:OG | 1.85 | 0.93 |
| 3:X:2948[A]:ASP:OD1 | 3:X:2950[A]:THR:OG1 | 1.85 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2932[A]:PRO:HA | 3:a:2935[A]:ILE:CD1 | 1.99 | 0.93 |
| 3:d:2948[A]:ASP:OD1 | 3:d:2950[A]:THR:OG1 | 1.85 | 0.93 |
| 3:d:2968[A]:GLN:HB2 | 3:d:2972[A]:GLY:HA2 | 1.47 | 0.93 |
| 3:C:2969[B]:TYR:HE2 | 3:L:3120[B]:HIS:NE2 | 1.62 | 0.93 |
| 3:C:3158[B]:PHE:CE2 | 3:L:3153[B]:LYS:CE | 2.50 | 0.93 |
| 3:C:3172[B]:SER:HB2 | 3:L:3150[B]:LYS:C | 1.94 | 0.93 |
| 3:C:3283[A]:ILE:HG21 | 3:C:3305[A]:ILE:HD11 | 1.51 | 0.93 |
| 3:F:2932[A]:PRO:HA | 3:F:2935[A]:ILE:CD1 | 1.99 | 0.93 |
| 3:F:2948[A]:ASP:OD1 | 3:F:2950[A]:THR:OG1 | 1.85 | 0.93 |
| 3:F:2969[A]:TYR:HD2 | 3:F:2971[A]:ASP:H | 1.02 | 0.93 |
| 3:F:3174[B]:GLY:HA3 | 3:a:3154[B]:PRO:HB3 | 1.48 | 0.93 |
| 3:I:2967[B]:CYS:HA | 3:R:2981[B]:GLY:HA3 | 1.51 | 0.93 |
| 3:O:2963[B]:MET:HE1 | 3:X:2975[B]:PHE:CD2 | 2.03 | 0.93 |
| 3:O:3252[B]:TYR:HB2 | 3:X:3156[B]:MET:SD | 2.09 | 0.93 |
| 3:R:2932[B]:PRO:HA | 3:R:2935[B]:ILE:CD1 | 1.99 | 0.93 |
| 3:U:3152[B]:LYS:CB | 3:d:3154[B]:PRO:CB | 2.47 | 0.93 |
| 3:a:2979[A]:GLN:CG | 3:a:3155[A]:MET:HE1 | 1.97 | 0.93 |
| 3:a:2988[A]:TRP:HE3 | 3:a:2989[A]:HIS:HD1 | 1.14 | 0.93 |
| 3:a:3284[A]:LYS:HE2 | 3:a:3284[A]:LYS:HA | 1.48 | 0.93 |
| 3:d:3298[A]:ASN:HB2 | 3:d:3300[A]:LEU:HD23 | 1.50 | 0.93 |
| 3:C:3079[B]:CYS:SG | 3:L:3161[B]:GLU:HG2 | 0.80 | 0.93 |
| 3:C:3258[B]:PHE:CZ | 3:L:2968[B]:GLN:NE2 | 2.37 | 0.93 |
| 2:H:2797:LYS:HZ1 | 3:I:3028[A]:PRO:HD3 | 1.14 | 0.93 |
| 3:O:3134[A]:GLN:O | 3:O:3137[A]:ARG:N | 2.02 | 0.93 |
| 3:O:3253[B]:GLU:HG3 | 3:X:3161[B]:GLU:OE2 | 1.69 | 0.93 |
| 3:O:3298[B]:ASN:HB2 | 3:O:3300[B]:LEU:HD23 | 1.50 | 0.93 |
| 3:R:3134[A]:GLN:O | 3:R:3137[A]:ARG:N | 2.02 | 0.93 |
| 3:U:3283[B]:ILE:HG21 | 3:U:3305[B]:ILE:HD11 | 1.51 | 0.93 |
| 3:X:2932[B]:PRO:HA | 3:X:2935[B]:ILE:CD1 | 1.99 | 0.93 |
| 3:C:2963[A]:MET:HG2 | 3:C:3108[A]:HIS:CD2 | 2.04 | 0.93 |
| 3:C:2967[B]:CYS:N | 3:L:3256[B]:TRP:CD1 | 2.22 | 0.93 |
| 3:C:2979[B]:GLN:HE22 | 3:L:2979[B]:GLN:HE22 | 0.97 | 0.93 |
| 3:C:3154[B]:PRO:HD3 | 3:L:3174[B]:GLY:HA2 | 1.02 | 0.93 |
| 3:C:3158[B]:PHE:CE2 | 3:L:3153[B]:LYS:NZ | 2.36 | 0.93 |
| 3:C:3298[B]:ASN:HB2 | 3:C:3300[B]:LEU:HD23 | 1.50 | 0.93 |
| 3:F:2965[B]:LEU:HD12 | 3:a:3256[B]:TRP:HE1 | 1.30 | 0.93 |
| 3:F:3106[A]:THR:O | 3:F:3110[A]:THR:OG1 | 1.85 | 0.93 |
| 3:I:3254[B]:MET:HG3 | 3:R:2966[B]:SER:HB2 | 0.93 | 0.93 |
| 3:L:2932[A]:PRO:HA | 3:L:2935[A]:ILE:HD12 | 1.51 | 0.93 |
| 3:O:2932[B]:PRO:HA | 3:O:2935[B]:ILE:CD1 | 1.99 | 0.93 |
| 3:O:3038[B]:ILE:HD13 | 3:X:2969[B]:TYR:HE2 | 1.27 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3106[B]:THR:O | 3:X:3110[B]:THR:OG1 | 1.85 | 0.93 |
| 3:a:3298[A]:ASN:HB2 | 3:a:3300[A]:LEU:HD23 | 1.51 | 0.93 |
| 3:d:2960[B]:PHE:HD2 | 3:d:3157[B]:PRO:CG | 1.82 | 0.93 |
| 3:C:2932[B]:PRO:HA | 3:C:2935[B]:ILE:CD1 | 1.99 | 0.93 |
| 3:C:2946[B]:GLN:O | 3:C:3037[B]:TYR:OH | 1.85 | 0.93 |
| 3:C:2965[A]:LEU:HD11 | 3:C:2975[A]:PHE:H | 1.31 | 0.93 |
| 3:C:2967[B]:CYS:H | 3:L:3256[B]:TRP:CD1 | 1.66 | 0.93 |
| 3:C:3106[B]:THR:O | 3:C:3110[B]:THR:OG1 | 1.85 | 0.93 |
| 3:C:3259[B]:ASP:OD2 | 3:L:3162[B]:ASP:CG | 2.11 | 0.93 |
| 3:F:2960[B]:PHE:HD2 | 3:F:3157[B]:PRO:CG | 1.82 | 0.93 |
| 3:F:2963[A]:MET:HG2 | 3:F:3108[A]:HIS:CD2 | 2.04 | 0.93 |
| 3:F:3149[B]:ASN:HD22 | 3:a:3163[B]:ASN:CG | 1.78 | 0.93 |
| 3:I:3134[A]:GLN:O | 3:I:3137[A]:ARG:N | 2.02 | 0.93 |
| 3:I:3149[B]:ASN:OD1 | 3:R:3169[B]:LYS:HG3 | 1.69 | 0.93 |
| 3:L:2932[B]:PRO:HA | 3:L:2935[B]:ILE:HD12 | 1.51 | 0.93 |
| 3:L:3096[A]:VAL:HG11 | 3:L:3115[A]:LEU:CD1 | 1.99 | 0.93 |
| 3:L:3283[B]:ILE:HG21 | 3:L:3305[B]:ILE:HD11 | 1.51 | 0.93 |
| 3:R:2948[A]:ASP:N | 3:R:2949[A]:LYS:HA | 1.81 | 0.93 |
| 3:U:2980[B]:HIS:HB2 | 3:d:2969[B]:TYR:HE1 | 1.34 | 0.93 |
| 3:U:3096[A]:VAL:HG11 | 3:U:3115[A]:LEU:CD1 | 1.99 | 0.93 |
| 3:X:2963[A]:MET:HG2 | 3:X:3108[A]:HIS:CD2 | 2.04 | 0.93 |
| 2:Z:2472:ASN:CB | 4:MA:1:NAG:H82 | 1.98 | 0.93 |
| 3:d:2931[A]:THR:OG1 | 3:d:2934[A]:GLU:OE2 | 1.85 | 0.93 |
| 3:C:2932[B]:PRO:HA | 3:C:2935[B]:ILE:HD12 | 1.51 | 0.92 |
| 3:C:2960[B]:PHE:HD2 | 3:C:3157[B]:PRO:CG | 1.82 | 0.92 |
| 3:F:2976[B]:ALA:HB3 | 3:a:3252[B]:TYR:O | 1.69 | 0.92 |
| 3:F:3221[B]:ALA:HB3 | 3:a:2964[B]:PRO:CB | 1.99 | 0.92 |
| 3:I:2969[A]:TYR:CE2 | 3:I:2970[A]:PRO:HG2 | 2.05 | 0.92 |
| 3:I:3160[B]:SER:N | 3:R:3150[B]:LYS:HD3 | 1.76 | 0.92 |
| 3:I:3163[B]:ASN:HB2 | 3:R:3150[B]:LYS:HE3 | 0.94 | 0.92 |
| 3:I:3298[A]:ASN:HB2 | 3:I:3300[A]:LEU:N | 1.78 | 0.92 |
| 3:U:3074[A]:GLU:OE1 | 3:U:3212[A]:ARG:NH2 | 2.03 | 0.92 |
| 3:X:2932[A]:PRO:HA | 3:X:2935[A]:ILE:CD1 | 1.99 | 0.92 |
| 3:C:3090[B]:ASN:CG | 3:L:2972[B]:GLY:CA | 2.36 | 0.92 |
| 3:F:2946[A]:GLN:O | 3:F:3037[A]:TYR:OH | 1.85 | 0.92 |
| 3:I:2982[B]:MET:CE | 3:R:2967[B]:CYS:SG | 2.58 | 0.92 |
| 3:I:2989[B]:HIS:NE2 | 3:R:2969[B]:TYR:HA | 1.83 | 0.92 |
| 3:O:3102[B]:TYR:CA | 3:X:2971[B]:ASP:HA | 1.98 | 0.92 |
| 3:R:3134[B]:GLN:O | 3:R:3137[B]:ARG:N | 2.02 | 0.92 |
| 3:U:2963[A]:MET:HG2 | 3:U:3108[A]:HIS:CD2 | 2.04 | 0.92 |
| 3:U:2971[B]:ASP:O | 3:d:3247[B]:VAL:CG1 | 2.16 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3169[B]:LYS:O | 3:d:3148[B]:ILE:HG22 | 1.69 | 0.92 |
| 3:U:3256[B]:TRP:HE3 | 3:d:2969[B]:TYR:HB3 | 1.31 | 0.92 |
| 3:d:2979[B]:GLN:CG | 3:d:3155[B]:MET:HE1 | 1.97 | 0.92 |
| 3:C:2956[A]:LYS:O | 3:C:2960[A]:PHE:HE1 | 1.22 | 0.92 |
| 3:C:3252[B]:TYR:CE2 | 3:L:3223[B]:GLY:O | 2.22 | 0.92 |
| 3:F:3298[B]:ASN:HB2 | 3:F:3300[B]:LEU:HD23 | 1.50 | 0.92 |
| 3:L:2935[B]:ILE:HD13 | 3:L:2936[B]:GLU:H | 1.35 | 0.92 |
| 3:L:2963[B]:MET:HG2 | 3:L:3108[B]:HIS:CD2 | 2.04 | 0.92 |
| 3:L:3169[B]:LYS:O | 3:L:3172[B]:SER:OG | 1.85 | 0.92 |
| 3:O:2963[A]:MET:HG2 | 3:O:3108[A]:HIS:CD2 | 2.04 | 0.92 |
| 3:O:3169[A]:LYS:O | 3:O:3172[A]:SER:OG | 1.85 | 0.92 |
| 3:R:2931[B]:THR:N | 3:R:2934[B]:GLU:OE2 | 2.02 | 0.92 |
| 3:R:3096[B]:VAL:HG11 | 3:R:3115[B]:LEU:CD1 | 1.99 | 0.92 |
| 3:U:3134[A]:GLN:O | 3:U:3137[A]:ARG:N | 2.02 | 0.92 |
| 3:X:3096[A]:VAL:HG11 | 3:X:3115[A]:LEU:CD1 | 1.99 | 0.92 |
| 3:X:3106[A]:THR:O | 3:X:3110[A]:THR:OG1 | 1.85 | 0.92 |
| 3:a:3298[B]:ASN:HB2 | 3:a:3300[B]:LEU:N | 1.78 | 0.92 |
| 3:d:2948[B]:ASP:HB3 | 3:d:2949[B]:LYS:HA | 1.52 | 0.92 |
| 3:d:2948[B]:ASP:OD1 | 3:d:2950[B]:THR:OG1 | 1.85 | 0.92 |
| 3:d:3074[B]:GLU:OE1 | 3:d:3212[B]:ARG:NH2 | 2.03 | 0.92 |
| 3:C:2969[A]:TYR:CE2 | 3:C:2970[A]:PRO:HG2 | 2.05 | 0.92 |
| 3:C:3096[B]:VAL:HG11 | 3:C:3115[B]:LEU:CD1 | 1.99 | 0.92 |
| 3:F:2931[A]:THR:N | 3:F:2934[A]:GLU:OE2 | 2.02 | 0.92 |
| 3:F:3074[A]:GLU:OE1 | 3:F:3212[A]:ARG:NH2 | 2.03 | 0.92 |
| 3:F:3096[A]:VAL:HG11 | 3:F:3115[A]:LEU:CD1 | 2.00 | 0.92 |
| 3:I:2931[B]:THR:OG1 | 3:I:2934[B]:GLU:OE2 | 1.85 | 0.92 |
| 3:I:3155[B]:MET:N | 3:R:3153[B]:LYS:O | 1.99 | 0.92 |
| 3:L:2979[B]:GLN:CG | 3:L:3155[B]:MET:HE1 | 1.97 | 0.92 |
| 3:O:2970[B]:PRO:HD2 | 3:X:2991[B]:LEU:HB2 | 1.17 | 0.92 |
| 3:O:3154[B]:PRO:HG3 | 3:X:3175[B]:TYR:CB | 1.95 | 0.92 |
| 3:O:3283[B]:ILE:HG21 | 3:O:3305[B]:ILE:HD11 | 1.51 | 0.92 |
| 3:R:2979[A]:GLN:CG | 3:R:3155[A]:MET:HE1 | 1.97 | 0.92 |
| 3:U:3169[A]:LYS:O | 3:U:3172[A]:SER:OG | 1.85 | 0.92 |
| 3:X:2965[B]:LEU:HD11 | 3:X:2975[B]:PHE:H | 1.32 | 0.92 |
| 3:a:3134[B]:GLN:O | 3:a:3137[B]:ARG:N | 2.02 | 0.92 |
| 3:d:2931[B]:THR:N | 3:d:2934[B]:GLU:OE2 | 2.02 | 0.92 |
| 3:d:3134[B]:GLN:O | 3:d:3137[B]:ARG:N | 2.02 | 0.92 |
| 3:C:2931[B]:THR:OG1 | 3:C:2934[B]:GLU:OE2 | 1.85 | 0.92 |
| 3:C:3134[B]:GLN:O | 3:C:3137[B]:ARG:N | 2.02 | 0.92 |
| 3:C:3154[B]:PRO:HB3 | 3:L:3174[B]:GLY:HA3 | 0.92 | 0.92 |
| 3:F:3120[B]:HIS:CD2 | 3:a:2969[B]:TYR:CE2 | 2.57 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2982[B]:MET:CE | 3:R:2977[B]:CYS:HB2 | 1.99 | 0.92 |
| 3:I:3074[B]:GLU:OE1 | 3:I:3212[B]:ARG:NH2 | 2.03 | 0.92 |
| 3:I:3096[A]:VAL:HG11 | 3:I:3115[A]:LEU:CD1 | 2.00 | 0.92 |
| 3:I:3148[B]:ILE:O | 3:R:3169[B]:LYS:C | 2.02 | 0.92 |
| 3:L:2931[A]:THR:N | 3:L:2934[A]:GLU:OE2 | 2.02 | 0.92 |
| 3:O:2948[A]:ASP:HB3 | 3:O:2949[A]:LYS:HA | 1.52 | 0.92 |
| 3:O:2969[A]:TYR:CE2 | 3:O:2970[A]:PRO:HG2 | 2.05 | 0.92 |
| 3:O:3161[B]:GLU:CD | 3:X:3151[B]:LEU:HD11 | 1.94 | 0.92 |
| 2:Q:2800:LYS:O | 3:R:3023[A]:ILE:HD11 | 1.69 | 0.92 |
| 3:R:2963[A]:MET:HG2 | 3:R:3108[A]:HIS:CD2 | 2.04 | 0.92 |
| 3:R:2963[B]:MET:HG2 | 3:R:3108[B]:HIS:CD2 | 2.04 | 0.92 |
| 3:R:3284[B]:LYS:HE2 | 3:R:3284[B]:LYS:HA | 1.48 | 0.92 |
| 3:U:2946[B]:GLN:O | 3:U:3037[B]:TYR:OH | 1.85 | 0.92 |
| 3:U:3134[B]:GLN:O | 3:U:3137[B]:ARG:N | 2.02 | 0.92 |
| 3:U:3169[B]:LYS:HG3 | 3:d:3147[B]:GLU:CB | 1.99 | 0.92 |
| 2:W:2800:LYS:O | 3:X:3023[A]:ILE:HD13 | 1.69 | 0.92 |
| 3:X:2935[B]:ILE:HD13 | 3:X:2936[B]:GLU:H | 1.35 | 0.92 |
| 1:Y:1655:SER:HB3 | 3:d:3007[B]:ILE:HG23 | 1.49 | 0.92 |
| 3:a:3169[A]:LYS:O | 3:a:3172[A]:SER:OG | 1.85 | 0.92 |
| 3:d:3283[A]:ILE:HG21 | 3:d:3305[A]:ILE:HD11 | 1.51 | 0.92 |
| 3:C:3153[B]:LYS:C | 3:L:3155[B]:MET:HG3 | 1.69 | 0.92 |
| 3:F:3298[A]:ASN:HB2 | 3:F:3300[A]:LEU:N | 1.78 | 0.92 |
| 3:I:2965[B]:LEU:HD11 | 3:I:2975[B]:PHE:H | 1.31 | 0.92 |
| 3:I:2969[B]:TYR:CE2 | 3:I:2970[B]:PRO:HG2 | 2.05 | 0.92 |
| 3:I:3096[B]:VAL:HG11 | 3:I:3115[B]:LEU:CD1 | 1.99 | 0.92 |
| 3:I:3147[A]:GLU:HB2 | 3:I:3149[A]:ASN:CG | 1.95 | 0.92 |
| 3:I:3155[B]:MET:CB | 3:R:3153[B]:LYS:CD | 2.34 | 0.92 |
| 3:I:3298[A]:ASN:HB2 | 3:I:3300[A]:LEU:HD23 | 1.51 | 0.92 |
| 3:L:2965[A]:LEU:HD11 | 3:L:2975[A]:PHE:N | 1.85 | 0.92 |
| 3:L:3147[A]:GLU:HB2 | 3:L:3149[A]:ASN:CG | 1.95 | 0.92 |
| 3:U:2932[B]:PRO:HA | 3:U:2935[B]:ILE:CD1 | 1.99 | 0.92 |
| 3:U:3106[A]:THR:O | 3:U:3110[A]:THR:OG1 | 1.85 | 0.92 |
| 3:U:3156[B]:MET:HE1 | 3:d:2982[B]:MET:SD | 1.54 | 0.92 |
| 3:X:2935[A]:ILE:HD13 | 3:X:2936[A]:GLU:H | 1.35 | 0.92 |
| 3:X:2948[B]:ASP:HB3 | 3:X:2949[B]:LYS:HA | 1.52 | 0.92 |
| 3:d:2932[B]:PRO:HA | 3:d:2935[B]:ILE:HD12 | 1.51 | 0.92 |
| 3:C:3150[B]:LYS:N | 3:L:3172[B]:SER:HB3 | 1.84 | 0.92 |
| 3:C:3298[A]:ASN:HB2 | 3:C:3300[A]:LEU:HD23 | 1.50 | 0.92 |
| 3:F:3283[A]:ILE:HG21 | 3:F:3305[A]:ILE:HD11 | 1.51 | 0.92 |
| 3:I:2963[A]:MET:HG2 | 3:I:3108[A]:HIS:CD2 | 2.03 | 0.92 |
| 3:I:2963[B]:MET:HG2 | 3:I:3108[B]:HIS:CD2 | 2.04 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2979[A]:GLN:CG | 3:I:3155[A]:MET:HE1 | 1.97 | 0.92 |
| 3:I:3074[A]:GLU:OE1 | 3:I:3212[A]:ARG:NH2 | 2.03 | 0.92 |
| 3:I:3284[A]:LYS:HA | 3:I:3284[A]:LYS:HE2 | 1.48 | 0.92 |
| 3:L:2932[B]:PRO:HA | 3:L:2935[B]:ILE:CD1 | 1.99 | 0.92 |
| 3:O:2963[B]:MET:HG2 | 3:O:3108[B]:HIS:CD2 | 2.04 | 0.92 |
| 3:O:2979[B]:GLN:CG | 3:O:3155[B]:MET:HE1 | 1.97 | 0.92 |
| 3:O:3159[B]:SER:C | 3:X:3148[B]:ILE:O | 2.11 | 0.92 |
| 3:R:3147[A]:GLU:HB2 | 3:R:3149[A]:ASN:CG | 1.95 | 0.92 |
| 3:U:3074[B]:GLU:OE1 | 3:U:3212[B]:ARG:NH2 | 2.03 | 0.92 |
| 3:a:3096[A]:VAL:HG11 | 3:a:3115[A]:LEU:CD1 | 1.99 | 0.92 |
| 3:a:3283[B]:ILE:HG21 | 3:a:3305[B]:ILE:HD11 | 1.51 | 0.92 |
| 3:d:3096[B]:VAL:HG11 | 3:d:3115[B]:LEU:CD1 | 1.99 | 0.92 |
| 3:F:2983[B]:VAL:CB | 3:a:3161[B]:GLU:N | 2.33 | 0.92 |
| 3:F:3256[B]:TRP:CB | 3:a:2966[B]:SER:C | 2.43 | 0.92 |
| 3:F:3298[A]:ASN:HB2 | 3:F:3300[A]:LEU:HD23 | 1.50 | 0.92 |
| 3:I:2932[A]:PRO:HA | 3:I:2935[A]:ILE:CD1 | 1.99 | 0.92 |
| 3:I:2960[A]:PHE:HD2 | 3:I:3157[A]:PRO:CG | 1.82 | 0.92 |
| 3:I:2960[B]:PHE:HD2 | 3:I:3157[B]:PRO:CG | 1.82 | 0.92 |
| 3:I:3150[B]:LYS:HE3 | 3:R:3163[B]:ASN:HB3 | 1.48 | 0.92 |
| 3:I:3220[B]:ARG:HG3 | 3:I:3220[B]:ARG:HH11 | 1.35 | 0.92 |
| 3:I:3255[B]:PRO:CG | 3:R:2962[B]:GLY:C | 2.43 | 0.92 |
| 3:L:2963[A]:MET:HG2 | 3:L:3108[A]:HIS:CD2 | 2.04 | 0.92 |
| 3:L:3169[A]:LYS:O | 3:L:3172[A]:SER:OG | 1.85 | 0.92 |
| 3:O:2960[A]:PHE:HD2 | 3:O:3157[A]:PRO:CG | 1.82 | 0.92 |
| 3:O:3074[A]:GLU:OE1 | 3:O:3212[A]:ARG:NH2 | 2.02 | 0.92 |
| 3:R:2931[A]:THR:N | 3:R:2934[A]:GLU:OE2 | 2.02 | 0.92 |
| 3:R:2969[A]:TYR:CE2 | 3:R:2970[A]:PRO:HG2 | 2.05 | 0.92 |
| 3:R:3298[A]:ASN:HB2 | 3:R:3300[A]:LEU:HD23 | 1.50 | 0.92 |
| 3:U:2960[B]:PHE:HD2 | 3:U:3157[B]:PRO:CG | 1.82 | 0.92 |
| 3:U:2963[B]:MET:HG2 | 3:U:3108[B]:HIS:CD2 | 2.04 | 0.92 |
| 3:U:2979[A]:GLN:CG | 3:U:3155[A]:MET:HE1 | 1.97 | 0.92 |
| 3:X:2948[A]:ASP:N | 3:X:2949[A]:LYS:HA | 1.81 | 0.92 |
| 3:X:3134[A]:GLN:O | 3:X:3137[A]:ARG:N | 2.02 | 0.92 |
| 3:a:2935[B]:ILE:HD13 | 3:a:2936[B]:GLU:H | 1.35 | 0.92 |
| 3:a:2960[A]:PHE:HD2 | 3:a:3157[A]:PRO:CG | 1.82 | 0.92 |
| 3:a:3134[A]:GLN:O | 3:a:3137[A]:ARG:N | 2.02 | 0.92 |
| 3:C:3156[B]:MET:HA | 3:L:3150[B]:LYS:HD3 | 1.50 | 0.92 |
| 3:C:3220[A]:ARG:HG3 | 3:C:3220[A]:ARG:HH11 | 1.35 | 0.92 |
| 3:F:2966[B]:SER:C | 3:a:3256[B]:TRP:CB | 2.33 | 0.92 |
| 3:F:3096[B]:VAL:HG11 | 3:F:3115[B]:LEU:CD1 | 1.99 | 0.92 |
| 3:F:3134[B]:GLN:O | 3:F:3137[B]:ARG:N | 2.02 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3298[B]:ASN:HB2 | 3:F:3300[B]:LEU:N | 1.78 | 0.92 |
| 3:I:3163[B]:ASN:O | 3:R:3149[B]:ASN:ND2 | 2.02 | 0.92 |
| 3:L:3298[B]:ASN:HB2 | 3:L:3300[B]:LEU:HD23 | 1.50 | 0.92 |
| 3:O:2931[B]:THR:N | 3:O:2934[B]:GLU:OE2 | 2.02 | 0.92 |
| 3:O:2971[B]:ASP:N | 3:X:2988[B]:TRP:O | 2.02 | 0.92 |
| 3:O:3096[A]:VAL:HG11 | 3:O:3115[A]:LEU:CD1 | 1.99 | 0.92 |
| 3:O:3108[B]:HIS:HB3 | 3:X:2969[B]:TYR:O | 1.64 | 0.92 |
| 2:Q:2867:PRO:HG3 | 3:R:2932[A]:PRO:HG2 | 1.50 | 0.92 |
| 3:R:3074[A]:GLU:OE1 | 3:R:3212[A]:ARG:NH2 | 2.03 | 0.92 |
| 3:U:2970[B]:PRO:CB | 3:d:2980[B]:HIS:HB3 | 1.68 | 0.92 |
| 3:U:3162[B]:ASP:OD1 | 3:d:3260[B]:ARG:NH1 | 2.02 | 0.92 |
| 3:U:3220[B]:ARG:HA | 3:d:2973[B]:THR:N | 1.84 | 0.92 |
| 3:X:2960[B]:PHE:HD2 | 3:X:3157[B]:PRO:CG | 1.82 | 0.92 |
| 3:X:2965[A]:LEU:HD11 | 3:X:2975[A]:PHE:N | 1.85 | 0.92 |
| 3:X:2979[B]:GLN:CG | 3:X:3155[B]:MET:HE1 | 1.97 | 0.92 |
| 3:X:3147[A]:GLU:HB2 | 3:X:3149[A]:ASN:CG | 1.95 | 0.92 |
| 3:a:2963[B]:MET:HG2 | 3:a:3108[B]:HIS:CD2 | 2.04 | 0.92 |
| 3:a:2969[B]:TYR:CE2 | 3:a:2970[B]:PRO:HG2 | 2.05 | 0.92 |
| 3:C:2963[B]:MET:HG2 | 3:C:3108[B]:HIS:CD2 | 2.04 | 0.92 |
| 3:C:3169[B]:LYS:O | 3:L:3152[B]:LYS:CG | 2.18 | 0.92 |
| 3:C:3298[A]:ASN:HB2 | 3:C:3300[A]:LEU:N | 1.78 | 0.92 |
| 3:F:2960[A]:PHE:HD2 | 3:F:3157[A]:PRO:CG | 1.82 | 0.92 |
| 3:F:3169[B]:LYS:O | 3:a:3152[B]:LYS:HB2 | 1.69 | 0.92 |
| 3:F:3251[B]:ASP:CB | 3:a:3251[B]:ASP:CG | 2.42 | 0.92 |
| 3:I:2932[B]:PRO:HA | 3:I:2935[B]:ILE:CD1 | 1.99 | 0.92 |
| 3:I:2982[B]:MET:CE | 3:R:2977[B]:CYS:CB | 2.48 | 0.92 |
| 3:L:2965[B]:LEU:HD11 | 3:L:2975[B]:PHE:N | 1.85 | 0.92 |
| 3:O:2931[A]:THR:N | 3:O:2934[A]:GLU:OE2 | 2.02 | 0.92 |
| 3:O:2970[B]:PRO:HD3 | 3:X:2991[B]:LEU:HD13 | 1.50 | 0.92 |
| 3:O:2974[B]:ALA:HB3 | 3:X:2977[B]:CYS:C | 1.92 | 0.92 |
| 3:O:3096[B]:VAL:HG11 | 3:O:3115[B]:LEU:CD1 | 2.00 | 0.92 |
| 3:O:3220[B]:ARG:HH11 | 3:O:3220[B]:ARG:HG3 | 1.35 | 0.92 |
| 3:R:2935[A]:ILE:HD13 | 3:R:2936[A]:GLU:H | 1.35 | 0.92 |
| 3:R:2960[A]:PHE:HD2 | 3:R:3157[A]:PRO:CG | 1.82 | 0.92 |
| 3:R:2960[B]:PHE:HD2 | 3:R:3157[B]:PRO:CG | 1.82 | 0.92 |
| 3:X:2931[A]:THR:N | 3:X:2934[A]:GLU:OE2 | 2.02 | 0.92 |
| 3:X:2969[A]:TYR:CE2 | 3:X:2970[A]:PRO:HG2 | 2.05 | 0.92 |
| 3:X:3074[B]:GLU:OE1 | 3:X:3212[B]:ARG:NH2 | 2.03 | 0.92 |
| 3:a:3220[B]:ARG:HG3 | 3:a:3220[B]:ARG:HH11 | 1.35 | 0.92 |
| 3:d:3298[B]:ASN:HB2 | 3:d:3300[B]:LEU:HD23 | 1.50 | 0.92 |
| 3:C:2931[B]:THR:N | 3:C:2934[B]:GLU:OE2 | 2.02 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2960[A]:PHE:HD2 | 3:C:3157[A]:PRO:CG | 1.82 | 0.91 |
| 3:C:3120[B]:HIS:CD2 | 3:L:2969[B]:TYR:OH | 2.22 | 0.91 |
| 3:F:2932[A]:PRO:HA | 3:F:2935[A]:ILE:HD12 | 1.51 | 0.91 |
| 3:F:3074[B]:GLU:OE1 | 3:F:3212[B]:ARG:NH2 | 2.03 | 0.91 |
| 3:I:2931[A]:THR:N | 3:I:2934[A]:GLU:OE2 | 2.02 | 0.91 |
| 3:I:2979[B]:GLN:C | 3:R:2967[B]:CYS:CB | 2.39 | 0.91 |
| 3:L:2960[B]:PHE:HD2 | 3:L:3157[B]:PRO:CG | 1.82 | 0.91 |
| 3:O:2951[B]:ASP:OD2 | 3:O:2952[B]:ALA:N | 2.03 | 0.91 |
| 3:O:2969[B]:TYR:HD2 | 3:O:2971[B]:ASP:H | 1.02 | 0.91 |
| 3:O:3255[B]:PRO:CD | 3:X:3169[B]:LYS:HG3 | 2.00 | 0.91 |
| 3:R:2932[A]:PRO:HA | 3:R:2935[A]:ILE:HD12 | 1.51 | 0.91 |
| 3:R:3074[B]:GLU:OE1 | 3:R:3212[B]:ARG:NH2 | 2.03 | 0.91 |
| 3:R:3096[A]:VAL:HG11 | 3:R:3115[A]:LEU:CD1 | 1.99 | 0.91 |
| 3:R:3220[A]:ARG:HG3 | 3:R:3220[A]:ARG:HH11 | 1.35 | 0.91 |
| 3:U:2965[B]:LEU:HD11 | 3:U:2975[B]:PHE:H | 1.31 | 0.91 |
| 3:U:3254[B]:MET:CE | 3:d:3254[B]:MET:HB3 | 2.00 | 0.91 |
| 3:X:2948[B]:ASP:N | 3:X:2949[B]:LYS:HA | 1.81 | 0.91 |
| 3:X:2956[B]:LYS:O | 3:X:2960[B]:PHE:HE1 | 1.22 | 0.91 |
| 3:X:3096[B]:VAL:HG11 | 3:X:3115[B]:LEU:CD1 | 2.00 | 0.91 |
| 3:X:3283[B]:ILE:HG21 | 3:X:3305[B]:ILE:HD11 | 1.51 | 0.91 |
| 1:b:1582:ASN:HB3 | 1:b:1583:CYS:HB2 | 1.53 | 0.91 |
| 3:d:3134[A]:GLN:O | 3:d:3137[A]:ARG:N | 2.01 | 0.91 |
| 3:C:2951[B]:ASP:OD2 | 3:C:2952[B]:ALA:N | 2.03 | 0.91 |
| 3:C:2965[A]:LEU:HD11 | 3:C:2975[A]:PHE:N | 1.85 | 0.91 |
| 3:C:2982[B]:MET:SD | 3:L:3156[B]:MET:C | 2.53 | 0.91 |
| 3:C:3172[B]:SER:CB | 3:L:3150[B]:LYS:CA | 2.48 | 0.91 |
| 3:F:2974[B]:ALA:N | 3:a:3249[B]:GLY:N | 2.10 | 0.91 |
| 3:F:3147[A]:GLU:HB2 | 3:F:3149[A]:ASN:CG | 1.95 | 0.91 |
| 3:F:3153[B]:LYS:HE3 | 3:a:3158[B]:PHE:N | 1.85 | 0.91 |
| 3:F:3173[B]:THR:OG1 | 3:a:3173[B]:THR:HG23 | 1.70 | 0.91 |
| 3:I:3220[A]:ARG:HH11 | 3:I:3220[A]:ARG:HG3 | 1.35 | 0.91 |
| 3:L:2969[A]:TYR:CE2 | 3:L:2970[A]:PRO:HG2 | 2.05 | 0.91 |
| 3:L:3134[B]:GLN:O | 3:L:3137[B]:ARG:N | 2.02 | 0.91 |
| 3:L:3220[A]:ARG:HH11 | 3:L:3220[A]:ARG:HG3 | 1.35 | 0.91 |
| 3:O:3147[A]:GLU:HB2 | 3:O:3149[A]:ASN:CG | 1.95 | 0.91 |
| 3:U:2935[A]:ILE:HD13 | 3:U:2936[A]:GLU:H | 1.35 | 0.91 |
| 3:U:3096[B]:VAL:HG11 | 3:U:3115[B]:LEU:CD1 | 1.99 | 0.91 |
| 3:U:3152[B]:LYS:HG3 | 3:d:3154[B]:PRO:HB3 | 0.92 | 0.91 |
| 3:U:3256[B]:TRP:CB | 3:d:2975[B]:PHE:CE1 | 2.48 | 0.91 |
| 3:U:3283[A]:ILE:HG21 | 3:U:3305[A]:ILE:HD11 | 1.51 | 0.91 |
| 3:U:3298[B]:ASN:HB2 | 3:U:3300[B]:LEU:HD23 | 1.50 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2956[A]:LYS:O | 3:X:2960[A]:PHE:HE1 | 1.22 | 0.91 |
| 3:X:2960[A]:PHE:HD2 | 3:X:3157[A]:PRO:CG | 1.82 | 0.91 |
| 3:X:3169[A]:LYS:O | 3:X:3172[A]:SER:OG | 1.85 | 0.91 |
| 3:X:3298[A]:ASN:HB2 | 3:X:3300[A]:LEU:HD23 | 1.50 | 0.91 |
| 1:Y:1617:LYS:CE | 3:d:3180[B]:TYR:CE2 | 2.52 | 0.91 |
| 3:a:2931[A]:THR:N | 3:a:2934[A]:GLU:OE2 | 2.02 | 0.91 |
| 3:a:3096[B]:VAL:HG11 | 3:a:3115[B]:LEU:CD1 | 1.99 | 0.91 |
| 3:a:3147[A]:GLU:HB2 | 3:a:3149[A]:ASN:CG | 1.95 | 0.91 |
| 3:d:2932[A]:PRO:HA | 3:d:2935[A]:ILE:HD12 | 1.51 | 0.91 |
| 3:d:2935[B]:ILE:HD13 | 3:d:2936[B]:GLU:H | 1.35 | 0.91 |
| 3:d:2960[A]:PHE:HD2 | 3:d:3157[A]:PRO:CG | 1.82 | 0.91 |
| 3:d:3217[A]:PHE:HZ | 3:d:3230[A]:PHE:CE1 | 1.89 | 0.91 |
| 3:C:2988[A]:TRP:HE3 | 3:C:2989[A]:HIS:HD1 | 1.14 | 0.91 |
| 3:C:3150[B]:LYS:HZ2 | 3:L:3160[B]:SER:CB | 1.77 | 0.91 |
| 3:C:3169[A]:LYS:O | 3:C:3172[A]:SER:OG | 1.85 | 0.91 |
| 3:F:2931[B]:THR:N | 3:F:2934[B]:GLU:OE2 | 2.02 | 0.91 |
| 3:F:2932[B]:PRO:HA | 3:F:2935[B]:ILE:CD1 | 1.99 | 0.91 |
| 3:F:3153[B]:LYS:CE | 3:a:3158[B]:PHE:H | 1.83 | 0.91 |
| 3:L:2948[B]:ASP:N | 3:L:2949[B]:LYS:HA | 1.81 | 0.91 |
| 3:L:3147[B]:GLU:HB2 | 3:L:3149[B]:ASN:CG | 1.95 | 0.91 |
| 3:L:3298[A]:ASN:HB2 | 3:L:3300[A]:LEU:HD23 | 1.51 | 0.91 |
| 3:O:2932[A]:PRO:HA | 3:O:2935[A]:ILE:CD1 | 1.99 | 0.91 |
| 3:R:2932[A]:PRO:HA | 3:R:2935[A]:ILE:CD1 | 1.99 | 0.91 |
| 3:U:3147[A]:GLU:HB2 | 3:U:3149[A]:ASN:CG | 1.95 | 0.91 |
| 3:X:2951[A]:ASP:OD2 | 3:X:2952[A]:ALA:N | 2.03 | 0.91 |
| 3:X:2979[A]:GLN:CG | 3:X:3155[A]:MET:HE1 | 1.97 | 0.91 |
| 3:a:2960[B]:PHE:HD2 | 3:a:3157[B]:PRO:CG | 1.82 | 0.91 |
| 3:a:2969[A]:TYR:CE2 | 3:a:2970[A]:PRO:HG2 | 2.05 | 0.91 |
| 3:a:3074[A]:GLU:OE1 | 3:a:3212[A]:ARG:NH2 | 2.03 | 0.91 |
| 3:d:2963[A]:MET:HG2 | 3:d:3108[A]:HIS:CD2 | 2.04 | 0.91 |
| 3:d:2969[B]:TYR:CE2 | 3:d:2970[B]:PRO:HG2 | 2.05 | 0.91 |
| 3:C:2932[A]:PRO:HA | 3:C:2935[A]:ILE:HD12 | 1.51 | 0.91 |
| 3:C:2951[A]:ASP:OD2 | 3:C:2952[A]:ALA:N | 2.03 | 0.91 |
| 3:C:2982[B]:MET:SD | 3:L:3157[B]:PRO:N | 2.42 | 0.91 |
| 3:F:2951[A]:ASP:OD2 | 3:F:2952[A]:ALA:N | 2.04 | 0.91 |
| 3:F:2965[B]:LEU:HD11 | 3:F:2975[B]:PHE:N | 1.85 | 0.91 |
| 3:F:2969[A]:TYR:CE2 | 3:F:2970[A]:PRO:HG2 | 2.05 | 0.91 |
| 3:I:2970[B]:PRO:N | 3:R:2989[B]:HIS:NE2 | 2.18 | 0.91 |
| 3:I:2988[B]:TRP:HE3 | 3:I:2989[B]:HIS:HD1 | 1.14 | 0.91 |
| 3:I:3134[B]:GLN:O | 3:I:3137[B]:ARG:N | 2.02 | 0.91 |
| 3:O:3147[B]:GLU:HB2 | 3:O:3149[B]:ASN:CG | 1.95 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3158[B]:PHE:N | 3:X:3152[B]:LYS:CG | 2.20 | 0.91 |
| 3:O:3253[B]:GLU:CD | 3:X:3161[B]:GLU:OE2 | 2.13 | 0.91 |
| 3:X:2932[B]:PRO:HA | 3:X:2935[B]:ILE:HD12 | 1.51 | 0.91 |
| 3:a:2951[A]:ASP:OD2 | 3:a:2952[A]:ALA:N | 2.03 | 0.91 |
| 3:a:2951[B]:ASP:OD2 | 3:a:2952[B]:ALA:N | 2.03 | 0.91 |
| 3:a:3283[A]:ILE:HG21 | 3:a:3305[A]:ILE:HD11 | 1.51 | 0.91 |
| 3:d:2931[A]:THR:N | 3:d:2934[A]:GLU:OE2 | 2.02 | 0.91 |
| 1:A:1161:ILE:HD11 | 1:A:1196:ILE:HD11 | 1.53 | 0.91 |
| 3:C:2968[B]:GLN:O | 3:L:2985[B]:PHE:HD2 | 1.48 | 0.91 |
| 3:C:2988[B]:TRP:CD1 | 3:L:3153[B]:LYS:NZ | 2.35 | 0.91 |
| 3:C:3096[A]:VAL:HG11 | 3:C:3115[A]:LEU:CD1 | 1.99 | 0.91 |
| 3:C:3252[B]:TYR:CE1 | 3:L:3223[B]:GLY:C | 2.48 | 0.91 |
| 3:F:2948[A]:ASP:HB3 | 3:F:2949[A]:LYS:HA | 1.52 | 0.91 |
| 3:F:3090[B]:ASN:HA | 3:a:2971[B]:ASP:O | 1.69 | 0.91 |
| 3:F:3153[B]:LYS:HD2 | 3:a:3155[B]:MET:C | 1.94 | 0.91 |
| 3:I:3147[B]:GLU:HB2 | 3:I:3149[B]:ASN:CG | 1.95 | 0.91 |
| 3:I:3251[B]:ASP:CA | 3:R:3251[B]:ASP:HB3 | 1.99 | 0.91 |
| 3:I:3298[B]:ASN:ND2 | 3:I:3301[B]:PRO:CA | 2.34 | 0.91 |
| 3:L:2931[B]:THR:N | 3:L:2934[B]:GLU:OE2 | 2.02 | 0.91 |
| 3:L:3074[A]:GLU:OE1 | 3:L:3212[A]:ARG:NH2 | 2.03 | 0.91 |
| 1:M:1582:ASN:HB3 | 1:M:1583:CYS:HB2 | 1.52 | 0.91 |
| 3:U:2931[B]:THR:N | 3:U:2934[B]:GLU:OE2 | 2.02 | 0.91 |
| 3:U:2960[A]:PHE:HD2 | 3:U:3157[A]:PRO:CG | 1.82 | 0.91 |
| 3:U:2968[B]:GLN:OE1 | 3:d:3258[B]:PHE:N | 2.04 | 0.91 |
| 3:X:2931[B]:THR:N | 3:X:2934[B]:GLU:OE2 | 2.02 | 0.91 |
| 3:d:3074[A]:GLU:OE1 | 3:d:3212[A]:ARG:NH2 | 2.02 | 0.91 |
| 3:C:2931[A]:THR:N | 3:C:2934[A]:GLU:OE2 | 2.02 | 0.91 |
| 3:C:2969[B]:TYR:O | 3:L:2985[B]:PHE:CE2 | 2.21 | 0.91 |
| 3:C:3074[A]:GLU:OE1 | 3:C:3212[A]:ARG:NH2 | 2.02 | 0.91 |
| 3:C:3153[B]:LYS:HB3 | 3:L:3155[B]:MET:CA | 1.78 | 0.91 |
| 3:F:2932[B]:PRO:HA | 3:F:2935[B]:ILE:HD12 | 1.51 | 0.91 |
| 3:F:3134[A]:GLN:O | 3:F:3137[A]:ARG:N | 2.02 | 0.91 |
| 3:F:3153[B]:LYS:HD2 | 3:a:3155[B]:MET:HB3 | 1.46 | 0.91 |
| 3:F:3162[B]:ASP:OD2 | 3:a:3258[B]:PHE:HA | 1.71 | 0.91 |
| 3:F:3252[B]:TYR:N | 3:a:3108[B]:HIS:CE1 | 2.39 | 0.91 |
| 3:F:3255[B]:PRO:HB3 | 3:a:2964[B]:PRO:CB | 1.97 | 0.91 |
| 3:I:3162[B]:ASP:OD2 | 3:R:3258[B]:PHE:HA | 1.70 | 0.91 |
| 3:I:3283[A]:ILE:HG21 | 3:I:3305[A]:ILE:HD11 | 1.52 | 0.91 |
| 3:O:2935[A]:ILE:HD13 | 3:O:2936[A]:GLU:H | 1.35 | 0.91 |
| 3:O:2951[A]:ASP:OD2 | 3:O:2952[A]:ALA:N | 2.03 | 0.91 |
| 3:O:2965[B]:LEU:HD11 | 3:O:2975[B]:PHE:N | 1.85 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3134[B]:GLN:O | 3:O:3137[B]:ARG:N | 2.02 | 0.91 |
| 3:O:3169[B]:LYS:HE3 | 3:X:3148[B]:ILE:CA | 1.57 | 0.91 |
| 2:Q:2867:PRO:HG3 | 3:R:2932[A]:PRO:CG | 2.01 | 0.91 |
| 3:R:2965[B]:LEU:HD11 | 3:R:2975[B]:PHE:H | 1.31 | 0.91 |
| 3:R:3298[B]:ASN:HB2 | 3:R:3300[B]:LEU:HD23 | 1.50 | 0.91 |
| 3:U:2969[B]:TYR:CE2 | 3:U:2970[B]:PRO:HG2 | 2.05 | 0.91 |
| 3:X:3134[B]:GLN:O | 3:X:3137[B]:ARG:N | 2.02 | 0.91 |
| 3:a:2931[B]:THR:N | 3:a:2934[B]:GLU:OE2 | 2.02 | 0.91 |
| 3:C:2932[A]:PRO:HA | 3:C:2935[A]:ILE:CD1 | 1.99 | 0.91 |
| 3:C:3284[A]:LYS:HE2 | 3:C:3284[A]:LYS:HA | 1.49 | 0.91 |
| 3:F:3153[B]:LYS:HZ1 | 3:a:3157[B]:PRO:N | 1.67 | 0.91 |
| 3:F:3163[B]:ASN:HB2 | 3:a:3150[B]:LYS:HE3 | 1.51 | 0.91 |
| 3:I:2951[A]:ASP:OD2 | 3:I:2952[A]:ALA:N | 2.03 | 0.91 |
| 3:I:3162[B]:ASP:CB | 3:R:3259[B]:ASP:HB3 | 2.00 | 0.91 |
| 3:L:2948[B]:ASP:HB3 | 3:L:2949[B]:LYS:HA | 1.52 | 0.91 |
| 3:L:3074[B]:GLU:OE1 | 3:L:3212[B]:ARG:NH2 | 2.02 | 0.91 |
| 3:L:3096[B]:VAL:HG11 | 3:L:3115[B]:LEU:CD1 | 1.99 | 0.91 |
| 3:O:2965[A]:LEU:HD11 | 3:O:2975[A]:PHE:N | 1.85 | 0.91 |
| 3:O:3074[B]:GLU:OE1 | 3:O:3212[B]:ARG:NH2 | 2.03 | 0.91 |
| 3:O:3283[A]:ILE:HG21 | 3:O:3305[A]:ILE:HD11 | 1.51 | 0.91 |
| 3:U:2951[A]:ASP:OD2 | 3:U:2952[A]:ALA:N | 2.04 | 0.91 |
| 3:U:3147[B]:GLU:HB2 | 3:U:3149[B]:ASN:CG | 1.95 | 0.91 |
| 3:U:3170[B]:ALA:HA | 3:d:3148[B]:ILE:HG21 | 0.93 | 0.91 |
| 3:U:3298[A]:ASN:HB2 | 3:U:3300[A]:LEU:HD23 | 1.51 | 0.91 |
| 3:X:3074[A]:GLU:OE1 | 3:X:3212[A]:ARG:NH2 | 2.03 | 0.91 |
| 3:X:3283[A]:ILE:HG21 | 3:X:3305[A]:ILE:HD11 | 1.51 | 0.91 |
| 3:X:3298[B]:ASN:HB2 | 3:X:3300[B]:LEU:N | 1.78 | 0.91 |
| 3:a:2932[A]:PRO:HA | 3:a:2935[A]:ILE:HD12 | 1.51 | 0.91 |
| 3:d:2965[B]:LEU:HD11 | 3:d:2975[B]:PHE:N | 1.85 | 0.91 |
| 3:d:3283[B]:ILE:HG21 | 3:d:3305[B]:ILE:HD11 | 1.51 | 0.91 |
| 3:C:2948[B]:ASP:HB3 | 3:C:2949[B]:LYS:HA | 1.52 | 0.91 |
| 3:C:2979[B]:GLN:CG | 3:C:3155[B]:MET:HE1 | 1.97 | 0.91 |
| 3:C:3158[B]:PHE:O | 3:L:3149[B]:ASN:CB | 2.19 | 0.91 |
| 3:C:3255[B]:PRO:CG | 3:L:2959[B]:SER:O | 2.17 | 0.91 |
| 3:F:2935[B]:ILE:HD13 | 3:F:2936[B]:GLU:H | 1.35 | 0.91 |
| 3:F:2951[B]:ASP:OD2 | 3:F:2952[B]:ALA:N | 2.03 | 0.91 |
| 3:F:2979[B]:GLN:CG | 3:F:3155[B]:MET:HE1 | 1.97 | 0.91 |
| 3:F:3253[B]:GLU:CA | 3:a:2976[B]:ALA:N | 2.33 | 0.91 |
| 3:F:3255[B]:PRO:HB3 | 3:a:2964[B]:PRO:HB2 | 1.53 | 0.91 |
| 3:I:2961[B]:HIS:CE1 | 3:I:2980[B]:HIS:HE2 | 1.77 | 0.91 |
| 3:L:2951[A]:ASP:OD2 | 3:L:2952[A]:ALA:N | 2.03 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2935[B]:ILE:HD13 | 3:O:2936[B]:GLU:H | 1.35 | 0.91 |
| 3:U:2931[A]:THR:N | 3:U:2934[A]:GLU:OE2 | 2.02 | 0.91 |
| 3:U:2972[B]:GLY:C | 3:d:3247[B]:VAL:CG1 | 2.44 | 0.91 |
| 3:d:2948[A]:ASP:HB3 | 3:d:2949[A]:LYS:HA | 1.52 | 0.91 |
| 3:d:2951[B]:ASP:OD2 | 3:d:2952[B]:ALA:N | 2.03 | 0.91 |
| 3:d:2969[A]:TYR:CE2 | 3:d:2970[A]:PRO:HG2 | 2.05 | 0.91 |
| 3:d:3147[A]:GLU:HB2 | 3:d:3149[A]:ASN:CG | 1.95 | 0.91 |
| 3:C:3172[B]:SER:HB3 | 3:L:3150[B]:LYS:HA | 1.50 | 0.91 |
| 3:F:3147[B]:GLU:HB2 | 3:F:3149[B]:ASN:CG | 1.95 | 0.91 |
| 3:F:3155[B]:MET:CG | 3:a:3154[B]:PRO:N | 2.33 | 0.91 |
| 3:I:2965[B]:LEU:HD11 | 3:I:2975[B]:PHE:N | 1.85 | 0.91 |
| 3:O:3220[A]:ARG:HG3 | 3:O:3220[A]:ARG:HH11 | 1.35 | 0.91 |
| 3:R:2948[B]:ASP:HB3 | 3:R:2949[B]:LYS:HA | 1.52 | 0.91 |
| 3:X:2951[B]:ASP:OD2 | 3:X:2952[B]:ALA:N | 2.03 | 0.91 |
| 3:a:3298[B]:ASN:HB2 | 3:a:3300[B]:LEU:HD23 | 1.50 | 0.91 |
| 3:C:2965[B]:LEU:HD11 | 3:C:2975[B]:PHE:N | 1.85 | 0.91 |
| 3:C:3147[B]:GLU:HB2 | 3:C:3149[B]:ASN:CG | 1.95 | 0.91 |
| 3:F:3169[B]:LYS:HE2 | 3:a:3147[B]:GLU:N | 1.82 | 0.91 |
| 3:F:3217[A]:PHE:HZ | 3:F:3230[A]:PHE:CE1 | 1.89 | 0.91 |
| 3:I:2970[B]:PRO:N | 3:R:2989[B]:HIS:CD2 | 2.38 | 0.91 |
| 3:I:2976[B]:ALA:HB3 | 3:R:3252[B]:TYR:O | 1.71 | 0.91 |
| 3:I:3090[B]:ASN:HB3 | 3:R:2972[B]:GLY:CA | 2.00 | 0.91 |
| 3:L:2948[A]:ASP:HB3 | 3:L:2949[A]:LYS:HA | 1.52 | 0.91 |
| 3:R:3220[B]:ARG:HH11 | 3:R:3220[B]:ARG:HG3 | 1.35 | 0.91 |
| 3:U:2948[A]:ASP:HB3 | 3:U:2949[A]:LYS:HA | 1.52 | 0.91 |
| 3:U:3155[B]:MET:H | 3:d:3150[B]:LYS:HA | 1.14 | 0.91 |
| 3:U:3230[B]:PHE:HB2 | 3:U:3243[B]:GLY:N | 1.86 | 0.91 |
| 3:a:2965[B]:LEU:HD11 | 3:a:2975[B]:PHE:N | 1.85 | 0.91 |
| 3:d:3096[A]:VAL:HG11 | 3:d:3115[A]:LEU:CD1 | 1.99 | 0.91 |
| 3:C:3156[B]:MET:CB | 3:L:2982[B]:MET:CG | 2.46 | 0.90 |
| 3:C:3163[B]:ASN:ND2 | 3:L:3149[B]:ASN:CG | 2.19 | 0.90 |
| 3:C:3298[A]:ASN:ND2 | 3:C:3301[A]:PRO:CA | 2.34 | 0.90 |
| 3:F:2979[A]:GLN:HE21 | 3:F:3155[A]:MET:HE3 | 1.37 | 0.90 |
| 3:F:3298[B]:ASN:ND2 | 3:F:3301[B]:PRO:CA | 2.34 | 0.90 |
| 3:I:2935[B]:ILE:HD13 | 3:I:2936[B]:GLU:H | 1.35 | 0.90 |
| 3:I:3149[B]:ASN:OD1 | 3:R:3169[B]:LYS:CD | 2.17 | 0.90 |
| 3:I:3150[B]:LYS:HZ3 | 3:R:3160[B]:SER:HB3 | 1.29 | 0.90 |
| 3:I:3173[B]:THR:O | 3:R:3154[B]:PRO:CD | 2.19 | 0.90 |
| 3:I:3173[B]:THR:C | 3:R:3154[B]:PRO:HD3 | 1.96 | 0.90 |
| 3:O:2974[B]:ALA:HB3 | 3:X:2977[B]:CYS:CA | 2.01 | 0.90 |
| 3:O:3196[A]:THR:HB | 3:O:3198[A]:PRO:HD2 | 1.54 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2932[B]:PRO:HA | 3:R:2935[B]:ILE:HD12 | 1.51 | 0.90 |
| 3:R:2951[B]:ASP:OD2 | 3:R:2952[B]:ALA:N | 2.03 | 0.90 |
| 3:R:2965[A]:LEU:HD11 | 3:R:2975[A]:PHE:N | 1.85 | 0.90 |
| 3:R:3283[A]:ILE:HG21 | 3:R:3305[A]:ILE:HD11 | 1.51 | 0.90 |
| 3:R:3298[A]:ASN:ND2 | 3:R:3301[A]:PRO:CA | 2.34 | 0.90 |
| 3:U:2935[B]:ILE:HD13 | 3:U:2936[B]:GLU:H | 1.35 | 0.90 |
| 3:U:3220[B]:ARG:HG3 | 3:U:3220[B]:ARG:HH11 | 1.35 | 0.90 |
| 3:X:3230[A]:PHE:HB2 | 3:X:3243[A]:GLY:N | 1.86 | 0.90 |
| 3:a:2965[A]:LEU:HD11 | 3:a:2975[A]:PHE:H | 1.31 | 0.90 |
| 3:a:3298[A]:ASN:ND2 | 3:a:3301[A]:PRO:CA | 2.34 | 0.90 |
| 3:a:3298[B]:ASN:ND2 | 3:a:3301[B]:PRO:CA | 2.34 | 0.90 |
| 3:C:3174[B]:GLY:HA3 | 3:L:3154[B]:PRO:CB | 2.00 | 0.90 |
| 3:F:3155[B]:MET:CG | 3:a:3153[B]:LYS:HG2 | 2.00 | 0.90 |
| 3:F:3230[A]:PHE:HB2 | 3:F:3243[A]:GLY:N | 1.87 | 0.90 |
| 3:I:2967[B]:CYS:HA | 3:R:2981[B]:GLY:CA | 1.94 | 0.90 |
| 3:I:3298[A]:ASN:ND2 | 3:I:3301[A]:PRO:CA | 2.34 | 0.90 |
| 3:L:2951[B]:ASP:OD2 | 3:L:2952[B]:ALA:N | 2.03 | 0.90 |
| 3:O:3157[B]:PRO:O | 3:X:3148[B]:ILE:O | 1.87 | 0.90 |
| 3:R:2988[A]:TRP:HE3 | 3:R:2989[A]:HIS:HD1 | 1.14 | 0.90 |
| 3:U:2969[A]:TYR:CE2 | 3:U:2970[A]:PRO:HG2 | 2.05 | 0.90 |
| 3:U:3153[B]:LYS:HB3 | 3:d:3153[B]:LYS:CG | 2.00 | 0.90 |
| 3:U:3160[B]:SER:O | 3:d:3147[B]:GLU:OE2 | 1.55 | 0.90 |
| 3:U:3196[A]:THR:HB | 3:U:3198[A]:PRO:HD2 | 1.54 | 0.90 |
| 3:U:3298[A]:ASN:ND2 | 3:U:3301[A]:PRO:CA | 2.34 | 0.90 |
| 3:a:2948[A]:ASP:HB3 | 3:a:2949[A]:LYS:HA | 1.52 | 0.90 |
| 3:C:2967[B]:CYS:HB3 | 3:L:2982[B]:MET:H | 1.29 | 0.90 |
| 3:C:2974[B]:ALA:CA | 3:L:3249[B]:GLY:HA2 | 2.01 | 0.90 |
| 3:C:3074[B]:GLU:OE1 | 3:C:3212[B]:ARG:NH2 | 2.02 | 0.90 |
| 3:C:3134[A]:GLN:O | 3:C:3137[A]:ARG:N | 2.02 | 0.90 |
| 3:C:3147[A]:GLU:HB2 | 3:C:3149[A]:ASN:CG | 1.95 | 0.90 |
| 1:D:695:TYR:HH | 1:D:703:TYR:HD1 | 1.07 | 0.90 |
| 3:F:2975[B]:PHE:CG | 3:a:3107[B]:LEU:HD11 | 2.04 | 0.90 |
| 3:F:3255[B]:PRO:HB2 | 3:a:2959[B]:SER:HB2 | 1.51 | 0.90 |
| 3:F:3283[B]:ILE:HG21 | 3:F:3305[B]:ILE:HD11 | 1.51 | 0.90 |
| 3:I:2931[B]:THR:N | 3:I:2934[B]:GLU:OE2 | 2.02 | 0.90 |
| 3:I:3298[B]:ASN:HB2 | 3:I:3300[B]:LEU:HD23 | 1.51 | 0.90 |
| 3:L:2979[B]:GLN:HE21 | 3:L:3155[B]:MET:HE3 | 1.36 | 0.90 |
| 3:R:2935[B]:ILE:HD13 | 3:R:2936[B]:GLU:H | 1.35 | 0.90 |
| 3:U:2951[B]:ASP:OD2 | 3:U:2952[B]:ALA:N | 2.03 | 0.90 |
| 3:U:3254[B]:MET:CE | 3:d:3254[B]:MET:CB | 2.45 | 0.90 |
| 3:X:2965[B]:LEU:HD11 | 3:X:2975[B]:PHE:N | 1.85 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3298[B]:ASN:HB2 | 3:X:3300[B]:LEU:HD23 | 1.51 | 0.90 |
| 3:d:2951[A]:ASP:OD2 | 3:d:2952[A]:ALA:N | 2.04 | 0.90 |
| 3:d:2988[B]:TRP:HE3 | 3:d:2989[B]:HIS:HD1 | 1.14 | 0.90 |
| 3:d:3230[A]:PHE:HB2 | 3:d:3243[A]:GLY:N | 1.87 | 0.90 |
| 3:C:3196[B]:THR:HB | 3:C:3198[B]:PRO:HD2 | 1.54 | 0.90 |
| 3:I:2975[B]:PHE:HZ | 3:R:2961[B]:HIS:CB | 1.85 | 0.90 |
| 3:I:2978[B]:CYS:O | 3:R:2977[B]:CYS:SG | 2.28 | 0.90 |
| 3:I:2988[B]:TRP:CH2 | 3:R:2975[B]:PHE:HE2 | 1.88 | 0.90 |
| 3:O:2971[B]:ASP:N | 3:X:2991[B]:LEU:N | 2.19 | 0.90 |
| 3:F:2969[B]:TYR:CE2 | 3:F:2970[B]:PRO:HG2 | 2.05 | 0.90 |
| 3:F:3150[B]:LYS:HZ2 | 3:a:3160[B]:SER:HB3 | 1.10 | 0.90 |
| 3:I:3172[B]:SER:HB3 | 3:R:3150[B]:LYS:C | 1.96 | 0.90 |
| 3:O:3160[B]:SER:CA | 3:X:3151[B]:LEU:HD12 | 2.01 | 0.90 |
| 3:R:3230[B]:PHE:HB2 | 3:R:3243[B]:GLY:N | 1.87 | 0.90 |
| 3:U:3220[B]:ARG:HA | 3:d:2973[B]:THR:HA | 0.91 | 0.90 |
| 3:a:2935[A]:ILE:HD13 | 3:a:2936[A]:GLU:H | 1.35 | 0.90 |
| 3:C:3153[B]:LYS:NZ | 3:L:2988[B]:TRP:CD1 | 2.40 | 0.90 |
| 3:F:2948[A]:ASP:N | 3:F:2949[A]:LYS:HA | 1.81 | 0.90 |
| 3:I:2935[A]:ILE:HD13 | 3:I:2936[A]:GLU:H | 1.35 | 0.90 |
| 3:I:3169[B]:LYS:C | 3:R:3148[B]:ILE:O | 2.14 | 0.90 |
| 3:I:3196[A]:THR:HB | 3:I:3198[A]:PRO:HD2 | 1.53 | 0.90 |
| 3:I:3230[B]:PHE:HB2 | 3:I:3243[B]:GLY:N | 1.87 | 0.90 |
| 3:L:2988[A]:TRP:HE3 | 3:L:2989[A]:HIS:HD1 | 1.14 | 0.90 |
| 3:L:3298[B]:ASN:ND2 | 3:L:3301[B]:PRO:CA | 2.34 | 0.90 |
| 3:O:3160[B]:SER:CB | 3:X:3151[B]:LEU:N | 2.30 | 0.90 |
| 3:R:3283[B]:ILE:HG21 | 3:R:3305[B]:ILE:HD11 | 1.51 | 0.90 |
| 3:U:3162[B]:ASP:CA | 3:d:3260[B]:ARG:NH1 | 2.28 | 0.90 |
| 3:U:3220[A]:ARG:HH11 | 3:U:3220[A]:ARG:HG3 | 1.35 | 0.90 |
| 3:X:2948[A]:ASP:HB3 | 3:X:2949[A]:LYS:HA | 1.52 | 0.90 |
| 3:a:2965[A]:LEU:HD11 | 3:a:2975[A]:PHE:N | 1.85 | 0.90 |
| 3:C:3148[B]:ILE:C | 3:L:3169[B]:LYS:C | 2.37 | 0.90 |
| 3:I:3283[B]:ILE:HG21 | 3:I:3305[B]:ILE:HD11 | 1.51 | 0.90 |
| 3:R:2979[B]:GLN:CG | 3:R:3155[B]:MET:HE1 | 1.97 | 0.90 |
| 3:U:2967[B]:CYS:HB2 | 3:d:3256[B]:TRP:CB | 2.00 | 0.90 |
| 3:U:3153[B]:LYS:HE2 | 3:d:2979[B]:GLN:HE22 | 0.74 | 0.90 |
| 3:U:3298[B]:ASN:ND2 | 3:U:3301[B]:PRO:CA | 2.34 | 0.90 |
| 3:X:2932[A]:PRO:HA | 3:X:2935[A]:ILE:HD12 | 1.51 | 0.90 |
| 3:X:3220[B]:ARG:HG3 | 3:X:3220[B]:ARG:HH11 | 1.35 | 0.90 |
| 3:a:2988[B]:TRP:HE3 | 3:a:2989[B]:HIS:HD1 | 1.13 | 0.90 |
| 3:C:3223[B]:GLY:O | 3:L:3252[B]:TYR:CE1 | 2.24 | 0.90 |
| 3:C:3230[B]:PHE:HB2 | 3:C:3243[B]:GLY:N | 1.87 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:806:ASN:HD22 | 6:k:1:NAG:H83 | 1.36 | 0.90 |
| 3:F:2965[A]:LEU:HD11 | 3:F:2975[A]:PHE:N | 1.85 | 0.90 |
| 3:F:2965[B]:LEU:O | 3:a:3221[B]:ALA:HB2 | 1.72 | 0.90 |
| 3:F:2970[B]:PRO:HD3 | 3:a:2989[B]:HIS:ND1 | 1.86 | 0.90 |
| 3:F:2982[B]:MET:CE | 3:a:2966[B]:SER:CB | 2.49 | 0.90 |
| 3:F:3298[A]:ASN:ND2 | 3:F:3301[A]:PRO:CA | 2.34 | 0.90 |
| 1:G:1582:ASN:HB3 | 1:G:1583:CYS:HB2 | 1.53 | 0.90 |
| 2:H:2868:GLU:OE2 | 3:I:2932[A]:PRO:C | 2.14 | 0.90 |
| 3:I:2966[B]:SER:C | 3:R:3256[B]:TRP:CG | 2.39 | 0.90 |
| 3:I:2967[B]:CYS:SG | 3:R:2982[B]:MET:CG | 2.60 | 0.90 |
| 3:L:3230[A]:PHE:HB2 | 3:L:3243[A]:GLY:N | 1.86 | 0.90 |
| 3:L:3283[A]:ILE:HG21 | 3:L:3305[A]:ILE:HD11 | 1.51 | 0.90 |
| 3:O:2932[A]:PRO:HA | 3:O:2935[A]:ILE:HD12 | 1.51 | 0.90 |
| 3:O:2932[B]:PRO:HA | 3:O:2935[B]:ILE:HD12 | 1.51 | 0.90 |
| 3:O:2973[B]:THR:CB | 3:X:3158[B]:PHE:CE2 | 2.54 | 0.90 |
| 3:O:3230[B]:PHE:HB2 | 3:O:3243[B]:GLY:N | 1.87 | 0.90 |
| 3:U:2948[B]:ASP:HB3 | 3:U:2949[B]:LYS:HA | 1.52 | 0.90 |
| 3:a:3196[A]:THR:HB | 3:a:3198[A]:PRO:HD2 | 1.53 | 0.90 |
| 3:d:3298[B]:ASN:ND2 | 3:d:3301[B]:PRO:CA | 2.34 | 0.90 |
| 3:C:2979[A]:GLN:HE21 | 3:C:3155[A]:MET:HE3 | 1.36 | 0.90 |
| 3:C:3220[B]:ARG:HH11 | 3:C:3220[B]:ARG:HG3 | 1.35 | 0.90 |
| 3:C:3223[B]:GLY:O | 3:L:3252[B]:TYR:CZ | 2.24 | 0.90 |
| 3:I:3153[B]:LYS:CD | 3:R:3155[B]:MET:CB | 2.46 | 0.90 |
| 3:L:3220[B]:ARG:HH11 | 3:L:3220[B]:ARG:HG3 | 1.35 | 0.90 |
| 3:O:2964[B]:PRO:HA | 3:X:2975[B]:PHE:HE2 | 1.37 | 0.90 |
| 3:O:2965[B]:LEU:HD11 | 3:X:2979[B]:GLN:NE2 | 1.86 | 0.90 |
| 3:O:3298[A]:ASN:HB2 | 3:O:3300[A]:LEU:N | 1.78 | 0.90 |
| 3:R:2951[A]:ASP:OD2 | 3:R:2952[A]:ALA:N | 2.04 | 0.90 |
| 3:R:3196[A]:THR:HB | 3:R:3198[A]:PRO:HD2 | 1.53 | 0.90 |
| 3:U:2932[A]:PRO:HA | 3:U:2935[A]:ILE:HD12 | 1.51 | 0.90 |
| 3:U:2988[A]:TRP:HE3 | 3:U:2989[A]:HIS:HD1 | 1.14 | 0.90 |
| 3:U:3252[B]:TYR:HE2 | 3:d:3222[B]:ILE:HD12 | 1.37 | 0.90 |
| 3:X:3298[B]:ASN:ND2 | 3:X:3301[B]:PRO:CA | 2.34 | 0.90 |
| 3:d:2965[A]:LEU:HD11 | 3:d:2975[A]:PHE:H | 1.32 | 0.90 |
| 3:d:3298[A]:ASN:HB2 | 3:d:3300[A]:LEU:N | 1.78 | 0.90 |
| 3:C:3252[B]:TYR:HB3 | 3:L:3253[B]:GLU:HB3 | 1.52 | 0.90 |
| 3:F:2948[B]:ASP:HB3 | 3:F:2949[B]:LYS:HA | 1.52 | 0.90 |
| 3:F:2967[B]:CYS:SG | 3:a:2982[B]:MET:HG2 | 2.11 | 0.90 |
| 3:F:3024[A]:LEU:CD1 | 3:F:3025[A]:VAL:H | 1.83 | 0.90 |
| 3:F:3196[B]:THR:HB | 3:F:3198[B]:PRO:HD2 | 1.54 | 0.90 |
| 3:F:3220[B]:ARG:HG3 | 3:F:3220[B]:ARG:HH11 | 1.35 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2968[B]:GLN:HG3 | 3:R:3086[B]:GLU:HG3 | 1.53 | 0.90 |
| 3:I:3255[B]:PRO:CG | 3:R:2964[B]:PRO:HD2 | 2.02 | 0.90 |
| 3:L:3217[B]:PHE:HZ | 3:L:3230[B]:PHE:CE1 | 1.89 | 0.90 |
| 3:O:2970[B]:PRO:HG2 | 3:X:2990[B]:ARG:C | 1.97 | 0.90 |
| 3:O:3230[A]:PHE:HB2 | 3:O:3243[A]:GLY:N | 1.87 | 0.90 |
| 3:R:3147[B]:GLU:HB2 | 3:R:3149[B]:ASN:CG | 1.95 | 0.90 |
| 1:Y:1616:LYS:C | 3:d:3187[B]:TYR:HB2 | 1.96 | 0.90 |
| 2:Z:2472:ASN:HB3 | 4:MA:1:NAG:C8 | 2.01 | 0.90 |
| 3:a:2979[B]:GLN:HE21 | 3:a:3155[B]:MET:HE3 | 1.37 | 0.90 |
| 3:a:3074[B]:GLU:OE1 | 3:a:3212[B]:ARG:NH2 | 2.03 | 0.90 |
| 3:a:3217[A]:PHE:HZ | 3:a:3230[A]:PHE:CE1 | 1.89 | 0.90 |
| 3:d:3298[A]:ASN:ND2 | 3:d:3301[A]:PRO:CA | 2.34 | 0.90 |
| 3:C:3248[B]:LEU:HB2 | 3:L:2972[B]:GLY:C | 1.96 | 0.89 |
| 3:F:2935[A]:ILE:HD13 | 3:F:2936[A]:GLU:H | 1.35 | 0.89 |
| 3:F:3155[B]:MET:H | 3:a:3153[B]:LYS:C | 1.80 | 0.89 |
| 3:I:2965[A]:LEU:HD11 | 3:I:2975[A]:PHE:N | 1.85 | 0.89 |
| 3:I:3173[B]:THR:C | 3:R:3154[B]:PRO:CD | 2.44 | 0.89 |
| 3:O:2965[B]:LEU:HB3 | 3:X:3254[B]:MET:SD | 2.12 | 0.89 |
| 3:U:3257[B]:ALA:H | 3:d:2968[B]:GLN:HA | 0.73 | 0.89 |
| 3:a:3196[B]:THR:HB | 3:a:3198[B]:PRO:HD2 | 1.54 | 0.89 |
| 3:d:3217[B]:PHE:HZ | 3:d:3230[B]:PHE:CE1 | 1.89 | 0.89 |
| 3:d:3220[A]:ARG:HH11 | 3:d:3220[A]:ARG:HG3 | 1.35 | 0.89 |
| 3:C:2988[A]:TRP:HE3 | 3:C:2989[A]:HIS:ND1 | 1.70 | 0.89 |
| 3:I:2948[A]:ASP:HB3 | 3:I:2949[A]:LYS:HA | 1.52 | 0.89 |
| 3:I:2979[B]:GLN:CG | 3:I:3155[B]:MET:HE1 | 1.97 | 0.89 |
| 3:L:3298[A]:ASN:ND2 | 3:L:3301[A]:PRO:CA | 2.34 | 0.89 |
| 3:R:2948[A]:ASP:HB3 | 3:R:2949[A]:LYS:HA | 1.52 | 0.89 |
| 3:R:2988[A]:TRP:HE3 | 3:R:2989[A]:HIS:ND1 | 1.70 | 0.89 |
| 3:U:3256[B]:TRP:HB3 | 3:d:2975[B]:PHE:CE1 | 2.04 | 0.89 |
| 3:X:3220[A]:ARG:HH11 | 3:X:3220[A]:ARG:HG3 | 1.35 | 0.89 |
| 3:d:2965[A]:LEU:HD11 | 3:d:2975[A]:PHE:N | 1.85 | 0.89 |
| 3:d:2988[B]:TRP:HE3 | 3:d:2989[B]:HIS:ND1 | 1.70 | 0.89 |
| 3:C:2988[B]:TRP:HE3 | 3:C:2989[B]:HIS:HD1 | 1.14 | 0.89 |
| 3:C:3283[B]:ILE:HG21 | 3:C:3305[B]:ILE:HD11 | 1.51 | 0.89 |
| 3:F:2969[B]:TYR:C | 3:a:2989[B]:HIS:NE2 | 2.31 | 0.89 |
| 3:I:2951[B]:ASP:OD2 | 3:I:2952[B]:ALA:N | 2.03 | 0.89 |
| 3:L:2988[A]:TRP:HE3 | 3:L:2989[A]:HIS:ND1 | 1.70 | 0.89 |
| 3:L:3230[B]:PHE:HB2 | 3:L:3243[B]:GLY:N | 1.87 | 0.89 |
| 3:O:2969[B]:TYR:HD1 | 3:X:3158[B]:PHE:CD1 | 1.80 | 0.89 |
| 3:O:2988[A]:TRP:HE3 | 3:O:2989[A]:HIS:ND1 | 1.70 | 0.89 |
| 1:P:1582:ASN:HB3 | 1:P:1583:CYS:HB2 | 1.54 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2967[B]:CYS:C | 3:d:3256[B]:TRP:HB2 | 1.97 | 0.89 |
| 3:U:3196[B]:THR:HB | 3:U:3198[B]:PRO:HD2 | 1.53 | 0.89 |
| 2:c:2800:LYS:O | 3:d:3023[A]:ILE:CD1 | 2.19 | 0.89 |
| 3:d:3196[B]:THR:HB | 3:d:3198[B]:PRO:HD2 | 1.54 | 0.89 |
| 3:d:3230[B]:PHE:HB2 | 3:d:3243[B]:GLY:N | 1.87 | 0.89 |
| 3:C:2935[A]:ILE:HD13 | 3:C:2936[A]:GLU:H | 1.35 | 0.89 |
| 3:C:2968[B]:GLN:HE21 | 3:L:3086[B]:GLU:HB3 | 1.37 | 0.89 |
| 3:C:2972[B]:GLY:HA3 | 3:L:3090[B]:ASN:CG | 1.96 | 0.89 |
| 3:F:3148[B]:ILE:O | 3:a:3169[B]:LYS:C | 2.13 | 0.89 |
| 1:M:427:ASP:OD2 | 1:M:518:LYS:NZ | 2.05 | 0.89 |
| 3:O:3298[A]:ASN:ND2 | 3:O:3301[A]:PRO:CA | 2.34 | 0.89 |
| 3:R:3298[B]:ASN:ND2 | 3:R:3301[B]:PRO:CA | 2.34 | 0.89 |
| 3:U:2932[B]:PRO:HA | 3:U:2935[B]:ILE:HD12 | 1.51 | 0.89 |
| 3:U:3230[A]:PHE:HB2 | 3:U:3243[A]:GLY:N | 1.87 | 0.89 |
| 3:a:2948[B]:ASP:HB3 | 3:a:2949[B]:LYS:HA | 1.52 | 0.89 |
| 2:c:2470:ALA:HB2 | 2:c:2476:LEU:HD21 | 1.54 | 0.89 |
| 3:C:2969[B]:TYR:HA | 3:L:2989[B]:HIS:NE2 | 1.88 | 0.89 |
| 3:C:3298[B]:ASN:ND2 | 3:C:3301[B]:PRO:CA | 2.34 | 0.89 |
| 3:I:2948[B]:ASP:HB3 | 3:I:2949[B]:LYS:HA | 1.52 | 0.89 |
| 3:I:2956[A]:LYS:O | 3:I:2960[A]:PHE:HE1 | 1.22 | 0.89 |
| 3:I:2988[B]:TRP:HE3 | 3:I:2989[B]:HIS:ND1 | 1.70 | 0.89 |
| 3:I:3151[B]:LEU:N | 3:R:3159[B]:SER:HA | 1.86 | 0.89 |
| 3:R:2988[B]:TRP:HE3 | 3:R:2989[B]:HIS:ND1 | 1.70 | 0.89 |
| 3:R:3230[A]:PHE:HB2 | 3:R:3243[A]:GLY:N | 1.87 | 0.89 |
| 3:U:2964[B]:PRO:HA | 3:d:3220[B]:ARG:HH22 | 1.37 | 0.89 |
| 3:U:2965[B]:LEU:HD11 | 3:U:2975[B]:PHE:N | 1.85 | 0.89 |
| 3:U:2975[B]:PHE:HE2 | 3:d:3254[B]:MET:HG3 | 0.73 | 0.89 |
| 3:X:2988[B]:TRP:HE3 | 3:X:2989[B]:HIS:ND1 | 1.70 | 0.89 |
| 3:a:2979[A]:GLN:HE21 | 3:a:3155[A]:MET:HE3 | 1.36 | 0.89 |
| 3:C:2988[B]:TRP:HE3 | 3:C:2989[B]:HIS:ND1 | 1.70 | 0.89 |
| 3:C:3108[B]:HIS:HE1 | 3:L:3251[B]:ASP:OD1 | 1.56 | 0.89 |
| 3:C:3154[B]:PRO:O | 3:L:3155[B]:MET:HG2 | 1.73 | 0.89 |
| 3:F:2982[B]:MET:SD | 3:a:2967[B]:CYS:SG | 2.70 | 0.89 |
| 3:I:2976[B]:ALA:CB | 3:R:3252[B]:TYR:O | 2.19 | 0.89 |
| 3:I:3153[B]:LYS:HB3 | 3:R:3155[B]:MET:O | 1.73 | 0.89 |
| 3:I:3163[B]:ASN:CG | 3:R:3149[B]:ASN:ND2 | 2.31 | 0.89 |
| 3:O:2965[B]:LEU:HD13 | 3:X:2979[B]:GLN:NE2 | 1.62 | 0.89 |
| 3:O:3196[B]:THR:H | 3:O:3199[B]:GLN:HB2 | 1.38 | 0.89 |
| 3:O:3298[A]:ASN:HB2 | 3:O:3300[A]:LEU:HD23 | 1.50 | 0.89 |
| 3:U:2965[A]:LEU:HD11 | 3:U:2975[A]:PHE:N | 1.85 | 0.89 |
| 3:U:2988[B]:TRP:HE3 | 3:U:2989[B]:HIS:ND1 | 1.70 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3217[A]:PHE:HZ | 3:X:3230[A]:PHE:CE1 | 1.89 | 0.89 |
| 3:a:3230[B]:PHE:HB2 | 3:a:3243[B]:GLY:N | 1.86 | 0.89 |
| 3:C:3172[B]:SER:H | 3:L:3152[B]:LYS:HB2 | 1.31 | 0.89 |
| 3:F:2948[B]:ASP:N | 3:F:2949[B]:LYS:HA | 1.81 | 0.89 |
| 3:I:2989[B]:HIS:CD2 | 3:R:2970[B]:PRO:CA | 2.55 | 0.89 |
| 3:U:3169[B]:LYS:CG | 3:d:3147[B]:GLU:CA | 2.51 | 0.89 |
| 3:X:3298[A]:ASN:ND2 | 3:X:3301[A]:PRO:CA | 2.34 | 0.89 |
| 2:Z:2800:LYS:O | 3:a:3023[A]:ILE:HD13 | 1.72 | 0.89 |
| 3:d:3013[B]:ASP:HA | 3:d:3122[B]:ASN:ND2 | 1.88 | 0.89 |
| 1:A:180:ASN:HD22 | 1:A:344:LEU:HD22 | 1.38 | 0.89 |
| 3:C:2948[A]:ASP:HB3 | 3:C:2949[A]:LYS:HA | 1.52 | 0.89 |
| 3:C:2959[B]:SER:O | 3:L:3255[B]:PRO:CB | 2.20 | 0.89 |
| 3:C:2974[B]:ALA:HB3 | 3:L:3249[B]:GLY:HA3 | 0.89 | 0.89 |
| 3:F:2967[B]:CYS:HA | 3:a:2981[B]:GLY:CA | 1.92 | 0.89 |
| 3:F:3149[B]:ASN:HD22 | 3:a:3163[B]:ASN:CB | 1.81 | 0.89 |
| 3:F:3196[A]:THR:HB | 3:F:3198[A]:PRO:HD2 | 1.54 | 0.89 |
| 3:F:3230[B]:PHE:HB2 | 3:F:3243[B]:GLY:N | 1.87 | 0.89 |
| 3:I:3273[B]:LEU:HB2 | 3:I:3275[B]:LEU:HD13 | 1.55 | 0.89 |
| 3:a:3220[A]:ARG:HH11 | 3:a:3220[A]:ARG:HG3 | 1.35 | 0.89 |
| 3:a:3273[B]:LEU:HB2 | 3:a:3275[B]:LEU:HD13 | 1.55 | 0.89 |
| 8:0:1:NAG:H61 | 8:0:2:NAG:HN2 | 1.37 | 0.89 |
| 3:F:2979[B]:GLN:HE21 | 3:F:3155[B]:MET:HE3 | 1.36 | 0.89 |
| 3:F:3013[B]:ASP:HA | 3:F:3122[B]:ASN:ND2 | 1.88 | 0.89 |
| 3:I:3273[A]:LEU:HB2 | 3:I:3275[A]:LEU:HD13 | 1.55 | 0.89 |
| 3:L:2935[A]:ILE:HD13 | 3:L:2936[A]:GLU:H | 1.35 | 0.89 |
| 3:O:3298[B]:ASN:ND2 | 3:O:3301[B]:PRO:CA | 2.34 | 0.89 |
| 3:R:2965[B]:LEU:HD11 | 3:R:2975[B]:PHE:N | 1.85 | 0.89 |
| 6:GA:1:NAG:H4 | 6:GA:2:NAG:C7 | 2.02 | 0.89 |
| 3:C:3153[B]:LYS:HB3 | 3:L:3155[B]:MET:H | 1.38 | 0.89 |
| 3:C:3159[B]:SER:HG | 3:L:3150[B]:LYS:C | 1.80 | 0.89 |
| 3:C:3273[A]:LEU:HB2 | 3:C:3275[A]:LEU:HD13 | 1.55 | 0.89 |
| 2:E:2800:LYS:O | 3:F:3023[A]:ILE:HD13 | 1.73 | 0.89 |
| 3:F:2966[B]:SER:CA | 3:a:3256[B]:TRP:CB | 2.51 | 0.89 |
| 3:F:3220[A]:ARG:HH11 | 3:F:3220[A]:ARG:HG3 | 1.35 | 0.89 |
| 3:F:3273[B]:LEU:HB2 | 3:F:3275[B]:LEU:HD13 | 1.55 | 0.89 |
| 3:I:3298[B]:ASN:HB2 | 3:I:3300[B]:LEU:N | 1.78 | 0.89 |
| 3:U:2993[A]:MET:O | 3:U:2997[A]:GLU:N | 2.07 | 0.89 |
| 3:X:3230[B]:PHE:HB2 | 3:X:3243[B]:GLY:N | 1.87 | 0.89 |
| 1:Y:1612:THR:O | 3:d:3186[B]:GLU:HB3 | 1.73 | 0.89 |
| 3:d:2935[A]:ILE:HD13 | 3:d:2936[A]:GLU:H | 1.35 | 0.89 |
| 6:LA:1:NAG:O4 | 6:LA:2:NAG:O7 | 1.89 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3149[B]:ASN:CG | 3:L:3163[B]:ASN:HD22 | 1.80 | 0.88 |
| 3:F:3160[B]:SER:C | 3:a:3150[B]:LYS:HZ2 | 1.80 | 0.88 |
| 3:F:3273[A]:LEU:HB2 | 3:F:3275[A]:LEU:HD13 | 1.55 | 0.88 |
| 3:I:2993[A]:MET:O | 3:I:2997[A]:GLU:N | 2.07 | 0.88 |
| 3:I:2993[B]:MET:O | 3:I:2997[B]:GLU:N | 2.07 | 0.88 |
| 3:O:2974[B]:ALA:HB2 | 3:X:2977[B]:CYS:C | 1.97 | 0.88 |
| 3:O:3159[B]:SER:C | 3:X:3148[B]:ILE:HA | 1.98 | 0.88 |
| 3:U:3013[B]:ASP:HA | 3:U:3122[B]:ASN:ND2 | 1.88 | 0.88 |
| 3:d:3196[A]:THR:HB | 3:d:3198[A]:PRO:HD2 | 1.54 | 0.88 |
| 3:C:2971[B]:ASP:HB3 | 3:L:3089[B]:HIS:CE1 | 2.06 | 0.88 |
| 3:C:2993[B]:MET:O | 3:C:2997[B]:GLU:N | 2.07 | 0.88 |
| 3:C:3154[B]:PRO:CB | 3:L:3151[B]:LEU:O | 2.20 | 0.88 |
| 3:C:3230[A]:PHE:HB2 | 3:C:3243[A]:GLY:N | 1.87 | 0.88 |
| 3:C:3287[B]:ILE:O | 3:C:3295[B]:LEU:HA | 1.73 | 0.88 |
| 3:F:2966[B]:SER:HA | 3:a:3256[B]:TRP:CA | 2.03 | 0.88 |
| 3:F:2993[A]:MET:O | 3:F:2997[A]:GLU:N | 2.07 | 0.88 |
| 3:F:3108[B]:HIS:HE1 | 3:a:3251[B]:ASP:OD1 | 1.52 | 0.88 |
| 3:I:2988[A]:TRP:HE3 | 3:I:2989[A]:HIS:ND1 | 1.70 | 0.88 |
| 3:I:3153[B]:LYS:HB2 | 3:R:3158[B]:PHE:CB | 2.03 | 0.88 |
| 3:I:3154[B]:PRO:HD3 | 3:R:3173[B]:THR:O | 1.73 | 0.88 |
| 3:O:2948[B]:ASP:N | 3:O:2949[B]:LYS:HA | 1.81 | 0.88 |
| 3:O:2979[B]:GLN:HE21 | 3:O:3155[B]:MET:HE3 | 1.36 | 0.88 |
| 3:a:2988[A]:TRP:HE3 | 3:a:2989[A]:HIS:ND1 | 1.70 | 0.88 |
| 3:a:3013[B]:ASP:HA | 3:a:3122[B]:ASN:ND2 | 1.88 | 0.88 |
| 3:C:3162[B]:ASP:CA | 3:L:3147[B]:GLU:OE1 | 1.94 | 0.88 |
| 3:F:3252[B]:TYR:CE2 | 3:a:3250[B]:GLY:HA2 | 2.03 | 0.88 |
| 3:I:2975[B]:PHE:CD1 | 3:R:3107[B]:LEU:CG | 2.49 | 0.88 |
| 3:L:3196[B]:THR:HB | 3:L:3198[B]:PRO:HD2 | 1.54 | 0.88 |
| 3:O:2988[B]:TRP:HE3 | 3:O:2989[B]:HIS:ND1 | 1.70 | 0.88 |
| 3:a:2932[B]:PRO:HA | 3:a:2935[B]:ILE:HD12 | 1.51 | 0.88 |
| 3:d:3273[B]:LEU:HB2 | 3:d:3275[B]:LEU:HD13 | 1.55 | 0.88 |
| 3:C:2979[B]:GLN:HE21 | 3:C:3155[B]:MET:HE3 | 1.36 | 0.88 |
| 3:C:2983[B]:VAL:CB | 3:L:3160[B]:SER:HA | 2.03 | 0.88 |
| 3:F:3252[B]:TYR:CA | 3:a:3108[B]:HIS:NE2 | 2.37 | 0.88 |
| 3:I:3013[A]:ASP:HA | 3:I:3122[A]:ASN:ND2 | 1.88 | 0.88 |
| 3:I:3153[B]:LYS:HE3 | 3:R:3158[B]:PHE:H | 1.37 | 0.88 |
| 3:I:3222[A]:ILE:HD12 | 3:I:3223[A]:GLY:N | 1.89 | 0.88 |
| 3:L:2993[B]:MET:O | 3:L:2997[B]:GLU:N | 2.07 | 0.88 |
| 3:R:3196[B]:THR:HB | 3:R:3198[B]:PRO:HD2 | 1.54 | 0.88 |
| 3:R:3222[A]:ILE:HD12 | 3:R:3223[A]:GLY:N | 1.89 | 0.88 |
| 3:X:3196[B]:THR:HB | 3:X:3198[B]:PRO:HD2 | 1.54 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3273[A]:LEU:HB2 | 3:X:3275[A]:LEU:HD13 | 1.55 | 0.88 |
| 3:X:3287[A]:ILE:O | 3:X:3295[A]:LEU:HA | 1.73 | 0.88 |
| 3:a:3287[A]:ILE:O | 3:a:3295[A]:LEU:HA | 1.73 | 0.88 |
| 3:d:3298[B]:ASN:HB2 | 3:d:3300[B]:LEU:N | 1.78 | 0.88 |
| 1:A:1582:ASN:HB3 | 1:A:1583:CYS:HB2 | 1.55 | 0.88 |
| 3:F:3169[B]:LYS:HE2 | 3:a:3147[B]:GLU:H | 1.36 | 0.88 |
| 1:G:387:ASN:ND2 | 4:o:1:NAG:O6 | 2.06 | 0.88 |
| 3:I:3287[B]:ILE:O | 3:I:3295[B]:LEU:HA | 1.74 | 0.88 |
| 3:L:3013[B]:ASP:HA | 3:L:3122[B]:ASN:ND2 | 1.88 | 0.88 |
| 3:O:2974[B]:ALA:HB3 | 3:X:2977[B]:CYS:HB3 | 1.55 | 0.88 |
| 3:O:2993[B]:MET:O | 3:O:2997[B]:GLU:N | 2.06 | 0.88 |
| 3:O:3255[B]:PRO:HA | 3:X:3161[B]:GLU:CA | 2.02 | 0.88 |
| 3:O:3273[B]:LEU:HB2 | 3:O:3275[B]:LEU:HD13 | 1.55 | 0.88 |
| 3:U:2967[B]:CYS:HB2 | 3:d:3256[B]:TRP:CA | 2.04 | 0.88 |
| 3:U:3013[A]:ASP:HA | 3:U:3122[A]:ASN:ND2 | 1.88 | 0.88 |
| 3:U:3222[A]:ILE:HD12 | 3:U:3223[A]:GLY:N | 1.89 | 0.88 |
| 3:U:3252[B]:TYR:O | 3:d:3255[B]:PRO:CG | 2.22 | 0.88 |
| 3:a:3230[A]:PHE:HB2 | 3:a:3243[A]:GLY:N | 1.87 | 0.88 |
| 3:d:2988[A]:TRP:HE3 | 3:d:2989[A]:HIS:ND1 | 1.70 | 0.88 |
| 3:d:3273[A]:LEU:HB2 | 3:d:3275[A]:LEU:HD13 | 1.55 | 0.88 |
| 3:C:3287[A]:ILE:O | 3:C:3295[A]:LEU:HA | 1.73 | 0.88 |
| 3:F:2943[B]:ALA:O | 3:F:2946[B]:GLN:HG3 | 1.74 | 0.88 |
| 3:F:3155[B]:MET:CB | 3:a:3153[B]:LYS:HD3 | 2.00 | 0.88 |
| 3:F:3256[B]:TRP:NE1 | 3:a:2965[B]:LEU:HD12 | 1.87 | 0.88 |
| 3:I:3013[B]:ASP:HA | 3:I:3122[B]:ASN:ND2 | 1.88 | 0.88 |
| 3:O:2948[B]:ASP:HB3 | 3:O:2949[B]:LYS:HA | 1.52 | 0.88 |
| 3:O:3108[B]:HIS:CB | 3:X:2970[B]:PRO:N | 2.28 | 0.88 |
| 3:O:3173[A]:THR:HB | 3:O:3176[A]:LYS:CD | 2.04 | 0.88 |
| 3:R:3287[A]:ILE:O | 3:R:3295[A]:LEU:HA | 1.73 | 0.88 |
| 3:U:2979[B]:GLN:HE21 | 3:U:3155[B]:MET:HE3 | 1.36 | 0.88 |
| 3:a:3273[A]:LEU:HB2 | 3:a:3275[A]:LEU:HD13 | 1.55 | 0.88 |
| 3:d:2997[A]:GLU:OE2 | 3:d:3009[A]:ILE:HG13 | 1.74 | 0.88 |
| 3:C:2948[B]:ASP:OD1 | 3:C:2950[B]:THR:N | 2.07 | 0.88 |
| 3:C:3196[A]:THR:HB | 3:C:3198[A]:PRO:HD2 | 1.54 | 0.88 |
| 3:F:2988[B]:TRP:HE3 | 3:F:2989[B]:HIS:ND1 | 1.70 | 0.88 |
| 3:I:3217[A]:PHE:HZ | 3:I:3230[A]:PHE:CE1 | 1.89 | 0.88 |
| 3:I:3250[B]:GLY:HA2 | 3:R:3252[B]:TYR:CE2 | 2.06 | 0.88 |
| 3:L:3273[B]:LEU:HB2 | 3:L:3275[B]:LEU:HD13 | 1.55 | 0.88 |
| 3:O:2970[B]:PRO:CG | 3:X:2990[B]:ARG:C | 2.47 | 0.88 |
| 3:O:2979[A]:GLN:HE21 | 3:O:3155[A]:MET:HE3 | 1.36 | 0.88 |
| 3:O:3013[A]:ASP:HA | 3:O:3122[A]:ASN:ND2 | 1.88 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3254[B]:MET:O | 3:d:2975[B]:PHE:CE1 | 2.27 | 0.88 |
| 3:X:2988[A]:TRP:HE3 | 3:X:2989[A]:HIS:ND1 | 1.70 | 0.88 |
| 3:X:3173[A]:THR:HB | 3:X:3176[A]:LYS:CD | 2.04 | 0.88 |
| 3:a:2948[A]:ASP:OD1 | 3:a:2950[A]:THR:N | 2.07 | 0.88 |
| 1:b:587:PHE:O | 1:b:651:ARG:NH2 | 2.06 | 0.88 |
| 3:d:2979[A]:GLN:HE21 | 3:d:3155[A]:MET:HE3 | 1.36 | 0.88 |
| 3:C:2982[B]:MET:CG | 3:L:3156[B]:MET:CG | 2.41 | 0.88 |
| 3:C:3217[B]:PHE:HZ | 3:C:3230[B]:PHE:CE1 | 1.89 | 0.88 |
| 3:F:2948[A]:ASP:OD1 | 3:F:2950[A]:THR:N | 2.07 | 0.88 |
| 3:F:2993[B]:MET:O | 3:F:2997[B]:GLU:N | 2.07 | 0.88 |
| 3:F:2997[B]:GLU:OE2 | 3:F:3009[B]:ILE:HG13 | 1.74 | 0.88 |
| 3:F:3013[A]:ASP:HA | 3:F:3122[A]:ASN:ND2 | 1.88 | 0.88 |
| 3:F:3163[B]:ASN:N | 3:a:3147[B]:GLU:OE1 | 2.06 | 0.88 |
| 3:F:3173[A]:THR:HB | 3:F:3176[A]:LYS:CD | 2.04 | 0.88 |
| 3:I:2961[B]:HIS:CB | 3:R:2975[B]:PHE:HZ | 1.86 | 0.88 |
| 3:I:3230[A]:PHE:HB2 | 3:I:3243[A]:GLY:N | 1.87 | 0.88 |
| 3:L:2997[A]:GLU:OE2 | 3:L:3009[A]:ILE:HG13 | 1.74 | 0.88 |
| 3:L:3173[B]:THR:HB | 3:L:3176[B]:LYS:CD | 2.04 | 0.88 |
| 3:O:2943[A]:ALA:O | 3:O:2946[A]:GLN:HG3 | 1.74 | 0.88 |
| 3:R:2948[A]:ASP:OD1 | 3:R:2950[A]:THR:N | 2.07 | 0.88 |
| 3:U:3253[B]:GLU:CA | 3:d:3255[B]:PRO:HG3 | 2.02 | 0.88 |
| 3:d:2948[B]:ASP:OD1 | 3:d:2950[B]:THR:N | 2.07 | 0.88 |
| 3:C:3013[B]:ASP:HA | 3:C:3122[B]:ASN:ND2 | 1.88 | 0.88 |
| 3:I:2948[B]:ASP:OD1 | 3:I:2950[B]:THR:N | 2.07 | 0.88 |
| 3:I:2967[B]:CYS:SG | 3:R:2982[B]:MET:HG2 | 2.14 | 0.88 |
| 3:O:2997[A]:GLU:OE2 | 3:O:3009[A]:ILE:HG13 | 1.74 | 0.88 |
| 3:U:2948[A]:ASP:OD1 | 3:U:2950[A]:THR:N | 2.07 | 0.88 |
| 3:U:2957[A]:ILE:HA | 3:U:2960[A]:PHE:CE1 | 2.09 | 0.88 |
| 3:U:2965[B]:LEU:CD1 | 3:d:3220[B]:ARG:HA | 1.93 | 0.88 |
| 3:U:2988[A]:TRP:HE3 | 3:U:2989[A]:HIS:ND1 | 1.70 | 0.88 |
| 3:U:2997[B]:GLU:OE2 | 3:U:3009[B]:ILE:HG13 | 1.74 | 0.88 |
| 3:U:3222[B]:ILE:HD12 | 3:U:3223[B]:GLY:N | 1.89 | 0.88 |
| 3:a:2988[B]:TRP:HE3 | 3:a:2989[B]:HIS:ND1 | 1.70 | 0.88 |
| 3:a:3013[A]:ASP:HA | 3:a:3122[A]:ASN:ND2 | 1.88 | 0.88 |
| 3:a:3287[B]:ILE:O | 3:a:3295[B]:LEU:HA | 1.73 | 0.88 |
| 3:C:2943[B]:ALA:O | 3:C:2946[B]:GLN:HG3 | 1.74 | 0.88 |
| 3:C:3174[B]:GLY:CA | 3:L:3154[B]:PRO:CB | 2.52 | 0.88 |
| 3:F:2966[B]:SER:CA | 3:a:3256[B]:TRP:HB3 | 2.04 | 0.88 |
| 3:F:2971[B]:ASP:O | 3:a:3090[B]:ASN:CB | 2.22 | 0.88 |
| 3:F:2992[B]:TYR:HE2 | 3:a:2969[B]:TYR:HE1 | 1.21 | 0.88 |
| 3:I:2979[B]:GLN:HE21 | 3:I:3155[B]:MET:HE3 | 1.36 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:2948[B]:ASP:OD1 | 3:L:2950[B]:THR:N | 2.07 | 0.88 |
| 3:L:3222[A]:ILE:HD12 | 3:L:3223[A]:GLY:N | 1.89 | 0.88 |
| 3:O:3157[B]:PRO:C | 3:X:3152[B]:LYS:CG | 2.47 | 0.88 |
| 3:U:2948[B]:ASP:OD1 | 3:U:2950[B]:THR:N | 2.07 | 0.88 |
| 3:U:2979[A]:GLN:HE21 | 3:U:3155[A]:MET:HE3 | 1.36 | 0.88 |
| 3:U:3254[B]:MET:HB3 | 3:d:3254[B]:MET:HA | 1.28 | 0.88 |
| 3:X:2957[B]:ILE:HA | 3:X:2960[B]:PHE:CE1 | 2.09 | 0.88 |
| 3:X:3287[B]:ILE:O | 3:X:3295[B]:LEU:HA | 1.73 | 0.88 |
| 3:a:3176[A]:LYS:O | 3:a:3177[A]:SER:OG | 1.92 | 0.88 |
| 3:d:3222[A]:ILE:HD12 | 3:d:3223[A]:GLY:N | 1.89 | 0.88 |
| 1:A:119:LYS:HB3 | 1:A:120:LYS:HA | 1.54 | 0.87 |
| 3:C:3173[B]:THR:HB | 3:C:3176[B]:LYS:CG | 2.05 | 0.87 |
| 3:C:3176[A]:LYS:O | 3:C:3177[A]:SER:OG | 1.92 | 0.87 |
| 3:F:3169[B]:LYS:HZ2 | 3:a:3149[B]:ASN:HD21 | 1.22 | 0.87 |
| 3:F:3173[B]:THR:HA | 3:a:3153[B]:LYS:C | 1.98 | 0.87 |
| 3:F:3287[B]:ILE:O | 3:F:3295[B]:LEU:HA | 1.74 | 0.87 |
| 3:I:3173[B]:THR:HB | 3:I:3176[B]:LYS:CG | 2.05 | 0.87 |
| 3:L:2957[A]:ILE:HA | 3:L:2960[A]:PHE:CE1 | 2.09 | 0.87 |
| 3:L:3092[A]:ILE:O | 3:L:3096[A]:VAL:HG23 | 1.75 | 0.87 |
| 3:O:3092[B]:ILE:O | 3:O:3096[B]:VAL:HG23 | 1.74 | 0.87 |
| 3:R:2957[B]:ILE:HA | 3:R:2960[B]:PHE:CE1 | 2.09 | 0.87 |
| 3:R:3173[A]:THR:HB | 3:R:3176[A]:LYS:CG | 2.04 | 0.87 |
| 3:U:3176[A]:LYS:O | 3:U:3177[A]:SER:OG | 1.92 | 0.87 |
| 3:U:3287[B]:ILE:O | 3:U:3295[B]:LEU:HA | 1.73 | 0.87 |
| 3:a:2979[B]:GLN:CG | 3:a:3155[B]:MET:HE1 | 1.97 | 0.87 |
| 3:d:3196[A]:THR:H | 3:d:3199[A]:GLN:HB2 | 1.38 | 0.87 |
| 4:JA:1:NAG:O4 | 4:JA:2:NAG:O7 | 1.92 | 0.87 |
| 2:B:2345:ASN:H | 2:E:2515:ARG:HD3 | 1.39 | 0.87 |
| 3:C:2957[B]:ILE:HA | 3:C:2960[B]:PHE:CE1 | 2.09 | 0.87 |
| 3:C:3253[B]:GLU:HB2 | 3:L:2976[B]:ALA:H | 1.34 | 0.87 |
| 3:C:3273[B]:LEU:HB2 | 3:C:3275[B]:LEU:HD13 | 1.55 | 0.87 |
| 3:I:2943[A]:ALA:O | 3:I:2946[A]:GLN:HG3 | 1.74 | 0.87 |
| 3:I:3173[A]:THR:HB | 3:I:3176[A]:LYS:CD | 2.04 | 0.87 |
| 3:I:3173[B]:THR:OG1 | 3:R:3173[B]:THR:HG21 | 1.72 | 0.87 |
| 3:L:3217[A]:PHE:HZ | 3:L:3230[A]:PHE:CE1 | 1.89 | 0.87 |
| 3:L:3222[B]:ILE:HD12 | 3:L:3223[B]:GLY:N | 1.89 | 0.87 |
| 2:N:2800:LYS:O | 3:O:3023[A]:ILE:HD11 | 1.72 | 0.87 |
| 3:O:2976[B]:ALA:CA | 3:X:3156[B]:MET:HG2 | 2.04 | 0.87 |
| 3:O:3273[A]:LEU:HB2 | 3:O:3275[A]:LEU:HD13 | 1.55 | 0.87 |
| 3:R:2993[B]:MET:O | 3:R:2997[B]:GLU:N | 2.07 | 0.87 |
| 3:R:3013[A]:ASP:HA | 3:R:3122[A]:ASN:ND2 | 1.88 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3092[B]:ILE:O | 3:R:3096[B]:VAL:HG23 | 1.75 | 0.87 |
| 3:U:2948[B]:ASP:N | 3:U:2949[B]:LYS:HA | 1.81 | 0.87 |
| 3:U:3092[B]:ILE:O | 3:U:3096[B]:VAL:HG23 | 1.75 | 0.87 |
| 3:U:3273[B]:LEU:HB2 | 3:U:3275[B]:LEU:HD13 | 1.55 | 0.87 |
| 3:X:3173[B]:THR:HB | 3:X:3176[B]:LYS:CD | 2.04 | 0.87 |
| 3:a:2943[A]:ALA:O | 3:a:2946[A]:GLN:HG3 | 1.74 | 0.87 |
| 3:d:2943[B]:ALA:O | 3:d:2946[B]:GLN:HG3 | 1.74 | 0.87 |
| 3:d:2993[A]:MET:O | 3:d:2997[A]:GLU:N | 2.07 | 0.87 |
| 3:d:2997[B]:GLU:OE2 | 3:d:3009[B]:ILE:HG13 | 1.74 | 0.87 |
| 3:C:3225[B]:SER:O | 3:C:3290[B]:ILE:HG23 | 1.75 | 0.87 |
| 3:F:2988[A]:TRP:HE3 | 3:F:2989[A]:HIS:ND1 | 1.70 | 0.87 |
| 3:F:3196[B]:THR:H | 3:F:3199[B]:GLN:HB2 | 1.38 | 0.87 |
| 3:F:3223[B]:GLY:HA3 | 3:a:2963[B]:MET:HE1 | 1.56 | 0.87 |
| 3:O:2979[A]:GLN:CG | 3:O:3155[A]:MET:HE1 | 1.97 | 0.87 |
| 3:O:3173[B]:THR:HB | 3:O:3176[B]:LYS:CG | 2.05 | 0.87 |
| 3:U:2975[B]:PHE:CD2 | 3:d:3256[B]:TRP:CD1 | 2.55 | 0.87 |
| 3:U:3173[B]:THR:HG23 | 3:d:3152[B]:LYS:O | 1.74 | 0.87 |
| 3:U:3287[A]:ILE:O | 3:U:3295[A]:LEU:HA | 1.73 | 0.87 |
| 3:X:3013[B]:ASP:HA | 3:X:3122[B]:ASN:ND2 | 1.88 | 0.87 |
| 3:X:3176[A]:LYS:O | 3:X:3177[A]:SER:OG | 1.92 | 0.87 |
| 3:a:3092[B]:ILE:O | 3:a:3096[B]:VAL:HG23 | 1.75 | 0.87 |
| 3:d:3176[B]:LYS:O | 3:d:3177[B]:SER:OG | 1.92 | 0.87 |
| 3:C:3090[B]:ASN:HB3 | 3:L:2972[B]:GLY:CA | 1.93 | 0.87 |
| 3:C:3092[A]:ILE:O | 3:C:3096[A]:VAL:HG23 | 1.74 | 0.87 |
| 3:C:3173[A]:THR:HB | 3:C:3176[A]:LYS:CG | 2.05 | 0.87 |
| 3:C:3217[A]:PHE:HZ | 3:C:3230[A]:PHE:CE1 | 1.89 | 0.87 |
| 3:F:2970[B]:PRO:CA | 3:a:2989[B]:HIS:CD2 | 2.57 | 0.87 |
| 3:F:2997[A]:GLU:OE2 | 3:F:3009[A]:ILE:HG13 | 1.74 | 0.87 |
| 3:F:3173[B]:THR:HB | 3:F:3176[B]:LYS:CD | 2.04 | 0.87 |
| 3:F:3217[B]:PHE:HZ | 3:F:3230[B]:PHE:CE1 | 1.89 | 0.87 |
| 2:H:2797:LYS:NZ | 3:I:3028[A]:PRO:CD | 2.36 | 0.87 |
| 3:I:3092[B]:ILE:O | 3:I:3096[B]:VAL:HG23 | 1.74 | 0.87 |
| 3:I:3196[B]:THR:HB | 3:I:3198[B]:PRO:HD2 | 1.54 | 0.87 |
| 3:I:3222[B]:ILE:HD12 | 3:I:3223[B]:GLY:N | 1.89 | 0.87 |
| 3:I:3225[A]:SER:O | 3:I:3290[A]:ILE:HG23 | 1.74 | 0.87 |
| 3:I:3256[B]:TRP:HE1 | 3:R:2965[B]:LEU:CG | 1.86 | 0.87 |
| 3:L:3173[A]:THR:HB | 3:L:3176[A]:LYS:CD | 2.04 | 0.87 |
| 3:O:3038[B]:ILE:CD1 | 3:X:2969[B]:TYR:CZ | 2.57 | 0.87 |
| 3:O:3156[B]:MET:HG2 | 3:X:3173[B]:THR:CG2 | 2.04 | 0.87 |
| 3:O:3160[B]:SER:OG | 3:X:3150[B]:LYS:CB | 2.18 | 0.87 |
| 3:O:3176[A]:LYS:O | 3:O:3177[A]:SER:OG | 1.92 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3222[B]:ILE:N | 3:X:3161[B]:GLU:HB2 | 1.89 | 0.87 |
| 3:R:2965[B]:LEU:HD11 | 3:R:2974[B]:ALA:HA | 1.57 | 0.87 |
| 3:R:3176[A]:LYS:O | 3:R:3177[A]:SER:OG | 1.92 | 0.87 |
| 3:R:3225[B]:SER:O | 3:R:3290[B]:ILE:HG23 | 1.74 | 0.87 |
| 3:U:2975[B]:PHE:CD1 | 3:d:3255[B]:PRO:HA | 1.91 | 0.87 |
| 3:U:3173[B]:THR:HB | 3:U:3176[B]:LYS:CG | 2.05 | 0.87 |
| 3:X:2948[A]:ASP:OD1 | 3:X:2950[A]:THR:N | 2.07 | 0.87 |
| 3:X:2979[A]:GLN:HE21 | 3:X:3155[A]:MET:HE3 | 1.36 | 0.87 |
| 3:X:3013[A]:ASP:HA | 3:X:3122[A]:ASN:ND2 | 1.88 | 0.87 |
| 3:X:3173[A]:THR:HB | 3:X:3176[A]:LYS:CG | 2.05 | 0.87 |
| 3:X:3222[A]:ILE:HD12 | 3:X:3223[A]:GLY:N | 1.89 | 0.87 |
| 1:Y:497:GLN:HG2 | 1:Y:683:THR:HG21 | 1.57 | 0.87 |
| 3:d:2979[B]:GLN:HE21 | 3:d:3155[B]:MET:HE3 | 1.36 | 0.87 |
| 3:d:3287[A]:ILE:O | 3:d:3295[A]:LEU:HA | 1.73 | 0.87 |
| 3:C:2993[A]:MET:O | 3:C:2997[A]:GLU:N | 2.07 | 0.87 |
| 3:C:3283[A]:ILE:CG2 | 3:C:3305[A]:ILE:HD11 | 2.05 | 0.87 |
| 3:F:2968[B]:GLN:OE1 | 3:a:2981[B]:GLY:HA2 | 1.72 | 0.87 |
| 3:L:2948[A]:ASP:N | 3:L:2949[A]:LYS:HA | 1.81 | 0.87 |
| 3:L:2988[B]:TRP:HE3 | 3:L:2989[B]:HIS:ND1 | 1.70 | 0.87 |
| 3:O:2957[A]:ILE:HA | 3:O:2960[A]:PHE:CE1 | 2.09 | 0.87 |
| 3:O:2997[B]:GLU:OE2 | 3:O:3009[B]:ILE:HG13 | 1.74 | 0.87 |
| 3:O:3108[B]:HIS:HB2 | 3:X:2969[B]:TYR:O | 1.73 | 0.87 |
| 3:O:3287[B]:ILE:O | 3:O:3295[B]:LEU:HA | 1.73 | 0.87 |
| 3:U:3173[B]:THR:HB | 3:U:3176[B]:LYS:CD | 2.04 | 0.87 |
| 3:X:2993[A]:MET:O | 3:X:2997[A]:GLU:N | 2.07 | 0.87 |
| 3:X:3293[B]:LYS:CD | 3:X:3294[B]:SER:CB | 2.53 | 0.87 |
| 3:d:3173[B]:THR:HB | 3:d:3176[B]:LYS:CD | 2.04 | 0.87 |
| 3:C:2976[B]:ALA:N | 3:L:3253[B]:GLU:CB | 2.38 | 0.87 |
| 3:C:3293[B]:LYS:CD | 3:C:3294[B]:SER:CB | 2.53 | 0.87 |
| 3:F:2948[B]:ASP:OD1 | 3:F:2950[B]:THR:N | 2.07 | 0.87 |
| 3:F:3092[A]:ILE:O | 3:F:3096[A]:VAL:HG23 | 1.74 | 0.87 |
| 3:I:2933[B]:SER:HB3 | 3:I:2936[B]:GLU:HB3 | 1.57 | 0.87 |
| 3:I:2957[A]:ILE:HA | 3:I:2960[A]:PHE:CE1 | 2.09 | 0.87 |
| 3:I:3196[A]:THR:HB | 1:J:416:ASN:ND2 | 1.87 | 0.87 |
| 3:L:2943[B]:ALA:O | 3:L:2946[B]:GLN:HG3 | 1.74 | 0.87 |
| 3:L:2997[B]:GLU:OE2 | 3:L:3009[B]:ILE:HG13 | 1.74 | 0.87 |
| 3:L:3176[B]:LYS:O | 3:L:3177[B]:SER:OG | 1.92 | 0.87 |
| 3:L:3225[A]:SER:O | 3:L:3290[A]:ILE:HG23 | 1.75 | 0.87 |
| 3:L:3273[A]:LEU:HB2 | 3:L:3275[A]:LEU:HD13 | 1.55 | 0.87 |
| 3:L:3293[A]:LYS:CD | 3:L:3294[A]:SER:CB | 2.53 | 0.87 |
| 3:O:2948[A]:ASP:OD1 | 3:O:2950[A]:THR:N | 2.07 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2977[B]:CYS:N | 3:X:3154[B]:PRO:O | 2.07 | 0.87 |
| 3:O:3173[B]:THR:HB | 3:O:3176[B]:LYS:CD | 2.04 | 0.87 |
| 3:O:3176[B]:LYS:O | 3:O:3177[B]:SER:OG | 1.92 | 0.87 |
| 3:R:2943[B]:ALA:O | 3:R:2946[B]:GLN:HG3 | 1.74 | 0.87 |
| 3:R:2957[A]:ILE:HA | 3:R:2960[A]:PHE:CE1 | 2.09 | 0.87 |
| 3:R:3273[A]:LEU:HB2 | 3:R:3275[A]:LEU:HD13 | 1.55 | 0.87 |
| 3:R:3283[B]:ILE:CG2 | 3:R:3305[B]:ILE:HD11 | 2.05 | 0.87 |
| 3:R:3287[B]:ILE:O | 3:R:3295[B]:LEU:HA | 1.73 | 0.87 |
| 3:U:2965[A]:LEU:HD11 | 3:U:2974[A]:ALA:HA | 1.57 | 0.87 |
| 3:U:3173[A]:THR:HB | 3:U:3176[A]:LYS:CG | 2.05 | 0.87 |
| 3:X:2957[A]:ILE:HA | 3:X:2960[A]:PHE:CE1 | 2.10 | 0.87 |
| 3:X:3196[A]:THR:HB | 3:X:3198[A]:PRO:HD2 | 1.54 | 0.87 |
| 3:X:3225[B]:SER:O | 3:X:3290[B]:ILE:HG23 | 1.75 | 0.87 |
| 3:a:2997[A]:GLU:OE2 | 3:a:3009[A]:ILE:HG13 | 1.74 | 0.87 |
| 3:a:3173[A]:THR:HB | 3:a:3176[A]:LYS:CG | 2.05 | 0.87 |
| 3:d:2943[A]:ALA:O | 3:d:2946[A]:GLN:HG3 | 1.74 | 0.87 |
| 3:d:3173[A]:THR:HB | 3:d:3176[A]:LYS:CD | 2.04 | 0.87 |
| 3:d:3173[A]:THR:HB | 3:d:3176[A]:LYS:CG | 2.05 | 0.87 |
| 3:C:3124[A]:ASP:OD2 | 3:C:3185[A]:TYR:OH | 1.93 | 0.87 |
| 3:C:3248[B]:LEU:CD2 | 3:L:2971[B]:ASP:CG | 2.48 | 0.87 |
| 3:F:2957[B]:ILE:HA | 3:F:2960[B]:PHE:CE1 | 2.10 | 0.87 |
| 3:F:3156[B]:MET:CB | 3:a:2982[B]:MET:CG | 2.52 | 0.87 |
| 3:F:3283[B]:ILE:CG2 | 3:F:3305[B]:ILE:HD11 | 2.05 | 0.87 |
| 3:L:2965[B]:LEU:HD11 | 3:L:2974[B]:ALA:HA | 1.57 | 0.87 |
| 3:L:3092[B]:ILE:O | 3:L:3096[B]:VAL:HG23 | 1.75 | 0.87 |
| 3:L:3287[A]:ILE:O | 3:L:3295[A]:LEU:HA | 1.73 | 0.87 |
| 3:O:2948[B]:ASP:OD1 | 3:O:2950[B]:THR:N | 2.07 | 0.87 |
| 3:O:3284[A]:LYS:HD3 | 3:O:3285[A]:VAL:H | 1.39 | 0.87 |
| 1:P:550:ILE:N | 1:P:557:VAL:O | 2.07 | 0.87 |
| 3:R:2948[B]:ASP:OD1 | 3:R:2950[B]:THR:N | 2.07 | 0.87 |
| 3:R:2979[B]:GLN:HE21 | 3:R:3155[B]:MET:HE3 | 1.36 | 0.87 |
| 3:U:2965[B]:LEU:O | 3:d:3257[B]:ALA:CB | 2.18 | 0.87 |
| 3:U:3293[A]:LYS:CD | 3:U:3294[A]:SER:CB | 2.53 | 0.87 |
| 3:X:2993[B]:MET:O | 3:X:2997[B]:GLU:N | 2.07 | 0.87 |
| 3:X:2997[A]:GLU:OE2 | 3:X:3009[A]:ILE:HG13 | 1.74 | 0.87 |
| 3:X:2997[B]:GLU:OE2 | 3:X:3009[B]:ILE:HG13 | 1.74 | 0.87 |
| 1:Y:1612:THR:O | 3:d:3186[B]:GLU:CB | 2.23 | 0.87 |
| 3:a:2943[B]:ALA:O | 3:a:2946[B]:GLN:HG3 | 1.74 | 0.87 |
| 3:d:2993[B]:MET:O | 3:d:2997[B]:GLU:N | 2.07 | 0.87 |
| 3:d:3222[B]:ILE:HD12 | 3:d:3223[B]:GLY:N | 1.89 | 0.87 |
| 3:C:2935[B]:ILE:HD13 | 3:C:2936[B]:GLU:H | 1.35 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2957[A]:ILE:HA | 3:C:2960[A]:PHE:CE1 | 2.10 | 0.87 |
| 3:C:2971[B]:ASP:OD1 | 3:L:3248[B]:LEU:HD22 | 1.74 | 0.87 |
| 3:C:3013[A]:ASP:HA | 3:C:3122[A]:ASN:ND2 | 1.88 | 0.87 |
| 3:F:2956[A]:LYS:O | 3:F:2960[A]:PHE:HE1 | 1.22 | 0.87 |
| 3:F:2965[A]:LEU:HD11 | 3:F:2974[A]:ALA:HA | 1.57 | 0.87 |
| 3:F:3155[B]:MET:HB3 | 3:a:3153[B]:LYS:HD2 | 1.54 | 0.87 |
| 3:I:2933[A]:SER:HB3 | 3:I:2936[A]:GLU:HB3 | 1.57 | 0.87 |
| 3:I:2979[A]:GLN:HE21 | 3:I:3155[A]:MET:HE3 | 1.36 | 0.87 |
| 3:I:2997[A]:GLU:OE2 | 3:I:3009[A]:ILE:HG13 | 1.74 | 0.87 |
| 3:L:2993[A]:MET:O | 3:L:2997[A]:GLU:N | 2.07 | 0.87 |
| 3:L:3283[A]:ILE:CG2 | 3:L:3305[A]:ILE:HD11 | 2.05 | 0.87 |
| 3:O:3101[B]:PRO:C | 3:X:2971[B]:ASP:CA | 2.46 | 0.87 |
| 3:R:2979[A]:GLN:HE21 | 3:R:3155[A]:MET:HE3 | 1.37 | 0.87 |
| 3:R:3173[B]:THR:HB | 3:R:3176[B]:LYS:CD | 2.04 | 0.87 |
| 3:R:3225[A]:SER:O | 3:R:3290[A]:ILE:HG23 | 1.74 | 0.87 |
| 3:U:3254[B]:MET:HA | 3:d:3254[B]:MET:CA | 2.05 | 0.87 |
| 3:U:3283[B]:ILE:CG2 | 3:U:3305[B]:ILE:HD11 | 2.05 | 0.87 |
| 3:X:3196[A]:THR:H | 3:X:3199[A]:GLN:HB2 | 1.38 | 0.87 |
| 3:a:2993[B]:MET:O | 3:a:2997[B]:GLU:N | 2.06 | 0.87 |
| 3:a:3173[A]:THR:HB | 3:a:3176[A]:LYS:CD | 2.04 | 0.87 |
| 3:a:3222[A]:ILE:HD12 | 3:a:3223[A]:GLY:N | 1.89 | 0.87 |
| 3:d:3287[B]:ILE:O | 3:d:3295[B]:LEU:HA | 1.74 | 0.87 |
| 6:CA:1:NAG:H61 | 6:CA:2:NAG:C7 | 2.04 | 0.87 |
| 3:C:2948[A]:ASP:N | 3:C:2949[A]:LYS:HA | 1.81 | 0.87 |
| 3:C:3156[B]:MET:O | 3:L:3153[B]:LYS:NZ | 2.06 | 0.87 |
| 3:F:2965[B]:LEU:HD11 | 3:F:2974[B]:ALA:HA | 1.57 | 0.87 |
| 3:F:3284[A]:LYS:HD3 | 3:F:3285[A]:VAL:H | 1.39 | 0.87 |
| 3:F:3287[A]:ILE:O | 3:F:3295[A]:LEU:HA | 1.74 | 0.87 |
| 3:I:2957[B]:ILE:HA | 3:I:2960[B]:PHE:CE1 | 2.10 | 0.87 |
| 3:I:2977[B]:CYS:CB | 3:R:2982[B]:MET:HE3 | 2.05 | 0.87 |
| 3:I:3172[B]:SER:H | 3:R:3152[B]:LYS:HB2 | 0.71 | 0.87 |
| 3:I:3173[B]:THR:HB | 3:I:3176[B]:LYS:CD | 2.04 | 0.87 |
| 3:I:3176[A]:LYS:O | 3:I:3177[A]:SER:OG | 1.92 | 0.87 |
| 1:J:566:ARG:HA | 1:J:567:LEU:HD22 | 1.56 | 0.87 |
| 3:L:2933[B]:SER:HB3 | 3:L:2936[B]:GLU:HB3 | 1.57 | 0.87 |
| 3:L:3013[A]:ASP:HA | 3:L:3122[A]:ASN:ND2 | 1.88 | 0.87 |
| 3:O:2943[B]:ALA:O | 3:O:2946[B]:GLN:HG3 | 1.74 | 0.87 |
| 3:O:3013[B]:ASP:HA | 3:O:3122[B]:ASN:ND2 | 1.88 | 0.87 |
| 3:O:3092[A]:ILE:O | 3:O:3096[A]:VAL:HG23 | 1.75 | 0.87 |
| 3:R:2956[B]:LYS:O | 3:R:2960[B]:PHE:HE1 | 1.22 | 0.87 |
| 3:R:2993[A]:MET:O | 3:R:2997[A]:GLU:N | 2.07 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3173[B]:THR:HB | 3:R:3176[B]:LYS:CG | 2.05 | 0.87 |
| 3:X:2948[B]:ASP:OD1 | 3:X:2950[B]:THR:N | 2.07 | 0.87 |
| 3:X:3283[A]:ILE:CG2 | 3:X:3305[A]:ILE:HD11 | 2.05 | 0.87 |
| 1:Y:1616:LYS:HD3 | 3:d:3188[B]:ASP:H | 1.39 | 0.87 |
| 3:a:2965[A]:LEU:HD11 | 3:a:2974[A]:ALA:HA | 1.57 | 0.87 |
| 3:a:3124[A]:ASP:OD2 | 3:a:3185[A]:TYR:OH | 1.93 | 0.87 |
| 3:a:3225[A]:SER:O | 3:a:3290[A]:ILE:HG23 | 1.75 | 0.87 |
| 3:d:2933[B]:SER:HB3 | 3:d:2936[B]:GLU:HB3 | 1.57 | 0.87 |
| 3:d:2957[B]:ILE:HA | 3:d:2960[B]:PHE:CE1 | 2.09 | 0.87 |
| 3:C:2997[A]:GLU:OE2 | 3:C:3009[A]:ILE:HG13 | 1.74 | 0.86 |
| 3:C:3222[A]:ILE:HD12 | 3:C:3223[A]:GLY:N | 1.89 | 0.86 |
| 3:F:3222[A]:ILE:HD12 | 3:F:3223[A]:GLY:N | 1.89 | 0.86 |
| 3:F:3256[B]:TRP:CG | 3:a:2966[B]:SER:C | 2.53 | 0.86 |
| 3:L:2943[A]:ALA:O | 3:L:2946[A]:GLN:HG3 | 1.74 | 0.86 |
| 3:L:3176[A]:LYS:O | 3:L:3177[A]:SER:OG | 1.92 | 0.86 |
| 3:O:2933[A]:SER:HB3 | 3:O:2936[A]:GLU:HB3 | 1.57 | 0.86 |
| 3:O:2993[A]:MET:O | 3:O:2997[A]:GLU:N | 2.07 | 0.86 |
| 3:O:3173[A]:THR:HB | 3:O:3176[A]:LYS:CG | 2.04 | 0.86 |
| 3:O:3283[B]:ILE:CG2 | 3:O:3305[B]:ILE:HD11 | 2.05 | 0.86 |
| 3:U:2971[B]:ASP:O | 3:d:3248[B]:LEU:N | 2.08 | 0.86 |
| 3:U:3153[B]:LYS:HD2 | 3:d:3153[B]:LYS:CD | 2.05 | 0.86 |
| 3:U:3173[A]:THR:HB | 3:U:3176[A]:LYS:CD | 2.04 | 0.86 |
| 3:X:3092[A]:ILE:O | 3:X:3096[A]:VAL:HG23 | 1.75 | 0.86 |
| 3:a:3124[B]:ASP:OD2 | 3:a:3185[B]:TYR:OH | 1.93 | 0.86 |
| 3:a:3173[B]:THR:HB | 3:a:3176[B]:LYS:CD | 2.04 | 0.86 |
| 3:d:3013[A]:ASP:HA | 3:d:3122[A]:ASN:ND2 | 1.88 | 0.86 |
| 3:d:3225[A]:SER:O | 3:d:3290[A]:ILE:HG23 | 1.75 | 0.86 |
| 3:d:3225[B]:SER:O | 3:d:3290[B]:ILE:HG23 | 1.75 | 0.86 |
| 3:d:3283[A]:ILE:CG2 | 3:d:3305[A]:ILE:HD11 | 2.05 | 0.86 |
| 3:F:2933[A]:SER:HB3 | 3:F:2936[A]:GLU:HB3 | 1.57 | 0.86 |
| 3:F:2943[A]:ALA:O | 3:F:2946[A]:GLN:HG3 | 1.74 | 0.86 |
| 3:F:2989[A]:HIS:O | 3:F:2992[A]:TYR:N | 2.08 | 0.86 |
| 3:F:3255[B]:PRO:O | 3:a:2966[B]:SER:OG | 1.93 | 0.86 |
| 3:I:2943[B]:ALA:O | 3:I:2946[B]:GLN:HG3 | 1.74 | 0.86 |
| 3:I:2969[B]:TYR:OH | 3:R:3116[B]:PHE:HD1 | 1.33 | 0.86 |
| 3:I:3283[B]:ILE:CG2 | 3:I:3305[B]:ILE:HD11 | 2.05 | 0.86 |
| 3:L:3196[A]:THR:HB | 3:L:3198[A]:PRO:HD2 | 1.53 | 0.86 |
| 3:L:3218[A]:LEU:C | 3:L:3219[A]:LEU:HD22 | 2.01 | 0.86 |
| 3:L:3283[B]:ILE:CG2 | 3:L:3305[B]:ILE:HD11 | 2.05 | 0.86 |
| 3:O:2948[A]:ASP:N | 3:O:2949[A]:LYS:HA | 1.81 | 0.86 |
| 3:O:2989[A]:HIS:O | 3:O:2992[A]:TYR:N | 2.09 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3222[B]:ILE:HD12 | 3:O:3223[B]:GLY:N | 1.89 | 0.86 |
| 3:O:3225[B]:SER:O | 3:O:3290[B]:ILE:HG23 | 1.75 | 0.86 |
| 3:O:3287[A]:ILE:O | 3:O:3295[A]:LEU:HA | 1.73 | 0.86 |
| 3:R:2956[A]:LYS:O | 3:R:2960[A]:PHE:HE1 | 1.22 | 0.86 |
| 3:R:3222[B]:ILE:HD12 | 3:R:3223[B]:GLY:N | 1.89 | 0.86 |
| 3:R:3273[B]:LEU:HB2 | 3:R:3275[B]:LEU:HD13 | 1.55 | 0.86 |
| 3:U:2993[B]:MET:O | 3:U:2997[B]:GLU:N | 2.07 | 0.86 |
| 3:U:3092[A]:ILE:O | 3:U:3096[A]:VAL:HG23 | 1.74 | 0.86 |
| 3:U:3160[B]:SER:OG | 3:d:3259[B]:ASP:CG | 2.17 | 0.86 |
| 3:U:3225[B]:SER:O | 3:U:3290[B]:ILE:HG23 | 1.74 | 0.86 |
| 3:a:2989[A]:HIS:O | 3:a:2992[A]:TYR:N | 2.08 | 0.86 |
| 3:d:2965[B]:LEU:HD11 | 3:d:2974[B]:ALA:HA | 1.57 | 0.86 |
| 3:d:3220[B]:ARG:HH11 | 3:d:3220[B]:ARG:HG3 | 1.35 | 0.86 |
| 3:C:2948[A]:ASP:OD1 | 3:C:2950[A]:THR:N | 2.07 | 0.86 |
| 3:C:2971[B]:ASP:CG | 3:L:3248[B]:LEU:HD22 | 1.99 | 0.86 |
| 3:F:3147[B]:GLU:HG3 | 3:a:3160[B]:SER:O | 1.72 | 0.86 |
| 3:F:3161[B]:GLU:CA | 3:a:3147[B]:GLU:HG2 | 2.02 | 0.86 |
| 3:F:3173[B]:THR:HB | 3:F:3176[B]:LYS:CG | 2.04 | 0.86 |
| 3:F:3283[A]:ILE:CG2 | 3:F:3305[A]:ILE:HD11 | 2.05 | 0.86 |
| 3:I:2959[B]:SER:CA | 3:R:3255[B]:PRO:CB | 2.45 | 0.86 |
| 3:I:2965[A]:LEU:HD11 | 3:I:2974[A]:ALA:HA | 1.57 | 0.86 |
| 3:I:3221[B]:ALA:CB | 3:R:2964[B]:PRO:CA | 2.53 | 0.86 |
| 3:L:2979[A]:GLN:HE21 | 3:L:3155[A]:MET:HE3 | 1.36 | 0.86 |
| 3:O:3038[B]:ILE:HG12 | 3:X:2969[B]:TYR:HH | 1.39 | 0.86 |
| 3:O:3153[B]:LYS:CG | 3:X:3176[B]:LYS:NZ | 2.37 | 0.86 |
| 3:U:3082[B]:GLU:OE1 | 3:d:2970[B]:PRO:CB | 2.20 | 0.86 |
| 3:U:3257[B]:ALA:HB2 | 3:d:2973[B]:THR:C | 1.99 | 0.86 |
| 3:a:2952[A]:ALA:HB3 | 3:a:2953[A]:GLY:O | 1.75 | 0.86 |
| 3:d:2989[B]:HIS:O | 3:d:2992[B]:TYR:N | 2.08 | 0.86 |
| 3:d:3283[B]:ILE:CG2 | 3:d:3305[B]:ILE:HD11 | 2.05 | 0.86 |
| 3:C:2943[A]:ALA:O | 3:C:2946[A]:GLN:HG3 | 1.74 | 0.86 |
| 3:C:2965[B]:LEU:HD11 | 3:C:2974[B]:ALA:HA | 1.57 | 0.86 |
| 3:F:2983[B]:VAL:HG21 | 3:a:3161[B]:GLU:CB | 2.05 | 0.86 |
| 3:F:2983[B]:VAL:HG23 | 3:a:3160[B]:SER:CB | 2.04 | 0.86 |
| 3:F:2989[B]:HIS:O | 3:F:2992[B]:TYR:N | 2.08 | 0.86 |
| 3:I:3248[B]:LEU:CB | 3:R:2972[B]:GLY:C | 2.45 | 0.86 |
| 3:I:3283[A]:ILE:CG2 | 3:I:3305[A]:ILE:HD11 | 2.05 | 0.86 |
| 3:I:3287[A]:ILE:O | 3:I:3295[A]:LEU:HA | 1.73 | 0.86 |
| 3:L:2957[B]:ILE:HA | 3:L:2960[B]:PHE:CE1 | 2.10 | 0.86 |
| 3:L:2989[B]:HIS:O | 3:L:2992[B]:TYR:N | 2.08 | 0.86 |
| 3:L:3173[B]:THR:HB | 3:L:3176[B]:LYS:CG | 2.04 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:126:GLY:HA3 | 1:M:127:GLU:HB3 | 1.58 | 0.86 |
| 3:O:3225[A]:SER:O | 3:O:3290[A]:ILE:HG23 | 1.75 | 0.86 |
| 3:R:2989[B]:HIS:O | 3:R:2992[B]:TYR:N | 2.08 | 0.86 |
| 3:U:2943[A]:ALA:O | 3:U:2946[A]:GLN:HG3 | 1.74 | 0.86 |
| 3:U:2943[B]:ALA:O | 3:U:2946[B]:GLN:HG3 | 1.74 | 0.86 |
| 3:U:3153[B]:LYS:CD | 3:d:3153[B]:LYS:HD2 | 2.05 | 0.86 |
| 3:U:3218[B]:LEU:C | 3:U:3219[B]:LEU:HD22 | 2.01 | 0.86 |
| 2:W:2507:ARG:HA | 2:W:2779:ASP:HB2 | 1.57 | 0.86 |
| 3:X:3092[B]:ILE:O | 3:X:3096[B]:VAL:HG23 | 1.74 | 0.86 |
| 3:X:3273[B]:LEU:HB2 | 3:X:3275[B]:LEU:HD13 | 1.55 | 0.86 |
| 3:a:2948[B]:ASP:OD1 | 3:a:2950[B]:THR:N | 2.07 | 0.86 |
| 3:a:2957[A]:ILE:HA | 3:a:2960[A]:PHE:CE1 | 2.10 | 0.86 |
| 3:a:3196[B]:THR:H | 3:a:3199[B]:GLN:HB2 | 1.37 | 0.86 |
| 3:C:2933[A]:SER:HB3 | 3:C:2936[A]:GLU:HB3 | 1.57 | 0.86 |
| 3:C:2952[A]:ALA:HB3 | 3:C:2953[A]:GLY:O | 1.76 | 0.86 |
| 3:C:3024[A]:LEU:CD1 | 3:C:3025[A]:VAL:H | 1.83 | 0.86 |
| 3:C:3173[A]:THR:HB | 3:C:3176[A]:LYS:CD | 2.04 | 0.86 |
| 3:C:3222[B]:ILE:HD12 | 3:C:3223[B]:GLY:N | 1.89 | 0.86 |
| 3:F:2952[A]:ALA:HB3 | 3:F:2953[A]:GLY:O | 1.76 | 0.86 |
| 3:F:3092[B]:ILE:O | 3:F:3096[B]:VAL:HG23 | 1.75 | 0.86 |
| 3:F:3222[B]:ILE:HD12 | 3:F:3223[B]:GLY:N | 1.89 | 0.86 |
| 3:I:2989[A]:HIS:O | 3:I:2992[A]:TYR:N | 2.08 | 0.86 |
| 3:L:2948[A]:ASP:OD1 | 3:L:2950[A]:THR:N | 2.07 | 0.86 |
| 3:L:3196[A]:THR:H | 3:L:3199[A]:GLN:HB2 | 1.37 | 0.86 |
| 1:M:906:HIS:CD2 | 9:M:2104:CUO:O1 | 2.26 | 0.86 |
| 3:O:3293[A]:LYS:CD | 3:O:3294[A]:SER:CB | 2.53 | 0.86 |
| 3:R:3013[B]:ASP:HA | 3:R:3122[B]:ASN:ND2 | 1.88 | 0.86 |
| 3:R:3176[B]:LYS:O | 3:R:3177[B]:SER:OG | 1.92 | 0.86 |
| 3:R:3218[A]:LEU:C | 3:R:3219[A]:LEU:HD22 | 2.01 | 0.86 |
| 3:U:2989[A]:HIS:O | 3:U:2992[A]:TYR:N | 2.08 | 0.86 |
| 3:U:3225[A]:SER:O | 3:U:3290[A]:ILE:HG23 | 1.75 | 0.86 |
| 3:d:3092[B]:ILE:O | 3:d:3096[B]:VAL:HG23 | 1.75 | 0.86 |
| 3:d:3293[B]:LYS:CD | 3:d:3294[B]:SER:CB | 2.53 | 0.86 |
| 3:C:2967[B]:CYS:CB | 3:L:2982[B]:MET:N | 2.37 | 0.86 |
| 3:C:3093[B]:HIS:NE2 | 3:L:2969[B]:TYR:CE2 | 2.44 | 0.86 |
| 3:C:3150[B]:LYS:N | 3:L:3172[B]:SER:CB | 2.35 | 0.86 |
| 3:C:3225[A]:SER:O | 3:C:3290[A]:ILE:HG23 | 1.75 | 0.86 |
| 3:C:3253[B]:GLU:CB | 3:L:2975[B]:PHE:C | 2.43 | 0.86 |
| 3:C:3293[A]:LYS:CD | 3:C:3294[A]:SER:CB | 2.53 | 0.86 |
| 3:C:3298[B]:ASN:HB2 | 3:C:3300[B]:LEU:N | 1.78 | 0.86 |
| 1:G:456:GLN:NE2 | 1:G:549:PRO:O | 2.08 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3160[B]:SER:CA | 3:R:3150[B]:LYS:HD2 | 2.05 | 0.86 |
| 3:I:3173[A]:THR:HB | 3:I:3176[A]:LYS:CG | 2.04 | 0.86 |
| 3:I:3196[A]:THR:H | 3:I:3199[A]:GLN:HB2 | 1.37 | 0.86 |
| 3:I:3225[B]:SER:O | 3:I:3290[B]:ILE:HG23 | 1.75 | 0.86 |
| 1:J:2:LEU:HD21 | 1:J:81:VAL:HG21 | 1.57 | 0.86 |
| 3:L:2989[A]:HIS:O | 3:L:2992[A]:TYR:N | 2.08 | 0.86 |
| 3:O:3163[B]:ASN:HA | 3:X:3149[B]:ASN:HB3 | 1.55 | 0.86 |
| 3:R:2943[A]:ALA:O | 3:R:2946[A]:GLN:HG3 | 1.74 | 0.86 |
| 3:R:3173[A]:THR:HB | 3:R:3176[A]:LYS:CD | 2.04 | 0.86 |
| 3:U:3176[B]:LYS:O | 3:U:3177[B]:SER:OG | 1.92 | 0.86 |
| 3:U:3284[B]:LYS:HD3 | 3:U:3285[B]:VAL:H | 1.39 | 0.86 |
| 3:X:2943[B]:ALA:O | 3:X:2946[B]:GLN:HG3 | 1.74 | 0.86 |
| 3:X:2952[A]:ALA:HB3 | 3:X:2953[A]:GLY:O | 1.76 | 0.86 |
| 3:X:3173[B]:THR:HB | 3:X:3176[B]:LYS:CG | 2.04 | 0.86 |
| 3:a:2997[B]:GLU:OE2 | 3:a:3009[B]:ILE:HG13 | 1.74 | 0.86 |
| 3:a:3092[A]:ILE:O | 3:a:3096[A]:VAL:HG23 | 1.75 | 0.86 |
| 3:a:3225[B]:SER:O | 3:a:3290[B]:ILE:HG23 | 1.75 | 0.86 |
| 3:d:2948[A]:ASP:OD1 | 3:d:2950[A]:THR:N | 2.07 | 0.86 |
| 3:d:2952[A]:ALA:HB3 | 3:d:2953[A]:GLY:O | 1.76 | 0.86 |
| 3:d:2957[A]:ILE:HA | 3:d:2960[A]:PHE:CE1 | 2.09 | 0.86 |
| 3:C:2989[B]:HIS:O | 3:C:2992[B]:TYR:N | 2.08 | 0.86 |
| 3:C:3196[B]:THR:H | 3:C:3199[B]:GLN:HB2 | 1.38 | 0.86 |
| 3:C:3253[B]:GLU:HA | 3:L:3253[B]:GLU:HA | 1.57 | 0.86 |
| 3:F:2957[A]:ILE:HA | 3:F:2960[A]:PHE:CE1 | 2.10 | 0.86 |
| 3:F:2965[B]:LEU:HB3 | 3:a:3256[B]:TRP:NE1 | 1.89 | 0.86 |
| 3:F:3161[B]:GLU:CB | 3:a:3079[B]:CYS:SG | 2.63 | 0.86 |
| 3:F:3225[B]:SER:O | 3:F:3290[B]:ILE:HG23 | 1.74 | 0.86 |
| 3:I:3248[B]:LEU:HD11 | 3:R:2973[B]:THR:HG23 | 1.57 | 0.86 |
| 3:I:3257[B]:ALA:HB3 | 3:R:2956[B]:LYS:HD2 | 1.58 | 0.86 |
| 3:O:2957[B]:ILE:HA | 3:O:2960[B]:PHE:CE1 | 2.10 | 0.86 |
| 3:O:2970[B]:PRO:HB2 | 3:X:2990[B]:ARG:C | 1.81 | 0.86 |
| 3:O:3160[B]:SER:CB | 3:X:3149[B]:ASN:OD1 | 2.20 | 0.86 |
| 3:O:3251[B]:ASP:CB | 3:X:2968[B]:GLN:OE1 | 2.23 | 0.86 |
| 3:U:2957[B]:ILE:HA | 3:U:2960[B]:PHE:CE1 | 2.10 | 0.86 |
| 3:U:3255[B]:PRO:CD | 3:d:3252[B]:TYR:C | 2.47 | 0.86 |
| 3:a:3173[B]:THR:HB | 3:a:3176[B]:LYS:CG | 2.05 | 0.86 |
| 3:d:3092[A]:ILE:O | 3:d:3096[A]:VAL:HG23 | 1.75 | 0.86 |
| 2:B:2394:VAL:H | 2:B:2448:THR:HG22 | 1.41 | 0.86 |
| 3:C:3156[B]:MET:HB3 | 3:L:2982[B]:MET:CB | 1.96 | 0.86 |
| 3:C:3252[B]:TYR:CB | 3:L:3253[B]:GLU:HB3 | 1.99 | 0.86 |
| 3:F:3173[A]:THR:HB | 3:F:3176[A]:LYS:CG | 2.05 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3284[B]:LYS:HD3 | 3:I:3285[B]:VAL:H | 1.39 | 0.86 |
| 1:J:329:ARG:HB2 | 1:M:1583:CYS:H | 1.39 | 0.86 |
| 3:L:3287[B]:ILE:O | 3:L:3295[B]:LEU:HA | 1.73 | 0.86 |
| 1:M:1427:HIS:HD1 | 1:M:1461:VAL:HG21 | 1.38 | 0.86 |
| 3:O:3217[A]:PHE:HZ | 3:O:3230[A]:PHE:CE1 | 1.89 | 0.86 |
| 3:R:3124[B]:ASP:OD2 | 3:R:3185[B]:TYR:OH | 1.93 | 0.86 |
| 3:R:3217[A]:PHE:HZ | 3:R:3230[A]:PHE:CE1 | 1.89 | 0.86 |
| 3:R:3218[B]:LEU:C | 3:R:3219[B]:LEU:HD22 | 2.01 | 0.86 |
| 3:U:3124[A]:ASP:OD2 | 3:U:3185[A]:TYR:OH | 1.93 | 0.86 |
| 3:U:3156[B]:MET:HE3 | 3:d:2982[B]:MET:SD | 1.46 | 0.86 |
| 3:X:3196[B]:THR:H | 3:X:3199[B]:GLN:HB2 | 1.38 | 0.86 |
| 1:Y:1546:LYS:HG2 | 3:d:3001[B]:LYS:HE3 | 1.52 | 0.86 |
| 3:a:2933[B]:SER:HB3 | 3:a:2936[B]:GLU:HB3 | 1.57 | 0.86 |
| 3:a:3222[B]:ILE:HD12 | 3:a:3223[B]:GLY:N | 1.89 | 0.86 |
| 3:d:2933[A]:SER:HB3 | 3:d:2936[A]:GLU:HB3 | 1.57 | 0.86 |
| 3:d:2965[A]:LEU:HD11 | 3:d:2974[A]:ALA:HA | 1.57 | 0.86 |
| 3:d:3173[B]:THR:HB | 3:d:3176[B]:LYS:CG | 2.05 | 0.86 |
| 3:C:2983[B]:VAL:CG2 | 3:L:3160[B]:SER:OG | 2.23 | 0.86 |
| 3:C:3154[B]:PRO:HD3 | 3:L:3173[B]:THR:C | 2.01 | 0.86 |
| 3:C:3218[A]:LEU:C | 3:C:3219[A]:LEU:HD22 | 2.01 | 0.86 |
| 3:C:3218[B]:LEU:C | 3:C:3219[B]:LEU:HD22 | 2.01 | 0.86 |
| 3:F:3176[B]:LYS:O | 3:F:3177[B]:SER:OG | 1.92 | 0.86 |
| 3:F:3225[A]:SER:O | 3:F:3290[A]:ILE:HG23 | 1.75 | 0.86 |
| 3:I:2948[A]:ASP:OD1 | 3:I:2950[A]:THR:N | 2.07 | 0.86 |
| 3:L:3218[B]:LEU:C | 3:L:3219[B]:LEU:HD22 | 2.01 | 0.86 |
| 3:L:3293[B]:LYS:CD | 3:L:3294[B]:SER:CB | 2.53 | 0.86 |
| 3:O:2933[B]:SER:HB3 | 3:O:2936[B]:GLU:HB3 | 1.57 | 0.86 |
| 3:O:3218[A]:LEU:C | 3:O:3219[A]:LEU:HD22 | 2.01 | 0.86 |
| 3:O:3298[A]:ASN:HA | 3:O:3299[A]:LEU:CB | 2.06 | 0.86 |
| 3:O:3298[B]:ASN:HB2 | 3:O:3300[B]:LEU:N | 1.78 | 0.86 |
| 1:P:1140:ASN:ND2 | 1:P:1236:TYR:OH | 2.09 | 0.86 |
| 3:R:3298[A]:ASN:HA | 3:R:3299[A]:LEU:CB | 2.06 | 0.86 |
| 3:X:2952[B]:ALA:HA | 3:X:2956[B]:LYS:CB | 2.06 | 0.86 |
| 3:X:2989[A]:HIS:O | 3:X:2992[A]:TYR:N | 2.08 | 0.86 |
| 3:X:3176[B]:LYS:O | 3:X:3177[B]:SER:OG | 1.92 | 0.86 |
| 3:X:3225[A]:SER:O | 3:X:3290[A]:ILE:HG23 | 1.74 | 0.86 |
| 3:a:2956[A]:LYS:O | 3:a:2960[A]:PHE:HE1 | 1.22 | 0.86 |
| 3:a:2957[B]:ILE:HA | 3:a:2960[B]:PHE:CE1 | 2.10 | 0.86 |
| 3:a:2965[B]:LEU:HD11 | 3:a:2974[B]:ALA:HA | 1.57 | 0.86 |
| 3:a:3283[A]:ILE:CG2 | 3:a:3305[A]:ILE:HD11 | 2.05 | 0.86 |
| 3:d:2948[A]:ASP:N | 3:d:2949[A]:LYS:HA | 1.81 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2933[B]:SER:HB3 | 3:C:2936[B]:GLU:HB3 | 1.57 | 0.86 |
| 3:F:2969[B]:TYR:CD1 | 3:a:2961[B]:HIS:ND1 | 2.13 | 0.86 |
| 3:F:3176[A]:LYS:O | 3:F:3177[A]:SER:OG | 1.92 | 0.86 |
| 3:F:3218[B]:LEU:C | 3:F:3219[B]:LEU:HD22 | 2.01 | 0.86 |
| 3:I:2997[B]:GLU:OE2 | 3:I:3009[B]:ILE:HG13 | 1.74 | 0.86 |
| 3:I:3153[B]:LYS:HB3 | 3:R:3155[B]:MET:HB2 | 1.56 | 0.86 |
| 3:I:3154[B]:PRO:CG | 3:R:3174[B]:GLY:HA2 | 2.05 | 0.86 |
| 3:I:3162[B]:ASP:HA | 3:R:3259[B]:ASP:HB3 | 1.58 | 0.86 |
| 3:I:3284[A]:LYS:HD3 | 3:I:3285[A]:VAL:H | 1.39 | 0.86 |
| 3:L:3225[B]:SER:O | 3:L:3290[B]:ILE:HG23 | 1.74 | 0.86 |
| 3:O:2989[B]:HIS:O | 3:O:2992[B]:TYR:N | 2.08 | 0.86 |
| 3:O:3172[B]:SER:HB3 | 3:X:3152[B]:LYS:HE2 | 1.58 | 0.86 |
| 3:O:3196[B]:THR:HB | 3:O:3198[B]:PRO:HD2 | 1.54 | 0.86 |
| 3:R:2952[B]:ALA:HB3 | 3:R:2953[B]:GLY:O | 1.76 | 0.86 |
| 3:R:3124[A]:ASP:OD2 | 3:R:3185[A]:TYR:OH | 1.93 | 0.86 |
| 3:U:3169[B]:LYS:CE | 3:d:3147[B]:GLU:CA | 2.52 | 0.86 |
| 3:X:2933[B]:SER:HB3 | 3:X:2936[B]:GLU:HB3 | 1.57 | 0.86 |
| 3:X:2965[A]:LEU:HD11 | 3:X:2974[A]:ALA:HA | 1.57 | 0.86 |
| 3:X:3218[A]:LEU:C | 3:X:3219[A]:LEU:HD22 | 2.01 | 0.86 |
| 3:C:2952[B]:ALA:HA | 3:C:2956[B]:LYS:CB | 2.06 | 0.85 |
| 3:C:2982[B]:MET:SD | 3:L:3157[B]:PRO:CA | 2.63 | 0.85 |
| 3:C:2997[B]:GLU:OE2 | 3:C:3009[B]:ILE:HG13 | 1.74 | 0.85 |
| 3:C:3079[B]:CYS:SG | 3:L:3161[B]:GLU:HB3 | 2.16 | 0.85 |
| 2:E:2800:LYS:O | 3:F:3023[A]:ILE:HD11 | 1.73 | 0.85 |
| 3:F:2983[B]:VAL:HG23 | 3:a:3161[B]:GLU:N | 1.90 | 0.85 |
| 3:F:3153[B]:LYS:NZ | 3:a:3156[B]:MET:C | 2.33 | 0.85 |
| 3:F:3155[B]:MET:SD | 3:a:3154[B]:PRO:HG2 | 2.16 | 0.85 |
| 3:F:3293[B]:LYS:CD | 3:F:3294[B]:SER:CB | 2.53 | 0.85 |
| 3:L:2952[B]:ALA:HA | 3:L:2956[B]:LYS:CB | 2.06 | 0.85 |
| 3:L:2965[A]:LEU:HD11 | 3:L:2974[A]:ALA:HA | 1.57 | 0.85 |
| 3:O:3218[B]:LEU:C | 3:O:3219[B]:LEU:HD22 | 2.01 | 0.85 |
| 3:R:2997[A]:GLU:OE2 | 3:R:3009[A]:ILE:HG13 | 1.74 | 0.85 |
| 3:U:2971[B]:ASP:CA | 3:d:3090[B]:ASN:ND2 | 2.22 | 0.85 |
| 3:U:2997[A]:GLU:OE2 | 3:U:3009[A]:ILE:HG13 | 1.74 | 0.85 |
| 3:U:3273[A]:LEU:HB2 | 3:U:3275[A]:LEU:HD13 | 1.55 | 0.85 |
| 3:X:3222[B]:ILE:HD12 | 3:X:3223[B]:GLY:N | 1.89 | 0.85 |
| 3:X:3298[A]:ASN:HA | 3:X:3299[A]:LEU:CB | 2.06 | 0.85 |
| 3:d:2989[A]:HIS:O | 3:d:2992[A]:TYR:N | 2.08 | 0.85 |
| 3:d:3124[A]:ASP:OD2 | 3:d:3185[A]:TYR:OH | 1.93 | 0.85 |
| 3:C:3090[B]:ASN:CB | 3:L:2972[B]:GLY:CA | 2.52 | 0.85 |
| 1:D:497:GLN:HG2 | 1:D:683:THR:HG21 | 1.56 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3256[B]:TRP:CB | 3:a:2966[B]:SER:CA | 2.36 | 0.85 |
| 3:I:2977[B]:CYS:SG | 3:R:2979[B]:GLN:HA | 2.15 | 0.85 |
| 3:I:3151[B]:LEU:H | 3:R:3169[B]:LYS:HG2 | 1.40 | 0.85 |
| 3:I:3153[B]:LYS:NZ | 3:R:3157[B]:PRO:CD | 2.38 | 0.85 |
| 3:I:3218[B]:LEU:C | 3:I:3219[B]:LEU:HD22 | 2.01 | 0.85 |
| 3:O:3156[B]:MET:HG3 | 3:X:3173[B]:THR:HG23 | 1.58 | 0.85 |
| 3:O:3222[A]:ILE:HD12 | 3:O:3223[A]:GLY:N | 1.89 | 0.85 |
| 1:P:1033:LEU:HA | 1:P:1036:SER:HB3 | 1.55 | 0.85 |
| 3:R:2956[A]:LYS:C | 3:R:2960[A]:PHE:CE1 | 2.47 | 0.85 |
| 3:R:2965[A]:LEU:HD11 | 3:R:2974[A]:ALA:HA | 1.57 | 0.85 |
| 3:R:3298[B]:ASN:HA | 3:R:3299[B]:LEU:CB | 2.06 | 0.85 |
| 3:U:2933[A]:SER:HB3 | 3:U:2936[A]:GLU:HB3 | 1.57 | 0.85 |
| 3:U:2965[B]:LEU:CD2 | 3:d:3220[B]:ARG:HH11 | 1.88 | 0.85 |
| 3:U:2989[B]:HIS:O | 3:U:2992[B]:TYR:N | 2.08 | 0.85 |
| 3:X:2948[B]:ASP:CB | 3:X:2953[B]:GLY:HA3 | 2.07 | 0.85 |
| 3:a:2993[A]:MET:O | 3:a:2997[A]:GLU:N | 2.07 | 0.85 |
| 3:d:3284[A]:LYS:HD3 | 3:d:3285[A]:VAL:H | 1.39 | 0.85 |
| 3:d:3298[A]:ASN:HA | 3:d:3299[A]:LEU:CB | 2.06 | 0.85 |
| 3:C:3173[B]:THR:HB | 3:C:3176[B]:LYS:CD | 2.04 | 0.85 |
| 3:C:3283[B]:ILE:CG2 | 3:C:3305[B]:ILE:HD11 | 2.05 | 0.85 |
| 1:D:567:LEU:HB2 | 1:D:609:TRP:CD1 | 2.10 | 0.85 |
| 3:F:3256[B]:TRP:CA | 3:a:2966[B]:SER:HA | 2.06 | 0.85 |
| 3:I:2948[B]:ASP:N | 3:I:2949[B]:LYS:HA | 1.81 | 0.85 |
| 3:I:3163[B]:ASN:CG | 3:R:3149[B]:ASN:HD22 | 1.82 | 0.85 |
| 3:I:3255[B]:PRO:CB | 3:R:2959[B]:SER:CB | 2.49 | 0.85 |
| 3:L:2952[A]:ALA:HB3 | 3:L:2953[A]:GLY:O | 1.76 | 0.85 |
| 3:L:3173[A]:THR:HB | 3:L:3176[A]:LYS:CG | 2.05 | 0.85 |
| 3:O:3283[A]:ILE:CG2 | 3:O:3305[A]:ILE:HD11 | 2.05 | 0.85 |
| 3:R:3092[A]:ILE:O | 3:R:3096[A]:VAL:HG23 | 1.75 | 0.85 |
| 3:X:2943[A]:ALA:O | 3:X:2946[A]:GLN:HG3 | 1.74 | 0.85 |
| 3:X:3124[A]:ASP:OD2 | 3:X:3185[A]:TYR:OH | 1.93 | 0.85 |
| 3:X:3217[B]:PHE:HZ | 3:X:3230[B]:PHE:CE1 | 1.89 | 0.85 |
| 3:X:3293[A]:LYS:CD | 3:X:3294[A]:SER:CB | 2.53 | 0.85 |
| 3:a:2952[B]:ALA:HB3 | 3:a:2953[B]:GLY:O | 1.76 | 0.85 |
| 3:a:3217[B]:PHE:HZ | 3:a:3230[B]:PHE:CE1 | 1.89 | 0.85 |
| 3:a:3298[B]:ASN:HA | 3:a:3299[B]:LEU:CB | 2.06 | 0.85 |
| 3:d:2948[B]:ASP:CB | 3:d:2953[B]:GLY:HA3 | 2.07 | 0.85 |
| 3:d:3124[B]:ASP:OD2 | 3:d:3185[B]:TYR:OH | 1.93 | 0.85 |
| 3:C:3153[B]:LYS:HE3 | 3:L:3158[B]:PHE:CD2 | 2.10 | 0.85 |
| 3:F:3124[B]:ASP:OD2 | 3:F:3185[B]:TYR:OH | 1.93 | 0.85 |
| 3:I:3092[A]:ILE:O | 3:I:3096[A]:VAL:HG23 | 1.74 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3124[B]:ASP:OD2 | 3:L:3185[B]:TYR:OH | 1.93 | 0.85 |
| 3:L:3196[B]:THR:H | 3:L:3199[B]:GLN:HB2 | 1.38 | 0.85 |
| 3:R:2989[A]:HIS:O | 3:R:2992[A]:TYR:N | 2.08 | 0.85 |
| 3:R:2997[B]:GLU:OE2 | 3:R:3009[B]:ILE:HG13 | 1.74 | 0.85 |
| 3:U:3283[A]:ILE:CG2 | 3:U:3305[A]:ILE:HD11 | 2.05 | 0.85 |
| 3:U:3284[A]:LYS:HD3 | 3:U:3285[A]:VAL:H | 1.39 | 0.85 |
| 3:X:3298[B]:ASN:HA | 3:X:3299[B]:LEU:CB | 2.06 | 0.85 |
| 3:a:2952[A]:ALA:HA | 3:a:2956[A]:LYS:CB | 2.06 | 0.85 |
| 3:a:2989[B]:HIS:O | 3:a:2992[B]:TYR:N | 2.08 | 0.85 |
| 3:a:3176[B]:LYS:O | 3:a:3177[B]:SER:OG | 1.92 | 0.85 |
| 3:F:2985[B]:PHE:HZ | 3:a:2970[B]:PRO:HA | 1.37 | 0.85 |
| 3:F:3159[B]:SER:OG | 3:a:2984[B]:THR:CG2 | 2.11 | 0.85 |
| 3:F:3256[B]:TRP:CB | 3:a:2966[B]:SER:O | 2.24 | 0.85 |
| 3:I:3124[B]:ASP:OD2 | 3:I:3185[B]:TYR:OH | 1.93 | 0.85 |
| 3:I:3176[B]:LYS:O | 3:I:3177[B]:SER:OG | 1.92 | 0.85 |
| 1:J:1427:HIS:CE1 | 1:J:1458:HIS:NE2 | 2.43 | 0.85 |
| 3:L:3089[A]:HIS:ND1 | 3:L:3119[A]:HIS:NE2 | 2.25 | 0.85 |
| 3:L:3124[A]:ASP:OD2 | 3:L:3185[A]:TYR:OH | 1.93 | 0.85 |
| 3:L:3298[A]:ASN:HA | 3:L:3299[A]:LEU:CB | 2.06 | 0.85 |
| 3:R:2952[B]:ALA:HA | 3:R:2956[B]:LYS:CB | 2.06 | 0.85 |
| 1:V:456:GLN:HG2 | 1:V:551:GLU:HB2 | 1.58 | 0.85 |
| 3:d:2952[B]:ALA:HA | 3:d:2956[B]:LYS:CB | 2.06 | 0.85 |
| 3:d:3089[B]:HIS:ND1 | 3:d:3119[B]:HIS:NE2 | 2.25 | 0.85 |
| 3:C:2978[B]:CYS:H | 3:L:3254[B]:MET:HB3 | 1.02 | 0.85 |
| 3:C:2989[A]:HIS:O | 3:C:2992[A]:TYR:N | 2.08 | 0.85 |
| 3:C:3124[B]:ASP:OD2 | 3:C:3185[B]:TYR:OH | 1.93 | 0.85 |
| 3:C:3176[B]:LYS:O | 3:C:3177[B]:SER:OG | 1.92 | 0.85 |
| 3:F:3124[A]:ASP:OD2 | 3:F:3185[A]:TYR:OH | 1.93 | 0.85 |
| 3:F:3174[B]:GLY:N | 3:a:3154[B]:PRO:CD | 2.40 | 0.85 |
| 3:I:2956[B]:LYS:O | 3:I:2960[B]:PHE:HE1 | 1.22 | 0.85 |
| 3:I:3150[B]:LYS:HE3 | 3:R:3163[B]:ASN:HB2 | 0.87 | 0.85 |
| 3:I:3218[A]:LEU:C | 3:I:3219[A]:LEU:HD22 | 2.01 | 0.85 |
| 3:L:2948[B]:ASP:CB | 3:L:2953[B]:GLY:HA3 | 2.07 | 0.85 |
| 1:M:497:GLN:HG2 | 1:M:683:THR:HG21 | 1.57 | 0.85 |
| 3:O:2965[B]:LEU:N | 3:X:3254[B]:MET:HE1 | 1.92 | 0.85 |
| 3:O:2967[B]:CYS:SG | 3:X:3153[B]:LYS:CB | 2.53 | 0.85 |
| 3:O:2970[B]:PRO:CB | 3:X:2990[B]:ARG:C | 2.44 | 0.85 |
| 3:O:3298[B]:ASN:HA | 3:O:3299[B]:LEU:CB | 2.06 | 0.85 |
| 3:R:2933[A]:SER:HB3 | 3:R:2936[A]:GLU:HB3 | 1.57 | 0.85 |
| 3:R:3283[A]:ILE:CG2 | 3:R:3305[A]:ILE:HD11 | 2.05 | 0.85 |
| 3:U:3154[B]:PRO:C | 3:d:3150[B]:LYS:HG2 | 2.02 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3298[B]:ASN:HA | 3:U:3299[B]:LEU:CB | 2.06 | 0.85 |
| 1:Y:1546:LYS:HG3 | 3:d:3001[B]:LYS:HG3 | 1.56 | 0.85 |
| 2:Z:2344:LEU:HD13 | 2:c:2515:ARG:HA | 1.57 | 0.85 |
| 3:d:3089[A]:HIS:ND1 | 3:d:3119[A]:HIS:NE2 | 2.25 | 0.85 |
| 3:F:2952[A]:ALA:HA | 3:F:2956[A]:LYS:CB | 2.06 | 0.85 |
| 3:F:3218[A]:LEU:C | 3:F:3219[A]:LEU:HD22 | 2.01 | 0.85 |
| 3:F:3298[B]:ASN:HA | 3:F:3299[B]:LEU:CB | 2.06 | 0.85 |
| 2:H:2797:LYS:HZ1 | 3:I:3028[A]:PRO:CD | 1.89 | 0.85 |
| 3:I:3150[B]:LYS:HB3 | 3:R:3160[B]:SER:N | 1.90 | 0.85 |
| 3:O:2952[A]:ALA:HA | 3:O:2956[A]:LYS:CB | 2.06 | 0.85 |
| 3:O:3038[B]:ILE:CD1 | 3:X:2969[B]:TYR:CE2 | 2.54 | 0.85 |
| 3:O:3124[B]:ASP:OD2 | 3:O:3185[B]:TYR:OH | 1.93 | 0.85 |
| 3:R:2952[A]:ALA:HA | 3:R:2956[A]:LYS:CB | 2.06 | 0.85 |
| 3:a:3218[B]:LEU:C | 3:a:3219[B]:LEU:HD22 | 2.01 | 0.85 |
| 3:a:3283[B]:ILE:CG2 | 3:a:3305[B]:ILE:HD11 | 2.05 | 0.85 |
| 3:C:2948[B]:ASP:CB | 3:C:2953[B]:GLY:HA3 | 2.07 | 0.85 |
| 3:C:3092[B]:ILE:O | 3:C:3096[B]:VAL:HG23 | 1.75 | 0.85 |
| 3:C:3149[B]:ASN:CG | 3:L:3163[B]:ASN:ND2 | 2.32 | 0.85 |
| 3:C:3172[B]:SER:OG | 3:L:3152[B]:LYS:CG | 2.24 | 0.85 |
| 3:C:3258[B]:PHE:CZ | 3:L:2968[B]:GLN:CD | 2.54 | 0.85 |
| 3:I:2952[B]:ALA:HB3 | 3:I:2953[B]:GLY:O | 1.76 | 0.85 |
| 3:I:2989[B]:HIS:O | 3:I:2992[B]:TYR:N | 2.09 | 0.85 |
| 3:I:3163[B]:ASN:H | 3:R:3147[B]:GLU:CD | 1.85 | 0.85 |
| 3:I:3251[B]:ASP:C | 3:R:3252[B]:TYR:HB2 | 2.00 | 0.85 |
| 3:L:2952[A]:ALA:HA | 3:L:2956[A]:LYS:CB | 2.06 | 0.85 |
| 3:O:2933[B]:SER:CB | 3:O:2936[B]:GLU:HB3 | 2.07 | 0.85 |
| 3:O:2948[A]:ASP:CB | 3:O:2953[A]:GLY:HA3 | 2.07 | 0.85 |
| 3:O:3254[B]:MET:HE3 | 3:X:3172[B]:SER:CB | 2.06 | 0.85 |
| 3:R:2948[B]:ASP:N | 3:R:2949[B]:LYS:HA | 1.81 | 0.85 |
| 3:U:2952[A]:ALA:HB3 | 3:U:2953[A]:GLY:O | 1.76 | 0.85 |
| 3:U:3257[B]:ALA:N | 3:d:2969[B]:TYR:N | 2.24 | 0.85 |
| 3:U:3293[B]:LYS:CD | 3:U:3294[B]:SER:CB | 2.53 | 0.85 |
| 3:X:2933[A]:SER:HB3 | 3:X:2936[A]:GLU:HB3 | 1.57 | 0.85 |
| 3:X:2933[B]:SER:CB | 3:X:2936[B]:GLU:HB3 | 2.07 | 0.85 |
| 3:a:2948[A]:ASP:CB | 3:a:2953[A]:GLY:HA3 | 2.07 | 0.85 |
| 3:a:3089[A]:HIS:ND1 | 3:a:3119[A]:HIS:NE2 | 2.25 | 0.85 |
| 3:a:3185[B]:TYR:CE2 | 3:a:3187[B]:TYR:CE2 | 2.65 | 0.85 |
| 3:a:3218[A]:LEU:C | 3:a:3219[A]:LEU:HD22 | 2.01 | 0.85 |
| 3:d:2948[B]:ASP:N | 3:d:2949[B]:LYS:HA | 1.81 | 0.85 |
| 3:C:2933[B]:SER:CB | 3:C:2936[B]:GLU:HB3 | 2.07 | 0.85 |
| 3:C:3149[B]:ASN:O | 3:L:3168[B]:THR:C | 2.12 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3156[B]:MET:SD | 3:L:2979[B]:GLN:HG3 | 2.17 | 0.85 |
| 3:C:3185[A]:TYR:CE2 | 3:C:3187[A]:TYR:CE2 | 2.65 | 0.85 |
| 3:I:3173[B]:THR:C | 3:R:3154[B]:PRO:N | 2.35 | 0.85 |
| 3:L:2933[A]:SER:HB3 | 3:L:2936[A]:GLU:HB3 | 1.57 | 0.85 |
| 2:N:2556:TYR:HE1 | 2:N:2845:PRO:HD2 | 1.38 | 0.85 |
| 3:O:2952[A]:ALA:HB3 | 3:O:2953[A]:GLY:O | 1.76 | 0.85 |
| 3:O:2956[B]:LYS:C | 3:O:2960[B]:PHE:CE1 | 2.47 | 0.85 |
| 3:O:2976[B]:ALA:H | 3:X:3156[B]:MET:HG2 | 1.10 | 0.85 |
| 3:O:3169[B]:LYS:HG3 | 3:X:3148[B]:ILE:HG21 | 1.04 | 0.85 |
| 3:R:3089[A]:HIS:ND1 | 3:R:3119[A]:HIS:NE2 | 2.25 | 0.85 |
| 3:R:3185[B]:TYR:CE2 | 3:R:3187[B]:TYR:CE2 | 2.65 | 0.85 |
| 3:U:2952[B]:ALA:HB3 | 3:U:2953[B]:GLY:O | 1.76 | 0.85 |
| 3:U:3185[B]:TYR:CE2 | 3:U:3187[B]:TYR:CE2 | 2.65 | 0.85 |
| 3:X:3089[B]:HIS:ND1 | 3:X:3119[B]:HIS:NE2 | 2.25 | 0.85 |
| 3:X:3124[B]:ASP:OD2 | 3:X:3185[B]:TYR:OH | 1.93 | 0.85 |
| 3:X:3283[B]:ILE:CG2 | 3:X:3305[B]:ILE:HD11 | 2.05 | 0.85 |
| 2:c:2549:PRO:HD2 | 2:c:2554:PRO:HB3 | 1.57 | 0.85 |
| 3:d:2952[A]:ALA:HA | 3:d:2956[A]:LYS:CB | 2.06 | 0.85 |
| 3:d:3218[B]:LEU:C | 3:d:3219[B]:LEU:HD22 | 2.01 | 0.85 |
| 3:F:2952[B]:ALA:HB3 | 3:F:2953[B]:GLY:O | 1.76 | 0.85 |
| 3:F:3162[B]:ASP:HB3 | 3:a:3259[B]:ASP:CA | 2.07 | 0.85 |
| 3:F:3174[B]:GLY:HA3 | 3:a:3154[B]:PRO:CB | 2.03 | 0.85 |
| 3:I:2933[A]:SER:CB | 3:I:2936[A]:GLU:HB3 | 2.07 | 0.85 |
| 3:I:2965[B]:LEU:CD1 | 3:R:3256[B]:TRP:HE1 | 1.88 | 0.85 |
| 3:I:2969[B]:TYR:C | 3:R:2989[B]:HIS:NE2 | 2.35 | 0.85 |
| 3:I:3124[A]:ASP:OD2 | 3:I:3185[A]:TYR:OH | 1.93 | 0.85 |
| 3:L:2952[B]:ALA:HB3 | 3:L:2953[B]:GLY:O | 1.76 | 0.85 |
| 3:L:3298[B]:ASN:HA | 3:L:3299[B]:LEU:CB | 2.06 | 0.85 |
| 3:O:3169[B]:LYS:HB2 | 3:X:3148[B]:ILE:HG21 | 1.57 | 0.85 |
| 3:O:3185[B]:TYR:CE2 | 3:O:3187[B]:TYR:CE2 | 2.65 | 0.85 |
| 3:O:3293[B]:LYS:CD | 3:O:3294[B]:SER:CB | 2.53 | 0.85 |
| 3:R:3284[A]:LYS:HD3 | 3:R:3285[A]:VAL:H | 1.40 | 0.85 |
| 3:U:2933[B]:SER:HB3 | 3:U:2936[B]:GLU:HB3 | 1.57 | 0.85 |
| 3:U:2965[B]:LEU:HA | 3:d:3220[B]:ARG:NH1 | 1.92 | 0.85 |
| 3:U:3152[B]:LYS:C | 3:d:3152[B]:LYS:O | 2.19 | 0.85 |
| 3:U:3256[B]:TRP:HD1 | 3:d:2975[B]:PHE:CE1 | 1.93 | 0.85 |
| 3:X:2952[A]:ALA:HA | 3:X:2956[A]:LYS:CB | 2.06 | 0.85 |
| 3:X:3089[A]:HIS:ND1 | 3:X:3119[A]:HIS:NE2 | 2.25 | 0.85 |
| 3:X:3218[B]:LEU:C | 3:X:3219[B]:LEU:HD22 | 2.01 | 0.85 |
| 3:d:2952[B]:ALA:HB3 | 3:d:2953[B]:GLY:O | 1.76 | 0.85 |
| 3:d:3176[A]:LYS:O | 3:d:3177[A]:SER:OG | 1.92 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3218[A]:LEU:C | 3:d:3219[A]:LEU:HD22 | 2.01 | 0.85 |
| 4:MA:1:NAG:H61 | 4:MA:2:NAG:C1 | 2.07 | 0.85 |
| 3:C:3149[B]:ASN:C | 3:L:3172[B]:SER:HB3 | 2.02 | 0.84 |
| 3:C:3173[B]:THR:OG1 | 3:L:3152[B]:LYS:CA | 2.24 | 0.84 |
| 3:C:3185[B]:TYR:CE2 | 3:C:3187[B]:TYR:CE2 | 2.65 | 0.84 |
| 3:C:3298[B]:ASN:HA | 3:C:3299[B]:LEU:CB | 2.06 | 0.84 |
| 3:F:2966[B]:SER:HA | 3:a:3256[B]:TRP:HB3 | 1.56 | 0.84 |
| 3:L:3089[B]:HIS:ND1 | 3:L:3119[B]:HIS:NE2 | 2.25 | 0.84 |
| 3:L:3284[A]:LYS:HD3 | 3:L:3285[A]:VAL:H | 1.39 | 0.84 |
| 3:O:2952[B]:ALA:HB3 | 3:O:2953[B]:GLY:O | 1.76 | 0.84 |
| 3:O:2965[A]:LEU:HD11 | 3:O:2974[A]:ALA:HA | 1.57 | 0.84 |
| 3:R:2952[A]:ALA:HB3 | 3:R:2953[A]:GLY:O | 1.76 | 0.84 |
| 3:R:2955[A]:GLN:CD | 3:R:3037[A]:TYR:CE1 | 2.55 | 0.84 |
| 3:U:2952[A]:ALA:HA | 3:U:2956[A]:LYS:CB | 2.06 | 0.84 |
| 3:U:3169[B]:LYS:HE2 | 3:d:3147[B]:GLU:HA | 1.59 | 0.84 |
| 3:U:3185[A]:TYR:CE2 | 3:U:3187[A]:TYR:CE2 | 2.65 | 0.84 |
| 3:X:2965[B]:LEU:HD11 | 3:X:2974[B]:ALA:HA | 1.57 | 0.84 |
| 3:a:3089[B]:HIS:ND1 | 3:a:3119[B]:HIS:NE2 | 2.25 | 0.84 |
| 3:a:3284[A]:LYS:HD3 | 3:a:3285[A]:VAL:H | 1.39 | 0.84 |
| 1:b:497:GLN:HG2 | 1:b:683:THR:HG21 | 1.57 | 0.84 |
| 3:d:3185[B]:TYR:CE2 | 3:d:3187[B]:TYR:CE2 | 2.65 | 0.84 |
| 3:C:2933[A]:SER:CB | 3:C:2936[A]:GLU:HB3 | 2.07 | 0.84 |
| 3:C:2952[B]:ALA:HB3 | 3:C:2953[B]:GLY:O | 1.76 | 0.84 |
| 3:C:2982[B]:MET:SD | 3:L:3157[B]:PRO:HA | 2.17 | 0.84 |
| 3:F:2952[B]:ALA:HA | 3:F:2956[B]:LYS:CB | 2.06 | 0.84 |
| 3:F:3089[A]:HIS:ND1 | 3:F:3119[A]:HIS:NE2 | 2.25 | 0.84 |
| 3:F:3153[B]:LYS:HZ2 | 3:a:3156[B]:MET:C | 1.84 | 0.84 |
| 3:I:3293[B]:LYS:CD | 3:I:3294[B]:SER:CB | 2.53 | 0.84 |
| 3:I:3298[A]:ASN:HA | 3:I:3299[A]:LEU:CB | 2.06 | 0.84 |
| 3:O:3038[B]:ILE:CG2 | 3:X:2969[B]:TYR:OH | 2.22 | 0.84 |
| 3:O:3124[A]:ASP:OD2 | 3:O:3185[A]:TYR:OH | 1.93 | 0.84 |
| 3:R:2948[A]:ASP:CB | 3:R:2953[A]:GLY:HA3 | 2.07 | 0.84 |
| 3:R:3293[B]:LYS:CD | 3:R:3294[B]:SER:CB | 2.53 | 0.84 |
| 1:S:871:GLN:HE22 | 1:S:964:ILE:HG13 | 1.40 | 0.84 |
| 3:U:3217[B]:PHE:HZ | 3:U:3230[B]:PHE:CE1 | 1.89 | 0.84 |
| 3:U:3252[B]:TYR:O | 3:d:3255[B]:PRO:HB3 | 1.77 | 0.84 |
| 3:a:2933[A]:SER:CB | 3:a:2936[A]:GLU:HB3 | 2.07 | 0.84 |
| 3:C:2955[B]:GLN:CD | 3:C:3037[B]:TYR:CE1 | 2.55 | 0.84 |
| 3:C:2965[A]:LEU:HD11 | 3:C:2974[A]:ALA:HA | 1.57 | 0.84 |
| 3:C:3284[A]:LYS:HD3 | 3:C:3285[A]:VAL:H | 1.39 | 0.84 |
| 3:F:2933[B]:SER:HB3 | 3:F:2936[B]:GLU:HB3 | 1.57 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2948[A]:ASP:CB | 3:F:2953[A]:GLY:HA3 | 2.07 | 0.84 |
| 3:I:2952[B]:ALA:HA | 3:I:2956[B]:LYS:CB | 2.06 | 0.84 |
| 3:I:3089[A]:HIS:ND1 | 3:I:3119[A]:HIS:NE2 | 2.25 | 0.84 |
| 3:I:3149[B]:ASN:ND2 | 3:R:3163[B]:ASN:HB3 | 1.92 | 0.84 |
| 3:O:2948[B]:ASP:CB | 3:O:2953[B]:GLY:HA3 | 2.07 | 0.84 |
| 3:O:3038[B]:ILE:HG23 | 3:X:2969[B]:TYR:CE1 | 2.10 | 0.84 |
| 3:O:3251[B]:ASP:HB3 | 3:X:2967[B]:CYS:HA | 0.90 | 0.84 |
| 3:U:2955[B]:GLN:CD | 3:U:3037[B]:TYR:CE1 | 2.55 | 0.84 |
| 3:U:3169[B]:LYS:HE3 | 3:d:3147[B]:GLU:HB3 | 1.59 | 0.84 |
| 3:U:3218[A]:LEU:C | 3:U:3219[A]:LEU:HD22 | 2.01 | 0.84 |
| 3:a:2933[B]:SER:CB | 3:a:2936[B]:GLU:HB3 | 2.07 | 0.84 |
| 3:d:3230[A]:PHE:CB | 3:d:3243[A]:GLY:HA2 | 2.06 | 0.84 |
| 3:F:2933[B]:SER:CB | 3:F:2936[B]:GLU:HB3 | 2.07 | 0.84 |
| 3:F:2971[B]:ASP:O | 3:a:3090[B]:ASN:CA | 2.24 | 0.84 |
| 3:F:3153[B]:LYS:CB | 3:a:3155[B]:MET:O | 2.24 | 0.84 |
| 3:F:3185[A]:TYR:CE2 | 3:F:3187[A]:TYR:CE2 | 2.65 | 0.84 |
| 3:I:2982[B]:MET:CG | 3:R:3156[B]:MET:HB2 | 2.07 | 0.84 |
| 3:I:3185[A]:TYR:CE2 | 3:I:3187[A]:TYR:CE2 | 2.65 | 0.84 |
| 3:L:2955[A]:GLN:CD | 3:L:3037[A]:TYR:CE1 | 2.55 | 0.84 |
| 1:M:401:VAL:HG22 | 1:M:662:SER:HB3 | 1.59 | 0.84 |
| 3:O:3196[A]:THR:H | 3:O:3199[A]:GLN:HB2 | 1.37 | 0.84 |
| 3:U:2952[B]:ALA:HA | 3:U:2956[B]:LYS:CB | 2.06 | 0.84 |
| 3:U:2969[B]:TYR:CE1 | 3:d:2978[B]:CYS:SG | 2.71 | 0.84 |
| 1:Y:883:CYS:N | 1:Y:894:CYS:SG | 2.51 | 0.84 |
| 3:a:2952[B]:ALA:HA | 3:a:2956[B]:LYS:CB | 2.06 | 0.84 |
| 3:F:2970[B]:PRO:CB | 3:a:2989[B]:HIS:CD2 | 2.59 | 0.84 |
| 3:F:3089[B]:HIS:ND1 | 3:F:3119[B]:HIS:NE2 | 2.25 | 0.84 |
| 3:F:3159[B]:SER:CB | 3:a:2984[B]:THR:HG23 | 1.85 | 0.84 |
| 3:I:2952[A]:ALA:HA | 3:I:2956[A]:LYS:CB | 2.06 | 0.84 |
| 3:I:2965[B]:LEU:HD11 | 3:I:2974[B]:ALA:HA | 1.57 | 0.84 |
| 3:I:3157[B]:PRO:HD3 | 3:R:3254[B]:MET:HE2 | 1.57 | 0.84 |
| 3:I:3185[B]:TYR:CE2 | 3:I:3187[B]:TYR:CE2 | 2.65 | 0.84 |
| 3:I:3230[A]:PHE:CB | 3:I:3243[A]:GLY:HA2 | 2.06 | 0.84 |
| 3:L:2948[A]:ASP:CB | 3:L:2953[A]:GLY:HA3 | 2.07 | 0.84 |
| 3:L:3185[A]:TYR:CE2 | 3:L:3187[A]:TYR:CE2 | 2.65 | 0.84 |
| 3:U:3196[B]:THR:H | 3:U:3199[B]:GLN:HB2 | 1.37 | 0.84 |
| 3:U:3298[A]:ASN:HA | 3:U:3299[A]:LEU:CB | 2.06 | 0.84 |
| 3:X:2955[B]:GLN:CD | 3:X:3037[B]:TYR:CE1 | 2.55 | 0.84 |
| 3:a:3298[A]:ASN:HA | 3:a:3299[A]:LEU:CB | 2.06 | 0.84 |
| 3:d:2956[B]:LYS:O | 3:d:2960[B]:PHE:HE1 | 1.22 | 0.84 |
| 3:C:3222[B]:ILE:CD1 | 3:L:2963[B]:MET:HE1 | 2.05 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2933[A]:SER:CB | 3:F:2936[A]:GLU:HB3 | 2.07 | 0.84 |
| 3:F:3185[B]:TYR:CE2 | 3:F:3187[B]:TYR:CE2 | 2.65 | 0.84 |
| 3:F:3298[A]:ASN:HA | 3:F:3299[A]:LEU:CB | 2.06 | 0.84 |
| 3:I:3089[B]:HIS:CD2 | 3:R:2972[B]:GLY:N | 2.46 | 0.84 |
| 3:L:3185[B]:TYR:CE2 | 3:L:3187[B]:TYR:CE2 | 2.65 | 0.84 |
| 3:O:2956[B]:LYS:O | 3:O:2960[B]:PHE:HE1 | 1.22 | 0.84 |
| 3:O:3255[B]:PRO:HD3 | 3:X:3158[B]:PHE:O | 1.76 | 0.84 |
| 1:P:392:PRO:HB2 | 1:P:394:GLN:HG2 | 1.60 | 0.84 |
| 3:U:2970[B]:PRO:O | 3:d:3086[B]:GLU:HG2 | 1.77 | 0.84 |
| 3:U:3217[A]:PHE:HZ | 3:U:3230[A]:PHE:CE1 | 1.89 | 0.84 |
| 3:X:3185[A]:TYR:CE2 | 3:X:3187[A]:TYR:CE2 | 2.65 | 0.84 |
| 3:X:3212[B]:ARG:HG3 | 3:X:3212[B]:ARG:HH11 | 1.43 | 0.84 |
| 3:a:2933[A]:SER:HB3 | 3:a:2936[A]:GLU:HB3 | 1.57 | 0.84 |
| 3:a:2948[B]:ASP:CB | 3:a:2953[B]:GLY:HA3 | 2.07 | 0.84 |
| 3:a:3196[A]:THR:H | 3:a:3199[A]:GLN:HB2 | 1.37 | 0.84 |
| 3:d:2933[B]:SER:CB | 3:d:2936[B]:GLU:HB3 | 2.07 | 0.84 |
| 3:C:3089[B]:HIS:ND1 | 3:C:3119[B]:HIS:NE2 | 2.25 | 0.84 |
| 3:C:3152[B]:LYS:H | 3:L:3172[B]:SER:CB | 1.90 | 0.84 |
| 3:F:2965[B]:LEU:HD13 | 3:a:3256[B]:TRP:HE1 | 1.38 | 0.84 |
| 3:F:2975[B]:PHE:HZ | 3:a:2961[B]:HIS:CA | 1.88 | 0.84 |
| 3:I:2948[A]:ASP:CB | 3:I:2953[A]:GLY:HA3 | 2.07 | 0.84 |
| 3:I:2948[B]:ASP:CB | 3:I:2953[B]:GLY:HA3 | 2.07 | 0.84 |
| 3:I:2952[A]:ALA:HB3 | 3:I:2953[A]:GLY:O | 1.76 | 0.84 |
| 3:I:3162[B]:ASP:CB | 3:R:3259[B]:ASP:H | 1.89 | 0.84 |
| 3:I:3170[B]:ALA:N | 3:R:3148[B]:ILE:O | 2.10 | 0.84 |
| 3:I:3217[B]:PHE:HZ | 3:I:3230[B]:PHE:CE1 | 1.89 | 0.84 |
| 3:L:3089[B]:HIS:HE1 | 3:L:3119[B]:HIS:CD2 | 1.96 | 0.84 |
| 3:O:2968[B]:GLN:CD | 3:X:2984[B]:THR:OG1 | 2.20 | 0.84 |
| 3:O:3089[B]:HIS:HE1 | 3:O:3119[B]:HIS:CD2 | 1.96 | 0.84 |
| 3:U:2956[A]:LYS:O | 3:U:2960[A]:PHE:HE1 | 1.22 | 0.84 |
| 3:U:2979[A]:GLN:CG | 3:U:3155[A]:MET:CE | 2.56 | 0.84 |
| 3:U:3124[B]:ASP:OD2 | 3:U:3185[B]:TYR:OH | 1.93 | 0.84 |
| 3:X:2948[A]:ASP:CB | 3:X:2953[A]:GLY:HA3 | 2.07 | 0.84 |
| 3:X:3176[A]:LYS:HE2 | 3:X:3176[A]:LYS:H | 1.43 | 0.84 |
| 3:X:3284[B]:LYS:HD3 | 3:X:3285[B]:VAL:H | 1.40 | 0.84 |
| 3:a:2948[B]:ASP:N | 3:a:2949[B]:LYS:HA | 1.81 | 0.84 |
| 3:a:2979[A]:GLN:CG | 3:a:3155[A]:MET:CE | 2.56 | 0.84 |
| 3:L:3212[B]:ARG:HH11 | 3:L:3212[B]:ARG:HG3 | 1.43 | 0.84 |
| 1:P:456:GLN:HG2 | 1:P:551:GLU:HB2 | 1.57 | 0.84 |
| 3:R:3089[A]:HIS:HE1 | 3:R:3119[A]:HIS:CD2 | 1.96 | 0.84 |
| 3:U:2948[B]:ASP:CB | 3:U:2953[B]:GLY:HA3 | 2.07 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3089[B]:HIS:HE1 | 3:X:3119[B]:HIS:CD2 | 1.96 | 0.84 |
| 3:X:3173[A]:THR:HG22 | 3:X:3174[A]:GLY:N | 1.93 | 0.84 |
| 2:Z:2648:ALA:HA | 2:Z:2654:SER:HB2 | 1.60 | 0.84 |
| 3:a:2948[A]:ASP:N | 3:a:2949[A]:LYS:HA | 1.81 | 0.84 |
| 3:a:3293[A]:LYS:CD | 3:a:3294[A]:SER:CB | 2.53 | 0.84 |
| 3:d:3293[A]:LYS:CD | 3:d:3294[A]:SER:CB | 2.53 | 0.84 |
| 3:C:2985[B]:PHE:CD2 | 3:L:2968[B]:GLN:O | 2.30 | 0.84 |
| 3:C:3154[B]:PRO:N | 3:L:3174[B]:GLY:N | 2.24 | 0.84 |
| 3:F:2966[B]:SER:O | 3:a:3256[B]:TRP:CG | 2.23 | 0.84 |
| 3:F:2969[B]:TYR:CE2 | 3:a:3120[B]:HIS:NE2 | 2.45 | 0.84 |
| 3:F:3196[A]:THR:H | 3:F:3199[A]:GLN:HB2 | 1.38 | 0.84 |
| 3:I:3160[B]:SER:O | 3:R:3150[B]:LYS:HD2 | 1.76 | 0.84 |
| 3:O:2979[B]:GLN:CG | 3:O:3155[B]:MET:CE | 2.56 | 0.84 |
| 3:O:3089[B]:HIS:ND1 | 3:O:3119[B]:HIS:NE2 | 2.25 | 0.84 |
| 3:O:3176[B]:LYS:HE2 | 3:O:3176[B]:LYS:H | 1.43 | 0.84 |
| 3:R:2933[A]:SER:CB | 3:R:2936[A]:GLU:HB3 | 2.07 | 0.84 |
| 3:U:2948[A]:ASP:CB | 3:U:2953[A]:GLY:HA3 | 2.07 | 0.84 |
| 1:Y:1546:LYS:HG3 | 3:d:3001[B]:LYS:CE | 2.03 | 0.84 |
| 3:d:2933[A]:SER:CB | 3:d:2936[A]:GLU:HB3 | 2.07 | 0.84 |
| 3:d:3185[A]:TYR:CE2 | 3:d:3187[A]:TYR:CE2 | 2.65 | 0.84 |
| 3:C:2948[A]:ASP:CB | 3:C:2953[A]:GLY:HA3 | 2.07 | 0.84 |
| 3:C:3158[B]:PHE:O | 3:L:3149[B]:ASN:CG | 2.21 | 0.84 |
| 3:C:3160[B]:SER:HA | 3:L:2983[B]:VAL:CB | 2.06 | 0.84 |
| 3:I:3173[B]:THR:HG1 | 3:R:3173[B]:THR:HG23 | 0.71 | 0.84 |
| 3:L:2933[B]:SER:CB | 3:L:2936[B]:GLU:HB3 | 2.07 | 0.84 |
| 3:O:3176[A]:LYS:HE2 | 3:O:3176[A]:LYS:H | 1.43 | 0.84 |
| 3:R:2933[B]:SER:HB3 | 3:R:2936[B]:GLU:HB3 | 1.57 | 0.84 |
| 3:R:3173[A]:THR:HG22 | 3:R:3174[A]:GLY:N | 1.93 | 0.84 |
| 3:U:3155[B]:MET:HA | 3:d:3150[B]:LYS:HG2 | 1.58 | 0.84 |
| 3:X:2933[A]:SER:CB | 3:X:2936[A]:GLU:HB3 | 2.07 | 0.84 |
| 3:X:3185[B]:TYR:CE2 | 3:X:3187[B]:TYR:CE2 | 2.65 | 0.84 |
| 2:c:2267:HIS:HD2 | 2:c:2297:HIS:HE1 | 1.26 | 0.84 |
| 3:C:2968[B]:GLN:HE22 | 3:L:3258[B]:PHE:HZ | 1.03 | 0.83 |
| 3:C:3089[A]:HIS:ND1 | 3:C:3119[A]:HIS:NE2 | 2.25 | 0.83 |
| 3:C:3093[B]:HIS:NE2 | 3:L:2969[B]:TYR:CD2 | 2.46 | 0.83 |
| 3:C:3147[B]:GLU:CD | 3:L:3163[B]:ASN:H | 1.85 | 0.83 |
| 3:C:3150[B]:LYS:HZ2 | 3:L:3160[B]:SER:HB3 | 1.26 | 0.83 |
| 3:F:2959[B]:SER:HB2 | 3:a:3255[B]:PRO:CB | 2.07 | 0.83 |
| 3:F:3256[B]:TRP:N | 3:a:2965[B]:LEU:C | 2.36 | 0.83 |
| 3:I:2933[B]:SER:CB | 3:I:2936[B]:GLU:HB3 | 2.07 | 0.83 |
| 3:I:3089[B]:HIS:ND1 | 3:I:3119[B]:HIS:NE2 | 2.25 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3212[A]:ARG:HH11 | 3:I:3212[A]:ARG:HG3 | 1.43 | 0.83 |
| 3:O:2956[A]:LYS:C | 3:O:2960[A]:PHE:CE1 | 2.47 | 0.83 |
| 3:O:2979[A]:GLN:CG | 3:O:3155[A]:MET:CE | 2.56 | 0.83 |
| 3:O:3156[B]:MET:CG | 3:X:3173[B]:THR:CG2 | 2.56 | 0.83 |
| 3:O:3284[B]:LYS:HD3 | 3:O:3285[B]:VAL:H | 1.40 | 0.83 |
| 3:U:2933[B]:SER:CB | 3:U:2936[B]:GLU:HB3 | 2.07 | 0.83 |
| 3:U:3212[A]:ARG:HH11 | 3:U:3212[A]:ARG:HG3 | 1.42 | 0.83 |
| 3:X:3216[B]:GLY:HA2 | 3:X:3262[B]:PHE:O | 1.78 | 0.83 |
| 3:a:3173[B]:THR:HG22 | 3:a:3174[B]:GLY:N | 1.93 | 0.83 |
| 3:a:3185[A]:TYR:CE2 | 3:a:3187[A]:TYR:CE2 | 2.65 | 0.83 |
| 3:d:2979[A]:GLN:CG | 3:d:3155[A]:MET:CE | 2.55 | 0.83 |
| 3:C:3284[B]:LYS:HD3 | 3:C:3285[B]:VAL:H | 1.40 | 0.83 |
| 3:F:2948[B]:ASP:N | 3:F:2949[B]:LYS:CA | 2.41 | 0.83 |
| 3:O:2933[A]:SER:CB | 3:O:2936[A]:GLU:HB3 | 2.07 | 0.83 |
| 3:O:2955[B]:GLN:CD | 3:O:3037[B]:TYR:CE1 | 2.55 | 0.83 |
| 3:O:2969[B]:TYR:HB2 | 3:X:3158[B]:PHE:CE1 | 2.13 | 0.83 |
| 3:O:2975[B]:PHE:CE2 | 3:X:3172[B]:SER:CA | 2.60 | 0.83 |
| 3:O:3157[B]:PRO:O | 3:X:3150[B]:LYS:N | 2.11 | 0.83 |
| 3:O:3157[B]:PRO:C | 3:X:3152[B]:LYS:CB | 2.50 | 0.83 |
| 3:O:3216[B]:GLY:HA2 | 3:O:3262[B]:PHE:O | 1.78 | 0.83 |
| 3:R:3089[B]:HIS:ND1 | 3:R:3119[B]:HIS:NE2 | 2.25 | 0.83 |
| 3:R:3196[B]:THR:H | 3:R:3199[B]:GLN:HB2 | 1.37 | 0.83 |
| 3:U:2956[A]:LYS:C | 3:U:2960[A]:PHE:CE1 | 2.47 | 0.83 |
| 3:U:2965[B]:LEU:CD1 | 3:d:3220[B]:ARG:CB | 2.27 | 0.83 |
| 3:U:3156[B]:MET:HE1 | 3:d:2982[B]:MET:HG2 | 1.58 | 0.83 |
| 3:U:3171[B]:HIS:HA | 3:d:3152[B]:LYS:NZ | 1.93 | 0.83 |
| 3:X:3230[A]:PHE:CB | 3:X:3243[A]:GLY:HA2 | 2.06 | 0.83 |
| 1:Y:1543:ILE:HA | 3:d:3001[B]:LYS:HE2 | 1.58 | 0.83 |
| 3:d:2948[A]:ASP:CB | 3:d:2953[A]:GLY:HA3 | 2.07 | 0.83 |
| 3:C:2969[B]:TYR:O | 3:L:2985[B]:PHE:CZ | 2.26 | 0.83 |
| 3:C:3222[B]:ILE:N | 3:L:2965[B]:LEU:HB2 | 1.94 | 0.83 |
| 3:C:3230[A]:PHE:CB | 3:C:3243[A]:GLY:HA2 | 2.06 | 0.83 |
| 3:F:2948[B]:ASP:CB | 3:F:2953[B]:GLY:HA3 | 2.07 | 0.83 |
| 1:G:1339:SER:HB3 | 1:G:1340:GLY:HA2 | 1.60 | 0.83 |
| 3:I:3230[B]:PHE:CB | 3:I:3243[B]:GLY:HA2 | 2.06 | 0.83 |
| 3:L:3176[B]:LYS:HE2 | 3:L:3176[B]:LYS:H | 1.43 | 0.83 |
| 3:O:2973[B]:THR:CB | 3:X:3158[B]:PHE:HE2 | 1.86 | 0.83 |
| 3:O:3185[A]:TYR:CE2 | 3:O:3187[A]:TYR:CE2 | 2.65 | 0.83 |
| 3:U:2965[A]:LEU:HG | 3:U:2974[A]:ALA:HB1 | 1.61 | 0.83 |
| 3:U:2965[B]:LEU:HD11 | 3:d:3256[B]:TRP:O | 1.78 | 0.83 |
| 3:U:2979[B]:GLN:CG | 3:U:3155[B]:MET:CE | 2.56 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3153[B]:LYS:CE | 3:d:2979[B]:GLN:NE2 | 2.27 | 0.83 |
| 3:U:3255[B]:PRO:CG | 3:d:3252[B]:TYR:O | 2.12 | 0.83 |
| 1:Y:1078:ARG:NH2 | 2:c:2877:ILE:O | 2.11 | 0.83 |
| 3:a:3089[B]:HIS:HE1 | 3:a:3119[B]:HIS:CD2 | 1.96 | 0.83 |
| 3:d:3216[B]:GLY:HA2 | 3:d:3262[B]:PHE:O | 1.78 | 0.83 |
| 3:C:2952[A]:ALA:HA | 3:C:2956[A]:LYS:CB | 2.06 | 0.83 |
| 3:C:3172[B]:SER:CB | 3:L:3152[B]:LYS:N | 2.41 | 0.83 |
| 2:E:2545:SER:HA | 2:E:2546:LEU:HB2 | 1.59 | 0.83 |
| 3:I:3298[B]:ASN:HA | 3:I:3299[B]:LEU:CB | 2.06 | 0.83 |
| 3:O:3162[B]:ASP:OD2 | 3:X:3150[B]:LYS:CD | 2.27 | 0.83 |
| 3:O:3212[A]:ARG:HG3 | 3:O:3212[A]:ARG:HH11 | 1.43 | 0.83 |
| 3:R:2948[A]:ASP:N | 3:R:2949[A]:LYS:CA | 2.41 | 0.83 |
| 3:R:2948[B]:ASP:CB | 3:R:2953[B]:GLY:HA3 | 2.07 | 0.83 |
| 3:R:3230[A]:PHE:CB | 3:R:3243[A]:GLY:HA2 | 2.06 | 0.83 |
| 3:U:2967[B]:CYS:C | 3:d:3256[B]:TRP:CB | 2.52 | 0.83 |
| 3:U:3089[B]:HIS:ND1 | 3:U:3119[B]:HIS:NE2 | 2.25 | 0.83 |
| 2:W:2569:TRP:HD1 | 2:W:2746:MET:HG2 | 1.42 | 0.83 |
| 3:X:2952[B]:ALA:HB3 | 3:X:2953[B]:GLY:O | 1.76 | 0.83 |
| 3:d:3089[A]:HIS:HE1 | 3:d:3119[A]:HIS:CD2 | 1.96 | 0.83 |
| 3:d:3298[B]:ASN:HA | 3:d:3299[B]:LEU:CB | 2.06 | 0.83 |
| 3:C:3149[B]:ASN:HB3 | 3:L:3163[B]:ASN:HD21 | 1.43 | 0.83 |
| 3:F:2965[B]:LEU:HG | 3:F:2974[B]:ALA:HB1 | 1.61 | 0.83 |
| 3:F:3155[B]:MET:HB2 | 3:a:3153[B]:LYS:CB | 2.08 | 0.83 |
| 3:F:3173[B]:THR:HG22 | 3:F:3174[B]:GLY:N | 1.93 | 0.83 |
| 3:I:2955[A]:GLN:CD | 3:I:3037[A]:TYR:CE1 | 2.55 | 0.83 |
| 3:I:2956[A]:LYS:C | 3:I:2960[A]:PHE:CE1 | 2.47 | 0.83 |
| 3:I:3216[B]:GLY:HA2 | 3:I:3262[B]:PHE:O | 1.78 | 0.83 |
| 3:L:2948[B]:ASP:N | 3:L:2949[B]:LYS:CA | 2.41 | 0.83 |
| 3:L:2965[A]:LEU:CG | 3:L:2974[A]:ALA:HB1 | 2.09 | 0.83 |
| 3:L:2979[A]:GLN:CG | 3:L:3155[A]:MET:CE | 2.56 | 0.83 |
| 3:O:3173[B]:THR:HG22 | 3:O:3174[B]:GLY:N | 1.93 | 0.83 |
| 3:O:3272[A]:HIS:CD2 | 1:P:1542:ARG:NH2 | 2.46 | 0.83 |
| 3:R:2948[B]:ASP:N | 3:R:2949[B]:LYS:CA | 2.41 | 0.83 |
| 3:U:3259[B]:ASP:CA | 3:d:2968[B]:GLN:HE21 | 1.92 | 0.83 |
| 3:X:3176[B]:LYS:HE2 | 3:X:3176[B]:LYS:H | 1.43 | 0.83 |
| 3:X:3216[A]:GLY:HA2 | 3:X:3262[A]:PHE:O | 1.78 | 0.83 |
| 3:a:3089[A]:HIS:HE1 | 3:a:3119[A]:HIS:CD2 | 1.96 | 0.83 |
| 3:a:3284[B]:LYS:HD3 | 3:a:3285[B]:VAL:H | 1.39 | 0.83 |
| 3:d:3173[A]:THR:HG22 | 3:d:3174[A]:GLY:N | 1.93 | 0.83 |
| 3:d:3173[B]:THR:HG22 | 3:d:3174[B]:GLY:N | 1.93 | 0.83 |
| 3:d:3284[B]:LYS:HD3 | 3:d:3285[B]:VAL:H | 1.39 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3153[B]:LYS:NZ | 3:L:2988[B]:TRP:NE1 | 2.27 | 0.83 |
| 3:F:3212[B]:ARG:HH11 | 3:F:3212[B]:ARG:HG3 | 1.43 | 0.83 |
| 3:F:3293[A]:LYS:CD | 3:F:3294[A]:SER:CB | 2.53 | 0.83 |
| 3:L:3216[B]:GLY:HA2 | 3:L:3262[B]:PHE:O | 1.78 | 0.83 |
| 3:O:2965[B]:LEU:H | 3:X:3254[B]:MET:HE3 | 1.41 | 0.83 |
| 3:O:2970[B]:PRO:C | 3:X:2988[B]:TRP:C | 2.40 | 0.83 |
| 3:O:3157[B]:PRO:C | 3:X:3152[B]:LYS:HB2 | 1.89 | 0.83 |
| 3:O:3253[B]:GLU:CG | 3:X:3161[B]:GLU:OE2 | 2.25 | 0.83 |
| 3:R:2965[B]:LEU:HG | 3:R:2974[B]:ALA:HB1 | 1.61 | 0.83 |
| 3:U:2975[B]:PHE:CE1 | 3:d:3256[B]:TRP:CD1 | 2.65 | 0.83 |
| 3:U:3089[A]:HIS:ND1 | 3:U:3119[A]:HIS:NE2 | 2.25 | 0.83 |
| 3:U:3155[B]:MET:O | 3:d:3149[B]:ASN:HB2 | 1.76 | 0.83 |
| 3:X:2951[A]:ASP:OD2 | 3:X:2953[A]:GLY:HA2 | 1.79 | 0.83 |
| 3:d:2948[A]:ASP:N | 3:d:2949[A]:LYS:CA | 2.41 | 0.83 |
| 3:d:2955[B]:GLN:CD | 3:d:3037[B]:TYR:CE1 | 2.55 | 0.83 |
| 3:C:2951[A]:ASP:OD2 | 3:C:2953[A]:GLY:HA2 | 1.79 | 0.83 |
| 3:C:2965[A]:LEU:CG | 3:C:2974[A]:ALA:HB1 | 2.09 | 0.83 |
| 3:C:3155[B]:MET:SD | 3:L:3154[B]:PRO:CD | 2.66 | 0.83 |
| 3:F:2965[A]:LEU:CG | 3:F:2974[A]:ALA:HB1 | 2.09 | 0.83 |
| 3:F:3228[A]:VAL:HG21 | 3:F:3245[A]:PHE:CE2 | 2.14 | 0.83 |
| 3:F:3253[B]:GLU:HA | 3:a:3252[B]:TYR:O | 1.78 | 0.83 |
| 3:I:3089[A]:HIS:HE1 | 3:I:3119[A]:HIS:CD2 | 1.96 | 0.83 |
| 3:L:2933[A]:SER:CB | 3:L:2936[A]:GLU:HB3 | 2.07 | 0.83 |
| 3:L:3089[A]:HIS:HE1 | 3:L:3119[A]:HIS:CD2 | 1.96 | 0.83 |
| 3:R:3284[B]:LYS:HD3 | 3:R:3285[B]:VAL:H | 1.39 | 0.83 |
| 3:a:2965[A]:LEU:CG | 3:a:2974[A]:ALA:HB1 | 2.09 | 0.83 |
| 3:a:3024[A]:LEU:CD1 | 3:a:3025[A]:VAL:H | 1.83 | 0.83 |
| 3:a:3176[A]:LYS:HE2 | 3:a:3176[A]:LYS:H | 1.43 | 0.83 |
| 3:d:2965[A]:LEU:CG | 3:d:2974[A]:ALA:HB1 | 2.09 | 0.83 |
| 3:d:3212[A]:ARG:HH11 | 3:d:3212[A]:ARG:HG3 | 1.43 | 0.83 |
| 3:C:3089[B]:HIS:HE1 | 3:C:3119[B]:HIS:CD2 | 1.96 | 0.83 |
| 3:C:3156[B]:MET:HE3 | 3:L:2979[B]:GLN:HG3 | 1.53 | 0.83 |
| 3:C:3212[B]:ARG:HH11 | 3:C:3212[B]:ARG:HG3 | 1.43 | 0.83 |
| 3:C:3298[A]:ASN:HA | 3:C:3299[A]:LEU:CB | 2.06 | 0.83 |
| 3:F:2971[B]:ASP:O | 3:a:3090[B]:ASN:HB3 | 1.79 | 0.83 |
| 3:F:3089[B]:HIS:HE1 | 3:F:3119[B]:HIS:CD2 | 1.96 | 0.83 |
| 3:F:3107[B]:LEU:HD11 | 3:a:2975[B]:PHE:HD1 | 0.75 | 0.83 |
| 3:F:3176[B]:LYS:H | 3:F:3176[B]:LYS:HE2 | 1.43 | 0.83 |
| 3:F:3253[B]:GLU:CB | 3:a:2975[B]:PHE:C | 2.50 | 0.83 |
| 3:I:2979[A]:GLN:CG | 3:I:3155[A]:MET:CE | 2.56 | 0.83 |
| 3:I:2989[B]:HIS:CE1 | 3:R:2969[B]:TYR:CA | 2.58 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3089[B]:HIS:HE1 | 3:I:3119[B]:HIS:CD2 | 1.96 | 0.83 |
| 3:I:3161[B]:GLU:HG2 | 3:R:3079[B]:CYS:HA | 1.60 | 0.83 |
| 3:O:2952[B]:ALA:HA | 3:O:2956[B]:LYS:CB | 2.06 | 0.83 |
| 3:O:2965[B]:LEU:HD11 | 3:O:2974[B]:ALA:HA | 1.57 | 0.83 |
| 3:O:2975[B]:PHE:CE2 | 3:X:3172[B]:SER:HB3 | 2.14 | 0.83 |
| 3:O:3251[B]:ASP:HB2 | 3:X:2968[B]:GLN:CD | 2.04 | 0.83 |
| 3:R:3185[A]:TYR:CE2 | 3:R:3187[A]:TYR:CE2 | 2.65 | 0.83 |
| 1:S:589:GLN:HG2 | 1:S:594:ASP:HB3 | 1.60 | 0.83 |
| 3:U:2965[A]:LEU:CG | 3:U:2974[A]:ALA:HB1 | 2.09 | 0.83 |
| 3:U:3176[B]:LYS:HE2 | 3:U:3176[B]:LYS:H | 1.43 | 0.83 |
| 3:U:3216[B]:GLY:HA2 | 3:U:3262[B]:PHE:O | 1.78 | 0.83 |
| 3:U:3259[B]:ASP:CG | 3:U:3260[B]:ARG:HG2 | 2.04 | 0.83 |
| 3:U:3265[A]:ASP:OD1 | 3:U:3267[A]:SER:OG | 1.97 | 0.83 |
| 1:Y:1365:TYR:HD1 | 1:Y:1372:ILE:HG22 | 1.44 | 0.83 |
| 1:Y:1546:LYS:CB | 3:d:3001[B]:LYS:HZ1 | 1.83 | 0.83 |
| 3:a:2965[B]:LEU:HG | 3:a:2974[B]:ALA:HB1 | 1.61 | 0.83 |
| 3:d:3176[B]:LYS:HE2 | 3:d:3176[B]:LYS:H | 1.43 | 0.83 |
| 3:d:3265[B]:ASP:OD1 | 3:d:3267[B]:SER:OG | 1.97 | 0.83 |
| 6:GA:2:NAG:C6 | 6:GA:3:BMA:C1 | 2.57 | 0.83 |
| 3:C:2964[B]:PRO:C | 3:L:3255[B]:PRO:HB3 | 2.04 | 0.83 |
| 3:C:3149[B]:ASN:HB2 | 3:L:3163[B]:ASN:ND2 | 1.93 | 0.83 |
| 3:F:2979[B]:GLN:CG | 3:F:3155[B]:MET:CE | 2.56 | 0.83 |
| 3:F:3152[B]:LYS:HD2 | 3:a:3170[B]:ALA:O | 0.88 | 0.83 |
| 3:F:3265[B]:ASP:OD1 | 3:F:3267[B]:SER:OG | 1.97 | 0.83 |
| 3:I:2966[B]:SER:HB3 | 3:R:2982[B]:MET:CE | 2.08 | 0.83 |
| 3:I:3259[B]:ASP:CG | 3:I:3260[B]:ARG:HG2 | 2.04 | 0.83 |
| 3:L:2956[A]:LYS:O | 3:L:2960[A]:PHE:HE1 | 1.22 | 0.83 |
| 3:L:2965[A]:LEU:HG | 3:L:2974[A]:ALA:HB1 | 1.61 | 0.83 |
| 3:O:3089[A]:HIS:ND1 | 3:O:3119[A]:HIS:NE2 | 2.25 | 0.83 |
| 3:R:3217[B]:PHE:HZ | 3:R:3230[B]:PHE:CE1 | 1.89 | 0.83 |
| 3:R:3259[B]:ASP:CG | 3:R:3260[B]:ARG:HG2 | 2.04 | 0.83 |
| 1:S:423:ARG:NH1 | 1:S:500:ASN:OD1 | 2.12 | 0.83 |
| 3:U:2972[B]:GLY:C | 3:d:3247[B]:VAL:HG13 | 2.01 | 0.83 |
| 3:U:2975[B]:PHE:CD1 | 3:d:3256[B]:TRP:NE1 | 2.45 | 0.83 |
| 3:U:3120[A]:HIS:HA | 3:U:3123[A]:THR:OG1 | 1.79 | 0.83 |
| 3:X:2965[A]:LEU:CG | 3:X:2974[A]:ALA:HB1 | 2.09 | 0.83 |
| 1:Y:1656:ASP:H | 3:d:3006[B]:LYS:HB2 | 1.43 | 0.83 |
| 2:c:2661:MET:HB3 | 2:c:2798:GLN:HE22 | 1.43 | 0.83 |
| 3:d:3298[B]:ASN:HB3 | 3:d:3300[B]:LEU:CD2 | 2.09 | 0.83 |
| 3:C:2965[A]:LEU:HG | 3:C:2974[A]:ALA:HB1 | 1.61 | 0.83 |
| 3:C:2965[B]:LEU:HG | 3:C:2974[B]:ALA:HB1 | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3216[B]:GLY:HA2 | 3:C:3262[B]:PHE:O | 1.78 | 0.83 |
| 3:C:3222[B]:ILE:H | 3:L:2965[B]:LEU:HB2 | 1.44 | 0.83 |
| 3:F:3253[B]:GLU:OE1 | 3:a:2974[B]:ALA:CB | 2.19 | 0.83 |
| 3:I:2965[A]:LEU:HG | 3:I:2974[A]:ALA:HB1 | 1.61 | 0.83 |
| 3:I:3259[A]:ASP:CG | 3:I:3260[A]:ARG:HG2 | 2.04 | 0.83 |
| 3:L:3176[A]:LYS:HE2 | 3:L:3176[A]:LYS:H | 1.43 | 0.83 |
| 3:O:3265[A]:ASP:OD1 | 3:O:3267[A]:SER:OG | 1.97 | 0.83 |
| 2:Q:2867:PRO:HG2 | 3:R:2932[A]:PRO:HG2 | 1.58 | 0.83 |
| 3:R:2965[A]:LEU:HG | 3:R:2974[A]:ALA:HB1 | 1.61 | 0.83 |
| 3:R:3120[A]:HIS:HA | 3:R:3123[A]:THR:OG1 | 1.79 | 0.83 |
| 3:U:2933[A]:SER:CB | 3:U:2936[A]:GLU:HB3 | 2.07 | 0.83 |
| 3:U:3176[A]:LYS:HE2 | 3:U:3176[A]:LYS:H | 1.43 | 0.83 |
| 3:X:2965[A]:LEU:HG | 3:X:2974[A]:ALA:HB1 | 1.61 | 0.83 |
| 3:X:3284[A]:LYS:HD3 | 3:X:3285[A]:VAL:H | 1.39 | 0.83 |
| 3:a:2955[B]:GLN:CD | 3:a:3037[B]:TYR:CE1 | 2.55 | 0.83 |
| 3:a:2956[B]:LYS:O | 3:a:2960[B]:PHE:HE1 | 1.22 | 0.83 |
| 3:a:3196[A]:THR:CG2 | 1:b:416:ASN:CG | 2.47 | 0.83 |
| 3:d:2951[B]:ASP:OD2 | 3:d:2953[B]:GLY:HA2 | 1.79 | 0.83 |
| 3:d:2965[A]:LEU:HG | 3:d:2974[A]:ALA:HB1 | 1.61 | 0.83 |
| 8:0:1:NAG:C6 | 8:0:2:NAG:HN2 | 1.92 | 0.83 |
| 3:C:3120[B]:HIS:HA | 3:C:3123[B]:THR:OG1 | 1.79 | 0.82 |
| 3:C:3172[B]:SER:HB2 | 3:L:3152[B]:LYS:H | 1.42 | 0.82 |
| 2:E:2625:LEU:HG | 2:E:2626:ARG:HG2 | 1.60 | 0.82 |
| 3:F:2966[B]:SER:CB | 3:a:3255[B]:PRO:O | 2.27 | 0.82 |
| 3:F:3160[B]:SER:HB3 | 3:a:3150[B]:LYS:HZ3 | 0.76 | 0.82 |
| 3:F:3183[B]:LEU:H | 3:F:3184[B]:ASN:HA | 1.44 | 0.82 |
| 3:F:3228[B]:VAL:HG21 | 3:F:3245[B]:PHE:CE2 | 2.14 | 0.82 |
| 3:F:3255[B]:PRO:HG3 | 3:a:2964[B]:PRO:N | 1.94 | 0.82 |
| 3:I:2948[A]:ASP:N | 3:I:2949[A]:LYS:HA | 1.81 | 0.82 |
| 3:I:2965[B]:LEU:HG | 3:I:2974[B]:ALA:HB1 | 1.61 | 0.82 |
| 3:I:3212[B]:ARG:HG3 | 3:I:3212[B]:ARG:HH11 | 1.43 | 0.82 |
| 3:I:3293[A]:LYS:CD | 3:I:3294[A]:SER:CB | 2.53 | 0.82 |
| 3:L:3173[A]:THR:HG22 | 3:L:3174[A]:GLY:N | 1.93 | 0.82 |
| 3:L:3228[A]:VAL:HG21 | 3:L:3245[A]:PHE:CE2 | 2.14 | 0.82 |
| 3:O:2965[A]:LEU:HG | 3:O:2974[A]:ALA:HB1 | 1.61 | 0.82 |
| 3:O:3089[A]:HIS:HE1 | 3:O:3119[A]:HIS:CD2 | 1.96 | 0.82 |
| 3:R:2965[A]:LEU:CG | 3:R:2974[A]:ALA:HB1 | 2.09 | 0.82 |
| 3:R:2965[B]:LEU:CG | 3:R:2974[B]:ALA:HB1 | 2.09 | 0.82 |
| 3:R:3024[A]:LEU:CD1 | 3:R:3025[A]:VAL:H | 1.84 | 0.82 |
| 3:R:3259[A]:ASP:CG | 3:R:3260[A]:ARG:HG2 | 2.04 | 0.82 |
| 3:R:3293[A]:LYS:CD | 3:R:3294[A]:SER:CB | 2.53 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3196[A]:THR:H | 3:U:3199[A]:GLN:HB2 | 1.37 | 0.82 |
| 3:U:3228[B]:VAL:HG21 | 3:U:3245[B]:PHE:CE2 | 2.14 | 0.82 |
| 2:W:2808:PHE:HZ | 2:W:2821:LEU:HD13 | 1.43 | 0.82 |
| 3:X:2952[A]:ALA:HB3 | 3:X:2953[A]:GLY:CA | 2.09 | 0.82 |
| 3:X:3183[A]:LEU:H | 3:X:3184[A]:ASN:HA | 1.44 | 0.82 |
| 3:X:3230[B]:PHE:CB | 3:X:3243[B]:GLY:HA2 | 2.06 | 0.82 |
| 3:X:3259[A]:ASP:CG | 3:X:3260[A]:ARG:HG2 | 2.04 | 0.82 |
| 3:a:3173[A]:THR:HG22 | 3:a:3174[A]:GLY:N | 1.93 | 0.82 |
| 2:B:2877:ILE:H | 1:D:1078:ARG:HH12 | 1.21 | 0.82 |
| 3:C:2951[B]:ASP:OD2 | 3:C:2953[B]:GLY:HA2 | 1.79 | 0.82 |
| 3:F:3216[B]:GLY:HA2 | 3:F:3262[B]:PHE:O | 1.78 | 0.82 |
| 3:F:3259[A]:ASP:CG | 3:F:3260[A]:ARG:HG2 | 2.04 | 0.82 |
| 1:J:497:GLN:HG2 | 1:J:683:THR:HG21 | 1.59 | 0.82 |
| 3:O:2952[B]:ALA:HB3 | 3:O:2953[B]:GLY:CA | 2.10 | 0.82 |
| 3:O:2975[B]:PHE:HE2 | 3:X:3172[B]:SER:HA | 1.44 | 0.82 |
| 3:O:3230[B]:PHE:CB | 3:O:3243[B]:GLY:HA2 | 2.06 | 0.82 |
| 3:O:3259[A]:ASP:CG | 3:O:3260[A]:ARG:HG2 | 2.04 | 0.82 |
| 1:P:497:GLN:HG2 | 1:P:683:THR:HG21 | 1.61 | 0.82 |
| 3:R:2933[B]:SER:CB | 3:R:2936[B]:GLU:HB3 | 2.07 | 0.82 |
| 3:R:2955[B]:GLN:CD | 3:R:3037[B]:TYR:CE1 | 2.55 | 0.82 |
| 3:U:3183[A]:LEU:H | 3:U:3184[A]:ASN:HA | 1.44 | 0.82 |
| 3:U:3183[B]:LEU:H | 3:U:3184[B]:ASN:HA | 1.44 | 0.82 |
| 3:X:3228[A]:VAL:HG21 | 3:X:3245[A]:PHE:CE2 | 2.14 | 0.82 |
| 3:d:2965[B]:LEU:HG | 3:d:2974[B]:ALA:HB1 | 1.61 | 0.82 |
| 3:d:3183[B]:LEU:H | 3:d:3184[B]:ASN:HA | 1.44 | 0.82 |
| 3:d:3230[B]:PHE:CB | 3:d:3243[B]:GLY:HA2 | 2.06 | 0.82 |
| 3:C:3089[A]:HIS:HE1 | 3:C:3119[A]:HIS:CD2 | 1.96 | 0.82 |
| 3:C:3147[B]:GLU:HG2 | 3:L:3161[B]:GLU:HA | 0.83 | 0.82 |
| 3:C:3153[B]:LYS:CE | 3:L:3158[B]:PHE:HD2 | 1.57 | 0.82 |
| 3:C:3183[A]:LEU:H | 3:C:3184[A]:ASN:HA | 1.44 | 0.82 |
| 3:F:2951[A]:ASP:OD2 | 3:F:2953[A]:GLY:HA2 | 1.79 | 0.82 |
| 3:F:2965[B]:LEU:CG | 3:F:2974[B]:ALA:HB1 | 2.09 | 0.82 |
| 3:F:2968[B]:GLN:CG | 3:a:2981[B]:GLY:H | 1.92 | 0.82 |
| 3:F:3163[B]:ASN:HB3 | 3:a:3150[B]:LYS:CE | 2.09 | 0.82 |
| 3:F:3259[B]:ASP:CG | 3:F:3260[B]:ARG:HG2 | 2.04 | 0.82 |
| 3:I:2951[A]:ASP:OD2 | 3:I:2953[A]:GLY:HA2 | 1.79 | 0.82 |
| 3:I:3120[B]:HIS:HA | 3:I:3123[B]:THR:OG1 | 1.79 | 0.82 |
| 3:L:2965[B]:LEU:CG | 3:L:2974[B]:ALA:HB1 | 2.09 | 0.82 |
| 3:L:3023[A]:ILE:O | 3:L:3026[A]:THR:N | 2.11 | 0.82 |
| 3:L:3259[B]:ASP:CG | 3:L:3260[B]:ARG:HG2 | 2.04 | 0.82 |
| 3:O:2951[A]:ASP:OD2 | 3:O:2953[A]:GLY:HA2 | 1.79 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3120[A]:HIS:HA | 3:O:3123[A]:THR:OG1 | 1.79 | 0.82 |
| 3:O:3216[A]:GLY:HA2 | 3:O:3262[A]:PHE:O | 1.78 | 0.82 |
| 3:O:3217[B]:PHE:HZ | 3:O:3230[B]:PHE:CE1 | 1.89 | 0.82 |
| 1:P:1584:GLY:HA3 | 1:S:329:ARG:HG2 | 1.61 | 0.82 |
| 3:R:3228[B]:VAL:HG21 | 3:R:3245[B]:PHE:CE2 | 2.14 | 0.82 |
| 3:R:3265[B]:ASP:OD1 | 3:R:3267[B]:SER:OG | 1.97 | 0.82 |
| 3:R:3298[A]:ASN:HB3 | 3:R:3300[A]:LEU:CD2 | 2.09 | 0.82 |
| 3:U:2948[A]:ASP:N | 3:U:2949[A]:LYS:HA | 1.81 | 0.82 |
| 3:U:2956[B]:LYS:O | 3:U:2960[B]:PHE:HE1 | 1.22 | 0.82 |
| 3:U:3089[B]:HIS:HE1 | 3:U:3119[B]:HIS:CD2 | 1.96 | 0.82 |
| 3:U:3298[A]:ASN:HB3 | 3:U:3300[A]:LEU:CD2 | 2.09 | 0.82 |
| 3:X:2989[B]:HIS:O | 3:X:2992[B]:TYR:N | 2.08 | 0.82 |
| 3:X:3173[B]:THR:HG22 | 3:X:3174[B]:GLY:N | 1.93 | 0.82 |
| 3:a:2951[B]:ASP:OD2 | 3:a:2953[B]:GLY:HA2 | 1.79 | 0.82 |
| 3:a:3259[B]:ASP:CG | 3:a:3260[B]:ARG:HG2 | 2.04 | 0.82 |
| 3:d:2956[A]:LYS:O | 3:d:2960[A]:PHE:HE1 | 1.22 | 0.82 |
| 1:A:497:GLN:HG2 | 1:A:683:THR:HG21 | 1.58 | 0.82 |
| 3:C:3153[B]:LYS:C | 3:L:3173[B]:THR:HA | 1.95 | 0.82 |
| 3:C:3223[B]:GLY:O | 3:L:3252[B]:TYR:CD1 | 2.33 | 0.82 |
| 3:C:3252[B]:TYR:HB2 | 3:L:3253[B]:GLU:HG2 | 1.61 | 0.82 |
| 3:F:2965[A]:LEU:HG | 3:F:2974[A]:ALA:HB1 | 1.61 | 0.82 |
| 3:F:3120[A]:HIS:HA | 3:F:3123[A]:THR:OG1 | 1.79 | 0.82 |
| 3:F:3189[A]:ASN:CG | 3:F:3191[A]:ASN:HD21 | 1.87 | 0.82 |
| 3:F:3216[A]:GLY:HA2 | 3:F:3262[A]:PHE:O | 1.78 | 0.82 |
| 3:I:2969[B]:TYR:HA | 3:R:2989[B]:HIS:CE1 | 2.14 | 0.82 |
| 3:I:3189[A]:ASN:CG | 3:I:3191[A]:ASN:HD21 | 1.87 | 0.82 |
| 3:I:3228[B]:VAL:HG21 | 3:I:3245[B]:PHE:CE2 | 2.14 | 0.82 |
| 3:L:2965[B]:LEU:HG | 3:L:2974[B]:ALA:HB1 | 1.61 | 0.82 |
| 3:L:3298[B]:ASN:HB3 | 3:L:3300[B]:LEU:CD2 | 2.09 | 0.82 |
| 3:O:2965[B]:LEU:CG | 3:O:2974[B]:ALA:HB1 | 2.09 | 0.82 |
| 3:O:2969[B]:TYR:HB2 | 3:X:3158[B]:PHE:CD1 | 2.13 | 0.82 |
| 3:O:3298[B]:ASN:HB3 | 3:O:3300[B]:LEU:CD2 | 2.09 | 0.82 |
| 3:R:2951[B]:ASP:OD2 | 3:R:2953[B]:GLY:HA2 | 1.79 | 0.82 |
| 1:S:1498:ASN:OD1 | 5:AA:1:NAG:H82 | 1.79 | 0.82 |
| 3:U:3089[A]:HIS:HE1 | 3:U:3119[A]:HIS:CD2 | 1.96 | 0.82 |
| 3:X:3189[B]:ASN:CG | 3:X:3191[B]:ASN:HD21 | 1.87 | 0.82 |
| 3:X:3298[A]:ASN:HB3 | 3:X:3300[A]:LEU:CD2 | 2.10 | 0.82 |
| 3:a:3120[B]:HIS:HA | 3:a:3123[B]:THR:OG1 | 1.79 | 0.82 |
| 3:a:3183[B]:LEU:H | 3:a:3184[B]:ASN:HA | 1.44 | 0.82 |
| 3:d:3189[A]:ASN:CG | 3:d:3191[A]:ASN:HD21 | 1.87 | 0.82 |
| 3:d:3228[A]:VAL:HG21 | 3:d:3245[A]:PHE:CE2 | 2.14 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:NA:1:NAG:H61 | 6:NA:2:NAG:HN2 | 1.44 | 0.82 |
| 3:C:2982[B]:MET:HB2 | 3:L:3156[B]:MET:HB3 | 1.59 | 0.82 |
| 3:C:3162[B]:ASP:CG | 3:L:3259[B]:ASP:OD2 | 2.16 | 0.82 |
| 2:E:2161:GLN:OE1 | 2:E:2345:ASN:ND2 | 2.13 | 0.82 |
| 3:F:2951[B]:ASP:OD2 | 3:F:2953[B]:GLY:HA2 | 1.79 | 0.82 |
| 3:F:2992[B]:TYR:CE2 | 3:a:2969[B]:TYR:HE1 | 1.96 | 0.82 |
| 3:F:3284[B]:LYS:HD3 | 3:F:3285[B]:VAL:H | 1.39 | 0.82 |
| 3:I:2965[A]:LEU:CG | 3:I:2974[A]:ALA:HB1 | 2.09 | 0.82 |
| 3:I:2965[B]:LEU:CG | 3:I:2974[B]:ALA:HB1 | 2.09 | 0.82 |
| 3:I:2966[B]:SER:CA | 3:R:3256[B]:TRP:HB3 | 2.08 | 0.82 |
| 3:I:2989[B]:HIS:NE2 | 3:R:2970[B]:PRO:CD | 2.39 | 0.82 |
| 3:I:3093[B]:HIS:HD2 | 3:R:2973[B]:THR:OG1 | 1.62 | 0.82 |
| 3:I:3173[A]:THR:HG22 | 3:I:3174[A]:GLY:N | 1.93 | 0.82 |
| 3:L:2951[B]:ASP:OD2 | 3:L:2953[B]:GLY:HA2 | 1.79 | 0.82 |
| 3:L:2956[B]:LYS:O | 3:L:2960[B]:PHE:HE1 | 1.22 | 0.82 |
| 3:L:3216[A]:GLY:HA2 | 3:L:3262[A]:PHE:O | 1.78 | 0.82 |
| 3:L:3265[B]:ASP:OD1 | 3:L:3267[B]:SER:OG | 1.97 | 0.82 |
| 3:O:3212[B]:ARG:HH11 | 3:O:3212[B]:ARG:HG3 | 1.43 | 0.82 |
| 3:R:3176[A]:LYS:HE2 | 3:R:3176[A]:LYS:H | 1.43 | 0.82 |
| 3:U:2952[B]:ALA:HB3 | 3:U:2953[B]:GLY:CA | 2.10 | 0.82 |
| 3:U:3120[B]:HIS:HA | 3:U:3123[B]:THR:OG1 | 1.79 | 0.82 |
| 3:a:3228[A]:VAL:HG21 | 3:a:3245[A]:PHE:CE2 | 2.14 | 0.82 |
| 3:a:3265[A]:ASP:OD1 | 3:a:3267[A]:SER:OG | 1.97 | 0.82 |
| 3:d:3089[B]:HIS:HE1 | 3:d:3119[B]:HIS:CD2 | 1.96 | 0.82 |
| 3:d:3228[B]:VAL:HG21 | 3:d:3245[B]:PHE:CE2 | 2.14 | 0.82 |
| 3:C:2952[B]:ALA:HB3 | 3:C:2953[B]:GLY:CA | 2.10 | 0.82 |
| 3:F:2965[B]:LEU:HD12 | 3:a:3256[B]:TRP:NE1 | 1.94 | 0.82 |
| 3:F:3154[B]:PRO:HD3 | 3:a:3173[B]:THR:C | 2.05 | 0.82 |
| 3:F:3251[B]:ASP:HB2 | 3:a:3251[B]:ASP:HB3 | 1.54 | 0.82 |
| 3:I:2965[B]:LEU:CD2 | 3:I:2974[B]:ALA:HB1 | 2.10 | 0.82 |
| 3:I:2983[B]:VAL:HG23 | 3:R:3160[B]:SER:OG | 1.78 | 0.82 |
| 3:L:3173[B]:THR:HG22 | 3:L:3174[B]:GLY:N | 1.93 | 0.82 |
| 3:O:2951[B]:ASP:OD2 | 3:O:2953[B]:GLY:HA2 | 1.79 | 0.82 |
| 3:O:2965[A]:LEU:CG | 3:O:2974[A]:ALA:HB1 | 2.09 | 0.82 |
| 3:O:3120[B]:HIS:HA | 3:O:3123[B]:THR:OG1 | 1.79 | 0.82 |
| 3:O:3173[A]:THR:HG22 | 3:O:3174[A]:GLY:N | 1.93 | 0.82 |
| 3:O:3253[B]:GLU:HG3 | 3:X:3160[B]:SER:CA | 2.08 | 0.82 |
| 3:U:3173[B]:THR:HG22 | 3:U:3174[B]:GLY:N | 1.93 | 0.82 |
| 3:X:2951[B]:ASP:OD2 | 3:X:2953[B]:GLY:HA2 | 1.79 | 0.82 |
| 2:Z:2867:PRO:HG2 | 3:a:2932[A]:PRO:HG2 | 0.83 | 0.82 |
| 3:a:2965[B]:LEU:CG | 3:a:2974[B]:ALA:HB1 | 2.09 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2951[A]:ASP:OD2 | 3:d:2953[A]:GLY:HA2 | 1.79 | 0.82 |
| 3:d:3183[A]:LEU:H | 3:d:3184[A]:ASN:HA | 1.44 | 0.82 |
| 3:C:2952[A]:ALA:HB3 | 3:C:2953[A]:GLY:CA | 2.10 | 0.82 |
| 3:C:2956[B]:LYS:O | 3:C:2960[B]:PHE:CD1 | 2.33 | 0.82 |
| 3:C:3172[B]:SER:CB | 3:L:3149[B]:ASN:O | 2.27 | 0.82 |
| 3:C:3173[B]:THR:HG22 | 3:C:3174[B]:GLY:N | 1.93 | 0.82 |
| 3:C:3216[A]:GLY:HA2 | 3:C:3262[A]:PHE:O | 1.78 | 0.82 |
| 3:C:3259[B]:ASP:CG | 3:C:3260[B]:ARG:HG2 | 2.04 | 0.82 |
| 3:C:3265[B]:ASP:OD1 | 3:C:3267[B]:SER:OG | 1.97 | 0.82 |
| 3:F:3089[A]:HIS:HE1 | 3:F:3119[A]:HIS:CD2 | 1.96 | 0.82 |
| 3:F:3189[B]:ASN:CG | 3:F:3191[B]:ASN:HD21 | 1.88 | 0.82 |
| 3:I:2979[B]:GLN:C | 3:R:2967[B]:CYS:HB3 | 1.96 | 0.82 |
| 3:I:3153[B]:LYS:CG | 3:R:3155[B]:MET:CB | 2.55 | 0.82 |
| 3:I:3189[B]:ASN:CG | 3:I:3191[B]:ASN:HD21 | 1.87 | 0.82 |
| 3:I:3248[B]:LEU:CD1 | 3:R:2973[B]:THR:HG23 | 2.06 | 0.82 |
| 3:L:3120[B]:HIS:HA | 3:L:3123[B]:THR:OG1 | 1.79 | 0.82 |
| 3:O:2965[B]:LEU:HB3 | 3:X:3254[B]:MET:CE | 2.02 | 0.82 |
| 3:O:2965[B]:LEU:CD2 | 3:O:2974[B]:ALA:HB1 | 2.10 | 0.82 |
| 3:O:3023[B]:ILE:O | 3:O:3026[B]:THR:N | 2.11 | 0.82 |
| 3:O:3228[B]:VAL:HG21 | 3:O:3245[B]:PHE:CE2 | 2.14 | 0.82 |
| 3:R:3173[B]:THR:HG22 | 3:R:3174[B]:GLY:N | 1.93 | 0.82 |
| 3:U:2951[B]:ASP:OD2 | 3:U:2953[B]:GLY:HA2 | 1.79 | 0.82 |
| 3:U:3259[A]:ASP:CG | 3:U:3260[A]:ARG:HG2 | 2.04 | 0.82 |
| 3:X:2965[B]:LEU:CG | 3:X:2974[B]:ALA:HB1 | 2.09 | 0.82 |
| 1:Y:1576:THR:HG22 | 3:d:3196[B]:THR:CG2 | 2.10 | 0.82 |
| 1:Y:1655:SER:O | 3:d:3006[B]:LYS:NZ | 2.13 | 0.82 |
| 3:a:3120[A]:HIS:HA | 3:a:3123[A]:THR:OG1 | 1.79 | 0.82 |
| 3:a:3216[B]:GLY:HA2 | 3:a:3262[B]:PHE:O | 1.78 | 0.82 |
| 3:d:2955[A]:GLN:CD | 3:d:3037[A]:TYR:CE1 | 2.55 | 0.82 |
| 3:d:3023[B]:ILE:O | 3:d:3026[B]:THR:N | 2.11 | 0.82 |
| 3:F:2952[A]:ALA:HB3 | 3:F:2953[A]:GLY:CA | 2.10 | 0.82 |
| 3:I:2956[A]:LYS:O | 3:I:2960[A]:PHE:CD1 | 2.33 | 0.82 |
| 3:L:3228[B]:VAL:HG21 | 3:L:3245[B]:PHE:CE2 | 2.14 | 0.82 |
| 3:O:2965[B]:LEU:H | 3:X:3254[B]:MET:CE | 1.92 | 0.82 |
| 3:R:3216[A]:GLY:HA2 | 3:R:3262[A]:PHE:O | 1.78 | 0.82 |
| 1:S:979:LEU:HB3 | 1:S:980:TYR:HA | 1.61 | 0.82 |
| 3:U:2951[A]:ASP:OD2 | 3:U:2953[A]:GLY:HA2 | 1.79 | 0.82 |
| 3:d:3216[A]:GLY:HA2 | 3:d:3262[A]:PHE:O | 1.78 | 0.82 |
| 1:A:883:CYS:N | 1:A:894:CYS:SG | 2.53 | 0.82 |
| 3:C:2965[B]:LEU:CG | 3:C:2974[B]:ALA:HB1 | 2.09 | 0.82 |
| 3:C:3196[A]:THR:H | 3:C:3199[A]:GLN:HB2 | 1.37 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3212[A]:ARG:HG3 | 3:C:3212[A]:ARG:HH11 | 1.43 | 0.82 |
| 3:C:3228[B]:VAL:HG21 | 3:C:3245[B]:PHE:CE2 | 2.14 | 0.82 |
| 3:C:3265[A]:ASP:OD1 | 3:C:3267[A]:SER:OG | 1.97 | 0.82 |
| 3:C:3298[B]:ASN:HB3 | 3:C:3300[B]:LEU:CD2 | 2.09 | 0.82 |
| 3:F:3154[B]:PRO:HG3 | 3:a:3174[B]:GLY:HA2 | 1.62 | 0.82 |
| 3:I:2952[B]:ALA:HB3 | 3:I:2953[B]:GLY:CA | 2.10 | 0.82 |
| 3:I:2966[B]:SER:O | 3:R:3256[B]:TRP:HB3 | 1.80 | 0.82 |
| 3:L:3027[A]:GLU:OE2 | 3:L:3028[A]:PRO:HD2 | 1.80 | 0.82 |
| 3:O:3027[A]:GLU:OE2 | 3:O:3028[A]:PRO:HD2 | 1.80 | 0.82 |
| 3:O:3183[A]:LEU:H | 3:O:3184[A]:ASN:HA | 1.44 | 0.82 |
| 3:R:2951[A]:ASP:OD2 | 3:R:2953[A]:GLY:HA2 | 1.79 | 0.82 |
| 3:R:3298[B]:ASN:HB3 | 3:R:3300[B]:LEU:CD2 | 2.09 | 0.82 |
| 3:U:3104[A]:MET:CA | 3:U:3110[A]:THR:HG23 | 2.10 | 0.82 |
| 3:X:3089[A]:HIS:HE1 | 3:X:3119[A]:HIS:CD2 | 1.96 | 0.82 |
| 3:a:2956[A]:LYS:O | 3:a:2960[A]:PHE:CD1 | 2.33 | 0.82 |
| 3:d:2952[B]:ALA:HB3 | 3:d:2953[B]:GLY:CA | 2.10 | 0.82 |
| 3:d:3259[A]:ASP:CG | 3:d:3260[A]:ARG:HG2 | 2.04 | 0.82 |
| 3:C:2956[B]:LYS:O | 3:C:2960[B]:PHE:HE1 | 1.22 | 0.82 |
| 3:C:3161[B]:GLU:OE2 | 3:L:2983[B]:VAL:CB | 2.04 | 0.82 |
| 3:C:3173[A]:THR:HG22 | 3:C:3174[A]:GLY:N | 1.93 | 0.82 |
| 3:C:3223[B]:GLY:O | 3:L:3252[B]:TYR:CE2 | 2.33 | 0.82 |
| 3:C:3259[A]:ASP:CG | 3:C:3260[A]:ARG:HG2 | 2.04 | 0.82 |
| 3:F:2972[B]:GLY:HA3 | 3:a:3090[B]:ASN:CB | 2.08 | 0.82 |
| 3:I:2967[B]:CYS:SG | 3:R:2982[B]:MET:CE | 2.67 | 0.82 |
| 3:I:2968[B]:GLN:NE2 | 3:R:3086[B]:GLU:CG | 1.86 | 0.82 |
| 3:I:2985[B]:PHE:CZ | 3:R:2970[B]:PRO:HA | 2.15 | 0.82 |
| 3:I:3173[B]:THR:HG22 | 3:I:3174[B]:GLY:N | 1.93 | 0.82 |
| 3:I:3265[A]:ASP:OD1 | 3:I:3267[A]:SER:OG | 1.97 | 0.82 |
| 3:L:3189[A]:ASN:CG | 3:L:3191[A]:ASN:HD21 | 1.87 | 0.82 |
| 2:N:2868:GLU:OE2 | 3:O:2932[A]:PRO:C | 2.15 | 0.82 |
| 3:O:2965[A]:LEU:CD2 | 3:O:2974[A]:ALA:HB1 | 2.10 | 0.82 |
| 3:O:3154[B]:PRO:HD2 | 3:X:3176[B]:LYS:HE3 | 1.61 | 0.82 |
| 3:O:3183[B]:LEU:H | 3:O:3184[B]:ASN:HA | 1.44 | 0.82 |
| 3:O:3189[B]:ASN:CG | 3:O:3191[B]:ASN:HD21 | 1.87 | 0.82 |
| 3:U:2956[B]:LYS:O | 3:U:2960[B]:PHE:CD1 | 2.33 | 0.82 |
| 3:U:3150[B]:LYS:O | 3:d:3153[B]:LYS:HG2 | 1.80 | 0.82 |
| 3:U:3189[A]:ASN:CG | 3:U:3191[A]:ASN:HD21 | 1.87 | 0.82 |
| 3:X:2956[B]:LYS:O | 3:X:2960[B]:PHE:CD1 | 2.33 | 0.82 |
| 3:X:3298[B]:ASN:HB3 | 3:X:3300[B]:LEU:CD2 | 2.10 | 0.82 |
| 3:d:2948[B]:ASP:N | 3:d:2949[B]:LYS:CA | 2.41 | 0.82 |
| 3:d:3259[B]:ASP:CG | 3:d:3260[B]:ARG:HG2 | 2.04 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3158[B]:PHE:O | 3:L:3149[B]:ASN:HB2 | 1.80 | 0.81 |
| 3:C:3230[B]:PHE:CB | 3:C:3243[B]:GLY:HA2 | 2.06 | 0.81 |
| 3:I:2965[A]:LEU:CD2 | 3:I:2974[A]:ALA:HB1 | 2.10 | 0.81 |
| 3:I:2979[B]:GLN:CG | 3:I:3155[B]:MET:CE | 2.56 | 0.81 |
| 3:I:3027[B]:GLU:OE2 | 3:I:3028[B]:PRO:HD2 | 1.80 | 0.81 |
| 2:K:2409:ALA:HB2 | 2:K:2468:ILE:HD12 | 1.59 | 0.81 |
| 3:L:2948[A]:ASP:N | 3:L:2949[A]:LYS:CA | 2.41 | 0.81 |
| 3:L:2965[B]:LEU:CD2 | 3:L:2974[B]:ALA:HB1 | 2.10 | 0.81 |
| 3:O:3255[B]:PRO:HB3 | 3:X:3161[B]:GLU:O | 1.79 | 0.81 |
| 3:O:3298[A]:ASN:HB3 | 3:O:3300[A]:LEU:CD2 | 2.09 | 0.81 |
| 3:R:3023[A]:ILE:O | 3:R:3026[A]:THR:N | 2.11 | 0.81 |
| 3:U:2955[A]:GLN:CD | 3:U:3037[A]:TYR:CE1 | 2.55 | 0.81 |
| 3:U:2956[A]:LYS:O | 3:U:2960[A]:PHE:CD1 | 2.33 | 0.81 |
| 3:U:3254[B]:MET:HE2 | 3:d:3254[B]:MET:HE3 | 1.55 | 0.81 |
| 3:U:3298[B]:ASN:HB3 | 3:U:3300[B]:LEU:CD2 | 2.09 | 0.81 |
| 2:W:2556:TYR:HE1 | 2:W:2845:PRO:HD2 | 1.44 | 0.81 |
| 3:X:3183[B]:LEU:H | 3:X:3184[B]:ASN:HA | 1.44 | 0.81 |
| 3:X:3228[B]:VAL:HG21 | 3:X:3245[B]:PHE:CE2 | 2.14 | 0.81 |
| 3:a:2948[B]:ASP:N | 3:a:2949[B]:LYS:CA | 2.41 | 0.81 |
| 3:a:2955[A]:GLN:CD | 3:a:3037[A]:TYR:CE1 | 2.55 | 0.81 |
| 3:a:2965[A]:LEU:HG | 3:a:2974[A]:ALA:HB1 | 1.61 | 0.81 |
| 3:a:3216[A]:GLY:HA2 | 3:a:3262[A]:PHE:O | 1.78 | 0.81 |
| 3:a:3293[B]:LYS:CD | 3:a:3294[B]:SER:CB | 2.53 | 0.81 |
| 3:d:2965[B]:LEU:CG | 3:d:2974[B]:ALA:HB1 | 2.09 | 0.81 |
| 3:C:3104[A]:MET:CA | 3:C:3110[A]:THR:HG23 | 2.10 | 0.81 |
| 3:F:3120[B]:HIS:HA | 3:F:3123[B]:THR:OG1 | 1.79 | 0.81 |
| 3:F:3147[B]:GLU:CD | 3:a:3163[B]:ASN:N | 2.36 | 0.81 |
| 3:I:3255[B]:PRO:HG3 | 3:R:2964[B]:PRO:N | 1.95 | 0.81 |
| 3:I:3298[B]:ASN:HB3 | 3:I:3300[B]:LEU:CD2 | 2.09 | 0.81 |
| 3:R:2956[B]:LYS:O | 3:R:2960[B]:PHE:CD1 | 2.33 | 0.81 |
| 3:R:2979[B]:GLN:CG | 3:R:3155[B]:MET:CE | 2.56 | 0.81 |
| 3:U:2963[B]:MET:N | 3:U:3108[B]:HIS:O | 2.13 | 0.81 |
| 3:U:3173[B]:THR:CG2 | 3:d:3152[B]:LYS:C | 2.49 | 0.81 |
| 3:X:2965[B]:LEU:HG | 3:X:2974[B]:ALA:HB1 | 1.61 | 0.81 |
| 3:a:2939[B]:ARG:HB3 | 3:a:3032[B]:PRO:HG2 | 1.63 | 0.81 |
| 3:a:2952[B]:ALA:HB3 | 3:a:2953[B]:GLY:CA | 2.10 | 0.81 |
| 3:a:3189[B]:ASN:CG | 3:a:3191[B]:ASN:HD21 | 1.87 | 0.81 |
| 3:a:3259[A]:ASP:CG | 3:a:3260[A]:ARG:HG2 | 2.04 | 0.81 |
| 3:d:3104[B]:MET:CA | 3:d:3110[B]:THR:HG23 | 2.10 | 0.81 |
| 3:d:3189[B]:ASN:CG | 3:d:3191[B]:ASN:HD21 | 1.87 | 0.81 |
| 3:d:3212[B]:ARG:HG3 | 3:d:3212[B]:ARG:HH11 | 1.43 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2974[B]:ALA:HB3 | 3:L:3249[B]:GLY:HA2 | 0.81 | 0.81 |
| 3:C:2979[B]:GLN:CG | 3:C:3155[B]:MET:CE | 2.56 | 0.81 |
| 3:C:3027[B]:GLU:OE2 | 3:C:3028[B]:PRO:HD2 | 1.80 | 0.81 |
| 3:C:3120[A]:HIS:HA | 3:C:3123[A]:THR:OG1 | 1.79 | 0.81 |
| 3:C:3149[B]:ASN:O | 3:L:3172[B]:SER:CB | 2.29 | 0.81 |
| 3:C:3172[B]:SER:CB | 3:L:3150[B]:LYS:C | 2.53 | 0.81 |
| 3:C:3176[B]:LYS:HE2 | 3:C:3176[B]:LYS:H | 1.43 | 0.81 |
| 3:C:3228[A]:VAL:HG21 | 3:C:3245[A]:PHE:CE2 | 2.14 | 0.81 |
| 3:F:2952[B]:ALA:HB3 | 3:F:2953[B]:GLY:CA | 2.10 | 0.81 |
| 3:F:2955[B]:GLN:CD | 3:F:3037[B]:TYR:CE1 | 2.55 | 0.81 |
| 3:F:2961[B]:HIS:CA | 3:a:2975[B]:PHE:HZ | 1.89 | 0.81 |
| 3:F:2963[A]:MET:N | 3:F:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:F:2971[B]:ASP:N | 9:F:3401[B]:CUO:O2 | 2.14 | 0.81 |
| 3:F:3173[A]:THR:HG22 | 3:F:3174[A]:GLY:N | 1.93 | 0.81 |
| 3:F:3176[A]:LYS:HE2 | 3:F:3176[A]:LYS:H | 1.43 | 0.81 |
| 3:F:3298[B]:ASN:HB3 | 3:F:3300[B]:LEU:CD2 | 2.09 | 0.81 |
| 3:I:2962[B]:GLY:O | 3:R:3255[B]:PRO:HD3 | 1.79 | 0.81 |
| 3:I:2963[B]:MET:N | 3:I:3108[B]:HIS:O | 2.14 | 0.81 |
| 3:I:3176[B]:LYS:HE2 | 3:I:3176[B]:LYS:H | 1.43 | 0.81 |
| 3:I:3298[A]:ASN:HB3 | 3:I:3300[A]:LEU:CD2 | 2.09 | 0.81 |
| 3:L:3027[B]:GLU:OE2 | 3:L:3028[B]:PRO:HD2 | 1.80 | 0.81 |
| 3:L:3120[A]:HIS:HA | 3:L:3123[A]:THR:OG1 | 1.79 | 0.81 |
| 3:L:3183[B]:LEU:H | 3:L:3184[B]:ASN:HA | 1.44 | 0.81 |
| 3:O:2939[B]:ARG:HB3 | 3:O:3032[B]:PRO:HG2 | 1.63 | 0.81 |
| 3:O:2963[A]:MET:N | 3:O:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:O:2965[B]:LEU:HG | 3:O:2974[B]:ALA:HB1 | 1.61 | 0.81 |
| 3:O:3228[A]:VAL:HG21 | 3:O:3245[A]:PHE:CE2 | 2.14 | 0.81 |
| 3:R:2952[A]:ALA:HB3 | 3:R:2953[A]:GLY:CA | 2.09 | 0.81 |
| 3:R:2952[B]:ALA:HB3 | 3:R:2953[B]:GLY:CA | 2.10 | 0.81 |
| 3:R:2965[A]:LEU:CD2 | 3:R:2974[A]:ALA:HB1 | 2.10 | 0.81 |
| 3:R:3027[B]:GLU:OE2 | 3:R:3028[B]:PRO:HD2 | 1.80 | 0.81 |
| 3:R:3120[B]:HIS:HA | 3:R:3123[B]:THR:OG1 | 1.79 | 0.81 |
| 3:R:3176[B]:LYS:HE2 | 3:R:3176[B]:LYS:H | 1.43 | 0.81 |
| 3:R:3265[A]:ASP:OD1 | 3:R:3267[A]:SER:OG | 1.97 | 0.81 |
| 3:U:2963[A]:MET:N | 3:U:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:U:2965[B]:LEU:HG | 3:U:2974[B]:ALA:HB1 | 1.61 | 0.81 |
| 3:U:3169[B]:LYS:O | 3:d:3148[B]:ILE:CA | 2.27 | 0.81 |
| 3:U:3216[A]:GLY:HA2 | 3:U:3262[A]:PHE:O | 1.78 | 0.81 |
| 1:V:589:GLN:HG2 | 1:V:594:ASP:HB3 | 1.62 | 0.81 |
| 3:X:2965[B]:LEU:CD2 | 3:X:2974[B]:ALA:HB1 | 2.10 | 0.81 |
| 3:X:3176[B]:LYS:HB3 | 3:X:3176[B]:LYS:HZ2 | 1.42 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3259[B]:ASP:CG | 3:X:3260[B]:ARG:HG2 | 2.04 | 0.81 |
| 3:a:3023[B]:ILE:O | 3:a:3026[B]:THR:N | 2.11 | 0.81 |
| 3:a:3189[A]:ASN:CG | 3:a:3191[A]:ASN:HD21 | 1.87 | 0.81 |
| 3:a:3212[A]:ARG:HG3 | 3:a:3212[A]:ARG:HH11 | 1.43 | 0.81 |
| 3:a:3228[B]:VAL:HG21 | 3:a:3245[B]:PHE:CE2 | 2.14 | 0.81 |
| 3:a:3230[A]:PHE:CB | 3:a:3243[A]:GLY:HA2 | 2.06 | 0.81 |
| 3:d:3120[A]:HIS:HA | 3:d:3123[A]:THR:OG1 | 1.79 | 0.81 |
| 3:d:3298[A]:ASN:HB3 | 3:d:3300[A]:LEU:CD2 | 2.09 | 0.81 |
| 3:C:3155[B]:MET:HG2 | 3:L:3154[B]:PRO:O | 1.81 | 0.81 |
| 3:C:3161[B]:GLU:HG3 | 3:L:3146[B]:CYS:C | 2.06 | 0.81 |
| 3:F:2948[A]:ASP:N | 3:F:2949[A]:LYS:CA | 2.41 | 0.81 |
| 3:F:2965[A]:LEU:CD2 | 3:F:2974[A]:ALA:HB1 | 2.10 | 0.81 |
| 3:F:2966[B]:SER:OG | 3:a:3255[B]:PRO:O | 1.99 | 0.81 |
| 3:F:2977[B]:CYS:O | 3:a:3254[B]:MET:HE3 | 0.92 | 0.81 |
| 3:F:3150[B]:LYS:HZ3 | 3:a:3160[B]:SER:HB3 | 1.02 | 0.81 |
| 3:F:3161[B]:GLU:HA | 3:a:3147[B]:GLU:HG3 | 1.61 | 0.81 |
| 3:F:3248[B]:LEU:HB3 | 3:a:2972[B]:GLY:C | 2.05 | 0.81 |
| 3:F:3298[A]:ASN:HB3 | 3:F:3300[A]:LEU:CD2 | 2.10 | 0.81 |
| 3:I:2983[B]:VAL:CB | 3:R:3160[B]:SER:HA | 2.09 | 0.81 |
| 3:L:2952[A]:ALA:HB3 | 3:L:2953[A]:GLY:CA | 2.10 | 0.81 |
| 3:L:2952[B]:ALA:HB3 | 3:L:2953[B]:GLY:CA | 2.09 | 0.81 |
| 3:O:2963[B]:MET:N | 3:O:3108[B]:HIS:O | 2.13 | 0.81 |
| 3:O:3109[B]:TYR:CE2 | 3:X:2969[B]:TYR:C | 2.58 | 0.81 |
| 3:O:3189[A]:ASN:CG | 3:O:3191[A]:ASN:HD21 | 1.87 | 0.81 |
| 3:R:3089[B]:HIS:HE1 | 3:R:3119[B]:HIS:CD2 | 1.96 | 0.81 |
| 3:R:3212[A]:ARG:HG3 | 3:R:3212[A]:ARG:HH11 | 1.43 | 0.81 |
| 3:R:3228[A]:VAL:HG21 | 3:R:3245[A]:PHE:CE2 | 2.14 | 0.81 |
| 2:T:2545:SER:HA | 2:T:2546:LEU:HB2 | 1.62 | 0.81 |
| 3:U:2975[B]:PHE:CG | 3:d:3256[B]:TRP:CG | 2.67 | 0.81 |
| 3:U:3162[B]:ASP:HA | 3:d:3260[B]:ARG:HH12 | 1.43 | 0.81 |
| 3:U:3228[A]:VAL:HG21 | 3:U:3245[A]:PHE:CE2 | 2.14 | 0.81 |
| 3:X:2948[A]:ASP:N | 3:X:2949[A]:LYS:CA | 2.41 | 0.81 |
| 3:X:2969[B]:TYR:CE2 | 3:X:2970[B]:PRO:HG2 | 2.05 | 0.81 |
| 3:X:3120[A]:HIS:HA | 3:X:3123[A]:THR:OG1 | 1.79 | 0.81 |
| 3:X:3120[B]:HIS:HA | 3:X:3123[B]:THR:OG1 | 1.79 | 0.81 |
| 3:X:3189[A]:ASN:CG | 3:X:3191[A]:ASN:HD21 | 1.87 | 0.81 |
| 3:a:3104[A]:MET:CA | 3:a:3110[A]:THR:HG23 | 2.10 | 0.81 |
| 3:a:3298[B]:ASN:HB3 | 3:a:3300[B]:LEU:CD2 | 2.10 | 0.81 |
| 3:C:2939[A]:ARG:HB3 | 3:C:3032[A]:PRO:HG2 | 1.63 | 0.81 |
| 3:C:2939[B]:ARG:HB3 | 3:C:3032[B]:PRO:HG2 | 1.63 | 0.81 |
| 3:C:2979[B]:GLN:HG3 | 3:L:3156[B]:MET:SD | 2.20 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3023[A]:ILE:O | 3:C:3026[A]:THR:N | 2.11 | 0.81 |
| 3:C:3189[A]:ASN:CG | 3:C:3191[A]:ASN:HD21 | 1.87 | 0.81 |
| 3:F:3027[B]:GLU:OE2 | 3:F:3028[B]:PRO:HD2 | 1.80 | 0.81 |
| 3:I:3027[A]:GLU:OE2 | 3:I:3028[A]:PRO:HD2 | 1.80 | 0.81 |
| 3:I:3120[A]:HIS:HA | 3:I:3123[A]:THR:OG1 | 1.79 | 0.81 |
| 3:L:2963[A]:MET:N | 3:L:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:L:3212[A]:ARG:HH11 | 3:L:3212[A]:ARG:HG3 | 1.43 | 0.81 |
| 3:L:3284[B]:LYS:HD3 | 3:L:3285[B]:VAL:H | 1.39 | 0.81 |
| 3:L:3298[A]:ASN:HB3 | 3:L:3300[A]:LEU:CD2 | 2.09 | 0.81 |
| 3:O:2955[A]:GLN:CD | 3:O:3037[A]:TYR:CE1 | 2.55 | 0.81 |
| 3:O:3265[B]:ASP:OD1 | 3:O:3267[B]:SER:OG | 1.97 | 0.81 |
| 1:P:387:ASN:ND2 | 6:3:1:NAG:O7 | 2.13 | 0.81 |
| 3:R:2963[B]:MET:N | 3:R:3108[B]:HIS:O | 2.14 | 0.81 |
| 3:R:3183[A]:LEU:H | 3:R:3184[A]:ASN:HA | 1.44 | 0.81 |
| 3:R:3183[B]:LEU:H | 3:R:3184[B]:ASN:HA | 1.44 | 0.81 |
| 3:R:3216[B]:GLY:HA2 | 3:R:3262[B]:PHE:O | 1.78 | 0.81 |
| 3:U:2967[B]:CYS:HB2 | 3:d:3256[B]:TRP:HB2 | 1.61 | 0.81 |
| 3:a:2963[A]:MET:N | 3:a:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:a:2963[B]:MET:N | 3:a:3108[B]:HIS:O | 2.13 | 0.81 |
| 3:d:2952[A]:ALA:HB3 | 3:d:2953[A]:GLY:CA | 2.10 | 0.81 |
| 3:d:3027[A]:GLU:OE2 | 3:d:3028[A]:PRO:HD2 | 1.80 | 0.81 |
| 3:C:2955[A]:GLN:CD | 3:C:3037[A]:TYR:CE1 | 2.55 | 0.81 |
| 3:F:3255[B]:PRO:C | 3:a:2966[B]:SER:N | 2.38 | 0.81 |
| 3:I:3154[B]:PRO:HD2 | 3:R:3155[B]:MET:SD | 2.21 | 0.81 |
| 3:I:3160[B]:SER:CB | 3:R:3150[B]:LYS:HZ3 | 1.91 | 0.81 |
| 3:I:3183[B]:LEU:H | 3:I:3184[B]:ASN:HA | 1.44 | 0.81 |
| 3:I:3228[A]:VAL:HG21 | 3:I:3245[A]:PHE:CE2 | 2.14 | 0.81 |
| 3:I:3265[B]:ASP:OD1 | 3:I:3267[B]:SER:OG | 1.97 | 0.81 |
| 1:J:401:VAL:HG22 | 1:J:662:SER:HB3 | 1.62 | 0.81 |
| 3:L:2951[A]:ASP:OD2 | 3:L:2953[A]:GLY:HA2 | 1.79 | 0.81 |
| 3:L:3259[A]:ASP:CG | 3:L:3260[A]:ARG:HG2 | 2.04 | 0.81 |
| 3:O:3160[B]:SER:HB2 | 3:X:3151[B]:LEU:N | 1.80 | 0.81 |
| 3:O:3259[B]:ASP:CG | 3:O:3260[B]:ARG:HG2 | 2.04 | 0.81 |
| 3:R:3189[A]:ASN:CG | 3:R:3191[A]:ASN:HD21 | 1.87 | 0.81 |
| 3:R:3212[B]:ARG:HH11 | 3:R:3212[B]:ARG:HG3 | 1.43 | 0.81 |
| 1:S:527:LEU:O | 1:S:561:ARG:NH1 | 2.12 | 0.81 |
| 3:X:2963[B]:MET:N | 3:X:3108[B]:HIS:O | 2.13 | 0.81 |
| 3:a:2952[A]:ALA:HB3 | 3:a:2953[A]:GLY:CA | 2.10 | 0.81 |
| 3:a:3176[B]:LYS:H | 3:a:3176[B]:LYS:HE2 | 1.43 | 0.81 |
| 3:d:2963[A]:MET:N | 3:d:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:d:3027[B]:GLU:OE2 | 3:d:3028[B]:PRO:HD2 | 1.80 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3120[B]:HIS:HA | 3:d:3123[B]:THR:OG1 | 1.79 | 0.81 |
| 3:C:2956[A]:LYS:O | 3:C:2960[A]:PHE:CD1 | 2.33 | 0.81 |
| 3:C:2963[A]:MET:N | 3:C:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:C:3176[A]:LYS:HE2 | 3:C:3176[A]:LYS:H | 1.43 | 0.81 |
| 3:F:3025[A]:VAL:CG2 | 3:F:3047[A]:ARG:HH12 | 1.94 | 0.81 |
| 3:F:3025[B]:VAL:CG2 | 3:F:3047[B]:ARG:HH12 | 1.94 | 0.81 |
| 3:F:3265[A]:ASP:OD1 | 3:F:3267[A]:SER:OG | 1.97 | 0.81 |
| 3:I:3104[B]:MET:CA | 3:I:3110[B]:THR:HG23 | 2.10 | 0.81 |
| 3:I:3180[A]:TYR:O | 3:I:3183[A]:LEU:HD22 | 1.81 | 0.81 |
| 3:I:3216[A]:GLY:HA2 | 3:I:3262[A]:PHE:O | 1.78 | 0.81 |
| 3:O:2952[A]:ALA:HB3 | 3:O:2953[A]:GLY:CA | 2.09 | 0.81 |
| 3:O:3169[B]:LYS:CA | 3:X:3148[B]:ILE:HG21 | 2.10 | 0.81 |
| 3:O:3180[B]:TYR:O | 3:O:3183[B]:LEU:HD22 | 1.81 | 0.81 |
| 3:R:2939[A]:ARG:HB3 | 3:R:3032[A]:PRO:HG2 | 1.63 | 0.81 |
| 3:R:3027[A]:GLU:OE2 | 3:R:3028[A]:PRO:HD2 | 1.80 | 0.81 |
| 3:U:3265[B]:ASP:OD1 | 3:U:3267[B]:SER:OG | 1.97 | 0.81 |
| 2:W:2823:ILE:HG13 | 2:W:2830:GLN:HE22 | 1.46 | 0.81 |
| 3:X:2952[B]:ALA:HB3 | 3:X:2953[B]:GLY:CA | 2.10 | 0.81 |
| 3:X:2955[A]:GLN:CD | 3:X:3037[A]:TYR:CE1 | 2.55 | 0.81 |
| 3:X:3180[A]:TYR:O | 3:X:3183[A]:LEU:HD22 | 1.81 | 0.81 |
| 3:a:2951[A]:ASP:OD2 | 3:a:2953[A]:GLY:HA2 | 1.79 | 0.81 |
| 3:a:3212[B]:ARG:HH11 | 3:a:3212[B]:ARG:HG3 | 1.43 | 0.81 |
| 3:C:3149[B]:ASN:HB3 | 3:L:3163[B]:ASN:ND2 | 1.95 | 0.81 |
| 3:C:3180[A]:TYR:O | 3:C:3183[A]:LEU:HD22 | 1.81 | 0.81 |
| 1:D:1641:THR:HG21 | 1:D:1644:ILE:HD11 | 1.63 | 0.81 |
| 3:F:2956[B]:LYS:O | 3:F:2960[B]:PHE:CD1 | 2.33 | 0.81 |
| 3:F:2963[B]:MET:N | 3:F:3108[B]:HIS:O | 2.14 | 0.81 |
| 3:F:3101[A]:PRO:O | 3:F:3106[A]:THR:HG21 | 1.81 | 0.81 |
| 3:F:3104[A]:MET:CA | 3:F:3110[A]:THR:HG23 | 2.10 | 0.81 |
| 3:F:3157[B]:PRO:CB | 3:a:2982[B]:MET:SD | 2.68 | 0.81 |
| 3:I:2963[A]:MET:N | 3:I:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:I:3172[B]:SER:CB | 3:R:3150[B]:LYS:O | 2.29 | 0.81 |
| 3:I:3180[B]:TYR:O | 3:I:3183[B]:LEU:HD22 | 1.81 | 0.81 |
| 3:L:2955[B]:GLN:CD | 3:L:3037[B]:TYR:CE1 | 2.55 | 0.81 |
| 3:L:2965[A]:LEU:CD2 | 3:L:2974[A]:ALA:HB1 | 2.10 | 0.81 |
| 3:L:3025[A]:VAL:CG2 | 3:L:3047[A]:ARG:HH12 | 1.94 | 0.81 |
| 3:L:3180[B]:TYR:O | 3:L:3183[B]:LEU:HD22 | 1.81 | 0.81 |
| 3:L:3265[A]:ASP:OD1 | 3:L:3267[A]:SER:OG | 1.97 | 0.81 |
| 3:O:3104[A]:MET:CA | 3:O:3110[A]:THR:HG23 | 2.10 | 0.81 |
| 3:R:2963[A]:MET:N | 3:R:3108[A]:HIS:O | 2.14 | 0.81 |
| 3:U:3173[A]:THR:HG22 | 3:U:3174[A]:GLY:N | 1.93 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2956[A]:LYS:O | 3:X:2960[A]:PHE:CD1 | 2.33 | 0.81 |
| 3:X:3212[A]:ARG:HH11 | 3:X:3212[A]:ARG:HG3 | 1.43 | 0.81 |
| 3:X:3265[B]:ASP:OD1 | 3:X:3267[B]:SER:OG | 1.97 | 0.81 |
| 3:F:2939[B]:ARG:HB3 | 3:F:3032[B]:PRO:HG2 | 1.63 | 0.81 |
| 3:F:3231[A]:ASP:N | 3:F:3284[A]:LYS:O | 2.14 | 0.81 |
| 2:H:2472:ASN:ND2 | 4:s:1:NAG:H61 | 1.90 | 0.81 |
| 2:H:2868:GLU:CD | 3:I:2933[A]:SER:H | 1.88 | 0.81 |
| 3:I:3255[B]:PRO:HG3 | 3:R:2962[B]:GLY:C | 2.05 | 0.81 |
| 3:L:3230[A]:PHE:CB | 3:L:3243[A]:GLY:HA2 | 2.06 | 0.81 |
| 3:L:3231[A]:ASP:N | 3:L:3284[A]:LYS:O | 2.14 | 0.81 |
| 3:O:3023[A]:ILE:O | 3:O:3026[A]:THR:N | 2.11 | 0.81 |
| 3:O:3024[B]:LEU:CD1 | 3:O:3025[B]:VAL:H | 1.83 | 0.81 |
| 3:O:3027[B]:GLU:OE2 | 3:O:3028[B]:PRO:HD2 | 1.80 | 0.81 |
| 3:R:3180[A]:TYR:O | 3:R:3183[A]:LEU:HD22 | 1.81 | 0.81 |
| 3:R:3231[A]:ASP:N | 3:R:3284[A]:LYS:O | 2.14 | 0.81 |
| 3:U:2952[A]:ALA:HB3 | 3:U:2953[A]:GLY:CA | 2.10 | 0.81 |
| 3:U:2973[B]:THR:HG22 | 3:d:3222[B]:ILE:HG23 | 1.63 | 0.81 |
| 3:U:3152[B]:LYS:NZ | 3:d:3172[B]:SER:OG | 2.14 | 0.81 |
| 3:U:3176[B]:LYS:HG3 | 3:d:3152[B]:LYS:HZ2 | 1.44 | 0.81 |
| 3:X:3025[B]:VAL:CG2 | 3:X:3047[B]:ARG:HH12 | 1.94 | 0.81 |
| 3:X:3027[B]:GLU:OE2 | 3:X:3028[B]:PRO:HD2 | 1.80 | 0.81 |
| 3:a:3104[B]:MET:CA | 3:a:3110[B]:THR:HG23 | 2.10 | 0.81 |
| 3:a:3231[B]:ASP:N | 3:a:3284[B]:LYS:O | 2.14 | 0.81 |
| 3:a:3265[B]:ASP:OD1 | 3:a:3267[B]:SER:OG | 1.97 | 0.81 |
| 3:d:2965[B]:LEU:CD2 | 3:d:2974[B]:ALA:HB1 | 2.10 | 0.81 |
| 3:d:3231[B]:ASP:N | 3:d:3284[B]:LYS:O | 2.14 | 0.81 |
| 3:d:3265[A]:ASP:OD1 | 3:d:3267[A]:SER:OG | 1.97 | 0.81 |
| 3:C:3298[A]:ASN:HB3 | 3:C:3300[A]:LEU:CD2 | 2.09 | 0.81 |
| 3:F:2977[B]:CYS:CB | 3:a:2982[B]:MET:CE | 2.59 | 0.81 |
| 3:F:3162[B]:ASP:HB3 | 3:a:3259[B]:ASP:N | 1.96 | 0.81 |
| 3:I:2939[B]:ARG:HB3 | 3:I:3032[B]:PRO:HG2 | 1.63 | 0.81 |
| 3:I:3101[B]:PRO:O | 3:I:3106[B]:THR:HG21 | 1.81 | 0.81 |
| 3:I:3108[B]:HIS:HE1 | 3:R:3251[B]:ASP:OD1 | 1.59 | 0.81 |
| 3:I:3150[B]:LYS:C | 3:R:3172[B]:SER:HB3 | 2.06 | 0.81 |
| 3:O:3163[B]:ASN:CB | 3:X:3149[B]:ASN:N | 2.30 | 0.81 |
| 3:O:3180[A]:TYR:O | 3:O:3183[A]:LEU:HD22 | 1.81 | 0.81 |
| 3:R:3101[A]:PRO:O | 3:R:3106[A]:THR:HG21 | 1.81 | 0.81 |
| 1:S:1636:ASN:ND2 | 1:S:1639:LYS:HD2 | 1.95 | 0.81 |
| 3:X:3265[A]:ASP:OD1 | 3:X:3267[A]:SER:OG | 1.97 | 0.81 |
| 3:a:2948[A]:ASP:N | 3:a:2949[A]:LYS:CA | 2.41 | 0.81 |
| 3:a:2965[A]:LEU:CD2 | 3:a:2974[A]:ALA:HB1 | 2.10 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3298[A]:ASN:HB3 | 3:a:3300[A]:LEU:CD2 | 2.09 | 0.81 |
| 3:d:3025[B]:VAL:CG2 | 3:d:3047[B]:ARG:HH12 | 1.94 | 0.81 |
| 3:C:2948[B]:ASP:N | 3:C:2949[B]:LYS:HA | 1.81 | 0.80 |
| 3:C:3025[B]:VAL:CG2 | 3:C:3047[B]:ARG:HH12 | 1.94 | 0.80 |
| 3:C:3160[B]:SER:C | 3:L:2983[B]:VAL:HG21 | 2.06 | 0.80 |
| 3:F:3023[B]:ILE:O | 3:F:3026[B]:THR:N | 2.11 | 0.80 |
| 3:F:3027[A]:GLU:OE2 | 3:F:3028[A]:PRO:HD2 | 1.80 | 0.80 |
| 3:F:3183[A]:LEU:H | 3:F:3184[A]:ASN:HA | 1.44 | 0.80 |
| 3:F:3231[B]:ASP:N | 3:F:3284[B]:LYS:O | 2.14 | 0.80 |
| 3:I:2939[A]:ARG:HB3 | 3:I:3032[A]:PRO:HG2 | 1.63 | 0.80 |
| 3:I:2951[B]:ASP:OD2 | 3:I:2953[B]:GLY:HA2 | 1.79 | 0.80 |
| 3:I:2952[A]:ALA:HB3 | 3:I:2953[A]:GLY:CA | 2.10 | 0.80 |
| 3:I:2956[B]:LYS:O | 3:I:2960[B]:PHE:CD1 | 2.33 | 0.80 |
| 3:I:2966[B]:SER:O | 3:R:3256[B]:TRP:CB | 2.29 | 0.80 |
| 3:I:3180[B]:TYR:HB2 | 3:I:3183[B]:LEU:HD22 | 1.63 | 0.80 |
| 1:J:1636:ASN:OD1 | 6:w:1:NAG:H82 | 1.81 | 0.80 |
| 3:L:3101[B]:PRO:O | 3:L:3106[B]:THR:HG21 | 1.81 | 0.80 |
| 3:L:3189[B]:ASN:CG | 3:L:3191[B]:ASN:HD21 | 1.87 | 0.80 |
| 3:O:3101[A]:PRO:O | 3:O:3106[A]:THR:HG21 | 1.81 | 0.80 |
| 3:U:3180[A]:TYR:O | 3:U:3183[A]:LEU:HD22 | 1.81 | 0.80 |
| 3:X:2965[A]:LEU:CD2 | 3:X:2974[A]:ALA:HB1 | 2.10 | 0.80 |
| 1:b:1442:MET:HE1 | 1:b:1454:PHE:HA | 1.63 | 0.80 |
| 3:C:3023[B]:ILE:O | 3:C:3026[B]:THR:N | 2.11 | 0.80 |
| 3:C:3027[A]:GLU:OE2 | 3:C:3028[A]:PRO:HD2 | 1.80 | 0.80 |
| 3:C:3169[B]:LYS:CE | 3:L:3149[B]:ASN:OD1 | 2.29 | 0.80 |
| 3:C:3174[B]:GLY:CA | 3:L:3154[B]:PRO:CD | 2.50 | 0.80 |
| 3:C:3183[B]:LEU:H | 3:C:3184[B]:ASN:HA | 1.44 | 0.80 |
| 3:C:3231[B]:ASP:N | 3:C:3284[B]:LYS:O | 2.14 | 0.80 |
| 3:F:2965[B]:LEU:CD2 | 3:F:2974[B]:ALA:HB1 | 2.10 | 0.80 |
| 3:F:3104[B]:MET:CA | 3:F:3110[B]:THR:HG23 | 2.10 | 0.80 |
| 3:F:3174[B]:GLY:H | 3:a:3154[B]:PRO:HB3 | 0.99 | 0.80 |
| 3:F:3180[A]:TYR:O | 3:F:3183[A]:LEU:HD22 | 1.81 | 0.80 |
| 3:L:2963[B]:MET:N | 3:L:3108[B]:HIS:O | 2.14 | 0.80 |
| 3:L:3025[B]:VAL:CG2 | 3:L:3047[B]:ARG:HH12 | 1.94 | 0.80 |
| 3:R:3025[B]:VAL:CG2 | 3:R:3047[B]:ARG:HH12 | 1.94 | 0.80 |
| 3:U:2965[B]:LEU:CD2 | 3:U:2974[B]:ALA:HB1 | 2.10 | 0.80 |
| 3:U:3025[B]:VAL:CG2 | 3:U:3047[B]:ARG:HH12 | 1.94 | 0.80 |
| 3:U:3231[A]:ASP:N | 3:U:3284[A]:LYS:O | 2.14 | 0.80 |
| 3:a:2969[B]:TYR:HB3 | 3:a:2971[B]:ASP:OD1 | 1.82 | 0.80 |
| 3:a:3027[A]:GLU:OE2 | 3:a:3028[A]:PRO:HD2 | 1.80 | 0.80 |
| 3:a:3027[B]:GLU:OE2 | 3:a:3028[B]:PRO:HD2 | 1.80 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3180[A]:TYR:O | 3:a:3183[A]:LEU:HD22 | 1.81 | 0.80 |
| 3:d:3180[A]:TYR:HB2 | 3:d:3183[A]:LEU:HD22 | 1.63 | 0.80 |
| 3:C:2956[B]:LYS:C | 3:C:2960[B]:PHE:CE1 | 2.47 | 0.80 |
| 3:C:2965[B]:LEU:CD2 | 3:C:2974[B]:ALA:HB1 | 2.10 | 0.80 |
| 3:C:2969[A]:TYR:HB3 | 3:C:2971[A]:ASP:OD1 | 1.82 | 0.80 |
| 3:C:3147[B]:GLU:OE1 | 3:L:3162[B]:ASP:CA | 2.30 | 0.80 |
| 3:C:3172[B]:SER:CB | 3:L:3150[B]:LYS:N | 2.45 | 0.80 |
| 3:C:3180[B]:TYR:O | 3:C:3183[B]:LEU:HD22 | 1.81 | 0.80 |
| 3:C:3189[B]:ASN:CG | 3:C:3191[B]:ASN:HD21 | 1.87 | 0.80 |
| 1:D:1574:VAL:H | 1:G:329:ARG:HH12 | 1.29 | 0.80 |
| 3:F:2976[B]:ALA:CB | 3:a:3252[B]:TYR:O | 2.28 | 0.80 |
| 3:I:3155[B]:MET:CE | 3:R:3156[B]:MET:HG2 | 2.12 | 0.80 |
| 3:I:3176[A]:LYS:HE2 | 3:I:3176[A]:LYS:H | 1.43 | 0.80 |
| 3:L:2939[A]:ARG:HB3 | 3:L:3032[A]:PRO:HG2 | 1.62 | 0.80 |
| 3:L:3101[A]:PRO:O | 3:L:3106[A]:THR:HG21 | 1.81 | 0.80 |
| 3:O:2939[A]:ARG:HB3 | 3:O:3032[A]:PRO:HG2 | 1.63 | 0.80 |
| 3:O:2956[B]:LYS:O | 3:O:2960[B]:PHE:CD1 | 2.33 | 0.80 |
| 3:O:3180[A]:TYR:HB2 | 3:O:3183[A]:LEU:HD22 | 1.63 | 0.80 |
| 3:O:3231[A]:ASP:N | 3:O:3284[A]:LYS:O | 2.14 | 0.80 |
| 3:R:3025[A]:VAL:CG2 | 3:R:3047[A]:ARG:HH12 | 1.94 | 0.80 |
| 3:X:2963[A]:MET:N | 3:X:3108[A]:HIS:O | 2.14 | 0.80 |
| 3:X:2965[B]:LEU:HD11 | 3:X:2974[B]:ALA:CA | 2.11 | 0.80 |
| 3:X:3180[A]:TYR:HB2 | 3:X:3183[A]:LEU:HD22 | 1.63 | 0.80 |
| 3:X:3231[A]:ASP:N | 3:X:3284[A]:LYS:O | 2.14 | 0.80 |
| 1:Y:1617:LYS:HE2 | 3:d:3180[B]:TYR:CE2 | 2.15 | 0.80 |
| 3:a:2956[B]:LYS:O | 3:a:2960[B]:PHE:CD1 | 2.33 | 0.80 |
| 3:d:2963[B]:MET:N | 3:d:3108[B]:HIS:O | 2.14 | 0.80 |
| 3:d:2965[A]:LEU:CD2 | 3:d:2974[A]:ALA:HB1 | 2.10 | 0.80 |
| 3:d:3176[A]:LYS:HE2 | 3:d:3176[A]:LYS:H | 1.43 | 0.80 |
| 3:C:2963[B]:MET:N | 3:C:3108[B]:HIS:O | 2.14 | 0.80 |
| 3:C:2965[A]:LEU:CD2 | 3:C:2974[A]:ALA:HB1 | 2.10 | 0.80 |
| 3:C:3231[A]:ASP:N | 3:C:3284[A]:LYS:O | 2.14 | 0.80 |
| 3:F:3155[B]:MET:HG3 | 3:a:3154[B]:PRO:CD | 2.11 | 0.80 |
| 3:I:2973[B]:THR:HG23 | 3:R:3248[B]:LEU:HD11 | 1.63 | 0.80 |
| 3:I:2975[B]:PHE:CZ | 3:R:2961[B]:HIS:CD2 | 2.68 | 0.80 |
| 3:I:3149[B]:ASN:OD1 | 3:R:3169[B]:LYS:NZ | 2.15 | 0.80 |
| 3:I:3223[B]:GLY:HA3 | 3:R:2963[B]:MET:CE | 2.09 | 0.80 |
| 3:I:3231[A]:ASP:N | 3:I:3284[A]:LYS:O | 2.14 | 0.80 |
| 3:L:2965[A]:LEU:HD11 | 3:L:2974[A]:ALA:CA | 2.12 | 0.80 |
| 3:O:2956[A]:LYS:O | 3:O:2960[A]:PHE:CD1 | 2.33 | 0.80 |
| 3:O:3255[B]:PRO:CA | 3:X:3161[B]:GLU:HA | 2.12 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2952[A]:ALA:CB | 3:R:2953[A]:GLY:C | 2.48 | 0.80 |
| 3:R:3231[B]:ASP:N | 3:R:3284[B]:LYS:O | 2.14 | 0.80 |
| 1:S:497:GLN:HG2 | 1:S:683:THR:HG21 | 1.63 | 0.80 |
| 3:U:2974[B]:ALA:HB1 | 3:d:3220[B]:ARG:CG | 2.10 | 0.80 |
| 3:U:3152[B]:LYS:HB2 | 3:d:3154[B]:PRO:CB | 2.08 | 0.80 |
| 3:U:3180[A]:TYR:HB2 | 3:U:3183[A]:LEU:HD22 | 1.63 | 0.80 |
| 3:d:2956[B]:LYS:O | 3:d:2960[B]:PHE:CD1 | 2.33 | 0.80 |
| 3:d:3101[B]:PRO:O | 3:d:3106[B]:THR:HG21 | 1.81 | 0.80 |
| 3:C:3223[B]:GLY:C | 3:L:3252[B]:TYR:CE1 | 2.60 | 0.80 |
| 3:F:2975[B]:PHE:CD1 | 3:a:3107[B]:LEU:HD21 | 2.16 | 0.80 |
| 3:F:2980[B]:HIS:N | 3:a:2967[B]:CYS:CB | 2.44 | 0.80 |
| 3:F:3180[B]:TYR:O | 3:F:3183[B]:LEU:HD22 | 1.81 | 0.80 |
| 3:F:3251[B]:ASP:OD1 | 3:a:3108[B]:HIS:CE1 | 2.35 | 0.80 |
| 3:I:2948[A]:ASP:N | 3:I:2949[A]:LYS:CA | 2.41 | 0.80 |
| 3:I:2969[A]:TYR:HB3 | 3:I:2971[A]:ASP:OD1 | 1.82 | 0.80 |
| 3:I:2969[B]:TYR:HB3 | 3:I:2971[B]:ASP:OD1 | 1.82 | 0.80 |
| 3:I:3101[A]:PRO:O | 3:I:3106[A]:THR:HG21 | 1.81 | 0.80 |
| 3:O:2965[B]:LEU:N | 3:X:3254[B]:MET:CE | 2.43 | 0.80 |
| 3:O:3101[B]:PRO:O | 3:O:3106[B]:THR:HG21 | 1.81 | 0.80 |
| 3:O:3104[B]:MET:CA | 3:O:3110[B]:THR:HG23 | 2.10 | 0.80 |
| 3:R:3180[B]:TYR:O | 3:R:3183[B]:LEU:HD22 | 1.81 | 0.80 |
| 3:U:2965[A]:LEU:CD2 | 3:U:2974[A]:ALA:HB1 | 2.10 | 0.80 |
| 3:U:3152[B]:LYS:O | 3:d:3153[B]:LYS:N | 2.03 | 0.80 |
| 3:X:3025[A]:VAL:CG2 | 3:X:3047[A]:ARG:HH12 | 1.94 | 0.80 |
| 3:X:3101[A]:PRO:O | 3:X:3106[A]:THR:HG21 | 1.81 | 0.80 |
| 1:Y:1656:ASP:C | 3:d:2937[B]:ASN:ND2 | 2.38 | 0.80 |
| 3:a:2965[A]:LEU:HD11 | 3:a:2974[A]:ALA:CA | 2.12 | 0.80 |
| 3:a:3101[A]:PRO:O | 3:a:3106[A]:THR:HG21 | 1.81 | 0.80 |
| 3:a:3183[A]:LEU:H | 3:a:3184[A]:ASN:HA | 1.44 | 0.80 |
| 3:C:3152[B]:LYS:HB2 | 3:L:3172[B]:SER:H | 1.43 | 0.80 |
| 3:C:3163[B]:ASN:CB | 3:L:3149[B]:ASN:ND2 | 2.30 | 0.80 |
| 1:D:115:GLY:HA2 | 1:D:116:LYS:HB2 | 1.64 | 0.80 |
| 3:I:3169[B]:LYS:NZ | 3:R:3149[B]:ASN:OD1 | 2.14 | 0.80 |
| 1:P:589:GLN:HG2 | 1:P:594:ASP:HB3 | 1.62 | 0.80 |
| 3:R:3101[B]:PRO:O | 3:R:3106[B]:THR:HG21 | 1.81 | 0.80 |
| 3:U:2956[B]:LYS:C | 3:U:2960[B]:PHE:CE1 | 2.47 | 0.80 |
| 3:U:3101[A]:PRO:O | 3:U:3106[A]:THR:HG21 | 1.81 | 0.80 |
| 3:X:3023[A]:ILE:O | 3:X:3026[A]:THR:N | 2.11 | 0.80 |
| 1:Y:855:ARG:O | 1:Y:957:ASN:ND2 | 2.15 | 0.80 |
| 1:Y:1620:LEU:C | 3:d:3189[B]:ASN:HD22 | 1.89 | 0.80 |
| 3:a:2939[A]:ARG:HB3 | 3:a:3032[A]:PRO:HG2 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3101[B]:PRO:O | 3:a:3106[B]:THR:HG21 | 1.81 | 0.80 |
| 3:d:2969[A]:TYR:HB3 | 3:d:2971[A]:ASP:OD1 | 1.82 | 0.80 |
| 3:I:3152[B]:LYS:CB | 3:R:3171[B]:HIS:C | 2.55 | 0.80 |
| 3:I:3162[B]:ASP:HB3 | 3:R:3259[B]:ASP:CA | 2.11 | 0.80 |
| 2:K:2870:LEU:HD21 | 2:K:2901:LEU:HD23 | 1.63 | 0.80 |
| 3:R:3196[A]:THR:H | 3:R:3199[A]:GLN:HB2 | 1.37 | 0.80 |
| 3:U:2939[B]:ARG:HB3 | 3:U:3032[B]:PRO:HG2 | 1.63 | 0.80 |
| 3:U:2965[B]:LEU:HD23 | 3:d:3220[B]:ARG:CD | 2.10 | 0.80 |
| 3:U:3189[B]:ASN:CG | 3:U:3191[B]:ASN:HD21 | 1.88 | 0.80 |
| 3:X:2939[B]:ARG:HB3 | 3:X:3032[B]:PRO:HG2 | 1.63 | 0.80 |
| 3:X:3231[B]:ASP:N | 3:X:3284[B]:LYS:O | 2.14 | 0.80 |
| 2:Z:2867:PRO:CD | 3:a:2932[A]:PRO:HG2 | 2.11 | 0.80 |
| 3:C:2979[B]:GLN:HE22 | 3:L:2979[B]:GLN:NE2 | 1.79 | 0.80 |
| 3:F:2973[B]:THR:HG23 | 3:a:3248[B]:LEU:CD1 | 2.10 | 0.80 |
| 3:F:3153[B]:LYS:CB | 3:a:3158[B]:PHE:HB2 | 2.11 | 0.80 |
| 3:F:3230[A]:PHE:CB | 3:F:3243[A]:GLY:HA2 | 2.06 | 0.80 |
| 3:I:3183[A]:LEU:H | 3:I:3184[A]:ASN:HA | 1.44 | 0.80 |
| 3:O:2972[B]:GLY:O | 3:X:2979[B]:GLN:CB | 2.30 | 0.80 |
| 3:R:2939[B]:ARG:HB3 | 3:R:3032[B]:PRO:HG2 | 1.63 | 0.80 |
| 3:R:2956[A]:LYS:O | 3:R:2960[A]:PHE:CD1 | 2.33 | 0.80 |
| 3:R:3180[A]:TYR:HB2 | 3:R:3183[A]:LEU:HD22 | 1.63 | 0.80 |
| 3:R:3189[B]:ASN:CG | 3:R:3191[B]:ASN:HD21 | 1.87 | 0.80 |
| 3:U:3023[B]:ILE:O | 3:U:3026[B]:THR:N | 2.11 | 0.80 |
| 3:U:3101[B]:PRO:O | 3:U:3106[B]:THR:HG21 | 1.82 | 0.80 |
| 3:U:3152[B]:LYS:C | 3:d:3152[B]:LYS:C | 2.41 | 0.80 |
| 3:U:3212[B]:ARG:HG3 | 3:U:3212[B]:ARG:HH11 | 1.43 | 0.80 |
| 3:X:3027[A]:GLU:OE2 | 3:X:3028[A]:PRO:HD2 | 1.80 | 0.80 |
| 1:Y:1397:LEU:O | 1:Y:1400:ASN:ND2 | 2.15 | 0.80 |
| 3:a:3025[B]:VAL:CG2 | 3:a:3047[B]:ARG:HH12 | 1.94 | 0.80 |
| 2:c:2394:VAL:H | 2:c:2448:THR:HG22 | 1.47 | 0.80 |
| 3:d:3180[B]:TYR:O | 3:d:3183[B]:LEU:HD22 | 1.81 | 0.80 |
| 3:C:2965[A]:LEU:HD11 | 3:C:2974[A]:ALA:CA | 2.12 | 0.80 |
| 3:C:2966[B]:SER:O | 3:L:2981[B]:GLY:O | 2.00 | 0.80 |
| 3:C:2983[B]:VAL:CG2 | 3:L:3160[B]:SER:C | 2.48 | 0.80 |
| 3:F:3153[B]:LYS:HD2 | 3:a:3155[B]:MET:CA | 2.10 | 0.80 |
| 3:I:2965[A]:LEU:HD11 | 3:I:2974[A]:ALA:CA | 2.12 | 0.80 |
| 3:L:2969[B]:TYR:HB3 | 3:L:2971[B]:ASP:OD1 | 1.82 | 0.80 |
| 3:L:3183[A]:LEU:H | 3:L:3184[A]:ASN:HA | 1.44 | 0.80 |
| 3:O:2968[B]:GLN:HB2 | 3:X:2988[B]:TRP:H | 1.47 | 0.80 |
| 3:R:2969[A]:TYR:HB3 | 3:R:2971[A]:ASP:OD1 | 1.82 | 0.80 |
| 3:R:3135[A]:LYS:CG | 3:R:3141[A]:TYR:CD1 | 2.65 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1618:LEU:HD22 | 3:X:3136[B]:TYR:CE2 | 2.17 | 0.80 |
| 3:U:3025[A]:VAL:CG2 | 3:U:3047[A]:ARG:HH12 | 1.94 | 0.80 |
| 3:U:3027[A]:GLU:OE2 | 3:U:3028[A]:PRO:HD2 | 1.80 | 0.80 |
| 3:U:3027[B]:GLU:OE2 | 3:U:3028[B]:PRO:HD2 | 1.80 | 0.80 |
| 3:U:3104[B]:MET:CA | 3:U:3110[B]:THR:HG23 | 2.10 | 0.80 |
| 1:V:497:GLN:HG2 | 1:V:683:THR:HG21 | 1.63 | 0.80 |
| 1:V:961:SER:HB2 | 1:V:973:ARG:HA | 1.64 | 0.80 |
| 3:X:2969[A]:TYR:HB3 | 3:X:2971[A]:ASP:OD1 | 1.82 | 0.80 |
| 3:a:2956[A]:LYS:C | 3:a:2960[A]:PHE:CE1 | 2.47 | 0.80 |
| 3:a:3231[A]:ASP:N | 3:a:3284[A]:LYS:O | 2.14 | 0.80 |
| 3:d:3196[B]:THR:H | 3:d:3199[B]:GLN:HB2 | 1.38 | 0.80 |
| 3:d:3231[A]:ASP:N | 3:d:3284[A]:LYS:O | 2.14 | 0.80 |
| 3:C:2948[A]:ASP:N | 3:C:2949[A]:LYS:CA | 2.41 | 0.80 |
| 3:C:2968[B]:GLN:HG2 | 3:L:2981[B]:GLY:N | 1.97 | 0.80 |
| 3:C:2982[B]:MET:CB | 3:L:3156[B]:MET:HB2 | 1.85 | 0.80 |
| 3:C:3154[B]:PRO:HB2 | 3:L:3151[B]:LEU:CA | 2.11 | 0.80 |
| 3:C:3180[B]:TYR:HB2 | 3:C:3183[B]:LEU:HD22 | 1.63 | 0.80 |
| 3:F:2939[A]:ARG:HB3 | 3:F:3032[A]:PRO:HG2 | 1.63 | 0.80 |
| 3:F:2981[B]:GLY:N | 3:a:2968[B]:GLN:OE1 | 2.15 | 0.80 |
| 3:F:3150[B]:LYS:HE3 | 3:a:3163[B]:ASN:HB3 | 1.64 | 0.80 |
| 3:I:2965[B]:LEU:HD11 | 3:I:2974[B]:ALA:CA | 2.12 | 0.80 |
| 3:I:3135[B]:LYS:CG | 3:I:3141[B]:TYR:CD1 | 2.65 | 0.80 |
| 3:I:3158[B]:PHE:HB2 | 3:R:3153[B]:LYS:HB2 | 1.64 | 0.80 |
| 3:L:2956[A]:LYS:O | 3:L:2960[A]:PHE:CD1 | 2.33 | 0.80 |
| 3:L:3231[B]:ASP:N | 3:L:3284[B]:LYS:O | 2.14 | 0.80 |
| 3:R:2965[A]:LEU:HD11 | 3:R:2974[A]:ALA:CA | 2.12 | 0.80 |
| 3:U:2965[A]:LEU:HD11 | 3:U:2974[A]:ALA:CA | 2.12 | 0.80 |
| 3:U:3180[B]:TYR:O | 3:U:3183[B]:LEU:HD22 | 1.81 | 0.80 |
| 1:b:415:VAL:HB | 1:b:697:ALA:HB2 | 1.63 | 0.80 |
| 3:C:2969[B]:TYR:HB3 | 3:C:2971[B]:ASP:OD1 | 1.82 | 0.79 |
| 3:C:2988[B]:TRP:CD1 | 3:L:3153[B]:LYS:HD3 | 2.10 | 0.79 |
| 3:C:3171[B]:HIS:C | 3:L:3152[B]:LYS:HB2 | 2.06 | 0.79 |
| 3:C:3180[A]:TYR:HB2 | 3:C:3183[A]:LEU:HD22 | 1.63 | 0.79 |
| 3:F:2955[A]:GLN:CD | 3:F:3037[A]:TYR:CE1 | 2.55 | 0.79 |
| 3:F:2979[A]:GLN:CG | 3:F:3155[A]:MET:CE | 2.56 | 0.79 |
| 3:F:2982[B]:MET:SD | 3:a:3157[B]:PRO:HB3 | 2.21 | 0.79 |
| 3:F:3154[B]:PRO:CB | 3:a:3174[B]:GLY:CA | 2.60 | 0.79 |
| 2:H:2868:GLU:CD | 3:I:2933[A]:SER:N | 2.40 | 0.79 |
| 3:I:2982[B]:MET:HE1 | 3:R:2966[B]:SER:HB3 | 1.63 | 0.79 |
| 3:I:3255[B]:PRO:HG2 | 3:R:2959[B]:SER:HA | 1.64 | 0.79 |
| 3:O:2965[A]:LEU:HD11 | 3:O:2974[A]:ALA:CA | 2.12 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2949[A]:LYS:O | 3:R:2949[A]:LYS:NZ | 2.15 | 0.79 |
| 3:U:2965[B]:LEU:HD23 | 3:d:3220[B]:ARG:HD3 | 1.63 | 0.79 |
| 3:U:2969[A]:TYR:HB3 | 3:U:2971[A]:ASP:OD1 | 1.82 | 0.79 |
| 3:U:3169[B]:LYS:HE3 | 3:d:3147[B]:GLU:CB | 2.13 | 0.79 |
| 3:U:3231[B]:ASP:N | 3:U:3284[B]:LYS:O | 2.14 | 0.79 |
| 3:X:2939[A]:ARG:HB3 | 3:X:3032[A]:PRO:HG2 | 1.63 | 0.79 |
| 3:X:3101[B]:PRO:O | 3:X:3106[B]:THR:HG21 | 1.81 | 0.79 |
| 3:a:3135[A]:LYS:CG | 3:a:3141[A]:TYR:CD1 | 2.65 | 0.79 |
| 1:b:456:GLN:NE2 | 1:b:549:PRO:O | 2.15 | 0.79 |
| 3:d:2965[B]:LEU:HD11 | 3:d:2974[B]:ALA:CA | 2.12 | 0.79 |
| 3:C:3101[A]:PRO:O | 3:C:3106[A]:THR:HG21 | 1.81 | 0.79 |
| 3:C:3147[B]:GLU:OE1 | 3:L:3162[B]:ASP:N | 1.98 | 0.79 |
| 3:C:3162[B]:ASP:OD1 | 3:L:3259[B]:ASP:OD2 | 1.98 | 0.79 |
| 3:F:2956[B]:LYS:O | 3:F:2960[B]:PHE:HE1 | 1.22 | 0.79 |
| 3:F:3135[A]:LYS:CG | 3:F:3141[A]:TYR:CD1 | 2.65 | 0.79 |
| 3:I:2961[B]:HIS:ND1 | 3:R:2975[B]:PHE:CE1 | 2.50 | 0.79 |
| 3:I:2965[B]:LEU:HB3 | 3:R:3256[B]:TRP:CE2 | 2.14 | 0.79 |
| 3:I:3104[A]:MET:CA | 3:I:3110[A]:THR:HG23 | 2.10 | 0.79 |
| 3:I:3196[B]:THR:H | 3:I:3199[B]:GLN:HB2 | 1.38 | 0.79 |
| 3:L:3180[A]:TYR:O | 3:L:3183[A]:LEU:HD22 | 1.81 | 0.79 |
| 3:O:2949[A]:LYS:O | 3:O:2949[A]:LYS:NZ | 2.16 | 0.79 |
| 3:O:3135[B]:LYS:CG | 3:O:3141[B]:TYR:CD1 | 2.65 | 0.79 |
| 3:R:2965[B]:LEU:HD11 | 3:R:2974[B]:ALA:CA | 2.12 | 0.79 |
| 3:U:3135[A]:LYS:CG | 3:U:3141[A]:TYR:CD1 | 2.65 | 0.79 |
| 3:U:3135[B]:LYS:CG | 3:U:3141[B]:TYR:CD1 | 2.65 | 0.79 |
| 3:U:3176[B]:LYS:CD | 3:d:3152[B]:LYS:CD | 2.54 | 0.79 |
| 3:d:2949[B]:LYS:O | 3:d:2949[B]:LYS:NZ | 2.16 | 0.79 |
| 3:C:2965[B]:LEU:O | 3:L:3256[B]:TRP:CA | 2.19 | 0.79 |
| 3:C:3090[B]:ASN:HD22 | 3:L:2972[B]:GLY:CA | 1.76 | 0.79 |
| 3:F:2964[B]:PRO:C | 3:a:3221[B]:ALA:HB3 | 2.08 | 0.79 |
| 3:F:2965[B]:LEU:HD11 | 3:F:2974[B]:ALA:CA | 2.12 | 0.79 |
| 3:F:3149[B]:ASN:ND2 | 3:a:3163[B]:ASN:CG | 2.39 | 0.79 |
| 3:F:3180[B]:TYR:HB2 | 3:F:3183[B]:LEU:HD22 | 1.63 | 0.79 |
| 3:F:3212[A]:ARG:HG3 | 3:F:3212[A]:ARG:HH11 | 1.43 | 0.79 |
| 3:I:3023[B]:ILE:O | 3:I:3026[B]:THR:N | 2.11 | 0.79 |
| 1:M:915:ASN:ND2 | 1:M:1095:MET:SD | 2.56 | 0.79 |
| 3:O:2948[A]:ASP:N | 3:O:2949[A]:LYS:CA | 2.41 | 0.79 |
| 3:O:3109[B]:TYR:CD1 | 3:X:2969[B]:TYR:C | 2.56 | 0.79 |
| 3:U:2948[B]:ASP:N | 3:U:2949[B]:LYS:CA | 2.41 | 0.79 |
| 3:U:3180[B]:TYR:HB2 | 3:U:3183[B]:LEU:HD22 | 1.63 | 0.79 |
| 3:X:3180[B]:TYR:O | 3:X:3183[B]:LEU:HD22 | 1.81 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2965[B]:LEU:HD11 | 3:a:2974[B]:ALA:CA | 2.12 | 0.79 |
| 3:d:3101[A]:PRO:O | 3:d:3106[A]:THR:HG21 | 1.81 | 0.79 |
| 1:A:456:GLN:NE2 | 1:A:549:PRO:O | 2.16 | 0.79 |
| 3:C:2963[B]:MET:HE1 | 3:L:3223[B]:GLY:N | 1.97 | 0.79 |
| 3:C:2965[B]:LEU:HD11 | 3:C:2974[B]:ALA:CA | 2.12 | 0.79 |
| 3:C:3101[B]:PRO:O | 3:C:3106[B]:THR:HG21 | 1.81 | 0.79 |
| 3:F:2984[B]:THR:HG23 | 3:a:3159[B]:SER:HB3 | 0.80 | 0.79 |
| 3:F:3151[B]:LEU:HB2 | 3:F:3175[B]:TYR:CD2 | 2.18 | 0.79 |
| 3:I:2963[B]:MET:CE | 3:R:3223[B]:GLY:HA3 | 2.10 | 0.79 |
| 3:R:3148[A]:ILE:O | 3:R:3152[A]:LYS:HE3 | 1.83 | 0.79 |
| 3:R:3151[B]:LEU:HB2 | 3:R:3175[B]:TYR:CD2 | 2.18 | 0.79 |
| 3:a:3025[A]:VAL:HG23 | 3:a:3033[A]:PHE:O | 1.83 | 0.79 |
| 3:a:3180[B]:TYR:O | 3:a:3183[B]:LEU:HD22 | 1.81 | 0.79 |
| 3:d:2939[B]:ARG:HB3 | 3:d:3032[B]:PRO:HG2 | 1.63 | 0.79 |
| 3:d:3025[B]:VAL:HG23 | 3:d:3033[B]:PHE:O | 1.83 | 0.79 |
| 3:C:2979[A]:GLN:CG | 3:C:3155[A]:MET:CE | 2.56 | 0.79 |
| 3:C:3149[B]:ASN:ND2 | 3:L:3163[B]:ASN:HB3 | 1.97 | 0.79 |
| 3:C:3151[A]:LEU:HB2 | 3:C:3175[A]:TYR:CD2 | 2.18 | 0.79 |
| 3:F:2965[A]:LEU:HD11 | 3:F:2974[A]:ALA:CA | 2.12 | 0.79 |
| 3:F:3101[B]:PRO:O | 3:F:3106[B]:THR:HG21 | 1.81 | 0.79 |
| 3:F:3148[A]:ILE:O | 3:F:3152[A]:LYS:HE3 | 1.83 | 0.79 |
| 3:F:3173[B]:THR:C | 3:a:3154[B]:PRO:N | 2.41 | 0.79 |
| 2:H:2868:GLU:CD | 3:I:2932[A]:PRO:C | 2.49 | 0.79 |
| 3:I:3160[B]:SER:CB | 3:R:2983[B]:VAL:HG23 | 2.07 | 0.79 |
| 3:L:2965[B]:LEU:HD11 | 3:L:2974[B]:ALA:CA | 2.12 | 0.79 |
| 3:L:3135[A]:LYS:CG | 3:L:3141[A]:TYR:CD1 | 2.65 | 0.79 |
| 3:O:2969[A]:TYR:HB3 | 3:O:2971[A]:ASP:OD1 | 1.82 | 0.79 |
| 3:O:3173[B]:THR:CB | 3:O:3176[B]:LYS:HD2 | 2.13 | 0.79 |
| 3:U:3025[B]:VAL:HG23 | 3:U:3033[B]:PHE:O | 1.83 | 0.79 |
| 3:U:3156[B]:MET:SD | 3:d:2982[B]:MET:HB3 | 2.22 | 0.79 |
| 3:X:2948[B]:ASP:N | 3:X:2949[B]:LYS:CA | 2.41 | 0.79 |
| 3:X:2979[A]:GLN:CG | 3:X:3155[A]:MET:CE | 2.56 | 0.79 |
| 3:a:3180[B]:TYR:HB2 | 3:a:3183[B]:LEU:HD22 | 1.64 | 0.79 |
| 3:d:2956[A]:LYS:O | 3:d:2960[A]:PHE:CD1 | 2.33 | 0.79 |
| 3:d:2979[B]:GLN:CG | 3:d:3155[B]:MET:CE | 2.55 | 0.79 |
| 3:d:3180[A]:TYR:O | 3:d:3183[A]:LEU:HD22 | 1.81 | 0.79 |
| 3:C:3150[B]:LYS:HZ3 | 3:L:3160[B]:SER:HB2 | 0.62 | 0.79 |
| 3:C:3151[B]:LEU:HB2 | 3:C:3175[B]:TYR:CD2 | 2.18 | 0.79 |
| 3:C:3151[B]:LEU:O | 3:L:3154[B]:PRO:HB3 | 1.81 | 0.79 |
| 3:C:3252[B]:TYR:CD1 | 3:L:3223[B]:GLY:O | 2.35 | 0.79 |
| 3:C:3255[B]:PRO:CA | 3:L:2964[B]:PRO:O | 2.30 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2969[B]:TYR:HB3 | 3:F:2971[B]:ASP:OD1 | 1.82 | 0.79 |
| 3:F:3153[B]:LYS:HB3 | 3:a:3155[B]:MET:HB2 | 1.58 | 0.79 |
| 1:G:1063:ARG:HB3 | 1:G:1065:LYS:HD2 | 1.61 | 0.79 |
| 3:I:2976[B]:ALA:N | 3:R:3253[B]:GLU:CB | 2.38 | 0.79 |
| 3:I:3158[B]:PHE:HB2 | 3:R:3153[B]:LYS:CB | 2.13 | 0.79 |
| 3:I:3180[A]:TYR:HB2 | 3:I:3183[A]:LEU:HD22 | 1.63 | 0.79 |
| 3:L:2979[B]:GLN:CG | 3:L:3155[B]:MET:CE | 2.56 | 0.79 |
| 2:N:2180:TRP:HB2 | 2:N:2243:LEU:HD13 | 1.64 | 0.79 |
| 3:O:2969[B]:TYR:HB3 | 3:O:2971[B]:ASP:OD1 | 1.82 | 0.79 |
| 1:S:1275:ARG:HH12 | 1:S:1357:ARG:HH12 | 1.26 | 0.79 |
| 3:a:2969[A]:TYR:HB3 | 3:a:2971[A]:ASP:OD1 | 1.82 | 0.79 |
| 3:d:2939[A]:ARG:HB3 | 3:d:3032[A]:PRO:HG2 | 1.63 | 0.79 |
| 3:F:3135[B]:LYS:CG | 3:F:3141[B]:TYR:CD1 | 2.65 | 0.79 |
| 3:F:3151[A]:LEU:HB2 | 3:F:3175[A]:TYR:CD2 | 2.18 | 0.79 |
| 3:I:2974[B]:ALA:H | 3:R:3249[B]:GLY:N | 1.79 | 0.79 |
| 3:I:2982[B]:MET:CE | 3:R:2966[B]:SER:CB | 2.55 | 0.79 |
| 3:I:3148[B]:ILE:O | 3:I:3152[B]:LYS:HE3 | 1.83 | 0.79 |
| 3:I:3156[B]:MET:H | 3:R:2979[B]:GLN:NE2 | 1.79 | 0.79 |
| 3:L:2952[A]:ALA:CB | 3:L:2953[A]:GLY:C | 2.48 | 0.79 |
| 3:L:3151[B]:LEU:HB2 | 3:L:3175[B]:TYR:CD2 | 2.18 | 0.79 |
| 3:O:2956[A]:LYS:O | 3:O:2960[A]:PHE:HE1 | 1.22 | 0.79 |
| 3:O:3231[B]:ASP:N | 3:O:3284[B]:LYS:O | 2.14 | 0.79 |
| 3:O:3255[B]:PRO:HG3 | 3:X:3163[B]:ASN:HB3 | 1.62 | 0.79 |
| 3:R:3180[B]:TYR:HB2 | 3:R:3183[B]:LEU:HD22 | 1.64 | 0.79 |
| 1:V:1137:LYS:HA | 1:V:1141:ARG:HH12 | 1.47 | 0.79 |
| 1:V:1140:ASN:ND2 | 1:V:1236:TYR:OH | 2.16 | 0.79 |
| 3:a:3025[A]:VAL:CG2 | 3:a:3047[A]:ARG:HH12 | 1.94 | 0.79 |
| 1:b:550:ILE:N | 1:b:557:VAL:O | 2.16 | 0.79 |
| 3:d:2965[A]:LEU:HD11 | 3:d:2974[A]:ALA:CA | 2.12 | 0.79 |
| 3:d:3023[A]:ILE:O | 3:d:3026[A]:THR:N | 2.11 | 0.79 |
| 3:d:3025[A]:VAL:CG2 | 3:d:3047[A]:ARG:HH12 | 1.94 | 0.79 |
| 3:C:3255[B]:PRO:HB2 | 3:L:2959[B]:SER:C | 2.07 | 0.79 |
| 3:C:3256[B]:TRP:CZ2 | 3:L:2965[B]:LEU:CG | 2.47 | 0.79 |
| 3:F:2977[B]:CYS:CB | 3:a:2982[B]:MET:HE3 | 2.12 | 0.79 |
| 3:F:3230[B]:PHE:CB | 3:F:3243[B]:GLY:HA2 | 2.06 | 0.79 |
| 1:G:724:LYS:HA | 1:G:728:ARG:HH12 | 1.47 | 0.79 |
| 2:H:2797:LYS:HZ3 | 3:I:3028[A]:PRO:HD3 | 1.48 | 0.79 |
| 3:I:2949[B]:LYS:O | 3:I:2949[B]:LYS:NZ | 2.16 | 0.79 |
| 3:I:3025[B]:VAL:CG2 | 3:I:3047[B]:ARG:HH12 | 1.94 | 0.79 |
| 3:I:3162[B]:ASP:CA | 3:R:3259[B]:ASP:HB3 | 2.13 | 0.79 |
| 3:I:3231[B]:ASP:N | 3:I:3284[B]:LYS:O | 2.14 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2625:LEU:HD13 | 2:K:2626:ARG:HG2 | 1.64 | 0.79 |
| 3:L:2956[B]:LYS:O | 3:L:2960[B]:PHE:CD1 | 2.33 | 0.79 |
| 3:L:2956[B]:LYS:C | 3:L:2960[B]:PHE:CE1 | 2.47 | 0.79 |
| 3:O:3025[B]:VAL:HG23 | 3:O:3033[B]:PHE:O | 1.83 | 0.79 |
| 3:O:3173[A]:THR:CB | 3:O:3176[A]:LYS:HD2 | 2.13 | 0.79 |
| 3:R:2949[B]:LYS:O | 3:R:2949[B]:LYS:NZ | 2.16 | 0.79 |
| 3:R:3135[B]:LYS:CG | 3:R:3141[B]:TYR:CD1 | 2.65 | 0.79 |
| 3:R:3151[A]:LEU:HB2 | 3:R:3175[A]:TYR:CD2 | 2.18 | 0.79 |
| 3:U:3148[B]:ILE:O | 3:U:3152[B]:LYS:HE3 | 1.83 | 0.79 |
| 3:U:3256[B]:TRP:HB2 | 3:d:2969[B]:TYR:H | 1.44 | 0.79 |
| 3:X:3151[A]:LEU:HB2 | 3:X:3175[A]:TYR:CD2 | 2.18 | 0.79 |
| 3:d:3148[B]:ILE:O | 3:d:3152[B]:LYS:HE3 | 1.83 | 0.79 |
| 3:C:2965[B]:LEU:HB3 | 3:L:3256[B]:TRP:CZ2 | 1.72 | 0.79 |
| 3:F:2969[A]:TYR:HB3 | 3:F:2971[A]:ASP:OD1 | 1.82 | 0.79 |
| 3:F:3161[B]:GLU:CA | 3:a:3147[B]:GLU:HG3 | 2.12 | 0.79 |
| 3:I:2955[B]:GLN:CD | 3:I:3037[B]:TYR:CE1 | 2.55 | 0.79 |
| 3:I:2956[B]:LYS:HD2 | 3:R:3257[B]:ALA:CB | 2.13 | 0.79 |
| 3:I:2975[B]:PHE:CE2 | 3:R:2961[B]:HIS:HA | 2.18 | 0.79 |
| 1:J:589:GLN:HG2 | 1:J:594:ASP:HB3 | 1.65 | 0.79 |
| 3:L:2939[B]:ARG:HB3 | 3:L:3032[B]:PRO:HG2 | 1.63 | 0.79 |
| 3:L:3025[B]:VAL:HG23 | 3:L:3033[B]:PHE:O | 1.83 | 0.79 |
| 3:L:3148[A]:ILE:O | 3:L:3152[A]:LYS:HE3 | 1.83 | 0.79 |
| 3:O:2965[B]:LEU:HD11 | 3:O:2974[B]:ALA:CA | 2.12 | 0.79 |
| 3:O:3153[B]:LYS:NZ | 3:X:3170[B]:ALA:O | 2.13 | 0.79 |
| 2:Q:2114:ARG:HH12 | 2:Q:2120:GLU:HG3 | 1.47 | 0.79 |
| 3:U:2980[B]:HIS:HB3 | 3:d:2969[B]:TYR:OH | 1.83 | 0.79 |
| 3:U:3256[B]:TRP:C | 3:d:2969[B]:TYR:H | 1.90 | 0.79 |
| 3:X:3135[B]:LYS:CG | 3:X:3141[B]:TYR:CD1 | 2.65 | 0.79 |
| 3:a:2979[B]:GLN:CG | 3:a:3155[B]:MET:CE | 2.56 | 0.79 |
| 3:a:3135[B]:LYS:CG | 3:a:3141[B]:TYR:CD1 | 2.65 | 0.79 |
| 3:a:3173[A]:THR:CB | 3:a:3176[A]:LYS:HD2 | 2.13 | 0.79 |
| 3:d:3180[B]:TYR:HB2 | 3:d:3183[B]:LEU:HD22 | 1.63 | 0.79 |
| 3:C:2952[A]:ALA:CB | 3:C:2953[A]:GLY:C | 2.48 | 0.79 |
| 3:C:2988[B]:TRP:HD1 | 3:L:3153[B]:LYS:CD | 1.95 | 0.79 |
| 3:C:3025[A]:VAL:CG2 | 3:C:3047[A]:ARG:HH12 | 1.94 | 0.79 |
| 3:C:3025[A]:VAL:HG23 | 3:C:3033[A]:PHE:O | 1.83 | 0.79 |
| 3:C:3104[B]:MET:CA | 3:C:3110[B]:THR:HG23 | 2.10 | 0.79 |
| 3:C:3148[B]:ILE:O | 3:C:3152[B]:LYS:HE3 | 1.83 | 0.79 |
| 3:F:3150[B]:LYS:O | 3:a:3159[B]:SER:OG | 1.82 | 0.79 |
| 3:F:3170[B]:ALA:O | 3:a:3152[B]:LYS:HB3 | 1.82 | 0.79 |
| 3:I:3173[B]:THR:CB | 3:I:3176[B]:LYS:HD2 | 2.13 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:210:HIS:HA | 1:J:213:VAL:HG22 | 1.64 | 0.79 |
| 3:L:3180[A]:TYR:HB2 | 3:L:3183[A]:LEU:HD22 | 1.63 | 0.79 |
| 3:O:3135[A]:LYS:CG | 3:O:3141[A]:TYR:CD1 | 2.65 | 0.79 |
| 3:O:3148[B]:ILE:O | 3:O:3152[B]:LYS:HE3 | 1.83 | 0.79 |
| 3:O:3180[B]:TYR:HB2 | 3:O:3183[B]:LEU:HD22 | 1.64 | 0.79 |
| 3:O:3196[A]:THR:HG21 | 1:P:416:ASN:CG | 2.06 | 0.79 |
| 3:R:2969[B]:TYR:HB3 | 3:R:2971[B]:ASP:OD1 | 1.82 | 0.79 |
| 3:U:2971[B]:ASP:O | 3:d:3247[B]:VAL:HG13 | 1.82 | 0.79 |
| 3:a:3151[A]:LEU:HB2 | 3:a:3175[A]:TYR:CD2 | 2.18 | 0.79 |
| 3:a:3185[B]:TYR:HE2 | 3:a:3187[B]:TYR:CE2 | 2.01 | 0.79 |
| 3:d:3024[B]:LEU:CD1 | 3:d:3025[B]:VAL:H | 1.83 | 0.79 |
| 3:d:3135[B]:LYS:CG | 3:d:3141[B]:TYR:CD1 | 2.65 | 0.79 |
| 3:d:3173[A]:THR:CB | 3:d:3176[A]:LYS:HD2 | 2.13 | 0.79 |
| 3:C:3135[B]:LYS:CG | 3:C:3141[B]:TYR:CD1 | 2.65 | 0.78 |
| 3:C:3150[B]:LYS:H | 3:L:3169[B]:LYS:HG2 | 1.46 | 0.78 |
| 3:F:3173[A]:THR:CB | 3:F:3176[A]:LYS:HD2 | 2.13 | 0.78 |
| 3:I:2949[A]:LYS:O | 3:I:2949[A]:LYS:NZ | 2.16 | 0.78 |
| 3:I:2982[B]:MET:HB3 | 3:R:3160[B]:SER:HB2 | 1.65 | 0.78 |
| 3:I:2989[B]:HIS:HD2 | 3:R:2970[B]:PRO:CA | 1.96 | 0.78 |
| 3:I:3153[B]:LYS:C | 3:R:3155[B]:MET:H | 1.90 | 0.78 |
| 3:I:3155[B]:MET:HB2 | 3:R:3153[B]:LYS:CB | 2.13 | 0.78 |
| 3:L:3230[B]:PHE:CB | 3:L:3243[B]:GLY:HA2 | 2.06 | 0.78 |
| 3:O:3148[A]:ILE:O | 3:O:3152[A]:LYS:HE3 | 1.83 | 0.78 |
| 3:U:3151[A]:LEU:HB2 | 3:U:3175[A]:TYR:CD2 | 2.18 | 0.78 |
| 3:U:3173[B]:THR:CB | 3:U:3176[B]:LYS:HD2 | 2.13 | 0.78 |
| 3:X:2949[A]:LYS:NZ | 3:X:2949[A]:LYS:O | 2.16 | 0.78 |
| 3:X:2965[A]:LEU:HD11 | 3:X:2974[A]:ALA:CA | 2.12 | 0.78 |
| 3:X:3025[B]:VAL:HG23 | 3:X:3033[B]:PHE:O | 1.83 | 0.78 |
| 3:X:3180[B]:TYR:HB2 | 3:X:3183[B]:LEU:HD22 | 1.63 | 0.78 |
| 1:Y:1551:ASP:OD1 | 3:d:3007[B]:ILE:HD13 | 1.82 | 0.78 |
| 3:d:3135[A]:LYS:CG | 3:d:3141[A]:TYR:CD1 | 2.65 | 0.78 |
| 3:C:2949[B]:LYS:NZ | 3:C:2949[B]:LYS:O | 2.16 | 0.78 |
| 3:C:3159[B]:SER:CB | 3:L:2984[B]:THR:HG21 | 1.96 | 0.78 |
| 3:C:3258[B]:PHE:CZ | 3:L:2968[B]:GLN:OE1 | 2.36 | 0.78 |
| 3:F:2985[B]:PHE:HE2 | 3:a:2969[B]:TYR:O | 1.66 | 0.78 |
| 3:F:3180[A]:TYR:HB2 | 3:F:3183[A]:LEU:HD22 | 1.64 | 0.78 |
| 3:F:3254[B]:MET:HG3 | 3:a:2966[B]:SER:CB | 2.08 | 0.78 |
| 3:I:2948[B]:ASP:N | 3:I:2949[B]:LYS:CA | 2.41 | 0.78 |
| 3:I:2961[A]:HIS:HD2 | 3:I:2988[A]:TRP:HZ3 | 1.32 | 0.78 |
| 3:I:2964[B]:PRO:HB2 | 3:R:3255[B]:PRO:HB3 | 1.63 | 0.78 |
| 3:I:2982[B]:MET:HE3 | 3:R:2977[B]:CYS:HB3 | 1.64 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3024[A]:LEU:CD1 | 3:I:3025[A]:VAL:H | 1.84 | 0.78 |
| 3:L:2949[A]:LYS:O | 3:L:2949[A]:LYS:NZ | 2.16 | 0.78 |
| 3:L:3185[A]:TYR:HE2 | 3:L:3187[A]:TYR:CE2 | 2.01 | 0.78 |
| 3:O:2970[B]:PRO:CG | 3:X:2991[B]:LEU:HB2 | 2.03 | 0.78 |
| 3:U:3153[B]:LYS:CD | 3:d:2979[B]:GLN:NE2 | 2.47 | 0.78 |
| 3:U:3256[B]:TRP:CB | 3:d:2969[B]:TYR:N | 2.46 | 0.78 |
| 1:V:527:LEU:HD22 | 1:V:629:MET:HG3 | 1.66 | 0.78 |
| 1:V:1046:HIS:HA | 1:V:1049:VAL:HB | 1.64 | 0.78 |
| 1:Y:1616:LYS:HD3 | 3:d:3188[B]:ASP:CA | 2.11 | 0.78 |
| 2:Z:2545:SER:HA | 2:Z:2546:LEU:HB2 | 1.65 | 0.78 |
| 3:a:3025[B]:VAL:HG23 | 3:a:3033[B]:PHE:O | 1.83 | 0.78 |
| 2:c:2166:LEU:HA | 2:c:2169:HIS:HB2 | 1.65 | 0.78 |
| 3:C:3135[A]:LYS:CG | 3:C:3141[A]:TYR:CD1 | 2.65 | 0.78 |
| 1:D:567:LEU:HB2 | 1:D:609:TRP:HD1 | 1.45 | 0.78 |
| 3:F:2952[B]:ALA:CB | 3:F:2953[B]:GLY:C | 2.48 | 0.78 |
| 3:F:2965[B]:LEU:CA | 3:a:3221[B]:ALA:CB | 2.49 | 0.78 |
| 3:F:2985[B]:PHE:HE2 | 3:a:2969[B]:TYR:C | 1.90 | 0.78 |
| 3:I:2961[B]:HIS:HD2 | 3:I:2988[B]:TRP:HZ3 | 1.31 | 0.78 |
| 3:L:3104[B]:MET:CA | 3:L:3110[B]:THR:HG23 | 2.10 | 0.78 |
| 3:O:2952[A]:ALA:CB | 3:O:2953[A]:GLY:C | 2.48 | 0.78 |
| 3:O:2975[B]:PHE:C | 3:X:3156[B]:MET:HG3 | 2.06 | 0.78 |
| 3:O:3025[A]:VAL:HG23 | 3:O:3033[A]:PHE:O | 1.83 | 0.78 |
| 3:O:3025[B]:VAL:CG2 | 3:O:3047[B]:ARG:HH12 | 1.94 | 0.78 |
| 1:P:979:LEU:HB2 | 1:P:980:TYR:HA | 1.65 | 0.78 |
| 3:R:3025[A]:VAL:HG23 | 3:R:3033[A]:PHE:O | 1.83 | 0.78 |
| 3:R:3173[A]:THR:CB | 3:R:3176[A]:LYS:HD2 | 2.13 | 0.78 |
| 3:U:2949[B]:LYS:NZ | 3:U:2949[B]:LYS:O | 2.16 | 0.78 |
| 3:U:3148[A]:ILE:O | 3:U:3152[A]:LYS:HE3 | 1.83 | 0.78 |
| 3:U:3151[B]:LEU:HB2 | 3:U:3175[B]:TYR:CD2 | 2.18 | 0.78 |
| 3:U:3160[B]:SER:CB | 3:d:3259[B]:ASP:HB3 | 2.12 | 0.78 |
| 3:U:3185[A]:TYR:HE2 | 3:U:3187[A]:TYR:CE2 | 2.01 | 0.78 |
| 3:X:3135[A]:LYS:CG | 3:X:3141[A]:TYR:CD1 | 2.65 | 0.78 |
| 3:X:3173[B]:THR:CB | 3:X:3176[B]:LYS:HD2 | 2.13 | 0.78 |
| 2:Z:2898:LYS:HE2 | 2:Z:2898:LYS:H | 1.48 | 0.78 |
| 3:C:3141[A]:TYR:HD2 | 3:C:3142[A]:ASN:H | 0.78 | 0.78 |
| 3:C:3159[B]:SER:CB | 3:L:3150[B]:LYS:C | 2.57 | 0.78 |
| 3:F:2961[B]:HIS:HD2 | 3:F:2988[B]:TRP:HZ3 | 1.31 | 0.78 |
| 3:F:3025[B]:VAL:HG23 | 3:F:3033[B]:PHE:O | 1.83 | 0.78 |
| 3:F:3185[A]:TYR:HE2 | 3:F:3187[A]:TYR:CE2 | 2.01 | 0.78 |
| 3:I:2966[B]:SER:HB2 | 3:R:3254[B]:MET:HG3 | 0.85 | 0.78 |
| 3:I:3135[A]:LYS:CG | 3:I:3141[A]:TYR:CD1 | 2.65 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:2952[B]:ALA:CB | 3:L:2953[B]:GLY:C | 2.48 | 0.78 |
| 3:L:2979[B]:GLN:NE2 | 3:L:3155[B]:MET:CE | 2.47 | 0.78 |
| 3:O:3141[A]:TYR:HD2 | 3:O:3142[A]:ASN:H | 0.78 | 0.78 |
| 1:P:161:ASN:OD1 | 1:P:174:GLN:NE2 | 2.16 | 0.78 |
| 3:R:2979[A]:GLN:CG | 3:R:3155[A]:MET:CE | 2.56 | 0.78 |
| 3:R:3185[A]:TYR:HE2 | 3:R:3187[A]:TYR:CE2 | 2.02 | 0.78 |
| 3:R:3259[B]:ASP:OD2 | 3:R:3260[B]:ARG:HG2 | 1.84 | 0.78 |
| 3:U:2949[A]:LYS:O | 3:U:2949[A]:LYS:NZ | 2.16 | 0.78 |
| 3:U:2965[B]:LEU:CA | 3:d:3220[B]:ARG:HH11 | 1.70 | 0.78 |
| 3:X:3185[B]:TYR:HE2 | 3:X:3187[B]:TYR:CE2 | 2.02 | 0.78 |
| 3:a:2949[B]:LYS:O | 3:a:2949[B]:LYS:NZ | 2.16 | 0.78 |
| 3:F:2956[A]:LYS:O | 3:F:2960[A]:PHE:CD1 | 2.33 | 0.78 |
| 3:F:3185[B]:TYR:HE2 | 3:F:3187[B]:TYR:CE2 | 2.01 | 0.78 |
| 3:I:3141[A]:TYR:HD2 | 3:I:3142[A]:ASN:H | 0.78 | 0.78 |
| 3:I:3148[A]:ILE:O | 3:I:3152[A]:LYS:HE3 | 1.83 | 0.78 |
| 3:I:3150[B]:LYS:HB2 | 3:R:3169[B]:LYS:HG3 | 1.64 | 0.78 |
| 3:L:2969[A]:TYR:HB3 | 3:L:2971[A]:ASP:OD1 | 1.82 | 0.78 |
| 3:L:3185[B]:TYR:HE2 | 3:L:3187[B]:TYR:CE2 | 2.01 | 0.78 |
| 3:O:3151[B]:LEU:HB2 | 3:O:3175[B]:TYR:CD2 | 2.18 | 0.78 |
| 3:O:3159[B]:SER:C | 3:X:3148[B]:ILE:C | 2.51 | 0.78 |
| 1:S:573:LYS:HB3 | 1:S:574:GLY:HA2 | 1.66 | 0.78 |
| 1:S:1618:LEU:HD22 | 3:X:3136[B]:TYR:HE2 | 1.49 | 0.78 |
| 2:T:2184:MET:HE3 | 2:T:2231:LEU:HG | 1.65 | 0.78 |
| 3:U:3169[B]:LYS:HE3 | 3:d:3147[B]:GLU:HA | 1.61 | 0.78 |
| 3:U:3255[B]:PRO:HG2 | 3:d:3252[B]:TYR:CB | 2.13 | 0.78 |
| 3:U:3259[A]:ASP:OD2 | 3:U:3260[A]:ARG:HG2 | 1.84 | 0.78 |
| 1:Y:1546:LYS:HB2 | 3:d:3001[B]:LYS:HZ1 | 0.95 | 0.78 |
| 3:a:3023[A]:ILE:O | 3:a:3026[A]:THR:N | 2.11 | 0.78 |
| 3:a:3151[B]:LEU:HB2 | 3:a:3175[B]:TYR:CD2 | 2.18 | 0.78 |
| 3:d:3259[A]:ASP:OD2 | 3:d:3260[A]:ARG:HG2 | 1.84 | 0.78 |
| 3:C:2981[B]:GLY:N | 3:L:2968[B]:GLN:HG2 | 1.97 | 0.78 |
| 3:C:3173[B]:THR:CB | 3:C:3176[B]:LYS:HD2 | 2.13 | 0.78 |
| 3:I:3025[A]:VAL:HG23 | 3:I:3033[A]:PHE:O | 1.83 | 0.78 |
| 3:I:3151[A]:LEU:HB2 | 3:I:3175[A]:TYR:CD2 | 2.18 | 0.78 |
| 3:I:3185[B]:TYR:HE2 | 3:I:3187[B]:TYR:CE2 | 2.01 | 0.78 |
| 1:J:1137:LYS:HA | 1:J:1141:ARG:HH12 | 1.48 | 0.78 |
| 3:L:3173[A]:THR:CB | 3:L:3176[A]:LYS:HD2 | 2.13 | 0.78 |
| 3:L:3259[B]:ASP:OD2 | 3:L:3260[B]:ARG:HG2 | 1.84 | 0.78 |
| 3:O:2979[A]:GLN:NE2 | 3:O:3155[A]:MET:CE | 2.47 | 0.78 |
| 3:R:2961[A]:HIS:HD2 | 3:R:2988[A]:TRP:HZ3 | 1.31 | 0.78 |
| 3:U:2948[A]:ASP:N | 3:U:2949[A]:LYS:CA | 2.41 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2975[B]:PHE:N | 3:d:3256[B]:TRP:O | 2.16 | 0.78 |
| 3:U:2982[B]:MET:C | 3:d:2970[B]:PRO:HD3 | 2.00 | 0.78 |
| 3:U:3169[B]:LYS:CD | 3:d:3147[B]:GLU:CA | 2.61 | 0.78 |
| 3:U:3259[B]:ASP:OD2 | 3:U:3260[B]:ARG:HG2 | 1.84 | 0.78 |
| 3:X:3141[A]:TYR:HD2 | 3:X:3142[A]:ASN:H | 0.78 | 0.78 |
| 3:d:2949[A]:LYS:O | 3:d:2949[A]:LYS:NZ | 2.16 | 0.78 |
| 3:d:3173[B]:THR:CB | 3:d:3176[B]:LYS:HD2 | 2.13 | 0.78 |
| 2:B:2867:PRO:HG2 | 3:C:2932[A]:PRO:CG | 2.14 | 0.78 |
| 3:C:3155[B]:MET:CE | 3:L:3154[B]:PRO:O | 2.31 | 0.78 |
| 3:C:3256[B]:TRP:CE2 | 3:L:2965[B]:LEU:C | 2.52 | 0.78 |
| 3:F:3160[B]:SER:OG | 3:a:2982[B]:MET:CA | 2.30 | 0.78 |
| 3:I:3141[B]:TYR:HD2 | 3:I:3142[B]:ASN:H | 0.78 | 0.78 |
| 3:L:3104[A]:MET:CA | 3:L:3110[A]:THR:HG23 | 2.10 | 0.78 |
| 3:L:3173[B]:THR:CB | 3:L:3176[B]:LYS:HD2 | 2.13 | 0.78 |
| 3:O:3185[B]:TYR:HE2 | 3:O:3187[B]:TYR:CE2 | 2.01 | 0.78 |
| 3:O:3259[B]:ASP:OD2 | 3:O:3260[B]:ARG:HG2 | 1.84 | 0.78 |
| 3:R:3023[B]:ILE:O | 3:R:3026[B]:THR:N | 2.11 | 0.78 |
| 3:R:3173[B]:THR:CB | 3:R:3176[B]:LYS:HD2 | 2.13 | 0.78 |
| 3:U:2939[A]:ARG:HB3 | 3:U:3032[A]:PRO:HG2 | 1.63 | 0.78 |
| 3:U:3025[A]:VAL:HG23 | 3:U:3033[A]:PHE:O | 1.83 | 0.78 |
| 3:a:2979[A]:GLN:NE2 | 3:a:3155[A]:MET:CE | 2.47 | 0.78 |
| 3:a:3259[B]:ASP:OD2 | 3:a:3260[B]:ARG:HG2 | 1.84 | 0.78 |
| 4:q:2:NAG:H83 | 4:q:2:NAG:H3 | 1.66 | 0.78 |
| 3:C:2961[B]:HIS:HD2 | 3:C:2988[B]:TRP:HZ3 | 1.31 | 0.78 |
| 3:C:2965[B]:LEU:O | 3:L:3256[B]:TRP:CE3 | 2.13 | 0.78 |
| 1:D:1296:VAL:HB | 1:D:1446:ASP:HB3 | 1.65 | 0.78 |
| 3:F:2949[A]:LYS:O | 3:F:2949[A]:LYS:NZ | 2.16 | 0.78 |
| 3:I:2979[B]:GLN:NE2 | 3:I:3155[B]:MET:CE | 2.47 | 0.78 |
| 3:L:3148[B]:ILE:O | 3:L:3152[B]:LYS:HE3 | 1.83 | 0.78 |
| 1:P:142:ARG:NH1 | 1:P:340:GLN:OE1 | 2.16 | 0.78 |
| 3:R:3259[A]:ASP:OD2 | 3:R:3260[A]:ARG:HG2 | 1.84 | 0.78 |
| 2:T:2711:HIS:HA | 2:T:2714:VAL:HG22 | 1.66 | 0.78 |
| 3:U:3173[A]:THR:CB | 3:U:3176[A]:LYS:HD2 | 2.13 | 0.78 |
| 3:U:3256[B]:TRP:HB3 | 3:d:2975[B]:PHE:CZ | 2.18 | 0.78 |
| 3:U:3284[A]:LYS:CD | 3:U:3285[A]:VAL:N | 2.47 | 0.78 |
| 3:X:2949[B]:LYS:O | 3:X:2949[B]:LYS:NZ | 2.16 | 0.78 |
| 3:X:3151[B]:LEU:HB2 | 3:X:3175[B]:TYR:CD2 | 2.18 | 0.78 |
| 1:Y:898:GLY:HA2 | 1:Y:1186:TRP:HB2 | 1.64 | 0.78 |
| 2:c:2638:ARG:NH1 | 2:c:2704:ASP:OD1 | 2.16 | 0.78 |
| 3:d:3151[A]:LEU:HB2 | 3:d:3175[A]:TYR:CD2 | 2.18 | 0.78 |
| 1:A:401:VAL:HG22 | 1:A:662:SER:HB3 | 1.66 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3093[B]:HIS:ND1 | 3:L:2971[B]:ASP:HB3 | 1.72 | 0.78 |
| 3:C:3150[B]:LYS:HD3 | 3:L:3156[B]:MET:HA | 1.66 | 0.78 |
| 3:C:3185[A]:TYR:HE2 | 3:C:3187[A]:TYR:CE2 | 2.01 | 0.78 |
| 3:F:3173[B]:THR:CB | 3:F:3176[B]:LYS:HD2 | 2.13 | 0.78 |
| 3:I:3153[B]:LYS:HD3 | 3:R:2988[B]:TRP:CD1 | 2.18 | 0.78 |
| 3:I:3259[B]:ASP:OD2 | 3:I:3260[B]:ARG:HG2 | 1.84 | 0.78 |
| 3:L:2949[B]:LYS:O | 3:L:2949[B]:LYS:NZ | 2.16 | 0.78 |
| 3:O:2963[B]:MET:HE1 | 3:X:2975[B]:PHE:HB2 | 1.65 | 0.78 |
| 3:R:3025[B]:VAL:HG23 | 3:R:3033[B]:PHE:O | 1.83 | 0.78 |
| 3:U:2969[B]:TYR:HB3 | 3:U:2971[B]:ASP:OD1 | 1.82 | 0.78 |
| 3:U:3252[B]:TYR:O | 3:d:3255[B]:PRO:CB | 2.32 | 0.78 |
| 1:V:401:VAL:HG22 | 1:V:662:SER:HB3 | 1.65 | 0.78 |
| 3:X:3104[A]:MET:CA | 3:X:3110[A]:THR:HG23 | 2.10 | 0.78 |
| 3:X:3259[B]:ASP:OD2 | 3:X:3260[B]:ARG:HG2 | 1.84 | 0.78 |
| 3:a:2961[A]:HIS:HD2 | 3:a:2988[A]:TRP:HZ3 | 1.31 | 0.78 |
| 3:C:2974[B]:ALA:HB2 | 3:L:3249[B]:GLY:HA3 | 1.66 | 0.78 |
| 3:C:2979[A]:GLN:NE2 | 3:C:3155[A]:MET:CE | 2.47 | 0.78 |
| 3:C:3154[B]:PRO:CB | 3:L:3151[B]:LEU:C | 2.57 | 0.78 |
| 3:C:3173[A]:THR:CB | 3:C:3176[A]:LYS:HD2 | 2.13 | 0.78 |
| 3:C:3259[A]:ASP:OD2 | 3:C:3260[A]:ARG:HG2 | 1.84 | 0.78 |
| 3:F:2949[B]:LYS:O | 3:F:2949[B]:LYS:NZ | 2.16 | 0.78 |
| 3:I:2979[A]:GLN:NE2 | 3:I:3155[A]:MET:CE | 2.47 | 0.78 |
| 3:I:2988[B]:TRP:CH2 | 3:R:2975[B]:PHE:CE2 | 2.71 | 0.78 |
| 3:L:3180[B]:TYR:HB2 | 3:L:3183[B]:LEU:HD22 | 1.63 | 0.78 |
| 3:O:2976[B]:ALA:C | 3:X:3154[B]:PRO:O | 2.27 | 0.78 |
| 3:O:3151[A]:LEU:HB2 | 3:O:3175[A]:TYR:CD2 | 2.18 | 0.78 |
| 3:R:3104[A]:MET:CA | 3:R:3110[A]:THR:HG23 | 2.10 | 0.78 |
| 3:R:3148[B]:ILE:O | 3:R:3152[B]:LYS:HE3 | 1.83 | 0.78 |
| 1:S:19:GLN:NE2 | 1:S:121:ASN:OD1 | 2.17 | 0.78 |
| 3:U:2965[B]:LEU:CD1 | 3:d:3220[B]:ARG:C | 2.57 | 0.78 |
| 3:U:3141[A]:TYR:HD2 | 3:U:3142[A]:ASN:H | 0.78 | 0.78 |
| 3:U:3154[B]:PRO:HG3 | 3:d:2984[B]:THR:HG23 | 1.64 | 0.78 |
| 3:X:3025[A]:VAL:HG23 | 3:X:3033[A]:PHE:O | 1.83 | 0.78 |
| 3:a:3148[B]:ILE:O | 3:a:3152[B]:LYS:HE3 | 1.83 | 0.78 |
| 3:a:3173[B]:THR:CB | 3:a:3176[B]:LYS:HD2 | 2.13 | 0.78 |
| 3:a:3259[A]:ASP:OD2 | 3:a:3260[A]:ARG:HG2 | 1.84 | 0.78 |
| 3:d:3148[A]:ILE:O | 3:d:3152[A]:LYS:HE3 | 1.83 | 0.78 |
| 3:d:3185[B]:TYR:HE2 | 3:d:3187[B]:TYR:CE2 | 2.01 | 0.78 |
| 2:B:2107:LEU:HD23 | 2:B:2208:PRO:HB2 | 1.64 | 0.77 |
| 3:C:2982[B]:MET:N | 3:L:2967[B]:CYS:HB3 | 1.99 | 0.77 |
| 3:C:3149[B]:ASN:O | 3:L:3172[B]:SER:HB3 | 1.83 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3172[B]:SER:OG | 3:L:3152[B]:LYS:N | 2.15 | 0.77 |
| 3:F:3259[A]:ASP:OD2 | 3:F:3260[A]:ARG:HG2 | 1.84 | 0.77 |
| 3:I:3023[A]:ILE:O | 3:I:3026[A]:THR:N | 2.11 | 0.77 |
| 3:I:3148[B]:ILE:O | 3:R:3170[B]:ALA:N | 2.17 | 0.77 |
| 3:I:3149[B]:ASN:CB | 3:R:3163[B]:ASN:CG | 2.55 | 0.77 |
| 3:L:2948[A]:ASP:H | 3:L:2949[A]:LYS:CA | 1.98 | 0.77 |
| 3:L:3135[B]:LYS:CG | 3:L:3141[B]:TYR:CD1 | 2.65 | 0.77 |
| 3:L:3284[B]:LYS:CD | 3:L:3285[B]:VAL:N | 2.47 | 0.77 |
| 3:O:3230[A]:PHE:CB | 3:O:3243[A]:GLY:HA2 | 2.06 | 0.77 |
| 3:U:2979[B]:GLN:NE2 | 3:U:3155[B]:MET:CE | 2.47 | 0.77 |
| 3:U:3284[B]:LYS:CD | 3:U:3285[B]:VAL:N | 2.47 | 0.77 |
| 3:U:3306[B]:LEU:HD12 | 3:U:3307[B]:PHE:N | 2.00 | 0.77 |
| 3:C:3255[B]:PRO:HD2 | 3:L:2960[B]:PHE:C | 2.10 | 0.77 |
| 3:C:3284[B]:LYS:CD | 3:C:3285[B]:VAL:N | 2.47 | 0.77 |
| 3:F:3023[A]:ILE:O | 3:F:3026[A]:THR:N | 2.11 | 0.77 |
| 3:F:3147[B]:GLU:H | 3:a:3161[B]:GLU:HA | 1.48 | 0.77 |
| 3:I:3151[B]:LEU:HB2 | 3:I:3175[B]:TYR:CD2 | 2.18 | 0.77 |
| 1:J:325:THR:OG1 | 1:J:332:ASP:N | 2.17 | 0.77 |
| 3:L:3025[A]:VAL:HG23 | 3:L:3033[A]:PHE:O | 1.83 | 0.77 |
| 3:L:3141[A]:TYR:HD2 | 3:L:3142[A]:ASN:H | 0.78 | 0.77 |
| 3:L:3151[A]:LEU:HB2 | 3:L:3175[A]:TYR:CD2 | 2.18 | 0.77 |
| 1:M:456:GLN:NE2 | 1:M:549:PRO:O | 2.17 | 0.77 |
| 1:M:1280:GLN:HE22 | 1:M:1337:ARG:HB3 | 1.47 | 0.77 |
| 2:N:2528:LYS:NZ | 2:N:2626:ARG:O | 2.16 | 0.77 |
| 3:R:2956[B]:LYS:C | 3:R:2960[B]:PHE:CE1 | 2.47 | 0.77 |
| 1:V:1442:MET:HE1 | 1:V:1454:PHE:HA | 1.66 | 0.77 |
| 3:a:2949[A]:LYS:O | 3:a:2949[A]:LYS:NZ | 2.16 | 0.77 |
| 3:a:3180[A]:TYR:HB2 | 3:a:3183[A]:LEU:HD22 | 1.64 | 0.77 |
| 3:F:2955[A]:GLN:CD | 3:F:3037[A]:TYR:HE1 | 1.92 | 0.77 |
| 3:F:2985[B]:PHE:CE2 | 3:a:2969[B]:TYR:O | 2.37 | 0.77 |
| 3:F:3153[B]:LYS:HB3 | 3:a:3155[B]:MET:CB | 2.06 | 0.77 |
| 3:I:3160[B]:SER:HA | 3:R:2983[B]:VAL:CA | 2.14 | 0.77 |
| 3:I:3173[A]:THR:CB | 3:I:3176[A]:LYS:HD2 | 2.13 | 0.77 |
| 3:L:2961[B]:HIS:HD2 | 3:L:2988[B]:TRP:HZ3 | 1.32 | 0.77 |
| 3:O:2968[B]:GLN:HA | 3:X:2988[B]:TRP:CD1 | 2.20 | 0.77 |
| 3:O:2969[B]:TYR:HA | 3:X:2991[B]:LEU:HD22 | 1.67 | 0.77 |
| 3:O:3185[A]:TYR:HE2 | 3:O:3187[A]:TYR:CE2 | 2.01 | 0.77 |
| 3:R:3284[A]:LYS:CD | 3:R:3285[A]:VAL:N | 2.47 | 0.77 |
| 3:R:3284[B]:LYS:CD | 3:R:3285[B]:VAL:N | 2.47 | 0.77 |
| 1:S:161:ASN:ND2 | 1:S:174:GLN:OE1 | 2.17 | 0.77 |
| 3:U:2955[B]:GLN:CD | 3:U:3037[B]:TYR:HE1 | 1.92 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2952[A]:ALA:CB | 3:X:2953[A]:GLY:C | 2.48 | 0.77 |
| 3:X:3284[B]:LYS:CD | 3:X:3285[B]:VAL:N | 2.47 | 0.77 |
| 3:d:3259[B]:ASP:OD2 | 3:d:3260[B]:ARG:HG2 | 1.84 | 0.77 |
| 3:C:3148[A]:ILE:O | 3:C:3152[A]:LYS:HE3 | 1.83 | 0.77 |
| 3:C:3155[B]:MET:HG3 | 3:L:3154[B]:PRO:N | 1.92 | 0.77 |
| 3:C:3252[B]:TYR:OH | 3:L:3224[B]:GLN:HA | 1.85 | 0.77 |
| 3:F:2965[B]:LEU:C | 3:a:3255[B]:PRO:HA | 2.08 | 0.77 |
| 3:F:3148[B]:ILE:O | 3:F:3152[B]:LYS:HE3 | 1.83 | 0.77 |
| 3:I:2963[B]:MET:HE1 | 3:R:3223[B]:GLY:CA | 2.10 | 0.77 |
| 3:I:2975[B]:PHE:CE1 | 3:R:2961[B]:HIS:O | 2.37 | 0.77 |
| 3:I:2983[B]:VAL:HB | 3:R:3160[B]:SER:HA | 1.65 | 0.77 |
| 3:I:3120[B]:HIS:NE2 | 3:R:2969[B]:TYR:CD2 | 2.53 | 0.77 |
| 3:I:3150[B]:LYS:C | 3:R:3172[B]:SER:CB | 2.57 | 0.77 |
| 3:L:3113[B]:ASP:CG | 3:L:3114[B]:PRO:CD | 2.56 | 0.77 |
| 3:L:3306[B]:LEU:HD12 | 3:L:3307[B]:PHE:N | 2.00 | 0.77 |
| 3:O:2948[A]:ASP:H | 3:O:2949[A]:LYS:CA | 1.98 | 0.77 |
| 3:O:2948[B]:ASP:N | 3:O:2949[B]:LYS:CA | 2.41 | 0.77 |
| 3:O:2949[B]:LYS:NZ | 3:O:2949[B]:LYS:O | 2.16 | 0.77 |
| 3:O:2975[B]:PHE:CE2 | 3:X:3172[B]:SER:HA | 2.17 | 0.77 |
| 3:R:3185[B]:TYR:HE2 | 3:R:3187[B]:TYR:CE2 | 2.01 | 0.77 |
| 1:S:724:LYS:HA | 1:S:728:ARG:HH12 | 1.49 | 0.77 |
| 3:U:3220[B]:ARG:CG | 3:d:2973[B]:THR:HG22 | 2.15 | 0.77 |
| 3:X:3259[A]:ASP:OD2 | 3:X:3260[A]:ARG:HG2 | 1.84 | 0.77 |
| 3:a:2979[B]:GLN:NE2 | 3:a:3155[B]:MET:CE | 2.47 | 0.77 |
| 3:a:3306[A]:LEU:HD12 | 3:a:3307[A]:PHE:N | 2.00 | 0.77 |
| 3:d:3211[A]:ASP:HB3 | 3:d:3309[A]:PRO:HA | 1.67 | 0.77 |
| 3:C:2955[A]:GLN:CD | 3:C:3037[A]:TYR:HE1 | 1.92 | 0.77 |
| 3:C:3152[B]:LYS:HB2 | 3:L:3171[B]:HIS:C | 2.09 | 0.77 |
| 3:C:3306[A]:LEU:HD12 | 3:C:3307[A]:PHE:N | 2.00 | 0.77 |
| 3:F:2961[B]:HIS:HB3 | 3:F:3111[B]:SER:OG | 1.85 | 0.77 |
| 3:F:2966[B]:SER:N | 3:a:3255[B]:PRO:C | 2.43 | 0.77 |
| 3:F:3141[A]:TYR:HD2 | 3:F:3142[A]:ASN:H | 0.78 | 0.77 |
| 3:F:3159[B]:SER:OG | 3:a:3150[B]:LYS:O | 2.02 | 0.77 |
| 3:F:3284[B]:LYS:CD | 3:F:3285[B]:VAL:N | 2.47 | 0.77 |
| 3:I:2937[A]:ASN:HB2 | 3:I:3006[A]:LYS:CE | 2.14 | 0.77 |
| 3:I:2975[B]:PHE:CE1 | 3:R:2961[B]:HIS:ND1 | 2.53 | 0.77 |
| 3:L:2961[A]:HIS:HD2 | 3:L:2988[A]:TRP:HZ3 | 1.31 | 0.77 |
| 3:O:2937[B]:ASN:CB | 3:O:3006[B]:LYS:HE2 | 2.14 | 0.77 |
| 3:O:2952[B]:ALA:CB | 3:O:2953[B]:GLY:C | 2.48 | 0.77 |
| 1:P:2:LEU:HD21 | 1:P:81:VAL:HG21 | 1.66 | 0.77 |
| 3:X:3173[A]:THR:CB | 3:X:3176[A]:LYS:HD2 | 2.13 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3306[B]:LEU:HD12 | 3:X:3307[B]:PHE:N | 2.00 | 0.77 |
| 3:a:3148[A]:ILE:O | 3:a:3152[A]:LYS:HE3 | 1.83 | 0.77 |
| 2:c:2554:PRO:HA | 2:c:2555:GLU:HB3 | 1.67 | 0.77 |
| 1:A:1583:CYS:H | 1:b:329:ARG:HB3 | 1.49 | 0.77 |
| 3:C:2981[B]:GLY:HA2 | 3:L:2968[B]:GLN:OE1 | 1.83 | 0.77 |
| 3:C:3185[B]:TYR:HE2 | 3:C:3187[B]:TYR:CE2 | 2.01 | 0.77 |
| 3:F:3025[A]:VAL:HG23 | 3:F:3033[A]:PHE:O | 1.83 | 0.77 |
| 3:F:3158[B]:PHE:H | 3:a:3153[B]:LYS:CE | 1.96 | 0.77 |
| 3:I:3025[B]:VAL:HG23 | 3:I:3033[B]:PHE:O | 1.83 | 0.77 |
| 3:I:3154[B]:PRO:HB3 | 3:R:3174[B]:GLY:HA3 | 1.64 | 0.77 |
| 2:N:2549:PRO:HD3 | 2:N:2556:TYR:HD2 | 1.50 | 0.77 |
| 3:U:3185[B]:TYR:HE2 | 3:U:3187[B]:TYR:CE2 | 2.01 | 0.77 |
| 3:U:3254[B]:MET:HE1 | 3:d:3254[B]:MET:HE1 | 1.59 | 0.77 |
| 3:U:3306[A]:LEU:HD12 | 3:U:3307[A]:PHE:N | 2.00 | 0.77 |
| 1:Y:401:VAL:HG22 | 1:Y:662:SER:HB3 | 1.65 | 0.77 |
| 3:d:3025[A]:VAL:HG23 | 3:d:3033[A]:PHE:O | 1.83 | 0.77 |
| 3:d:3104[A]:MET:CA | 3:d:3110[A]:THR:HG23 | 2.10 | 0.77 |
| 3:d:3151[B]:LEU:HB2 | 3:d:3175[B]:TYR:CD2 | 2.18 | 0.77 |
| 3:C:2937[A]:ASN:HB2 | 3:C:3006[A]:LYS:CE | 2.14 | 0.77 |
| 3:F:2979[B]:GLN:NE2 | 3:F:3155[B]:MET:CE | 2.47 | 0.77 |
| 3:I:3090[B]:ASN:CA | 3:R:2971[B]:ASP:O | 2.31 | 0.77 |
| 3:I:3306[B]:LEU:HD12 | 3:I:3307[B]:PHE:N | 2.00 | 0.77 |
| 2:K:2236:ALA:HB3 | 2:K:2239:LYS:HB2 | 1.66 | 0.77 |
| 3:L:3211[B]:ASP:HB3 | 3:L:3309[B]:PRO:HA | 1.67 | 0.77 |
| 3:O:3259[A]:ASP:OD2 | 3:O:3260[A]:ARG:HG2 | 1.84 | 0.77 |
| 3:R:2961[B]:HIS:HB3 | 3:R:3111[B]:SER:OG | 1.85 | 0.77 |
| 3:R:2979[B]:GLN:NE2 | 3:R:3155[B]:MET:CE | 2.47 | 0.77 |
| 1:S:1617:LYS:CE | 3:X:3135[B]:LYS:NZ | 2.43 | 0.77 |
| 3:U:2948[B]:ASP:HB3 | 3:U:2949[B]:LYS:CA | 2.15 | 0.77 |
| 3:U:2964[B]:PRO:C | 3:d:3220[B]:ARG:HH12 | 1.92 | 0.77 |
| 3:X:2961[B]:HIS:HD2 | 3:X:2988[B]:TRP:HZ3 | 1.31 | 0.77 |
| 1:Y:567:LEU:N | 1:Y:568:PHE:HA | 2.00 | 0.77 |
| 3:a:2961[B]:HIS:HB3 | 3:a:3111[B]:SER:OG | 1.85 | 0.77 |
| 3:C:2961[A]:HIS:HB3 | 3:C:3111[A]:SER:OG | 1.85 | 0.77 |
| 3:C:3089[B]:HIS:ND1 | 3:L:2971[B]:ASP:HA | 1.95 | 0.77 |
| 3:C:3211[A]:ASP:HB3 | 3:C:3309[A]:PRO:HA | 1.67 | 0.77 |
| 3:F:2961[A]:HIS:HD2 | 3:F:2988[A]:TRP:HZ3 | 1.32 | 0.77 |
| 3:F:3161[B]:GLU:HB3 | 3:a:3079[B]:CYS:SG | 2.25 | 0.77 |
| 3:F:3259[B]:ASP:OD2 | 3:F:3260[B]:ARG:HG2 | 1.84 | 0.77 |
| 3:I:2962[B]:GLY:C | 3:R:3255[B]:PRO:HG3 | 2.09 | 0.77 |
| 3:I:2964[B]:PRO:HB3 | 3:R:3221[B]:ALA:HB3 | 1.65 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2973[B]:THR:HG21 | 3:R:3106[B]:THR:C | 2.09 | 0.77 |
| 1:J:164:GLU:O | 1:J:297:ARG:NH2 | 2.17 | 0.77 |
| 3:L:2961[B]:HIS:HB3 | 3:L:3111[B]:SER:OG | 1.85 | 0.77 |
| 3:L:3306[A]:LEU:HD12 | 3:L:3307[A]:PHE:N | 2.00 | 0.77 |
| 3:O:3025[A]:VAL:CG2 | 3:O:3047[A]:ARG:HH12 | 1.94 | 0.77 |
| 3:R:2979[A]:GLN:NE2 | 3:R:3155[A]:MET:CE | 2.47 | 0.77 |
| 3:R:3211[B]:ASP:HB3 | 3:R:3309[B]:PRO:HA | 1.67 | 0.77 |
| 3:U:2969[B]:TYR:HH | 3:d:3107[B]:LEU:HD12 | 1.49 | 0.77 |
| 3:U:3211[B]:ASP:HB3 | 3:U:3309[B]:PRO:HA | 1.67 | 0.77 |
| 3:X:2948[A]:ASP:HB3 | 3:X:2949[A]:LYS:CA | 2.15 | 0.77 |
| 3:X:2961[A]:HIS:HD2 | 3:X:2988[A]:TRP:HZ3 | 1.31 | 0.77 |
| 3:X:3141[B]:TYR:HD2 | 3:X:3142[B]:ASN:H | 0.78 | 0.77 |
| 3:X:3148[A]:ILE:O | 3:X:3152[A]:LYS:HE3 | 1.83 | 0.77 |
| 3:X:3288[B]:MET:HG2 | 3:X:3295[B]:LEU:HD21 | 1.67 | 0.77 |
| 3:X:3306[A]:LEU:HD12 | 3:X:3307[A]:PHE:N | 2.00 | 0.77 |
| 3:a:2961[A]:HIS:HB3 | 3:a:3111[A]:SER:OG | 1.85 | 0.77 |
| 3:a:3211[B]:ASP:HB3 | 3:a:3309[B]:PRO:HA | 1.67 | 0.77 |
| 3:a:3284[A]:LYS:CD | 3:a:3285[A]:VAL:N | 2.47 | 0.77 |
| 3:d:2948[A]:ASP:HB3 | 3:d:2949[A]:LYS:CA | 2.15 | 0.77 |
| 3:d:2956[A]:LYS:C | 3:d:2960[A]:PHE:CE1 | 2.47 | 0.77 |
| 4:HA:1:NAG:O7 | 4:HA:1:NAG:O3 | 2.02 | 0.77 |
| 3:C:3156[B]:MET:CG | 3:L:2982[B]:MET:HG3 | 2.14 | 0.77 |
| 3:C:3172[B]:SER:HB2 | 3:L:3152[B]:LYS:N | 1.99 | 0.77 |
| 3:F:2961[B]:HIS:CG | 3:a:2975[B]:PHE:CZ | 2.73 | 0.77 |
| 3:F:2966[B]:SER:N | 3:a:3255[B]:PRO:CA | 2.48 | 0.77 |
| 3:F:3169[B]:LYS:HZ2 | 3:a:3149[B]:ASN:ND2 | 1.80 | 0.77 |
| 3:F:3306[A]:LEU:HD12 | 3:F:3307[A]:PHE:N | 2.00 | 0.77 |
| 3:I:2961[A]:HIS:HB3 | 3:I:3111[A]:SER:OG | 1.85 | 0.77 |
| 3:I:2969[B]:TYR:CE2 | 3:R:3120[B]:HIS:CD2 | 2.72 | 0.77 |
| 2:K:2394:VAL:H | 2:K:2448:THR:HG22 | 1.50 | 0.77 |
| 3:O:3284[A]:LYS:CD | 3:O:3285[A]:VAL:N | 2.47 | 0.77 |
| 3:O:3288[A]:MET:HG2 | 3:O:3295[A]:LEU:HD21 | 1.67 | 0.77 |
| 3:U:2969[B]:TYR:N | 3:d:3256[B]:TRP:NE1 | 2.32 | 0.77 |
| 3:U:3288[A]:MET:HG2 | 3:U:3295[A]:LEU:HD21 | 1.67 | 0.77 |
| 3:X:3113[B]:ASP:CG | 3:X:3114[B]:PRO:CD | 2.56 | 0.77 |
| 1:Y:105:VAL:HG12 | 1:Y:123:PHE:HB3 | 1.67 | 0.77 |
| 3:a:3288[B]:MET:HG2 | 3:a:3295[B]:LEU:HD21 | 1.67 | 0.77 |
| 3:a:3306[B]:LEU:HD12 | 3:a:3307[B]:PHE:N | 2.00 | 0.77 |
| 3:d:2952[B]:ALA:HA | 3:d:2956[B]:LYS:HB3 | 1.67 | 0.77 |
| 3:d:2979[B]:GLN:NE2 | 3:d:3155[B]:MET:CE | 2.47 | 0.77 |
| 3:C:3151[B]:LEU:HA | 3:L:3154[B]:PRO:HB2 | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3212[B]:ARG:HG3 | 3:C:3212[B]:ARG:NH1 | 2.00 | 0.77 |
| 1:D:1170:MET:HB3 | 1:D:1203:MET:HE2 | 1.65 | 0.77 |
| 3:F:2965[B]:LEU:H | 3:a:3221[B]:ALA:HB1 | 0.96 | 0.77 |
| 3:F:2980[B]:HIS:N | 3:a:2967[B]:CYS:HB2 | 1.99 | 0.77 |
| 3:F:3211[A]:ASP:HB3 | 3:F:3309[A]:PRO:HA | 1.67 | 0.77 |
| 3:F:3220[A]:ARG:HG3 | 3:F:3220[A]:ARG:NH1 | 1.98 | 0.77 |
| 3:I:3025[A]:VAL:CG2 | 3:I:3047[A]:ARG:HH12 | 1.94 | 0.77 |
| 3:I:3204[A]:LEU:O | 3:I:3208[A]:GLN:HG3 | 1.85 | 0.77 |
| 3:I:3284[A]:LYS:CD | 3:I:3285[A]:VAL:N | 2.47 | 0.77 |
| 3:L:2948[A]:ASP:HB3 | 3:L:2949[A]:LYS:CA | 2.15 | 0.77 |
| 3:L:3023[B]:ILE:O | 3:L:3026[B]:THR:N | 2.11 | 0.77 |
| 3:O:2967[B]:CYS:C | 3:X:2979[B]:GLN:HG2 | 1.91 | 0.77 |
| 3:U:3086[B]:GLU:CD | 3:d:2970[B]:PRO:CG | 2.57 | 0.77 |
| 3:U:3254[B]:MET:CE | 3:d:3254[B]:MET:HB2 | 2.09 | 0.77 |
| 3:X:2955[A]:GLN:CD | 3:X:3037[A]:TYR:HE1 | 1.93 | 0.77 |
| 3:a:2948[B]:ASP:HB3 | 3:a:2949[B]:LYS:CA | 2.15 | 0.77 |
| 3:d:3306[B]:LEU:HD12 | 3:d:3307[B]:PHE:N | 2.00 | 0.77 |
| 3:C:2979[B]:GLN:NE2 | 3:C:3155[B]:MET:CE | 2.47 | 0.76 |
| 3:C:3152[B]:LYS:N | 3:L:3172[B]:SER:OG | 2.16 | 0.76 |
| 3:F:3248[B]:LEU:CB | 3:a:2972[B]:GLY:C | 2.58 | 0.76 |
| 3:I:2961[B]:HIS:HB3 | 3:I:3111[B]:SER:OG | 1.85 | 0.76 |
| 3:I:3211[A]:ASP:HB3 | 3:I:3309[A]:PRO:HA | 1.67 | 0.76 |
| 3:I:3211[B]:ASP:HB3 | 3:I:3309[B]:PRO:HA | 1.67 | 0.76 |
| 3:L:3259[A]:ASP:OD2 | 3:L:3260[A]:ARG:HG2 | 1.84 | 0.76 |
| 3:L:3307[B]:PHE:CE1 | 3:L:3309[B]:PRO:HG3 | 2.16 | 0.76 |
| 1:M:1301:PRO:O | 1:M:1494:ARG:NH2 | 2.18 | 0.76 |
| 3:O:2961[B]:HIS:HD2 | 3:O:2988[B]:TRP:HZ3 | 1.31 | 0.76 |
| 3:O:3160[B]:SER:CA | 3:X:3151[B]:LEU:H | 1.97 | 0.76 |
| 3:R:2948[B]:ASP:H | 3:R:2949[B]:LYS:CA | 1.98 | 0.76 |
| 2:T:2800:LYS:HB3 | 3:U:3023[A]:ILE:HD11 | 1.67 | 0.76 |
| 3:U:3162[B]:ASP:CB | 3:d:3260[B]:ARG:NH1 | 2.48 | 0.76 |
| 1:V:1636:ASN:HB3 | 1:V:1639:LYS:HD3 | 1.67 | 0.76 |
| 3:X:2979[A]:GLN:NE2 | 3:X:3155[A]:MET:CE | 2.47 | 0.76 |
| 3:X:3104[B]:MET:CA | 3:X:3110[B]:THR:HG23 | 2.10 | 0.76 |
| 3:X:3185[A]:TYR:HE2 | 3:X:3187[A]:TYR:CE2 | 2.01 | 0.76 |
| 3:a:2961[B]:HIS:HD2 | 3:a:2988[B]:TRP:HZ3 | 1.31 | 0.76 |
| 3:a:3220[B]:ARG:HG3 | 3:a:3220[B]:ARG:NH1 | 1.98 | 0.76 |
| 1:b:456:GLN:HG2 | 1:b:551:GLU:HB2 | 1.67 | 0.76 |
| 3:d:2952[A]:ALA:HA | 3:d:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:C:3025[B]:VAL:HG23 | 3:C:3033[B]:PHE:O | 1.83 | 0.76 |
| 3:C:3156[B]:MET:CB | 3:L:2982[B]:MET:SD | 2.64 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2948[B]:ASP:HB3 | 3:F:2949[B]:LYS:CA | 2.15 | 0.76 |
| 3:F:2979[A]:GLN:NE2 | 3:F:3155[A]:MET:CE | 2.47 | 0.76 |
| 3:F:3152[B]:LYS:HB2 | 3:a:3172[B]:SER:CA | 2.14 | 0.76 |
| 3:F:3251[B]:ASP:C | 3:a:3251[B]:ASP:HB3 | 2.10 | 0.76 |
| 1:G:417:MET:SD | 3:L:3199[A]:GLN:NE2 | 2.58 | 0.76 |
| 3:I:2961[B]:HIS:CG | 3:R:2975[B]:PHE:CE1 | 2.74 | 0.76 |
| 3:I:2970[B]:PRO:CD | 3:R:2989[B]:HIS:NE2 | 2.47 | 0.76 |
| 3:I:3155[B]:MET:SD | 3:R:3154[B]:PRO:CG | 2.71 | 0.76 |
| 3:O:2967[B]:CYS:CB | 3:X:3155[B]:MET:HG2 | 2.04 | 0.76 |
| 3:O:3163[B]:ASN:CB | 3:X:3149[B]:ASN:CB | 2.62 | 0.76 |
| 3:O:3306[A]:LEU:HD12 | 3:O:3307[A]:PHE:N | 2.00 | 0.76 |
| 3:R:3141[A]:TYR:HD2 | 3:R:3142[A]:ASN:H | 0.78 | 0.76 |
| 3:R:3288[B]:MET:HG2 | 3:R:3295[B]:LEU:HD21 | 1.67 | 0.76 |
| 2:T:2546:LEU:H | 2:T:2557:ALA:HA | 1.49 | 0.76 |
| 3:U:3219[B]:LEU:C | 3:d:2971[B]:ASP:O | 2.27 | 0.76 |
| 3:U:3254[B]:MET:HB3 | 3:d:3254[B]:MET:HB2 | 1.65 | 0.76 |
| 3:X:2956[A]:LYS:C | 3:X:2960[A]:PHE:CE1 | 2.47 | 0.76 |
| 3:X:3023[B]:ILE:O | 3:X:3026[B]:THR:N | 2.11 | 0.76 |
| 3:a:2937[A]:ASN:HB2 | 3:a:3006[A]:LYS:CE | 2.14 | 0.76 |
| 3:a:3204[A]:LEU:O | 3:a:3208[A]:GLN:HG3 | 1.86 | 0.76 |
| 1:A:324:PRO:HG2 | 1:A:376:ASN:HD21 | 1.50 | 0.76 |
| 3:C:2955[B]:GLN:CD | 3:C:3037[B]:TYR:HE1 | 1.92 | 0.76 |
| 3:C:3149[B]:ASN:C | 3:L:3172[B]:SER:CB | 2.57 | 0.76 |
| 3:C:3159[B]:SER:HA | 3:L:3151[B]:LEU:N | 2.01 | 0.76 |
| 3:F:2955[B]:GLN:CD | 3:F:3037[B]:TYR:HE1 | 1.92 | 0.76 |
| 3:F:2961[A]:HIS:HB3 | 3:F:3111[A]:SER:OG | 1.85 | 0.76 |
| 3:F:3288[B]:MET:HG2 | 3:F:3295[B]:LEU:HD21 | 1.67 | 0.76 |
| 3:I:2988[B]:TRP:CE3 | 3:I:2989[B]:HIS:ND1 | 2.53 | 0.76 |
| 3:L:2988[A]:TRP:CE3 | 3:L:2989[A]:HIS:ND1 | 2.53 | 0.76 |
| 3:L:3024[A]:LEU:CD1 | 3:L:3025[A]:VAL:H | 1.84 | 0.76 |
| 3:L:3204[A]:LEU:O | 3:L:3208[A]:GLN:HG3 | 1.86 | 0.76 |
| 3:L:3212[B]:ARG:HG3 | 3:L:3212[B]:ARG:NH1 | 2.00 | 0.76 |
| 3:O:2952[B]:ALA:HA | 3:O:2956[B]:LYS:HB3 | 1.67 | 0.76 |
| 3:O:2961[A]:HIS:HD2 | 3:O:2988[A]:TRP:HZ3 | 1.31 | 0.76 |
| 3:O:2979[B]:GLN:NE2 | 3:O:3155[B]:MET:CE | 2.47 | 0.76 |
| 3:O:3108[B]:HIS:CB | 3:X:2970[B]:PRO:CA | 2.63 | 0.76 |
| 3:O:3211[A]:ASP:HB3 | 3:O:3309[A]:PRO:HA | 1.67 | 0.76 |
| 3:R:3230[B]:PHE:CB | 3:R:3243[B]:GLY:HA2 | 2.06 | 0.76 |
| 3:U:2961[B]:HIS:HB3 | 3:U:3111[B]:SER:OG | 1.85 | 0.76 |
| 3:U:3256[B]:TRP:HE3 | 3:d:2973[B]:THR:H | 1.34 | 0.76 |
| 3:X:3148[B]:ILE:O | 3:X:3152[B]:LYS:HE3 | 1.83 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:2135:PRO:O | 2:Z:2140:ARG:NH2 | 2.18 | 0.76 |
| 3:d:2948[B]:ASP:HB3 | 3:d:2949[B]:LYS:CA | 2.15 | 0.76 |
| 3:d:2961[A]:HIS:HB3 | 3:d:3111[A]:SER:OG | 1.85 | 0.76 |
| 3:d:3211[B]:ASP:HB3 | 3:d:3309[B]:PRO:HA | 1.67 | 0.76 |
| 3:d:3306[A]:LEU:HD12 | 3:d:3307[A]:PHE:N | 2.00 | 0.76 |
| 1:A:1442:MET:HE1 | 1:A:1454:PHE:HA | 1.67 | 0.76 |
| 3:C:2937[A]:ASN:CB | 3:C:3006[A]:LYS:HE2 | 2.14 | 0.76 |
| 3:C:3113[B]:ASP:CG | 3:C:3114[B]:PRO:CD | 2.56 | 0.76 |
| 3:F:3147[A]:GLU:HB2 | 3:F:3149[A]:ASN:OD1 | 1.86 | 0.76 |
| 3:F:3180[B]:TYR:HB2 | 3:F:3183[B]:LEU:CD2 | 2.16 | 0.76 |
| 2:H:2168:ARG:NH1 | 2:K:2587:SER:OG | 2.18 | 0.76 |
| 3:I:2948[A]:ASP:HB3 | 3:I:2949[A]:LYS:CA | 2.15 | 0.76 |
| 3:I:3147[A]:GLU:HB2 | 3:I:3149[A]:ASN:OD1 | 1.86 | 0.76 |
| 3:I:3185[A]:TYR:HE2 | 3:I:3187[A]:TYR:CE2 | 2.01 | 0.76 |
| 3:I:3253[B]:GLU:CB | 3:R:2975[B]:PHE:C | 2.58 | 0.76 |
| 1:J:456:GLN:NE2 | 1:J:549:PRO:O | 2.17 | 0.76 |
| 2:K:2545:SER:HA | 2:K:2546:LEU:HG | 1.68 | 0.76 |
| 3:L:3288[A]:MET:HG2 | 3:L:3295[A]:LEU:HD21 | 1.67 | 0.76 |
| 3:O:3284[B]:LYS:CD | 3:O:3285[B]:VAL:N | 2.47 | 0.76 |
| 3:R:3147[A]:GLU:HB2 | 3:R:3149[A]:ASN:OD1 | 1.86 | 0.76 |
| 3:R:3204[A]:LEU:O | 3:R:3208[A]:GLN:HG3 | 1.86 | 0.76 |
| 3:R:3211[A]:ASP:HB3 | 3:R:3309[A]:PRO:HA | 1.67 | 0.76 |
| 3:R:3307[B]:PHE:CE1 | 3:R:3309[B]:PRO:HG3 | 2.16 | 0.76 |
| 3:U:2948[A]:ASP:H | 3:U:2949[A]:LYS:CA | 1.98 | 0.76 |
| 3:U:2973[B]:THR:CG2 | 3:d:3222[B]:ILE:HG23 | 2.15 | 0.76 |
| 3:U:2979[A]:GLN:NE2 | 3:U:3155[A]:MET:CE | 2.47 | 0.76 |
| 3:U:3147[A]:GLU:HB2 | 3:U:3149[A]:ASN:OD1 | 1.86 | 0.76 |
| 1:V:1372:ILE:HD11 | 1:Y:1392:ASP:HB2 | 1.66 | 0.76 |
| 3:X:3204[B]:LEU:O | 3:X:3208[B]:GLN:HG3 | 1.86 | 0.76 |
| 3:X:3211[B]:ASP:HB3 | 3:X:3309[B]:PRO:HA | 1.67 | 0.76 |
| 3:a:3113[A]:ASP:CG | 3:a:3114[A]:PRO:CD | 2.56 | 0.76 |
| 3:d:3204[B]:LEU:O | 3:d:3208[B]:GLN:HG3 | 1.86 | 0.76 |
| 1:A:22:LEU:HG | 1:A:122:VAL:HG11 | 1.68 | 0.76 |
| 3:C:2949[A]:LYS:O | 3:C:2949[A]:LYS:NZ | 2.16 | 0.76 |
| 3:C:2952[B]:ALA:HA | 3:C:2956[B]:LYS:HB3 | 1.67 | 0.76 |
| 3:C:2961[A]:HIS:HD2 | 3:C:2988[A]:TRP:HZ3 | 1.32 | 0.76 |
| 3:C:3306[B]:LEU:HD12 | 3:C:3307[B]:PHE:N | 2.00 | 0.76 |
| 3:F:2965[B]:LEU:CB | 3:a:3256[B]:TRP:NE1 | 2.49 | 0.76 |
| 3:F:2979[B]:GLN:C | 3:a:2967[B]:CYS:CB | 2.59 | 0.76 |
| 3:F:3180[A]:TYR:HB2 | 3:F:3183[A]:LEU:CD2 | 2.16 | 0.76 |
| 3:I:2974[B]:ALA:N | 3:R:3249[B]:GLY:N | 2.30 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3180[A]:TYR:HB2 | 3:I:3183[A]:LEU:CD2 | 2.16 | 0.76 |
| 3:I:3256[B]:TRP:HB3 | 3:R:2966[B]:SER:C | 2.10 | 0.76 |
| 3:I:3256[B]:TRP:CZ2 | 3:R:2965[B]:LEU:HB3 | 2.19 | 0.76 |
| 3:L:3212[A]:ARG:HG3 | 3:L:3212[A]:ARG:NH1 | 2.00 | 0.76 |
| 3:O:2961[A]:HIS:HB3 | 3:O:3111[A]:SER:OG | 1.85 | 0.76 |
| 3:O:3163[B]:ASN:HD22 | 3:X:3148[B]:ILE:HG22 | 1.50 | 0.76 |
| 3:O:3204[A]:LEU:O | 3:O:3208[A]:GLN:HG3 | 1.85 | 0.76 |
| 3:O:3307[A]:PHE:CE1 | 3:O:3309[A]:PRO:HG3 | 2.16 | 0.76 |
| 3:R:2988[B]:TRP:CE3 | 3:R:2989[B]:HIS:ND1 | 2.53 | 0.76 |
| 3:R:3306[A]:LEU:HD12 | 3:R:3307[A]:PHE:N | 2.00 | 0.76 |
| 3:U:2961[B]:HIS:HD2 | 3:U:2988[B]:TRP:HZ3 | 1.31 | 0.76 |
| 3:U:3204[B]:LEU:O | 3:U:3208[B]:GLN:HG3 | 1.86 | 0.76 |
| 3:U:3230[B]:PHE:CB | 3:U:3243[B]:GLY:HA2 | 2.06 | 0.76 |
| 3:X:3288[A]:MET:HG2 | 3:X:3295[A]:LEU:HD21 | 1.67 | 0.76 |
| 3:a:2952[A]:ALA:HA | 3:a:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:a:3180[A]:TYR:HB2 | 3:a:3183[A]:LEU:CD2 | 2.16 | 0.76 |
| 3:d:3185[A]:TYR:HE2 | 3:d:3187[A]:TYR:CE2 | 2.01 | 0.76 |
| 3:C:2948[A]:ASP:HB3 | 3:C:2949[A]:LYS:CA | 2.15 | 0.76 |
| 3:C:2988[A]:TRP:CE3 | 3:C:2989[A]:HIS:ND1 | 2.53 | 0.76 |
| 3:C:3156[B]:MET:HG2 | 3:L:2984[B]:THR:OG1 | 1.86 | 0.76 |
| 3:F:2965[B]:LEU:C | 3:a:3221[B]:ALA:HB2 | 2.10 | 0.76 |
| 3:F:3306[B]:LEU:HD12 | 3:F:3307[B]:PHE:N | 2.00 | 0.76 |
| 3:I:2952[A]:ALA:CB | 3:I:2953[A]:GLY:C | 2.48 | 0.76 |
| 3:I:3107[B]:LEU:HD21 | 3:R:2975[B]:PHE:HA | 1.67 | 0.76 |
| 3:L:2952[A]:ALA:HA | 3:L:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:O:2971[B]:ASP:H | 3:X:2991[B]:LEU:N | 1.82 | 0.76 |
| 3:O:2971[B]:ASP:O | 3:X:2988[B]:TRP:HE3 | 1.68 | 0.76 |
| 3:R:3114[A]:PRO:HD2 | 3:R:3115[A]:LEU:H | 1.51 | 0.76 |
| 3:R:3180[B]:TYR:HB2 | 3:R:3183[B]:LEU:CD2 | 2.16 | 0.76 |
| 3:U:3150[B]:LYS:HG2 | 3:d:3156[B]:MET:HG2 | 1.66 | 0.76 |
| 3:U:3204[A]:LEU:O | 3:U:3208[A]:GLN:HG3 | 1.86 | 0.76 |
| 3:U:3230[A]:PHE:CB | 3:U:3243[A]:GLY:HA2 | 2.06 | 0.76 |
| 3:X:3220[B]:ARG:HG3 | 3:X:3220[B]:ARG:NH1 | 1.98 | 0.76 |
| 3:a:2952[B]:ALA:CB | 3:a:2953[B]:GLY:C | 2.48 | 0.76 |
| 3:a:3147[A]:GLU:HB2 | 3:a:3149[A]:ASN:OD1 | 1.86 | 0.76 |
| 3:d:2937[A]:ASN:HB2 | 3:d:3006[A]:LYS:CE | 2.14 | 0.76 |
| 3:d:3180[B]:TYR:HB2 | 3:d:3183[B]:LEU:CD2 | 2.16 | 0.76 |
| 1:A:550:ILE:N | 1:A:557:VAL:O | 2.15 | 0.76 |
| 3:C:2985[B]:PHE:CZ | 3:L:2969[B]:TYR:C | 2.58 | 0.76 |
| 3:C:2988[B]:TRP:CE3 | 3:C:2989[B]:HIS:ND1 | 2.53 | 0.76 |
| 3:C:3158[B]:PHE:O | 3:L:3150[B]:LYS:N | 2.05 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3253[B]:GLU:CG | 3:L:2976[B]:ALA:HB2 | 2.14 | 0.76 |
| 3:F:2952[B]:ALA:HA | 3:F:2956[B]:LYS:HB3 | 1.67 | 0.76 |
| 3:F:2956[B]:LYS:C | 3:F:2960[B]:PHE:CE1 | 2.47 | 0.76 |
| 3:F:3220[B]:ARG:HG3 | 3:F:3220[B]:ARG:NH1 | 1.98 | 0.76 |
| 3:I:2956[B]:LYS:C | 3:I:2960[B]:PHE:CE1 | 2.47 | 0.76 |
| 3:I:2974[B]:ALA:HB1 | 3:R:3253[B]:GLU:OE1 | 1.84 | 0.76 |
| 1:J:723:ALA:O | 1:J:728:ARG:NH1 | 2.19 | 0.76 |
| 3:L:2948[B]:ASP:H | 3:L:2949[B]:LYS:CA | 1.98 | 0.76 |
| 3:L:2955[B]:GLN:CD | 3:L:3037[B]:TYR:HE1 | 1.92 | 0.76 |
| 1:M:1210:LYS:HA | 1:M:1211:TYR:CB | 2.15 | 0.76 |
| 3:O:3141[B]:TYR:HD2 | 3:O:3142[B]:ASN:H | 0.78 | 0.76 |
| 3:R:2948[A]:ASP:HB3 | 3:R:2949[A]:LYS:CA | 2.15 | 0.76 |
| 3:R:2948[B]:ASP:HB3 | 3:R:2949[B]:LYS:CA | 2.15 | 0.76 |
| 1:S:898:GLY:HA2 | 1:S:1186:TRP:HB2 | 1.66 | 0.76 |
| 3:U:3180[B]:TYR:HB2 | 3:U:3183[B]:LEU:CD2 | 2.16 | 0.76 |
| 3:X:2937[B]:ASN:CB | 3:X:3006[B]:LYS:HE2 | 2.14 | 0.76 |
| 3:X:2952[A]:ALA:HA | 3:X:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:X:2952[B]:ALA:HA | 3:X:2956[B]:LYS:HB3 | 1.67 | 0.76 |
| 3:X:2961[A]:HIS:HB3 | 3:X:3111[A]:SER:OG | 1.85 | 0.76 |
| 3:X:2961[B]:HIS:HB3 | 3:X:3111[B]:SER:OG | 1.85 | 0.76 |
| 3:X:3089[B]:HIS:HD1 | 3:X:3119[B]:HIS:CE1 | 2.04 | 0.76 |
| 3:a:3147[B]:GLU:HB2 | 3:a:3149[B]:ASN:CG | 1.95 | 0.76 |
| 3:a:3180[B]:TYR:HB2 | 3:a:3183[B]:LEU:CD2 | 2.16 | 0.76 |
| 3:d:3196[B]:THR:H | 3:d:3199[B]:GLN:CD | 1.94 | 0.76 |
| 3:C:3114[B]:PRO:HD2 | 3:C:3115[B]:LEU:H | 1.51 | 0.76 |
| 3:C:3172[B]:SER:CB | 3:L:3149[B]:ASN:C | 2.58 | 0.76 |
| 3:F:2952[A]:ALA:HA | 3:F:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:F:2975[B]:PHE:HA | 3:a:3107[B]:LEU:CD2 | 2.15 | 0.76 |
| 3:F:3120[A]:HIS:O | 3:F:3121[A]:SER:C | 2.29 | 0.76 |
| 3:F:3154[B]:PRO:HD3 | 3:a:3173[B]:THR:O | 1.86 | 0.76 |
| 3:F:3255[B]:PRO:HG3 | 3:a:2962[B]:GLY:C | 2.10 | 0.76 |
| 3:I:2971[B]:ASP:OD1 | 3:I:2973[B]:THR:OG1 | 2.04 | 0.76 |
| 3:I:3153[B]:LYS:CE | 3:R:3158[B]:PHE:H | 1.98 | 0.76 |
| 3:I:3196[B]:THR:H | 3:I:3199[B]:GLN:CD | 1.94 | 0.76 |
| 3:I:3221[B]:ALA:HB3 | 3:R:2964[B]:PRO:CA | 2.12 | 0.76 |
| 3:I:3259[A]:ASP:OD2 | 3:I:3260[A]:ARG:HG2 | 1.84 | 0.76 |
| 3:I:3306[A]:LEU:HD12 | 3:I:3307[A]:PHE:N | 2.00 | 0.76 |
| 3:L:2961[A]:HIS:HB3 | 3:L:3111[A]:SER:OG | 1.85 | 0.76 |
| 3:O:3089[A]:HIS:HD1 | 3:O:3119[A]:HIS:CE1 | 2.04 | 0.76 |
| 3:O:3114[B]:PRO:HD2 | 3:O:3115[B]:LEU:H | 1.51 | 0.76 |
| 3:O:3204[B]:LEU:O | 3:O:3208[B]:GLN:HG3 | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3196[B]:THR:H | 3:R:3199[B]:GLN:CD | 1.94 | 0.76 |
| 3:U:2965[B]:LEU:HD13 | 3:d:3256[B]:TRP:O | 1.85 | 0.76 |
| 3:U:2970[B]:PRO:CA | 3:d:3086[B]:GLU:CD | 2.43 | 0.76 |
| 3:X:3114[B]:PRO:HD2 | 3:X:3115[B]:LEU:H | 1.51 | 0.76 |
| 3:d:2971[A]:ASP:OD1 | 3:d:2973[A]:THR:OG1 | 2.04 | 0.76 |
| 3:C:2952[A]:ALA:HA | 3:C:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:C:3252[B]:TYR:CE2 | 3:L:3249[B]:GLY:O | 2.35 | 0.76 |
| 2:E:2394:VAL:H | 2:E:2448:THR:HG22 | 1.50 | 0.76 |
| 3:F:2948[A]:ASP:HB3 | 3:F:2949[A]:LYS:CA | 2.15 | 0.76 |
| 3:F:3150[B]:LYS:HG2 | 3:a:3158[B]:PHE:HA | 1.63 | 0.76 |
| 3:I:2969[B]:TYR:CE2 | 3:R:3120[B]:HIS:NE2 | 2.48 | 0.76 |
| 3:I:3255[B]:PRO:CB | 3:R:2959[B]:SER:CA | 2.64 | 0.76 |
| 3:L:2988[B]:TRP:CE3 | 3:L:2989[B]:HIS:ND1 | 2.53 | 0.76 |
| 3:L:3089[A]:HIS:HD1 | 3:L:3119[A]:HIS:CE1 | 2.04 | 0.76 |
| 3:L:3220[A]:ARG:HG3 | 3:L:3220[A]:ARG:NH1 | 1.98 | 0.76 |
| 3:O:2971[B]:ASP:OD1 | 3:O:2973[B]:THR:OG1 | 2.04 | 0.76 |
| 1:P:1296:VAL:HB | 1:P:1446:ASP:HB3 | 1.66 | 0.76 |
| 3:R:2930[B]:LEU:H | 3:R:2930[B]:LEU:CD2 | 1.98 | 0.76 |
| 3:R:2952[A]:ALA:HA | 3:R:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:a:3212[A]:ARG:HG3 | 3:a:3212[A]:ARG:NH1 | 2.00 | 0.76 |
| 3:a:3288[A]:MET:HG2 | 3:a:3295[A]:LEU:HD21 | 1.67 | 0.76 |
| 1:b:1358:LEU:HD23 | 1:b:1456:LEU:HD21 | 1.68 | 0.76 |
| 3:d:3180[A]:TYR:HB2 | 3:d:3183[A]:LEU:CD2 | 2.16 | 0.76 |
| 4:q:2:NAG:H83 | 4:q:2:NAG:C3 | 2.16 | 0.76 |
| 3:C:3089[B]:HIS:HD1 | 3:C:3119[B]:HIS:CE1 | 2.04 | 0.76 |
| 3:F:2971[A]:ASP:OD1 | 3:F:2973[A]:THR:OG1 | 2.04 | 0.76 |
| 3:F:2971[B]:ASP:OD1 | 3:a:3248[B]:LEU:CD2 | 2.34 | 0.76 |
| 3:F:3089[A]:HIS:HD1 | 3:F:3119[A]:HIS:CE1 | 2.04 | 0.76 |
| 3:F:3114[B]:PRO:HD2 | 3:F:3115[B]:LEU:H | 1.51 | 0.76 |
| 3:I:2948[A]:ASP:H | 3:I:2949[A]:LYS:CA | 1.98 | 0.76 |
| 3:I:3114[B]:PRO:HD2 | 3:I:3115[B]:LEU:H | 1.51 | 0.76 |
| 3:I:3180[B]:TYR:HB2 | 3:I:3183[B]:LEU:CD2 | 2.16 | 0.76 |
| 3:I:3204[B]:LEU:O | 3:I:3208[B]:GLN:HG3 | 1.86 | 0.76 |
| 3:I:3255[B]:PRO:HD3 | 3:R:2962[B]:GLY:C | 2.11 | 0.76 |
| 3:I:3288[A]:MET:HG2 | 3:I:3295[A]:LEU:HD21 | 1.67 | 0.76 |
| 3:L:3089[B]:HIS:HD1 | 3:L:3119[B]:HIS:CE1 | 2.04 | 0.76 |
| 3:L:3114[B]:PRO:HD2 | 3:L:3115[B]:LEU:H | 1.51 | 0.76 |
| 3:L:3220[B]:ARG:HG3 | 3:L:3220[B]:ARG:NH1 | 1.98 | 0.76 |
| 3:O:2948[B]:ASP:H | 3:O:2949[B]:LYS:CA | 1.98 | 0.76 |
| 3:O:2952[A]:ALA:HA | 3:O:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:O:2955[A]:GLN:CD | 3:O:3037[A]:TYR:HE1 | 1.92 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2961[B]:HIS:HB3 | 3:O:3111[B]:SER:OG | 1.85 | 0.76 |
| 3:R:2952[B]:ALA:CB | 3:R:2953[B]:GLY:C | 2.48 | 0.76 |
| 3:R:2988[A]:TRP:CE3 | 3:R:2989[A]:HIS:ND1 | 2.53 | 0.76 |
| 3:U:2930[B]:LEU:H | 3:U:2930[B]:LEU:CD2 | 1.97 | 0.76 |
| 3:U:2952[A]:ALA:HA | 3:U:2956[A]:LYS:HB3 | 1.67 | 0.76 |
| 3:U:2961[A]:HIS:HB3 | 3:U:3111[A]:SER:OG | 1.85 | 0.76 |
| 3:U:3023[A]:ILE:O | 3:U:3026[A]:THR:N | 2.11 | 0.76 |
| 3:X:2948[A]:ASP:H | 3:X:2949[A]:LYS:CA | 1.98 | 0.76 |
| 3:X:2988[B]:TRP:CE3 | 3:X:2989[B]:HIS:ND1 | 2.53 | 0.76 |
| 3:X:3114[A]:PRO:HD2 | 3:X:3115[A]:LEU:H | 1.51 | 0.76 |
| 1:Y:14:GLU:O | 1:Y:17:ASN:ND2 | 2.18 | 0.76 |
| 3:a:2955[A]:GLN:CD | 3:a:3037[A]:TYR:HE1 | 1.92 | 0.76 |
| 3:a:3220[A]:ARG:HG3 | 3:a:3220[A]:ARG:NH1 | 1.98 | 0.76 |
| 1:b:439:LEU:HD23 | 1:b:509:ILE:HD12 | 1.68 | 0.76 |
| 3:d:2961[B]:HIS:HD2 | 3:d:2988[B]:TRP:HZ3 | 1.31 | 0.76 |
| 3:d:3089[A]:HIS:HD1 | 3:d:3119[A]:HIS:CE1 | 2.04 | 0.76 |
| 3:d:3113[A]:ASP:CG | 3:d:3114[A]:PRO:CD | 2.56 | 0.76 |
| 3:C:3089[A]:HIS:HD1 | 3:C:3119[A]:HIS:CE1 | 2.04 | 0.75 |
| 3:C:3259[B]:ASP:OD2 | 3:C:3260[B]:ARG:HG2 | 1.84 | 0.75 |
| 3:F:2937[A]:ASN:CB | 3:F:3006[A]:LYS:HE2 | 2.14 | 0.75 |
| 3:F:3174[B]:GLY:N | 3:a:3154[B]:PRO:CG | 2.47 | 0.75 |
| 3:I:2967[B]:CYS:SG | 3:R:2982[B]:MET:HE2 | 2.26 | 0.75 |
| 3:L:3120[B]:HIS:O | 3:L:3121[B]:SER:C | 2.29 | 0.75 |
| 3:O:2968[B]:GLN:HG2 | 3:X:2984[B]:THR:CB | 2.16 | 0.75 |
| 3:O:2969[B]:TYR:CD1 | 3:X:3158[B]:PHE:HD1 | 1.97 | 0.75 |
| 3:O:2969[B]:TYR:HB2 | 3:X:3158[B]:PHE:CZ | 2.19 | 0.75 |
| 3:O:3156[B]:MET:HE2 | 3:X:3173[B]:THR:CG2 | 1.94 | 0.75 |
| 3:O:3180[B]:TYR:HB2 | 3:O:3183[B]:LEU:CD2 | 2.16 | 0.75 |
| 3:R:2937[B]:ASN:HB2 | 3:R:3006[B]:LYS:CE | 2.14 | 0.75 |
| 3:R:2965[B]:LEU:CD2 | 3:R:2974[B]:ALA:HB1 | 2.10 | 0.75 |
| 1:S:1046:HIS:HA | 1:S:1049:VAL:HB | 1.67 | 0.75 |
| 3:a:2955[B]:GLN:CD | 3:a:3037[B]:TYR:HE1 | 1.92 | 0.75 |
| 3:a:3185[A]:TYR:HE2 | 3:a:3187[A]:TYR:CE2 | 2.01 | 0.75 |
| 3:d:2979[A]:GLN:NE2 | 3:d:3155[A]:MET:CE | 2.47 | 0.75 |
| 3:d:3288[A]:MET:HG2 | 3:d:3295[A]:LEU:HD21 | 1.67 | 0.75 |
| 3:C:3024[B]:LEU:CD1 | 3:C:3025[B]:VAL:H | 1.84 | 0.75 |
| 3:C:3180[B]:TYR:HB2 | 3:C:3183[B]:LEU:CD2 | 2.16 | 0.75 |
| 3:C:3204[B]:LEU:O | 3:C:3208[B]:GLN:HG3 | 1.86 | 0.75 |
| 3:C:3288[A]:MET:HG2 | 3:C:3295[A]:LEU:HD21 | 1.67 | 0.75 |
| 3:F:2971[B]:ASP:OD1 | 3:F:2973[B]:THR:OG1 | 2.04 | 0.75 |
| 3:F:2981[B]:GLY:H | 3:a:2968[B]:GLN:CD | 1.94 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3170[B]:ALA:O | 3:a:3152[B]:LYS:CB | 2.33 | 0.75 |
| 1:G:92:TRP:O | 1:G:212:ASN:ND2 | 2.20 | 0.75 |
| 3:I:3288[B]:MET:HG2 | 3:I:3295[B]:LEU:HD21 | 1.67 | 0.75 |
| 1:J:975:PRO:HG2 | 1:J:1024:GLY:HA3 | 1.67 | 0.75 |
| 3:L:3288[B]:MET:HG2 | 3:L:3295[B]:LEU:HD21 | 1.67 | 0.75 |
| 3:O:2948[A]:ASP:HB3 | 3:O:2949[A]:LYS:CA | 2.15 | 0.75 |
| 3:O:2948[B]:ASP:HB3 | 3:O:2949[B]:LYS:CA | 2.15 | 0.75 |
| 3:O:2988[B]:TRP:CE3 | 3:O:2989[B]:HIS:ND1 | 2.53 | 0.75 |
| 3:R:3180[A]:TYR:HB2 | 3:R:3183[A]:LEU:CD2 | 2.16 | 0.75 |
| 3:U:3156[B]:MET:SD | 3:d:2982[B]:MET:HA | 2.26 | 0.75 |
| 3:U:3288[B]:MET:HG2 | 3:U:3295[B]:LEU:HD21 | 1.67 | 0.75 |
| 1:V:456:GLN:NE2 | 1:V:549:PRO:O | 2.19 | 0.75 |
| 1:Y:1612:THR:O | 3:d:3186[B]:GLU:CG | 2.32 | 0.75 |
| 1:b:718:ARG:NH1 | 1:b:830:ASN:OD1 | 2.17 | 0.75 |
| 3:d:2961[A]:HIS:HD2 | 3:d:2988[A]:TRP:HZ3 | 1.32 | 0.75 |
| 3:d:2961[B]:HIS:HB3 | 3:d:3111[B]:SER:OG | 1.85 | 0.75 |
| 3:d:3114[B]:PRO:HD2 | 3:d:3115[B]:LEU:H | 1.51 | 0.75 |
| 3:C:2930[A]:LEU:H | 3:C:2930[A]:LEU:CD2 | 1.98 | 0.75 |
| 3:C:2961[B]:HIS:HB3 | 3:C:3111[B]:SER:OG | 1.85 | 0.75 |
| 3:C:3090[B]:ASN:HB3 | 3:L:2972[B]:GLY:C | 2.10 | 0.75 |
| 3:C:3150[B]:LYS:N | 3:L:3172[B]:SER:OG | 2.19 | 0.75 |
| 3:C:3172[B]:SER:HG | 3:L:3152[B]:LYS:HG3 | 1.49 | 0.75 |
| 3:C:3174[B]:GLY:CA | 3:L:3154[B]:PRO:CG | 2.63 | 0.75 |
| 1:D:1046:HIS:HA | 1:D:1049:VAL:HB | 1.69 | 0.75 |
| 1:D:1240:ILE:HG23 | 1:D:1247:ARG:HG3 | 1.66 | 0.75 |
| 3:F:3149[B]:ASN:HB3 | 3:a:3163[B]:ASN:ND2 | 1.98 | 0.75 |
| 3:F:3162[B]:ASP:CA | 3:a:3259[B]:ASP:HB3 | 2.15 | 0.75 |
| 3:F:3173[B]:THR:CA | 3:a:3153[B]:LYS:C | 2.58 | 0.75 |
| 3:F:3196[B]:THR:H | 3:F:3199[B]:GLN:CD | 1.94 | 0.75 |
| 3:I:2971[A]:ASP:OD1 | 3:I:2973[A]:THR:OG1 | 2.04 | 0.75 |
| 3:I:3113[A]:ASP:CG | 3:I:3114[A]:PRO:CD | 2.56 | 0.75 |
| 3:L:3141[B]:TYR:HD2 | 3:L:3142[B]:ASN:H | 0.78 | 0.75 |
| 3:L:3180[A]:TYR:HB2 | 3:L:3183[A]:LEU:CD2 | 2.16 | 0.75 |
| 3:L:3211[A]:ASP:HB3 | 3:L:3309[A]:PRO:HA | 1.67 | 0.75 |
| 1:M:999:LEU:O | 1:M:1063:ARG:NH2 | 2.20 | 0.75 |
| 3:O:2954[B]:TYR:O | 3:O:2957[B]:ILE:HG22 | 1.87 | 0.75 |
| 3:O:3120[B]:HIS:O | 3:O:3121[B]:SER:C | 2.29 | 0.75 |
| 3:O:3180[A]:TYR:HB2 | 3:O:3183[A]:LEU:CD2 | 2.16 | 0.75 |
| 3:R:2952[B]:ALA:HA | 3:R:2956[B]:LYS:HB3 | 1.67 | 0.75 |
| 3:R:2961[A]:HIS:HB3 | 3:R:3111[A]:SER:OG | 1.85 | 0.75 |
| 3:R:3114[B]:PRO:HD2 | 3:R:3115[B]:LEU:H | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3204[B]:LEU:O | 3:R:3208[B]:GLN:HG3 | 1.86 | 0.75 |
| 3:U:2969[B]:TYR:H | 3:d:3256[B]:TRP:NE1 | 1.81 | 0.75 |
| 3:U:2988[B]:TRP:CE3 | 3:U:2989[B]:HIS:ND1 | 2.53 | 0.75 |
| 3:U:3038[B]:ILE:HG22 | 3:U:3040[B]:VAL:HG22 | 1.68 | 0.75 |
| 3:U:3089[B]:HIS:HD1 | 3:U:3119[B]:HIS:CE1 | 2.04 | 0.75 |
| 3:U:3180[A]:TYR:HB2 | 3:U:3183[A]:LEU:CD2 | 2.16 | 0.75 |
| 3:U:3212[A]:ARG:HG3 | 3:U:3212[A]:ARG:NH1 | 2.00 | 0.75 |
| 3:X:3180[A]:TYR:HB2 | 3:X:3183[A]:LEU:CD2 | 2.16 | 0.75 |
| 3:a:2948[A]:ASP:HB3 | 3:a:2949[A]:LYS:CA | 2.15 | 0.75 |
| 3:a:3038[A]:ILE:HG22 | 3:a:3040[A]:VAL:HG22 | 1.68 | 0.75 |
| 3:d:2954[B]:TYR:O | 3:d:2957[B]:ILE:HG22 | 1.87 | 0.75 |
| 3:d:3204[A]:LEU:O | 3:d:3208[A]:GLN:HG3 | 1.86 | 0.75 |
| 1:A:979:LEU:HB3 | 1:A:980:TYR:HA | 1.69 | 0.75 |
| 3:C:3079[B]:CYS:CA | 3:L:3161[B]:GLU:HG2 | 2.16 | 0.75 |
| 3:F:3204[A]:LEU:O | 3:F:3208[A]:GLN:HG3 | 1.86 | 0.75 |
| 3:F:3293[A]:LYS:HB2 | 3:F:3294[A]:SER:HB2 | 0.82 | 0.75 |
| 1:G:527:LEU:HD21 | 1:G:632:LEU:HD12 | 1.68 | 0.75 |
| 3:I:3114[A]:PRO:HD2 | 3:I:3115[A]:LEU:H | 1.51 | 0.75 |
| 3:L:3114[A]:PRO:HD2 | 3:L:3115[A]:LEU:H | 1.51 | 0.75 |
| 3:O:3147[B]:GLU:HB2 | 3:O:3149[B]:ASN:OD1 | 1.86 | 0.75 |
| 3:O:3255[B]:PRO:CA | 3:X:3160[B]:SER:C | 2.50 | 0.75 |
| 3:R:2955[A]:GLN:CD | 3:R:3037[A]:TYR:HE1 | 1.92 | 0.75 |
| 3:R:3141[B]:TYR:HD2 | 3:R:3142[B]:ASN:H | 0.78 | 0.75 |
| 3:U:2975[B]:PHE:CD2 | 3:d:3255[B]:PRO:O | 2.32 | 0.75 |
| 3:U:3114[B]:PRO:HD2 | 3:U:3115[B]:LEU:H | 1.51 | 0.75 |
| 3:X:2948[B]:ASP:HB3 | 3:X:2949[B]:LYS:CA | 2.15 | 0.75 |
| 3:X:3089[A]:HIS:HD1 | 3:X:3119[A]:HIS:CE1 | 2.04 | 0.75 |
| 3:a:3089[A]:HIS:HD1 | 3:a:3119[A]:HIS:CE1 | 2.04 | 0.75 |
| 3:a:3089[B]:HIS:HD1 | 3:a:3119[B]:HIS:CE1 | 2.04 | 0.75 |
| 3:a:3204[B]:LEU:O | 3:a:3208[B]:GLN:HG3 | 1.86 | 0.75 |
| 3:a:3230[B]:PHE:CB | 3:a:3243[B]:GLY:HA2 | 2.06 | 0.75 |
| 3:d:3196[A]:THR:H | 3:d:3199[A]:GLN:CD | 1.94 | 0.75 |
| 3:d:3220[A]:ARG:HG3 | 3:d:3220[A]:ARG:NH1 | 1.98 | 0.75 |
| 3:C:2954[B]:TYR:O | 3:C:2957[B]:ILE:HG22 | 1.87 | 0.75 |
| 3:C:3204[A]:LEU:O | 3:C:3208[A]:GLN:HG3 | 1.86 | 0.75 |
| 3:C:3288[B]:MET:HG2 | 3:C:3295[B]:LEU:HD21 | 1.67 | 0.75 |
| 3:F:2984[B]:THR:HG23 | 3:a:3159[B]:SER:CB | 1.75 | 0.75 |
| 3:F:3038[B]:ILE:HG22 | 3:F:3040[B]:VAL:HG22 | 1.68 | 0.75 |
| 3:F:3120[B]:HIS:O | 3:F:3121[B]:SER:C | 2.29 | 0.75 |
| 3:I:2948[B]:ASP:HB3 | 3:I:2949[B]:LYS:CA | 2.15 | 0.75 |
| 3:I:2954[A]:TYR:O | 3:I:2957[A]:ILE:HG22 | 1.87 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2965[B]:LEU:HA | 3:R:3253[B]:GLU:HG3 | 1.69 | 0.75 |
| 3:I:2968[B]:GLN:CG | 3:R:3086[B]:GLU:CG | 2.53 | 0.75 |
| 3:I:2982[B]:MET:HE3 | 3:R:2977[B]:CYS:SG | 2.26 | 0.75 |
| 3:I:3137[B]:ARG:HB3 | 3:I:3139[B]:LEU:CD2 | 2.17 | 0.75 |
| 3:L:2937[A]:ASN:HB2 | 3:L:3006[A]:LYS:CE | 2.14 | 0.75 |
| 3:L:3180[B]:TYR:HB2 | 3:L:3183[B]:LEU:CD2 | 2.16 | 0.75 |
| 3:O:2969[B]:TYR:OH | 3:X:2991[B]:LEU:O | 1.94 | 0.75 |
| 3:O:2969[B]:TYR:HB2 | 3:X:3158[B]:PHE:CG | 2.22 | 0.75 |
| 3:O:2974[B]:ALA:CB | 3:X:2977[B]:CYS:CA | 2.62 | 0.75 |
| 3:O:3162[B]:ASP:N | 3:X:3149[B]:ASN:OD1 | 2.15 | 0.75 |
| 3:O:3255[B]:PRO:HA | 3:X:3160[B]:SER:C | 2.12 | 0.75 |
| 3:O:3288[B]:MET:HG2 | 3:O:3295[B]:LEU:HD21 | 1.67 | 0.75 |
| 3:O:3306[B]:LEU:HD12 | 3:O:3307[B]:PHE:N | 2.00 | 0.75 |
| 2:Q:2124:SER:HB2 | 2:Q:2129:PRO:HG2 | 1.67 | 0.75 |
| 3:R:3113[A]:ASP:CG | 3:R:3114[A]:PRO:CD | 2.56 | 0.75 |
| 3:R:3220[A]:ARG:HG3 | 3:R:3220[A]:ARG:NH1 | 1.98 | 0.75 |
| 3:R:3306[B]:LEU:HD12 | 3:R:3307[B]:PHE:N | 2.00 | 0.75 |
| 3:U:2948[A]:ASP:HB3 | 3:U:2949[A]:LYS:CA | 2.15 | 0.75 |
| 3:U:3169[B]:LYS:CG | 3:d:3147[B]:GLU:HA | 2.14 | 0.75 |
| 3:U:3219[B]:LEU:HD22 | 3:U:3219[B]:LEU:N | 2.02 | 0.75 |
| 3:X:2956[B]:LYS:C | 3:X:2960[B]:PHE:CE1 | 2.47 | 0.75 |
| 3:a:2952[B]:ALA:HA | 3:a:2956[B]:LYS:HB3 | 1.67 | 0.75 |
| 3:a:3038[B]:ILE:HG22 | 3:a:3040[B]:VAL:HG22 | 1.68 | 0.75 |
| 3:a:3284[B]:LYS:CD | 3:a:3285[B]:VAL:N | 2.47 | 0.75 |
| 3:C:2948[B]:ASP:HB3 | 3:C:2949[B]:LYS:CA | 2.15 | 0.75 |
| 3:C:2979[B]:GLN:HG3 | 3:L:3156[B]:MET:CG | 2.17 | 0.75 |
| 3:C:2982[B]:MET:CB | 3:L:3156[B]:MET:CG | 2.64 | 0.75 |
| 3:F:3204[B]:LEU:O | 3:F:3208[B]:GLN:HG3 | 1.86 | 0.75 |
| 3:F:3254[B]:MET:CB | 3:a:2966[B]:SER:OG | 2.35 | 0.75 |
| 3:F:3288[A]:MET:HG2 | 3:F:3295[A]:LEU:HD21 | 1.67 | 0.75 |
| 2:H:2400:LEU:HB2 | 2:H:2439:PHE:HD2 | 1.50 | 0.75 |
| 3:I:2954[B]:TYR:O | 3:I:2957[B]:ILE:HG22 | 1.87 | 0.75 |
| 3:I:3089[A]:HIS:HD1 | 3:I:3119[A]:HIS:CE1 | 2.04 | 0.75 |
| 3:I:3219[B]:LEU:HD22 | 3:I:3219[B]:LEU:N | 2.02 | 0.75 |
| 3:L:2954[B]:TYR:O | 3:L:2957[B]:ILE:HG22 | 1.87 | 0.75 |
| 3:L:2955[A]:GLN:CD | 3:L:3037[A]:TYR:HE1 | 1.92 | 0.75 |
| 3:O:2971[A]:ASP:OD1 | 3:O:2973[A]:THR:OG1 | 2.04 | 0.75 |
| 3:O:2976[B]:ALA:HB2 | 3:X:3156[B]:MET:CE | 2.15 | 0.75 |
| 3:O:3089[B]:HIS:HD1 | 3:O:3119[B]:HIS:CE1 | 2.04 | 0.75 |
| 3:O:3147[A]:GLU:HB2 | 3:O:3149[A]:ASN:OD1 | 1.86 | 0.75 |
| 3:O:3219[A]:LEU:HD22 | 3:O:3219[A]:LEU:N | 2.02 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2961[A]:HIS:HD2 | 3:U:2988[A]:TRP:HZ3 | 1.32 | 0.75 |
| 3:U:3219[A]:LEU:HD22 | 3:U:3219[A]:LEU:N | 2.02 | 0.75 |
| 1:V:907:ARG:NH2 | 1:V:1106:PHE:O | 2.20 | 0.75 |
| 2:W:2472:ASN:ND2 | 4:HA:1:NAG:H61 | 1.99 | 0.75 |
| 2:W:2823:ILE:O | 2:W:2830:GLN:NE2 | 2.20 | 0.75 |
| 3:X:3147[A]:GLU:HB2 | 3:X:3149[A]:ASN:OD1 | 1.86 | 0.75 |
| 3:a:3212[B]:ARG:HG3 | 3:a:3212[B]:ARG:NH1 | 2.00 | 0.75 |
| 1:b:392:PRO:HB2 | 1:b:394:GLN:HG2 | 1.68 | 0.75 |
| 3:d:3114[A]:PRO:HD2 | 3:d:3115[A]:LEU:H | 1.51 | 0.75 |
| 3:d:3288[B]:MET:HG2 | 3:d:3295[B]:LEU:HD21 | 1.67 | 0.75 |
| 3:C:2948[A]:ASP:H | 3:C:2949[A]:LYS:CA | 1.98 | 0.75 |
| 3:C:3211[B]:ASP:HB3 | 3:C:3309[B]:PRO:HA | 1.67 | 0.75 |
| 3:F:2965[B]:LEU:HB3 | 3:a:3256[B]:TRP:CE2 | 2.20 | 0.75 |
| 3:F:2968[B]:GLN:OE1 | 3:a:2981[B]:GLY:CA | 2.34 | 0.75 |
| 3:F:3212[B]:ARG:HG3 | 3:F:3212[B]:ARG:NH1 | 2.00 | 0.75 |
| 3:I:2937[B]:ASN:HB2 | 3:I:3006[B]:LYS:CE | 2.14 | 0.75 |
| 3:I:2952[A]:ALA:HA | 3:I:2956[A]:LYS:HB3 | 1.67 | 0.75 |
| 3:I:2955[A]:GLN:CD | 3:I:3037[A]:TYR:HE1 | 1.92 | 0.75 |
| 3:I:3159[B]:SER:C | 3:R:3150[B]:LYS:CD | 2.60 | 0.75 |
| 3:I:3250[B]:GLY:CA | 3:R:3252[B]:TYR:CE2 | 2.40 | 0.75 |
| 3:L:3147[A]:GLU:CG | 3:L:3149[A]:ASN:HD21 | 2.00 | 0.75 |
| 3:L:3196[B]:THR:H | 3:L:3199[B]:GLN:CD | 1.94 | 0.75 |
| 1:M:1046:HIS:HA | 1:M:1049:VAL:HB | 1.69 | 0.75 |
| 3:O:3012[B]:TRP:O | 3:O:3122[B]:ASN:ND2 | 2.20 | 0.75 |
| 3:O:3196[A]:THR:H | 3:O:3199[A]:GLN:CD | 1.94 | 0.75 |
| 3:R:2937[A]:ASN:CB | 3:R:3006[A]:LYS:HE2 | 2.14 | 0.75 |
| 3:R:3038[B]:ILE:HG22 | 3:R:3040[B]:VAL:HG22 | 1.68 | 0.75 |
| 3:U:2937[B]:ASN:HB2 | 3:U:3006[B]:LYS:CE | 2.14 | 0.75 |
| 3:X:3176[B]:LYS:HE2 | 3:X:3176[B]:LYS:N | 2.02 | 0.75 |
| 3:X:3196[B]:THR:H | 3:X:3199[B]:GLN:CD | 1.94 | 0.75 |
| 3:C:2954[A]:TYR:O | 3:C:2957[A]:ILE:HG22 | 1.87 | 0.75 |
| 3:C:3196[B]:THR:H | 3:C:3199[B]:GLN:CD | 1.94 | 0.75 |
| 3:F:2952[B]:ALA:HA | 3:F:2956[B]:LYS:HB2 | 1.69 | 0.75 |
| 3:F:2966[B]:SER:C | 3:a:3256[B]:TRP:HD1 | 1.54 | 0.75 |
| 3:F:2969[B]:TYR:HA | 3:a:2989[B]:HIS:CE1 | 2.20 | 0.75 |
| 3:F:2982[B]:MET:SD | 3:a:3157[B]:PRO:CB | 2.75 | 0.75 |
| 3:F:2983[B]:VAL:CG2 | 3:a:3160[B]:SER:C | 2.59 | 0.75 |
| 3:F:3153[B]:LYS:CA | 3:a:3155[B]:MET:HG3 | 2.16 | 0.75 |
| 3:I:2962[B]:GLY:C | 3:R:3255[B]:PRO:CG | 2.60 | 0.75 |
| 3:I:3120[A]:HIS:O | 3:I:3121[A]:SER:C | 2.29 | 0.75 |
| 3:I:3137[A]:ARG:HB3 | 3:I:3139[A]:LEU:CD2 | 2.17 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3153[B]:LYS:HZ2 | 3:R:3157[B]:PRO:HD2 | 1.51 | 0.75 |
| 3:L:2979[A]:GLN:NE2 | 3:L:3155[A]:MET:CE | 2.47 | 0.75 |
| 1:P:499:GLU:HG3 | 1:P:511:VAL:HG12 | 1.67 | 0.75 |
| 3:R:2930[A]:LEU:H | 3:R:2930[A]:LEU:CD2 | 1.98 | 0.75 |
| 3:U:2969[B]:TYR:HE1 | 3:d:3107[B]:LEU:HD11 | 0.90 | 0.75 |
| 3:U:2973[B]:THR:N | 3:d:3247[B]:VAL:CG1 | 2.50 | 0.75 |
| 3:X:3137[A]:ARG:HB3 | 3:X:3139[A]:LEU:CD2 | 2.17 | 0.75 |
| 3:X:3180[B]:TYR:HB2 | 3:X:3183[B]:LEU:CD2 | 2.16 | 0.75 |
| 3:a:2971[A]:ASP:OD1 | 3:a:2973[A]:THR:OG1 | 2.04 | 0.75 |
| 3:a:3141[A]:TYR:HD2 | 3:a:3142[A]:ASN:H | 0.78 | 0.75 |
| 3:a:3147[A]:GLU:CG | 3:a:3149[A]:ASN:HD21 | 2.00 | 0.75 |
| 3:a:3211[A]:ASP:HB3 | 3:a:3309[A]:PRO:HA | 1.67 | 0.75 |
| 3:d:2937[B]:ASN:HB2 | 3:d:3006[B]:LYS:CE | 2.13 | 0.75 |
| 3:d:2954[A]:TYR:O | 3:d:2957[A]:ILE:HG22 | 1.87 | 0.75 |
| 3:d:3120[A]:HIS:O | 3:d:3121[A]:SER:C | 2.29 | 0.75 |
| 3:d:3137[A]:ARG:HB3 | 3:d:3139[A]:LEU:CD2 | 2.17 | 0.75 |
| 3:d:3137[A]:ARG:HB3 | 3:d:3139[A]:LEU:HD23 | 1.69 | 0.75 |
| 3:d:3147[A]:GLU:HB2 | 3:d:3149[A]:ASN:OD1 | 1.86 | 0.75 |
| 3:d:3284[B]:LYS:CD | 3:d:3285[B]:VAL:N | 2.47 | 0.75 |
| 2:B:2867:PRO:HG2 | 3:C:2932[A]:PRO:HG2 | 1.69 | 0.75 |
| 3:C:3137[A]:ARG:HB3 | 3:C:3139[A]:LEU:HD23 | 1.69 | 0.75 |
| 3:C:3137[B]:ARG:HB3 | 3:C:3139[B]:LEU:CD2 | 2.17 | 0.75 |
| 3:F:2988[B]:TRP:CE3 | 3:F:2989[B]:HIS:ND1 | 2.53 | 0.75 |
| 3:F:2992[B]:TYR:HE2 | 3:a:2969[B]:TYR:CE1 | 2.03 | 0.75 |
| 3:F:3176[A]:LYS:HE2 | 3:F:3176[A]:LYS:N | 2.02 | 0.75 |
| 3:I:2952[A]:ALA:HA | 3:I:2956[A]:LYS:HB2 | 1.69 | 0.75 |
| 3:I:3107[B]:LEU:CD1 | 3:R:2975[B]:PHE:CD1 | 2.41 | 0.75 |
| 3:I:3147[B]:GLU:HB2 | 3:I:3149[B]:ASN:OD1 | 1.86 | 0.75 |
| 3:I:3154[B]:PRO:HG3 | 3:R:3174[B]:GLY:HA2 | 1.67 | 0.75 |
| 3:L:3137[A]:ARG:HB3 | 3:L:3139[A]:LEU:CD2 | 2.17 | 0.75 |
| 3:L:3176[B]:LYS:HE2 | 3:L:3176[B]:LYS:N | 2.02 | 0.75 |
| 3:O:3137[B]:ARG:HB3 | 3:O:3139[B]:LEU:CD2 | 2.17 | 0.75 |
| 3:R:3104[B]:MET:CA | 3:R:3110[B]:THR:HG23 | 2.10 | 0.75 |
| 3:U:3141[B]:TYR:HD2 | 3:U:3142[B]:ASN:H | 0.78 | 0.75 |
| 3:U:3255[B]:PRO:CD | 3:d:3253[B]:GLU:C | 2.59 | 0.75 |
| 3:X:2971[A]:ASP:OD1 | 3:X:2973[A]:THR:OG1 | 2.04 | 0.75 |
| 3:X:3196[A]:THR:H | 3:X:3199[A]:GLN:CD | 1.94 | 0.75 |
| 3:X:3204[A]:LEU:O | 3:X:3208[A]:GLN:HG3 | 1.86 | 0.75 |
| 3:X:3307[A]:PHE:CE1 | 3:X:3309[A]:PRO:HG3 | 2.16 | 0.75 |
| 2:c:2625:LEU:HA | 2:c:2638:ARG:HH12 | 1.51 | 0.75 |
| 3:d:2955[A]:GLN:CD | 3:d:3037[A]:TYR:HE1 | 1.92 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3038[A]:ILE:HG22 | 3:d:3040[A]:VAL:HG22 | 1.68 | 0.75 |
| 3:d:3089[B]:HIS:HD1 | 3:d:3119[B]:HIS:CE1 | 2.04 | 0.75 |
| 3:d:3137[B]:ARG:HB3 | 3:d:3139[B]:LEU:CD2 | 2.17 | 0.75 |
| 3:C:3180[A]:TYR:HB2 | 3:C:3183[A]:LEU:CD2 | 2.16 | 0.74 |
| 3:C:3219[A]:LEU:HD22 | 3:C:3219[A]:LEU:N | 2.02 | 0.74 |
| 3:C:3219[B]:LEU:HD22 | 3:C:3219[B]:LEU:N | 2.02 | 0.74 |
| 3:F:2983[B]:VAL:HG23 | 3:a:3160[B]:SER:CA | 2.17 | 0.74 |
| 3:F:3149[B]:ASN:CB | 3:a:3163[B]:ASN:CG | 2.60 | 0.74 |
| 3:F:3153[B]:LYS:HD3 | 3:a:2988[B]:TRP:CD1 | 2.22 | 0.74 |
| 3:F:3223[B]:GLY:CA | 3:a:2963[B]:MET:HE1 | 2.17 | 0.74 |
| 3:I:3174[B]:GLY:N | 3:R:3154[B]:PRO:CA | 2.49 | 0.74 |
| 3:I:3176[B]:LYS:HE2 | 3:I:3176[B]:LYS:N | 2.02 | 0.74 |
| 3:I:3220[A]:ARG:HG3 | 3:I:3220[A]:ARG:NH1 | 1.98 | 0.74 |
| 3:I:3293[B]:LYS:HB2 | 3:I:3294[B]:SER:HB2 | 0.82 | 0.74 |
| 1:J:1627:ARG:NH2 | 1:J:1629:GLU:OE1 | 2.19 | 0.74 |
| 3:L:2954[A]:TYR:O | 3:L:2957[A]:ILE:HG22 | 1.87 | 0.74 |
| 3:L:3204[B]:LEU:O | 3:L:3208[B]:GLN:HG3 | 1.86 | 0.74 |
| 3:O:2952[A]:ALA:HA | 3:O:2956[A]:LYS:HB2 | 1.69 | 0.74 |
| 3:O:3211[B]:ASP:HB3 | 3:O:3309[B]:PRO:HA | 1.67 | 0.74 |
| 3:R:2971[B]:ASP:N | 9:R:3401[B]:CUO:O2 | 2.19 | 0.74 |
| 3:R:3137[A]:ARG:HB3 | 3:R:3139[A]:LEU:HD23 | 1.69 | 0.74 |
| 3:R:3288[A]:MET:HG2 | 3:R:3295[A]:LEU:HD21 | 1.67 | 0.74 |
| 3:X:2952[A]:ALA:HA | 3:X:2956[A]:LYS:HB2 | 1.69 | 0.74 |
| 3:X:3211[A]:ASP:HB3 | 3:X:3309[A]:PRO:HA | 1.67 | 0.74 |
| 3:a:3114[B]:PRO:HD2 | 3:a:3115[B]:LEU:H | 1.51 | 0.74 |
| 3:d:2969[B]:TYR:HD2 | 3:d:2971[B]:ASP:N | 1.84 | 0.74 |
| 3:d:3120[B]:HIS:O | 3:d:3121[B]:SER:C | 2.29 | 0.74 |
| 3:d:3212[B]:ARG:HG3 | 3:d:3212[B]:ARG:NH1 | 2.00 | 0.74 |
| 3:C:3114[A]:PRO:HD2 | 3:C:3115[A]:LEU:H | 1.51 | 0.74 |
| 1:D:806:ASN:ND2 | 6:k:1:NAG:H83 | 2.02 | 0.74 |
| 3:F:2979[B]:GLN:C | 3:a:2967[B]:CYS:HB3 | 2.12 | 0.74 |
| 3:F:3012[A]:TRP:O | 3:F:3122[A]:ASN:ND2 | 2.20 | 0.74 |
| 3:F:3137[A]:ARG:HB3 | 3:F:3139[A]:LEU:HD23 | 1.69 | 0.74 |
| 3:I:2971[B]:ASP:N | 9:I:3401[B]:CUO:O2 | 2.20 | 0.74 |
| 3:I:3150[B]:LYS:NZ | 3:R:3162[B]:ASP:O | 2.19 | 0.74 |
| 3:I:3155[B]:MET:O | 3:I:3159[B]:SER:N | 2.20 | 0.74 |
| 3:I:3219[A]:LEU:HD22 | 3:I:3219[A]:LEU:N | 2.02 | 0.74 |
| 3:L:2952[B]:ALA:HA | 3:L:2956[B]:LYS:HB3 | 1.67 | 0.74 |
| 3:L:3012[B]:TRP:O | 3:L:3122[B]:ASN:ND2 | 2.20 | 0.74 |
| 3:O:2965[A]:LEU:HD21 | 3:O:2974[A]:ALA:HB1 | 1.70 | 0.74 |
| 3:O:2968[B]:GLN:HB3 | 3:X:2979[B]:GLN:HB3 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3219[B]:LEU:HD22 | 3:O:3219[B]:LEU:N | 2.02 | 0.74 |
| 3:R:2971[A]:ASP:OD1 | 3:R:2973[A]:THR:OG1 | 2.04 | 0.74 |
| 3:U:2952[A]:ALA:HA | 3:U:2956[A]:LYS:HB2 | 1.69 | 0.74 |
| 3:U:2965[B]:LEU:CG | 3:U:2974[B]:ALA:HB1 | 2.09 | 0.74 |
| 3:U:3082[B]:GLU:CD | 3:d:2970[B]:PRO:HB3 | 2.12 | 0.74 |
| 3:U:3114[A]:PRO:HD2 | 3:U:3115[A]:LEU:H | 1.51 | 0.74 |
| 3:X:2954[A]:TYR:O | 3:X:2957[A]:ILE:HG22 | 1.87 | 0.74 |
| 3:X:3012[A]:TRP:O | 3:X:3122[A]:ASN:ND2 | 2.20 | 0.74 |
| 3:X:3307[B]:PHE:CE1 | 3:X:3309[B]:PRO:HG3 | 2.16 | 0.74 |
| 3:a:3196[A]:THR:H | 3:a:3199[A]:GLN:CD | 1.94 | 0.74 |
| 3:d:3012[B]:TRP:O | 3:d:3122[B]:ASN:ND2 | 2.20 | 0.74 |
| 3:d:3176[B]:LYS:HE2 | 3:d:3176[B]:LYS:N | 2.02 | 0.74 |
| 1:A:527:LEU:O | 1:A:561:ARG:NH1 | 2.19 | 0.74 |
| 1:A:1063:ARG:HB3 | 1:A:1065:LYS:HD2 | 1.68 | 0.74 |
| 3:C:2969[B]:TYR:HD2 | 3:C:2971[B]:ASP:N | 1.84 | 0.74 |
| 3:C:3137[B]:ARG:HB3 | 3:C:3139[B]:LEU:HD23 | 1.69 | 0.74 |
| 3:C:3147[B]:GLU:CG | 3:C:3149[B]:ASN:HD21 | 2.00 | 0.74 |
| 3:C:3284[A]:LYS:CD | 3:C:3285[A]:VAL:N | 2.47 | 0.74 |
| 3:F:3038[A]:ILE:HG22 | 3:F:3040[A]:VAL:HG22 | 1.68 | 0.74 |
| 3:F:3089[B]:HIS:HD1 | 3:F:3119[B]:HIS:CE1 | 2.04 | 0.74 |
| 3:F:3113[A]:ASP:CG | 3:F:3114[A]:PRO:CD | 2.56 | 0.74 |
| 3:F:3113[B]:ASP:CG | 3:F:3114[B]:PRO:CD | 2.56 | 0.74 |
| 3:F:3147[A]:GLU:CG | 3:F:3149[A]:ASN:HD21 | 2.00 | 0.74 |
| 3:F:3176[B]:LYS:HE2 | 3:F:3176[B]:LYS:N | 2.02 | 0.74 |
| 3:F:3219[B]:LEU:HD22 | 3:F:3219[B]:LEU:N | 2.02 | 0.74 |
| 2:H:2142:ALA:HB2 | 2:H:2433:THR:HG23 | 1.68 | 0.74 |
| 3:I:3024[B]:LEU:CD1 | 3:I:3025[B]:VAL:H | 1.83 | 0.74 |
| 3:I:3038[A]:ILE:HG22 | 3:I:3040[A]:VAL:HG22 | 1.68 | 0.74 |
| 3:I:3089[B]:HIS:HD1 | 3:I:3119[B]:HIS:CE1 | 2.04 | 0.74 |
| 3:I:3137[A]:ARG:HB3 | 3:I:3139[A]:LEU:HD23 | 1.69 | 0.74 |
| 3:I:3137[B]:ARG:HB3 | 3:I:3139[B]:LEU:HD23 | 1.69 | 0.74 |
| 3:I:3157[B]:PRO:HD3 | 3:R:3254[B]:MET:CE | 2.16 | 0.74 |
| 3:L:2948[B]:ASP:HB3 | 3:L:2949[B]:LYS:CA | 2.15 | 0.74 |
| 3:L:3196[A]:THR:H | 3:L:3199[A]:GLN:CD | 1.94 | 0.74 |
| 3:O:2969[B]:TYR:HB3 | 3:X:2988[B]:TRP:O | 1.88 | 0.74 |
| 3:O:3137[A]:ARG:HB3 | 3:O:3139[A]:LEU:HD23 | 1.69 | 0.74 |
| 3:O:3222[B]:ILE:N | 3:X:3161[B]:GLU:CB | 2.40 | 0.74 |
| 3:U:3170[B]:ALA:N | 3:d:3148[B]:ILE:HB | 2.03 | 0.74 |
| 3:X:2952[B]:ALA:CB | 3:X:2953[B]:GLY:C | 2.48 | 0.74 |
| 3:X:2969[A]:TYR:O | 3:X:2972[A]:GLY:N | 2.21 | 0.74 |
| 3:X:2969[B]:TYR:O | 3:X:2972[B]:GLY:N | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3155[B]:MET:O | 3:X:3159[B]:SER:N | 2.20 | 0.74 |
| 3:a:3114[A]:PRO:HD2 | 3:a:3115[A]:LEU:H | 1.51 | 0.74 |
| 3:a:3137[A]:ARG:HB3 | 3:a:3139[A]:LEU:HD23 | 1.69 | 0.74 |
| 3:a:3155[A]:MET:O | 3:a:3159[A]:SER:N | 2.20 | 0.74 |
| 3:C:3153[B]:LYS:O | 3:L:3154[B]:PRO:C | 2.29 | 0.74 |
| 3:F:2954[B]:TYR:O | 3:F:2957[B]:ILE:HG22 | 1.87 | 0.74 |
| 3:F:2988[A]:TRP:CE3 | 3:F:2989[A]:HIS:ND1 | 2.53 | 0.74 |
| 3:F:3137[A]:ARG:HB3 | 3:F:3139[A]:LEU:CD2 | 2.17 | 0.74 |
| 3:F:3211[B]:ASP:HB3 | 3:F:3309[B]:PRO:HA | 1.67 | 0.74 |
| 1:G:1145:THR:HG1 | 1:G:1233:SER:HG | 1.33 | 0.74 |
| 3:I:2952[B]:ALA:HA | 3:I:2956[B]:LYS:HB3 | 1.67 | 0.74 |
| 3:I:2977[B]:CYS:CB | 3:R:2982[B]:MET:CE | 2.65 | 0.74 |
| 3:I:3012[A]:TRP:O | 3:I:3122[A]:ASN:ND2 | 2.20 | 0.74 |
| 3:I:3012[B]:TRP:O | 3:I:3122[B]:ASN:ND2 | 2.20 | 0.74 |
| 3:L:3219[B]:LEU:HD22 | 3:L:3219[B]:LEU:N | 2.02 | 0.74 |
| 3:R:2954[B]:TYR:O | 3:R:2957[B]:ILE:HG22 | 1.87 | 0.74 |
| 3:R:2963[A]:MET:HG2 | 3:R:3108[A]:HIS:CG | 2.23 | 0.74 |
| 3:R:3012[A]:TRP:O | 3:R:3122[A]:ASN:ND2 | 2.20 | 0.74 |
| 3:R:3089[B]:HIS:HD1 | 3:R:3119[B]:HIS:CE1 | 2.04 | 0.74 |
| 3:R:3134[A]:GLN:HG3 | 3:R:3139[A]:LEU:HB2 | 1.70 | 0.74 |
| 3:R:3147[A]:GLU:CG | 3:R:3149[A]:ASN:HD21 | 2.00 | 0.74 |
| 3:R:3219[B]:LEU:HD22 | 3:R:3219[B]:LEU:N | 2.02 | 0.74 |
| 3:U:2988[A]:TRP:CE3 | 3:U:2989[A]:HIS:ND1 | 2.53 | 0.74 |
| 3:U:3137[A]:ARG:HB3 | 3:U:3139[A]:LEU:CD2 | 2.17 | 0.74 |
| 3:U:3147[A]:GLU:CG | 3:U:3149[A]:ASN:HD21 | 2.00 | 0.74 |
| 3:X:3176[A]:LYS:HE2 | 3:X:3176[A]:LYS:N | 2.02 | 0.74 |
| 1:Y:133:LYS:HE3 | 1:Y:134:VAL:H | 1.53 | 0.74 |
| 3:a:2952[B]:ALA:HA | 3:a:2956[B]:LYS:HB2 | 1.69 | 0.74 |
| 3:a:3137[A]:ARG:HB3 | 3:a:3139[A]:LEU:CD2 | 2.17 | 0.74 |
| 3:a:3147[B]:GLU:CG | 3:a:3149[B]:ASN:HD21 | 2.00 | 0.74 |
| 3:a:3219[B]:LEU:HD22 | 3:a:3219[B]:LEU:N | 2.02 | 0.74 |
| 1:b:1228:LEU:HB3 | 1:b:1229:LYS:HB2 | 1.69 | 0.74 |
| 3:d:2952[B]:ALA:HA | 3:d:2956[B]:LYS:HB2 | 1.69 | 0.74 |
| 3:d:2988[A]:TRP:CE3 | 3:d:2989[A]:HIS:ND1 | 2.53 | 0.74 |
| 3:d:3038[B]:ILE:HG22 | 3:d:3040[B]:VAL:HG22 | 1.68 | 0.74 |
| 3:d:3141[A]:TYR:HD2 | 3:d:3142[A]:ASN:H | 0.78 | 0.74 |
| 3:d:3155[A]:MET:O | 3:d:3159[A]:SER:N | 2.21 | 0.74 |
| 3:C:3012[A]:TRP:O | 3:C:3122[A]:ASN:ND2 | 2.20 | 0.74 |
| 3:C:3137[A]:ARG:HB3 | 3:C:3139[A]:LEU:CD2 | 2.17 | 0.74 |
| 3:C:3147[A]:GLU:HB2 | 3:C:3149[A]:ASN:OD1 | 1.86 | 0.74 |
| 3:C:3152[B]:LYS:CB | 3:L:3173[B]:THR:N | 2.30 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3196[A]:THR:H | 3:C:3199[A]:GLN:CD | 1.94 | 0.74 |
| 3:F:2937[B]:ASN:HB2 | 3:F:3006[B]:LYS:CE | 2.14 | 0.74 |
| 3:F:2963[B]:MET:HG2 | 3:F:3108[B]:HIS:CG | 2.23 | 0.74 |
| 3:F:3137[B]:ARG:HB3 | 3:F:3139[B]:LEU:CD2 | 2.17 | 0.74 |
| 3:I:2963[A]:MET:HG2 | 3:I:3108[A]:HIS:CG | 2.23 | 0.74 |
| 3:I:2974[B]:ALA:N | 3:R:3248[B]:LEU:C | 2.45 | 0.74 |
| 3:I:2988[A]:TRP:CE3 | 3:I:2989[A]:HIS:ND1 | 2.53 | 0.74 |
| 3:I:3155[B]:MET:HE1 | 3:R:3156[B]:MET:HG2 | 1.67 | 0.74 |
| 3:I:3196[A]:THR:HG21 | 1:J:416:ASN:HD22 | 0.68 | 0.74 |
| 3:I:3307[A]:PHE:CE1 | 3:I:3309[A]:PRO:HG3 | 2.16 | 0.74 |
| 1:J:1392:ASP:HB2 | 1:M:1372:ILE:HD11 | 1.70 | 0.74 |
| 3:O:3038[B]:ILE:CB | 3:X:2969[B]:TYR:OH | 2.35 | 0.74 |
| 3:O:3159[B]:SER:C | 3:X:3148[B]:ILE:CA | 2.60 | 0.74 |
| 1:P:240:PHE:HA | 1:P:263:ALA:HB3 | 1.69 | 0.74 |
| 1:P:1357:ARG:HH11 | 1:P:1357:ARG:HB3 | 1.53 | 0.74 |
| 3:R:2952[A]:ALA:HA | 3:R:2956[A]:LYS:HB2 | 1.70 | 0.74 |
| 3:R:2961[B]:HIS:HD2 | 3:R:2988[B]:TRP:HZ3 | 1.31 | 0.74 |
| 3:R:2969[B]:TYR:O | 3:R:2972[B]:GLY:N | 2.20 | 0.74 |
| 3:R:2971[B]:ASP:OD1 | 3:R:2973[B]:THR:OG1 | 2.04 | 0.74 |
| 3:R:3113[B]:ASP:CG | 3:R:3114[B]:PRO:CD | 2.56 | 0.74 |
| 3:U:2954[B]:TYR:O | 3:U:2957[B]:ILE:HG22 | 1.87 | 0.74 |
| 3:U:2971[A]:ASP:OD1 | 3:U:2973[A]:THR:OG1 | 2.04 | 0.74 |
| 3:U:3147[B]:GLU:HB2 | 3:U:3149[B]:ASN:OD1 | 1.86 | 0.74 |
| 3:U:3155[B]:MET:O | 3:U:3159[B]:SER:N | 2.20 | 0.74 |
| 3:U:3156[B]:MET:CE | 3:d:2982[B]:MET:CB | 2.66 | 0.74 |
| 3:U:3256[B]:TRP:CG | 3:d:2975[B]:PHE:CE1 | 2.75 | 0.74 |
| 3:X:2937[A]:ASN:CB | 3:X:3006[A]:LYS:HE2 | 2.14 | 0.74 |
| 3:X:2952[B]:ALA:HA | 3:X:2956[B]:LYS:HB2 | 1.70 | 0.74 |
| 3:X:2963[B]:MET:HG2 | 3:X:3108[B]:HIS:CG | 2.23 | 0.74 |
| 3:X:2965[A]:LEU:HD21 | 3:X:2974[A]:ALA:HB1 | 1.69 | 0.74 |
| 3:X:3038[A]:ILE:HG22 | 3:X:3040[A]:VAL:HG22 | 1.68 | 0.74 |
| 3:X:3212[B]:ARG:HG3 | 3:X:3212[B]:ARG:NH1 | 2.00 | 0.74 |
| 1:Y:136:ALA:O | 1:Y:193:SER:OG | 2.04 | 0.74 |
| 3:a:2954[A]:TYR:O | 3:a:2957[A]:ILE:HG22 | 1.87 | 0.74 |
| 3:a:2954[B]:TYR:O | 3:a:2957[B]:ILE:HG22 | 1.87 | 0.74 |
| 3:a:2971[B]:ASP:OD1 | 3:a:2973[B]:THR:OG1 | 2.04 | 0.74 |
| 3:d:2937[B]:ASN:CB | 3:d:3006[B]:LYS:HE2 | 2.14 | 0.74 |
| 3:d:2952[A]:ALA:HA | 3:d:2956[A]:LYS:HB2 | 1.69 | 0.74 |
| 3:d:2955[B]:GLN:CD | 3:d:3037[B]:TYR:HE1 | 1.92 | 0.74 |
| 3:d:2965[B]:LEU:HD21 | 3:d:2974[B]:ALA:HB1 | 1.70 | 0.74 |
| 8:0:2:NAG:O3 | 8:0:3:BMA:H2 | 1.86 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2963[A]:MET:HG2 | 3:C:3108[A]:HIS:CG | 2.23 | 0.74 |
| 3:C:3012[B]:TRP:O | 3:C:3122[B]:ASN:ND2 | 2.20 | 0.74 |
| 3:C:3113[A]:ASP:CG | 3:C:3114[A]:PRO:CD | 2.56 | 0.74 |
| 3:F:3147[B]:GLU:CG | 3:F:3149[B]:ASN:HD21 | 2.00 | 0.74 |
| 3:F:3155[A]:MET:O | 3:F:3159[A]:SER:N | 2.20 | 0.74 |
| 2:H:2869:ALA:O | 2:H:2875:SER:OG | 2.05 | 0.74 |
| 3:I:2971[B]:ASP:O | 3:R:3093[B]:HIS:CG | 2.40 | 0.74 |
| 3:I:3120[B]:HIS:O | 3:I:3121[B]:SER:C | 2.29 | 0.74 |
| 3:I:3196[A]:THR:H | 3:I:3199[A]:GLN:CD | 1.94 | 0.74 |
| 3:I:3256[B]:TRP:NE1 | 3:R:2965[B]:LEU:CD1 | 2.50 | 0.74 |
| 1:J:187:GLY:HA3 | 1:J:195:SER:HB3 | 1.70 | 0.74 |
| 3:O:2954[A]:TYR:O | 3:O:2957[A]:ILE:HG22 | 1.87 | 0.74 |
| 3:O:3147[A]:GLU:CG | 3:O:3149[A]:ASN:HD21 | 2.00 | 0.74 |
| 3:O:3159[B]:SER:O | 3:X:3148[B]:ILE:CA | 2.30 | 0.74 |
| 3:O:3163[B]:ASN:HB2 | 3:X:3149[B]:ASN:CB | 2.17 | 0.74 |
| 3:O:3196[B]:THR:H | 3:O:3199[B]:GLN:CD | 1.94 | 0.74 |
| 3:R:3089[A]:HIS:HD1 | 3:R:3119[A]:HIS:CE1 | 2.04 | 0.74 |
| 3:U:2963[A]:MET:HG2 | 3:U:3108[A]:HIS:CG | 2.23 | 0.74 |
| 3:U:3157[B]:PRO:O | 3:d:3147[B]:GLU:OE1 | 2.06 | 0.74 |
| 3:U:3211[A]:ASP:HB3 | 3:U:3309[A]:PRO:HA | 1.67 | 0.74 |
| 3:X:2955[B]:GLN:CD | 3:X:3037[B]:TYR:HE1 | 1.92 | 0.74 |
| 3:a:2988[B]:TRP:CE3 | 3:a:2989[B]:HIS:ND1 | 2.53 | 0.74 |
| 2:c:2570:HIS:HD2 | 2:c:2711:HIS:CE1 | 2.05 | 0.74 |
| 3:d:2948[A]:ASP:H | 3:d:2949[A]:LYS:CA | 1.98 | 0.74 |
| 3:d:2969[A]:TYR:O | 3:d:2972[A]:GLY:N | 2.20 | 0.74 |
| 3:d:3307[B]:PHE:CE1 | 3:d:3309[B]:PRO:HG3 | 2.16 | 0.74 |
| 1:A:1187:LYS:HD3 | 2:E:2897:PRO:HG3 | 1.70 | 0.74 |
| 3:C:2965[A]:LEU:HD21 | 3:C:2974[A]:ALA:HB1 | 1.70 | 0.74 |
| 3:C:3155[B]:MET:O | 3:C:3159[B]:SER:N | 2.20 | 0.74 |
| 3:F:2937[B]:ASN:CB | 3:F:3006[B]:LYS:HE2 | 2.14 | 0.74 |
| 3:F:3134[A]:GLN:HG3 | 3:F:3139[A]:LEU:HB2 | 1.70 | 0.74 |
| 3:L:2971[A]:ASP:OD1 | 3:L:2973[A]:THR:OG1 | 2.04 | 0.74 |
| 3:L:3137[A]:ARG:HB3 | 3:L:3139[A]:LEU:HD23 | 1.69 | 0.74 |
| 3:L:3219[A]:LEU:HD22 | 3:L:3219[A]:LEU:N | 2.02 | 0.74 |
| 3:O:2955[B]:GLN:CD | 3:O:3037[B]:TYR:HE1 | 1.92 | 0.74 |
| 3:O:3134[A]:GLN:HG3 | 3:O:3139[A]:LEU:HB2 | 1.70 | 0.74 |
| 3:O:3147[B]:GLU:CG | 3:O:3149[B]:ASN:HD21 | 2.00 | 0.74 |
| 3:O:3155[A]:MET:O | 3:O:3159[A]:SER:N | 2.20 | 0.74 |
| 3:O:3176[A]:LYS:HE2 | 3:O:3176[A]:LYS:N | 2.02 | 0.74 |
| 3:O:3252[B]:TYR:HB3 | 3:X:3156[B]:MET:CB | 2.13 | 0.74 |
| 3:R:2965[B]:LEU:HD21 | 3:R:2974[B]:ALA:HB1 | 1.70 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3137[B]:ARG:HB3 | 3:R:3139[B]:LEU:HD23 | 1.69 | 0.74 |
| 3:R:3176[A]:LYS:HE2 | 3:R:3176[A]:LYS:N | 2.02 | 0.74 |
| 3:U:2952[B]:ALA:HA | 3:U:2956[B]:LYS:HB3 | 1.67 | 0.74 |
| 3:U:2954[A]:TYR:O | 3:U:2957[A]:ILE:HG22 | 1.87 | 0.74 |
| 3:U:2967[B]:CYS:CB | 3:d:3256[B]:TRP:HB2 | 2.18 | 0.74 |
| 3:U:2982[B]:MET:O | 3:d:2970[B]:PRO:HD3 | 1.87 | 0.74 |
| 3:U:3137[B]:ARG:HB3 | 3:U:3139[B]:LEU:CD2 | 2.17 | 0.74 |
| 3:U:3137[B]:ARG:HB3 | 3:U:3139[B]:LEU:HD23 | 1.69 | 0.74 |
| 3:U:3155[A]:MET:O | 3:U:3159[A]:SER:N | 2.20 | 0.74 |
| 3:U:3220[B]:ARG:HG3 | 3:U:3220[B]:ARG:NH1 | 1.98 | 0.74 |
| 3:U:3254[B]:MET:HB2 | 3:d:3254[B]:MET:HA | 1.66 | 0.74 |
| 3:U:3255[B]:PRO:CB | 3:d:2974[B]:ALA:O | 2.36 | 0.74 |
| 3:X:3012[B]:TRP:O | 3:X:3122[B]:ASN:ND2 | 2.20 | 0.74 |
| 3:X:3038[B]:ILE:HG22 | 3:X:3040[B]:VAL:HG22 | 1.68 | 0.74 |
| 3:X:3137[B]:ARG:HB3 | 3:X:3139[B]:LEU:CD2 | 2.17 | 0.74 |
| 3:X:3220[A]:ARG:HG3 | 3:X:3220[A]:ARG:NH1 | 1.98 | 0.74 |
| 3:a:2965[B]:LEU:HD21 | 3:a:2974[B]:ALA:HB1 | 1.70 | 0.74 |
| 3:d:2937[A]:ASN:CB | 3:d:3006[A]:LYS:HE2 | 2.14 | 0.74 |
| 3:C:2963[B]:MET:HG2 | 3:C:3108[B]:HIS:CG | 2.23 | 0.74 |
| 3:C:3147[A]:GLU:CG | 3:C:3149[A]:ASN:HD21 | 2.00 | 0.74 |
| 3:C:3158[B]:PHE:O | 3:L:3149[B]:ASN:C | 2.31 | 0.74 |
| 3:C:3307[B]:PHE:CE1 | 3:C:3309[B]:PRO:HG3 | 2.16 | 0.74 |
| 1:D:1631:GLU:OE1 | 1:G:328:LYS:NZ | 2.21 | 0.74 |
| 3:F:2954[A]:TYR:O | 3:F:2957[A]:ILE:HG22 | 1.87 | 0.74 |
| 3:F:3012[B]:TRP:O | 3:F:3122[B]:ASN:ND2 | 2.20 | 0.74 |
| 3:F:3155[B]:MET:O | 3:F:3159[B]:SER:N | 2.20 | 0.74 |
| 3:F:3173[B]:THR:CA | 3:a:3154[B]:PRO:N | 2.51 | 0.74 |
| 3:F:3284[A]:LYS:CD | 3:F:3285[A]:VAL:N | 2.47 | 0.74 |
| 2:K:2124:SER:HB2 | 2:K:2129:PRO:HG2 | 1.70 | 0.74 |
| 3:L:3038[A]:ILE:HG22 | 3:L:3040[A]:VAL:HG22 | 1.68 | 0.74 |
| 3:L:3038[B]:ILE:HG22 | 3:L:3040[B]:VAL:HG22 | 1.68 | 0.74 |
| 3:U:3212[B]:ARG:HG3 | 3:U:3212[B]:ARG:NH1 | 2.00 | 0.74 |
| 3:X:2954[B]:TYR:O | 3:X:2957[B]:ILE:HG22 | 1.87 | 0.74 |
| 3:X:2963[A]:MET:HG2 | 3:X:3108[A]:HIS:CG | 2.23 | 0.74 |
| 3:X:3120[A]:HIS:O | 3:X:3121[A]:SER:C | 2.29 | 0.74 |
| 3:X:3155[A]:MET:O | 3:X:3159[A]:SER:N | 2.20 | 0.74 |
| 3:a:3113[B]:ASP:CG | 3:a:3114[B]:PRO:CD | 2.56 | 0.74 |
| 1:b:460:GLU:OE2 | 1:b:1368:ARG:NH2 | 2.21 | 0.74 |
| 2:c:2806:ALA:HB2 | 2:c:2856:ILE:HD11 | 1.69 | 0.74 |
| 1:A:1302:SER:HB3 | 1:A:1303:GLU:HA | 1.68 | 0.74 |
| 3:C:2968[B]:GLN:HE21 | 3:L:3086[B]:GLU:CB | 2.00 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:2426:PHE:HB3 | 2:E:2445:MET:HE1 | 1.69 | 0.74 |
| 3:F:3114[A]:PRO:HD2 | 3:F:3115[A]:LEU:H | 1.51 | 0.74 |
| 3:F:3221[B]:ALA:HB3 | 3:a:2964[B]:PRO:HB3 | 1.68 | 0.74 |
| 3:I:2965[A]:LEU:HD21 | 3:I:2974[A]:ALA:HB1 | 1.70 | 0.74 |
| 3:L:3012[A]:TRP:O | 3:L:3122[A]:ASN:ND2 | 2.20 | 0.74 |
| 3:L:3093[B]:HIS:HE1 | 3:L:3119[B]:HIS:CD2 | 2.06 | 0.74 |
| 3:O:2930[B]:LEU:H | 3:O:2930[B]:LEU:CD2 | 1.97 | 0.74 |
| 3:O:3113[A]:ASP:CG | 3:O:3114[A]:PRO:CD | 2.56 | 0.74 |
| 3:O:3160[B]:SER:CA | 3:X:3151[B]:LEU:HG | 2.18 | 0.74 |
| 3:R:2955[B]:GLN:CD | 3:R:3037[B]:TYR:HE1 | 1.92 | 0.74 |
| 3:R:3012[B]:TRP:O | 3:R:3122[B]:ASN:ND2 | 2.20 | 0.74 |
| 3:R:3137[B]:ARG:HB3 | 3:R:3139[B]:LEU:CD2 | 2.17 | 0.74 |
| 3:U:2965[A]:LEU:HD21 | 3:U:2974[A]:ALA:HB1 | 1.69 | 0.74 |
| 3:U:3012[B]:TRP:O | 3:U:3122[B]:ASN:ND2 | 2.20 | 0.74 |
| 3:U:3089[A]:HIS:HD1 | 3:U:3119[A]:HIS:CE1 | 2.04 | 0.74 |
| 3:U:3093[A]:HIS:HE1 | 3:U:3119[A]:HIS:CD2 | 2.06 | 0.74 |
| 3:U:3113[A]:ASP:CG | 3:U:3114[A]:PRO:CD | 2.56 | 0.74 |
| 3:U:3176[A]:LYS:HE2 | 3:U:3176[A]:LYS:N | 2.02 | 0.74 |
| 3:U:3196[A]:THR:H | 3:U:3199[A]:GLN:CD | 1.94 | 0.74 |
| 3:U:3254[B]:MET:HB2 | 3:d:3254[B]:MET:HB3 | 1.70 | 0.74 |
| 3:U:3257[B]:ALA:H | 3:d:2968[B]:GLN:C | 1.95 | 0.74 |
| 3:X:2971[B]:ASP:OD1 | 3:X:2973[B]:THR:OG1 | 2.04 | 0.74 |
| 3:a:2988[A]:TRP:CE3 | 3:a:2989[A]:HIS:ND1 | 2.53 | 0.74 |
| 3:a:3012[A]:TRP:O | 3:a:3122[A]:ASN:ND2 | 2.20 | 0.74 |
| 3:a:3219[A]:LEU:HD22 | 3:a:3219[A]:LEU:N | 2.02 | 0.74 |
| 3:d:3093[A]:HIS:HE1 | 3:d:3119[A]:HIS:CD2 | 2.06 | 0.74 |
| 3:d:3293[A]:LYS:HB2 | 3:d:3294[A]:SER:HB2 | 0.82 | 0.74 |
| 4:t:1:NAG:H83 | 4:t:1:NAG:O3 | 1.88 | 0.74 |
| 1:A:105:VAL:HG12 | 1:A:123:PHE:HB3 | 1.70 | 0.74 |
| 1:A:589:GLN:HG2 | 1:A:594:ASP:HB3 | 1.68 | 0.74 |
| 1:A:1036:SER:OG | 1:A:1037:ALA:N | 2.20 | 0.74 |
| 3:C:2952[A]:ALA:HA | 3:C:2956[A]:LYS:HB2 | 1.70 | 0.74 |
| 3:C:2971[A]:ASP:OD1 | 3:C:2973[A]:THR:OG1 | 2.04 | 0.74 |
| 3:F:2956[A]:LYS:C | 3:F:2960[A]:PHE:CE1 | 2.47 | 0.74 |
| 3:F:2963[A]:MET:HG2 | 3:F:3108[A]:HIS:CG | 2.23 | 0.74 |
| 3:F:3163[B]:ASN:CB | 3:a:3150[B]:LYS:CE | 2.60 | 0.74 |
| 3:I:3147[B]:GLU:CG | 3:I:3149[B]:ASN:HD21 | 2.00 | 0.74 |
| 3:L:2952[B]:ALA:HA | 3:L:2956[B]:LYS:HB2 | 1.69 | 0.74 |
| 3:L:2963[A]:MET:HG2 | 3:L:3108[A]:HIS:CG | 2.23 | 0.74 |
| 3:L:3137[B]:ARG:HB3 | 3:L:3139[B]:LEU:CD2 | 2.17 | 0.74 |
| 3:L:3147[A]:GLU:HB2 | 3:L:3149[A]:ASN:OD1 | 1.86 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3147[B]:GLU:HB2 | 3:L:3149[B]:ASN:OD1 | 1.86 | 0.74 |
| 1:M:898:GLY:N | 1:M:899:MET:SD | 2.56 | 0.74 |
| 3:O:3025[A]:VAL:HG22 | 3:O:3047[A]:ARG:NH1 | 2.02 | 0.74 |
| 3:O:3137[A]:ARG:HB3 | 3:O:3139[A]:LEU:CD2 | 2.17 | 0.74 |
| 1:P:1301:PRO:HB3 | 1:P:1308:VAL:HG12 | 1.69 | 0.74 |
| 3:R:3137[A]:ARG:HB3 | 3:R:3139[A]:LEU:CD2 | 2.17 | 0.74 |
| 3:U:2937[B]:ASN:CB | 3:U:3006[B]:LYS:HE2 | 2.14 | 0.74 |
| 3:U:2975[B]:PHE:CE1 | 3:d:3253[B]:GLU:HG3 | 2.23 | 0.74 |
| 3:U:3134[B]:GLN:HG3 | 3:U:3139[B]:LEU:HB2 | 1.70 | 0.74 |
| 3:X:3212[A]:ARG:HG3 | 3:X:3212[A]:ARG:NH1 | 2.00 | 0.74 |
| 1:Y:1617:LYS:HE3 | 3:d:3180[B]:TYR:CE2 | 2.22 | 0.74 |
| 3:a:2963[A]:MET:HG2 | 3:a:3108[A]:HIS:CG | 2.23 | 0.74 |
| 3:d:3012[A]:TRP:O | 3:d:3122[A]:ASN:ND2 | 2.20 | 0.74 |
| 3:d:3137[B]:ARG:HB3 | 3:d:3139[B]:LEU:HD23 | 1.69 | 0.74 |
| 3:d:3141[B]:TYR:HD2 | 3:d:3142[B]:ASN:H | 0.78 | 0.74 |
| 3:C:2969[A]:TYR:HD2 | 3:C:2971[A]:ASP:N | 1.85 | 0.73 |
| 3:C:3038[B]:ILE:HG22 | 3:C:3040[B]:VAL:HG22 | 1.68 | 0.73 |
| 3:C:3212[A]:ARG:HG3 | 3:C:3212[A]:ARG:NH1 | 2.00 | 0.73 |
| 3:C:3223[B]:GLY:O | 3:L:3252[B]:TYR:CD2 | 2.40 | 0.73 |
| 3:C:3293[B]:LYS:HB2 | 3:C:3294[B]:SER:HB2 | 0.82 | 0.73 |
| 1:D:1161:ILE:HD11 | 1:D:1196:ILE:HD11 | 1.69 | 0.73 |
| 3:F:2937[A]:ASN:HB2 | 3:F:3006[A]:LYS:CE | 2.14 | 0.73 |
| 3:F:3089[B]:HIS:CD2 | 3:a:2972[B]:GLY:N | 2.55 | 0.73 |
| 3:F:3141[B]:TYR:HD2 | 3:F:3142[B]:ASN:H | 0.78 | 0.73 |
| 3:F:3153[B]:LYS:HZ3 | 3:a:3157[B]:PRO:HD2 | 1.49 | 0.73 |
| 3:F:3154[B]:PRO:CG | 3:a:3174[B]:GLY:HA2 | 2.16 | 0.73 |
| 3:F:3154[B]:PRO:C | 3:a:3153[B]:LYS:O | 2.31 | 0.73 |
| 3:F:3158[B]:PHE:N | 3:a:3153[B]:LYS:HE3 | 2.03 | 0.73 |
| 1:J:142:ARG:NH1 | 1:J:340:GLN:OE1 | 2.21 | 0.73 |
| 3:L:3155[A]:MET:O | 3:L:3159[A]:SER:N | 2.20 | 0.73 |
| 3:L:3176[A]:LYS:HE2 | 3:L:3176[A]:LYS:N | 2.02 | 0.73 |
| 3:L:3307[A]:PHE:CE1 | 3:L:3309[A]:PRO:HG3 | 2.16 | 0.73 |
| 3:O:3134[B]:GLN:HG3 | 3:O:3139[B]:LEU:HB2 | 1.70 | 0.73 |
| 1:S:573:LYS:HB3 | 1:S:574:GLY:CA | 2.18 | 0.73 |
| 3:U:2955[A]:GLN:CD | 3:U:3037[A]:TYR:HE1 | 1.92 | 0.73 |
| 3:X:2937[A]:ASN:HB2 | 3:X:3006[A]:LYS:CE | 2.14 | 0.73 |
| 3:X:3284[A]:LYS:CD | 3:X:3285[A]:VAL:N | 2.47 | 0.73 |
| 3:a:3120[B]:HIS:O | 3:a:3121[B]:SER:C | 2.29 | 0.73 |
| 3:a:3155[B]:MET:O | 3:a:3159[B]:SER:N | 2.20 | 0.73 |
| 3:a:3196[B]:THR:H | 3:a:3199[B]:GLN:CD | 1.94 | 0.73 |
| 3:C:2937[B]:ASN:HB2 | 3:C:3006[B]:LYS:CE | 2.14 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3038[A]:ILE:HG22 | 3:C:3040[A]:VAL:HG22 | 1.68 | 0.73 |
| 3:C:3172[B]:SER:OG | 3:L:3152[B]:LYS:CB | 2.36 | 0.73 |
| 1:D:1144:VAL:HB | 1:D:1196:ILE:HD12 | 1.70 | 0.73 |
| 3:F:3093[B]:HIS:HE1 | 3:F:3119[B]:HIS:CD2 | 2.06 | 0.73 |
| 3:F:3196[A]:THR:H | 3:F:3199[A]:GLN:CD | 1.94 | 0.73 |
| 3:I:3093[A]:HIS:HE1 | 3:I:3119[A]:HIS:CD2 | 2.06 | 0.73 |
| 3:I:3147[A]:GLU:CG | 3:I:3149[A]:ASN:HD21 | 2.00 | 0.73 |
| 3:I:3155[A]:MET:O | 3:I:3159[A]:SER:N | 2.20 | 0.73 |
| 3:I:3221[B]:ALA:HB1 | 3:R:2964[B]:PRO:CA | 2.13 | 0.73 |
| 3:I:3255[B]:PRO:CG | 3:R:2964[B]:PRO:CD | 2.66 | 0.73 |
| 3:I:3293[A]:LYS:HB2 | 3:I:3294[A]:SER:HB2 | 0.82 | 0.73 |
| 1:J:639:ARG:NH2 | 1:J:707:PHE:O | 2.21 | 0.73 |
| 2:K:2722:GLN:NE2 | 2:K:2769:PHE:O | 2.20 | 0.73 |
| 3:R:3093[A]:HIS:HE1 | 3:R:3119[A]:HIS:CD2 | 2.06 | 0.73 |
| 3:U:3012[A]:TRP:O | 3:U:3122[A]:ASN:ND2 | 2.20 | 0.73 |
| 3:U:3147[B]:GLU:CG | 3:U:3149[B]:ASN:HD21 | 2.00 | 0.73 |
| 3:U:3275[A]:LEU:N | 3:U:3275[A]:LEU:HD12 | 2.04 | 0.73 |
| 3:X:3134[A]:GLN:HG3 | 3:X:3139[A]:LEU:HB2 | 1.70 | 0.73 |
| 1:Y:1546:LYS:HG3 | 3:d:3001[B]:LYS:CG | 2.17 | 0.73 |
| 3:a:2948[B]:ASP:H | 3:a:2949[B]:LYS:CA | 1.98 | 0.73 |
| 3:a:2952[A]:ALA:HA | 3:a:2956[A]:LYS:HB2 | 1.70 | 0.73 |
| 3:a:3176[A]:LYS:HE2 | 3:a:3176[A]:LYS:N | 2.02 | 0.73 |
| 3:a:3176[B]:LYS:HE2 | 3:a:3176[B]:LYS:N | 2.02 | 0.73 |
| 3:d:2969[B]:TYR:O | 3:d:2972[B]:GLY:N | 2.21 | 0.73 |
| 3:d:3025[A]:VAL:HG22 | 3:d:3047[A]:ARG:NH1 | 2.01 | 0.73 |
| 3:d:3219[B]:LEU:HD22 | 3:d:3219[B]:LEU:N | 2.02 | 0.73 |
| 3:d:3307[A]:PHE:CE1 | 3:d:3309[A]:PRO:HG3 | 2.16 | 0.73 |
| 3:C:2937[B]:ASN:CB | 3:C:3006[B]:LYS:HE2 | 2.14 | 0.73 |
| 3:C:3176[B]:LYS:HE2 | 3:C:3176[B]:LYS:N | 2.02 | 0.73 |
| 3:F:2971[B]:ASP:OD2 | 3:a:3110[B]:THR:HG21 | 1.88 | 0.73 |
| 3:F:2975[B]:PHE:CZ | 3:a:2961[B]:HIS:CG | 2.75 | 0.73 |
| 3:F:3159[B]:SER:HG | 3:a:2984[B]:THR:HG21 | 1.52 | 0.73 |
| 3:I:2985[B]:PHE:HZ | 3:R:2970[B]:PRO:HA | 1.52 | 0.73 |
| 1:J:164:GLU:OE1 | 1:J:296:ARG:NH1 | 2.21 | 0.73 |
| 3:L:2968[A]:GLN:CB | 3:L:2972[A]:GLY:HA2 | 2.18 | 0.73 |
| 3:L:3137[B]:ARG:HB3 | 3:L:3139[B]:LEU:HD23 | 1.69 | 0.73 |
| 3:L:3155[B]:MET:O | 3:L:3159[B]:SER:N | 2.20 | 0.73 |
| 3:O:3089[B]:HIS:NE2 | 9:O:3401[B]:CUO:CU1 | 1.54 | 0.73 |
| 3:O:3093[B]:HIS:HE1 | 3:O:3119[B]:HIS:CD2 | 2.06 | 0.73 |
| 3:R:2937[A]:ASN:HB2 | 3:R:3006[A]:LYS:CE | 2.14 | 0.73 |
| 3:R:2968[B]:GLN:CB | 3:R:2972[B]:GLY:HA2 | 2.19 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3120[A]:HIS:O | 3:R:3121[A]:SER:C | 2.29 | 0.73 |
| 3:R:3155[A]:MET:O | 3:R:3159[A]:SER:N | 2.20 | 0.73 |
| 3:R:3275[A]:LEU:HD12 | 3:R:3275[A]:LEU:N | 2.04 | 0.73 |
| 3:U:2952[B]:ALA:HA | 3:U:2956[B]:LYS:HB2 | 1.69 | 0.73 |
| 3:U:3025[A]:VAL:HG22 | 3:U:3047[A]:ARG:NH1 | 2.02 | 0.73 |
| 3:U:3038[A]:ILE:HG22 | 3:U:3040[A]:VAL:HG22 | 1.68 | 0.73 |
| 3:U:3093[B]:HIS:HE1 | 3:U:3119[B]:HIS:CD2 | 2.06 | 0.73 |
| 3:X:3025[B]:VAL:HG22 | 3:X:3047[B]:ARG:NH1 | 2.02 | 0.73 |
| 3:X:3093[B]:HIS:HE1 | 3:X:3119[B]:HIS:CD2 | 2.06 | 0.73 |
| 3:X:3134[B]:GLN:HG3 | 3:X:3139[B]:LEU:HB2 | 1.70 | 0.73 |
| 3:a:3012[B]:TRP:O | 3:a:3122[B]:ASN:ND2 | 2.20 | 0.73 |
| 3:d:2963[B]:MET:HG2 | 3:d:3108[B]:HIS:CG | 2.23 | 0.73 |
| 3:d:3176[A]:LYS:HE2 | 3:d:3176[A]:LYS:N | 2.02 | 0.73 |
| 1:A:898:GLY:HA2 | 1:A:1186:TRP:HB2 | 1.68 | 0.73 |
| 3:C:3158[B]:PHE:HD2 | 3:L:3153[B]:LYS:NZ | 1.72 | 0.73 |
| 3:F:3275[B]:LEU:HD12 | 3:F:3275[B]:LEU:N | 2.04 | 0.73 |
| 3:I:2968[B]:GLN:CB | 3:I:2972[B]:GLY:HA2 | 2.18 | 0.73 |
| 1:J:572:SER:HB2 | 1:J:578:PHE:HB2 | 1.68 | 0.73 |
| 3:L:2965[B]:LEU:HD21 | 3:L:2974[B]:ALA:HB1 | 1.70 | 0.73 |
| 3:O:3038[B]:ILE:HD13 | 3:X:2969[B]:TYR:OH | 1.75 | 0.73 |
| 3:O:3114[A]:PRO:HD2 | 3:O:3115[A]:LEU:H | 1.51 | 0.73 |
| 3:O:3154[B]:PRO:CD | 3:X:3176[B]:LYS:CE | 2.64 | 0.73 |
| 3:O:3176[B]:LYS:HE2 | 3:O:3176[B]:LYS:N | 2.02 | 0.73 |
| 3:O:3196[A]:THR:HG21 | 1:P:416:ASN:HD21 | 1.50 | 0.73 |
| 3:R:3147[B]:GLU:CG | 3:R:3149[B]:ASN:HD21 | 2.00 | 0.73 |
| 1:S:1636:ASN:HD22 | 1:S:1639:LYS:CD | 2.01 | 0.73 |
| 3:U:3293[B]:LYS:HB2 | 3:U:3294[B]:SER:HB2 | 0.82 | 0.73 |
| 3:d:2965[A]:LEU:HD21 | 3:d:2974[A]:ALA:HB1 | 1.70 | 0.73 |
| 3:d:3155[B]:MET:O | 3:d:3159[B]:SER:N | 2.20 | 0.73 |
| 3:C:2966[B]:SER:HB2 | 3:L:2982[B]:MET:HE2 | 1.70 | 0.73 |
| 3:F:2974[B]:ALA:CB | 3:a:3253[B]:GLU:OE1 | 2.34 | 0.73 |
| 3:F:3156[B]:MET:C | 3:a:3153[B]:LYS:NZ | 2.45 | 0.73 |
| 3:I:2948[B]:ASP:H | 3:I:2949[B]:LYS:CA | 1.98 | 0.73 |
| 3:I:2955[B]:GLN:CD | 3:I:3037[B]:TYR:HE1 | 1.92 | 0.73 |
| 3:I:2983[B]:VAL:CG2 | 3:R:3162[B]:ASP:H | 2.01 | 0.73 |
| 3:I:3149[B]:ASN:CG | 3:R:3163[B]:ASN:HD22 | 1.96 | 0.73 |
| 3:I:3149[B]:ASN:ND2 | 3:R:3163[B]:ASN:ND2 | 2.34 | 0.73 |
| 3:I:3155[B]:MET:CG | 3:R:3153[B]:LYS:C | 2.56 | 0.73 |
| 3:L:3293[A]:LYS:HB2 | 3:L:3294[A]:SER:HB2 | 0.82 | 0.73 |
| 1:M:557:VAL:HG23 | 1:M:558:HIS:HA | 1.69 | 0.73 |
| 1:M:838:ARG:NH2 | 1:M:1112:PHE:O | 2.21 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3012[A]:TRP:O | 3:O:3122[A]:ASN:ND2 | 2.20 | 0.73 |
| 3:O:3113[B]:ASP:CG | 3:O:3114[B]:PRO:CD | 2.56 | 0.73 |
| 1:P:984:ASP:OD1 | 1:P:984:ASP:N | 2.22 | 0.73 |
| 3:R:3275[B]:LEU:HD12 | 3:R:3275[B]:LEU:N | 2.04 | 0.73 |
| 1:S:1617:LYS:CE | 3:X:3135[B]:LYS:HZ1 | 1.99 | 0.73 |
| 3:U:2963[B]:MET:HG2 | 3:U:3108[B]:HIS:CG | 2.23 | 0.73 |
| 3:U:2965[B]:LEU:CD2 | 3:d:3220[B]:ARG:HD3 | 2.17 | 0.73 |
| 2:W:2806:ALA:HB2 | 2:W:2856:ILE:HD11 | 1.70 | 0.73 |
| 3:X:3219[A]:LEU:HD22 | 3:X:3219[A]:LEU:N | 2.02 | 0.73 |
| 3:a:3134[B]:GLN:HG3 | 3:a:3139[B]:LEU:HB2 | 1.70 | 0.73 |
| 3:a:3137[B]:ARG:HB3 | 3:a:3139[B]:LEU:CD2 | 2.17 | 0.73 |
| 3:d:2968[A]:GLN:CB | 3:d:2972[A]:GLY:HA2 | 2.18 | 0.73 |
| 3:d:3275[B]:LEU:HD12 | 3:d:3275[B]:LEU:N | 2.04 | 0.73 |
| 3:C:3307[A]:PHE:CE1 | 3:C:3309[A]:PRO:HG3 | 2.16 | 0.73 |
| 1:D:1195:ASP:O | 1:D:1197:THR:N | 2.22 | 0.73 |
| 3:F:3134[B]:GLN:HG3 | 3:F:3139[B]:LEU:HB2 | 1.70 | 0.73 |
| 3:F:3137[B]:ARG:HB3 | 3:F:3139[B]:LEU:HD23 | 1.69 | 0.73 |
| 3:F:3155[B]:MET:CB | 3:a:3153[B]:LYS:HG2 | 2.06 | 0.73 |
| 3:I:2952[B]:ALA:CB | 3:I:2953[B]:GLY:C | 2.48 | 0.73 |
| 3:I:2963[B]:MET:HG2 | 3:I:3108[B]:HIS:CG | 2.23 | 0.73 |
| 3:I:2975[B]:PHE:CD1 | 3:R:3107[B]:LEU:HG | 2.22 | 0.73 |
| 3:I:2981[B]:GLY:H | 3:R:2968[B]:GLN:HG2 | 1.53 | 0.73 |
| 3:I:3093[B]:HIS:HE1 | 3:I:3119[B]:HIS:CD2 | 2.06 | 0.73 |
| 3:I:3150[B]:LYS:HZ2 | 3:R:3160[B]:SER:HB3 | 1.52 | 0.73 |
| 3:I:3159[B]:SER:O | 3:R:3150[B]:LYS:HB3 | 1.88 | 0.73 |
| 3:I:3171[B]:HIS:N | 3:R:3152[B]:LYS:HB2 | 1.88 | 0.73 |
| 3:I:3212[A]:ARG:HG3 | 3:I:3212[A]:ARG:NH1 | 2.00 | 0.73 |
| 3:I:3248[B]:LEU:HB3 | 3:R:2972[B]:GLY:C | 2.07 | 0.73 |
| 3:L:3025[A]:VAL:HG22 | 3:L:3047[A]:ARG:NH1 | 2.02 | 0.73 |
| 3:L:3134[A]:GLN:HG3 | 3:L:3139[A]:LEU:HB2 | 1.70 | 0.73 |
| 3:O:2963[A]:MET:HG2 | 3:O:3108[A]:HIS:CG | 2.23 | 0.73 |
| 3:O:3038[A]:ILE:HG22 | 3:O:3040[A]:VAL:HG22 | 1.68 | 0.73 |
| 3:O:3089[A]:HIS:NE2 | 9:O:3401[A]:CUO:CU1 | 1.54 | 0.73 |
| 3:R:2948[A]:ASP:H | 3:R:2949[A]:LYS:CA | 1.98 | 0.73 |
| 3:R:2963[B]:MET:HG2 | 3:R:3108[B]:HIS:CG | 2.23 | 0.73 |
| 3:R:3196[A]:THR:H | 3:R:3199[A]:GLN:CD | 1.94 | 0.73 |
| 3:U:3113[B]:ASP:CG | 3:U:3114[B]:PRO:CD | 2.56 | 0.73 |
| 3:U:3149[B]:ASN:O | 3:d:3154[B]:PRO:CB | 2.36 | 0.73 |
| 2:W:2252:GLU:OE2 | 2:W:2393:ARG:NH1 | 2.21 | 0.73 |
| 3:X:3275[B]:LEU:HD12 | 3:X:3275[B]:LEU:N | 2.04 | 0.73 |
| 3:d:2948[B]:ASP:H | 3:d:2949[B]:LYS:CA | 1.98 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2952[A]:ALA:CB | 3:d:2953[A]:GLY:C | 2.48 | 0.73 |
| 3:d:3284[A]:LYS:CD | 3:d:3285[A]:VAL:N | 2.47 | 0.73 |
| 6:GA:1:NAG:C4 | 6:GA:2:NAG:O7 | 2.33 | 0.73 |
| 3:C:2965[B]:LEU:HD21 | 3:C:2974[B]:ALA:HB1 | 1.70 | 0.73 |
| 3:C:3093[B]:HIS:HE1 | 3:C:3119[B]:HIS:CD2 | 2.06 | 0.73 |
| 3:C:3223[B]:GLY:O | 3:L:3252[B]:TYR:CG | 2.42 | 0.73 |
| 1:D:1209:ASP:OD1 | 1:D:1210:LYS:N | 2.21 | 0.73 |
| 3:F:2948[A]:ASP:H | 3:F:2949[A]:LYS:CA | 1.98 | 0.73 |
| 3:F:3172[B]:SER:N | 3:a:3152[B]:LYS:CB | 2.51 | 0.73 |
| 3:I:3134[B]:GLN:HG3 | 3:I:3139[B]:LEU:HB2 | 1.70 | 0.73 |
| 3:L:2937[A]:ASN:CB | 3:L:3006[A]:LYS:HE2 | 2.14 | 0.73 |
| 3:O:3212[A]:ARG:HG3 | 3:O:3212[A]:ARG:NH1 | 2.00 | 0.73 |
| 3:R:2954[A]:TYR:O | 3:R:2957[A]:ILE:HG22 | 1.87 | 0.73 |
| 1:S:456:GLN:NE2 | 1:S:549:PRO:O | 2.22 | 0.73 |
| 3:U:3154[B]:PRO:HA | 3:d:3153[B]:LYS:H | 1.53 | 0.73 |
| 3:X:3147[A]:GLU:CG | 3:X:3149[A]:ASN:HD21 | 2.00 | 0.73 |
| 3:d:3219[A]:LEU:HD22 | 3:d:3219[A]:LEU:N | 2.02 | 0.73 |
| 3:C:3154[B]:PRO:CB | 3:L:3151[B]:LEU:HA | 2.18 | 0.73 |
| 3:C:3154[B]:PRO:HG3 | 3:L:3174[B]:GLY:CA | 2.13 | 0.73 |
| 3:C:3174[B]:GLY:N | 3:L:3154[B]:PRO:HD3 | 2.03 | 0.73 |
| 3:C:3176[A]:LYS:HE2 | 3:C:3176[A]:LYS:N | 2.02 | 0.73 |
| 3:C:3256[B]:TRP:C | 3:L:2965[B]:LEU:O | 2.30 | 0.73 |
| 1:D:1152:LYS:HB3 | 1:D:1181:GLU:HA | 1.71 | 0.73 |
| 3:F:2968[B]:GLN:CB | 3:F:2972[B]:GLY:HA2 | 2.19 | 0.73 |
| 3:F:3219[A]:LEU:HD22 | 3:F:3219[A]:LEU:N | 2.02 | 0.73 |
| 1:J:1442:MET:HE1 | 1:J:1454:PHE:HA | 1.70 | 0.73 |
| 3:L:3275[A]:LEU:HD12 | 3:L:3275[A]:LEU:N | 2.04 | 0.73 |
| 3:L:3293[B]:LYS:HB2 | 3:L:3294[B]:SER:HB2 | 0.82 | 0.73 |
| 3:O:2969[A]:TYR:O | 3:O:2972[A]:GLY:N | 2.20 | 0.73 |
| 3:O:3293[A]:LYS:HB2 | 3:O:3294[A]:SER:HB2 | 0.82 | 0.73 |
| 3:U:3176[A]:LYS:HB3 | 3:U:3176[A]:LYS:HZ2 | 1.53 | 0.73 |
| 3:U:3196[B]:THR:H | 3:U:3199[B]:GLN:CD | 1.94 | 0.73 |
| 3:U:3220[B]:ARG:CG | 3:d:2974[B]:ALA:H | 2.01 | 0.73 |
| 3:X:2968[B]:GLN:CB | 3:X:2972[B]:GLY:HA2 | 2.19 | 0.73 |
| 3:X:3024[B]:LEU:CD1 | 3:X:3025[B]:VAL:H | 1.83 | 0.73 |
| 3:X:3093[A]:HIS:HE1 | 3:X:3119[A]:HIS:CD2 | 2.06 | 0.73 |
| 3:X:3113[A]:ASP:CG | 3:X:3114[A]:PRO:CD | 2.56 | 0.73 |
| 3:a:3025[A]:VAL:HG22 | 3:a:3047[A]:ARG:NH1 | 2.01 | 0.73 |
| 3:a:3275[A]:LEU:HD12 | 3:a:3275[A]:LEU:N | 2.04 | 0.73 |
| 3:d:2963[A]:MET:HG2 | 3:d:3108[A]:HIS:CG | 2.23 | 0.73 |
| 3:d:2988[B]:TRP:CE3 | 3:d:2989[B]:HIS:ND1 | 2.53 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2971[B]:ASP:OD1 | 3:C:2973[B]:THR:OG1 | 2.04 | 0.73 |
| 3:C:3093[A]:HIS:HE1 | 3:C:3119[A]:HIS:CD2 | 2.06 | 0.73 |
| 3:C:3150[B]:LYS:N | 3:L:3169[B]:LYS:CG | 2.52 | 0.73 |
| 3:C:3285[A]:VAL:HG22 | 3:C:3286[A]:THR:N | 2.04 | 0.73 |
| 2:E:2889:ALA:N | 2:E:2890:VAL:HA | 2.03 | 0.73 |
| 3:F:2969[B]:TYR:HD2 | 3:F:2971[B]:ASP:N | 1.84 | 0.73 |
| 3:F:2970[B]:PRO:CD | 3:a:2989[B]:HIS:CG | 2.42 | 0.73 |
| 3:F:3093[A]:HIS:HE1 | 3:F:3119[A]:HIS:CD2 | 2.06 | 0.73 |
| 3:F:3162[B]:ASP:C | 3:a:3150[B]:LYS:HZ1 | 1.97 | 0.73 |
| 3:F:3170[B]:ALA:C | 3:a:3152[B]:LYS:CB | 2.62 | 0.73 |
| 2:H:2340:ALA:HB1 | 2:H:2341:PRO:HD2 | 1.70 | 0.73 |
| 3:I:2968[A]:GLN:CB | 3:I:2972[A]:GLY:HA2 | 2.18 | 0.73 |
| 3:I:3169[B]:LYS:O | 3:R:3152[B]:LYS:HB2 | 1.86 | 0.73 |
| 3:I:3174[B]:GLY:HA3 | 3:R:3154[B]:PRO:CB | 2.04 | 0.73 |
| 1:P:1358:LEU:HD23 | 1:P:1456:LEU:HD21 | 1.71 | 0.73 |
| 2:Q:2868:GLU:HG2 | 3:R:2932[A]:PRO:O | 1.89 | 0.73 |
| 3:R:3155[B]:MET:O | 3:R:3159[B]:SER:N | 2.20 | 0.73 |
| 3:R:3176[B]:LYS:HE2 | 3:R:3176[B]:LYS:N | 2.02 | 0.73 |
| 3:R:3220[B]:ARG:HG3 | 3:R:3220[B]:ARG:NH1 | 1.98 | 0.73 |
| 3:U:2952[B]:ALA:CB | 3:U:2953[B]:GLY:C | 2.48 | 0.73 |
| 1:V:1604:ASP:OD1 | 1:V:1605:ARG:NH1 | 2.22 | 0.73 |
| 3:X:3137[A]:ARG:HB3 | 3:X:3139[A]:LEU:HD23 | 1.69 | 0.73 |
| 2:Z:2515:ARG:HB3 | 2:c:2344:LEU:HB3 | 1.71 | 0.73 |
| 3:a:3134[A]:GLN:HG3 | 3:a:3139[A]:LEU:HB2 | 1.70 | 0.73 |
| 2:c:2180:TRP:HA | 2:c:2184:MET:HE3 | 1.70 | 0.73 |
| 3:d:2949[A]:LYS:O | 3:d:2953[A]:GLY:N | 2.22 | 0.73 |
| 3:d:3089[B]:HIS:NE2 | 9:d:3401[B]:CUO:CU1 | 1.54 | 0.73 |
| 3:C:2949[A]:LYS:O | 3:C:2953[A]:GLY:N | 2.22 | 0.73 |
| 3:C:3149[B]:ASN:CG | 3:L:3158[B]:PHE:O | 2.32 | 0.73 |
| 1:D:17:ASN:HD21 | 1:D:86:THR:H | 1.37 | 0.73 |
| 3:F:2965[A]:LEU:HD21 | 3:F:2974[A]:ALA:HB1 | 1.70 | 0.73 |
| 3:F:2982[B]:MET:HG3 | 3:a:3156[B]:MET:HB2 | 1.71 | 0.73 |
| 1:G:838:ARG:HD3 | 1:G:918:ARG:HD3 | 1.71 | 0.73 |
| 3:I:3157[B]:PRO:HD2 | 3:R:3153[B]:LYS:NZ | 2.04 | 0.73 |
| 3:I:3172[B]:SER:HB2 | 3:R:3150[B]:LYS:O | 1.89 | 0.73 |
| 3:I:3176[A]:LYS:HE2 | 3:I:3176[A]:LYS:N | 2.02 | 0.73 |
| 3:I:3220[B]:ARG:HG3 | 3:I:3220[B]:ARG:NH1 | 1.98 | 0.73 |
| 3:I:3256[B]:TRP:HB3 | 3:R:2966[B]:SER:O | 1.89 | 0.73 |
| 9:I:3401[A]:CUO:CU1 | 3:R:3089[A]:HIS:NE2 | 1.54 | 0.73 |
| 3:O:3038[B]:ILE:HG22 | 3:O:3040[B]:VAL:HG22 | 1.68 | 0.73 |
| 3:O:3093[A]:HIS:HE1 | 3:O:3119[A]:HIS:CD2 | 2.06 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3163[B]:ASN:HB3 | 3:X:3148[B]:ILE:C | 2.14 | 0.73 |
| 3:O:3212[B]:ARG:HG3 | 3:O:3212[B]:ARG:NH1 | 2.00 | 0.73 |
| 1:P:557:VAL:HG23 | 1:P:558:HIS:HA | 1.71 | 0.73 |
| 3:R:2952[B]:ALA:HA | 3:R:2956[B]:LYS:HB2 | 1.69 | 0.73 |
| 3:U:2937[A]:ASN:HB2 | 3:U:3006[A]:LYS:CE | 2.14 | 0.73 |
| 3:U:2965[B]:LEU:HD21 | 3:U:2974[B]:ALA:HB1 | 1.70 | 0.73 |
| 3:U:3176[B]:LYS:HE2 | 3:U:3176[B]:LYS:N | 2.02 | 0.73 |
| 1:V:949:ASP:HB3 | 1:V:953:GLU:HB2 | 1.71 | 0.73 |
| 2:c:2524:LEU:HA | 2:c:2581:MET:HE1 | 1.70 | 0.73 |
| 3:d:3113[B]:ASP:CG | 3:d:3114[B]:PRO:CD | 2.56 | 0.73 |
| 3:d:3147[A]:GLU:CG | 3:d:3149[A]:ASN:HD21 | 2.01 | 0.73 |
| 3:d:3212[A]:ARG:HG3 | 3:d:3212[A]:ARG:NH1 | 2.00 | 0.73 |
| 3:C:2972[B]:GLY:HA2 | 3:L:3086[B]:GLU:HG2 | 1.71 | 0.72 |
| 9:C:3401[A]:CUO:CU1 | 3:L:3089[A]:HIS:NE2 | 1.54 | 0.72 |
| 1:D:1140:ASN:ND2 | 1:D:1236:TYR:OH | 2.22 | 0.72 |
| 3:F:2949[A]:LYS:O | 3:F:2953[A]:GLY:N | 2.22 | 0.72 |
| 3:F:2965[B]:LEU:HD21 | 3:F:2974[B]:ALA:HB1 | 1.69 | 0.72 |
| 3:F:3212[A]:ARG:HG3 | 3:F:3212[A]:ARG:NH1 | 2.00 | 0.72 |
| 3:L:3147[B]:GLU:CG | 3:L:3149[B]:ASN:HD21 | 2.00 | 0.72 |
| 3:L:3196[A]:THR:H | 3:L:3199[A]:GLN:CB | 2.02 | 0.72 |
| 3:L:3284[A]:LYS:CD | 3:L:3285[A]:VAL:N | 2.47 | 0.72 |
| 3:O:2952[B]:ALA:HA | 3:O:2956[B]:LYS:HB2 | 1.69 | 0.72 |
| 3:O:3137[B]:ARG:HB3 | 3:O:3139[B]:LEU:HD23 | 1.69 | 0.72 |
| 3:O:3255[B]:PRO:HD2 | 3:X:3169[B]:LYS:CG | 2.17 | 0.72 |
| 3:R:3038[A]:ILE:HG22 | 3:R:3040[A]:VAL:HG22 | 1.68 | 0.72 |
| 3:R:3133[A]:LEU:O | 3:R:3134[A]:GLN:C | 2.32 | 0.72 |
| 3:R:3133[B]:LEU:O | 3:R:3134[B]:GLN:C | 2.32 | 0.72 |
| 3:R:3219[A]:LEU:HD22 | 3:R:3219[A]:LEU:N | 2.02 | 0.72 |
| 3:U:3120[A]:HIS:O | 3:U:3121[A]:SER:C | 2.29 | 0.72 |
| 3:U:3159[B]:SER:HB2 | 3:d:3150[B]:LYS:HD2 | 1.50 | 0.72 |
| 3:X:2965[B]:LEU:HD21 | 3:X:2974[B]:ALA:HB1 | 1.69 | 0.72 |
| 3:X:3293[A]:LYS:HB2 | 3:X:3294[A]:SER:HB2 | 0.82 | 0.72 |
| 3:a:3093[A]:HIS:HE1 | 3:a:3119[A]:HIS:CD2 | 2.06 | 0.72 |
| 3:a:3093[B]:HIS:HE1 | 3:a:3119[B]:HIS:CD2 | 2.06 | 0.72 |
| 3:d:3134[A]:GLN:HG3 | 3:d:3139[A]:LEU:HB2 | 1.70 | 0.72 |
| 3:C:2952[B]:ALA:HA | 3:C:2956[B]:LYS:HB2 | 1.70 | 0.72 |
| 3:C:2972[B]:GLY:CA | 3:L:3090[B]:ASN:CG | 2.60 | 0.72 |
| 3:C:3133[A]:LEU:O | 3:C:3134[A]:GLN:C | 2.32 | 0.72 |
| 3:C:3141[B]:TYR:HD2 | 3:C:3142[B]:ASN:H | 0.78 | 0.72 |
| 3:C:3149[B]:ASN:HD22 | 3:L:3163[B]:ASN:CB | 2.01 | 0.72 |
| 3:C:3155[A]:MET:O | 3:C:3159[A]:SER:N | 2.20 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3196[A]:THR:H | 3:C:3199[A]:GLN:CB | 2.02 | 0.72 |
| 3:C:3196[B]:THR:H | 3:C:3199[B]:GLN:CB | 2.02 | 0.72 |
| 3:F:2975[B]:PHE:HZ | 3:a:2961[B]:HIS:CG | 2.06 | 0.72 |
| 3:F:2982[B]:MET:CG | 3:a:3156[B]:MET:HB2 | 2.18 | 0.72 |
| 3:F:2992[B]:TYR:CE2 | 3:a:2969[B]:TYR:CE1 | 2.77 | 0.72 |
| 3:F:3147[B]:GLU:N | 3:a:3161[B]:GLU:HA | 2.05 | 0.72 |
| 2:H:2650:GLY:HA3 | 2:H:2653:GLU:O | 1.89 | 0.72 |
| 3:I:3038[B]:ILE:HG22 | 3:I:3040[B]:VAL:HG22 | 1.68 | 0.72 |
| 3:I:3134[A]:GLN:HG3 | 3:I:3139[A]:LEU:HB2 | 1.70 | 0.72 |
| 3:I:3171[B]:HIS:C | 3:R:3152[B]:LYS:HB2 | 2.14 | 0.72 |
| 3:L:2969[A]:TYR:O | 3:L:2972[A]:GLY:N | 2.20 | 0.72 |
| 3:O:2969[B]:TYR:H | 3:X:2988[B]:TRP:CD1 | 2.08 | 0.72 |
| 3:O:2979[B]:GLN:HE21 | 3:O:3155[B]:MET:HE2 | 1.54 | 0.72 |
| 3:O:3285[B]:VAL:HG22 | 3:O:3286[B]:THR:N | 2.04 | 0.72 |
| 3:R:3134[B]:GLN:HG3 | 3:R:3139[B]:LEU:HB2 | 1.70 | 0.72 |
| 3:R:3196[B]:THR:H | 3:R:3199[B]:GLN:CB | 2.02 | 0.72 |
| 3:U:2930[A]:LEU:H | 3:U:2930[A]:LEU:CD2 | 1.98 | 0.72 |
| 3:U:2949[A]:LYS:O | 3:U:2953[A]:GLY:N | 2.22 | 0.72 |
| 3:U:3152[B]:LYS:CG | 3:d:3154[B]:PRO:CB | 2.48 | 0.72 |
| 3:U:3196[B]:THR:H | 3:U:3199[B]:GLN:CB | 2.02 | 0.72 |
| 2:W:2340:ALA:HB1 | 2:W:2341:PRO:HD2 | 1.71 | 0.72 |
| 3:a:2949[B]:LYS:O | 3:a:2953[B]:GLY:N | 2.22 | 0.72 |
| 3:a:2963[B]:MET:HG2 | 3:a:3108[B]:HIS:CG | 2.23 | 0.72 |
| 3:a:3285[B]:VAL:HG22 | 3:a:3286[B]:THR:N | 2.04 | 0.72 |
| 3:a:3307[A]:PHE:CE1 | 3:a:3309[A]:PRO:HG3 | 2.16 | 0.72 |
| 1:b:118:ALA:HB1 | 1:b:119:LYS:HA | 1.69 | 0.72 |
| 3:d:3093[B]:HIS:HE1 | 3:d:3119[B]:HIS:CD2 | 2.06 | 0.72 |
| 3:C:2984[B]:THR:HB | 3:L:3154[B]:PRO:HG2 | 1.70 | 0.72 |
| 3:C:3120[B]:HIS:O | 3:C:3121[B]:SER:C | 2.29 | 0.72 |
| 3:F:3196[B]:THR:H | 3:F:3199[B]:GLN:CB | 2.02 | 0.72 |
| 9:F:3401[A]:CUO:CU1 | 3:a:3089[A]:HIS:NE2 | 1.54 | 0.72 |
| 3:I:2981[B]:GLY:HA2 | 3:R:2968[B]:GLN:OE1 | 1.89 | 0.72 |
| 3:I:3113[B]:ASP:CG | 3:I:3114[B]:PRO:CD | 2.56 | 0.72 |
| 3:I:3163[B]:ASN:ND2 | 3:R:3149[B]:ASN:ND2 | 2.37 | 0.72 |
| 3:L:2949[B]:LYS:O | 3:L:2953[B]:GLY:N | 2.22 | 0.72 |
| 3:L:3093[A]:HIS:HE1 | 3:L:3119[A]:HIS:CD2 | 2.06 | 0.72 |
| 3:L:3285[B]:VAL:HG22 | 3:L:3286[B]:THR:N | 2.04 | 0.72 |
| 3:O:2963[B]:MET:HE3 | 3:X:2975[B]:PHE:CE1 | 2.24 | 0.72 |
| 3:U:2949[B]:LYS:O | 3:U:2953[B]:GLY:N | 2.22 | 0.72 |
| 3:X:3219[B]:LEU:HD22 | 3:X:3219[B]:LEU:N | 2.02 | 0.72 |
| 1:Y:1046:HIS:HA | 1:Y:1049:VAL:HB | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2965[A]:LEU:HD21 | 3:a:2974[A]:ALA:HB1 | 1.70 | 0.72 |
| 3:a:3196[B]:THR:H | 3:a:3199[B]:GLN:CB | 2.02 | 0.72 |
| 3:a:3293[A]:LYS:HD2 | 3:a:3293[A]:LYS:C | 2.15 | 0.72 |
| 3:d:2956[B]:LYS:C | 3:d:2960[B]:PHE:CE1 | 2.47 | 0.72 |
| 3:d:3089[A]:HIS:NE2 | 9:d:3401[A]:CUO:CU1 | 1.54 | 0.72 |
| 3:C:2968[B]:GLN:CB | 3:C:2972[B]:GLY:HA2 | 2.18 | 0.72 |
| 3:C:3153[B]:LYS:HE2 | 3:L:3158[B]:PHE:CE2 | 2.25 | 0.72 |
| 3:C:3220[B]:ARG:HG3 | 3:C:3220[B]:ARG:NH1 | 1.98 | 0.72 |
| 3:F:2969[A]:TYR:O | 3:F:2972[A]:GLY:N | 2.21 | 0.72 |
| 3:I:3196[A]:THR:HG21 | 1:J:416:ASN:CB | 2.19 | 0.72 |
| 3:I:3285[A]:VAL:HG22 | 3:I:3286[A]:THR:N | 2.04 | 0.72 |
| 3:O:2968[B]:GLN:OE1 | 3:X:2979[B]:GLN:HG3 | 1.90 | 0.72 |
| 3:O:2979[A]:GLN:HE21 | 3:O:3155[A]:MET:HE2 | 1.54 | 0.72 |
| 3:R:3120[B]:HIS:O | 3:R:3121[B]:SER:C | 2.29 | 0.72 |
| 1:S:755:PHE:HB2 | 1:S:788:LEU:HD21 | 1.69 | 0.72 |
| 3:U:3256[B]:TRP:HD1 | 3:d:2975[B]:PHE:HE1 | 1.25 | 0.72 |
| 1:V:142:ARG:NH1 | 1:V:340:GLN:OE1 | 2.23 | 0.72 |
| 2:W:2711:HIS:HA | 2:W:2714:VAL:HG22 | 1.71 | 0.72 |
| 3:X:2937[B]:ASN:HB2 | 3:X:3006[B]:LYS:CE | 2.14 | 0.72 |
| 3:X:2949[B]:LYS:O | 3:X:2953[B]:GLY:N | 2.22 | 0.72 |
| 3:X:3120[B]:HIS:O | 3:X:3121[B]:SER:C | 2.29 | 0.72 |
| 3:X:3137[B]:ARG:HB3 | 3:X:3139[B]:LEU:HD23 | 1.69 | 0.72 |
| 3:a:3293[B]:LYS:HB2 | 3:a:3294[B]:SER:HB2 | 0.82 | 0.72 |
| 1:b:444:GLU:HG3 | 1:b:544:PRO:HG3 | 1.70 | 0.72 |
| 3:C:3285[B]:VAL:HG22 | 3:C:3286[B]:THR:N | 2.04 | 0.72 |
| 3:F:3155[B]:MET:O | 3:a:3153[B]:LYS:HB3 | 1.90 | 0.72 |
| 3:I:2982[B]:MET:HE3 | 3:R:2967[B]:CYS:SG | 2.27 | 0.72 |
| 3:I:3156[B]:MET:CB | 3:R:2982[B]:MET:CG | 2.57 | 0.72 |
| 3:I:3293[A]:LYS:HD2 | 3:I:3293[A]:LYS:C | 2.15 | 0.72 |
| 3:I:3293[B]:LYS:HD2 | 3:I:3293[B]:LYS:C | 2.15 | 0.72 |
| 3:L:2968[B]:GLN:CB | 3:L:2972[B]:GLY:HA2 | 2.19 | 0.72 |
| 3:L:2969[B]:TYR:O | 3:L:2972[B]:GLY:N | 2.20 | 0.72 |
| 3:L:3133[B]:LEU:O | 3:L:3134[B]:GLN:C | 2.32 | 0.72 |
| 3:O:2963[B]:MET:HB2 | 3:X:2970[B]:PRO:CD | 2.19 | 0.72 |
| 3:O:3158[B]:PHE:O | 3:X:3148[B]:ILE:HG23 | 1.86 | 0.72 |
| 3:U:2968[A]:GLN:CB | 3:U:2972[A]:GLY:HA2 | 2.18 | 0.72 |
| 3:U:2969[A]:TYR:O | 3:U:2972[A]:GLY:N | 2.20 | 0.72 |
| 3:U:3171[B]:HIS:CA | 3:d:3152[B]:LYS:NZ | 2.52 | 0.72 |
| 3:X:3217[A]:PHE:HE1 | 3:X:3230[A]:PHE:HZ | 0.81 | 0.72 |
| 3:a:2979[A]:GLN:HE21 | 3:a:3155[A]:MET:HE2 | 1.54 | 0.72 |
| 3:a:3141[B]:TYR:HD2 | 3:a:3142[B]:ASN:H | 0.78 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3134[B]:GLN:HG3 | 3:d:3139[B]:LEU:HB2 | 1.70 | 0.72 |
| 1:A:1153:LYS:HB2 | 1:A:1155:LEU:HD23 | 1.72 | 0.72 |
| 1:A:1639:LYS:HB2 | 1:b:472:ASP:HB3 | 1.71 | 0.72 |
| 3:C:2935[B]:ILE:HD13 | 3:C:2936[B]:GLU:N | 2.05 | 0.72 |
| 3:C:2969[B]:TYR:CD2 | 3:L:3089[B]:HIS:NE2 | 2.58 | 0.72 |
| 3:C:3089[A]:HIS:NE2 | 9:L:3401[A]:CUO:CU1 | 1.54 | 0.72 |
| 3:C:3168[B]:THR:C | 3:L:3149[B]:ASN:O | 2.25 | 0.72 |
| 3:F:2977[B]:CYS:SG | 3:a:2978[B]:CYS:O | 2.48 | 0.72 |
| 3:F:3025[B]:VAL:HG22 | 3:F:3047[B]:ARG:NH1 | 2.01 | 0.72 |
| 1:G:589:GLN:HG2 | 1:G:594:ASP:HB3 | 1.71 | 0.72 |
| 3:I:2969[A]:TYR:O | 3:I:2972[A]:GLY:N | 2.21 | 0.72 |
| 3:I:3108[B]:HIS:CE1 | 3:R:3251[B]:ASP:CG | 2.67 | 0.72 |
| 3:I:3149[B]:ASN:HD22 | 3:R:3163[B]:ASN:CB | 1.97 | 0.72 |
| 3:I:3150[B]:LYS:CA | 3:R:3159[B]:SER:CA | 2.61 | 0.72 |
| 3:I:3275[A]:LEU:HD12 | 3:I:3275[A]:LEU:N | 2.04 | 0.72 |
| 1:J:417:MET:HG2 | 1:J:419:THR:HG23 | 1.71 | 0.72 |
| 1:J:836:GLN:HG3 | 1:J:838:ARG:HH21 | 1.53 | 0.72 |
| 3:O:2968[A]:GLN:CB | 3:O:2972[A]:GLY:HA2 | 2.18 | 0.72 |
| 3:O:3153[B]:LYS:HD3 | 3:X:3176[B]:LYS:HD3 | 0.92 | 0.72 |
| 3:O:3196[A]:THR:H | 3:O:3199[A]:GLN:CB | 2.02 | 0.72 |
| 3:R:2949[B]:LYS:O | 3:R:2953[B]:GLY:N | 2.22 | 0.72 |
| 2:T:2900:SER:HA | 1:V:1075:GLU:HG2 | 1.72 | 0.72 |
| 3:U:2968[B]:GLN:CB | 3:U:2972[B]:GLY:HA2 | 2.19 | 0.72 |
| 3:U:3293[A]:LYS:HD2 | 3:U:3293[A]:LYS:C | 2.15 | 0.72 |
| 2:Z:2900:SER:HA | 1:b:1075:GLU:HG2 | 1.71 | 0.72 |
| 3:a:2935[A]:ILE:HD13 | 3:a:2936[A]:GLU:N | 2.05 | 0.72 |
| 2:c:2149:ALA:HA | 2:c:2260:GLU:HG2 | 1.71 | 0.72 |
| 2:B:2851:ASN:ND2 | 1:D:1189:ASP:HB2 | 2.04 | 0.72 |
| 3:C:3134[B]:GLN:HG3 | 3:C:3139[B]:LEU:HB2 | 1.70 | 0.72 |
| 3:C:3169[B]:LYS:O | 3:L:3152[B]:LYS:CE | 2.37 | 0.72 |
| 3:F:2966[B]:SER:HA | 3:a:3256[B]:TRP:CG | 2.17 | 0.72 |
| 3:F:3283[A]:ILE:HD13 | 3:F:3283[A]:ILE:C | 2.15 | 0.72 |
| 3:I:2961[A]:HIS:HD2 | 3:I:2988[A]:TRP:CZ3 | 2.08 | 0.72 |
| 3:I:3285[B]:VAL:HG22 | 3:I:3286[B]:THR:N | 2.04 | 0.72 |
| 3:I:3307[B]:PHE:CE1 | 3:I:3309[B]:PRO:HG3 | 2.16 | 0.72 |
| 3:L:2956[A]:LYS:C | 3:L:2960[A]:PHE:CE1 | 2.47 | 0.72 |
| 3:L:2963[B]:MET:HG2 | 3:L:3108[B]:HIS:CG | 2.23 | 0.72 |
| 3:L:3134[B]:GLN:HG3 | 3:L:3139[B]:LEU:HB2 | 1.70 | 0.72 |
| 3:L:3228[A]:VAL:HG22 | 3:L:3245[A]:PHE:O | 1.90 | 0.72 |
| 3:L:3283[B]:ILE:HD13 | 3:L:3283[B]:ILE:C | 2.15 | 0.72 |
| 3:L:3293[B]:LYS:HD2 | 3:L:3293[B]:LYS:C | 2.15 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:965:ASP:OD2 | 1:M:968:GLY:N | 2.22 | 0.72 |
| 3:O:2949[A]:LYS:O | 3:O:2953[A]:GLY:N | 2.22 | 0.72 |
| 3:O:2969[B]:TYR:HB2 | 3:X:3158[B]:PHE:CE2 | 2.25 | 0.72 |
| 3:O:3157[B]:PRO:O | 3:X:3152[B]:LYS:HG3 | 1.89 | 0.72 |
| 3:O:3283[A]:ILE:C | 3:O:3283[A]:ILE:HD13 | 2.15 | 0.72 |
| 1:P:456:GLN:NE2 | 1:P:549:PRO:O | 2.21 | 0.72 |
| 3:R:2937[B]:ASN:CB | 3:R:3006[B]:LYS:HE2 | 2.14 | 0.72 |
| 3:R:3293[A]:LYS:HB2 | 3:R:3294[A]:SER:HB2 | 0.82 | 0.72 |
| 3:U:2969[B]:TYR:O | 3:U:2972[B]:GLY:N | 2.20 | 0.72 |
| 3:U:3024[A]:LEU:CD1 | 3:U:3025[A]:VAL:H | 1.84 | 0.72 |
| 3:U:3256[B]:TRP:CD2 | 3:d:2969[B]:TYR:CG | 2.76 | 0.72 |
| 3:d:3283[A]:ILE:HD13 | 3:d:3283[A]:ILE:C | 2.15 | 0.72 |
| 3:C:2948[B]:ASP:N | 3:C:2949[B]:LYS:CA | 2.41 | 0.72 |
| 3:F:2935[B]:ILE:HD13 | 3:F:2936[B]:GLU:N | 2.05 | 0.72 |
| 3:F:3173[B]:THR:OG1 | 3:a:3173[B]:THR:CG2 | 2.38 | 0.72 |
| 1:G:1485:ALA:HB3 | 1:G:1489:MET:HE2 | 1.72 | 0.72 |
| 3:I:3283[B]:ILE:C | 3:I:3283[B]:ILE:HD13 | 2.15 | 0.72 |
| 3:I:3284[B]:LYS:CD | 3:I:3285[B]:VAL:N | 2.47 | 0.72 |
| 3:O:2949[B]:LYS:O | 3:O:2953[B]:GLY:N | 2.22 | 0.72 |
| 3:O:2977[B]:CYS:CA | 3:X:3154[B]:PRO:O | 2.38 | 0.72 |
| 3:O:2988[A]:TRP:CE3 | 3:O:2989[A]:HIS:ND1 | 2.53 | 0.72 |
| 3:R:2965[A]:LEU:HD21 | 3:R:2974[A]:ALA:HB1 | 1.69 | 0.72 |
| 3:R:2979[A]:GLN:HE21 | 3:R:3155[A]:MET:HE2 | 1.54 | 0.72 |
| 3:R:3093[B]:HIS:HE1 | 3:R:3119[B]:HIS:CD2 | 2.06 | 0.72 |
| 3:R:3212[B]:ARG:HG3 | 3:R:3212[B]:ARG:NH1 | 2.00 | 0.72 |
| 1:S:1618:LEU:CD2 | 3:X:3136[B]:TYR:CE2 | 2.72 | 0.72 |
| 3:U:3134[A]:GLN:HG3 | 3:U:3139[A]:LEU:HB2 | 1.70 | 0.72 |
| 3:U:3149[B]:ASN:O | 3:d:3155[B]:MET:N | 2.22 | 0.72 |
| 3:U:3156[B]:MET:SD | 3:d:2982[B]:MET:CB | 2.77 | 0.72 |
| 3:U:3162[B]:ASP:N | 3:d:3260[B]:ARG:HH11 | 1.84 | 0.72 |
| 1:V:1520:GLN:HE21 | 1:V:1526:LYS:HG3 | 1.55 | 0.72 |
| 3:X:2949[A]:LYS:O | 3:X:2953[A]:GLY:N | 2.22 | 0.72 |
| 3:X:2988[A]:TRP:CE3 | 3:X:2989[A]:HIS:ND1 | 2.53 | 0.72 |
| 3:X:3196[A]:THR:H | 3:X:3199[A]:GLN:CB | 2.03 | 0.72 |
| 2:Z:2743:ALA:HB1 | 1:b:1210:LYS:HG2 | 1.72 | 0.72 |
| 2:Z:2867:PRO:HD2 | 3:a:2932[A]:PRO:HB2 | 1.71 | 0.72 |
| 3:a:2937[B]:ASN:HB2 | 3:a:3006[B]:LYS:CE | 2.14 | 0.72 |
| 3:a:3196[A]:THR:H | 3:a:3199[A]:GLN:CB | 2.02 | 0.72 |
| 3:a:3285[A]:VAL:HG22 | 3:a:3286[A]:THR:N | 2.04 | 0.72 |
| 3:d:2961[B]:HIS:HD2 | 3:d:2988[B]:TRP:CZ3 | 2.08 | 0.72 |
| 3:d:3133[B]:LEU:O | 3:d:3134[B]:GLN:C | 2.32 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3293[B]:LYS:HD2 | 3:d:3293[B]:LYS:C | 2.15 | 0.72 |
| 1:A:830:ASN:HA | 1:A:831:VAL:HB | 1.71 | 0.72 |
| 3:C:3134[A]:GLN:HG3 | 3:C:3139[A]:LEU:HB2 | 1.70 | 0.72 |
| 3:C:3275[A]:LEU:HD12 | 3:C:3275[A]:LEU:N | 2.04 | 0.72 |
| 3:C:3275[B]:LEU:HD12 | 3:C:3275[B]:LEU:N | 2.04 | 0.72 |
| 3:F:2961[B]:HIS:HD2 | 3:F:2988[B]:TRP:CZ3 | 2.08 | 0.72 |
| 3:F:3228[A]:VAL:HG22 | 3:F:3245[A]:PHE:O | 1.90 | 0.72 |
| 3:F:3275[A]:LEU:HD12 | 3:F:3275[A]:LEU:N | 2.04 | 0.72 |
| 3:I:2969[B]:TYR:O | 3:I:2972[B]:GLY:N | 2.21 | 0.72 |
| 3:I:3160[B]:SER:CB | 3:R:2983[B]:VAL:N | 2.40 | 0.72 |
| 3:I:3196[B]:THR:H | 3:I:3199[B]:GLN:CB | 2.02 | 0.72 |
| 3:L:2979[B]:GLN:HE21 | 3:L:3155[B]:MET:HE2 | 1.54 | 0.72 |
| 3:O:2968[B]:GLN:HE22 | 3:X:2985[B]:PHE:CA | 1.94 | 0.72 |
| 3:O:3133[B]:LEU:O | 3:O:3134[B]:GLN:C | 2.32 | 0.72 |
| 3:O:3228[A]:VAL:HG22 | 3:O:3245[A]:PHE:O | 1.90 | 0.72 |
| 3:O:3306[A]:LEU:HD12 | 3:O:3306[A]:LEU:C | 2.15 | 0.72 |
| 1:S:157:GLU:OE2 | 1:S:296:ARG:NH2 | 2.22 | 0.72 |
| 1:S:1019:HIS:NE2 | 1:S:1046:HIS:CE1 | 2.57 | 0.72 |
| 3:U:2965[B]:LEU:HD11 | 3:U:2974[B]:ALA:HA | 1.57 | 0.72 |
| 3:U:3228[A]:VAL:HG22 | 3:U:3245[A]:PHE:O | 1.90 | 0.72 |
| 3:X:3089[A]:HIS:NE2 | 9:X:3401[A]:CUO:CU1 | 1.54 | 0.72 |
| 3:d:3285[A]:VAL:HG22 | 3:d:3286[A]:THR:N | 2.04 | 0.72 |
| 3:C:3090[B]:ASN:CB | 3:L:2972[B]:GLY:C | 2.63 | 0.72 |
| 3:C:3120[A]:HIS:O | 3:C:3121[A]:SER:C | 2.29 | 0.72 |
| 3:F:2980[B]:HIS:CA | 3:a:2968[B]:GLN:HG2 | 2.19 | 0.72 |
| 3:F:3172[B]:SER:HB3 | 3:a:3150[B]:LYS:HA | 1.72 | 0.72 |
| 3:F:3307[B]:PHE:CE1 | 3:F:3309[B]:PRO:HG3 | 2.16 | 0.72 |
| 2:H:2727:HIS:HB2 | 2:H:2788:ILE:HD11 | 1.70 | 0.72 |
| 3:I:2933[B]:SER:O | 3:I:2936[B]:GLU:N | 2.23 | 0.72 |
| 3:I:2965[A]:LEU:HG | 3:I:2974[A]:ALA:CB | 2.20 | 0.72 |
| 3:I:2979[A]:GLN:HE21 | 3:I:3155[A]:MET:HE2 | 1.54 | 0.72 |
| 3:I:2982[B]:MET:HE2 | 3:R:2967[B]:CYS:SG | 2.30 | 0.72 |
| 3:I:3160[B]:SER:C | 3:R:3150[B]:LYS:HD2 | 2.13 | 0.72 |
| 3:L:2935[B]:ILE:HD13 | 3:L:2936[B]:GLU:N | 2.04 | 0.72 |
| 3:L:2965[A]:LEU:HD21 | 3:L:2974[A]:ALA:HB1 | 1.70 | 0.72 |
| 3:L:3228[B]:VAL:HG22 | 3:L:3245[B]:PHE:O | 1.90 | 0.72 |
| 1:M:804:ASP:OD1 | 1:M:805:VAL:N | 2.23 | 0.72 |
| 3:O:2933[B]:SER:O | 3:O:2936[B]:GLU:N | 2.23 | 0.72 |
| 3:O:3255[B]:PRO:CD | 3:X:3158[B]:PHE:O | 2.37 | 0.72 |
| 3:O:3285[A]:VAL:HG22 | 3:O:3286[A]:THR:N | 2.04 | 0.72 |
| 1:P:926:LEU:HD11 | 1:P:1043:MET:HB3 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q:2340:ALA:HB1 | 2:Q:2341:PRO:HD2 | 1.72 | 0.72 |
| 3:R:2961[B]:HIS:HD2 | 3:R:2988[B]:TRP:CZ3 | 2.08 | 0.72 |
| 3:R:3025[A]:VAL:HG22 | 3:R:3047[A]:ARG:NH1 | 2.02 | 0.72 |
| 3:U:3137[A]:ARG:HB3 | 3:U:3139[A]:LEU:HD23 | 1.69 | 0.72 |
| 3:U:3155[B]:MET:H | 3:d:3150[B]:LYS:CA | 1.93 | 0.72 |
| 3:U:3285[A]:VAL:HG22 | 3:U:3286[A]:THR:N | 2.04 | 0.72 |
| 3:U:3306[A]:LEU:HD12 | 3:U:3306[A]:LEU:C | 2.15 | 0.72 |
| 1:V:121:ASN:HD21 | 1:V:124:TYR:HB2 | 1.54 | 0.72 |
| 3:X:3306[B]:LEU:HD12 | 3:X:3306[B]:LEU:C | 2.15 | 0.72 |
| 3:a:2948[A]:ASP:H | 3:a:2949[A]:LYS:CA | 1.98 | 0.72 |
| 3:a:2968[B]:GLN:CB | 3:a:2972[B]:GLY:HA2 | 2.19 | 0.72 |
| 3:a:2969[A]:TYR:O | 3:a:2972[A]:GLY:N | 2.20 | 0.72 |
| 3:a:3306[A]:LEU:HD12 | 3:a:3306[A]:LEU:C | 2.15 | 0.72 |
| 3:a:3307[B]:PHE:CE1 | 3:a:3309[B]:PRO:HG3 | 2.16 | 0.72 |
| 1:b:1394:GLN:HG2 | 1:b:1395:PRO:HD2 | 1.72 | 0.72 |
| 3:d:2933[B]:SER:O | 3:d:2936[B]:GLU:N | 2.23 | 0.72 |
| 3:d:2952[B]:ALA:CB | 3:d:2953[B]:GLY:C | 2.48 | 0.72 |
| 3:d:3306[B]:LEU:HD12 | 3:d:3306[B]:LEU:C | 2.15 | 0.72 |
| 2:B:2547:MET:HB3 | 2:B:2558:CYS:HB2 | 1.72 | 0.71 |
| 3:C:2933[B]:SER:O | 3:C:2936[B]:GLU:N | 2.23 | 0.71 |
| 3:C:2949[B]:LYS:O | 3:C:2953[B]:GLY:N | 2.22 | 0.71 |
| 3:C:2974[B]:ALA:HB1 | 3:L:3253[B]:GLU:OE1 | 1.89 | 0.71 |
| 3:C:3283[A]:ILE:C | 3:C:3283[A]:ILE:HD13 | 2.15 | 0.71 |
| 3:C:3293[A]:LYS:HB2 | 3:C:3294[A]:SER:HB2 | 0.82 | 0.71 |
| 3:C:3293[A]:LYS:HD2 | 3:C:3293[A]:LYS:C | 2.15 | 0.71 |
| 3:C:3293[B]:LYS:HD2 | 3:C:3293[B]:LYS:C | 2.15 | 0.71 |
| 3:F:2930[A]:LEU:H | 3:F:2930[A]:LEU:CD2 | 1.98 | 0.71 |
| 3:F:2935[A]:ILE:HD13 | 3:F:2936[A]:GLU:N | 2.05 | 0.71 |
| 3:F:3133[B]:LEU:O | 3:F:3134[B]:GLN:C | 2.32 | 0.71 |
| 3:F:3173[B]:THR:HA | 3:a:3154[B]:PRO:N | 2.04 | 0.71 |
| 3:F:3293[B]:LYS:HD2 | 3:F:3293[B]:LYS:C | 2.15 | 0.71 |
| 1:G:965:ASP:OD1 | 1:G:965:ASP:N | 2.22 | 0.71 |
| 3:I:2949[B]:LYS:O | 3:I:2953[B]:GLY:N | 2.22 | 0.71 |
| 3:I:3152[B]:LYS:HB2 | 3:R:3171[B]:HIS:C | 2.09 | 0.71 |
| 3:I:3160[B]:SER:HA | 3:R:2983[B]:VAL:CB | 2.19 | 0.71 |
| 3:I:3306[B]:LEU:HD12 | 3:I:3306[B]:LEU:C | 2.15 | 0.71 |
| 1:J:1296:VAL:HB | 1:J:1446:ASP:HB3 | 1.72 | 0.71 |
| 3:L:3283[A]:ILE:C | 3:L:3283[A]:ILE:HD13 | 2.15 | 0.71 |
| 1:M:17:ASN:HD21 | 1:M:86:THR:H | 1.37 | 0.71 |
| 3:O:2969[A]:TYR:HD2 | 3:O:2971[A]:ASP:N | 1.84 | 0.71 |
| 3:O:2971[B]:ASP:OD1 | 3:X:3158[B]:PHE:CZ | 2.42 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2949[A]:LYS:O | 3:R:2953[A]:GLY:N | 2.22 | 0.71 |
| 3:R:2968[A]:GLN:CB | 3:R:2972[A]:GLY:HA2 | 2.19 | 0.71 |
| 3:U:2933[B]:SER:O | 3:U:2936[B]:GLU:N | 2.23 | 0.71 |
| 3:U:2935[B]:ILE:HD13 | 3:U:2936[B]:GLU:N | 2.05 | 0.71 |
| 3:U:2965[B]:LEU:HG | 3:U:2974[B]:ALA:CB | 2.20 | 0.71 |
| 3:U:2969[B]:TYR:CZ | 3:d:2980[B]:HIS:CE1 | 2.77 | 0.71 |
| 3:U:2975[B]:PHE:CE2 | 3:d:3256[B]:TRP:HD1 | 2.08 | 0.71 |
| 3:U:3161[B]:GLU:C | 3:d:3260[B]:ARG:NH1 | 2.48 | 0.71 |
| 3:U:3220[A]:ARG:HG3 | 3:U:3220[A]:ARG:NH1 | 1.98 | 0.71 |
| 3:X:3228[B]:VAL:HG22 | 3:X:3245[B]:PHE:O | 1.90 | 0.71 |
| 2:Z:2344:LEU:HB3 | 2:c:2515:ARG:HB3 | 1.72 | 0.71 |
| 3:a:2968[A]:GLN:CB | 3:a:2972[A]:GLY:HA2 | 2.18 | 0.71 |
| 3:a:3137[B]:ARG:HB3 | 3:a:3139[B]:LEU:HD23 | 1.69 | 0.71 |
| 3:a:3293[B]:LYS:HD2 | 3:a:3293[B]:LYS:C | 2.15 | 0.71 |
| 1:b:979:LEU:HB2 | 1:b:980:TYR:HB3 | 1.71 | 0.71 |
| 3:d:2961[A]:HIS:HD2 | 3:d:2988[A]:TRP:CZ3 | 2.08 | 0.71 |
| 3:d:3025[B]:VAL:HG22 | 3:d:3047[B]:ARG:NH1 | 2.02 | 0.71 |
| 3:d:3133[A]:LEU:O | 3:d:3134[A]:GLN:C | 2.32 | 0.71 |
| 3:d:3285[B]:VAL:HG22 | 3:d:3286[B]:THR:N | 2.04 | 0.71 |
| 3:d:3306[A]:LEU:HD12 | 3:d:3306[A]:LEU:C | 2.15 | 0.71 |
| 3:F:2952[A]:ALA:HA | 3:F:2956[A]:LYS:HB2 | 1.69 | 0.71 |
| 3:F:2961[A]:HIS:HD2 | 3:F:2988[A]:TRP:CZ3 | 2.08 | 0.71 |
| 3:F:2965[B]:LEU:HG | 3:F:2974[B]:ALA:CB | 2.21 | 0.71 |
| 3:F:3155[B]:MET:HG3 | 3:a:3153[B]:LYS:HG2 | 1.71 | 0.71 |
| 3:F:3285[A]:VAL:HG22 | 3:F:3286[A]:THR:N | 2.04 | 0.71 |
| 2:H:2541:GLY:O | 2:H:2545:SER:OG | 2.07 | 0.71 |
| 3:I:2935[B]:ILE:HD13 | 3:I:2936[B]:GLU:N | 2.05 | 0.71 |
| 3:I:2965[B]:LEU:HD21 | 3:I:2974[B]:ALA:HB1 | 1.69 | 0.71 |
| 3:I:2979[B]:GLN:HE21 | 3:I:3155[B]:MET:HE2 | 1.54 | 0.71 |
| 3:I:3159[B]:SER:C | 3:R:3150[B]:LYS:HD2 | 2.14 | 0.71 |
| 3:I:3196[A]:THR:HB | 1:J:416:ASN:HD21 | 1.53 | 0.71 |
| 3:L:3226[B]:ALA:HB1 | 3:L:3288[B]:MET:O | 1.91 | 0.71 |
| 3:O:2961[B]:HIS:HD2 | 3:O:2988[B]:TRP:CZ3 | 2.08 | 0.71 |
| 3:O:2965[B]:LEU:HD21 | 3:O:2974[B]:ALA:HB1 | 1.69 | 0.71 |
| 3:O:3251[B]:ASP:OD2 | 3:X:2968[B]:GLN:OE1 | 2.08 | 0.71 |
| 3:R:3169[A]:LYS:C | 3:R:3172[A]:SER:HG | 1.98 | 0.71 |
| 3:R:3283[B]:ILE:C | 3:R:3283[B]:ILE:HD13 | 2.15 | 0.71 |
| 3:R:3285[B]:VAL:HG22 | 3:R:3286[B]:THR:N | 2.04 | 0.71 |
| 3:R:3293[A]:LYS:HD2 | 3:R:3293[A]:LYS:C | 2.15 | 0.71 |
| 3:R:3293[B]:LYS:HD2 | 3:R:3293[B]:LYS:C | 2.15 | 0.71 |
| 3:U:2961[B]:HIS:HD2 | 3:U:2988[B]:TRP:CZ3 | 2.08 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3275[B]:LEU:HD12 | 3:a:3275[B]:LEU:N | 2.04 | 0.71 |
| 1:b:110:PHE:N | 1:b:119:LYS:O | 2.23 | 0.71 |
| 1:b:401:VAL:HG22 | 1:b:662:SER:HB3 | 1.72 | 0.71 |
| 3:d:2949[B]:LYS:O | 3:d:2953[B]:GLY:N | 2.22 | 0.71 |
| 3:d:3226[B]:ALA:HB1 | 3:d:3288[B]:MET:O | 1.90 | 0.71 |
| 3:C:2933[A]:SER:O | 3:C:2936[A]:GLU:N | 2.23 | 0.71 |
| 3:C:2935[A]:ILE:HD13 | 3:C:2936[A]:GLU:N | 2.05 | 0.71 |
| 3:C:2961[A]:HIS:HD2 | 3:C:2988[A]:TRP:CZ3 | 2.08 | 0.71 |
| 3:C:2969[A]:TYR:O | 3:C:2972[A]:GLY:N | 2.20 | 0.71 |
| 3:C:3133[B]:LEU:O | 3:C:3134[B]:GLN:C | 2.32 | 0.71 |
| 3:C:3160[B]:SER:HG | 3:L:2983[B]:VAL:CG2 | 2.04 | 0.71 |
| 3:C:3228[A]:VAL:HG22 | 3:C:3245[A]:PHE:O | 1.90 | 0.71 |
| 3:C:3306[B]:LEU:HD12 | 3:C:3306[B]:LEU:C | 2.15 | 0.71 |
| 3:F:2949[B]:LYS:O | 3:F:2953[B]:GLY:N | 2.22 | 0.71 |
| 3:F:2975[B]:PHE:CD1 | 3:a:3107[B]:LEU:CD2 | 2.72 | 0.71 |
| 3:F:3090[B]:ASN:HB3 | 3:a:2972[B]:GLY:HA3 | 1.72 | 0.71 |
| 3:I:2933[A]:SER:O | 3:I:2936[A]:GLU:N | 2.23 | 0.71 |
| 3:I:3275[B]:LEU:HD12 | 3:I:3275[B]:LEU:N | 2.04 | 0.71 |
| 3:I:3306[A]:LEU:HD12 | 3:I:3306[A]:LEU:C | 2.15 | 0.71 |
| 1:J:163:LEU:HD21 | 1:J:219:LEU:HD13 | 1.72 | 0.71 |
| 3:L:2933[A]:SER:O | 3:L:2936[A]:GLU:N | 2.23 | 0.71 |
| 3:L:2949[A]:LYS:O | 3:L:2953[A]:GLY:N | 2.22 | 0.71 |
| 3:L:2952[A]:ALA:HA | 3:L:2956[A]:LYS:HB2 | 1.69 | 0.71 |
| 3:L:2961[B]:HIS:HD2 | 3:L:2988[B]:TRP:CZ3 | 2.08 | 0.71 |
| 3:L:3120[A]:HIS:O | 3:L:3121[A]:SER:C | 2.29 | 0.71 |
| 1:M:1618:LEU:O | 3:R:3198[B]:PRO:HD3 | 1.90 | 0.71 |
| 3:O:2968[B]:GLN:CA | 3:X:2979[B]:GLN:HG2 | 2.19 | 0.71 |
| 3:O:3226[A]:ALA:HB1 | 3:O:3288[A]:MET:O | 1.91 | 0.71 |
| 3:O:3293[A]:LYS:HD2 | 3:O:3293[A]:LYS:C | 2.15 | 0.71 |
| 3:O:3307[B]:PHE:CE1 | 3:O:3309[B]:PRO:HG3 | 2.16 | 0.71 |
| 1:P:428:ILE:HD12 | 1:P:514:TRP:HB3 | 1.72 | 0.71 |
| 3:R:2933[A]:SER:O | 3:R:2936[A]:GLU:N | 2.23 | 0.71 |
| 3:R:3226[B]:ALA:HB1 | 3:R:3288[B]:MET:O | 1.90 | 0.71 |
| 3:R:3228[B]:VAL:HG22 | 3:R:3245[B]:PHE:O | 1.90 | 0.71 |
| 3:R:3283[A]:ILE:C | 3:R:3283[A]:ILE:HD13 | 2.15 | 0.71 |
| 3:R:3285[A]:VAL:HG22 | 3:R:3286[A]:THR:N | 2.04 | 0.71 |
| 3:U:2961[A]:HIS:HD2 | 3:U:2988[A]:TRP:CZ3 | 2.08 | 0.71 |
| 3:U:3089[B]:HIS:NE2 | 9:U:3401[B]:CUO:CU1 | 1.54 | 0.71 |
| 3:U:3196[A]:THR:H | 3:U:3199[A]:GLN:CB | 2.02 | 0.71 |
| 3:U:3256[B]:TRP:N | 3:d:2974[B]:ALA:O | 2.24 | 0.71 |
| 3:U:3275[B]:LEU:HD12 | 3:U:3275[B]:LEU:N | 2.04 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:1655:SER:C | 3:d:3006[B]:LYS:NZ | 2.48 | 0.71 |
| 3:a:3133[B]:LEU:O | 3:a:3134[B]:GLN:C | 2.32 | 0.71 |
| 3:a:3283[B]:ILE:C | 3:a:3283[B]:ILE:HD13 | 2.15 | 0.71 |
| 3:d:3196[A]:THR:H | 3:d:3199[A]:GLN:CB | 2.02 | 0.71 |
| 1:A:806:ASN:ND2 | 4:f:1:NAG:O7 | 2.23 | 0.71 |
| 2:B:2598:PRO:HG3 | 2:B:2651:GLN:HB3 | 1.71 | 0.71 |
| 3:C:2965[B]:LEU:HG | 3:C:2974[B]:ALA:CB | 2.21 | 0.71 |
| 3:C:3226[B]:ALA:HB1 | 3:C:3288[B]:MET:O | 1.91 | 0.71 |
| 3:F:3089[A]:HIS:NE2 | 9:a:3401[A]:CUO:CU1 | 1.54 | 0.71 |
| 3:F:3283[B]:ILE:C | 3:F:3283[B]:ILE:HD13 | 2.15 | 0.71 |
| 3:F:3306[A]:LEU:HD12 | 3:F:3306[A]:LEU:C | 2.15 | 0.71 |
| 3:F:3306[B]:LEU:HD12 | 3:F:3306[B]:LEU:C | 2.15 | 0.71 |
| 3:I:2961[B]:HIS:CE1 | 3:R:2975[B]:PHE:CE1 | 2.78 | 0.71 |
| 3:L:2933[B]:SER:O | 3:L:2936[B]:GLU:N | 2.23 | 0.71 |
| 3:L:3226[A]:ALA:HB1 | 3:L:3288[A]:MET:O | 1.91 | 0.71 |
| 3:L:3285[A]:VAL:HG22 | 3:L:3286[A]:THR:N | 2.04 | 0.71 |
| 2:N:2090:LYS:NZ | 2:N:2099:GLU:OE2 | 2.23 | 0.71 |
| 3:O:2933[A]:SER:O | 3:O:2936[A]:GLU:N | 2.23 | 0.71 |
| 3:O:3163[B]:ASN:CB | 3:X:3149[B]:ASN:HB3 | 2.20 | 0.71 |
| 3:O:3275[A]:LEU:HD12 | 3:O:3275[A]:LEU:N | 2.04 | 0.71 |
| 3:R:3161[B]:GLU:OE2 | 3:R:3161[B]:GLU:N | 1.88 | 0.71 |
| 1:S:164:GLU:OE2 | 1:S:301:ARG:NH2 | 2.22 | 0.71 |
| 3:U:2935[A]:ILE:HD13 | 3:U:2936[A]:GLU:N | 2.05 | 0.71 |
| 3:U:3285[B]:VAL:HG22 | 3:U:3286[B]:THR:N | 2.04 | 0.71 |
| 3:X:3196[B]:THR:H | 3:X:3199[B]:GLN:CB | 2.02 | 0.71 |
| 3:X:3228[A]:VAL:HG22 | 3:X:3245[A]:PHE:O | 1.90 | 0.71 |
| 3:X:3285[B]:VAL:HG22 | 3:X:3286[B]:THR:N | 2.04 | 0.71 |
| 3:X:3293[B]:LYS:HD2 | 3:X:3293[B]:LYS:C | 2.15 | 0.71 |
| 1:Y:2:LEU:HD21 | 1:Y:81:VAL:HG21 | 1.72 | 0.71 |
| 1:Y:1421:VAL:HG23 | 1:Y:1422:HIS:HD1 | 1.55 | 0.71 |
| 3:a:3133[A]:LEU:O | 3:a:3134[A]:GLN:C | 2.32 | 0.71 |
| 3:a:3283[A]:ILE:HD13 | 3:a:3283[A]:ILE:C | 2.15 | 0.71 |
| 1:b:884:PRO:HG2 | 1:b:888:ALA:HB2 | 1.73 | 0.71 |
| 3:C:3163[B]:ASN:HB3 | 3:L:3149[B]:ASN:HD21 | 1.56 | 0.71 |
| 3:F:2965[A]:LEU:HG | 3:F:2974[A]:ALA:CB | 2.20 | 0.71 |
| 3:F:2979[B]:GLN:HE21 | 3:F:3155[B]:MET:HE2 | 1.55 | 0.71 |
| 3:F:3025[A]:VAL:HG22 | 3:F:3047[A]:ARG:NH1 | 2.01 | 0.71 |
| 3:F:3133[A]:LEU:O | 3:F:3134[A]:GLN:C | 2.32 | 0.71 |
| 3:I:2937[B]:ASN:CB | 3:I:3006[B]:LYS:HE2 | 2.14 | 0.71 |
| 3:I:2952[B]:ALA:HA | 3:I:2956[B]:LYS:HB2 | 1.70 | 0.71 |
| 3:I:2964[B]:PRO:HB2 | 3:R:3221[B]:ALA:HB3 | 1.71 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2982[A]:MET:HE1 | 3:I:3254[A]:MET:HE2 | 1.73 | 0.71 |
| 3:I:3089[A]:HIS:NE2 | 9:R:3401[A]:CUO:CU1 | 1.54 | 0.71 |
| 3:I:3107[B]:LEU:CD2 | 3:R:2975[B]:PHE:HA | 2.21 | 0.71 |
| 3:I:3212[B]:ARG:HG3 | 3:I:3212[B]:ARG:NH1 | 2.00 | 0.71 |
| 3:L:3275[B]:LEU:HD12 | 3:L:3275[B]:LEU:N | 2.04 | 0.71 |
| 3:O:3041[B]:ALA:HB2 | 3:X:2971[B]:ASP:OD2 | 1.89 | 0.71 |
| 3:O:3163[B]:ASN:CA | 3:X:3149[B]:ASN:CB | 2.66 | 0.71 |
| 1:P:1636:ASN:HB3 | 1:P:1638:SER:O | 1.91 | 0.71 |
| 3:R:2965[A]:LEU:HG | 3:R:2974[A]:ALA:CB | 2.21 | 0.71 |
| 3:R:3147[B]:GLU:HB2 | 3:R:3149[B]:ASN:OD1 | 1.86 | 0.71 |
| 3:U:3133[A]:LEU:O | 3:U:3134[A]:GLN:C | 2.32 | 0.71 |
| 3:U:3228[B]:VAL:HG22 | 3:U:3245[B]:PHE:O | 1.90 | 0.71 |
| 3:U:3252[B]:TYR:C | 3:d:3255[B]:PRO:HG3 | 2.15 | 0.71 |
| 3:X:2933[B]:SER:O | 3:X:2936[B]:GLU:N | 2.23 | 0.71 |
| 3:X:2982[A]:MET:HE1 | 3:X:3254[A]:MET:HE2 | 1.73 | 0.71 |
| 3:X:3275[A]:LEU:HD12 | 3:X:3275[A]:LEU:N | 2.04 | 0.71 |
| 3:a:2952[A]:ALA:CB | 3:a:2953[A]:GLY:C | 2.48 | 0.71 |
| 3:a:2965[A]:LEU:HG | 3:a:2974[A]:ALA:CB | 2.21 | 0.71 |
| 3:a:2969[B]:TYR:O | 3:a:2972[B]:GLY:N | 2.20 | 0.71 |
| 2:B:2373:MET:HE3 | 2:B:2374:ASN:HB2 | 1.73 | 0.71 |
| 3:C:2968[B]:GLN:O | 3:L:2985[B]:PHE:CE2 | 2.44 | 0.71 |
| 3:C:3025[B]:VAL:HG22 | 3:C:3047[B]:ARG:NH1 | 2.01 | 0.71 |
| 3:C:3226[A]:ALA:HB1 | 3:C:3288[A]:MET:O | 1.91 | 0.71 |
| 3:C:3252[B]:TYR:CB | 3:L:3253[B]:GLU:CB | 2.68 | 0.71 |
| 3:C:3283[B]:ILE:HD13 | 3:C:3283[B]:ILE:C | 2.15 | 0.71 |
| 3:C:3306[A]:LEU:HD12 | 3:C:3306[A]:LEU:C | 2.15 | 0.71 |
| 3:F:2933[A]:SER:O | 3:F:2936[A]:GLU:N | 2.23 | 0.71 |
| 3:I:2935[A]:ILE:HD13 | 3:I:2936[A]:GLU:N | 2.05 | 0.71 |
| 3:I:2949[A]:LYS:O | 3:I:2953[A]:GLY:N | 2.22 | 0.71 |
| 3:I:3172[B]:SER:HB3 | 3:R:3150[B]:LYS:CA | 2.21 | 0.71 |
| 1:J:1140:ASN:ND2 | 1:J:1236:TYR:OH | 2.22 | 0.71 |
| 3:L:2930[A]:LEU:HD22 | 3:L:2930[A]:LEU:N | 2.02 | 0.71 |
| 3:L:3306[A]:LEU:HD12 | 3:L:3306[A]:LEU:C | 2.15 | 0.71 |
| 1:M:975:PRO:HG2 | 1:M:1024:GLY:HA3 | 1.73 | 0.71 |
| 3:O:3108[B]:HIS:CB | 3:X:2970[B]:PRO:HA | 2.20 | 0.71 |
| 3:O:3228[B]:VAL:HG22 | 3:O:3245[B]:PHE:O | 1.90 | 0.71 |
| 3:U:2965[A]:LEU:HG | 3:U:2974[A]:ALA:CB | 2.20 | 0.71 |
| 3:U:3169[B]:LYS:HE2 | 3:d:3146[B]:CYS:CB | 2.20 | 0.71 |
| 3:U:3293[B]:LYS:HD2 | 3:U:3293[B]:LYS:C | 2.15 | 0.71 |
| 3:X:2961[A]:HIS:HD2 | 3:X:2988[A]:TRP:CZ3 | 2.08 | 0.71 |
| 3:X:3283[B]:ILE:HD13 | 3:X:3283[B]:ILE:C | 2.15 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:1284:GLU:HG3 | 1:Y:1337:ARG:HH12 | 1.55 | 0.71 |
| 3:a:2949[A]:LYS:O | 3:a:2953[A]:GLY:N | 2.22 | 0.71 |
| 3:a:2961[A]:HIS:HD2 | 3:a:2988[A]:TRP:CZ3 | 2.08 | 0.71 |
| 1:b:972:SER:HA | 1:b:1028:VAL:HG22 | 1.70 | 0.71 |
| 3:d:3196[B]:THR:H | 3:d:3199[B]:GLN:CB | 2.02 | 0.71 |
| 3:d:3228[B]:VAL:HG22 | 3:d:3245[B]:PHE:O | 1.90 | 0.71 |
| 3:d:3283[B]:ILE:C | 3:d:3283[B]:ILE:HD13 | 2.15 | 0.71 |
| 3:C:2969[B]:TYR:HD2 | 3:L:3089[B]:HIS:NE2 | 1.87 | 0.71 |
| 3:F:3153[B]:LYS:NZ | 3:a:3157[B]:PRO:N | 2.31 | 0.71 |
| 3:F:3293[B]:LYS:HB2 | 3:F:3294[B]:SER:HB2 | 0.82 | 0.71 |
| 2:H:2180:TRP:HB2 | 2:H:2243:LEU:HD13 | 1.73 | 0.71 |
| 3:I:3226[A]:ALA:HB1 | 3:I:3288[A]:MET:O | 1.91 | 0.71 |
| 3:I:3228[A]:VAL:HG22 | 3:I:3245[A]:PHE:O | 1.90 | 0.71 |
| 3:I:3255[B]:PRO:HB2 | 3:R:2959[B]:SER:C | 2.13 | 0.71 |
| 3:O:3158[B]:PHE:H | 3:X:3152[B]:LYS:CB | 1.92 | 0.71 |
| 3:O:3160[B]:SER:OG | 3:X:3151[B]:LEU:HG | 1.89 | 0.71 |
| 3:R:3228[A]:VAL:HG22 | 3:R:3245[A]:PHE:O | 1.90 | 0.71 |
| 2:T:2133:PRO:HG2 | 2:T:2140:ARG:HA | 1.71 | 0.71 |
| 3:U:2970[B]:PRO:CA | 3:d:3086[B]:GLU:CG | 2.68 | 0.71 |
| 3:U:3283[A]:ILE:HD13 | 3:U:3283[A]:ILE:C | 2.15 | 0.71 |
| 3:X:3306[A]:LEU:HD12 | 3:X:3306[A]:LEU:C | 2.15 | 0.71 |
| 3:a:3120[A]:HIS:O | 3:a:3121[A]:SER:C | 2.29 | 0.71 |
| 3:a:3228[A]:VAL:HG22 | 3:a:3245[A]:PHE:O | 1.90 | 0.71 |
| 3:d:2935[B]:ILE:HD13 | 3:d:2936[B]:GLU:N | 2.05 | 0.71 |
| 3:d:2982[B]:MET:HE1 | 3:d:3254[B]:MET:HE2 | 1.73 | 0.71 |
| 3:C:3156[B]:MET:HE3 | 3:L:2979[B]:GLN:CG | 2.04 | 0.71 |
| 3:F:2933[B]:SER:O | 3:F:2936[B]:GLU:N | 2.23 | 0.71 |
| 3:F:3255[B]:PRO:CG | 3:a:2964[B]:PRO:N | 2.54 | 0.71 |
| 3:I:2960[B]:PHE:C | 3:R:3255[B]:PRO:HD2 | 2.16 | 0.71 |
| 3:I:2962[B]:GLY:O | 3:R:3255[B]:PRO:CD | 2.38 | 0.71 |
| 3:I:3228[B]:VAL:HG22 | 3:I:3245[B]:PHE:O | 1.90 | 0.71 |
| 3:I:3283[A]:ILE:HD13 | 3:I:3283[A]:ILE:C | 2.15 | 0.71 |
| 1:J:1152:LYS:NZ | 1:J:1180:SER:O | 2.21 | 0.71 |
| 3:L:2965[B]:LEU:HG | 3:L:2974[B]:ALA:CB | 2.20 | 0.71 |
| 3:O:2969[B]:TYR:HD2 | 3:O:2971[B]:ASP:N | 1.84 | 0.71 |
| 3:O:3275[B]:LEU:HD12 | 3:O:3275[B]:LEU:N | 2.04 | 0.71 |
| 3:O:3283[B]:ILE:HD13 | 3:O:3283[B]:ILE:C | 2.15 | 0.71 |
| 3:O:3306[B]:LEU:HD12 | 3:O:3306[B]:LEU:C | 2.15 | 0.71 |
| 1:P:975:PRO:HG2 | 1:P:1024:GLY:HA3 | 1.72 | 0.71 |
| 3:R:2935[A]:ILE:HD13 | 3:R:2936[A]:GLU:N | 2.05 | 0.71 |
| 1:S:1170:MET:HB3 | 1:S:1203:MET:HE2 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2970[B]:PRO:CA | 3:d:2980[B]:HIS:HB3 | 2.08 | 0.71 |
| 3:U:3283[B]:ILE:C | 3:U:3283[B]:ILE:HD13 | 2.15 | 0.71 |
| 3:X:2965[A]:LEU:HG | 3:X:2974[A]:ALA:CB | 2.20 | 0.71 |
| 3:X:3089[B]:HIS:NE2 | 9:X:3401[B]:CUO:CU1 | 1.54 | 0.71 |
| 3:a:2933[B]:SER:O | 3:a:2936[B]:GLU:N | 2.23 | 0.71 |
| 3:a:3306[B]:LEU:HD12 | 3:a:3306[B]:LEU:C | 2.15 | 0.71 |
| 2:B:2671:ASP:OD1 | 2:B:2850:ARG:NH1 | 2.23 | 0.71 |
| 3:C:2961[B]:HIS:HD2 | 3:C:2988[B]:TRP:CZ3 | 2.08 | 0.71 |
| 3:C:2964[B]:PRO:O | 3:L:3256[B]:TRP:N | 2.24 | 0.71 |
| 3:C:2969[B]:TYR:CA | 3:L:2989[B]:HIS:NE2 | 2.52 | 0.71 |
| 3:C:2979[B]:GLN:NE2 | 3:L:2979[B]:GLN:HE22 | 1.82 | 0.71 |
| 3:C:3228[B]:VAL:HG22 | 3:C:3245[B]:PHE:O | 1.90 | 0.71 |
| 3:C:3252[B]:TYR:HB2 | 3:L:3253[B]:GLU:CG | 2.20 | 0.71 |
| 2:E:2806:ALA:HB2 | 2:E:2856:ILE:HD11 | 1.73 | 0.71 |
| 3:F:2952[A]:ALA:CB | 3:F:2953[A]:GLY:C | 2.48 | 0.71 |
| 3:F:2968[A]:GLN:CB | 3:F:2972[A]:GLY:HA2 | 2.19 | 0.71 |
| 3:F:3160[B]:SER:OG | 3:a:2983[B]:VAL:N | 2.24 | 0.71 |
| 3:F:3248[B]:LEU:HB2 | 3:a:2972[B]:GLY:O | 1.88 | 0.71 |
| 3:L:3024[B]:LEU:CD1 | 3:L:3025[B]:VAL:H | 1.83 | 0.71 |
| 3:O:2935[A]:ILE:HD13 | 3:O:2936[A]:GLU:N | 2.05 | 0.71 |
| 3:O:2935[B]:ILE:HD13 | 3:O:2936[B]:GLU:N | 2.04 | 0.71 |
| 3:O:2969[B]:TYR:HE1 | 3:X:3168[B]:THR:HG22 | 1.55 | 0.71 |
| 3:O:3169[B]:LYS:C | 3:O:3172[B]:SER:HG | 1.98 | 0.71 |
| 3:R:3226[A]:ALA:HB1 | 3:R:3288[A]:MET:O | 1.91 | 0.71 |
| 3:X:2933[A]:SER:O | 3:X:2936[A]:GLU:N | 2.23 | 0.71 |
| 1:Y:439:LEU:HD23 | 1:Y:509:ILE:HD12 | 1.71 | 0.71 |
| 1:Y:1470:GLU:HG3 | 1:Y:1530:LEU:HD12 | 1.73 | 0.71 |
| 3:a:2933[A]:SER:O | 3:a:2936[A]:GLU:N | 2.23 | 0.71 |
| 1:b:127:GLU:N | 1:b:127:GLU:OE1 | 2.23 | 0.71 |
| 3:d:2933[A]:SER:O | 3:d:2936[A]:GLU:N | 2.23 | 0.71 |
| 3:d:2935[A]:ILE:HD13 | 3:d:2936[A]:GLU:N | 2.05 | 0.71 |
| 3:F:2973[B]:THR:HG21 | 3:a:3106[B]:THR:C | 2.15 | 0.71 |
| 3:F:3154[B]:PRO:HB3 | 3:a:3174[B]:GLY:HA3 | 1.72 | 0.71 |
| 3:F:3154[B]:PRO:CB | 3:a:3174[B]:GLY:N | 2.50 | 0.71 |
| 3:F:3226[B]:ALA:HB1 | 3:F:3288[B]:MET:O | 1.91 | 0.71 |
| 1:J:622:HIS:CE1 | 1:J:767:LYS:H | 2.09 | 0.71 |
| 3:L:2937[B]:ASN:CB | 3:L:3006[B]:LYS:HE2 | 2.14 | 0.71 |
| 3:L:2982[A]:MET:HE1 | 3:L:3254[A]:MET:HE2 | 1.73 | 0.71 |
| 3:O:3133[A]:LEU:O | 3:O:3134[A]:GLN:C | 2.32 | 0.71 |
| 3:R:2969[A]:TYR:O | 3:R:2972[A]:GLY:N | 2.20 | 0.71 |
| 3:R:2982[A]:MET:HE1 | 3:R:3254[A]:MET:HE2 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3066[B]:TYR:CD1 | 3:R:3193[B]:HIS:CE1 | 2.79 | 0.71 |
| 3:R:3306[A]:LEU:HD12 | 3:R:3306[A]:LEU:C | 2.15 | 0.71 |
| 3:R:3307[A]:PHE:CE1 | 3:R:3309[A]:PRO:HG3 | 2.16 | 0.71 |
| 3:X:2968[A]:GLN:CB | 3:X:2972[A]:GLY:HA2 | 2.18 | 0.71 |
| 3:X:3226[A]:ALA:HB1 | 3:X:3288[A]:MET:O | 1.90 | 0.71 |
| 3:X:3226[B]:ALA:HB1 | 3:X:3288[B]:MET:O | 1.90 | 0.71 |
| 2:Z:2867:PRO:CD | 3:a:2932[A]:PRO:CG | 2.69 | 0.71 |
| 3:a:2961[B]:HIS:HD2 | 3:a:2988[B]:TRP:CZ3 | 2.08 | 0.71 |
| 3:a:3066[B]:TYR:CD1 | 3:a:3193[B]:HIS:CE1 | 2.79 | 0.71 |
| 3:C:2974[B]:ALA:O | 3:L:3107[B]:LEU:CD1 | 2.33 | 0.70 |
| 1:D:1258:ARG:NH2 | 1:D:1332:ASP:OD1 | 2.23 | 0.70 |
| 3:F:2971[B]:ASP:C | 3:a:3248[B]:LEU:HD22 | 2.15 | 0.70 |
| 3:F:3162[B]:ASP:HA | 3:a:3259[B]:ASP:HB3 | 1.73 | 0.70 |
| 3:F:3293[A]:LYS:HD2 | 3:F:3293[A]:LYS:C | 2.15 | 0.70 |
| 3:I:3066[A]:TYR:CD1 | 3:I:3193[A]:HIS:CE1 | 2.79 | 0.70 |
| 3:I:3150[B]:LYS:HD2 | 3:R:3160[B]:SER:C | 2.16 | 0.70 |
| 3:I:3162[B]:ASP:CB | 3:R:3259[B]:ASP:N | 2.49 | 0.70 |
| 3:I:3166[B]:GLU:O | 3:R:3149[B]:ASN:HA | 1.90 | 0.70 |
| 3:I:3179[A]:ASP:OD1 | 3:I:3181[A]:GLN:HB2 | 1.91 | 0.70 |
| 3:I:3196[A]:THR:H | 3:I:3199[A]:GLN:CB | 2.02 | 0.70 |
| 3:I:3252[B]:TYR:CE2 | 3:R:3250[B]:GLY:HA2 | 2.26 | 0.70 |
| 3:L:3066[B]:TYR:CD1 | 3:L:3193[B]:HIS:CE1 | 2.79 | 0.70 |
| 3:R:2930[A]:LEU:HD22 | 3:R:2930[A]:LEU:N | 2.02 | 0.70 |
| 3:R:2961[A]:HIS:HD2 | 3:R:2988[A]:TRP:CZ3 | 2.08 | 0.70 |
| 3:U:3066[A]:TYR:CD1 | 3:U:3193[A]:HIS:CE1 | 2.79 | 0.70 |
| 3:U:3089[A]:HIS:NE2 | 9:U:3401[A]:CUO:CU1 | 1.54 | 0.70 |
| 3:U:3149[B]:ASN:O | 3:d:3154[B]:PRO:C | 2.33 | 0.70 |
| 3:U:3153[B]:LYS:HG3 | 3:d:2979[B]:GLN:HE21 | 1.54 | 0.70 |
| 3:U:3194[B]:GLY:C | 3:U:3195[B]:MET:HG2 | 2.16 | 0.70 |
| 3:U:3226[A]:ALA:HB1 | 3:U:3288[A]:MET:O | 1.91 | 0.70 |
| 1:V:1137:LYS:HG2 | 1:V:1240:ILE:HG13 | 1.73 | 0.70 |
| 3:X:2965[B]:LEU:HG | 3:X:2974[B]:ALA:CB | 2.21 | 0.70 |
| 3:X:2979[A]:GLN:HE21 | 3:X:3155[A]:MET:HE2 | 1.54 | 0.70 |
| 3:X:3133[B]:LEU:O | 3:X:3134[B]:GLN:C | 2.32 | 0.70 |
| 3:X:3179[B]:ASP:OD1 | 3:X:3181[B]:GLN:HB2 | 1.91 | 0.70 |
| 3:X:3221[B]:ALA:HB2 | 3:X:3256[B]:TRP:H | 1.56 | 0.70 |
| 3:X:3293[A]:LYS:HD2 | 3:X:3293[A]:LYS:C | 2.15 | 0.70 |
| 3:a:2979[B]:GLN:HE21 | 3:a:3155[B]:MET:HE2 | 1.55 | 0.70 |
| 3:a:3194[B]:GLY:C | 3:a:3195[B]:MET:HG2 | 2.16 | 0.70 |
| 3:d:2965[A]:LEU:HG | 3:d:2974[A]:ALA:CB | 2.21 | 0.70 |
| 1:A:1242:ASN:ND2 | 1:A:1245:GLU:OE2 | 2.23 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2982[A]:MET:HE1 | 3:C:3254[A]:MET:HE2 | 1.73 | 0.70 |
| 3:C:3066[B]:TYR:CD1 | 3:C:3193[B]:HIS:CE1 | 2.79 | 0.70 |
| 3:C:3156[B]:MET:CE | 3:L:2979[B]:GLN:CB | 2.15 | 0.70 |
| 3:C:3287[B]:ILE:O | 3:C:3287[B]:ILE:HD13 | 1.92 | 0.70 |
| 1:D:401:VAL:HG22 | 1:D:662:SER:HB3 | 1.73 | 0.70 |
| 3:F:2982[B]:MET:HE1 | 3:F:3254[B]:MET:HE2 | 1.72 | 0.70 |
| 3:F:3287[B]:ILE:O | 3:F:3287[B]:ILE:HD13 | 1.91 | 0.70 |
| 2:K:2556:TYR:HD1 | 2:K:2557:ALA:H | 1.39 | 0.70 |
| 3:L:2935[A]:ILE:HD13 | 3:L:2936[A]:GLU:N | 2.05 | 0.70 |
| 3:L:3293[A]:LYS:HD2 | 3:L:3293[A]:LYS:C | 2.15 | 0.70 |
| 3:O:2961[A]:HIS:HD2 | 3:O:2988[A]:TRP:CZ3 | 2.08 | 0.70 |
| 3:O:3221[B]:ALA:HB2 | 3:O:3256[B]:TRP:H | 1.56 | 0.70 |
| 3:O:3293[B]:LYS:HD2 | 3:O:3293[B]:LYS:C | 2.15 | 0.70 |
| 2:Q:2598:PRO:HD3 | 2:Q:2651:GLN:HB2 | 1.73 | 0.70 |
| 3:R:2933[B]:SER:O | 3:R:2936[B]:GLU:N | 2.23 | 0.70 |
| 3:U:2952[A]:ALA:H | 3:U:2953[A]:GLY:CA | 2.04 | 0.70 |
| 3:U:3066[B]:TYR:CD1 | 3:U:3193[B]:HIS:CE1 | 2.79 | 0.70 |
| 3:U:3120[B]:HIS:O | 3:U:3121[B]:SER:C | 2.29 | 0.70 |
| 3:U:3221[B]:ALA:HB2 | 3:U:3256[B]:TRP:H | 1.57 | 0.70 |
| 3:X:3066[A]:TYR:CD1 | 3:X:3193[A]:HIS:CE1 | 2.79 | 0.70 |
| 1:Y:1442:MET:HE1 | 1:Y:1454:PHE:HA | 1.74 | 0.70 |
| 3:a:3221[B]:ALA:HB2 | 3:a:3256[B]:TRP:H | 1.56 | 0.70 |
| 3:a:3293[A]:LYS:HB2 | 3:a:3294[A]:SER:HB2 | 0.82 | 0.70 |
| 3:d:2969[B]:TYR:HB3 | 3:d:2971[B]:ASP:OD1 | 1.82 | 0.70 |
| 3:d:3194[B]:GLY:C | 3:d:3195[B]:MET:HG2 | 2.16 | 0.70 |
| 3:d:3275[A]:LEU:HD12 | 3:d:3275[A]:LEU:N | 2.04 | 0.70 |
| 3:d:3293[A]:LYS:HD2 | 3:d:3293[A]:LYS:C | 2.15 | 0.70 |
| 3:C:2965[A]:LEU:HG | 3:C:2974[A]:ALA:CB | 2.21 | 0.70 |
| 3:F:2982[A]:MET:HE1 | 3:F:3254[A]:MET:HE2 | 1.73 | 0.70 |
| 3:F:3285[B]:VAL:HG22 | 3:F:3286[B]:THR:N | 2.04 | 0.70 |
| 3:I:2948[A]:ASP:CB | 3:I:2949[A]:LYS:HA | 2.16 | 0.70 |
| 3:I:3153[B]:LYS:HG2 | 3:R:3155[B]:MET:HB2 | 1.67 | 0.70 |
| 3:I:3254[B]:MET:CG | 3:R:2966[B]:SER:CB | 2.55 | 0.70 |
| 3:I:3287[A]:ILE:O | 3:I:3287[A]:ILE:HD13 | 1.92 | 0.70 |
| 1:M:456:GLN:HG2 | 1:M:551:GLU:HB2 | 1.72 | 0.70 |
| 3:O:2952[A]:ALA:H | 3:O:2953[A]:GLY:CA | 2.04 | 0.70 |
| 3:O:2982[A]:MET:HE1 | 3:O:3254[A]:MET:HE2 | 1.73 | 0.70 |
| 3:O:3194[B]:GLY:C | 3:O:3195[B]:MET:HG2 | 2.16 | 0.70 |
| 2:Q:2890:VAL:N | 2:Q:2891:LEU:HA | 2.07 | 0.70 |
| 3:R:2930[B]:LEU:HD22 | 3:R:2930[B]:LEU:N | 2.02 | 0.70 |
| 3:R:2965[B]:LEU:HG | 3:R:2974[B]:ALA:CB | 2.20 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3221[A]:ALA:HB2 | 3:R:3256[A]:TRP:H | 1.57 | 0.70 |
| 3:U:2965[B]:LEU:HD11 | 3:d:3221[B]:ALA:H | 0.62 | 0.70 |
| 3:U:2982[A]:MET:HE1 | 3:U:3254[A]:MET:HE2 | 1.72 | 0.70 |
| 3:U:3179[A]:ASP:OD1 | 3:U:3181[A]:GLN:HB2 | 1.91 | 0.70 |
| 3:X:2935[A]:ILE:HD13 | 3:X:2936[A]:GLU:N | 2.05 | 0.70 |
| 3:X:3025[A]:VAL:HG22 | 3:X:3047[A]:ARG:NH1 | 2.01 | 0.70 |
| 3:X:3283[A]:ILE:HD13 | 3:X:3283[A]:ILE:C | 2.15 | 0.70 |
| 3:a:2935[B]:ILE:HD13 | 3:a:2936[B]:GLU:N | 2.05 | 0.70 |
| 3:a:3221[A]:ALA:HB2 | 3:a:3256[A]:TRP:H | 1.56 | 0.70 |
| 3:a:3228[B]:VAL:HG22 | 3:a:3245[B]:PHE:O | 1.90 | 0.70 |
| 3:d:2982[A]:MET:HE1 | 3:d:3254[A]:MET:HE2 | 1.73 | 0.70 |
| 3:C:2948[A]:ASP:CB | 3:C:2949[A]:LYS:HA | 2.15 | 0.70 |
| 3:C:3154[B]:PRO:CD | 3:L:3173[B]:THR:C | 2.63 | 0.70 |
| 3:F:2959[B]:SER:CB | 3:a:3255[B]:PRO:CB | 2.66 | 0.70 |
| 3:F:2969[B]:TYR:O | 3:F:2972[B]:GLY:N | 2.21 | 0.70 |
| 3:F:2970[B]:PRO:CG | 3:a:2989[B]:HIS:CD2 | 2.74 | 0.70 |
| 3:F:2985[B]:PHE:CZ | 3:a:2970[B]:PRO:CA | 2.69 | 0.70 |
| 3:I:2937[A]:ASN:CB | 3:I:3006[A]:LYS:HE2 | 2.14 | 0.70 |
| 3:I:2982[B]:MET:HE1 | 3:I:3254[B]:MET:HE2 | 1.73 | 0.70 |
| 3:I:3066[B]:TYR:CD1 | 3:I:3193[B]:HIS:CE1 | 2.80 | 0.70 |
| 3:L:2965[A]:LEU:HG | 3:L:2974[A]:ALA:CB | 2.21 | 0.70 |
| 3:L:3306[B]:LEU:HD12 | 3:L:3306[B]:LEU:C | 2.15 | 0.70 |
| 3:O:2965[A]:LEU:HG | 3:O:2974[A]:ALA:CB | 2.21 | 0.70 |
| 3:O:2969[B]:TYR:HB2 | 3:X:3158[B]:PHE:CD2 | 2.26 | 0.70 |
| 3:O:3179[B]:ASP:OD1 | 3:O:3181[B]:GLN:HB2 | 1.92 | 0.70 |
| 3:O:3221[A]:ALA:HB2 | 3:O:3256[A]:TRP:H | 1.56 | 0.70 |
| 3:R:3173[B]:THR:CG2 | 3:R:3174[B]:GLY:N | 2.55 | 0.70 |
| 1:S:838:ARG:NH1 | 1:S:915:ASN:OD1 | 2.24 | 0.70 |
| 3:U:2933[A]:SER:O | 3:U:2936[A]:GLU:N | 2.23 | 0.70 |
| 3:U:3086[B]:GLU:CD | 3:d:2970[B]:PRO:HG2 | 2.16 | 0.70 |
| 3:U:3170[B]:ALA:C | 3:d:3148[B]:ILE:CG2 | 2.64 | 0.70 |
| 3:U:3306[B]:LEU:HD12 | 3:U:3306[B]:LEU:C | 2.15 | 0.70 |
| 3:X:2982[B]:MET:HE1 | 3:X:3254[B]:MET:HE2 | 1.73 | 0.70 |
| 3:d:2965[B]:LEU:HG | 3:d:2974[B]:ALA:CB | 2.20 | 0.70 |
| 3:d:3228[A]:VAL:HG22 | 3:d:3245[A]:PHE:O | 1.90 | 0.70 |
| 1:A:898:GLY:N | 1:A:899:MET:HA | 2.06 | 0.70 |
| 3:C:3179[A]:ASP:OD1 | 3:C:3181[A]:GLN:HB2 | 1.92 | 0.70 |
| 3:F:2960[B]:PHE:CA | 3:a:3255[B]:PRO:HD2 | 2.22 | 0.70 |
| 3:F:3066[A]:TYR:CD1 | 3:F:3193[A]:HIS:CE1 | 2.79 | 0.70 |
| 3:I:2961[B]:HIS:HD2 | 3:I:2988[B]:TRP:CZ3 | 2.08 | 0.70 |
| 3:I:2965[B]:LEU:HG | 3:I:2974[B]:ALA:CB | 2.20 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2969[B]:TYR:HD2 | 3:I:2971[B]:ASP:N | 1.84 | 0.70 |
| 3:I:2971[B]:ASP:O | 3:R:3090[B]:ASN:CA | 2.38 | 0.70 |
| 3:I:3194[A]:GLY:C | 3:I:3195[A]:MET:HG2 | 2.16 | 0.70 |
| 3:I:3221[B]:ALA:HB1 | 3:R:2965[B]:LEU:H | 0.87 | 0.70 |
| 3:L:3196[B]:THR:H | 3:L:3199[B]:GLN:CB | 2.02 | 0.70 |
| 1:M:871:GLN:NE2 | 1:M:964:ILE:O | 2.24 | 0.70 |
| 2:N:2130:PRO:HB2 | 2:N:2142:ALA:HB3 | 1.72 | 0.70 |
| 3:O:2975[B]:PHE:HD1 | 3:X:3156[B]:MET:C | 1.98 | 0.70 |
| 1:S:515:ASP:O | 1:S:518:LYS:NZ | 2.19 | 0.70 |
| 1:S:780:GLU:O | 1:S:782:THR:N | 2.24 | 0.70 |
| 3:U:3226[B]:ALA:HB1 | 3:U:3288[B]:MET:O | 1.90 | 0.70 |
| 3:X:2935[B]:ILE:HD13 | 3:X:2936[B]:GLU:N | 2.05 | 0.70 |
| 3:X:2948[B]:ASP:H | 3:X:2949[B]:LYS:CA | 1.98 | 0.70 |
| 3:X:3221[A]:ALA:HB2 | 3:X:3256[A]:TRP:H | 1.56 | 0.70 |
| 2:Z:2149:ALA:HA | 2:Z:2260:GLU:HG2 | 1.72 | 0.70 |
| 3:d:3194[A]:GLY:C | 3:d:3195[A]:MET:HG2 | 2.16 | 0.70 |
| 6:r:1:NAG:O3 | 6:r:2:NAG:C1 | 2.39 | 0.70 |
| 3:C:2968[A]:GLN:CB | 3:C:2972[A]:GLY:HA2 | 2.19 | 0.70 |
| 3:C:2979[B]:GLN:HE21 | 3:C:3155[B]:MET:HE2 | 1.55 | 0.70 |
| 3:C:3156[B]:MET:HB2 | 3:L:2982[B]:MET:HB3 | 1.59 | 0.70 |
| 3:C:3279[B]:ASP:OD1 | 3:C:3279[B]:ASP:N | 2.25 | 0.70 |
| 3:F:3066[B]:TYR:CD1 | 3:F:3193[B]:HIS:CE1 | 2.79 | 0.70 |
| 3:F:3155[B]:MET:O | 3:a:3153[B]:LYS:HE3 | 1.90 | 0.70 |
| 3:F:3179[B]:ASP:OD1 | 3:F:3181[B]:GLN:HB2 | 1.92 | 0.70 |
| 3:F:3228[B]:VAL:HG22 | 3:F:3245[B]:PHE:O | 1.90 | 0.70 |
| 3:F:3256[B]:TRP:NE1 | 3:a:2965[B]:LEU:HD13 | 2.07 | 0.70 |
| 3:F:3279[B]:ASP:OD1 | 3:F:3279[B]:ASP:N | 2.25 | 0.70 |
| 1:G:854:LEU:HD23 | 1:G:941:LEU:HD21 | 1.72 | 0.70 |
| 1:G:1442:MET:HE1 | 1:G:1454:PHE:HA | 1.72 | 0.70 |
| 3:I:2964[B]:PRO:CA | 3:R:3221[B]:ALA:CB | 2.69 | 0.70 |
| 3:I:3157[B]:PRO:HD3 | 3:R:2982[B]:MET:HE1 | 1.74 | 0.70 |
| 3:I:3173[A]:THR:CG2 | 3:I:3174[A]:GLY:N | 2.55 | 0.70 |
| 3:I:3255[B]:PRO:HG3 | 3:R:2963[B]:MET:C | 2.16 | 0.70 |
| 3:O:3252[B]:TYR:CB | 3:X:3156[B]:MET:SD | 2.79 | 0.70 |
| 2:Q:2564:PRO:HA | 2:Q:2673:GLU:HG3 | 1.73 | 0.70 |
| 3:R:3194[A]:GLY:C | 3:R:3195[A]:MET:HG2 | 2.16 | 0.70 |
| 3:U:2974[B]:ALA:HB1 | 3:d:3220[B]:ARG:CD | 2.20 | 0.70 |
| 3:U:3152[B]:LYS:HD2 | 3:d:3173[B]:THR:OG1 | 1.90 | 0.70 |
| 3:U:3179[B]:ASP:OD1 | 3:U:3181[B]:GLN:HB2 | 1.92 | 0.70 |
| 3:U:3194[A]:GLY:C | 3:U:3195[A]:MET:HG2 | 2.16 | 0.70 |
| 1:V:855:ARG:HH21 | 1:V:941:LEU:HA | 1.55 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3066[B]:TYR:CD1 | 3:X:3193[B]:HIS:CE1 | 2.79 | 0.70 |
| 3:X:3279[B]:ASP:OD1 | 3:X:3279[B]:ASP:N | 2.25 | 0.70 |
| 3:X:3284[A]:LYS:HA | 3:X:3284[A]:LYS:CE | 2.22 | 0.70 |
| 1:Y:848:VAL:O | 1:Y:852:ASN:ND2 | 2.24 | 0.70 |
| 1:Y:999:LEU:O | 1:Y:1063:ARG:NH2 | 2.24 | 0.70 |
| 2:Z:2225:ARG:HD2 | 2:Z:2274:LEU:HD22 | 1.74 | 0.70 |
| 1:b:2:LEU:HD21 | 1:b:81:VAL:HG21 | 1.72 | 0.70 |
| 3:d:3066[B]:TYR:CD1 | 3:d:3193[B]:HIS:CE1 | 2.79 | 0.70 |
| 3:C:2965[B]:LEU:CD1 | 3:C:2974[B]:ALA:HA | 2.22 | 0.70 |
| 3:C:3169[A]:LYS:C | 3:C:3172[A]:SER:HG | 1.99 | 0.70 |
| 3:F:2962[B]:GLY:O | 3:a:3255[B]:PRO:HD3 | 1.90 | 0.70 |
| 3:F:2963[B]:MET:HE1 | 3:a:3223[B]:GLY:HA3 | 1.73 | 0.70 |
| 1:G:911:LEU:O | 1:G:915:ASN:ND2 | 2.24 | 0.70 |
| 2:H:2605:LEU:O | 2:H:2622:ASN:ND2 | 2.25 | 0.70 |
| 3:I:3226[B]:ALA:HB1 | 3:I:3288[B]:MET:O | 1.91 | 0.70 |
| 1:J:262:LYS:NZ | 1:J:795:GLU:OE1 | 2.25 | 0.70 |
| 1:J:1170:MET:HB3 | 1:J:1203:MET:HE2 | 1.74 | 0.70 |
| 3:L:2933[A]:SER:C | 3:L:2935[A]:ILE:HD13 | 2.17 | 0.70 |
| 3:L:3113[A]:ASP:CG | 3:L:3114[A]:PRO:CD | 2.56 | 0.70 |
| 3:L:3221[A]:ALA:HB2 | 3:L:3256[A]:TRP:H | 1.56 | 0.70 |
| 3:O:3112[B]:TYR:CD2 | 3:X:2969[B]:TYR:OH | 2.45 | 0.70 |
| 3:R:2982[B]:MET:HE1 | 3:R:3254[B]:MET:HE2 | 1.73 | 0.70 |
| 3:R:3194[B]:GLY:C | 3:R:3195[B]:MET:HG2 | 2.16 | 0.70 |
| 3:R:3306[B]:LEU:HD12 | 3:R:3306[B]:LEU:C | 2.15 | 0.70 |
| 3:U:2937[A]:ASN:CB | 3:U:3006[A]:LYS:HE2 | 2.14 | 0.70 |
| 3:U:2969[B]:TYR:OH | 3:d:3107[B]:LEU:CD1 | 2.28 | 0.70 |
| 3:U:3173[A]:THR:CG2 | 3:U:3174[A]:GLY:N | 2.55 | 0.70 |
| 1:V:1033:LEU:HA | 1:V:1036:SER:HB3 | 1.74 | 0.70 |
| 3:X:2930[A]:LEU:H | 3:X:2930[A]:LEU:CD2 | 1.98 | 0.70 |
| 3:X:3194[B]:GLY:C | 3:X:3195[B]:MET:HG2 | 2.16 | 0.70 |
| 3:C:2933[A]:SER:C | 3:C:2935[A]:ILE:HD13 | 2.17 | 0.70 |
| 3:C:2952[B]:ALA:CB | 3:C:2953[B]:GLY:C | 2.48 | 0.70 |
| 3:C:3066[A]:TYR:CD1 | 3:C:3193[A]:HIS:CE1 | 2.79 | 0.70 |
| 3:F:2965[A]:LEU:CD1 | 3:F:2974[A]:ALA:HA | 2.22 | 0.70 |
| 3:F:2974[B]:ALA:HB1 | 3:a:3253[B]:GLU:CD | 2.12 | 0.70 |
| 3:F:3259[B]:ASP:HB3 | 3:a:3162[B]:ASP:HB3 | 0.78 | 0.70 |
| 3:F:3287[A]:ILE:O | 3:F:3287[A]:ILE:HD13 | 1.92 | 0.70 |
| 1:G:401:VAL:HG22 | 1:G:662:SER:HB3 | 1.74 | 0.70 |
| 1:G:619:SER:HB2 | 1:G:805:VAL:HG11 | 1.72 | 0.70 |
| 3:I:3255[B]:PRO:CG | 3:R:2962[B]:GLY:O | 2.38 | 0.70 |
| 1:J:757:VAL:HG21 | 1:J:781:ILE:HG22 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1215:LEU:HD13 | 1:J:1229:LYS:HE3 | 1.72 | 0.70 |
| 3:O:2937[A]:ASN:CB | 3:O:3006[A]:LYS:HE2 | 2.14 | 0.70 |
| 3:R:2933[A]:SER:C | 3:R:2935[A]:ILE:HD13 | 2.17 | 0.70 |
| 3:R:3196[A]:THR:H | 3:R:3199[A]:GLN:CB | 2.02 | 0.70 |
| 3:R:3221[B]:ALA:HB2 | 3:R:3256[B]:TRP:H | 1.56 | 0.70 |
| 3:R:3287[B]:ILE:O | 3:R:3287[B]:ILE:HD13 | 1.92 | 0.70 |
| 1:S:1000:GLU:HG2 | 1:S:1133:ILE:HG23 | 1.74 | 0.70 |
| 2:T:2826:GLU:HA | 2:T:2876:LYS:HE3 | 1.73 | 0.70 |
| 3:U:2933[B]:SER:C | 3:U:2935[B]:ILE:HD13 | 2.17 | 0.70 |
| 1:V:609:TRP:HZ3 | 1:V:761:ALA:HB2 | 1.56 | 0.70 |
| 1:V:1583:CYS:SG | 1:V:1584:GLY:N | 2.63 | 0.70 |
| 3:X:2933[A]:SER:C | 3:X:2935[A]:ILE:HD13 | 2.17 | 0.70 |
| 3:X:2961[B]:HIS:HD2 | 3:X:2988[B]:TRP:CZ3 | 2.08 | 0.70 |
| 3:a:3226[B]:ALA:HB1 | 3:a:3288[B]:MET:O | 1.91 | 0.70 |
| 2:B:2191:LEU:O | 2:B:2225:ARG:NH2 | 2.25 | 0.70 |
| 3:C:2965[A]:LEU:CD1 | 3:C:2974[A]:ALA:HA | 2.22 | 0.70 |
| 3:F:3090[B]:ASN:CA | 3:a:2971[B]:ASP:O | 2.39 | 0.70 |
| 3:F:3173[B]:THR:O | 3:a:3154[B]:PRO:CD | 2.24 | 0.70 |
| 3:I:3221[B]:ALA:HB2 | 3:I:3256[B]:TRP:H | 1.56 | 0.70 |
| 3:L:2930[B]:LEU:H | 3:L:2930[B]:LEU:CD2 | 1.98 | 0.70 |
| 3:L:2952[A]:ALA:H | 3:L:2953[A]:GLY:CA | 2.04 | 0.70 |
| 3:L:2965[A]:LEU:CD1 | 3:L:2974[A]:ALA:HA | 2.22 | 0.70 |
| 3:L:3025[B]:VAL:HG22 | 3:L:3047[B]:ARG:NH1 | 2.01 | 0.70 |
| 3:L:3133[A]:LEU:O | 3:L:3134[A]:GLN:C | 2.32 | 0.70 |
| 3:O:3066[B]:TYR:CD1 | 3:O:3193[B]:HIS:CE1 | 2.79 | 0.70 |
| 3:O:3196[B]:THR:H | 3:O:3199[B]:GLN:CB | 2.03 | 0.70 |
| 3:O:3226[B]:ALA:HB1 | 3:O:3288[B]:MET:O | 1.91 | 0.70 |
| 2:Q:2090:LYS:NZ | 2:Q:2099:GLU:OE2 | 2.25 | 0.70 |
| 1:S:456:GLN:HG2 | 1:S:551:GLU:HB3 | 1.74 | 0.70 |
| 3:U:2933[A]:SER:C | 3:U:2935[A]:ILE:HD13 | 2.17 | 0.70 |
| 3:U:3133[B]:LEU:O | 3:U:3134[B]:GLN:C | 2.32 | 0.70 |
| 3:U:3169[B]:LYS:CG | 3:d:3147[B]:GLU:CB | 2.70 | 0.70 |
| 3:U:3293[A]:LYS:HB2 | 3:U:3294[A]:SER:HB2 | 0.82 | 0.70 |
| 3:X:2952[A]:ALA:H | 3:X:2953[A]:GLY:CA | 2.04 | 0.70 |
| 3:X:3179[A]:ASP:OD1 | 3:X:3181[A]:GLN:HB2 | 1.92 | 0.70 |
| 3:a:2933[B]:SER:C | 3:a:2935[B]:ILE:HD13 | 2.17 | 0.70 |
| 3:a:2937[A]:ASN:CB | 3:a:3006[A]:LYS:HE2 | 2.14 | 0.70 |
| 3:a:2982[B]:MET:HE1 | 3:a:3254[B]:MET:HE2 | 1.73 | 0.70 |
| 3:a:3179[A]:ASP:OD1 | 3:a:3181[A]:GLN:HB2 | 1.92 | 0.70 |
| 3:a:3179[B]:ASP:OD1 | 3:a:3181[B]:GLN:HB2 | 1.92 | 0.70 |
| 3:a:3226[A]:ALA:HB1 | 3:a:3288[A]:MET:O | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3287[B]:ILE:O | 3:a:3287[B]:ILE:HD13 | 1.92 | 0.70 |
| 3:d:2979[B]:GLN:HE21 | 3:d:3155[B]:MET:HE2 | 1.55 | 0.70 |
| 3:d:3179[A]:ASP:OD1 | 3:d:3181[A]:GLN:HB2 | 1.92 | 0.70 |
| 4:n:1:NAG:O3 | 4:n:2:NAG:C7 | 2.40 | 0.70 |
| 3:C:2933[B]:SER:C | 3:C:2935[B]:ILE:HD13 | 2.17 | 0.70 |
| 3:C:2969[B]:TYR:O | 3:C:2972[B]:GLY:N | 2.20 | 0.70 |
| 3:C:3194[A]:GLY:C | 3:C:3195[A]:MET:HG2 | 2.16 | 0.70 |
| 1:D:724:LYS:HA | 1:D:728:ARG:HH11 | 1.57 | 0.70 |
| 3:F:3160[B]:SER:O | 3:a:3150[B]:LYS:CD | 2.40 | 0.70 |
| 3:F:3162[B]:ASP:CA | 3:a:3147[B]:GLU:OE1 | 2.36 | 0.70 |
| 3:I:2966[B]:SER:O | 3:R:3256[B]:TRP:CG | 2.44 | 0.70 |
| 3:I:3173[B]:THR:CG2 | 3:I:3174[B]:GLY:N | 2.55 | 0.70 |
| 3:L:2937[B]:ASN:HB2 | 3:L:3006[B]:LYS:CE | 2.14 | 0.70 |
| 3:L:2961[B]:HIS:HB3 | 3:L:3111[B]:SER:HG | 1.56 | 0.70 |
| 3:L:3173[B]:THR:CG2 | 3:L:3174[B]:GLY:N | 2.55 | 0.70 |
| 3:L:3179[B]:ASP:OD1 | 3:L:3181[B]:GLN:HB2 | 1.91 | 0.70 |
| 3:O:3169[B]:LYS:HE3 | 3:X:3148[B]:ILE:HA | 1.69 | 0.70 |
| 3:O:3169[B]:LYS:NZ | 3:X:3148[B]:ILE:H | 1.90 | 0.70 |
| 3:O:3254[B]:MET:CG | 3:X:3159[B]:SER:OG | 2.40 | 0.70 |
| 1:P:997:SER:O | 1:P:1001:GLN:NE2 | 2.24 | 0.70 |
| 1:S:1019:HIS:NE2 | 1:S:1046:HIS:HE1 | 1.90 | 0.70 |
| 2:T:2806:ALA:HB2 | 2:T:2856:ILE:HD11 | 1.74 | 0.70 |
| 3:U:3173[B]:THR:CG2 | 3:U:3174[B]:GLY:N | 2.55 | 0.70 |
| 3:U:3254[B]:MET:HB2 | 3:d:3254[B]:MET:CB | 2.22 | 0.70 |
| 3:U:3284[B]:LYS:HA | 3:U:3284[B]:LYS:CE | 2.22 | 0.70 |
| 3:U:3287[A]:ILE:O | 3:U:3287[A]:ILE:HD13 | 1.92 | 0.70 |
| 2:W:2166:LEU:HA | 2:W:2169:HIS:HB2 | 1.73 | 0.70 |
| 1:Y:1471:LEU:HD11 | 1:Y:1540:LEU:HD23 | 1.73 | 0.70 |
| 3:a:3196[A]:THR:HG21 | 1:b:416:ASN:CB | 2.20 | 0.70 |
| 3:C:3160[B]:SER:HA | 3:L:2983[B]:VAL:HB | 1.74 | 0.69 |
| 3:F:2964[B]:PRO:HB2 | 3:a:3255[B]:PRO:HB3 | 1.74 | 0.69 |
| 3:F:3090[B]:ASN:HB3 | 3:a:2971[B]:ASP:O | 1.92 | 0.69 |
| 3:F:3160[B]:SER:CA | 3:a:2983[B]:VAL:H | 2.05 | 0.69 |
| 3:F:3196[A]:THR:H | 3:F:3199[A]:GLN:CB | 2.02 | 0.69 |
| 3:I:2965[B]:LEU:CD1 | 3:I:2974[B]:ALA:HA | 2.22 | 0.69 |
| 3:L:2961[A]:HIS:HD2 | 3:L:2988[A]:TRP:CZ3 | 2.08 | 0.69 |
| 3:L:3287[B]:ILE:O | 3:L:3287[B]:ILE:HD13 | 1.92 | 0.69 |
| 3:O:2965[B]:LEU:HG | 3:O:2974[B]:ALA:CB | 2.21 | 0.69 |
| 3:O:2982[B]:MET:HE1 | 3:O:3254[B]:MET:HE2 | 1.72 | 0.69 |
| 3:O:3109[B]:TYR:CE2 | 3:X:2969[B]:TYR:O | 2.44 | 0.69 |
| 3:O:3120[A]:HIS:O | 3:O:3121[A]:SER:C | 2.29 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1582:ASN:HB3 | 1:S:1583:CYS:CB | 2.22 | 0.69 |
| 3:U:2980[B]:HIS:CB | 3:d:2969[B]:TYR:OH | 2.39 | 0.69 |
| 3:U:2982[B]:MET:HE1 | 3:U:3254[B]:MET:HE2 | 1.72 | 0.69 |
| 1:V:1390:ASP:HB3 | 1:Y:1372:ILE:HD11 | 1.74 | 0.69 |
| 3:X:2965[B]:LEU:CD1 | 3:X:2974[B]:ALA:HA | 2.22 | 0.69 |
| 3:X:3173[A]:THR:CG2 | 3:X:3174[A]:GLY:N | 2.55 | 0.69 |
| 1:Y:1576:THR:CG2 | 3:d:3196[B]:THR:HG21 | 2.22 | 0.69 |
| 3:a:3066[A]:TYR:CD1 | 3:a:3193[A]:HIS:CE1 | 2.79 | 0.69 |
| 3:d:2933[A]:SER:C | 3:d:2935[A]:ILE:HD13 | 2.17 | 0.69 |
| 2:B:2711:HIS:HA | 2:B:2714:VAL:HG22 | 1.74 | 0.69 |
| 3:C:3173[B]:THR:CG2 | 3:C:3174[B]:GLY:N | 2.55 | 0.69 |
| 3:C:3194[B]:GLY:C | 3:C:3195[B]:MET:HG2 | 2.16 | 0.69 |
| 3:I:3150[B]:LYS:HZ3 | 3:R:3160[B]:SER:CB | 2.04 | 0.69 |
| 3:I:3176[B]:LYS:HZ2 | 3:I:3176[B]:LYS:HB3 | 1.56 | 0.69 |
| 3:L:3179[A]:ASP:OD1 | 3:L:3181[A]:GLN:HB2 | 1.92 | 0.69 |
| 3:O:2965[B]:LEU:CD1 | 3:O:2974[B]:ALA:HA | 2.22 | 0.69 |
| 3:O:2965[B]:LEU:HD11 | 3:X:2979[B]:GLN:CD | 2.12 | 0.69 |
| 3:O:3066[A]:TYR:CD1 | 3:O:3193[A]:HIS:CE1 | 2.79 | 0.69 |
| 2:Q:2180:TRP:HB2 | 2:Q:2243:LEU:HD13 | 1.72 | 0.69 |
| 3:R:3173[A]:THR:CG2 | 3:R:3174[A]:GLY:N | 2.55 | 0.69 |
| 3:R:3230[A]:PHE:CB | 3:R:3243[A]:GLY:N | 2.56 | 0.69 |
| 3:U:3153[B]:LYS:CG | 3:d:3153[B]:LYS:HD2 | 2.22 | 0.69 |
| 1:V:337:ASP:OD1 | 1:V:337:ASP:N | 2.24 | 0.69 |
| 2:W:2890:VAL:N | 2:W:2891:LEU:HA | 2.06 | 0.69 |
| 3:X:3279[A]:ASP:OD1 | 3:X:3279[A]:ASP:N | 2.25 | 0.69 |
| 3:a:3176[B]:LYS:HZ2 | 3:a:3176[B]:LYS:HB3 | 1.58 | 0.69 |
| 3:a:3287[A]:ILE:O | 3:a:3287[A]:ILE:HD13 | 1.92 | 0.69 |
| 3:C:3147[B]:GLU:CG | 3:L:3160[B]:SER:C | 2.55 | 0.69 |
| 3:C:3169[B]:LYS:O | 3:L:3152[B]:LYS:HE3 | 1.91 | 0.69 |
| 3:F:3162[B]:ASP:CG | 3:a:3259[B]:ASP:H | 1.99 | 0.69 |
| 3:F:3174[B]:GLY:N | 3:a:3154[B]:PRO:HD3 | 2.01 | 0.69 |
| 3:F:3194[A]:GLY:C | 3:F:3195[A]:MET:HG2 | 2.16 | 0.69 |
| 3:F:3194[B]:GLY:C | 3:F:3195[B]:MET:HG2 | 2.16 | 0.69 |
| 3:F:3226[A]:ALA:HB1 | 3:F:3288[A]:MET:O | 1.91 | 0.69 |
| 3:F:3284[A]:LYS:HA | 3:F:3284[A]:LYS:CE | 2.22 | 0.69 |
| 1:G:1470:GLU:HG2 | 1:G:1537:ILE:HD12 | 1.73 | 0.69 |
| 3:I:3194[B]:GLY:C | 3:I:3195[B]:MET:HG2 | 2.16 | 0.69 |
| 3:I:3255[B]:PRO:CB | 3:R:2964[B]:PRO:HD2 | 2.22 | 0.69 |
| 1:M:984:ASP:OD1 | 1:M:985:PHE:N | 2.25 | 0.69 |
| 3:O:3173[A]:THR:CG2 | 3:O:3174[A]:GLY:N | 2.55 | 0.69 |
| 3:O:3220[A]:ARG:HG3 | 3:O:3220[A]:ARG:NH1 | 1.98 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3287[A]:ILE:O | 3:O:3287[A]:ILE:HD13 | 1.92 | 0.69 |
| 1:P:21:SER:HB2 | 1:P:83:HIS:O | 1.92 | 0.69 |
| 3:R:2933[B]:SER:C | 3:R:2935[B]:ILE:HD13 | 2.17 | 0.69 |
| 3:U:2980[B]:HIS:O | 3:d:2969[B]:TYR:CD1 | 2.26 | 0.69 |
| 3:U:3153[B]:LYS:CB | 3:d:3154[B]:PRO:O | 2.30 | 0.69 |
| 3:X:2933[B]:SER:C | 3:X:2935[B]:ILE:HD13 | 2.17 | 0.69 |
| 3:X:3287[B]:ILE:O | 3:X:3287[B]:ILE:HD13 | 1.92 | 0.69 |
| 3:a:2933[A]:SER:C | 3:a:2935[A]:ILE:HD13 | 2.17 | 0.69 |
| 3:a:2965[A]:LEU:CD1 | 3:a:2974[A]:ALA:HA | 2.22 | 0.69 |
| 3:a:2965[B]:LEU:CD1 | 3:a:2974[B]:ALA:HA | 2.22 | 0.69 |
| 1:A:678:ASN:O | 1:A:684:ARG:NH2 | 2.23 | 0.69 |
| 3:C:2930[B]:LEU:H | 3:C:2930[B]:LEU:CD2 | 1.98 | 0.69 |
| 3:C:3284[B]:LYS:HA | 3:C:3284[B]:LYS:CE | 2.22 | 0.69 |
| 3:F:2933[A]:SER:C | 3:F:2935[A]:ILE:HD13 | 2.17 | 0.69 |
| 3:F:2948[B]:ASP:H | 3:F:2949[B]:LYS:CA | 1.98 | 0.69 |
| 3:F:2962[B]:GLY:O | 3:a:3255[B]:PRO:CG | 2.40 | 0.69 |
| 3:F:2966[B]:SER:N | 3:a:3255[B]:PRO:HA | 2.07 | 0.69 |
| 3:F:3255[B]:PRO:HG3 | 3:a:2962[B]:GLY:O | 1.91 | 0.69 |
| 3:F:3307[A]:PHE:CE1 | 3:F:3309[A]:PRO:HG3 | 2.16 | 0.69 |
| 3:I:3133[A]:LEU:O | 3:I:3134[A]:GLN:C | 2.32 | 0.69 |
| 3:I:3230[B]:PHE:CB | 3:I:3243[B]:GLY:N | 2.56 | 0.69 |
| 3:I:3287[B]:ILE:O | 3:I:3287[B]:ILE:HD13 | 1.92 | 0.69 |
| 3:L:3066[A]:TYR:CD1 | 3:L:3193[A]:HIS:CE1 | 2.80 | 0.69 |
| 3:L:3077[B]:ASP:HB2 | 3:L:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:L:3287[A]:ILE:O | 3:L:3287[A]:ILE:HD13 | 1.92 | 0.69 |
| 1:M:1358:LEU:HD23 | 1:M:1456:LEU:HD21 | 1.74 | 0.69 |
| 3:O:2930[A]:LEU:H | 3:O:2930[A]:LEU:CD2 | 1.98 | 0.69 |
| 3:O:2961[B]:HIS:CE1 | 3:O:2980[B]:HIS:NE2 | 2.57 | 0.69 |
| 3:O:2965[A]:LEU:CD1 | 3:O:2974[A]:ALA:HA | 2.22 | 0.69 |
| 3:O:3154[B]:PRO:CD | 3:X:3176[B]:LYS:HE3 | 2.22 | 0.69 |
| 3:O:3284[B]:LYS:HA | 3:O:3284[B]:LYS:CE | 2.22 | 0.69 |
| 3:R:3077[B]:ASP:HB2 | 3:R:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:R:3230[B]:PHE:CB | 3:R:3243[B]:GLY:N | 2.56 | 0.69 |
| 3:R:3284[B]:LYS:HA | 3:R:3284[B]:LYS:CE | 2.22 | 0.69 |
| 1:S:723:ALA:O | 1:S:728:ARG:NH1 | 2.25 | 0.69 |
| 1:V:588:GLU:OE2 | 1:V:728:ARG:NH1 | 2.25 | 0.69 |
| 3:X:2930[B]:LEU:H | 3:X:2930[B]:LEU:CD2 | 1.98 | 0.69 |
| 3:X:3230[A]:PHE:CB | 3:X:3243[A]:GLY:N | 2.56 | 0.69 |
| 3:X:3230[B]:PHE:CB | 3:X:3243[B]:GLY:N | 2.56 | 0.69 |
| 3:a:2965[B]:LEU:HG | 3:a:2974[B]:ALA:CB | 2.21 | 0.69 |
| 1:b:588:GLU:OE2 | 1:b:728:ARG:NH1 | 2.17 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2933[B]:SER:C | 3:d:2935[B]:ILE:HD13 | 2.17 | 0.69 |
| 3:d:3066[A]:TYR:CD1 | 3:d:3193[A]:HIS:CE1 | 2.79 | 0.69 |
| 3:d:3077[B]:ASP:HB2 | 3:d:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:d:3169[B]:LYS:C | 3:d:3172[B]:SER:HG | 1.98 | 0.69 |
| 1:A:416:ASN:OD1 | 3:F:3196[A]:THR:HG21 | 1.92 | 0.69 |
| 1:A:567:LEU:HB3 | 1:A:571:PRO:HG2 | 1.72 | 0.69 |
| 3:C:2930[B]:LEU:HD22 | 3:C:2930[B]:LEU:N | 2.02 | 0.69 |
| 3:C:3179[B]:ASP:OD1 | 3:C:3181[B]:GLN:HB2 | 1.91 | 0.69 |
| 3:F:2933[B]:SER:C | 3:F:2935[B]:ILE:HD13 | 2.17 | 0.69 |
| 3:F:2966[B]:SER:HB2 | 3:F:2977[B]:CYS:CB | 2.21 | 0.69 |
| 3:F:2979[A]:GLN:HE21 | 3:F:3155[A]:MET:HE2 | 1.55 | 0.69 |
| 3:F:3077[B]:ASP:HB2 | 3:F:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:F:3159[B]:SER:HB3 | 3:a:2984[B]:THR:CB | 2.19 | 0.69 |
| 3:I:2937[A]:ASN:CB | 3:I:3006[A]:LYS:HD3 | 2.23 | 0.69 |
| 3:I:3161[B]:GLU:HG2 | 3:R:3079[B]:CYS:CA | 2.20 | 0.69 |
| 3:I:3179[B]:ASP:OD1 | 3:I:3181[B]:GLN:HB2 | 1.92 | 0.69 |
| 3:L:3284[A]:LYS:HA | 3:L:3284[A]:LYS:CE | 2.21 | 0.69 |
| 1:M:1239:GLY:O | 1:M:1242:ASN:ND2 | 2.25 | 0.69 |
| 3:O:2933[A]:SER:C | 3:O:2935[A]:ILE:HD13 | 2.17 | 0.69 |
| 3:O:2937[B]:ASN:HB2 | 3:O:3006[B]:LYS:CE | 2.14 | 0.69 |
| 3:O:3109[B]:TYR:CG | 3:X:2970[B]:PRO:N | 1.97 | 0.69 |
| 3:O:3230[B]:PHE:CB | 3:O:3243[B]:GLY:N | 2.56 | 0.69 |
| 2:Q:2166:LEU:HA | 2:Q:2169:HIS:HB2 | 1.73 | 0.69 |
| 3:R:2935[B]:ILE:HD13 | 3:R:2936[B]:GLU:N | 2.05 | 0.69 |
| 3:R:3179[A]:ASP:OD1 | 3:R:3181[A]:GLN:HB2 | 1.92 | 0.69 |
| 3:U:2948[B]:ASP:H | 3:U:2949[B]:LYS:CA | 1.98 | 0.69 |
| 3:U:2952[A]:ALA:CB | 3:U:2953[A]:GLY:C | 2.48 | 0.69 |
| 3:U:2979[B]:GLN:HE21 | 3:U:3155[B]:MET:HE2 | 1.54 | 0.69 |
| 3:U:3086[B]:GLU:CD | 3:d:2970[B]:PRO:HG3 | 2.12 | 0.69 |
| 3:U:3153[B]:LYS:HG3 | 3:d:3155[B]:MET:HE3 | 1.75 | 0.69 |
| 1:V:355:ALA:HA | 1:V:734:LEU:HD12 | 1.74 | 0.69 |
| 3:X:3285[A]:VAL:HG22 | 3:X:3286[A]:THR:N | 2.04 | 0.69 |
| 3:X:3287[A]:ILE:O | 3:X:3287[A]:ILE:HD13 | 1.92 | 0.69 |
| 3:a:3077[B]:ASP:HB2 | 3:a:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:d:2965[B]:LEU:CD1 | 3:d:2974[B]:ALA:HA | 2.22 | 0.69 |
| 3:d:3077[A]:ASP:HB2 | 3:d:3080[A]:ASP:OD2 | 1.93 | 0.69 |
| 3:d:3173[B]:THR:CG2 | 3:d:3174[B]:GLY:N | 2.55 | 0.69 |
| 3:d:3179[B]:ASP:OD1 | 3:d:3181[B]:GLN:HB2 | 1.92 | 0.69 |
| 3:C:3173[A]:THR:CG2 | 3:C:3174[A]:GLY:N | 2.55 | 0.69 |
| 3:C:3287[A]:ILE:O | 3:C:3287[A]:ILE:HD13 | 1.92 | 0.69 |
| 1:D:534:ASP:HB2 | 1:D:541:LYS:HE2 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2942[A]:LEU:HD13 | 3:F:3033[A]:PHE:CE1 | 2.28 | 0.69 |
| 3:F:2965[B]:LEU:CD1 | 3:F:2974[B]:ALA:HA | 2.22 | 0.69 |
| 3:F:2970[B]:PRO:CB | 3:a:2989[B]:HIS:HD2 | 2.04 | 0.69 |
| 3:F:3024[B]:LEU:CD1 | 3:F:3025[B]:VAL:H | 1.84 | 0.69 |
| 3:F:3169[B]:LYS:HZ3 | 3:a:3149[B]:ASN:ND2 | 1.87 | 0.69 |
| 3:I:2937[B]:ASN:CB | 3:I:3006[B]:LYS:HD3 | 2.23 | 0.69 |
| 3:I:2973[B]:THR:HG23 | 3:R:3248[B]:LEU:CD1 | 2.20 | 0.69 |
| 3:I:3160[B]:SER:CB | 3:R:2982[B]:MET:HB3 | 2.20 | 0.69 |
| 3:L:2933[B]:SER:C | 3:L:2935[B]:ILE:HD13 | 2.17 | 0.69 |
| 3:L:2937[A]:ASN:CB | 3:L:3006[A]:LYS:HD3 | 2.23 | 0.69 |
| 3:L:2965[B]:LEU:CD1 | 3:L:2974[B]:ALA:HA | 2.22 | 0.69 |
| 3:L:3230[B]:PHE:CB | 3:L:3243[B]:GLY:N | 2.56 | 0.69 |
| 3:O:3040[B]:VAL:HG21 | 3:X:2969[B]:TYR:CE1 | 2.11 | 0.69 |
| 3:O:3077[B]:ASP:HB2 | 3:O:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:O:3179[A]:ASP:OD1 | 3:O:3181[A]:GLN:HB2 | 1.92 | 0.69 |
| 3:O:3230[A]:PHE:CB | 3:O:3243[A]:GLY:N | 2.56 | 0.69 |
| 1:P:484:MET:HE2 | 1:P:663:GLU:HG3 | 1.73 | 0.69 |
| 2:Q:2797:LYS:HA | 2:Q:2800:LYS:HD3 | 1.75 | 0.69 |
| 3:R:2937[B]:ASN:CB | 3:R:3006[B]:LYS:HD3 | 2.23 | 0.69 |
| 3:R:3077[A]:ASP:HB2 | 3:R:3080[A]:ASP:OD2 | 1.93 | 0.69 |
| 3:U:3077[A]:ASP:HB2 | 3:U:3080[A]:ASP:OD2 | 1.93 | 0.69 |
| 2:W:2851:ASN:OD1 | 2:W:2851:ASN:N | 2.24 | 0.69 |
| 3:X:2942[A]:LEU:HD13 | 3:X:3033[A]:PHE:CE1 | 2.28 | 0.69 |
| 3:X:2942[B]:LEU:HD13 | 3:X:3033[B]:PHE:CE1 | 2.28 | 0.69 |
| 3:X:3077[B]:ASP:HB2 | 3:X:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:a:2937[B]:ASN:CB | 3:a:3006[B]:LYS:HD3 | 2.23 | 0.69 |
| 3:a:2937[B]:ASN:CB | 3:a:3006[B]:LYS:HE2 | 2.14 | 0.69 |
| 3:a:3173[A]:THR:CG2 | 3:a:3174[A]:GLY:N | 2.55 | 0.69 |
| 1:b:1063:ARG:HB3 | 1:b:1065:LYS:HD2 | 1.73 | 0.69 |
| 3:d:2937[B]:ASN:CB | 3:d:3006[B]:LYS:HD3 | 2.23 | 0.69 |
| 3:d:3226[A]:ALA:HB1 | 3:d:3288[A]:MET:O | 1.90 | 0.69 |
| 3:F:3077[A]:ASP:HB2 | 3:F:3080[A]:ASP:OD2 | 1.93 | 0.69 |
| 3:F:3156[B]:MET:CB | 3:a:2982[B]:MET:SD | 2.81 | 0.69 |
| 3:F:3173[A]:THR:CG2 | 3:F:3174[A]:GLY:N | 2.55 | 0.69 |
| 1:G:1046:HIS:HA | 1:G:1049:VAL:HB | 1.75 | 0.69 |
| 3:I:3077[B]:ASP:HB2 | 3:I:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:I:3110[A]:THR:O | 3:I:3112[A]:TYR:N | 2.26 | 0.69 |
| 3:I:3153[B]:LYS:HD2 | 3:R:3155[B]:MET:HB3 | 1.72 | 0.69 |
| 3:O:2937[A]:ASN:CB | 3:O:3006[A]:LYS:HD3 | 2.23 | 0.69 |
| 3:O:2966[B]:SER:HB2 | 3:O:2977[B]:CYS:HB2 | 1.39 | 0.69 |
| 3:O:3077[A]:ASP:HB2 | 3:O:3080[A]:ASP:OD2 | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3255[B]:PRO:CD | 3:X:3163[B]:ASN:HD22 | 2.06 | 0.69 |
| 2:Q:2546:LEU:H | 2:Q:2557:ALA:HA | 1.58 | 0.69 |
| 3:R:2942[A]:LEU:HD13 | 3:R:3033[A]:PHE:CE1 | 2.28 | 0.69 |
| 3:R:2965[B]:LEU:CD1 | 3:R:2974[B]:ALA:HA | 2.22 | 0.69 |
| 3:R:3066[A]:TYR:CD1 | 3:R:3193[A]:HIS:CE1 | 2.79 | 0.69 |
| 3:R:3179[B]:ASP:OD1 | 3:R:3181[B]:GLN:HB2 | 1.91 | 0.69 |
| 3:R:3212[A]:ARG:HG3 | 3:R:3212[A]:ARG:NH1 | 2.00 | 0.69 |
| 3:U:2937[A]:ASN:CB | 3:U:3006[A]:LYS:HD3 | 2.23 | 0.69 |
| 3:U:3024[B]:LEU:CD1 | 3:U:3025[B]:VAL:H | 1.84 | 0.69 |
| 1:Y:527:LEU:O | 1:Y:561:ARG:NH1 | 2.26 | 0.69 |
| 2:Z:2823:ILE:HD11 | 2:Z:2856:ILE:HD12 | 1.74 | 0.69 |
| 3:d:3221[A]:ALA:HB2 | 3:d:3256[A]:TRP:H | 1.56 | 0.69 |
| 3:d:3287[B]:ILE:O | 3:d:3287[B]:ILE:HD13 | 1.92 | 0.69 |
| 1:A:557:VAL:HG23 | 1:A:558:HIS:HA | 1.74 | 0.69 |
| 2:B:2240:GLN:HE21 | 2:B:2241:THR:H | 1.41 | 0.69 |
| 2:B:2550:THR:O | 2:B:2553:ALA:N | 2.22 | 0.69 |
| 3:C:2942[B]:LEU:HD13 | 3:C:3033[B]:PHE:CE1 | 2.28 | 0.69 |
| 3:C:2966[B]:SER:HB2 | 3:C:2977[B]:CYS:CB | 2.21 | 0.69 |
| 3:C:2975[B]:PHE:CE2 | 3:L:2979[B]:GLN:N | 2.57 | 0.69 |
| 3:C:2975[B]:PHE:O | 3:L:3256[B]:TRP:CD1 | 2.46 | 0.69 |
| 3:C:3110[A]:THR:O | 3:C:3112[A]:TYR:N | 2.26 | 0.69 |
| 3:C:3217[A]:PHE:HE1 | 3:C:3230[A]:PHE:HZ | 0.80 | 0.69 |
| 3:C:3220[A]:ARG:HG3 | 3:C:3220[A]:ARG:NH1 | 1.98 | 0.69 |
| 3:F:2942[B]:LEU:HD13 | 3:F:3033[B]:PHE:CE1 | 2.28 | 0.69 |
| 3:F:2968[B]:GLN:CG | 3:a:2981[B]:GLY:N | 2.54 | 0.69 |
| 3:F:2970[B]:PRO:HB3 | 3:a:2989[B]:HIS:CD2 | 2.28 | 0.69 |
| 3:F:3110[A]:THR:O | 3:F:3112[A]:TYR:N | 2.26 | 0.69 |
| 3:F:3169[B]:LYS:HE3 | 3:a:3150[B]:LYS:HB2 | 1.74 | 0.69 |
| 3:F:3179[A]:ASP:OD1 | 3:F:3181[A]:GLN:HB2 | 1.92 | 0.69 |
| 3:F:3221[B]:ALA:HB2 | 3:F:3256[B]:TRP:H | 1.56 | 0.69 |
| 3:I:2933[A]:SER:C | 3:I:2935[A]:ILE:HD13 | 2.17 | 0.69 |
| 3:I:2933[B]:SER:C | 3:I:2935[B]:ILE:HD13 | 2.17 | 0.69 |
| 3:I:2966[B]:SER:O | 3:R:2981[B]:GLY:HA3 | 1.93 | 0.69 |
| 3:I:3155[B]:MET:CB | 3:R:3153[B]:LYS:CG | 2.66 | 0.69 |
| 3:I:3158[B]:PHE:H | 3:R:3153[B]:LYS:NZ | 1.89 | 0.69 |
| 3:L:2942[A]:LEU:HD13 | 3:L:3033[A]:PHE:CE1 | 2.28 | 0.69 |
| 3:L:2966[B]:SER:HB2 | 3:L:2977[B]:CYS:CB | 2.21 | 0.69 |
| 3:L:2979[A]:GLN:HE21 | 3:L:3155[A]:MET:HE2 | 1.54 | 0.69 |
| 3:L:3110[B]:THR:O | 3:L:3112[B]:TYR:N | 2.26 | 0.69 |
| 2:N:2225:ARG:HD2 | 2:N:2274:LEU:HD22 | 1.74 | 0.69 |
| 3:O:2942[B]:LEU:HD13 | 3:O:3033[B]:PHE:CE1 | 2.28 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2952[B]:ALA:H | 3:O:2953[B]:GLY:CA | 2.04 | 0.69 |
| 3:O:2970[B]:PRO:HD2 | 3:X:2991[B]:LEU:CD2 | 2.22 | 0.69 |
| 3:O:2970[B]:PRO:CA | 3:X:2991[B]:LEU:N | 2.56 | 0.69 |
| 3:O:3156[B]:MET:CE | 3:X:3173[B]:THR:CG2 | 2.70 | 0.69 |
| 3:R:3025[B]:VAL:HG22 | 3:R:3047[B]:ARG:NH1 | 2.01 | 0.69 |
| 3:R:3089[B]:HIS:ND1 | 3:R:3119[B]:HIS:CE1 | 2.61 | 0.69 |
| 3:R:3287[A]:ILE:O | 3:R:3287[A]:ILE:HD13 | 1.92 | 0.69 |
| 3:U:2942[A]:LEU:HD13 | 3:U:3033[A]:PHE:CE1 | 2.28 | 0.69 |
| 3:U:2969[B]:TYR:HD2 | 3:U:2971[B]:ASP:N | 1.85 | 0.69 |
| 3:U:2969[B]:TYR:CE2 | 3:d:2980[B]:HIS:CD2 | 2.81 | 0.69 |
| 3:U:3307[B]:PHE:CE1 | 3:U:3309[B]:PRO:HG3 | 2.16 | 0.69 |
| 1:V:622:HIS:CE1 | 1:V:767:LYS:H | 2.10 | 0.69 |
| 1:V:944:GLU:O | 1:V:957:ASN:ND2 | 2.25 | 0.69 |
| 2:W:2868:GLU:OE1 | 3:X:2932[A]:PRO:C | 2.34 | 0.69 |
| 3:X:3077[A]:ASP:HB2 | 3:X:3080[A]:ASP:OD2 | 1.93 | 0.69 |
| 3:X:3110[B]:THR:O | 3:X:3112[B]:TYR:N | 2.26 | 0.69 |
| 3:X:3176[A]:LYS:HB3 | 3:X:3176[A]:LYS:NZ | 2.08 | 0.69 |
| 1:Y:1656:ASP:N | 3:d:3006[B]:LYS:HB2 | 2.06 | 0.69 |
| 2:Z:2267:HIS:HD2 | 2:Z:2297:HIS:HE1 | 1.40 | 0.69 |
| 3:a:2960[A]:PHE:HD1 | 3:a:2960[A]:PHE:H | 1.41 | 0.69 |
| 3:a:2982[A]:MET:HE1 | 3:a:3254[A]:MET:HE2 | 1.73 | 0.69 |
| 1:b:946:GLU:HG2 | 1:b:955:LYS:HD2 | 1.75 | 0.69 |
| 2:c:2191:LEU:O | 2:c:2225:ARG:NH2 | 2.25 | 0.69 |
| 3:d:2960[B]:PHE:H | 3:d:2960[B]:PHE:HD1 | 1.41 | 0.69 |
| 3:d:3176[B]:LYS:NZ | 3:d:3176[B]:LYS:HB3 | 2.08 | 0.69 |
| 3:d:3284[A]:LYS:HA | 3:d:3284[A]:LYS:CE | 2.22 | 0.69 |
| 3:C:2948[B]:ASP:H | 3:C:2949[B]:LYS:CA | 1.98 | 0.69 |
| 3:C:3150[B]:LYS:O | 3:L:3172[B]:SER:HB2 | 1.92 | 0.69 |
| 1:D:329:ARG:HB2 | 1:G:1583:CYS:H | 1.57 | 0.69 |
| 3:F:3110[B]:THR:O | 3:F:3112[B]:TYR:N | 2.26 | 0.69 |
| 3:I:3284[A]:LYS:HA | 3:I:3284[A]:LYS:CE | 2.22 | 0.69 |
| 3:O:2937[B]:ASN:CB | 3:O:3006[B]:LYS:HD3 | 2.23 | 0.69 |
| 3:O:3031[A]:ASN:OD1 | 3:O:3033[A]:PHE:N | 2.26 | 0.69 |
| 3:R:3089[A]:HIS:ND1 | 3:R:3119[A]:HIS:CE1 | 2.61 | 0.69 |
| 3:R:3110[B]:THR:O | 3:R:3112[B]:TYR:N | 2.26 | 0.69 |
| 1:S:460:GLU:HB3 | 1:S:465:PRO:HG2 | 1.74 | 0.69 |
| 3:U:2961[A]:HIS:HB3 | 3:U:3111[A]:SER:HG | 1.56 | 0.69 |
| 3:U:3176[B]:LYS:NZ | 3:U:3176[B]:LYS:HB3 | 2.08 | 0.69 |
| 3:U:3258[B]:PHE:C | 3:d:2968[B]:GLN:HE21 | 2.00 | 0.69 |
| 3:U:3287[B]:ILE:O | 3:U:3287[B]:ILE:HD13 | 1.92 | 0.69 |
| 3:X:2965[A]:LEU:CD1 | 3:X:2974[A]:ALA:HA | 2.22 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3230[A]:PHE:CB | 3:a:3243[A]:GLY:N | 2.56 | 0.69 |
| 2:c:2648:ALA:HA | 2:c:2654:SER:HB2 | 1.75 | 0.69 |
| 3:d:3220[A]:ARG:HG2 | 3:d:3221[A]:ALA:N | 2.08 | 0.69 |
| 3:C:2979[A]:GLN:HE21 | 3:C:3155[A]:MET:HE2 | 1.55 | 0.69 |
| 3:C:3154[B]:PRO:HB3 | 3:L:3151[B]:LEU:C | 2.17 | 0.69 |
| 3:C:3230[A]:PHE:CB | 3:C:3243[A]:GLY:N | 2.56 | 0.69 |
| 3:F:3031[A]:ASN:OD1 | 3:F:3033[A]:PHE:N | 2.26 | 0.69 |
| 3:F:3217[A]:PHE:HE1 | 3:F:3230[A]:PHE:HZ | 0.80 | 0.69 |
| 3:F:3256[B]:TRP:CZ2 | 3:a:2965[B]:LEU:HB3 | 2.25 | 0.69 |
| 3:F:3279[A]:ASP:OD1 | 3:F:3279[A]:ASP:N | 2.25 | 0.69 |
| 1:G:1650:ILE:HB | 2:K:2326:ILE:HG22 | 1.74 | 0.69 |
| 3:I:2966[B]:SER:HB2 | 3:I:2977[B]:CYS:CB | 2.21 | 0.69 |
| 3:I:2983[B]:VAL:HG22 | 3:R:3162[B]:ASP:OD1 | 1.92 | 0.69 |
| 3:I:3176[A]:LYS:HB3 | 3:I:3176[A]:LYS:NZ | 2.08 | 0.69 |
| 1:J:1148:LEU:HB2 | 1:J:1188:PHE:HD2 | 1.57 | 0.69 |
| 3:O:2968[B]:GLN:HB2 | 3:X:2988[B]:TRP:N | 2.08 | 0.69 |
| 3:O:3176[B]:LYS:HB3 | 3:O:3176[B]:LYS:NZ | 2.08 | 0.69 |
| 3:O:3255[B]:PRO:HB3 | 3:X:3161[B]:GLU:C | 2.18 | 0.69 |
| 3:O:3287[B]:ILE:O | 3:O:3287[B]:ILE:HD13 | 1.92 | 0.69 |
| 1:P:744:VAL:HG22 | 1:P:760:ILE:HG12 | 1.73 | 0.69 |
| 3:R:2942[B]:LEU:HD13 | 3:R:3033[B]:PHE:CE1 | 2.28 | 0.69 |
| 3:R:3293[B]:LYS:HB2 | 3:R:3294[B]:SER:HB2 | 0.82 | 0.69 |
| 3:U:2937[B]:ASN:CB | 3:U:3006[B]:LYS:HD3 | 2.23 | 0.69 |
| 3:U:3077[B]:ASP:HB2 | 3:U:3080[B]:ASP:OD2 | 1.93 | 0.69 |
| 3:U:3110[B]:THR:O | 3:U:3112[B]:TYR:N | 2.26 | 0.69 |
| 3:X:3089[B]:HIS:ND1 | 3:X:3119[B]:HIS:CE1 | 2.61 | 0.69 |
| 3:d:2966[A]:SER:HB2 | 3:d:2977[A]:CYS:CB | 2.21 | 0.69 |
| 3:d:3279[B]:ASP:OD1 | 3:d:3279[B]:ASP:N | 2.25 | 0.69 |
| 3:C:2942[A]:LEU:HD13 | 3:C:3033[A]:PHE:CE1 | 2.28 | 0.68 |
| 3:C:3077[A]:ASP:HB2 | 3:C:3080[A]:ASP:OD2 | 1.93 | 0.68 |
| 3:C:3160[B]:SER:HB2 | 3:L:3150[B]:LYS:HZ3 | 0.55 | 0.68 |
| 3:F:3031[B]:ASN:OD1 | 3:F:3033[B]:PHE:N | 2.27 | 0.68 |
| 1:G:210:HIS:HA | 1:G:213:VAL:HG22 | 1.74 | 0.68 |
| 3:I:2942[A]:LEU:HD13 | 3:I:3033[A]:PHE:CE1 | 2.28 | 0.68 |
| 3:I:2942[B]:LEU:HD13 | 3:I:3033[B]:PHE:CE1 | 2.28 | 0.68 |
| 3:I:3108[B]:HIS:HE1 | 3:R:3251[B]:ASP:CG | 2.00 | 0.68 |
| 3:L:3176[A]:LYS:NZ | 3:L:3176[A]:LYS:HB3 | 2.08 | 0.68 |
| 1:M:550:ILE:N | 1:M:557:VAL:O | 2.26 | 0.68 |
| 1:P:105:VAL:HG12 | 1:P:123:PHE:HB3 | 1.73 | 0.68 |
| 1:P:152:LYS:HE3 | 1:P:153:ASN:H | 1.58 | 0.68 |
| 3:R:2965[A]:LEU:CD1 | 3:R:2974[A]:ALA:HA | 2.22 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2937[B]:ASN:CB | 3:X:3006[B]:LYS:HD3 | 2.23 | 0.68 |
| 1:Y:958:PRO:HA | 1:Y:959:PHE:HB2 | 1.74 | 0.68 |
| 3:a:3230[B]:PHE:CB | 3:a:3243[B]:GLY:N | 2.56 | 0.68 |
| 3:d:2942[A]:LEU:HD13 | 3:d:3033[A]:PHE:CE1 | 2.28 | 0.68 |
| 3:d:2952[A]:ALA:H | 3:d:2953[A]:GLY:CA | 2.04 | 0.68 |
| 3:d:3173[A]:THR:CG2 | 3:d:3174[A]:GLY:N | 2.55 | 0.68 |
| 4:m:1:NAG:O3 | 4:m:2:NAG:N2 | 2.21 | 0.68 |
| 3:C:2964[B]:PRO:N | 3:L:3255[B]:PRO:HB3 | 2.08 | 0.68 |
| 3:F:3221[A]:ALA:HB2 | 3:F:3256[A]:TRP:H | 1.56 | 0.68 |
| 3:I:2965[A]:LEU:CD1 | 3:I:2974[A]:ALA:HA | 2.22 | 0.68 |
| 3:I:3217[B]:PHE:HE1 | 3:I:3230[B]:PHE:HZ | 0.80 | 0.68 |
| 3:I:3230[A]:PHE:CB | 3:I:3243[A]:GLY:N | 2.56 | 0.68 |
| 3:L:3031[A]:ASN:OD1 | 3:L:3033[A]:PHE:N | 2.27 | 0.68 |
| 3:O:2942[A]:LEU:HD13 | 3:O:3033[A]:PHE:CE1 | 2.28 | 0.68 |
| 3:O:3106[B]:THR:HG21 | 3:X:2970[B]:PRO:C | 2.18 | 0.68 |
| 3:O:3173[B]:THR:CG2 | 3:O:3174[B]:GLY:N | 2.55 | 0.68 |
| 1:P:105:VAL:HB | 1:P:137:ARG:HH22 | 1.58 | 0.68 |
| 1:P:1000:GLU:HG2 | 1:P:1133:ILE:HG23 | 1.75 | 0.68 |
| 2:T:2872:GLU:O | 1:V:1078:ARG:NH1 | 2.26 | 0.68 |
| 3:U:2952[B]:ALA:H | 3:U:2953[B]:GLY:CA | 2.04 | 0.68 |
| 3:U:2969[B]:TYR:OH | 3:d:2961[B]:HIS:CE1 | 2.46 | 0.68 |
| 3:U:3220[B]:ARG:HG2 | 3:d:2974[B]:ALA:H | 1.58 | 0.68 |
| 3:U:3221[A]:ALA:HB2 | 3:U:3256[A]:TRP:H | 1.57 | 0.68 |
| 1:V:439:LEU:HD23 | 1:V:509:ILE:HD12 | 1.72 | 0.68 |
| 2:W:2180:TRP:HB2 | 2:W:2243:LEU:HD13 | 1.75 | 0.68 |
| 3:a:3110[A]:THR:O | 3:a:3112[A]:TYR:N | 2.26 | 0.68 |
| 3:a:3176[A]:LYS:NZ | 3:a:3176[A]:LYS:HB3 | 2.08 | 0.68 |
| 3:a:3279[A]:ASP:OD1 | 3:a:3279[A]:ASP:N | 2.25 | 0.68 |
| 3:d:3287[A]:ILE:O | 3:d:3287[A]:ILE:HD13 | 1.92 | 0.68 |
| 1:A:1304:ASP:OD1 | 1:A:1305:GLY:N | 2.26 | 0.68 |
| 3:C:2979[A]:GLN:NE2 | 3:C:3155[A]:MET:HE2 | 2.09 | 0.68 |
| 3:C:3153[B]:LYS:HD3 | 3:L:2988[B]:TRP:HD1 | 1.56 | 0.68 |
| 3:C:3221[A]:ALA:HB2 | 3:C:3256[A]:TRP:H | 1.56 | 0.68 |
| 3:F:2966[A]:SER:HB2 | 3:F:2977[A]:CYS:CB | 2.21 | 0.68 |
| 3:F:2973[B]:THR:HG23 | 3:a:3248[B]:LEU:HD11 | 1.75 | 0.68 |
| 3:F:3230[A]:PHE:CB | 3:F:3243[A]:GLY:N | 2.56 | 0.68 |
| 1:G:355:ALA:HA | 1:G:734:LEU:HD12 | 1.74 | 0.68 |
| 1:G:1296:VAL:HB | 1:G:1446:ASP:HB3 | 1.75 | 0.68 |
| 2:H:2806:ALA:HB2 | 2:H:2856:ILE:HD11 | 1.75 | 0.68 |
| 3:I:3089[A]:HIS:ND1 | 3:I:3119[A]:HIS:CE1 | 2.61 | 0.68 |
| 3:I:3162[B]:ASP:C | 3:R:3150[B]:LYS:HZ1 | 2.00 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2794:LEU:HD12 | 2:K:2797:LYS:HD2 | 1.75 | 0.68 |
| 3:L:3089[A]:HIS:ND1 | 3:L:3119[A]:HIS:CE1 | 2.61 | 0.68 |
| 3:L:3176[B]:LYS:NZ | 3:L:3176[B]:LYS:HB3 | 2.08 | 0.68 |
| 3:L:3194[A]:GLY:C | 3:L:3195[A]:MET:HG2 | 2.16 | 0.68 |
| 3:O:2933[B]:SER:C | 3:O:2935[B]:ILE:HD13 | 2.17 | 0.68 |
| 3:O:3110[B]:THR:O | 3:O:3112[B]:TYR:N | 2.26 | 0.68 |
| 1:S:164:GLU:OE1 | 1:S:296:ARG:NH1 | 2.22 | 0.68 |
| 1:S:871:GLN:NE2 | 1:S:964:ILE:O | 2.26 | 0.68 |
| 1:S:1030:MET:HA | 1:S:1036:SER:HA | 1.75 | 0.68 |
| 3:U:2965[A]:LEU:CD1 | 3:U:2974[A]:ALA:HA | 2.22 | 0.68 |
| 3:U:3153[B]:LYS:HG3 | 3:d:2979[B]:GLN:NE2 | 2.08 | 0.68 |
| 3:X:3194[A]:GLY:C | 3:X:3195[A]:MET:HG2 | 2.16 | 0.68 |
| 1:Y:194:MET:HA | 1:Y:200:THR:HA | 1.75 | 0.68 |
| 3:a:3176[B]:LYS:HB3 | 3:a:3176[B]:LYS:NZ | 2.08 | 0.68 |
| 3:a:3284[A]:LYS:HA | 3:a:3284[A]:LYS:CE | 2.22 | 0.68 |
| 3:d:2942[B]:LEU:HD13 | 3:d:3033[B]:PHE:CE1 | 2.28 | 0.68 |
| 3:d:3284[B]:LYS:HA | 3:d:3284[B]:LYS:CE | 2.22 | 0.68 |
| 1:A:912:ASN:HD21 | 1:A:1091:ASN:HD21 | 1.41 | 0.68 |
| 3:C:3089[B]:HIS:ND1 | 3:C:3119[B]:HIS:CE1 | 2.61 | 0.68 |
| 3:C:3253[B]:GLU:HB2 | 3:L:2975[B]:PHE:CA | 2.23 | 0.68 |
| 3:F:2966[B]:SER:CB | 3:a:3254[B]:MET:CB | 2.71 | 0.68 |
| 2:H:2695:MET:HE1 | 2:H:2707:PHE:HB2 | 1.74 | 0.68 |
| 3:I:2961[B]:HIS:CE1 | 3:I:2980[B]:HIS:NE2 | 2.57 | 0.68 |
| 3:I:3077[A]:ASP:HB2 | 3:I:3080[A]:ASP:OD2 | 1.93 | 0.68 |
| 3:I:3110[B]:THR:HG21 | 3:R:2971[B]:ASP:OD2 | 1.93 | 0.68 |
| 3:L:2966[A]:SER:HB2 | 3:L:2977[A]:CYS:CB | 2.21 | 0.68 |
| 3:L:2969[A]:TYR:HD2 | 3:L:2971[A]:ASP:N | 1.84 | 0.68 |
| 3:L:3173[A]:THR:CG2 | 3:L:3174[A]:GLY:N | 2.55 | 0.68 |
| 3:O:3194[A]:GLY:C | 3:O:3195[A]:MET:HG2 | 2.16 | 0.68 |
| 1:P:46:ASP:OD2 | 1:P:249:ARG:NH2 | 2.26 | 0.68 |
| 3:R:2979[B]:GLN:HE21 | 3:R:3155[B]:MET:HE2 | 1.54 | 0.68 |
| 3:R:3176[A]:LYS:NZ | 3:R:3176[A]:LYS:HB3 | 2.08 | 0.68 |
| 3:U:2960[A]:PHE:HD1 | 3:U:2960[A]:PHE:H | 1.41 | 0.68 |
| 3:U:3089[A]:HIS:ND1 | 3:U:3119[A]:HIS:CE1 | 2.61 | 0.68 |
| 3:U:3230[A]:PHE:CB | 3:U:3243[A]:GLY:N | 2.56 | 0.68 |
| 3:X:3173[B]:THR:CG2 | 3:X:3174[B]:GLY:N | 2.55 | 0.68 |
| 3:a:3089[A]:HIS:ND1 | 3:a:3119[A]:HIS:CE1 | 2.61 | 0.68 |
| 3:a:3089[B]:HIS:ND1 | 3:a:3119[B]:HIS:CE1 | 2.61 | 0.68 |
| 3:d:2979[B]:GLN:NE2 | 3:d:3155[B]:MET:HE2 | 2.09 | 0.68 |
| 3:d:3110[A]:THR:O | 3:d:3112[A]:TYR:N | 2.26 | 0.68 |
| 1:A:460:GLU:HB3 | 1:A:465:PRO:HG2 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:830:ASN:HB3 | 1:A:832:LYS:N | 2.09 | 0.68 |
| 2:B:2573:TYR:HE2 | 2:B:2707:PHE:HE2 | 1.42 | 0.68 |
| 3:C:3150[B]:LYS:NZ | 3:L:3160[B]:SER:CA | 2.51 | 0.68 |
| 3:F:2937[B]:ASN:CB | 3:F:3006[B]:LYS:HD3 | 2.23 | 0.68 |
| 2:H:2191:LEU:O | 2:H:2225:ARG:NH2 | 2.25 | 0.68 |
| 3:I:2930[A]:LEU:HD22 | 3:I:2930[A]:LEU:N | 2.02 | 0.68 |
| 3:I:2975[B]:PHE:CZ | 3:R:2961[B]:HIS:ND1 | 2.62 | 0.68 |
| 2:K:2648:ALA:HA | 2:K:2654:SER:HB2 | 1.75 | 0.68 |
| 3:L:2930[A]:LEU:H | 3:L:2930[A]:LEU:CD2 | 1.98 | 0.68 |
| 3:L:3194[B]:GLY:C | 3:L:3195[B]:MET:HG2 | 2.16 | 0.68 |
| 2:N:2344:LEU:HB3 | 2:Q:2515:ARG:HB3 | 1.74 | 0.68 |
| 3:O:2930[B]:LEU:HD22 | 3:O:2930[B]:LEU:N | 2.02 | 0.68 |
| 3:O:3110[A]:THR:O | 3:O:3112[A]:TYR:N | 2.26 | 0.68 |
| 3:O:3169[A]:LYS:C | 3:O:3172[A]:SER:HG | 1.98 | 0.68 |
| 1:P:1414:THR:HG23 | 1:P:1477:LEU:HD13 | 1.76 | 0.68 |
| 3:R:3077[A]:ASP:CB | 3:R:3080[A]:ASP:OD2 | 2.42 | 0.68 |
| 2:T:2890:VAL:N | 2:T:2891:LEU:HA | 2.08 | 0.68 |
| 3:U:2960[B]:PHE:H | 3:U:2960[B]:PHE:HD1 | 1.41 | 0.68 |
| 3:X:2937[A]:ASN:CB | 3:X:3006[A]:LYS:HD3 | 2.23 | 0.68 |
| 3:X:3110[A]:THR:O | 3:X:3112[A]:TYR:N | 2.26 | 0.68 |
| 3:a:2942[A]:LEU:HD13 | 3:a:3033[A]:PHE:CE1 | 2.28 | 0.68 |
| 3:a:2942[B]:LEU:HD13 | 3:a:3033[B]:PHE:CE1 | 2.28 | 0.68 |
| 3:a:3194[A]:GLY:C | 3:a:3195[A]:MET:HG2 | 2.17 | 0.68 |
| 1:b:28:ASP:OD2 | 1:b:83:HIS:NE2 | 2.22 | 0.68 |
| 1:b:964:ILE:HG12 | 1:b:971:THR:HG22 | 1.76 | 0.68 |
| 2:c:2711:HIS:HA | 2:c:2714:VAL:HG22 | 1.76 | 0.68 |
| 3:d:2961[B]:HIS:CE1 | 3:d:2980[B]:HIS:NE2 | 2.57 | 0.68 |
| 3:C:2972[B]:GLY:HA2 | 3:L:3086[B]:GLU:CG | 2.24 | 0.68 |
| 3:C:3077[A]:ASP:CB | 3:C:3080[A]:ASP:OD2 | 2.42 | 0.68 |
| 3:C:3230[B]:PHE:CB | 3:C:3243[B]:GLY:N | 2.56 | 0.68 |
| 3:F:3161[B]:GLU:HG2 | 3:a:3079[B]:CYS:CB | 2.22 | 0.68 |
| 3:I:3089[B]:HIS:CD2 | 3:R:2971[B]:ASP:C | 2.70 | 0.68 |
| 3:I:3150[B]:LYS:HZ1 | 3:R:3162[B]:ASP:C | 2.01 | 0.68 |
| 3:I:3221[A]:ALA:HB2 | 3:I:3256[A]:TRP:H | 1.57 | 0.68 |
| 3:L:3077[A]:ASP:HB2 | 3:L:3080[A]:ASP:OD2 | 1.93 | 0.68 |
| 3:L:3176[A]:LYS:C | 3:L:3177[A]:SER:HG | 1.98 | 0.68 |
| 1:M:622:HIS:CE1 | 1:M:767:LYS:H | 2.12 | 0.68 |
| 2:N:2900:SER:HA | 1:P:1075:GLU:HG2 | 1.74 | 0.68 |
| 3:O:2937[A]:ASN:HB2 | 3:O:3006[A]:LYS:CE | 2.14 | 0.68 |
| 3:O:3108[B]:HIS:HB2 | 3:X:2970[B]:PRO:HA | 1.75 | 0.68 |
| 3:O:3220[B]:ARG:HG2 | 3:O:3221[B]:ALA:N | 2.09 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2966[B]:SER:HB2 | 3:R:2977[B]:CYS:CB | 2.21 | 0.68 |
| 2:W:2267:HIS:HD2 | 2:W:2297:HIS:HE1 | 1.42 | 0.68 |
| 3:X:3031[B]:ASN:OD1 | 3:X:3033[B]:PHE:N | 2.27 | 0.68 |
| 3:X:3284[B]:LYS:HA | 3:X:3284[B]:LYS:CE | 2.22 | 0.68 |
| 1:Y:1414:THR:HG23 | 1:Y:1477:LEU:HD13 | 1.74 | 0.68 |
| 3:a:2930[B]:LEU:H | 3:a:2930[B]:LEU:CD2 | 1.98 | 0.68 |
| 3:a:2952[B]:ALA:H | 3:a:2953[B]:GLY:CA | 2.04 | 0.68 |
| 3:d:3077[B]:ASP:CB | 3:d:3080[B]:ASP:OD2 | 2.42 | 0.68 |
| 3:d:3110[B]:THR:O | 3:d:3112[B]:TYR:N | 2.26 | 0.68 |
| 3:d:3176[A]:LYS:HB3 | 3:d:3176[A]:LYS:HZ2 | 1.59 | 0.68 |
| 3:d:3279[A]:ASP:OD1 | 3:d:3279[A]:ASP:N | 2.25 | 0.68 |
| 3:C:2937[B]:ASN:CB | 3:C:3006[B]:LYS:HD3 | 2.23 | 0.68 |
| 3:C:3031[B]:ASN:OD1 | 3:C:3033[B]:PHE:N | 2.26 | 0.68 |
| 3:C:3150[B]:LYS:C | 3:L:3159[B]:SER:OG | 2.37 | 0.68 |
| 3:C:3220[B]:ARG:HG2 | 3:C:3221[B]:ALA:N | 2.09 | 0.68 |
| 3:L:2937[B]:ASN:CB | 3:L:3006[B]:LYS:HD3 | 2.23 | 0.68 |
| 3:L:2948[B]:ASP:CB | 3:L:2949[B]:LYS:HA | 2.16 | 0.68 |
| 3:L:3089[B]:HIS:ND1 | 3:L:3119[B]:HIS:CE1 | 2.61 | 0.68 |
| 3:L:3230[A]:PHE:CB | 3:L:3243[A]:GLY:N | 2.56 | 0.68 |
| 3:O:2960[B]:PHE:HD1 | 3:O:2960[B]:PHE:H | 1.41 | 0.68 |
| 3:O:2968[B]:GLN:HG2 | 3:X:2984[B]:THR:HB | 1.75 | 0.68 |
| 3:O:2970[B]:PRO:CG | 3:X:2991[B]:LEU:HA | 1.99 | 0.68 |
| 3:O:3163[B]:ASN:HB3 | 3:X:3149[B]:ASN:CA | 1.99 | 0.68 |
| 3:O:3220[B]:ARG:HG3 | 3:O:3220[B]:ARG:NH1 | 1.98 | 0.68 |
| 3:U:3176[B]:LYS:HD3 | 3:d:3152[B]:LYS:HD2 | 1.74 | 0.68 |
| 3:U:3230[B]:PHE:CB | 3:U:3243[B]:GLY:N | 2.56 | 0.68 |
| 3:U:3284[A]:LYS:HA | 3:U:3284[A]:LYS:CE | 2.22 | 0.68 |
| 3:U:3307[A]:PHE:CE1 | 3:U:3309[A]:PRO:HG3 | 2.16 | 0.68 |
| 1:V:1304:ASP:N | 1:V:1305:GLY:HA2 | 2.08 | 0.68 |
| 3:X:2960[B]:PHE:H | 3:X:2960[B]:PHE:HD1 | 1.41 | 0.68 |
| 3:X:3031[A]:ASN:OD1 | 3:X:3033[A]:PHE:N | 2.26 | 0.68 |
| 3:X:3176[B]:LYS:NZ | 3:X:3176[B]:LYS:HB3 | 2.08 | 0.68 |
| 2:Z:2722:GLN:NE2 | 2:Z:2769:PHE:O | 2.24 | 0.68 |
| 3:a:3110[B]:THR:O | 3:a:3112[B]:TYR:N | 2.26 | 0.68 |
| 3:d:2937[A]:ASN:CB | 3:d:3006[A]:LYS:HD3 | 2.23 | 0.68 |
| 3:d:3089[A]:HIS:ND1 | 3:d:3119[A]:HIS:CE1 | 2.61 | 0.68 |
| 3:C:2971[B]:ASP:CG | 3:C:2973[B]:THR:OG1 | 2.37 | 0.68 |
| 3:C:3077[B]:ASP:HB2 | 3:C:3080[B]:ASP:OD2 | 1.93 | 0.68 |
| 3:F:2937[A]:ASN:CB | 3:F:3006[A]:LYS:HD3 | 2.23 | 0.68 |
| 3:F:2979[B]:GLN:NE2 | 3:F:3155[B]:MET:HE2 | 2.09 | 0.68 |
| 3:F:3089[B]:HIS:ND1 | 3:F:3119[B]:HIS:CE1 | 2.61 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3160[B]:SER:O | 3:a:3150[B]:LYS:HD2 | 1.71 | 0.68 |
| 3:F:3173[B]:THR:CG2 | 3:a:3173[B]:THR:OG1 | 2.42 | 0.68 |
| 3:I:2983[B]:VAL:CB | 3:R:3160[B]:SER:CA | 2.70 | 0.68 |
| 3:I:3077[A]:ASP:CB | 3:I:3080[A]:ASP:OD2 | 2.42 | 0.68 |
| 3:I:3107[B]:LEU:CG | 3:R:2975[B]:PHE:HD1 | 2.06 | 0.68 |
| 3:I:3133[B]:LEU:O | 3:I:3134[B]:GLN:C | 2.32 | 0.68 |
| 2:K:2824:CYS:HA | 2:K:2829:CYS:HA | 1.75 | 0.68 |
| 3:L:2960[A]:PHE:H | 3:L:2960[A]:PHE:HD1 | 1.41 | 0.68 |
| 3:L:2960[B]:PHE:HD1 | 3:L:2960[B]:PHE:H | 1.41 | 0.68 |
| 3:L:3110[A]:THR:O | 3:L:3112[A]:TYR:N | 2.26 | 0.68 |
| 2:N:2149:ALA:HA | 2:N:2260:GLU:HG2 | 1.75 | 0.68 |
| 3:O:2968[B]:GLN:HA | 3:X:2988[B]:TRP:HD1 | 1.58 | 0.68 |
| 3:O:2971[A]:ASP:CG | 3:O:2973[A]:THR:OG1 | 2.37 | 0.68 |
| 3:O:3024[A]:LEU:CD1 | 3:O:3025[A]:VAL:H | 1.83 | 0.68 |
| 3:O:3077[B]:ASP:CB | 3:O:3080[B]:ASP:OD2 | 2.42 | 0.68 |
| 3:O:3089[B]:HIS:ND1 | 3:O:3119[B]:HIS:CE1 | 2.61 | 0.68 |
| 2:Q:2172:ILE:HG13 | 2:Q:2173:VAL:HG13 | 1.74 | 0.68 |
| 2:Q:2903:TYR:OH | 3:R:2932[A]:PRO:HD2 | 1.94 | 0.68 |
| 3:R:2937[A]:ASN:CB | 3:R:3006[A]:LYS:HD3 | 2.23 | 0.68 |
| 3:R:2952[B]:ALA:H | 3:R:2953[B]:GLY:CA | 2.04 | 0.68 |
| 3:R:3077[B]:ASP:CB | 3:R:3080[B]:ASP:OD2 | 2.42 | 0.68 |
| 3:U:3110[A]:THR:O | 3:U:3112[A]:TYR:N | 2.26 | 0.68 |
| 3:U:3220[A]:ARG:HG2 | 3:U:3221[A]:ALA:N | 2.09 | 0.68 |
| 2:W:2235:PRO:HG3 | 2:W:2240:GLN:HE22 | 1.58 | 0.68 |
| 3:X:3089[A]:HIS:ND1 | 3:X:3119[A]:HIS:CE1 | 2.61 | 0.68 |
| 3:X:3298[A]:ASN:HA | 3:X:3299[A]:LEU:HB2 | 1.76 | 0.68 |
| 1:Y:1656:ASP:C | 3:d:3006[B]:LYS:HD2 | 2.19 | 0.68 |
| 3:a:3077[A]:ASP:HB2 | 3:a:3080[A]:ASP:OD2 | 1.93 | 0.68 |
| 3:a:3220[A]:ARG:HG2 | 3:a:3221[A]:ALA:N | 2.09 | 0.68 |
| 3:d:3031[A]:ASN:OD1 | 3:d:3033[A]:PHE:N | 2.26 | 0.68 |
| 3:d:3298[A]:ASN:HA | 3:d:3299[A]:LEU:HB2 | 1.76 | 0.68 |
| 1:A:1140:ASN:ND2 | 1:A:1236:TYR:OH | 2.27 | 0.68 |
| 2:B:2226:GLU:OE2 | 2:B:2277:LYS:N | 2.27 | 0.68 |
| 3:C:3110[B]:THR:O | 3:C:3112[B]:TYR:N | 2.26 | 0.68 |
| 3:C:3153[B]:LYS:O | 3:L:3155[B]:MET:N | 2.27 | 0.68 |
| 3:C:3298[B]:ASN:HA | 3:C:3299[B]:LEU:HB2 | 1.76 | 0.68 |
| 3:F:2979[A]:GLN:NE2 | 3:F:3155[A]:MET:HE2 | 2.09 | 0.68 |
| 3:F:3077[A]:ASP:CB | 3:F:3080[A]:ASP:OD2 | 2.42 | 0.68 |
| 3:F:3153[B]:LYS:HD3 | 3:a:2988[B]:TRP:HD1 | 1.58 | 0.68 |
| 3:F:3253[B]:GLU:CA | 3:a:3252[B]:TYR:O | 2.42 | 0.68 |
| 3:F:3298[B]:ASN:HA | 3:F:3299[B]:LEU:HB2 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:474:LEU:H | 1:G:474:LEU:HD13 | 1.59 | 0.68 |
| 3:I:3110[B]:THR:O | 3:I:3112[B]:TYR:N | 2.26 | 0.68 |
| 3:I:3221[B]:ALA:CB | 3:R:2965[B]:LEU:H | 1.77 | 0.68 |
| 3:I:3288[A]:MET:HA | 3:I:3295[A]:LEU:HG | 1.76 | 0.68 |
| 1:M:1078:ARG:NH2 | 2:Q:2875:SER:O | 2.26 | 0.68 |
| 1:M:1357:ARG:HH11 | 1:M:1357:ARG:HB3 | 1.59 | 0.68 |
| 2:N:2476:LEU:HG | 2:N:2480:LEU:HG | 1.76 | 0.68 |
| 3:O:3025[B]:VAL:HG22 | 3:O:3047[B]:ARG:NH1 | 2.01 | 0.68 |
| 3:O:3185[B]:TYR:C | 3:O:3186[B]:GLU:OE2 | 2.37 | 0.68 |
| 3:O:3298[B]:ASN:HA | 3:O:3299[B]:LEU:HB2 | 1.76 | 0.68 |
| 2:Q:2680:HIS:HD1 | 2:Q:2714:VAL:HG11 | 1.57 | 0.68 |
| 1:S:1617:LYS:HE2 | 3:X:3135[B]:LYS:HZ3 | 1.59 | 0.68 |
| 3:U:2965[B]:LEU:CG | 3:d:3220[B]:ARG:HH11 | 2.04 | 0.68 |
| 3:U:3031[A]:ASN:OD1 | 3:U:3033[A]:PHE:N | 2.26 | 0.68 |
| 3:U:3077[B]:ASP:CB | 3:U:3080[B]:ASP:OD2 | 2.42 | 0.68 |
| 3:U:3256[B]:TRP:HB3 | 3:d:2969[B]:TYR:HB2 | 1.62 | 0.68 |
| 3:X:3133[A]:LEU:O | 3:X:3134[A]:GLN:C | 2.32 | 0.68 |
| 1:Y:1620:LEU:HD12 | 3:d:3189[B]:ASN:CB | 2.21 | 0.68 |
| 3:a:3077[B]:ASP:CB | 3:a:3080[B]:ASP:OD2 | 2.42 | 0.68 |
| 3:a:3284[B]:LYS:HA | 3:a:3284[B]:LYS:CE | 2.21 | 0.68 |
| 1:b:11:THR:HG22 | 1:b:13:ASP:H | 1.58 | 0.68 |
| 3:d:2986[A]:PRO:HB2 | 3:d:3127[A]:TRP:CZ3 | 2.29 | 0.68 |
| 3:d:3230[B]:PHE:CB | 3:d:3243[B]:GLY:N | 2.56 | 0.68 |
| 3:C:2937[A]:ASN:CB | 3:C:3006[A]:LYS:HD3 | 2.23 | 0.68 |
| 3:C:3288[A]:MET:HA | 3:C:3295[A]:LEU:HG | 1.76 | 0.68 |
| 3:F:2965[B]:LEU:CB | 3:a:3256[B]:TRP:HE1 | 2.05 | 0.68 |
| 3:F:3173[B]:THR:CG2 | 3:F:3174[B]:GLY:N | 2.55 | 0.68 |
| 3:F:3249[B]:GLY:N | 3:a:2974[B]:ALA:H | 1.92 | 0.68 |
| 3:F:3288[A]:MET:HA | 3:F:3295[A]:LEU:HG | 1.76 | 0.68 |
| 3:L:2942[B]:LEU:HD13 | 3:L:3033[B]:PHE:CE1 | 2.28 | 0.68 |
| 3:L:3031[B]:ASN:OD1 | 3:L:3033[B]:PHE:N | 2.26 | 0.68 |
| 2:N:2597:MET:HE2 | 2:N:2598:PRO:HD2 | 1.74 | 0.68 |
| 3:O:3288[A]:MET:HA | 3:O:3295[A]:LEU:HG | 1.76 | 0.68 |
| 1:P:883:CYS:N | 1:P:894:CYS:SG | 2.67 | 0.68 |
| 3:R:2960[B]:PHE:H | 3:R:2960[B]:PHE:HD1 | 1.41 | 0.68 |
| 3:R:3031[B]:ASN:OD1 | 3:R:3033[B]:PHE:N | 2.26 | 0.68 |
| 3:U:2966[A]:SER:HB2 | 3:U:2977[A]:CYS:CB | 2.21 | 0.68 |
| 3:U:2973[B]:THR:CG2 | 3:d:3222[B]:ILE:CG2 | 2.65 | 0.68 |
| 3:U:2986[B]:PRO:HB2 | 3:U:3127[B]:TRP:CZ3 | 2.29 | 0.68 |
| 3:X:2986[B]:PRO:HB2 | 3:X:3127[B]:TRP:CZ3 | 2.29 | 0.68 |
| 3:X:3220[B]:ARG:HG2 | 3:X:3221[B]:ALA:N | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3298[B]:ASN:HA | 3:X:3299[B]:LEU:HB2 | 1.76 | 0.68 |
| 1:Y:418:ASP:OD1 | 1:Y:418:ASP:N | 2.26 | 0.68 |
| 2:Z:2236:ALA:HB3 | 2:Z:2239:LYS:HB2 | 1.76 | 0.68 |
| 3:a:2930[A]:LEU:HD22 | 3:a:2930[A]:LEU:N | 2.02 | 0.68 |
| 3:d:3230[A]:PHE:CB | 3:d:3243[A]:GLY:N | 2.56 | 0.68 |
| 3:d:3288[A]:MET:HA | 3:d:3295[A]:LEU:HG | 1.76 | 0.68 |
| 1:A:449:ASP:OD2 | 1:A:1280:GLN:NE2 | 2.28 | 0.67 |
| 1:A:1189:ASP:HA | 2:E:2809:LEU:HD12 | 1.76 | 0.67 |
| 3:C:2979[B]:GLN:NE2 | 3:C:3155[B]:MET:HE2 | 2.09 | 0.67 |
| 3:C:2986[A]:PRO:HB2 | 3:C:3127[A]:TRP:CZ3 | 2.30 | 0.67 |
| 3:C:3176[B]:LYS:HB3 | 3:C:3176[B]:LYS:NZ | 2.08 | 0.67 |
| 3:C:3288[B]:MET:HA | 3:C:3295[B]:LEU:HG | 1.76 | 0.67 |
| 3:F:2961[B]:HIS:CG | 3:a:2975[B]:PHE:HZ | 2.10 | 0.67 |
| 3:F:3154[B]:PRO:HB3 | 3:a:3174[B]:GLY:H | 1.52 | 0.67 |
| 3:F:3156[B]:MET:SD | 3:a:2982[B]:MET:HG3 | 2.34 | 0.67 |
| 3:F:3176[B]:LYS:NZ | 3:F:3176[B]:LYS:HB3 | 2.08 | 0.67 |
| 3:F:3298[A]:ASN:HA | 3:F:3299[A]:LEU:HB2 | 1.76 | 0.67 |
| 3:I:2971[B]:ASP:CG | 3:I:2973[B]:THR:OG1 | 2.37 | 0.67 |
| 3:I:3152[B]:LYS:CB | 3:R:3171[B]:HIS:N | 2.53 | 0.67 |
| 3:O:2965[B]:LEU:CG | 3:X:2979[B]:GLN:OE1 | 2.43 | 0.67 |
| 3:O:2986[A]:PRO:HB2 | 3:O:3127[A]:TRP:CZ3 | 2.30 | 0.67 |
| 3:O:3176[A]:LYS:HZ2 | 3:O:3176[A]:LYS:HB3 | 1.56 | 0.67 |
| 3:O:3298[B]:ASN:HB2 | 3:O:3299[B]:LEU:C | 2.20 | 0.67 |
| 1:P:556:GLY:H | 1:P:558:HIS:CE1 | 2.12 | 0.67 |
| 2:Q:2870:LEU:HA | 2:Q:2877:ILE:HD11 | 1.76 | 0.67 |
| 3:U:2942[B]:LEU:HD13 | 3:U:3033[B]:PHE:CE1 | 2.28 | 0.67 |
| 3:U:3185[A]:TYR:C | 3:U:3186[A]:GLU:OE2 | 2.37 | 0.67 |
| 1:V:804:ASP:OD1 | 1:V:805:VAL:N | 2.27 | 0.67 |
| 2:W:2650:GLY:N | 2:W:2651:GLN:HA | 2.09 | 0.67 |
| 2:Z:2890:VAL:N | 2:Z:2891:LEU:HA | 2.08 | 0.67 |
| 3:a:3031[A]:ASN:OD1 | 3:a:3033[A]:PHE:N | 2.27 | 0.67 |
| 2:c:2889:ALA:N | 2:c:2890:VAL:HA | 2.08 | 0.67 |
| 3:d:3176[A]:LYS:HB3 | 3:d:3176[A]:LYS:NZ | 2.08 | 0.67 |
| 3:d:3298[B]:ASN:HA | 3:d:3299[B]:LEU:HB2 | 1.76 | 0.67 |
| 1:A:566:ARG:HH12 | 1:A:743:ASN:HB3 | 1.58 | 0.67 |
| 3:C:3025[A]:VAL:HG22 | 3:C:3047[A]:ARG:NH1 | 2.02 | 0.67 |
| 3:C:3147[B]:GLU:HB2 | 3:C:3149[B]:ASN:ND2 | 2.09 | 0.67 |
| 3:C:3153[B]:LYS:HE2 | 3:L:3158[B]:PHE:CG | 2.25 | 0.67 |
| 3:C:3253[B]:GLU:CA | 3:L:3253[B]:GLU:HA | 2.24 | 0.67 |
| 1:D:238:ASN:OD1 | 1:D:238:ASN:N | 2.20 | 0.67 |
| 1:D:566:ARG:NH1 | 1:D:759:SER:OG | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:2124:SER:HB2 | 2:E:2129:PRO:HG2 | 1.75 | 0.67 |
| 3:F:2971[A]:ASP:CG | 3:F:2973[A]:THR:OG1 | 2.37 | 0.67 |
| 3:F:3149[B]:ASN:CG | 3:a:3163[B]:ASN:HD22 | 1.98 | 0.67 |
| 3:F:3255[B]:PRO:C | 3:a:2966[B]:SER:CA | 2.67 | 0.67 |
| 3:I:2977[B]:CYS:HB3 | 3:R:2982[B]:MET:HE3 | 1.75 | 0.67 |
| 3:L:2986[B]:PRO:HB2 | 3:L:3127[B]:TRP:CZ3 | 2.29 | 0.67 |
| 3:O:2971[B]:ASP:CG | 3:O:2973[B]:THR:OG1 | 2.37 | 0.67 |
| 3:O:2986[B]:PRO:HB2 | 3:O:3127[B]:TRP:CZ3 | 2.29 | 0.67 |
| 3:O:3256[B]:TRP:NE1 | 3:X:3161[B]:GLU:CD | 2.52 | 0.67 |
| 3:R:3110[A]:THR:O | 3:R:3112[A]:TYR:N | 2.26 | 0.67 |
| 3:U:2970[B]:PRO:N | 3:d:3086[B]:GLU:OE1 | 2.27 | 0.67 |
| 3:U:2974[B]:ALA:CB | 3:d:3220[B]:ARG:HG2 | 2.22 | 0.67 |
| 3:U:2979[B]:GLN:NE2 | 3:U:3155[B]:MET:HE2 | 2.09 | 0.67 |
| 3:U:3298[A]:ASN:HB2 | 3:U:3299[A]:LEU:C | 2.19 | 0.67 |
| 3:X:3011[A]:TYR:HB3 | 3:X:3121[A]:SER:HB2 | 1.77 | 0.67 |
| 3:X:3288[B]:MET:HA | 3:X:3295[B]:LEU:HG | 1.77 | 0.67 |
| 2:Z:2687:ILE:HD11 | 2:Z:2695:MET:HG2 | 1.75 | 0.67 |
| 3:a:2937[A]:ASN:CB | 3:a:3006[A]:LYS:HD3 | 2.23 | 0.67 |
| 3:a:3288[B]:MET:HA | 3:a:3295[B]:LEU:HG | 1.76 | 0.67 |
| 3:d:2965[A]:LEU:CD1 | 3:d:2974[A]:ALA:HA | 2.22 | 0.67 |
| 3:d:2971[A]:ASP:CG | 3:d:2973[A]:THR:OG1 | 2.37 | 0.67 |
| 3:C:2971[A]:ASP:CG | 3:C:2973[A]:THR:OG1 | 2.37 | 0.67 |
| 3:C:3031[A]:ASN:OD1 | 3:C:3033[A]:PHE:N | 2.26 | 0.67 |
| 3:C:3077[B]:ASP:CB | 3:C:3080[B]:ASP:OD2 | 2.42 | 0.67 |
| 3:C:3176[A]:LYS:HZ2 | 3:C:3176[A]:LYS:HB3 | 1.59 | 0.67 |
| 3:C:3185[B]:TYR:C | 3:C:3186[B]:GLU:OE2 | 2.37 | 0.67 |
| 3:C:3254[B]:MET:O | 3:L:2977[B]:CYS:N | 2.03 | 0.67 |
| 3:F:2986[A]:PRO:HB2 | 3:F:3127[A]:TRP:CZ3 | 2.30 | 0.67 |
| 1:G:492:ARG:HD2 | 1:G:692:VAL:HG13 | 1.76 | 0.67 |
| 1:G:1140:ASN:ND2 | 1:G:1236:TYR:OH | 2.28 | 0.67 |
| 2:H:2542:TYR:HA | 2:H:2547:MET:HE1 | 1.75 | 0.67 |
| 3:I:3077[B]:ASP:CB | 3:I:3080[B]:ASP:OD2 | 2.42 | 0.67 |
| 3:I:3150[B]:LYS:CB | 3:R:3169[B]:LYS:HG3 | 2.22 | 0.67 |
| 3:I:3150[B]:LYS:CG | 3:R:3158[B]:PHE:CA | 2.40 | 0.67 |
| 3:I:3220[B]:ARG:HG2 | 3:I:3221[B]:ALA:N | 2.08 | 0.67 |
| 3:I:3255[B]:PRO:HG2 | 3:R:2964[B]:PRO:HD2 | 1.74 | 0.67 |
| 3:L:2971[A]:ASP:CG | 3:L:2973[A]:THR:OG1 | 2.37 | 0.67 |
| 3:O:2961[A]:HIS:CE1 | 3:O:2980[A]:HIS:NE2 | 2.57 | 0.67 |
| 3:O:3254[B]:MET:CB | 3:X:3159[B]:SER:OG | 2.40 | 0.67 |
| 3:R:2971[A]:ASP:CG | 3:R:2973[A]:THR:OG1 | 2.37 | 0.67 |
| 3:R:2971[B]:ASP:CG | 3:R:2973[B]:THR:OG1 | 2.37 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2979[A]:GLN:NE2 | 3:R:3155[A]:MET:HE2 | 2.09 | 0.67 |
| 3:R:3176[B]:LYS:NZ | 3:R:3176[B]:LYS:HB3 | 2.08 | 0.67 |
| 3:R:3298[B]:ASN:HB2 | 3:R:3299[B]:LEU:C | 2.20 | 0.67 |
| 3:U:2969[A]:TYR:HD2 | 3:U:2971[A]:ASP:N | 1.85 | 0.67 |
| 3:U:3197[B]:ILE:HD12 | 1:V:1617:LYS:O | 1.94 | 0.67 |
| 3:U:3255[B]:PRO:HB2 | 3:d:2975[B]:PHE:CA | 2.21 | 0.67 |
| 3:U:3279[B]:ASP:OD1 | 3:U:3279[B]:ASP:N | 2.25 | 0.67 |
| 3:X:2971[A]:ASP:CG | 3:X:2973[A]:THR:OG1 | 2.37 | 0.67 |
| 2:Z:2457:LYS:O | 2:Z:2460:SER:OG | 2.12 | 0.67 |
| 3:a:3298[A]:ASN:HB2 | 3:a:3299[A]:LEU:C | 2.19 | 0.67 |
| 3:d:2986[B]:PRO:HB2 | 3:d:3127[B]:TRP:CZ3 | 2.30 | 0.67 |
| 3:d:3023[B]:ILE:HA | 3:d:3026[B]:THR:OG1 | 1.95 | 0.67 |
| 2:B:2554:PRO:HB3 | 2:B:2556:TYR:HB2 | 1.75 | 0.67 |
| 3:C:2982[B]:MET:HB2 | 3:L:3156[B]:MET:CG | 2.23 | 0.67 |
| 3:C:3160[B]:SER:CA | 3:L:2983[B]:VAL:HG21 | 2.13 | 0.67 |
| 3:F:2986[B]:PRO:HB2 | 3:F:3127[B]:TRP:CZ3 | 2.30 | 0.67 |
| 3:F:3089[A]:HIS:ND1 | 3:F:3119[A]:HIS:CE1 | 2.61 | 0.67 |
| 3:F:3220[A]:ARG:HG2 | 3:F:3221[A]:ALA:N | 2.09 | 0.67 |
| 3:F:3255[B]:PRO:HA | 3:a:2965[B]:LEU:CA | 2.18 | 0.67 |
| 3:F:3298[B]:ASN:HB2 | 3:F:3299[B]:LEU:C | 2.20 | 0.67 |
| 3:I:3185[A]:TYR:C | 3:I:3186[A]:GLU:OE2 | 2.37 | 0.67 |
| 3:I:3255[B]:PRO:HB3 | 3:R:2964[B]:PRO:CA | 2.20 | 0.67 |
| 3:I:3288[B]:MET:HA | 3:I:3295[B]:LEU:HG | 1.77 | 0.67 |
| 2:K:2690:HIS:ND1 | 2:K:2886:VAL:O | 2.23 | 0.67 |
| 3:L:2961[A]:HIS:HB3 | 3:L:3111[A]:SER:HG | 1.58 | 0.67 |
| 3:L:2979[A]:GLN:NE2 | 3:L:3155[A]:MET:HE2 | 2.09 | 0.67 |
| 3:L:3011[B]:TYR:HB3 | 3:L:3121[B]:SER:HB2 | 1.77 | 0.67 |
| 3:L:3137[B]:ARG:CB | 3:L:3139[B]:LEU:HD23 | 2.25 | 0.67 |
| 3:O:2971[B]:ASP:OD1 | 3:X:3158[B]:PHE:HZ | 1.78 | 0.67 |
| 3:O:3176[A]:LYS:HB3 | 3:O:3176[A]:LYS:NZ | 2.08 | 0.67 |
| 1:P:567:LEU:H | 1:P:571:PRO:HB3 | 1.59 | 0.67 |
| 1:P:588:GLU:HG3 | 1:P:724:LYS:HD2 | 1.76 | 0.67 |
| 3:R:3011[A]:TYR:HB3 | 3:R:3121[A]:SER:HB2 | 1.76 | 0.67 |
| 3:R:3288[B]:MET:HA | 3:R:3295[B]:LEU:HG | 1.76 | 0.67 |
| 3:U:2979[A]:GLN:NE2 | 3:U:3155[A]:MET:HE2 | 2.09 | 0.67 |
| 3:U:3169[B]:LYS:HE3 | 3:d:3147[B]:GLU:CA | 2.21 | 0.67 |
| 3:U:3170[B]:ALA:C | 3:d:3148[B]:ILE:HG22 | 2.18 | 0.67 |
| 3:a:2979[B]:GLN:NE2 | 3:a:3155[B]:MET:HE2 | 2.09 | 0.67 |
| 1:b:804:ASP:OD1 | 1:b:805:VAL:N | 2.28 | 0.67 |
| 1:b:871:GLN:NE2 | 1:b:964:ILE:O | 2.28 | 0.67 |
| 1:b:883:CYS:N | 1:b:894:CYS:SG | 2.66 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3031[B]:ASN:OD1 | 3:d:3033[B]:PHE:N | 2.27 | 0.67 |
| 2:B:2252:GLU:HG2 | 2:B:2385:ILE:HG23 | 1.75 | 0.67 |
| 3:C:2961[B]:HIS:HB2 | 3:C:2992[B]:TYR:CE2 | 2.30 | 0.67 |
| 3:C:3023[B]:ILE:HA | 3:C:3026[B]:THR:OG1 | 1.95 | 0.67 |
| 2:E:2340:ALA:HB1 | 2:E:2341:PRO:HD2 | 1.77 | 0.67 |
| 3:F:2962[B]:GLY:O | 3:a:3255[B]:PRO:HG3 | 1.94 | 0.67 |
| 3:F:2982[B]:MET:HE1 | 3:a:2977[B]:CYS:HB2 | 1.75 | 0.67 |
| 3:F:3252[B]:TYR:HA | 3:a:3108[B]:HIS:CD2 | 2.29 | 0.67 |
| 1:G:534:ASP:HB2 | 1:G:541:LYS:HE2 | 1.76 | 0.67 |
| 1:G:930:ASP:OD1 | 1:G:1051:ARG:NH2 | 2.27 | 0.67 |
| 3:I:3023[B]:ILE:HA | 3:I:3026[B]:THR:OG1 | 1.95 | 0.67 |
| 3:I:3176[B]:LYS:HB3 | 3:I:3176[B]:LYS:NZ | 2.08 | 0.67 |
| 3:I:3298[B]:ASN:HA | 3:I:3299[B]:LEU:HB2 | 1.76 | 0.67 |
| 3:L:3011[A]:TYR:HB3 | 3:L:3121[A]:SER:HB2 | 1.76 | 0.67 |
| 3:L:3023[B]:ILE:HA | 3:L:3026[B]:THR:OG1 | 1.95 | 0.67 |
| 3:L:3185[B]:TYR:C | 3:L:3186[B]:GLU:OE2 | 2.37 | 0.67 |
| 1:M:864:ASP:HB3 | 1:M:869:GLY:HA3 | 1.76 | 0.67 |
| 2:N:2370:MET:HE1 | 2:Q:2094:ARG:HD3 | 1.77 | 0.67 |
| 3:O:2969[B]:TYR:HD2 | 3:X:2988[B]:TRP:O | 1.78 | 0.67 |
| 3:O:3293[B]:LYS:HB2 | 3:O:3294[B]:SER:HB2 | 0.82 | 0.67 |
| 1:S:533:VAL:HG12 | 1:S:540:THR:HG22 | 1.76 | 0.67 |
| 3:U:2961[B]:HIS:CE1 | 3:U:2980[B]:HIS:NE2 | 2.57 | 0.67 |
| 3:U:3089[B]:HIS:ND1 | 3:U:3119[B]:HIS:CE1 | 2.61 | 0.67 |
| 3:X:2971[B]:ASP:CG | 3:X:2973[B]:THR:OG1 | 2.37 | 0.67 |
| 3:a:2986[A]:PRO:HB2 | 3:a:3127[A]:TRP:CZ3 | 2.30 | 0.67 |
| 3:a:3077[A]:ASP:CB | 3:a:3080[A]:ASP:OD2 | 2.42 | 0.67 |
| 3:d:2960[A]:PHE:HD1 | 3:d:2960[A]:PHE:H | 1.41 | 0.67 |
| 3:d:3137[B]:ARG:CB | 3:d:3139[B]:LEU:HD23 | 2.25 | 0.67 |
| 3:C:2986[B]:PRO:HB2 | 3:C:3127[B]:TRP:CZ3 | 2.30 | 0.67 |
| 3:C:3089[A]:HIS:ND1 | 3:C:3119[A]:HIS:CE1 | 2.61 | 0.67 |
| 3:C:3153[B]:LYS:C | 3:L:3173[B]:THR:CA | 2.65 | 0.67 |
| 3:C:3176[A]:LYS:HB3 | 3:C:3176[A]:LYS:NZ | 2.08 | 0.67 |
| 3:C:3220[A]:ARG:HG2 | 3:C:3221[A]:ALA:N | 2.09 | 0.67 |
| 3:C:3252[B]:TYR:CZ | 3:L:3223[B]:GLY:C | 2.72 | 0.67 |
| 2:E:2303:ARG:NH2 | 2:E:2372:GLU:O | 2.27 | 0.67 |
| 3:F:2980[B]:HIS:CB | 3:a:2968[B]:GLN:HG2 | 2.22 | 0.67 |
| 3:F:3108[B]:HIS:CD2 | 3:a:3252[B]:TYR:H | 2.08 | 0.67 |
| 3:F:3137[B]:ARG:CB | 3:F:3139[B]:LEU:HD23 | 2.25 | 0.67 |
| 3:F:3230[B]:PHE:CB | 3:F:3243[B]:GLY:N | 2.56 | 0.67 |
| 3:I:2986[A]:PRO:HB2 | 3:I:3127[A]:TRP:CZ3 | 2.29 | 0.67 |
| 3:I:3031[B]:ASN:OD1 | 3:I:3033[B]:PHE:N | 2.26 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3256[B]:TRP:CG | 3:R:2966[B]:SER:C | 2.60 | 0.67 |
| 1:J:479:CYS:HB3 | 1:J:670:PRO:HG3 | 1.76 | 0.67 |
| 2:K:2107:LEU:HD23 | 2:K:2208:PRO:HB2 | 1.76 | 0.67 |
| 2:K:2235:PRO:HG3 | 2:K:2240:GLN:HE22 | 1.58 | 0.67 |
| 3:L:2961[A]:HIS:HB2 | 3:L:2992[A]:TYR:CE2 | 2.30 | 0.67 |
| 3:L:3147[A]:GLU:HB2 | 3:L:3149[A]:ASN:ND2 | 2.09 | 0.67 |
| 1:M:46:ASP:OD2 | 1:M:249:ARG:NH2 | 2.28 | 0.67 |
| 2:N:2806:ALA:HB2 | 2:N:2856:ILE:HD11 | 1.77 | 0.67 |
| 3:O:2970[B]:PRO:C | 3:X:2991[B]:LEU:N | 2.52 | 0.67 |
| 3:O:2979[A]:GLN:NE2 | 3:O:3155[A]:MET:HE2 | 2.09 | 0.67 |
| 3:O:3031[B]:ASN:OD1 | 3:O:3033[B]:PHE:N | 2.26 | 0.67 |
| 3:R:2961[A]:HIS:HB2 | 3:R:2992[A]:TYR:CE2 | 2.30 | 0.67 |
| 3:R:2984[B]:THR:HG22 | 3:R:3151[B]:LEU:HD23 | 1.77 | 0.67 |
| 3:R:2986[B]:PRO:HB2 | 3:R:3127[B]:TRP:CZ3 | 2.30 | 0.67 |
| 3:R:3220[B]:ARG:HG2 | 3:R:3221[B]:ALA:N | 2.08 | 0.67 |
| 3:R:3279[B]:ASP:OD1 | 3:R:3279[B]:ASP:N | 2.25 | 0.67 |
| 3:U:3023[A]:ILE:HA | 3:U:3026[A]:THR:OG1 | 1.95 | 0.67 |
| 3:U:3077[A]:ASP:CB | 3:U:3080[A]:ASP:OD2 | 2.42 | 0.67 |
| 3:X:2984[A]:THR:HG22 | 3:X:3151[A]:LEU:HD23 | 1.77 | 0.67 |
| 3:X:3077[A]:ASP:CB | 3:X:3080[A]:ASP:OD2 | 2.42 | 0.67 |
| 3:X:3298[A]:ASN:HB2 | 3:X:3299[A]:LEU:C | 2.20 | 0.67 |
| 3:a:2986[B]:PRO:HB2 | 3:a:3127[B]:TRP:CZ3 | 2.30 | 0.67 |
| 3:a:3147[A]:GLU:HB2 | 3:a:3149[A]:ASN:ND2 | 2.09 | 0.67 |
| 2:c:2107:LEU:HD23 | 2:c:2208:PRO:HB2 | 1.77 | 0.67 |
| 2:B:2877:ILE:H | 1:D:1078:ARG:NH1 | 1.92 | 0.67 |
| 3:C:2960[A]:PHE:H | 3:C:2960[A]:PHE:HD1 | 1.41 | 0.67 |
| 3:C:3011[B]:TYR:HB3 | 3:C:3121[B]:SER:HB2 | 1.77 | 0.67 |
| 3:C:3156[B]:MET:CG | 3:L:2982[B]:MET:CG | 2.73 | 0.67 |
| 3:C:3298[B]:ASN:HB2 | 3:C:3299[B]:LEU:C | 2.20 | 0.67 |
| 1:D:1498:ASN:ND2 | 1:D:1500:THR:O | 2.27 | 0.67 |
| 3:F:3011[B]:TYR:HB3 | 3:F:3121[B]:SER:HB2 | 1.77 | 0.67 |
| 3:F:3023[A]:ILE:HA | 3:F:3026[A]:THR:OG1 | 1.95 | 0.67 |
| 3:F:3077[B]:ASP:CB | 3:F:3080[B]:ASP:OD2 | 2.42 | 0.67 |
| 3:F:3137[A]:ARG:CB | 3:F:3139[A]:LEU:HD23 | 2.25 | 0.67 |
| 3:I:2966[B]:SER:C | 3:R:3256[B]:TRP:HB3 | 2.20 | 0.67 |
| 3:I:3176[A]:LYS:HB3 | 3:I:3176[A]:LYS:HZ2 | 1.59 | 0.67 |
| 1:J:245:GLU:OE2 | 1:J:249:ARG:NH1 | 2.27 | 0.67 |
| 3:L:2930[B]:LEU:HD22 | 3:L:2930[B]:LEU:N | 2.02 | 0.67 |
| 3:L:2984[B]:THR:HG22 | 3:L:3151[B]:LEU:HD23 | 1.77 | 0.67 |
| 3:L:3023[A]:ILE:HA | 3:L:3026[A]:THR:OG1 | 1.95 | 0.67 |
| 3:O:3077[A]:ASP:CB | 3:O:3080[A]:ASP:OD2 | 2.42 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3137[B]:ARG:CB | 3:O:3139[B]:LEU:HD23 | 2.25 | 0.67 |
| 3:O:3255[B]:PRO:HA | 3:X:3161[B]:GLU:N | 2.09 | 0.67 |
| 1:P:1304:ASP:N | 1:P:1305:GLY:HA2 | 2.10 | 0.67 |
| 3:R:3023[A]:ILE:HA | 3:R:3026[A]:THR:OG1 | 1.95 | 0.67 |
| 1:S:11:THR:HG22 | 1:S:13:ASP:H | 1.58 | 0.67 |
| 3:U:3279[A]:ASP:OD1 | 3:U:3279[A]:ASP:N | 2.25 | 0.67 |
| 3:X:3220[A]:ARG:HG2 | 3:X:3221[A]:ALA:N | 2.08 | 0.67 |
| 1:Y:829:ALA:HA | 1:Y:830:ASN:C | 2.19 | 0.67 |
| 1:Y:1401:ARG:HD2 | 3:d:3182[B]:GLN:OE1 | 1.92 | 0.67 |
| 3:a:3211[B]:ASP:OD1 | 3:a:3211[B]:ASP:N | 2.27 | 0.67 |
| 1:b:1033:LEU:HD21 | 1:b:1183:GLU:HB3 | 1.76 | 0.67 |
| 1:b:1301:PRO:HB3 | 1:b:1308:VAL:HG22 | 1.77 | 0.67 |
| 3:F:3147[A]:GLU:HB2 | 3:F:3149[A]:ASN:ND2 | 2.10 | 0.67 |
| 3:F:3169[B]:LYS:C | 3:a:3152[B]:LYS:HG3 | 2.19 | 0.67 |
| 3:I:2960[A]:PHE:HD1 | 3:I:2960[A]:PHE:H | 1.41 | 0.67 |
| 3:I:2988[A]:TRP:CE3 | 3:I:2989[A]:HIS:CE1 | 2.83 | 0.67 |
| 3:I:3149[B]:ASN:HD22 | 3:R:3163[B]:ASN:C | 2.02 | 0.67 |
| 3:I:3255[B]:PRO:HB3 | 3:R:2964[B]:PRO:CD | 2.24 | 0.67 |
| 3:I:3298[A]:ASN:HD21 | 3:I:3301[A]:PRO:HA | 1.60 | 0.67 |
| 3:L:3169[A]:LYS:C | 3:L:3172[A]:SER:HG | 1.98 | 0.67 |
| 3:L:3220[A]:ARG:HG2 | 3:L:3221[A]:ALA:N | 2.08 | 0.67 |
| 3:O:3147[B]:GLU:HB2 | 3:O:3149[B]:ASN:ND2 | 2.09 | 0.67 |
| 3:O:3169[B]:LYS:HZ1 | 3:X:3148[B]:ILE:HB | 1.60 | 0.67 |
| 3:R:2960[A]:PHE:H | 3:R:2960[A]:PHE:HD1 | 1.41 | 0.67 |
| 3:R:3147[B]:GLU:HB2 | 3:R:3149[B]:ASN:ND2 | 2.09 | 0.67 |
| 1:S:401:VAL:HG22 | 1:S:662:SER:HB3 | 1.76 | 0.67 |
| 3:U:3031[B]:ASN:OD1 | 3:U:3033[B]:PHE:N | 2.26 | 0.67 |
| 3:U:3185[B]:TYR:C | 3:U:3186[B]:GLU:OE2 | 2.37 | 0.67 |
| 3:U:3254[B]:MET:HE3 | 3:d:3254[B]:MET:CE | 1.90 | 0.67 |
| 1:V:325:THR:OG1 | 1:V:329:ARG:O | 2.07 | 0.67 |
| 3:X:2965[A]:LEU:CD1 | 3:X:2975[A]:PHE:H | 2.08 | 0.67 |
| 3:X:2986[A]:PRO:HB2 | 3:X:3127[A]:TRP:CZ3 | 2.30 | 0.67 |
| 3:X:3298[B]:ASN:HB2 | 3:X:3299[B]:LEU:C | 2.20 | 0.67 |
| 1:Y:863:ALA:O | 1:Y:865:LYS:NZ | 2.27 | 0.67 |
| 3:a:2956[B]:LYS:C | 3:a:2960[B]:PHE:CE1 | 2.47 | 0.67 |
| 3:a:2969[A]:TYR:HD2 | 3:a:2971[A]:ASP:N | 1.85 | 0.67 |
| 3:a:2971[A]:ASP:CG | 3:a:2973[A]:THR:OG1 | 2.37 | 0.67 |
| 3:a:2971[B]:ASP:CG | 3:a:2973[B]:THR:OG1 | 2.37 | 0.67 |
| 3:a:2988[B]:TRP:CE3 | 3:a:2989[B]:HIS:CE1 | 2.83 | 0.67 |
| 3:a:3137[B]:ARG:CB | 3:a:3139[B]:LEU:HD23 | 2.25 | 0.67 |
| 3:d:3011[A]:TYR:HB3 | 3:d:3121[A]:SER:HB2 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3077[A]:ASP:CB | 3:d:3080[A]:ASP:OD2 | 2.42 | 0.67 |
| 3:d:3220[B]:ARG:HG2 | 3:d:3221[B]:ALA:N | 2.09 | 0.67 |
| 3:C:2930[A]:LEU:HD22 | 3:C:2930[A]:LEU:N | 2.02 | 0.67 |
| 3:C:2966[A]:SER:HB2 | 3:C:2977[A]:CYS:CB | 2.21 | 0.67 |
| 1:D:1520:GLN:HE21 | 1:D:1526:LYS:HG3 | 1.60 | 0.67 |
| 2:E:2525:LYS:HE2 | 2:E:2620:ILE:HG21 | 1.76 | 0.67 |
| 3:F:2969[A]:TYR:HD2 | 3:F:2971[A]:ASP:N | 1.84 | 0.67 |
| 3:F:2969[B]:TYR:CE1 | 3:a:2961[B]:HIS:CG | 2.80 | 0.67 |
| 3:F:2984[A]:THR:HG22 | 3:F:3151[A]:LEU:HD23 | 1.77 | 0.67 |
| 3:F:2988[B]:TRP:CH2 | 3:a:2975[B]:PHE:HE2 | 2.13 | 0.67 |
| 1:G:164:GLU:OE1 | 1:G:296:ARG:NH1 | 2.27 | 0.67 |
| 3:I:2979[B]:GLN:NE2 | 3:I:3155[B]:MET:HE2 | 2.09 | 0.67 |
| 3:I:3220[A]:ARG:HG2 | 3:I:3221[A]:ALA:N | 2.09 | 0.67 |
| 3:I:3221[B]:ALA:HB2 | 3:R:2965[B]:LEU:N | 2.05 | 0.67 |
| 3:L:2988[A]:TRP:CE3 | 3:L:2989[A]:HIS:CE1 | 2.83 | 0.67 |
| 3:L:3077[B]:ASP:CB | 3:L:3080[B]:ASP:OD2 | 2.42 | 0.67 |
| 3:L:3284[B]:LYS:HA | 3:L:3284[B]:LYS:CE | 2.22 | 0.67 |
| 3:O:2930[A]:LEU:HD22 | 3:O:2930[A]:LEU:N | 2.02 | 0.67 |
| 3:O:2988[B]:TRP:CE3 | 3:O:2989[B]:HIS:CE1 | 2.83 | 0.67 |
| 3:O:3137[A]:ARG:CB | 3:O:3139[A]:LEU:HD23 | 2.25 | 0.67 |
| 3:O:3284[A]:LYS:HA | 3:O:3284[A]:LYS:CE | 2.22 | 0.67 |
| 3:R:2957[B]:ILE:CA | 3:R:2960[B]:PHE:CE1 | 2.78 | 0.67 |
| 3:U:2975[B]:PHE:HE1 | 3:d:3253[B]:GLU:CD | 2.02 | 0.67 |
| 3:U:2975[B]:PHE:HE1 | 3:d:3253[B]:GLU:CG | 2.08 | 0.67 |
| 3:U:3011[A]:TYR:HB3 | 3:U:3121[A]:SER:HB2 | 1.77 | 0.67 |
| 3:U:3137[A]:ARG:CB | 3:U:3139[A]:LEU:HD23 | 2.25 | 0.67 |
| 2:W:2569:TRP:CD1 | 2:W:2746:MET:HG2 | 2.29 | 0.67 |
| 2:W:2800:LYS:HB3 | 3:X:3023[A]:ILE:HD13 | 1.77 | 0.67 |
| 3:X:2960[A]:PHE:H | 3:X:2960[A]:PHE:HD1 | 1.41 | 0.67 |
| 3:X:3011[B]:TYR:HB3 | 3:X:3121[B]:SER:HB2 | 1.77 | 0.67 |
| 3:X:3077[B]:ASP:CB | 3:X:3080[B]:ASP:OD2 | 2.42 | 0.67 |
| 1:Y:1616:LYS:HZ2 | 3:d:3188[B]:ASP:HA | 1.58 | 0.67 |
| 3:a:2960[B]:PHE:H | 3:a:2960[B]:PHE:HD1 | 1.41 | 0.67 |
| 3:a:2984[A]:THR:HG22 | 3:a:3151[A]:LEU:HD23 | 1.77 | 0.67 |
| 3:d:2930[B]:LEU:HD22 | 3:d:2930[B]:LEU:N | 2.02 | 0.67 |
| 3:d:3023[A]:ILE:HA | 3:d:3026[A]:THR:OG1 | 1.95 | 0.67 |
| 3:d:3147[A]:GLU:HB2 | 3:d:3149[A]:ASN:ND2 | 2.09 | 0.67 |
| 2:B:2226:GLU:N | 2:B:2226:GLU:OE1 | 2.28 | 0.67 |
| 3:C:2961[A]:HIS:HB2 | 3:C:2992[A]:TYR:CE2 | 2.30 | 0.67 |
| 3:F:2983[B]:VAL:H | 3:a:3160[B]:SER:CB | 2.07 | 0.67 |
| 3:F:3023[B]:ILE:HA | 3:F:3026[B]:THR:OG1 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3298[A]:ASN:HB2 | 3:F:3299[A]:LEU:C | 2.19 | 0.67 |
| 1:G:240:PHE:HA | 1:G:263:ALA:HB3 | 1.76 | 0.67 |
| 3:I:2961[A]:HIS:HB2 | 3:I:2992[A]:TYR:CE2 | 2.30 | 0.67 |
| 3:I:3011[B]:TYR:HB3 | 3:I:3121[B]:SER:HB2 | 1.77 | 0.67 |
| 3:I:3089[B]:HIS:ND1 | 3:I:3119[B]:HIS:CE1 | 2.61 | 0.67 |
| 3:I:3090[B]:ASN:CB | 3:R:2972[B]:GLY:HA3 | 2.20 | 0.67 |
| 3:I:3147[A]:GLU:HB2 | 3:I:3149[A]:ASN:ND2 | 2.09 | 0.67 |
| 1:M:92:TRP:O | 1:M:212:ASN:ND2 | 2.27 | 0.67 |
| 1:M:944:GLU:O | 1:M:957:ASN:ND2 | 2.28 | 0.67 |
| 2:N:2565:THR:HA | 2:N:2568:HIS:HD2 | 1.59 | 0.67 |
| 3:O:2961[B]:HIS:HB2 | 3:O:2992[B]:TYR:CE2 | 2.30 | 0.67 |
| 3:O:2963[B]:MET:CE | 3:X:2975[B]:PHE:CE1 | 2.78 | 0.67 |
| 3:O:3011[B]:TYR:HB3 | 3:O:3121[B]:SER:HB2 | 1.77 | 0.67 |
| 3:O:3220[A]:ARG:HG2 | 3:O:3221[A]:ALA:N | 2.09 | 0.67 |
| 3:O:3254[B]:MET:HG2 | 3:X:3159[B]:SER:OG | 1.95 | 0.67 |
| 3:O:3298[A]:ASN:HA | 3:O:3299[A]:LEU:HB2 | 1.76 | 0.67 |
| 3:R:2988[A]:TRP:CE3 | 3:R:2989[A]:HIS:CE1 | 2.83 | 0.67 |
| 3:R:2988[B]:TRP:CE3 | 3:R:2989[B]:HIS:CE1 | 2.83 | 0.67 |
| 2:T:2107:LEU:HA | 2:T:2110:MET:HG2 | 1.77 | 0.67 |
| 3:U:2961[A]:HIS:HB2 | 3:U:2992[A]:TYR:CE2 | 2.30 | 0.67 |
| 3:U:2961[B]:HIS:HB2 | 3:U:2992[B]:TYR:CE2 | 2.30 | 0.67 |
| 3:U:2971[B]:ASP:O | 3:d:3247[B]:VAL:C | 2.38 | 0.67 |
| 3:U:2986[A]:PRO:HB2 | 3:U:3127[A]:TRP:CZ3 | 2.29 | 0.67 |
| 3:U:3025[B]:VAL:HG22 | 3:U:3047[B]:ARG:NH1 | 2.01 | 0.67 |
| 3:X:2984[B]:THR:HG22 | 3:X:3151[B]:LEU:HD23 | 1.77 | 0.67 |
| 3:X:3185[A]:TYR:C | 3:X:3186[A]:GLU:OE2 | 2.37 | 0.67 |
| 3:a:3023[B]:ILE:HA | 3:a:3026[B]:THR:OG1 | 1.95 | 0.67 |
| 3:a:3185[A]:TYR:C | 3:a:3186[A]:GLU:OE2 | 2.38 | 0.67 |
| 3:a:3298[B]:ASN:CB | 3:a:3300[B]:LEU:CD2 | 2.61 | 0.67 |
| 3:a:3298[B]:ASN:HB2 | 3:a:3299[B]:LEU:C | 2.20 | 0.67 |
| 2:c:2800:LYS:HB3 | 3:d:3023[A]:ILE:HD13 | 1.77 | 0.67 |
| 3:d:3185[A]:TYR:C | 3:d:3186[A]:GLU:OE2 | 2.37 | 0.67 |
| 3:d:3217[A]:PHE:HE1 | 3:d:3230[A]:PHE:HZ | 0.80 | 0.67 |
| 6:r:1:NAG:H4 | 6:r:2:NAG:O7 | 1.94 | 0.67 |
| 1:D:1019:HIS:NE2 | 1:D:1046:HIS:CE1 | 2.63 | 0.66 |
| 2:E:2570:HIS:CD2 | 2:E:2711:HIS:HE1 | 2.13 | 0.66 |
| 2:E:2711:HIS:HA | 2:E:2714:VAL:HG22 | 1.77 | 0.66 |
| 3:F:2961[B]:HIS:HB2 | 3:F:2992[B]:TYR:CE2 | 2.30 | 0.66 |
| 3:F:2988[B]:TRP:CE3 | 3:F:2989[B]:HIS:CE1 | 2.83 | 0.66 |
| 3:I:2960[B]:PHE:H | 3:I:2960[B]:PHE:HD1 | 1.41 | 0.66 |
| 3:I:2970[B]:PRO:HA | 3:R:2985[B]:PHE:HZ | 1.60 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2984[A]:THR:HG22 | 3:I:3151[A]:LEU:HD23 | 1.77 | 0.66 |
| 3:I:3137[B]:ARG:CB | 3:I:3139[B]:LEU:HD23 | 2.25 | 0.66 |
| 3:L:3288[B]:MET:HA | 3:L:3295[B]:LEU:HG | 1.76 | 0.66 |
| 1:M:327:ASP:OD1 | 1:M:328:LYS:N | 2.27 | 0.66 |
| 3:O:3023[B]:ILE:HA | 3:O:3026[B]:THR:OG1 | 1.95 | 0.66 |
| 3:O:3149[B]:ASN:OD1 | 3:O:3150[B]:LYS:HB2 | 1.96 | 0.66 |
| 3:O:3196[B]:THR:OG1 | 3:O:3199[B]:GLN:CG | 2.44 | 0.66 |
| 3:O:3211[A]:ASP:OD1 | 3:O:3211[A]:ASP:N | 2.27 | 0.66 |
| 2:Q:2217:ILE:HG22 | 2:Q:2218:SER:H | 1.60 | 0.66 |
| 3:R:2961[B]:HIS:HB2 | 3:R:2992[B]:TYR:CE2 | 2.30 | 0.66 |
| 3:R:3176[A]:LYS:HB3 | 3:R:3176[A]:LYS:HZ2 | 1.60 | 0.66 |
| 3:R:3220[A]:ARG:HG2 | 3:R:3221[A]:ALA:N | 2.09 | 0.66 |
| 2:T:2107:LEU:HD23 | 2:T:2208:PRO:HB2 | 1.76 | 0.66 |
| 3:U:2971[A]:ASP:CG | 3:U:2973[A]:THR:OG1 | 2.37 | 0.66 |
| 3:U:2979[A]:GLN:HE21 | 3:U:3155[A]:MET:HE2 | 1.55 | 0.66 |
| 3:U:3176[A]:LYS:HB3 | 3:U:3176[A]:LYS:NZ | 2.09 | 0.66 |
| 3:U:3255[B]:PRO:CB | 3:d:2975[B]:PHE:HA | 2.20 | 0.66 |
| 1:V:492:ARG:NH1 | 1:V:701:TYR:OH | 2.27 | 0.66 |
| 3:X:2961[A]:HIS:HB2 | 3:X:2992[A]:TYR:CE2 | 2.30 | 0.66 |
| 3:X:2988[A]:TRP:CE3 | 3:X:2989[A]:HIS:CE1 | 2.83 | 0.66 |
| 3:X:3036[B]:GLY:O | 3:X:3044[B]:LYS:HA | 1.96 | 0.66 |
| 3:a:2979[A]:GLN:NE2 | 3:a:3155[A]:MET:HE2 | 2.09 | 0.66 |
| 3:a:3023[A]:ILE:HA | 3:a:3026[A]:THR:OG1 | 1.95 | 0.66 |
| 3:a:3185[B]:TYR:C | 3:a:3186[B]:GLU:OE2 | 2.37 | 0.66 |
| 3:d:3011[B]:TYR:HB3 | 3:d:3121[B]:SER:HB2 | 1.77 | 0.66 |
| 3:d:3259[B]:ASP:OD1 | 3:d:3260[B]:ARG:HD2 | 1.95 | 0.66 |
| 1:A:562:GLN:HG3 | 1:A:563:ILE:HG13 | 1.77 | 0.66 |
| 3:C:2956[A]:LYS:C | 3:C:2960[A]:PHE:CE1 | 2.47 | 0.66 |
| 3:F:2961[A]:HIS:HB2 | 3:F:2992[A]:TYR:CE2 | 2.30 | 0.66 |
| 3:F:3036[B]:GLY:O | 3:F:3044[B]:LYS:HA | 1.96 | 0.66 |
| 3:F:3155[B]:MET:CG | 3:a:3153[B]:LYS:C | 2.68 | 0.66 |
| 3:F:3185[B]:TYR:C | 3:F:3186[B]:GLU:OE2 | 2.37 | 0.66 |
| 2:H:2643:GLU:HA | 2:H:2646:ALA:HB3 | 1.75 | 0.66 |
| 3:I:2961[B]:HIS:HB2 | 3:I:2992[B]:TYR:CE2 | 2.30 | 0.66 |
| 3:I:2966[A]:SER:HB2 | 3:I:2977[A]:CYS:CB | 2.21 | 0.66 |
| 3:I:2967[B]:CYS:SG | 3:R:2982[B]:MET:HG3 | 2.34 | 0.66 |
| 3:I:2969[B]:TYR:CD1 | 3:R:2961[B]:HIS:ND1 | 2.44 | 0.66 |
| 3:I:2971[A]:ASP:CG | 3:I:2973[A]:THR:OG1 | 2.37 | 0.66 |
| 3:I:3093[B]:HIS:CD2 | 3:R:2973[B]:THR:OG1 | 2.44 | 0.66 |
| 3:L:3077[A]:ASP:CB | 3:L:3080[A]:ASP:OD2 | 2.42 | 0.66 |
| 3:L:3298[B]:ASN:HA | 3:L:3299[B]:LEU:HB2 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:2252:GLU:CD | 2:N:2393:ARG:HH12 | 2.03 | 0.66 |
| 3:O:2975[B]:PHE:CE2 | 3:X:3172[B]:SER:HB2 | 2.30 | 0.66 |
| 3:O:2994[B]:LYS:O | 3:O:2995[B]:GLN:C | 2.38 | 0.66 |
| 3:O:3023[A]:ILE:HA | 3:O:3026[A]:THR:OG1 | 1.95 | 0.66 |
| 1:P:965:ASP:N | 1:P:965:ASP:OD1 | 2.26 | 0.66 |
| 3:R:3011[B]:TYR:HB3 | 3:R:3121[B]:SER:HB2 | 1.77 | 0.66 |
| 3:U:3147[B]:GLU:HB2 | 3:U:3149[B]:ASN:ND2 | 2.09 | 0.66 |
| 3:U:3259[A]:ASP:OD1 | 3:U:3260[A]:ARG:HD2 | 1.96 | 0.66 |
| 3:U:3298[B]:ASN:HB2 | 3:U:3299[B]:LEU:C | 2.20 | 0.66 |
| 2:W:2823:ILE:HG22 | 2:W:2879:LEU:HG | 1.75 | 0.66 |
| 3:X:2961[B]:HIS:HB2 | 3:X:2992[B]:TYR:CE2 | 2.30 | 0.66 |
| 3:X:3147[A]:GLU:HB2 | 3:X:3149[A]:ASN:ND2 | 2.10 | 0.66 |
| 3:X:3298[B]:ASN:HD21 | 3:X:3301[B]:PRO:HA | 1.60 | 0.66 |
| 3:a:2952[A]:ALA:H | 3:a:2953[A]:GLY:CA | 2.04 | 0.66 |
| 3:a:2961[A]:HIS:HB2 | 3:a:2992[A]:TYR:CE2 | 2.30 | 0.66 |
| 3:a:3024[B]:LEU:CD1 | 3:a:3025[B]:VAL:H | 1.83 | 0.66 |
| 3:a:3031[B]:ASN:OD1 | 3:a:3033[B]:PHE:N | 2.27 | 0.66 |
| 3:a:3036[A]:GLY:O | 3:a:3044[A]:LYS:HA | 1.95 | 0.66 |
| 3:a:3217[A]:PHE:HE1 | 3:a:3230[A]:PHE:HZ | 0.80 | 0.66 |
| 3:d:2979[A]:GLN:HE21 | 3:d:3155[A]:MET:HE2 | 1.55 | 0.66 |
| 3:d:2984[A]:THR:HG22 | 3:d:3151[A]:LEU:HD23 | 1.77 | 0.66 |
| 3:C:2984[B]:THR:HG22 | 3:C:3151[B]:LEU:HD23 | 1.77 | 0.66 |
| 3:C:3023[A]:ILE:HA | 3:C:3026[A]:THR:OG1 | 1.95 | 0.66 |
| 3:C:3036[B]:GLY:O | 3:C:3044[B]:LYS:HA | 1.96 | 0.66 |
| 3:C:3137[A]:ARG:CB | 3:C:3139[A]:LEU:HD23 | 2.25 | 0.66 |
| 3:C:3154[B]:PRO:O | 3:L:3155[B]:MET:CG | 2.43 | 0.66 |
| 3:C:3155[B]:MET:HE2 | 3:L:3153[B]:LYS:HD3 | 1.77 | 0.66 |
| 3:F:3107[B]:LEU:CD1 | 3:a:2975[B]:PHE:CD1 | 2.52 | 0.66 |
| 3:F:3251[B]:ASP:CG | 3:a:3251[B]:ASP:CB | 2.67 | 0.66 |
| 3:F:3259[A]:ASP:OD1 | 3:F:3260[A]:ARG:HD2 | 1.96 | 0.66 |
| 1:G:1166:THR:N | 1:G:1167:ASP:HA | 2.08 | 0.66 |
| 3:I:3196[B]:THR:OG1 | 3:I:3199[B]:GLN:CG | 2.44 | 0.66 |
| 1:J:881:GLN:NE2 | 1:J:888:ALA:O | 2.28 | 0.66 |
| 3:L:2961[B]:HIS:HB2 | 3:L:2992[B]:TYR:CE2 | 2.30 | 0.66 |
| 3:L:3036[B]:GLY:O | 3:L:3044[B]:LYS:HA | 1.95 | 0.66 |
| 3:L:3137[A]:ARG:CB | 3:L:3139[A]:LEU:HD23 | 2.25 | 0.66 |
| 3:L:3185[A]:TYR:C | 3:L:3186[A]:GLU:OE2 | 2.37 | 0.66 |
| 3:L:3298[A]:ASN:HA | 3:L:3299[A]:LEU:HB2 | 1.76 | 0.66 |
| 3:O:2967[B]:CYS:N | 3:X:2979[B]:GLN:NE2 | 2.42 | 0.66 |
| 3:O:2971[B]:ASP:H | 3:X:2992[B]:TYR:H | 1.44 | 0.66 |
| 3:O:3185[A]:TYR:C | 3:O:3186[A]:GLU:OE2 | 2.37 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q:2500:ILE:HG12 | 2:Q:2501:PRO:HD2 | 1.76 | 0.66 |
| 3:U:3149[A]:ASN:OD1 | 3:U:3150[A]:LYS:HB2 | 1.96 | 0.66 |
| 3:U:3170[B]:ALA:O | 3:d:3152[B]:LYS:CE | 2.44 | 0.66 |
| 3:U:3259[B]:ASP:OD1 | 3:U:3260[B]:ARG:HD2 | 1.96 | 0.66 |
| 2:W:2142:ALA:HB2 | 2:W:2433:THR:HG23 | 1.77 | 0.66 |
| 3:X:3137[B]:ARG:CB | 3:X:3139[B]:LEU:HD23 | 2.25 | 0.66 |
| 3:a:3149[A]:ASN:OD1 | 3:a:3150[A]:LYS:HB2 | 1.96 | 0.66 |
| 1:b:949:ASP:HB2 | 1:b:953:GLU:HB2 | 1.76 | 0.66 |
| 2:c:2090:LYS:NZ | 2:c:2099:GLU:OE2 | 2.28 | 0.66 |
| 3:d:2933[B]:SER:O | 3:d:2936[B]:GLU:HB3 | 1.96 | 0.66 |
| 3:d:2961[A]:HIS:HB3 | 3:d:3111[A]:SER:HG | 1.59 | 0.66 |
| 3:d:2988[B]:TRP:CE3 | 3:d:2989[B]:HIS:CE1 | 2.83 | 0.66 |
| 3:d:3036[A]:GLY:O | 3:d:3044[A]:LYS:HA | 1.95 | 0.66 |
| 3:d:3137[A]:ARG:CB | 3:d:3139[A]:LEU:HD23 | 2.25 | 0.66 |
| 3:C:3036[A]:GLY:O | 3:C:3044[A]:LYS:HA | 1.95 | 0.66 |
| 3:F:2960[A]:PHE:HD1 | 3:F:2960[A]:PHE:H | 1.41 | 0.66 |
| 3:F:2960[B]:PHE:H | 3:F:2960[B]:PHE:HD1 | 1.41 | 0.66 |
| 3:F:2981[B]:GLY:N | 3:a:2968[B]:GLN:CG | 2.47 | 0.66 |
| 3:F:2988[A]:TRP:CE3 | 3:F:2989[A]:HIS:CE1 | 2.83 | 0.66 |
| 3:F:3284[B]:LYS:HA | 3:F:3284[B]:LYS:CE | 2.22 | 0.66 |
| 1:G:1263:LEU:HD11 | 1:G:1358:LEU:HD22 | 1.76 | 0.66 |
| 3:I:2966[B]:SER:HB3 | 3:I:2977[B]:CYS:HB2 | 1.78 | 0.66 |
| 3:I:2979[B]:GLN:OE1 | 3:R:2977[B]:CYS:SG | 2.53 | 0.66 |
| 3:I:2994[A]:LYS:O | 3:I:2995[A]:GLN:C | 2.38 | 0.66 |
| 3:I:3132[A]:ALA:HB1 | 3:I:3197[A]:ILE:CD1 | 2.26 | 0.66 |
| 3:I:3185[B]:TYR:C | 3:I:3186[B]:GLU:OE2 | 2.37 | 0.66 |
| 3:I:3252[B]:TYR:CG | 3:R:3108[B]:HIS:CE1 | 2.84 | 0.66 |
| 1:J:949:ASP:HB2 | 1:J:953:GLU:HB2 | 1.76 | 0.66 |
| 3:L:2957[A]:ILE:CA | 3:L:2960[A]:PHE:CE1 | 2.78 | 0.66 |
| 3:L:2984[A]:THR:HG22 | 3:L:3151[A]:LEU:HD23 | 1.77 | 0.66 |
| 3:L:3036[A]:GLY:O | 3:L:3044[A]:LYS:HA | 1.96 | 0.66 |
| 3:L:3149[B]:ASN:OD1 | 3:L:3150[B]:LYS:HB2 | 1.96 | 0.66 |
| 3:L:3288[A]:MET:HA | 3:L:3295[A]:LEU:HG | 1.76 | 0.66 |
| 3:O:2975[B]:PHE:HE2 | 3:X:3172[B]:SER:HB3 | 1.49 | 0.66 |
| 3:O:3036[A]:GLY:O | 3:O:3044[A]:LYS:HA | 1.96 | 0.66 |
| 3:O:3180[B]:TYR:CA | 3:O:3183[B]:LEU:HD22 | 2.26 | 0.66 |
| 3:O:3298[A]:ASN:HB2 | 3:O:3299[A]:LEU:C | 2.20 | 0.66 |
| 3:R:2965[A]:LEU:CD1 | 3:R:2975[A]:PHE:H | 2.08 | 0.66 |
| 3:R:3298[B]:ASN:HA | 3:R:3299[B]:LEU:HB2 | 1.76 | 0.66 |
| 1:S:1442:MET:HE1 | 1:S:1454:PHE:HA | 1.76 | 0.66 |
| 3:U:2967[B]:CYS:O | 3:d:3256[B]:TRP:CD2 | 2.47 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2970[B]:PRO:CB | 3:d:2985[B]:PHE:CE2 | 2.75 | 0.66 |
| 3:U:3150[B]:LYS:HA | 3:d:3154[B]:PRO:O | 1.94 | 0.66 |
| 3:U:3150[B]:LYS:CG | 3:d:3156[B]:MET:HG2 | 2.24 | 0.66 |
| 3:U:3196[B]:THR:OG1 | 3:U:3199[B]:GLN:CG | 2.44 | 0.66 |
| 3:U:3298[B]:ASN:HA | 3:U:3299[B]:LEU:HB2 | 1.76 | 0.66 |
| 1:V:240:PHE:HA | 1:V:263:ALA:HB3 | 1.77 | 0.66 |
| 1:V:450:LYS:HB3 | 1:V:454:GLY:HA3 | 1.75 | 0.66 |
| 3:X:3023[A]:ILE:HA | 3:X:3026[A]:THR:OG1 | 1.95 | 0.66 |
| 3:X:3137[A]:ARG:CB | 3:X:3139[A]:LEU:HD23 | 2.25 | 0.66 |
| 1:Y:1612:THR:C | 3:d:3186[B]:GLU:CB | 2.60 | 0.66 |
| 3:a:3036[B]:GLY:O | 3:a:3044[B]:LYS:HA | 1.95 | 0.66 |
| 3:a:3149[B]:ASN:OD1 | 3:a:3150[B]:LYS:HB2 | 1.96 | 0.66 |
| 3:a:3173[B]:THR:CG2 | 3:a:3174[B]:GLY:N | 2.55 | 0.66 |
| 3:d:3036[B]:GLY:O | 3:d:3044[B]:LYS:HA | 1.96 | 0.66 |
| 3:d:3180[B]:TYR:CA | 3:d:3183[B]:LEU:HD22 | 2.26 | 0.66 |
| 3:d:3196[B]:THR:OG1 | 3:d:3199[B]:GLN:CG | 2.44 | 0.66 |
| 1:A:516:TRP:HB2 | 1:A:579:LEU:HD13 | 1.77 | 0.66 |
| 3:C:2975[B]:PHE:CD2 | 3:L:2979[B]:GLN:N | 2.37 | 0.66 |
| 3:C:3153[B]:LYS:CE | 3:L:3158[B]:PHE:CE2 | 2.71 | 0.66 |
| 3:C:3185[A]:TYR:C | 3:C:3186[A]:GLU:OE2 | 2.37 | 0.66 |
| 3:F:3036[A]:GLY:O | 3:F:3044[A]:LYS:HA | 1.95 | 0.66 |
| 3:F:3157[B]:PRO:HB3 | 3:a:2982[B]:MET:SD | 2.34 | 0.66 |
| 3:F:3196[B]:THR:OG1 | 3:F:3199[B]:GLN:CG | 2.44 | 0.66 |
| 2:H:2251:LEU:O | 2:H:2315:ARG:NH2 | 2.27 | 0.66 |
| 3:I:2961[B]:HIS:HB3 | 3:I:3111[B]:SER:HG | 1.59 | 0.66 |
| 3:I:2970[B]:PRO:CA | 3:R:2989[B]:HIS:CD2 | 2.79 | 0.66 |
| 3:I:2979[A]:GLN:NE2 | 3:I:3155[A]:MET:HE2 | 2.09 | 0.66 |
| 3:I:3152[B]:LYS:HB3 | 3:R:3171[B]:HIS:CA | 2.25 | 0.66 |
| 1:J:875:ALA:O | 1:J:878:GLY:N | 2.20 | 0.66 |
| 1:J:1258:ARG:NH2 | 1:J:1332:ASP:OD1 | 2.29 | 0.66 |
| 3:L:2986[A]:PRO:HB2 | 3:L:3127[A]:TRP:CZ3 | 2.29 | 0.66 |
| 3:L:3147[B]:GLU:HB2 | 3:L:3149[B]:ASN:ND2 | 2.09 | 0.66 |
| 3:L:3180[A]:TYR:CA | 3:L:3183[A]:LEU:HD22 | 2.26 | 0.66 |
| 3:O:2933[B]:SER:O | 3:O:2936[B]:GLU:HB3 | 1.96 | 0.66 |
| 3:O:2961[A]:HIS:HB2 | 3:O:2992[A]:TYR:CE2 | 2.30 | 0.66 |
| 3:O:3011[A]:TYR:HB3 | 3:O:3121[A]:SER:HB2 | 1.77 | 0.66 |
| 3:O:3036[B]:GLY:O | 3:O:3044[B]:LYS:HA | 1.95 | 0.66 |
| 3:O:3253[B]:GLU:HG2 | 3:X:3160[B]:SER:OG | 1.96 | 0.66 |
| 2:Q:2824:CYS:HB2 | 2:Q:2878:ARG:HD2 | 1.77 | 0.66 |
| 3:R:3298[A]:ASN:HB2 | 3:R:3299[A]:LEU:C | 2.20 | 0.66 |
| 3:U:2966[B]:SER:HB2 | 3:U:2977[B]:CYS:CB | 2.21 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2984[A]:THR:HG22 | 3:U:3151[A]:LEU:HD23 | 1.77 | 0.66 |
| 3:U:2984[B]:THR:HG22 | 3:U:3151[B]:LEU:HD23 | 1.77 | 0.66 |
| 3:U:2994[A]:LYS:O | 3:U:2995[A]:GLN:C | 2.38 | 0.66 |
| 3:U:3147[A]:GLU:HB2 | 3:U:3149[A]:ASN:ND2 | 2.09 | 0.66 |
| 3:U:3155[B]:MET:N | 3:d:3150[B]:LYS:CB | 2.58 | 0.66 |
| 3:X:2933[A]:SER:O | 3:X:2936[A]:GLU:HB3 | 1.96 | 0.66 |
| 3:X:2988[B]:TRP:CE3 | 3:X:2989[B]:HIS:CE1 | 2.83 | 0.66 |
| 3:X:3132[A]:ALA:HB1 | 3:X:3197[A]:ILE:CD1 | 2.26 | 0.66 |
| 3:X:3259[B]:ASP:OD1 | 3:X:3260[B]:ARG:HD2 | 1.95 | 0.66 |
| 1:Y:1550:ARG:NE | 3:d:3008[B]:GLY:O | 2.29 | 0.66 |
| 3:a:2961[B]:HIS:HB2 | 3:a:2992[B]:TYR:CE2 | 2.30 | 0.66 |
| 3:a:3132[A]:ALA:HB1 | 3:a:3197[A]:ILE:CD1 | 2.26 | 0.66 |
| 1:b:1172:ALA:HB1 | 1:b:1196:ILE:HG13 | 1.78 | 0.66 |
| 3:d:2957[B]:ILE:CA | 3:d:2960[B]:PHE:CE1 | 2.78 | 0.66 |
| 3:d:2965[B]:LEU:CD1 | 3:d:2975[B]:PHE:H | 2.08 | 0.66 |
| 3:C:2988[B]:TRP:CE3 | 3:C:2989[B]:HIS:CE1 | 2.83 | 0.66 |
| 3:C:3132[A]:ALA:HB1 | 3:C:3197[A]:ILE:CD1 | 2.26 | 0.66 |
| 3:C:3132[B]:ALA:HB1 | 3:C:3197[B]:ILE:CD1 | 2.26 | 0.66 |
| 3:C:3298[A]:ASN:HB2 | 3:C:3299[A]:LEU:C | 2.20 | 0.66 |
| 1:D:930:ASP:OD1 | 1:D:1051:ARG:NH2 | 2.29 | 0.66 |
| 2:E:2252:GLU:HG2 | 2:E:2385:ILE:HG23 | 1.77 | 0.66 |
| 3:F:2971[B]:ASP:CG | 3:F:2973[B]:THR:OG1 | 2.37 | 0.66 |
| 3:F:3132[B]:ALA:HB1 | 3:F:3197[B]:ILE:CD1 | 2.26 | 0.66 |
| 3:F:3169[A]:LYS:C | 3:F:3172[A]:SER:HG | 2.00 | 0.66 |
| 3:F:3196[A]:THR:OG1 | 3:F:3199[A]:GLN:CG | 2.44 | 0.66 |
| 3:F:3248[B]:LEU:C | 3:a:2974[B]:ALA:N | 2.53 | 0.66 |
| 3:F:3259[B]:ASP:OD1 | 3:F:3260[B]:ARG:HD2 | 1.96 | 0.66 |
| 2:H:2415:PRO:HD3 | 2:H:2454:MET:HE1 | 1.77 | 0.66 |
| 2:H:2903:TYR:OH | 3:I:2932[A]:PRO:HD2 | 1.96 | 0.66 |
| 3:I:2964[B]:PRO:CB | 3:R:3221[B]:ALA:CB | 2.70 | 0.66 |
| 3:I:2986[B]:PRO:HB2 | 3:I:3127[B]:TRP:CZ3 | 2.30 | 0.66 |
| 3:I:2988[B]:TRP:CE3 | 3:I:2989[B]:HIS:CE1 | 2.83 | 0.66 |
| 3:I:3137[A]:ARG:CB | 3:I:3139[A]:LEU:HD23 | 2.25 | 0.66 |
| 3:I:3150[B]:LYS:HD2 | 3:R:3160[B]:SER:O | 1.96 | 0.66 |
| 3:I:3163[B]:ASN:CB | 3:R:3150[B]:LYS:NZ | 2.58 | 0.66 |
| 3:I:3259[B]:ASP:OD1 | 3:I:3260[B]:ARG:HD2 | 1.96 | 0.66 |
| 3:I:3298[B]:ASN:HB2 | 3:I:3299[B]:LEU:C | 2.19 | 0.66 |
| 1:J:1427:HIS:CE1 | 1:J:1458:HIS:HE2 | 2.13 | 0.66 |
| 3:L:3132[A]:ALA:HB1 | 3:L:3197[A]:ILE:CD1 | 2.26 | 0.66 |
| 3:L:3196[A]:THR:OG1 | 3:L:3199[A]:GLN:CG | 2.43 | 0.66 |
| 2:N:2472:ASN:ND2 | 4:2:1:NAG:O7 | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2988[A]:TRP:CE3 | 3:O:2989[A]:HIS:CE1 | 2.83 | 0.66 |
| 3:O:3038[B]:ILE:HG23 | 3:X:2969[B]:TYR:CZ | 2.26 | 0.66 |
| 3:O:3196[A]:THR:OG1 | 3:O:3199[A]:GLN:CG | 2.44 | 0.66 |
| 3:O:3259[B]:ASP:OD1 | 3:O:3260[B]:ARG:HD2 | 1.96 | 0.66 |
| 3:O:3279[A]:ASP:OD1 | 3:O:3279[A]:ASP:N | 2.25 | 0.66 |
| 1:P:673:PHE:HB3 | 1:P:677:LEU:HB2 | 1.78 | 0.66 |
| 3:R:2933[A]:SER:O | 3:R:2936[A]:GLU:HB3 | 1.96 | 0.66 |
| 3:R:2979[B]:GLN:NE2 | 3:R:3155[B]:MET:HE2 | 2.09 | 0.66 |
| 3:U:2994[B]:LYS:O | 3:U:2995[B]:GLN:C | 2.38 | 0.66 |
| 3:U:3154[B]:PRO:C | 3:d:3150[B]:LYS:CG | 2.67 | 0.66 |
| 3:X:3036[A]:GLY:O | 3:X:3044[A]:LYS:HA | 1.95 | 0.66 |
| 3:a:2957[A]:ILE:CA | 3:a:2960[A]:PHE:CE1 | 2.78 | 0.66 |
| 3:a:2988[A]:TRP:CE3 | 3:a:2989[A]:HIS:CE1 | 2.83 | 0.66 |
| 3:a:3011[A]:TYR:HB3 | 3:a:3121[A]:SER:HB2 | 1.77 | 0.66 |
| 3:a:3137[A]:ARG:CB | 3:a:3139[A]:LEU:HD23 | 2.25 | 0.66 |
| 3:a:3180[A]:TYR:CA | 3:a:3183[A]:LEU:HD22 | 2.26 | 0.66 |
| 3:a:3180[B]:TYR:CA | 3:a:3183[B]:LEU:HD22 | 2.26 | 0.66 |
| 3:a:3259[A]:ASP:OD1 | 3:a:3260[A]:ARG:HD2 | 1.96 | 0.66 |
| 3:d:2961[B]:HIS:HB2 | 3:d:2992[B]:TYR:CE2 | 2.30 | 0.66 |
| 3:d:3185[B]:TYR:C | 3:d:3186[B]:GLU:OE2 | 2.37 | 0.66 |
| 3:d:3293[B]:LYS:HB2 | 3:d:3294[B]:SER:HB2 | 0.82 | 0.66 |
| 3:d:3298[B]:ASN:HB2 | 3:d:3299[B]:LEU:C | 2.19 | 0.66 |
| 1:A:70:ARG:HA | 1:A:214:GLU:OE1 | 1.95 | 0.66 |
| 3:C:3161[B]:GLU:HA | 3:L:3147[B]:GLU:N | 2.09 | 0.66 |
| 3:C:3298[A]:ASN:HA | 3:C:3299[A]:LEU:HB2 | 1.76 | 0.66 |
| 3:F:2960[B]:PHE:C | 3:a:3255[B]:PRO:HD2 | 2.20 | 0.66 |
| 3:F:2965[A]:LEU:CD1 | 3:F:2975[A]:PHE:H | 2.08 | 0.66 |
| 3:F:3176[A]:LYS:NZ | 3:F:3176[A]:LYS:HB3 | 2.08 | 0.66 |
| 3:F:3180[A]:TYR:CA | 3:F:3183[A]:LEU:HD22 | 2.26 | 0.66 |
| 3:F:3185[A]:TYR:C | 3:F:3186[A]:GLU:OE2 | 2.37 | 0.66 |
| 3:F:3288[B]:MET:HA | 3:F:3295[B]:LEU:HG | 1.76 | 0.66 |
| 1:G:305:ASN:HB3 | 1:G:400:ILE:HG12 | 1.76 | 0.66 |
| 3:I:3298[A]:ASN:HB2 | 3:I:3299[A]:LEU:C | 2.20 | 0.66 |
| 3:L:2933[B]:SER:O | 3:L:2936[B]:GLU:HB3 | 1.96 | 0.66 |
| 3:L:3279[A]:ASP:N | 3:L:3279[A]:ASP:OD1 | 2.25 | 0.66 |
| 3:L:3298[B]:ASN:HB2 | 3:L:3299[B]:LEU:C | 2.20 | 0.66 |
| 1:M:533:VAL:HG12 | 1:M:540:THR:HG22 | 1.77 | 0.66 |
| 3:O:2969[B]:TYR:CB | 3:X:3158[B]:PHE:CE2 | 2.79 | 0.66 |
| 1:P:1315:GLY:HA3 | 1:P:1601:TRP:HB2 | 1.78 | 0.66 |
| 3:R:2986[A]:PRO:HB2 | 3:R:3127[A]:TRP:CZ3 | 2.30 | 0.66 |
| 3:R:3023[B]:ILE:HA | 3:R:3026[B]:THR:OG1 | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3137[A]:ARG:CB | 3:R:3139[A]:LEU:HD23 | 2.25 | 0.66 |
| 3:R:3137[B]:ARG:CB | 3:R:3139[B]:LEU:HD23 | 2.25 | 0.66 |
| 3:R:3288[A]:MET:HA | 3:R:3295[A]:LEU:HG | 1.77 | 0.66 |
| 3:U:2979[B]:GLN:HE22 | 3:d:3153[B]:LYS:HZ1 | 0.69 | 0.66 |
| 3:U:2988[A]:TRP:CE3 | 3:U:2989[A]:HIS:CE1 | 2.83 | 0.66 |
| 3:U:2988[B]:TRP:CE3 | 3:U:2989[B]:HIS:CE1 | 2.83 | 0.66 |
| 3:U:3036[B]:GLY:O | 3:U:3044[B]:LYS:HA | 1.95 | 0.66 |
| 3:U:3132[A]:ALA:HB1 | 3:U:3197[A]:ILE:CD1 | 2.26 | 0.66 |
| 3:U:3298[A]:ASN:HA | 3:U:3299[A]:LEU:HB2 | 1.76 | 0.66 |
| 1:V:105:VAL:HG12 | 1:V:123:PHE:HB3 | 1.77 | 0.66 |
| 1:V:1023:GLY:HA3 | 1:V:1031:ALA:HB2 | 1.77 | 0.66 |
| 3:X:2957[B]:ILE:CA | 3:X:2960[B]:PHE:CE1 | 2.78 | 0.66 |
| 3:a:2957[B]:ILE:CA | 3:a:2960[B]:PHE:CE1 | 2.78 | 0.66 |
| 1:b:324:PRO:HG2 | 1:b:376:ASN:HD21 | 1.61 | 0.66 |
| 3:d:3089[B]:HIS:ND1 | 3:d:3119[B]:HIS:CE1 | 2.61 | 0.66 |
| 3:d:3180[A]:TYR:CA | 3:d:3183[A]:LEU:HD22 | 2.26 | 0.66 |
| 1:A:221:GLN:NE2 | 1:A:267:PHE:O | 2.27 | 0.66 |
| 3:C:2964[B]:PRO:O | 3:L:3255[B]:PRO:C | 2.38 | 0.66 |
| 3:C:2966[A]:SER:HB3 | 3:C:2977[A]:CYS:HB2 | 1.78 | 0.66 |
| 3:C:3148[B]:ILE:HG22 | 3:L:3170[B]:ALA:HA | 1.77 | 0.66 |
| 3:C:3196[B]:THR:OG1 | 3:C:3199[B]:GLN:CG | 2.44 | 0.66 |
| 2:E:2799:LYS:HA | 2:E:2803:ARG:HH12 | 1.60 | 0.66 |
| 3:F:3147[B]:GLU:HB2 | 3:F:3149[B]:ASN:ND2 | 2.09 | 0.66 |
| 3:F:3149[A]:ASN:OD1 | 3:F:3150[A]:LYS:HB2 | 1.96 | 0.66 |
| 3:I:3031[A]:ASN:OD1 | 3:I:3033[A]:PHE:N | 2.26 | 0.66 |
| 3:I:3132[B]:ALA:HB1 | 3:I:3197[B]:ILE:CD1 | 2.26 | 0.66 |
| 3:I:3162[B]:ASP:C | 3:R:3150[B]:LYS:NZ | 2.54 | 0.66 |
| 3:O:2957[B]:ILE:CA | 3:O:2960[B]:PHE:CE1 | 2.78 | 0.66 |
| 3:O:2984[B]:THR:HG22 | 3:O:3151[B]:LEU:HD23 | 1.77 | 0.66 |
| 3:R:2982[A]:MET:CE | 3:R:3254[A]:MET:HE2 | 2.26 | 0.66 |
| 3:R:3031[A]:ASN:OD1 | 3:R:3033[A]:PHE:N | 2.26 | 0.66 |
| 3:R:3149[A]:ASN:OD1 | 3:R:3150[A]:LYS:HB2 | 1.96 | 0.66 |
| 1:S:1567:ASP:OD1 | 1:S:1591:SER:OG | 2.11 | 0.66 |
| 2:T:2090:LYS:NZ | 2:T:2099:GLU:OE2 | 2.28 | 0.66 |
| 3:U:3011[B]:TYR:HB3 | 3:U:3121[B]:SER:HB2 | 1.76 | 0.66 |
| 3:U:3023[B]:ILE:HA | 3:U:3026[B]:THR:OG1 | 1.95 | 0.66 |
| 3:X:2957[A]:ILE:CA | 3:X:2960[A]:PHE:CE1 | 2.78 | 0.66 |
| 1:Y:1546:LYS:CB | 3:d:3001[B]:LYS:HZ2 | 2.02 | 0.66 |
| 3:a:2982[B]:MET:CE | 3:a:3254[B]:MET:HE2 | 2.26 | 0.66 |
| 3:a:2984[B]:THR:HG22 | 3:a:3151[B]:LEU:HD23 | 1.77 | 0.66 |
| 3:a:3196[A]:THR:OG1 | 3:a:3199[A]:GLN:CG | 2.44 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3298[A]:ASN:HA | 3:a:3299[A]:LEU:HB2 | 1.77 | 0.66 |
| 3:a:3298[B]:ASN:HA | 3:a:3299[B]:LEU:HB2 | 1.76 | 0.66 |
| 3:d:2988[A]:TRP:CE3 | 3:d:2989[A]:HIS:CE1 | 2.83 | 0.66 |
| 2:B:2472:ASN:HD21 | 4:i:1:NAG:C7 | 2.08 | 0.66 |
| 3:C:2982[A]:MET:CE | 3:C:3254[A]:MET:HE2 | 2.26 | 0.66 |
| 3:C:3147[A]:GLU:HB2 | 3:C:3149[A]:ASN:ND2 | 2.10 | 0.66 |
| 1:D:110:PHE:N | 1:D:119:LYS:O | 2.29 | 0.66 |
| 1:D:1329:LEU:HB2 | 1:D:1507:THR:HG21 | 1.78 | 0.66 |
| 3:F:2937[B]:ASN:ND2 | 3:F:3006[B]:LYS:HD3 | 2.11 | 0.66 |
| 3:F:2965[B]:LEU:O | 3:a:3256[B]:TRP:N | 2.29 | 0.66 |
| 3:F:2965[B]:LEU:CG | 3:a:3256[B]:TRP:HE1 | 2.09 | 0.66 |
| 3:F:2970[B]:PRO:CA | 3:a:2989[B]:HIS:HD2 | 2.09 | 0.66 |
| 3:F:3155[B]:MET:C | 3:a:3153[B]:LYS:CD | 2.64 | 0.66 |
| 1:G:606:ILE:O | 1:G:610:THR:OG1 | 2.12 | 0.66 |
| 3:I:2937[B]:ASN:HD22 | 3:I:3006[B]:LYS:HD3 | 1.61 | 0.66 |
| 3:I:3116[B]:PHE:CE2 | 3:R:2969[B]:TYR:CG | 2.36 | 0.66 |
| 3:I:3147[B]:GLU:HB2 | 3:I:3149[B]:ASN:ND2 | 2.09 | 0.66 |
| 1:J:527:LEU:HD22 | 1:J:629:MET:HG3 | 1.77 | 0.66 |
| 2:K:2800:LYS:HB3 | 3:L:3023[A]:ILE:HD13 | 1.78 | 0.66 |
| 3:L:2933[A]:SER:O | 3:L:2936[A]:GLU:HB3 | 1.96 | 0.66 |
| 3:L:2937[A]:ASN:HB3 | 3:L:3006[A]:LYS:HD3 | 1.78 | 0.66 |
| 3:L:2988[B]:TRP:CE3 | 3:L:2989[B]:HIS:CE1 | 2.83 | 0.66 |
| 3:L:3132[B]:ALA:HB1 | 3:L:3197[B]:ILE:CD1 | 2.26 | 0.66 |
| 3:L:3180[B]:TYR:CA | 3:L:3183[B]:LEU:HD22 | 2.26 | 0.66 |
| 3:L:3259[B]:ASP:OD1 | 3:L:3260[B]:ARG:HD2 | 1.96 | 0.66 |
| 1:M:1617:LYS:O | 3:R:3197[B]:ILE:HD12 | 1.96 | 0.66 |
| 3:O:2960[A]:PHE:H | 3:O:2960[A]:PHE:HD1 | 1.41 | 0.66 |
| 3:O:3112[B]:TYR:CE2 | 3:X:2969[B]:TYR:OH | 2.46 | 0.66 |
| 3:O:3147[A]:GLU:HB2 | 3:O:3149[A]:ASN:ND2 | 2.09 | 0.66 |
| 1:P:1639:LYS:HD2 | 1:S:472:ASP:HB3 | 1.77 | 0.66 |
| 1:S:1639:LYS:HD2 | 4:BA:1:NAG:C1 | 2.26 | 0.66 |
| 3:U:2937[A]:ASN:ND2 | 3:U:3006[A]:LYS:HD3 | 2.11 | 0.66 |
| 3:U:3180[B]:TYR:CA | 3:U:3183[B]:LEU:HD22 | 2.26 | 0.66 |
| 3:X:2930[B]:LEU:HD22 | 3:X:2930[B]:LEU:N | 2.02 | 0.66 |
| 3:X:2952[B]:ALA:H | 3:X:2953[B]:GLY:CA | 2.04 | 0.66 |
| 1:Y:1348:TRP:HD1 | 1:Y:1403:LEU:HD13 | 1.61 | 0.66 |
| 3:a:2937[B]:ASN:HD22 | 3:a:3006[B]:LYS:HD3 | 1.61 | 0.66 |
| 3:a:3196[B]:THR:OG1 | 3:a:3199[B]:GLN:CG | 2.43 | 0.66 |
| 3:a:3220[B]:ARG:HG2 | 3:a:3221[B]:ALA:N | 2.09 | 0.66 |
| 3:d:2937[A]:ASN:ND2 | 3:d:3006[A]:LYS:HD3 | 2.11 | 0.66 |
| 3:d:2937[B]:ASN:ND2 | 3:d:3006[B]:LYS:HD3 | 2.11 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2952[B]:ALA:H | 3:d:2953[B]:GLY:CA | 2.04 | 0.66 |
| 3:d:2982[B]:MET:CE | 3:d:3254[B]:MET:HE2 | 2.26 | 0.66 |
| 3:d:3259[A]:ASP:OD1 | 3:d:3260[A]:ARG:HD2 | 1.96 | 0.66 |
| 3:C:2937[A]:ASN:HD22 | 3:C:3006[A]:LYS:HD3 | 1.61 | 0.66 |
| 3:C:2966[B]:SER:HB3 | 3:C:2977[B]:CYS:HB2 | 1.77 | 0.66 |
| 3:C:3152[B]:LYS:HB2 | 3:L:3173[B]:THR:N | 2.11 | 0.66 |
| 3:C:3180[B]:TYR:CA | 3:C:3183[B]:LEU:HD22 | 2.26 | 0.66 |
| 1:D:456:GLN:NE2 | 1:D:549:PRO:O | 2.29 | 0.66 |
| 1:D:518:LYS:NZ | 1:D:519:PRO:O | 2.29 | 0.66 |
| 2:E:2412:GLN:HG2 | 2:E:2422:GLU:HA | 1.77 | 0.66 |
| 3:F:2970[B]:PRO:HB3 | 3:a:2989[B]:HIS:HD2 | 1.58 | 0.66 |
| 3:F:3220[B]:ARG:HG2 | 3:F:3221[B]:ALA:N | 2.09 | 0.66 |
| 1:G:126:GLY:HA3 | 1:G:127:GLU:HG3 | 1.77 | 0.66 |
| 3:I:3150[B]:LYS:CE | 3:R:3163[B]:ASN:HB3 | 2.12 | 0.66 |
| 3:L:3220[B]:ARG:HG2 | 3:L:3221[B]:ALA:N | 2.08 | 0.66 |
| 2:N:2830:GLN:OE1 | 2:N:2863:ARG:NH1 | 2.27 | 0.66 |
| 3:O:2968[B]:GLN:CA | 3:X:2988[B]:TRP:CB | 2.67 | 0.66 |
| 3:O:3160[B]:SER:CA | 3:X:3151[B]:LEU:CD1 | 2.59 | 0.66 |
| 1:P:841:LYS:HA | 1:P:1117:ASP:HB2 | 1.78 | 0.66 |
| 3:R:3196[A]:THR:OG1 | 3:R:3199[A]:GLN:CG | 2.44 | 0.66 |
| 3:R:3196[B]:THR:OG1 | 3:R:3199[B]:GLN:CG | 2.44 | 0.66 |
| 1:S:1618:LEU:CD2 | 3:X:3136[B]:TYR:HE2 | 2.08 | 0.66 |
| 3:U:2930[B]:LEU:HD22 | 3:U:2930[B]:LEU:N | 2.02 | 0.66 |
| 3:U:2957[B]:ILE:CA | 3:U:2960[B]:PHE:CE1 | 2.78 | 0.66 |
| 3:U:3132[B]:ALA:HB1 | 3:U:3197[B]:ILE:CD1 | 2.26 | 0.66 |
| 3:U:3171[B]:HIS:HA | 3:d:3152[B]:LYS:HZ3 | 1.55 | 0.66 |
| 3:U:3217[B]:PHE:HB2 | 3:U:3219[B]:LEU:HD21 | 1.78 | 0.66 |
| 3:X:2937[B]:ASN:ND2 | 3:X:3006[B]:LYS:HD3 | 2.11 | 0.66 |
| 3:X:3151[A]:LEU:O | 3:X:3174[A]:GLY:HA3 | 1.96 | 0.66 |
| 3:X:3185[B]:TYR:C | 3:X:3186[B]:GLU:OE2 | 2.37 | 0.66 |
| 1:Y:1250:ILE:O | 1:Y:1473:ARG:NH2 | 2.29 | 0.66 |
| 3:a:3132[B]:ALA:HB1 | 3:a:3197[B]:ILE:CD1 | 2.26 | 0.66 |
| 3:a:3217[B]:PHE:HB2 | 3:a:3219[B]:LEU:HD21 | 1.78 | 0.66 |
| 3:d:2957[A]:ILE:CA | 3:d:2960[A]:PHE:CE1 | 2.78 | 0.66 |
| 3:d:3196[A]:THR:OG1 | 3:d:3199[A]:GLN:CG | 2.44 | 0.66 |
| 3:C:2957[B]:ILE:CA | 3:C:2960[B]:PHE:CE1 | 2.78 | 0.65 |
| 3:C:2968[B]:GLN:HE21 | 3:L:3086[B]:GLU:CG | 2.09 | 0.65 |
| 3:C:2988[A]:TRP:CE3 | 3:C:2989[A]:HIS:CE1 | 2.83 | 0.65 |
| 3:C:3217[B]:PHE:HE1 | 3:C:3230[B]:PHE:HZ | 0.80 | 0.65 |
| 3:C:3259[B]:ASP:OD1 | 3:C:3260[B]:ARG:HD2 | 1.96 | 0.65 |
| 2:E:2149:ALA:HA | 2:E:2260:GLU:HG2 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2961[B]:HIS:CD2 | 3:a:2975[B]:PHE:CZ | 2.83 | 0.65 |
| 3:F:3256[B]:TRP:N | 3:a:2965[B]:LEU:O | 2.17 | 0.65 |
| 3:I:2964[B]:PRO:CA | 3:R:3221[B]:ALA:HB1 | 2.24 | 0.65 |
| 3:I:2984[B]:THR:HG22 | 3:I:3151[B]:LEU:HD23 | 1.77 | 0.65 |
| 3:I:3298[A]:ASN:HA | 3:I:3299[A]:LEU:HB2 | 1.76 | 0.65 |
| 3:L:2957[B]:ILE:CA | 3:L:2960[B]:PHE:CE1 | 2.78 | 0.65 |
| 3:L:3259[A]:ASP:OD1 | 3:L:3260[A]:ARG:HD2 | 1.96 | 0.65 |
| 3:L:3298[B]:ASN:HD21 | 3:L:3301[B]:PRO:HA | 1.60 | 0.65 |
| 1:M:926:LEU:HD11 | 1:M:1043:MET:HB3 | 1.77 | 0.65 |
| 3:O:2937[A]:ASN:ND2 | 3:O:3006[A]:LYS:HD3 | 2.11 | 0.65 |
| 3:O:2937[B]:ASN:ND2 | 3:O:3006[B]:LYS:HD3 | 2.11 | 0.65 |
| 3:O:2973[B]:THR:C | 3:X:2979[B]:GLN:HB2 | 2.21 | 0.65 |
| 3:O:2982[B]:MET:CE | 3:O:3254[B]:MET:HE2 | 2.26 | 0.65 |
| 3:R:2937[B]:ASN:ND2 | 3:R:3006[B]:LYS:HD3 | 2.11 | 0.65 |
| 3:R:3036[A]:GLY:O | 3:R:3044[A]:LYS:HA | 1.95 | 0.65 |
| 3:R:3180[B]:TYR:CA | 3:R:3183[B]:LEU:HD22 | 2.26 | 0.65 |
| 2:T:2885:SER:HB3 | 2:T:2890:VAL:HG22 | 1.77 | 0.65 |
| 3:U:2933[B]:SER:O | 3:U:2936[B]:GLU:HB3 | 1.96 | 0.65 |
| 3:U:3180[A]:TYR:CA | 3:U:3183[A]:LEU:HD22 | 2.26 | 0.65 |
| 3:U:3196[A]:THR:OG1 | 3:U:3199[A]:GLN:CG | 2.44 | 0.65 |
| 1:V:1573:CYS:HB2 | 1:V:1627:ARG:HG2 | 1.78 | 0.65 |
| 3:X:2937[A]:ASN:ND2 | 3:X:3006[A]:LYS:HD3 | 2.11 | 0.65 |
| 1:Y:958:PRO:HB2 | 1:Y:960:PHE:N | 2.12 | 0.65 |
| 3:a:2933[B]:SER:O | 3:a:2936[B]:GLU:HB3 | 1.96 | 0.65 |
| 3:a:2937[A]:ASN:HB3 | 3:a:3006[A]:LYS:HD3 | 1.79 | 0.65 |
| 3:a:3151[B]:LEU:O | 3:a:3174[B]:GLY:HA3 | 1.97 | 0.65 |
| 3:d:3132[B]:ALA:HB1 | 3:d:3197[B]:ILE:CD1 | 2.26 | 0.65 |
| 1:A:70:ARG:NH1 | 1:A:266:LEU:O | 2.29 | 0.65 |
| 3:C:2933[B]:SER:O | 3:C:2936[B]:GLU:HB3 | 1.96 | 0.65 |
| 3:C:2937[B]:ASN:HD22 | 3:C:3006[B]:LYS:HD3 | 1.61 | 0.65 |
| 3:C:3011[A]:TYR:HB3 | 3:C:3121[A]:SER:HB2 | 1.77 | 0.65 |
| 3:C:3151[B]:LEU:O | 3:C:3174[B]:GLY:HA3 | 1.97 | 0.65 |
| 3:F:2957[A]:ILE:CA | 3:F:2960[A]:PHE:CE1 | 2.78 | 0.65 |
| 3:F:2984[B]:THR:HG22 | 3:F:3151[B]:LEU:HD23 | 1.77 | 0.65 |
| 3:F:3180[B]:TYR:CA | 3:F:3183[B]:LEU:HD22 | 2.26 | 0.65 |
| 3:F:3298[B]:ASN:HD21 | 3:F:3301[B]:PRO:HA | 1.60 | 0.65 |
| 3:I:2957[A]:ILE:CA | 3:I:2960[A]:PHE:CE1 | 2.78 | 0.65 |
| 3:I:3023[A]:ILE:HA | 3:I:3026[A]:THR:OG1 | 1.95 | 0.65 |
| 3:I:3149[A]:ASN:OD1 | 3:I:3150[A]:LYS:HB2 | 1.96 | 0.65 |
| 3:I:3171[B]:HIS:C | 3:R:3152[B]:LYS:CB | 2.68 | 0.65 |
| 3:I:3248[B]:LEU:C | 3:R:2974[B]:ALA:N | 2.54 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:2937[A]:ASN:ND2 | 3:L:3006[A]:LYS:HD3 | 2.11 | 0.65 |
| 3:L:3298[A]:ASN:HB2 | 3:L:3299[A]:LEU:C | 2.20 | 0.65 |
| 3:O:3151[A]:LEU:O | 3:O:3174[A]:GLY:HA3 | 1.96 | 0.65 |
| 3:O:3180[A]:TYR:CA | 3:O:3183[A]:LEU:HD22 | 2.26 | 0.65 |
| 3:O:3288[B]:MET:HA | 3:O:3295[B]:LEU:HG | 1.76 | 0.65 |
| 1:P:534:ASP:HB2 | 1:P:541:LYS:HE2 | 1.79 | 0.65 |
| 3:R:3036[B]:GLY:O | 3:R:3044[B]:LYS:HA | 1.96 | 0.65 |
| 3:R:3147[A]:GLU:HB2 | 3:R:3149[A]:ASN:ND2 | 2.09 | 0.65 |
| 3:U:2937[B]:ASN:ND2 | 3:U:3006[B]:LYS:HD3 | 2.11 | 0.65 |
| 3:U:2967[B]:CYS:HB2 | 3:d:3256[B]:TRP:HA | 1.79 | 0.65 |
| 3:U:2975[B]:PHE:HD2 | 3:d:3255[B]:PRO:O | 1.79 | 0.65 |
| 2:W:2687:ILE:HD11 | 2:W:2695:MET:HG2 | 1.79 | 0.65 |
| 3:X:2982[B]:MET:CE | 3:X:3254[B]:MET:HE2 | 2.26 | 0.65 |
| 3:X:3196[B]:THR:OG1 | 3:X:3199[B]:GLN:CG | 2.43 | 0.65 |
| 3:d:2951[B]:ASP:O | 3:d:2956[B]:LYS:CE | 2.45 | 0.65 |
| 3:C:2937[A]:ASN:ND2 | 3:C:3006[A]:LYS:HD3 | 2.11 | 0.65 |
| 1:D:1573:CYS:HB2 | 1:D:1627:ARG:HG2 | 1.79 | 0.65 |
| 3:F:2933[B]:SER:O | 3:F:2936[B]:GLU:HB3 | 1.96 | 0.65 |
| 3:F:2951[B]:ASP:O | 3:F:2956[B]:LYS:CE | 2.45 | 0.65 |
| 3:F:2952[A]:ALA:H | 3:F:2953[A]:GLY:CA | 2.04 | 0.65 |
| 3:F:2965[B]:LEU:CD1 | 3:F:2975[B]:PHE:H | 2.08 | 0.65 |
| 3:F:2982[B]:MET:HE3 | 3:a:2977[B]:CYS:HB3 | 1.76 | 0.65 |
| 3:F:3011[A]:TYR:HB3 | 3:F:3121[A]:SER:HB2 | 1.77 | 0.65 |
| 3:F:3149[B]:ASN:OD1 | 3:F:3150[B]:LYS:HB2 | 1.95 | 0.65 |
| 3:F:3255[B]:PRO:HG2 | 3:a:2962[B]:GLY:C | 2.19 | 0.65 |
| 3:I:2937[A]:ASN:HD22 | 3:I:3006[A]:LYS:HD3 | 1.61 | 0.65 |
| 3:I:3151[A]:LEU:O | 3:I:3174[A]:GLY:HA3 | 1.97 | 0.65 |
| 3:I:3171[B]:HIS:CA | 3:R:3152[B]:LYS:CB | 2.74 | 0.65 |
| 3:I:3180[A]:TYR:CA | 3:I:3183[A]:LEU:HD22 | 2.26 | 0.65 |
| 3:I:3196[A]:THR:OG1 | 3:I:3199[A]:GLN:CG | 2.44 | 0.65 |
| 3:I:3217[A]:PHE:HB2 | 3:I:3219[A]:LEU:HD21 | 1.78 | 0.65 |
| 1:J:450:LYS:HB3 | 1:J:454:GLY:HA3 | 1.79 | 0.65 |
| 1:J:898:GLY:N | 1:J:899:MET:HA | 2.10 | 0.65 |
| 3:L:2937[B]:ASN:ND2 | 3:L:3006[B]:LYS:HD3 | 2.11 | 0.65 |
| 1:M:1280:GLN:NE2 | 1:M:1337:ARG:HB3 | 2.10 | 0.65 |
| 3:O:2963[B]:MET:HG2 | 3:O:3108[B]:HIS:CG | 2.23 | 0.65 |
| 3:R:2933[B]:SER:O | 3:R:2936[B]:GLU:HB3 | 1.96 | 0.65 |
| 3:R:2969[A]:TYR:HD2 | 3:R:2971[A]:ASP:N | 1.84 | 0.65 |
| 3:R:3089[B]:HIS:CE1 | 3:R:3119[B]:HIS:CE1 | 2.81 | 0.65 |
| 3:R:3132[B]:ALA:HB1 | 3:R:3197[B]:ILE:CD1 | 2.26 | 0.65 |
| 3:R:3259[A]:ASP:OD1 | 3:R:3260[A]:ARG:HD2 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3259[B]:ASP:OD1 | 3:R:3260[B]:ARG:HD2 | 1.96 | 0.65 |
| 3:U:2951[A]:ASP:O | 3:U:2956[A]:LYS:CE | 2.45 | 0.65 |
| 3:U:3288[A]:MET:HA | 3:U:3295[A]:LEU:HG | 1.76 | 0.65 |
| 2:W:2889:ALA:N | 2:W:2890:VAL:HA | 2.12 | 0.65 |
| 3:X:2966[A]:SER:HB3 | 3:X:2977[A]:CYS:HB2 | 1.78 | 0.65 |
| 3:X:3293[B]:LYS:HB2 | 3:X:3294[B]:SER:HB2 | 0.82 | 0.65 |
| 1:Y:492:ARG:HD2 | 1:Y:692:VAL:HG22 | 1.78 | 0.65 |
| 1:Y:1140:ASN:ND2 | 1:Y:1236:TYR:OH | 2.30 | 0.65 |
| 3:a:3288[A]:MET:HA | 3:a:3295[A]:LEU:HG | 1.76 | 0.65 |
| 3:d:2961[A]:HIS:HB2 | 3:d:2992[A]:TYR:CE2 | 2.30 | 0.65 |
| 3:d:2979[A]:GLN:NE2 | 3:d:3155[A]:MET:HE2 | 2.09 | 0.65 |
| 3:d:3132[A]:ALA:HB1 | 3:d:3197[A]:ILE:CD1 | 2.26 | 0.65 |
| 3:C:3137[B]:ARG:CB | 3:C:3139[B]:LEU:HD23 | 2.25 | 0.65 |
| 3:C:3180[A]:TYR:CA | 3:C:3183[A]:LEU:HD22 | 2.26 | 0.65 |
| 3:C:3196[A]:THR:OG1 | 3:C:3199[A]:GLN:CG | 2.44 | 0.65 |
| 3:C:3284[A]:LYS:HA | 3:C:3284[A]:LYS:CE | 2.22 | 0.65 |
| 1:D:1019:HIS:NE2 | 1:D:1046:HIS:HE1 | 1.95 | 0.65 |
| 1:D:1153:LYS:HB2 | 1:D:1155:LEU:HD23 | 1.78 | 0.65 |
| 3:F:2937[B]:ASN:HB3 | 3:F:3006[B]:LYS:HD3 | 1.79 | 0.65 |
| 3:F:2957[B]:ILE:CA | 3:F:2960[B]:PHE:CE1 | 2.78 | 0.65 |
| 3:F:3248[B]:LEU:HD11 | 3:a:2973[B]:THR:HG23 | 1.78 | 0.65 |
| 2:H:2889:ALA:N | 2:H:2890:VAL:HA | 2.11 | 0.65 |
| 3:I:2933[A]:SER:O | 3:I:2936[A]:GLU:HB3 | 1.96 | 0.65 |
| 3:I:2957[B]:ILE:CA | 3:I:2960[B]:PHE:CE1 | 2.78 | 0.65 |
| 3:I:2970[B]:PRO:HA | 3:R:2985[B]:PHE:CZ | 2.31 | 0.65 |
| 3:I:2982[B]:MET:SD | 3:R:3157[B]:PRO:N | 2.70 | 0.65 |
| 3:I:3036[B]:GLY:O | 3:I:3044[B]:LYS:HA | 1.95 | 0.65 |
| 3:I:3150[B]:LYS:NZ | 3:R:3162[B]:ASP:C | 2.54 | 0.65 |
| 3:I:3217[B]:PHE:HB2 | 3:I:3219[B]:LEU:HD21 | 1.78 | 0.65 |
| 3:I:3256[B]:TRP:HE1 | 3:R:2965[B]:LEU:HB3 | 1.15 | 0.65 |
| 3:L:3066[B]:TYR:CE1 | 3:L:3193[B]:HIS:HE1 | 2.15 | 0.65 |
| 3:L:3149[A]:ASN:OD1 | 3:L:3150[A]:LYS:HB2 | 1.96 | 0.65 |
| 3:L:3217[A]:PHE:HB2 | 3:L:3219[A]:LEU:HD21 | 1.78 | 0.65 |
| 3:O:2965[B]:LEU:C | 3:X:3153[B]:LYS:HZ3 | 2.05 | 0.65 |
| 3:O:2966[A]:SER:HB3 | 3:O:2977[A]:CYS:HB2 | 1.78 | 0.65 |
| 3:O:3132[A]:ALA:HB1 | 3:O:3197[A]:ILE:CD1 | 2.26 | 0.65 |
| 3:O:3217[B]:PHE:HB2 | 3:O:3219[B]:LEU:HD21 | 1.78 | 0.65 |
| 3:O:3259[A]:ASP:OD1 | 3:O:3260[A]:ARG:HD2 | 1.96 | 0.65 |
| 1:P:1195:ASP:OD1 | 1:P:1196:ILE:N | 2.29 | 0.65 |
| 1:P:1280:GLN:HG2 | 1:P:1337:ARG:HD2 | 1.77 | 0.65 |
| 3:R:3285[B]:VAL:HG22 | 3:R:3286[B]:THR:H | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2933[A]:SER:O | 3:U:2936[A]:GLU:HB3 | 1.96 | 0.65 |
| 3:U:2937[A]:ASN:HD22 | 3:U:3006[A]:LYS:HD3 | 1.61 | 0.65 |
| 3:U:2937[B]:ASN:HD22 | 3:U:3006[B]:LYS:HD3 | 1.61 | 0.65 |
| 3:U:2973[B]:THR:N | 3:d:3247[B]:VAL:HG12 | 2.09 | 0.65 |
| 3:U:2975[B]:PHE:CE1 | 3:d:3253[B]:GLU:CG | 2.80 | 0.65 |
| 3:U:3151[B]:LEU:O | 3:U:3174[B]:GLY:HA3 | 1.97 | 0.65 |
| 2:W:2317:LEU:HB3 | 2:W:2318:PRO:HD2 | 1.79 | 0.65 |
| 3:X:2951[A]:ASP:O | 3:X:2956[A]:LYS:CE | 2.45 | 0.65 |
| 3:X:2979[A]:GLN:NE2 | 3:X:3155[A]:MET:HE2 | 2.09 | 0.65 |
| 3:X:3023[B]:ILE:HA | 3:X:3026[B]:THR:OG1 | 1.95 | 0.65 |
| 2:Z:2509:ILE:HD11 | 2:Z:2605:LEU:HD23 | 1.78 | 0.65 |
| 3:a:2966[B]:SER:HB2 | 3:a:2977[B]:CYS:CB | 2.21 | 0.65 |
| 3:a:3011[B]:TYR:HB3 | 3:a:3121[B]:SER:HB2 | 1.77 | 0.65 |
| 2:c:2867:PRO:HG2 | 3:d:2932[A]:PRO:HG2 | 1.73 | 0.65 |
| 3:d:2933[A]:SER:O | 3:d:2936[A]:GLU:HB3 | 1.96 | 0.65 |
| 3:d:2937[A]:ASN:HD22 | 3:d:3006[A]:LYS:HD3 | 1.62 | 0.65 |
| 3:d:2937[B]:ASN:HB3 | 3:d:3006[B]:LYS:HD3 | 1.79 | 0.65 |
| 3:d:3151[B]:LEU:O | 3:d:3174[B]:GLY:HA3 | 1.97 | 0.65 |
| 3:C:2937[B]:ASN:ND2 | 3:C:3006[B]:LYS:HD3 | 2.11 | 0.65 |
| 3:C:3151[A]:LEU:O | 3:C:3174[A]:GLY:HA3 | 1.97 | 0.65 |
| 3:C:3174[B]:GLY:HA2 | 3:L:3154[B]:PRO:HG3 | 1.79 | 0.65 |
| 3:C:3217[B]:PHE:HB2 | 3:C:3219[B]:LEU:HD21 | 1.78 | 0.65 |
| 3:F:2937[A]:ASN:ND2 | 3:F:3006[A]:LYS:HD3 | 2.11 | 0.65 |
| 3:F:2980[B]:HIS:HB3 | 3:a:2968[B]:GLN:HG2 | 1.75 | 0.65 |
| 3:F:3252[B]:TYR:O | 3:a:3252[B]:TYR:C | 2.40 | 0.65 |
| 3:I:2966[B]:SER:CB | 3:R:3254[B]:MET:CG | 2.54 | 0.65 |
| 3:I:3011[A]:TYR:HB3 | 3:I:3121[A]:SER:HB2 | 1.76 | 0.65 |
| 3:I:3169[A]:LYS:C | 3:I:3172[A]:SER:HG | 1.98 | 0.65 |
| 1:J:327:ASP:OD1 | 1:J:328:LYS:N | 2.27 | 0.65 |
| 1:J:1286:ARG:NH1 | 1:J:1333:GLU:OE1 | 2.30 | 0.65 |
| 2:K:2470:ALA:HB2 | 2:K:2476:LEU:HD11 | 1.77 | 0.65 |
| 3:L:3285[B]:VAL:HG22 | 3:L:3286[B]:THR:H | 1.62 | 0.65 |
| 1:M:1421:VAL:HG23 | 1:M:1422:HIS:HD1 | 1.61 | 0.65 |
| 2:N:2687:ILE:HD11 | 2:N:2695:MET:HG2 | 1.79 | 0.65 |
| 3:O:3089[A]:HIS:ND1 | 3:O:3119[A]:HIS:CE1 | 2.61 | 0.65 |
| 3:O:3156[B]:MET:HG2 | 3:X:3173[B]:THR:HG23 | 1.61 | 0.65 |
| 3:O:3169[B]:LYS:HZ1 | 3:X:3148[B]:ILE:CB | 2.05 | 0.65 |
| 1:P:891:LYS:HB3 | 1:P:892:TYR:CD2 | 2.31 | 0.65 |
| 1:P:1143:ALA:HA | 1:P:1195:ASP:HA | 1.77 | 0.65 |
| 2:Q:2394:VAL:H | 2:Q:2448:THR:HG22 | 1.60 | 0.65 |
| 3:R:2937[A]:ASN:HD22 | 3:R:3006[A]:LYS:HD3 | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2982[B]:MET:CE | 3:R:3254[B]:MET:HE2 | 2.26 | 0.65 |
| 3:R:3228[B]:VAL:HG21 | 3:R:3245[B]:PHE:CE1 | 2.32 | 0.65 |
| 3:R:3298[A]:ASN:HD21 | 3:R:3301[A]:PRO:HA | 1.60 | 0.65 |
| 1:S:1414:THR:HG23 | 1:S:1477:LEU:HD13 | 1.78 | 0.65 |
| 2:T:2252:GLU:O | 2:T:2389:ARG:NH2 | 2.28 | 0.65 |
| 3:U:2957[A]:ILE:CA | 3:U:2960[A]:PHE:CE1 | 2.78 | 0.65 |
| 3:U:3137[B]:ARG:CB | 3:U:3139[B]:LEU:HD23 | 2.25 | 0.65 |
| 3:U:3284[A]:LYS:CD | 3:U:3285[A]:VAL:H | 2.10 | 0.65 |
| 3:U:3288[B]:MET:HA | 3:U:3295[B]:LEU:HG | 1.76 | 0.65 |
| 3:X:3066[A]:TYR:CE1 | 3:X:3193[A]:HIS:HE1 | 2.15 | 0.65 |
| 3:X:3217[B]:PHE:HB2 | 3:X:3219[B]:LEU:HD21 | 1.78 | 0.65 |
| 3:X:3228[B]:VAL:HG21 | 3:X:3245[B]:PHE:CE1 | 2.32 | 0.65 |
| 1:Y:1621:ASN:N | 3:d:3189[B]:ASN:HD22 | 1.93 | 0.65 |
| 3:a:2982[A]:MET:CE | 3:a:3254[A]:MET:HE2 | 2.26 | 0.65 |
| 3:a:3259[B]:ASP:OD1 | 3:a:3260[B]:ARG:HD2 | 1.96 | 0.65 |
| 1:b:23:ARG:HD3 | 1:b:120:LYS:HG2 | 1.79 | 0.65 |
| 1:b:1086:LEU:HB3 | 1:b:1090:ILE:HD11 | 1.78 | 0.65 |
| 3:d:2984[B]:THR:HG22 | 3:d:3151[B]:LEU:HD23 | 1.77 | 0.65 |
| 3:d:3217[A]:PHE:HB2 | 3:d:3219[A]:LEU:HD21 | 1.79 | 0.65 |
| 1:A:1492:PRO:HB2 | 1:A:1497:SER:HB2 | 1.78 | 0.65 |
| 3:C:2988[B]:TRP:CD1 | 3:L:3153[B]:LYS:CE | 2.79 | 0.65 |
| 3:C:3149[B]:ASN:CB | 3:L:3158[B]:PHE:O | 2.45 | 0.65 |
| 3:C:3149[B]:ASN:OD1 | 3:C:3150[B]:LYS:HB2 | 1.96 | 0.65 |
| 3:C:3228[A]:VAL:HG21 | 3:C:3245[A]:PHE:CE1 | 2.32 | 0.65 |
| 3:F:2966[B]:SER:CB | 3:a:3254[B]:MET:HB2 | 2.26 | 0.65 |
| 3:F:2985[B]:PHE:CE2 | 3:a:2969[B]:TYR:C | 2.74 | 0.65 |
| 3:F:3155[B]:MET:N | 3:a:3153[B]:LYS:C | 2.47 | 0.65 |
| 3:F:3173[B]:THR:HG23 | 3:a:3173[B]:THR:OG1 | 1.95 | 0.65 |
| 3:F:3228[A]:VAL:HG21 | 3:F:3245[A]:PHE:CE1 | 2.32 | 0.65 |
| 3:I:2937[B]:ASN:ND2 | 3:I:3006[B]:LYS:HD3 | 2.11 | 0.65 |
| 3:I:3180[B]:TYR:CA | 3:I:3183[B]:LEU:HD22 | 2.26 | 0.65 |
| 1:J:1219:ASP:OD1 | 1:J:1223:ALA:N | 2.30 | 0.65 |
| 3:L:3200[A]:LEU:HD22 | 3:L:3204[A]:LEU:CD1 | 2.27 | 0.65 |
| 1:M:1060:GLN:OE1 | 1:M:1063:ARG:NH1 | 2.30 | 0.65 |
| 3:O:2933[A]:SER:O | 3:O:2936[A]:GLU:HB3 | 1.96 | 0.65 |
| 3:O:2937[A]:ASN:HB3 | 3:O:3006[A]:LYS:HD3 | 1.79 | 0.65 |
| 3:O:2957[A]:ILE:CA | 3:O:2960[A]:PHE:CE1 | 2.78 | 0.65 |
| 3:O:2984[A]:THR:HG22 | 3:O:3151[A]:LEU:HD23 | 1.77 | 0.65 |
| 3:O:3149[A]:ASN:OD1 | 3:O:3150[A]:LYS:HB2 | 1.96 | 0.65 |
| 3:O:3158[B]:PHE:O | 3:X:3148[B]:ILE:O | 2.13 | 0.65 |
| 3:O:3217[A]:PHE:HB2 | 3:O:3219[A]:LEU:HD21 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q:2545:SER:HA | 2:Q:2546:LEU:HB3 | 1.78 | 0.65 |
| 3:R:2984[A]:THR:HG22 | 3:R:3151[A]:LEU:HD23 | 1.77 | 0.65 |
| 3:R:3132[A]:ALA:HB1 | 3:R:3197[A]:ILE:CD1 | 2.26 | 0.65 |
| 3:R:3185[A]:TYR:C | 3:R:3186[A]:GLU:OE2 | 2.37 | 0.65 |
| 3:R:3217[B]:PHE:HB2 | 3:R:3219[B]:LEU:HD21 | 1.78 | 0.65 |
| 2:T:2403:PHE:HD1 | 2:T:2405:SER:H | 1.45 | 0.65 |
| 3:U:2982[A]:MET:CE | 3:U:3254[A]:MET:HE2 | 2.26 | 0.65 |
| 3:X:2937[B]:ASN:HD22 | 3:X:3006[B]:LYS:HD3 | 1.61 | 0.65 |
| 3:X:3288[A]:MET:HA | 3:X:3295[A]:LEU:HG | 1.76 | 0.65 |
| 3:a:2994[A]:LYS:O | 3:a:2995[A]:GLN:C | 2.38 | 0.65 |
| 3:a:3176[A]:LYS:HB3 | 3:a:3176[A]:LYS:HZ2 | 1.62 | 0.65 |
| 3:a:3228[A]:VAL:HG21 | 3:a:3245[A]:PHE:CE1 | 2.32 | 0.65 |
| 3:a:3298[A]:ASN:ND2 | 3:a:3301[A]:PRO:O | 2.30 | 0.65 |
| 3:d:2982[A]:MET:CE | 3:d:3254[A]:MET:HE2 | 2.26 | 0.65 |
| 3:d:3288[B]:MET:HA | 3:d:3295[B]:LEU:HG | 1.76 | 0.65 |
| 1:A:133:LYS:HG3 | 1:A:134:VAL:HG22 | 1.78 | 0.65 |
| 1:A:327:ASP:OD1 | 1:A:328:LYS:N | 2.29 | 0.65 |
| 2:B:2283:ASN:O | 2:B:2406:SER:OG | 2.07 | 0.65 |
| 3:C:3120[A]:HIS:HA | 3:C:3123[A]:THR:HG1 | 1.61 | 0.65 |
| 3:C:3154[B]:PRO:HD2 | 3:L:3155[B]:MET:SD | 2.37 | 0.65 |
| 3:C:3217[A]:PHE:HB2 | 3:C:3219[A]:LEU:HD21 | 1.79 | 0.65 |
| 3:C:3255[B]:PRO:HG2 | 3:L:2959[B]:SER:O | 1.96 | 0.65 |
| 3:F:2937[A]:ASN:HD22 | 3:F:3006[A]:LYS:HD3 | 1.62 | 0.65 |
| 3:F:2966[B]:SER:HB2 | 3:a:3254[B]:MET:CB | 2.26 | 0.65 |
| 3:F:3176[A]:LYS:HB3 | 3:F:3176[A]:LYS:HZ2 | 1.60 | 0.65 |
| 3:F:3298[B]:ASN:ND2 | 3:F:3301[B]:PRO:O | 2.30 | 0.65 |
| 3:I:2951[A]:ASP:O | 3:I:2956[A]:LYS:CE | 2.45 | 0.65 |
| 3:I:2965[B]:LEU:CD1 | 3:I:2975[B]:PHE:H | 2.08 | 0.65 |
| 3:I:2982[A]:MET:CE | 3:I:3254[A]:MET:HE2 | 2.26 | 0.65 |
| 3:I:3036[A]:GLY:O | 3:I:3044[A]:LYS:HA | 1.96 | 0.65 |
| 3:I:3171[B]:HIS:N | 3:R:3152[B]:LYS:CB | 2.45 | 0.65 |
| 3:I:3248[B]:LEU:HB2 | 3:R:2972[B]:GLY:C | 2.19 | 0.65 |
| 3:I:3256[B]:TRP:CB | 3:R:2966[B]:SER:O | 2.45 | 0.65 |
| 3:I:3259[A]:ASP:OD1 | 3:I:3260[A]:ARG:HD2 | 1.96 | 0.65 |
| 3:L:2979[B]:GLN:NE2 | 3:L:3155[B]:MET:HE2 | 2.09 | 0.65 |
| 3:L:3089[B]:HIS:CE1 | 3:L:3119[B]:HIS:CE1 | 2.81 | 0.65 |
| 3:L:3151[A]:LEU:O | 3:L:3174[A]:GLY:HA3 | 1.97 | 0.65 |
| 3:L:3196[B]:THR:OG1 | 3:L:3199[B]:GLN:CG | 2.44 | 0.65 |
| 3:L:3217[B]:PHE:HB2 | 3:L:3219[B]:LEU:HD21 | 1.78 | 0.65 |
| 1:M:664:VAL:HG12 | 1:M:690:THR:HG22 | 1.79 | 0.65 |
| 3:O:2965[B]:LEU:HD12 | 3:X:2979[B]:GLN:NE2 | 1.60 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2979[B]:GLN:NE2 | 3:O:3155[B]:MET:HE2 | 2.09 | 0.65 |
| 3:O:2994[A]:LYS:O | 3:O:2995[A]:GLN:C | 2.38 | 0.65 |
| 1:P:450:LYS:NZ | 1:P:1273:SER:OG | 2.26 | 0.65 |
| 1:P:1304:ASP:N | 1:P:1304:ASP:OD1 | 2.23 | 0.65 |
| 3:R:2957[A]:ILE:CA | 3:R:2960[A]:PHE:CE1 | 2.78 | 0.65 |
| 3:R:3180[A]:TYR:CA | 3:R:3183[A]:LEU:HD22 | 2.26 | 0.65 |
| 3:R:3217[A]:PHE:HB2 | 3:R:3219[A]:LEU:HD21 | 1.79 | 0.65 |
| 3:R:3298[A]:ASN:HA | 3:R:3299[A]:LEU:HB2 | 1.76 | 0.65 |
| 3:U:2965[B]:LEU:CD1 | 3:U:2975[B]:PHE:H | 2.08 | 0.65 |
| 3:U:3036[A]:GLY:O | 3:U:3044[A]:LYS:HA | 1.95 | 0.65 |
| 1:V:1631:GLU:OE1 | 1:Y:328:LYS:NZ | 2.29 | 0.65 |
| 3:X:3180[B]:TYR:CA | 3:X:3183[B]:LEU:HD22 | 2.26 | 0.65 |
| 1:b:1140:ASN:ND2 | 1:b:1236:TYR:OH | 2.30 | 0.65 |
| 3:d:3284[A]:LYS:CD | 3:d:3285[A]:VAL:H | 2.10 | 0.65 |
| 6:GA:1:NAG:O3 | 6:GA:2:NAG:N2 | 2.30 | 0.65 |
| 1:A:931:TRP:CG | 1:A:1018:ILE:HD11 | 2.32 | 0.65 |
| 3:C:3160[B]:SER:CB | 3:L:2983[B]:VAL:CG2 | 2.55 | 0.65 |
| 3:C:3169[B]:LYS:C | 3:C:3172[B]:SER:HG | 1.98 | 0.65 |
| 3:C:3298[A]:ASN:ND2 | 3:C:3301[A]:PRO:O | 2.30 | 0.65 |
| 3:C:3298[B]:ASN:ND2 | 3:C:3301[B]:PRO:O | 2.30 | 0.65 |
| 3:F:2982[A]:MET:CE | 3:F:3254[A]:MET:HE2 | 2.26 | 0.65 |
| 3:F:3066[B]:TYR:CE1 | 3:F:3193[B]:HIS:HE1 | 2.15 | 0.65 |
| 3:F:3217[B]:PHE:HE1 | 3:F:3230[B]:PHE:HZ | 0.80 | 0.65 |
| 1:G:580:TYR:O | 1:G:584:SER:OG | 2.14 | 0.65 |
| 3:I:2982[B]:MET:CE | 3:I:3254[B]:MET:HE2 | 2.26 | 0.65 |
| 3:I:3014[A]:TRP:CG | 3:I:3092[A]:ILE:HD11 | 2.32 | 0.65 |
| 3:I:3014[B]:TRP:CG | 3:I:3092[B]:ILE:HD11 | 2.32 | 0.65 |
| 3:I:3228[A]:VAL:HG21 | 3:I:3245[A]:PHE:CE1 | 2.32 | 0.65 |
| 3:I:3298[B]:ASN:ND2 | 3:I:3301[B]:PRO:O | 2.30 | 0.65 |
| 3:L:3176[B]:LYS:HB3 | 3:L:3176[B]:LYS:HZ2 | 1.60 | 0.65 |
| 3:L:3228[B]:VAL:HG21 | 3:L:3245[B]:PHE:CE1 | 2.32 | 0.65 |
| 3:L:3298[A]:ASN:HD21 | 3:L:3301[A]:PRO:HA | 1.60 | 0.65 |
| 3:O:3217[A]:PHE:HE1 | 3:O:3230[A]:PHE:HZ | 0.81 | 0.65 |
| 2:Q:2648:ALA:HA | 2:Q:2654:SER:HB2 | 1.78 | 0.65 |
| 3:R:2966[A]:SER:HB3 | 3:R:2977[A]:CYS:HB2 | 1.78 | 0.65 |
| 3:R:3014[B]:TRP:CG | 3:R:3092[B]:ILE:HD11 | 2.32 | 0.65 |
| 3:R:3149[B]:ASN:OD1 | 3:R:3150[B]:LYS:HB2 | 1.96 | 0.65 |
| 3:R:3284[A]:LYS:HA | 3:R:3284[A]:LYS:CE | 2.22 | 0.65 |
| 3:R:3285[A]:VAL:HG22 | 3:R:3286[A]:THR:H | 1.61 | 0.65 |
| 2:T:2638:ARG:NH2 | 2:T:2704:ASP:OD1 | 2.30 | 0.65 |
| 3:U:3066[B]:TYR:CE1 | 3:U:3193[B]:HIS:HE1 | 2.15 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W:2867:PRO:HB2 | 3:X:2932[A]:PRO:HG2 | 1.79 | 0.65 |
| 3:X:3180[A]:TYR:CB | 3:X:3183[A]:LEU:HD22 | 2.27 | 0.65 |
| 3:X:3259[A]:ASP:OD1 | 3:X:3260[A]:ARG:HD2 | 1.96 | 0.65 |
| 3:d:3285[B]:VAL:HG22 | 3:d:3286[B]:THR:H | 1.62 | 0.65 |
| 3:d:3298[A]:ASN:ND2 | 3:d:3301[A]:PRO:O | 2.30 | 0.65 |
| 1:A:930:ASP:OD1 | 1:A:1051:ARG:NH2 | 2.29 | 0.65 |
| 3:C:2957[A]:ILE:CA | 3:C:2960[A]:PHE:CE1 | 2.78 | 0.65 |
| 3:C:3149[A]:ASN:OD1 | 3:C:3150[A]:LYS:HB2 | 1.96 | 0.65 |
| 3:C:3248[B]:LEU:HD21 | 3:L:2971[B]:ASP:OD2 | 1.97 | 0.65 |
| 3:C:3285[A]:VAL:HG22 | 3:C:3286[A]:THR:H | 1.61 | 0.65 |
| 3:F:2961[B]:HIS:CA | 3:a:2975[B]:PHE:CZ | 2.69 | 0.65 |
| 3:F:3117[B]:TYR:O | 3:F:3120[B]:HIS:HB2 | 1.97 | 0.65 |
| 3:F:3200[B]:LEU:HD22 | 3:F:3204[B]:LEU:CD1 | 2.27 | 0.65 |
| 3:F:3217[B]:PHE:HB2 | 3:F:3219[B]:LEU:HD21 | 1.79 | 0.65 |
| 2:H:2509:ILE:HD11 | 2:H:2605:LEU:HD23 | 1.78 | 0.65 |
| 3:I:2965[B]:LEU:HB3 | 3:R:3256[B]:TRP:CZ2 | 2.31 | 0.65 |
| 3:I:3025[B]:VAL:HG22 | 3:I:3047[B]:ARG:NH1 | 2.02 | 0.65 |
| 1:J:1576:THR:H | 1:J:1581:GLU:HB3 | 1.60 | 0.65 |
| 3:L:2961[B]:HIS:CE1 | 3:L:2980[B]:HIS:NE2 | 2.57 | 0.65 |
| 3:L:2982[A]:MET:CE | 3:L:3254[A]:MET:HE2 | 2.26 | 0.65 |
| 3:L:3014[A]:TRP:CG | 3:L:3092[A]:ILE:HD11 | 2.32 | 0.65 |
| 1:M:460:GLU:HB3 | 1:M:465:PRO:HG2 | 1.79 | 0.65 |
| 3:O:2937[A]:ASN:HD22 | 3:O:3006[A]:LYS:HD3 | 1.61 | 0.65 |
| 3:O:2967[B]:CYS:C | 3:X:2979[B]:GLN:CG | 2.61 | 0.65 |
| 1:P:329:ARG:O | 1:S:1583:CYS:N | 2.29 | 0.65 |
| 1:P:883:CYS:O | 1:P:885:SER:OG | 2.14 | 0.65 |
| 2:Q:2109:ARG:NH1 | 2:Q:2169:HIS:O | 2.30 | 0.65 |
| 3:R:2937[B]:ASN:HD22 | 3:R:3006[B]:LYS:HD3 | 1.62 | 0.65 |
| 3:R:3180[A]:TYR:CB | 3:R:3183[A]:LEU:HD22 | 2.27 | 0.65 |
| 3:R:3185[B]:TYR:C | 3:R:3186[B]:GLU:OE2 | 2.37 | 0.65 |
| 1:S:545:PHE:O | 1:S:561:ARG:NH2 | 2.28 | 0.65 |
| 3:U:3228[B]:VAL:HG21 | 3:U:3245[B]:PHE:CE1 | 2.32 | 0.65 |
| 1:V:136:ALA:O | 1:V:193:SER:OG | 2.14 | 0.65 |
| 1:V:452:ILE:HD12 | 1:V:1367:SER:HB2 | 1.79 | 0.65 |
| 3:X:2982[A]:MET:CE | 3:X:3254[A]:MET:HE2 | 2.26 | 0.65 |
| 3:a:2966[B]:SER:HB3 | 3:a:2977[B]:CYS:HB2 | 1.78 | 0.65 |
| 3:a:2994[B]:LYS:O | 3:a:2995[B]:GLN:C | 2.38 | 0.65 |
| 3:a:3151[A]:LEU:O | 3:a:3174[A]:GLY:HA3 | 1.97 | 0.65 |
| 3:a:3228[B]:VAL:HG21 | 3:a:3245[B]:PHE:CE1 | 2.32 | 0.65 |
| 3:d:3298[A]:ASN:HB2 | 3:d:3299[A]:LEU:C | 2.20 | 0.65 |
| 8:0:1:NAG:C6 | 8:0:2:NAG:N2 | 2.59 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3153[B]:LYS:NZ | 3:L:2988[B]:TRP:HE1 | 1.93 | 0.65 |
| 3:C:3154[B]:PRO:CG | 3:L:3174[B]:GLY:HA3 | 2.09 | 0.65 |
| 3:C:3176[B]:LYS:HB3 | 3:C:3176[B]:LYS:HZ2 | 1.62 | 0.65 |
| 3:C:3232[A]:VAL:CG2 | 3:C:3273[A]:LEU:HD11 | 2.27 | 0.65 |
| 3:C:3251[B]:ASP:O | 3:L:3253[B]:GLU:N | 2.22 | 0.65 |
| 1:D:855:ARG:NH2 | 1:D:941:LEU:O | 2.30 | 0.65 |
| 2:E:2858:ASP:OD2 | 2:E:2862:LYS:NZ | 2.30 | 0.65 |
| 3:F:3170[B]:ALA:C | 3:a:3152[B]:LYS:CG | 2.70 | 0.65 |
| 3:F:3172[B]:SER:CB | 3:a:3150[B]:LYS:C | 2.70 | 0.65 |
| 3:F:3200[A]:LEU:HD22 | 3:F:3204[A]:LEU:CD1 | 2.27 | 0.65 |
| 2:H:2185:THR:HG23 | 2:H:2186:GLU:HG3 | 1.79 | 0.65 |
| 3:I:2937[B]:ASN:HB3 | 3:I:3006[B]:LYS:HD3 | 1.79 | 0.65 |
| 3:I:2955[B]:GLN:OE1 | 3:I:3037[B]:TYR:CE1 | 2.50 | 0.65 |
| 3:I:2965[B]:LEU:CA | 3:R:3221[B]:ALA:HB1 | 2.18 | 0.65 |
| 3:I:2966[B]:SER:C | 3:R:3256[B]:TRP:CB | 2.70 | 0.65 |
| 3:I:2975[B]:PHE:CZ | 3:R:2961[B]:HIS:O | 2.50 | 0.65 |
| 3:I:3146[B]:CYS:O | 3:R:3161[B]:GLU:HG3 | 1.97 | 0.65 |
| 3:I:3153[B]:LYS:HB3 | 3:R:3155[B]:MET:CB | 2.26 | 0.65 |
| 1:J:1182:ASN:HD22 | 1:J:1182:ASN:H | 1.44 | 0.65 |
| 3:L:2937[A]:ASN:HD22 | 3:L:3006[A]:LYS:HD3 | 1.62 | 0.65 |
| 1:M:450:LYS:NZ | 1:M:1273:SER:OG | 2.30 | 0.65 |
| 3:O:3066[B]:TYR:CE1 | 3:O:3193[B]:HIS:HE1 | 2.15 | 0.65 |
| 3:O:3089[B]:HIS:CE1 | 3:O:3119[B]:HIS:CE1 | 2.81 | 0.65 |
| 3:O:3124[A]:ASP:OD2 | 3:O:3187[A]:TYR:OH | 2.15 | 0.65 |
| 1:P:61:GLY:HA3 | 1:P:352:TRP:HB2 | 1.78 | 0.65 |
| 3:R:2951[B]:ASP:O | 3:R:2956[B]:LYS:CE | 2.45 | 0.65 |
| 3:R:3066[A]:TYR:CE1 | 3:R:3193[A]:HIS:HE1 | 2.15 | 0.65 |
| 3:R:3298[B]:ASN:HD21 | 3:R:3301[B]:PRO:HA | 1.60 | 0.65 |
| 3:U:3232[B]:VAL:CG2 | 3:U:3273[B]:LEU:HD11 | 2.27 | 0.65 |
| 3:U:3254[B]:MET:HB3 | 3:d:3254[B]:MET:C | 2.20 | 0.65 |
| 3:U:3298[B]:ASN:ND2 | 3:U:3301[B]:PRO:O | 2.30 | 0.65 |
| 3:X:3014[A]:TRP:CG | 3:X:3092[A]:ILE:HD11 | 2.32 | 0.65 |
| 3:X:3014[B]:TRP:CG | 3:X:3092[B]:ILE:HD11 | 2.32 | 0.65 |
| 3:X:3298[B]:ASN:ND2 | 3:X:3301[B]:PRO:O | 2.30 | 0.65 |
| 3:a:2937[A]:ASN:ND2 | 3:a:3006[A]:LYS:HD3 | 2.11 | 0.65 |
| 3:a:3025[B]:VAL:HG22 | 3:a:3047[B]:ARG:NH1 | 2.02 | 0.65 |
| 3:a:3066[B]:TYR:CE1 | 3:a:3193[B]:HIS:HE1 | 2.15 | 0.65 |
| 3:a:3117[B]:TYR:O | 3:a:3120[B]:HIS:HB2 | 1.97 | 0.65 |
| 3:a:3124[B]:ASP:OD2 | 3:a:3187[B]:TYR:OH | 2.15 | 0.65 |
| 3:a:3200[A]:LEU:HD22 | 3:a:3204[A]:LEU:CD1 | 2.27 | 0.65 |
| 3:a:3232[A]:VAL:CG2 | 3:a:3273[A]:LEU:HD11 | 2.27 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3232[B]:VAL:CG2 | 3:a:3273[B]:LEU:HD11 | 2.27 | 0.65 |
| 3:a:3284[A]:LYS:CD | 3:a:3285[A]:VAL:H | 2.09 | 0.65 |
| 3:a:3298[A]:ASN:CB | 3:a:3300[A]:LEU:CD2 | 2.61 | 0.65 |
| 3:d:2937[B]:ASN:HD22 | 3:d:3006[B]:LYS:HD3 | 1.62 | 0.65 |
| 3:d:3124[B]:ASP:OD2 | 3:d:3187[B]:TYR:OH | 2.15 | 0.65 |
| 4:m:1:NAG:H4 | 4:m:2:NAG:N2 | 2.11 | 0.65 |
| 1:A:1013:ILE:HD11 | 1:A:1175:PHE:CD2 | 2.31 | 0.64 |
| 1:A:1604:ASP:OD1 | 1:A:1605:ARG:NH1 | 2.30 | 0.64 |
| 3:C:3014[B]:TRP:CG | 3:C:3092[B]:ILE:HD11 | 2.32 | 0.64 |
| 1:D:984:ASP:N | 1:D:984:ASP:OD1 | 2.30 | 0.64 |
| 3:F:2933[A]:SER:O | 3:F:2936[A]:GLU:HB3 | 1.96 | 0.64 |
| 3:F:3124[B]:ASP:OD2 | 3:F:3187[B]:TYR:OH | 2.15 | 0.64 |
| 3:F:3151[B]:LEU:O | 3:F:3174[B]:GLY:HA3 | 1.97 | 0.64 |
| 3:F:3174[B]:GLY:H | 3:a:3154[B]:PRO:CB | 1.82 | 0.64 |
| 3:I:2960[B]:PHE:CA | 3:R:3255[B]:PRO:HD2 | 2.18 | 0.64 |
| 3:I:2969[A]:TYR:HD2 | 3:I:2971[A]:ASP:N | 1.84 | 0.64 |
| 3:I:3259[B]:ASP:N | 3:R:3162[B]:ASP:HB3 | 2.11 | 0.64 |
| 1:J:534:ASP:HB2 | 1:J:541:LYS:HE2 | 1.77 | 0.64 |
| 3:L:2994[A]:LYS:O | 3:L:2995[A]:GLN:C | 2.38 | 0.64 |
| 3:L:3151[B]:LEU:O | 3:L:3174[B]:GLY:HA3 | 1.97 | 0.64 |
| 3:L:3298[A]:ASN:ND2 | 3:L:3301[A]:PRO:O | 2.30 | 0.64 |
| 3:O:2951[A]:ASP:O | 3:O:2956[A]:LYS:CE | 2.45 | 0.64 |
| 3:O:3117[B]:TYR:O | 3:O:3120[B]:HIS:HB2 | 1.98 | 0.64 |
| 3:R:3298[B]:ASN:ND2 | 3:R:3301[B]:PRO:O | 2.30 | 0.64 |
| 3:U:3124[B]:ASP:OD2 | 3:U:3187[B]:TYR:OH | 2.15 | 0.64 |
| 3:U:3217[A]:PHE:HB2 | 3:U:3219[A]:LEU:HD21 | 1.79 | 0.64 |
| 3:U:3285[A]:VAL:HG22 | 3:U:3286[A]:THR:H | 1.62 | 0.64 |
| 3:X:2955[A]:GLN:OE1 | 3:X:3037[A]:TYR:CE1 | 2.51 | 0.64 |
| 3:X:3132[B]:ALA:HB1 | 3:X:3197[B]:ILE:CD1 | 2.26 | 0.64 |
| 3:X:3180[A]:TYR:CA | 3:X:3183[A]:LEU:HD22 | 2.26 | 0.64 |
| 3:X:3180[B]:TYR:CB | 3:X:3183[B]:LEU:HD22 | 2.27 | 0.64 |
| 3:X:3232[B]:VAL:CG2 | 3:X:3273[B]:LEU:HD11 | 2.27 | 0.64 |
| 1:Y:1613:ASP:OD1 | 3:d:3185[B]:TYR:C | 2.40 | 0.64 |
| 2:Z:2833:GLY:HA3 | 2:Z:2854:MET:HE1 | 1.79 | 0.64 |
| 3:a:2933[A]:SER:O | 3:a:2936[A]:GLU:HB3 | 1.96 | 0.64 |
| 3:a:2966[A]:SER:HB3 | 3:a:2977[A]:CYS:HB2 | 1.77 | 0.64 |
| 1:b:105:VAL:HB | 1:b:137:ARG:NH2 | 2.12 | 0.64 |
| 1:b:589:GLN:HG2 | 1:b:594:ASP:HB3 | 1.78 | 0.64 |
| 1:b:898:GLY:N | 1:b:899:MET:SD | 2.64 | 0.64 |
| 1:b:1296:VAL:HB | 1:b:1446:ASP:HB3 | 1.78 | 0.64 |
| 3:d:3120[A]:HIS:NE2 | 9:d:3401[A]:CUO:O1 | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3149[A]:ASN:OD1 | 3:d:3150[A]:LYS:HB2 | 1.96 | 0.64 |
| 3:d:3232[A]:VAL:CG2 | 3:d:3273[A]:LEU:HD11 | 2.27 | 0.64 |
| 3:d:3232[B]:VAL:CG2 | 3:d:3273[B]:LEU:HD11 | 2.27 | 0.64 |
| 1:A:1618:LEU:O | 3:F:3198[B]:PRO:HD3 | 1.98 | 0.64 |
| 3:C:2952[A]:ALA:H | 3:C:2953[A]:GLY:CA | 2.04 | 0.64 |
| 3:C:3066[A]:TYR:CE1 | 3:C:3193[A]:HIS:HE1 | 2.15 | 0.64 |
| 3:C:3149[B]:ASN:ND2 | 3:L:3163[B]:ASN:CB | 2.60 | 0.64 |
| 1:D:1013:ILE:HD11 | 1:D:1175:PHE:CD2 | 2.32 | 0.64 |
| 3:F:3217[A]:PHE:HB2 | 3:F:3219[A]:LEU:HD21 | 1.78 | 0.64 |
| 3:I:2930[B]:LEU:HD22 | 3:I:2930[B]:LEU:N | 2.02 | 0.64 |
| 3:I:3120[A]:HIS:NE2 | 9:R:3401[A]:CUO:O1 | 2.30 | 0.64 |
| 3:I:3251[B]:ASP:CB | 3:R:3251[B]:ASP:CG | 2.70 | 0.64 |
| 3:I:3298[A]:ASN:ND2 | 3:I:3301[A]:PRO:O | 2.30 | 0.64 |
| 3:L:2966[B]:SER:HB3 | 3:L:2977[B]:CYS:HB2 | 1.78 | 0.64 |
| 3:L:3200[B]:LEU:HD22 | 3:L:3204[B]:LEU:CD1 | 2.27 | 0.64 |
| 3:O:2951[B]:ASP:O | 3:O:2956[B]:LYS:CE | 2.45 | 0.64 |
| 3:O:2982[A]:MET:CE | 3:O:3254[A]:MET:HE2 | 2.26 | 0.64 |
| 3:O:3132[B]:ALA:HB1 | 3:O:3197[B]:ILE:CD1 | 2.26 | 0.64 |
| 3:O:3157[B]:PRO:HD3 | 3:X:3153[B]:LYS:HA | 1.80 | 0.64 |
| 3:O:3298[A]:ASN:ND2 | 3:O:3301[A]:PRO:O | 2.30 | 0.64 |
| 3:O:3298[B]:ASN:ND2 | 3:O:3301[B]:PRO:O | 2.30 | 0.64 |
| 3:R:3151[B]:LEU:O | 3:R:3174[B]:GLY:HA3 | 1.97 | 0.64 |
| 3:R:3232[B]:VAL:CG2 | 3:R:3273[B]:LEU:HD11 | 2.27 | 0.64 |
| 3:R:3298[A]:ASN:ND2 | 3:R:3301[A]:PRO:O | 2.30 | 0.64 |
| 1:S:573:LYS:HD2 | 1:S:574:GLY:HA2 | 1.77 | 0.64 |
| 3:U:2937[A]:ASN:HB3 | 3:U:3006[A]:LYS:HD3 | 1.78 | 0.64 |
| 3:U:3117[A]:TYR:O | 3:U:3120[A]:HIS:HB2 | 1.97 | 0.64 |
| 3:U:3228[A]:VAL:HG21 | 3:U:3245[A]:PHE:CE1 | 2.32 | 0.64 |
| 1:V:912:ASN:ND2 | 1:V:1093:ASP:OD2 | 2.30 | 0.64 |
| 1:V:1029:SER:OG | 1:V:1030:MET:N | 2.30 | 0.64 |
| 3:X:2961[A]:HIS:CE1 | 3:X:2980[A]:HIS:NE2 | 2.57 | 0.64 |
| 3:X:3149[A]:ASN:OD1 | 3:X:3150[A]:LYS:HB2 | 1.96 | 0.64 |
| 3:X:3232[A]:VAL:CG2 | 3:X:3273[A]:LEU:HD11 | 2.27 | 0.64 |
| 3:a:2951[A]:ASP:O | 3:a:2956[A]:LYS:CE | 2.45 | 0.64 |
| 3:d:2994[A]:LYS:O | 3:d:2995[A]:GLN:C | 2.38 | 0.64 |
| 3:d:3066[B]:TYR:HD1 | 3:d:3193[B]:HIS:CE1 | 2.16 | 0.64 |
| 3:d:3149[B]:ASN:OD1 | 3:d:3150[B]:LYS:HB2 | 1.96 | 0.64 |
| 3:d:3157[B]:PRO:O | 3:d:3160[B]:SER:N | 2.30 | 0.64 |
| 3:d:3217[B]:PHE:HB2 | 3:d:3219[B]:LEU:HD21 | 1.78 | 0.64 |
| 3:C:2971[B]:ASP:CB | 3:L:3089[B]:HIS:CE1 | 2.59 | 0.64 |
| 3:C:3180[A]:TYR:CB | 3:C:3183[A]:LEU:HD22 | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3259[A]:ASP:OD1 | 3:C:3260[A]:ARG:HD2 | 1.96 | 0.64 |
| 2:E:2142:ALA:HB1 | 2:E:2143:CYS:HB2 | 1.77 | 0.64 |
| 3:F:2937[B]:ASN:HD22 | 3:F:3006[B]:LYS:HD3 | 1.61 | 0.64 |
| 3:F:2975[B]:PHE:CE1 | 3:a:3107[B]:LEU:HG | 2.32 | 0.64 |
| 3:F:3014[A]:TRP:CG | 3:F:3092[A]:ILE:HD11 | 2.32 | 0.64 |
| 3:F:3014[B]:TRP:CG | 3:F:3092[B]:ILE:HD11 | 2.32 | 0.64 |
| 3:F:3180[A]:TYR:CB | 3:F:3183[A]:LEU:HD22 | 2.27 | 0.64 |
| 3:F:3255[B]:PRO:HB2 | 3:a:2959[B]:SER:CA | 2.28 | 0.64 |
| 3:I:2965[A]:LEU:CD1 | 3:I:2975[A]:PHE:H | 2.08 | 0.64 |
| 3:I:3180[A]:TYR:CB | 3:I:3183[A]:LEU:HD22 | 2.27 | 0.64 |
| 3:I:3259[B]:ASP:CA | 3:R:3162[B]:ASP:HB3 | 2.26 | 0.64 |
| 1:J:105:VAL:HG12 | 1:J:123:PHE:HB3 | 1.80 | 0.64 |
| 3:L:2951[A]:ASP:O | 3:L:2956[A]:LYS:CE | 2.45 | 0.64 |
| 3:L:2961[A]:HIS:CE1 | 3:L:2980[A]:HIS:NE2 | 2.57 | 0.64 |
| 3:L:3180[B]:TYR:CB | 3:L:3183[B]:LEU:HD22 | 2.27 | 0.64 |
| 3:L:3232[B]:VAL:CG2 | 3:L:3273[B]:LEU:HD11 | 2.27 | 0.64 |
| 3:O:2969[B]:TYR:CG | 3:X:3158[B]:PHE:HE1 | 2.12 | 0.64 |
| 3:O:3120[B]:HIS:NE2 | 9:O:3401[B]:CUO:O1 | 2.30 | 0.64 |
| 3:O:3180[A]:TYR:CB | 3:O:3183[A]:LEU:HD22 | 2.27 | 0.64 |
| 3:O:3253[B]:GLU:OE2 | 3:X:3161[B]:GLU:CD | 2.40 | 0.64 |
| 1:P:450:LYS:HB3 | 1:P:454:GLY:HA3 | 1.79 | 0.64 |
| 3:R:2955[B]:GLN:OE1 | 3:R:3037[B]:TYR:CE1 | 2.51 | 0.64 |
| 3:R:2966[A]:SER:HB2 | 3:R:2977[A]:CYS:CB | 2.21 | 0.64 |
| 1:S:1284:GLU:OE1 | 1:S:1337:ARG:NH1 | 2.30 | 0.64 |
| 3:U:2955[B]:GLN:OE1 | 3:U:3037[B]:TYR:CE1 | 2.51 | 0.64 |
| 3:U:3014[A]:TRP:CG | 3:U:3092[A]:ILE:HD11 | 2.32 | 0.64 |
| 3:U:3151[A]:LEU:O | 3:U:3174[A]:GLY:HA3 | 1.97 | 0.64 |
| 1:V:804:ASP:OD2 | 6:EA:1:NAG:O6 | 2.14 | 0.64 |
| 3:X:3298[A]:ASN:ND2 | 3:X:3301[A]:PRO:O | 2.30 | 0.64 |
| 3:a:2937[A]:ASN:HD22 | 3:a:3006[A]:LYS:HD3 | 1.61 | 0.64 |
| 3:a:2965[A]:LEU:CD1 | 3:a:2975[A]:PHE:H | 2.08 | 0.64 |
| 3:a:3200[B]:LEU:HD22 | 3:a:3204[B]:LEU:CD1 | 2.27 | 0.64 |
| 3:a:3279[B]:ASP:OD1 | 3:a:3279[B]:ASP:N | 2.25 | 0.64 |
| 3:d:2955[A]:GLN:OE1 | 3:d:3037[A]:TYR:CE1 | 2.51 | 0.64 |
| 3:d:3066[B]:TYR:CE1 | 3:d:3193[B]:HIS:HE1 | 2.15 | 0.64 |
| 1:A:533:VAL:HG12 | 1:A:540:THR:HG22 | 1.80 | 0.64 |
| 3:C:2937[B]:ASN:HB3 | 3:C:3006[B]:LYS:HD3 | 1.79 | 0.64 |
| 3:C:2955[A]:GLN:OE1 | 3:C:3037[A]:TYR:CE1 | 2.51 | 0.64 |
| 3:C:2975[B]:PHE:HD1 | 3:L:3107[B]:LEU:HD13 | 1.54 | 0.64 |
| 3:C:3066[B]:TYR:CE1 | 3:C:3193[B]:HIS:HE1 | 2.15 | 0.64 |
| 3:F:2954[A]:TYR:HA | 3:F:2957[A]:ILE:HG22 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3117[A]:TYR:O | 3:F:3120[A]:HIS:HB2 | 1.98 | 0.64 |
| 3:F:3151[A]:LEU:O | 3:F:3174[A]:GLY:HA3 | 1.97 | 0.64 |
| 3:F:3232[A]:VAL:CG2 | 3:F:3273[A]:LEU:HD11 | 2.27 | 0.64 |
| 3:F:3255[B]:PRO:CG | 3:a:2964[B]:PRO:HD2 | 2.27 | 0.64 |
| 3:F:3285[A]:VAL:HG22 | 3:F:3286[A]:THR:H | 1.62 | 0.64 |
| 1:G:164:GLU:HG3 | 1:G:297:ARG:HE | 1.63 | 0.64 |
| 3:I:2961[A]:HIS:CE1 | 3:I:2980[A]:HIS:NE2 | 2.57 | 0.64 |
| 3:I:3025[A]:VAL:HG22 | 3:I:3047[A]:ARG:NH1 | 2.01 | 0.64 |
| 3:I:3151[B]:LEU:O | 3:I:3174[B]:GLY:HA3 | 1.96 | 0.64 |
| 3:I:3153[B]:LYS:CB | 3:R:3155[B]:MET:CB | 2.71 | 0.64 |
| 3:L:3240[A]:THR:HG22 | 3:L:3241[A]:PHE:N | 2.13 | 0.64 |
| 3:L:3279[B]:ASP:OD1 | 3:L:3279[B]:ASP:N | 2.25 | 0.64 |
| 3:L:3285[A]:VAL:HG22 | 3:L:3286[A]:THR:H | 1.62 | 0.64 |
| 1:M:439:LEU:HD23 | 1:M:509:ILE:HD12 | 1.80 | 0.64 |
| 1:M:873:VAL:HA | 1:M:876:PHE:CE1 | 2.32 | 0.64 |
| 3:O:2937[B]:ASN:HB3 | 3:O:3006[B]:LYS:HD3 | 1.79 | 0.64 |
| 3:O:2969[B]:TYR:CD2 | 3:X:2988[B]:TRP:O | 2.50 | 0.64 |
| 3:O:3285[B]:VAL:HG22 | 3:O:3286[B]:THR:H | 1.62 | 0.64 |
| 1:P:325:THR:HB | 1:P:332:ASP:H | 1.62 | 0.64 |
| 2:Q:2687:ILE:HD11 | 2:Q:2695:MET:HG2 | 1.77 | 0.64 |
| 3:R:2961[B]:HIS:CE1 | 3:R:2980[B]:HIS:NE2 | 2.57 | 0.64 |
| 3:U:2937[B]:ASN:HB3 | 3:U:3006[B]:LYS:HD3 | 1.79 | 0.64 |
| 3:U:2969[B]:TYR:OH | 3:d:2980[B]:HIS:NE2 | 2.30 | 0.64 |
| 3:U:3149[B]:ASN:OD1 | 3:U:3150[B]:LYS:HB2 | 1.96 | 0.64 |
| 3:U:3157[B]:PRO:O | 3:U:3160[B]:SER:N | 2.30 | 0.64 |
| 3:U:3298[A]:ASN:ND2 | 3:U:3301[A]:PRO:O | 2.30 | 0.64 |
| 1:Y:1505:ARG:HG3 | 1:Y:1508:PHE:HB3 | 1.79 | 0.64 |
| 3:d:2930[A]:LEU:H | 3:d:2930[A]:LEU:CD2 | 1.98 | 0.64 |
| 3:d:3120[B]:HIS:NE2 | 9:d:3401[B]:CUO:O1 | 2.30 | 0.64 |
| 3:d:3200[A]:LEU:HD22 | 3:d:3204[A]:LEU:CD1 | 2.27 | 0.64 |
| 3:d:3228[B]:VAL:HG21 | 3:d:3245[B]:PHE:CE1 | 2.32 | 0.64 |
| 3:d:3298[B]:ASN:ND2 | 3:d:3301[B]:PRO:O | 2.30 | 0.64 |
| 6:LA:2:NAG:H62 | 6:LA:3:BMA:H2 | 1.80 | 0.64 |
| 3:C:2933[A]:SER:O | 3:C:2936[A]:GLU:HB3 | 1.96 | 0.64 |
| 3:C:2951[A]:ASP:O | 3:C:2956[A]:LYS:CE | 2.45 | 0.64 |
| 3:C:2984[A]:THR:HG22 | 3:C:3151[A]:LEU:HD23 | 1.77 | 0.64 |
| 3:C:3147[B]:GLU:CD | 3:L:3160[B]:SER:O | 2.40 | 0.64 |
| 3:C:3211[B]:ASP:OD1 | 3:C:3211[B]:ASP:N | 2.27 | 0.64 |
| 3:C:3252[B]:TYR:HB3 | 3:L:3253[B]:GLU:CB | 2.27 | 0.64 |
| 3:F:2955[B]:GLN:OE1 | 3:F:3037[B]:TYR:CE1 | 2.51 | 0.64 |
| 3:F:2982[B]:MET:CE | 3:F:3254[B]:MET:HE2 | 2.26 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2983[B]:VAL:HB | 3:a:3160[B]:SER:HA | 1.79 | 0.64 |
| 3:F:3252[B]:TYR:HE1 | 3:a:3251[B]:ASP:CG | 2.04 | 0.64 |
| 3:F:3298[A]:ASN:ND2 | 3:F:3301[A]:PRO:O | 2.30 | 0.64 |
| 1:G:834:ASP:OD1 | 1:G:834:ASP:N | 2.20 | 0.64 |
| 3:I:2969[B]:TYR:CA | 3:R:2989[B]:HIS:NE2 | 2.61 | 0.64 |
| 3:I:3066[B]:TYR:CE1 | 3:I:3193[B]:HIS:HE1 | 2.15 | 0.64 |
| 3:I:3149[B]:ASN:OD1 | 3:I:3150[B]:LYS:HB2 | 1.96 | 0.64 |
| 3:I:3200[A]:LEU:HD22 | 3:I:3204[A]:LEU:CD1 | 2.27 | 0.64 |
| 3:I:3200[B]:LEU:HD22 | 3:I:3204[B]:LEU:CD1 | 2.27 | 0.64 |
| 3:I:3228[B]:VAL:HG21 | 3:I:3245[B]:PHE:CE1 | 2.32 | 0.64 |
| 2:K:2549:PRO:HG2 | 2:K:2747:LYS:HD2 | 1.78 | 0.64 |
| 3:L:2937[B]:ASN:HD22 | 3:L:3006[B]:LYS:HD3 | 1.61 | 0.64 |
| 3:L:2965[A]:LEU:CD1 | 3:L:2975[A]:PHE:H | 2.08 | 0.64 |
| 3:L:3066[A]:TYR:CE1 | 3:L:3193[A]:HIS:HE1 | 2.15 | 0.64 |
| 3:L:3066[B]:TYR:HD1 | 3:L:3193[B]:HIS:CE1 | 2.16 | 0.64 |
| 1:M:260:ASN:OD1 | 1:M:271:HIS:NE2 | 2.30 | 0.64 |
| 2:N:2133:PRO:HD3 | 2:N:2142:ALA:HB2 | 1.78 | 0.64 |
| 2:N:2390:GLN:NE2 | 2:N:2494:GLN:O | 2.29 | 0.64 |
| 3:O:2937[B]:ASN:HD22 | 3:O:3006[B]:LYS:HD3 | 1.61 | 0.64 |
| 3:O:2957[B]:ILE:CA | 3:O:2960[B]:PHE:HE1 | 2.11 | 0.64 |
| 3:O:2965[A]:LEU:CD1 | 3:O:2975[A]:PHE:H | 2.08 | 0.64 |
| 3:O:3014[A]:TRP:CG | 3:O:3092[A]:ILE:HD11 | 2.32 | 0.64 |
| 1:P:588:GLU:OE2 | 1:P:728:ARG:NH2 | 2.30 | 0.64 |
| 3:R:2955[A]:GLN:OE1 | 3:R:3037[A]:TYR:CE1 | 2.51 | 0.64 |
| 3:R:2969[B]:TYR:HD2 | 3:R:2971[B]:ASP:N | 1.84 | 0.64 |
| 3:R:3066[B]:TYR:CE1 | 3:R:3193[B]:HIS:HE1 | 2.15 | 0.64 |
| 3:R:3200[A]:LEU:HD22 | 3:R:3204[A]:LEU:CD1 | 2.27 | 0.64 |
| 1:S:37:ILE:HD13 | 1:S:75:GLN:HG3 | 1.80 | 0.64 |
| 1:S:909:ILE:HG12 | 1:S:1084:PHE:HZ | 1.62 | 0.64 |
| 3:U:2982[B]:MET:CE | 3:U:3254[B]:MET:HE2 | 2.26 | 0.64 |
| 3:U:3180[A]:TYR:CB | 3:U:3183[A]:LEU:HD22 | 2.27 | 0.64 |
| 2:W:2548:CYS:O | 2:W:2554:PRO:HB3 | 1.97 | 0.64 |
| 3:X:2937[B]:ASN:HB3 | 3:X:3006[B]:LYS:HD3 | 1.79 | 0.64 |
| 3:X:3149[B]:ASN:OD1 | 3:X:3150[B]:LYS:HB2 | 1.96 | 0.64 |
| 3:X:3196[A]:THR:OG1 | 3:X:3199[A]:GLN:CG | 2.44 | 0.64 |
| 3:X:3200[B]:LEU:HD22 | 3:X:3204[B]:LEU:CD1 | 2.27 | 0.64 |
| 3:a:3217[B]:PHE:HE1 | 3:a:3230[B]:PHE:HZ | 0.81 | 0.64 |
| 3:d:2937[A]:ASN:HB3 | 3:d:3006[A]:LYS:HD3 | 1.78 | 0.64 |
| 3:d:3066[A]:TYR:HD1 | 3:d:3193[A]:HIS:CE1 | 2.16 | 0.64 |
| 1:A:157:GLU:OE2 | 1:A:296:ARG:NH2 | 2.31 | 0.64 |
| 3:C:3066[A]:TYR:HD1 | 3:C:3193[A]:HIS:CE1 | 2.16 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3285[B]:VAL:HG22 | 3:C:3286[B]:THR:H | 1.62 | 0.64 |
| 3:F:2951[A]:ASP:O | 3:F:2956[A]:LYS:CE | 2.45 | 0.64 |
| 3:F:2955[A]:GLN:OE1 | 3:F:3037[A]:TYR:CE1 | 2.51 | 0.64 |
| 3:F:2975[B]:PHE:HA | 3:a:3107[B]:LEU:HD21 | 1.79 | 0.64 |
| 3:F:3066[A]:TYR:HD1 | 3:F:3193[A]:HIS:CE1 | 2.16 | 0.64 |
| 3:F:3120[A]:HIS:NE2 | 9:a:3401[A]:CUO:O1 | 2.30 | 0.64 |
| 3:F:3132[A]:ALA:HB1 | 3:F:3197[A]:ILE:CD1 | 2.26 | 0.64 |
| 1:G:104:LEU:O | 1:G:121:ASN:ND2 | 2.30 | 0.64 |
| 1:G:127:GLU:HG2 | 1:G:135:THR:H | 1.61 | 0.64 |
| 3:I:2937[A]:ASN:ND2 | 3:I:3006[A]:LYS:HD3 | 2.11 | 0.64 |
| 3:I:2951[B]:ASP:O | 3:I:2956[B]:LYS:CE | 2.45 | 0.64 |
| 3:I:2954[A]:TYR:HA | 3:I:2957[A]:ILE:HG22 | 1.80 | 0.64 |
| 3:I:2975[B]:PHE:HA | 3:R:3107[B]:LEU:HD22 | 1.80 | 0.64 |
| 3:I:3066[A]:TYR:CE1 | 3:I:3193[A]:HIS:HE1 | 2.15 | 0.64 |
| 3:I:3089[B]:HIS:CE1 | 3:I:3119[B]:HIS:CE1 | 2.81 | 0.64 |
| 3:I:3163[B]:ASN:CB | 3:R:3149[B]:ASN:ND2 | 2.61 | 0.64 |
| 3:I:3256[B]:TRP:CB | 3:R:2966[B]:SER:C | 2.70 | 0.64 |
| 9:I:3401[A]:CUO:O1 | 3:R:3120[A]:HIS:NE2 | 2.30 | 0.64 |
| 1:J:118:ALA:HB1 | 1:J:119:LYS:HA | 1.79 | 0.64 |
| 3:L:2965[B]:LEU:CD1 | 3:L:2975[B]:PHE:H | 2.08 | 0.64 |
| 1:M:1164:ASP:CG | 1:M:1212:HIS:HE2 | 2.06 | 0.64 |
| 3:O:2955[A]:GLN:OE1 | 3:O:3037[A]:TYR:CE1 | 2.51 | 0.64 |
| 3:O:2965[B]:LEU:CD1 | 3:O:2975[B]:PHE:H | 2.08 | 0.64 |
| 3:O:2971[B]:ASP:N | 3:X:2992[B]:TYR:H | 1.96 | 0.64 |
| 3:O:3200[A]:LEU:HD22 | 3:O:3204[A]:LEU:CD1 | 2.27 | 0.64 |
| 3:O:3200[B]:LEU:HD22 | 3:O:3204[B]:LEU:CD1 | 2.27 | 0.64 |
| 3:O:3284[A]:LYS:CD | 3:O:3285[A]:VAL:H | 2.10 | 0.64 |
| 1:P:1355:LEU:HD11 | 1:P:1393:THR:HG21 | 1.77 | 0.64 |
| 3:R:3151[A]:LEU:O | 3:R:3174[A]:GLY:HA3 | 1.96 | 0.64 |
| 3:R:3180[B]:TYR:CB | 3:R:3183[B]:LEU:HD22 | 2.27 | 0.64 |
| 3:R:3228[A]:VAL:HG21 | 3:R:3245[A]:PHE:CE1 | 2.32 | 0.64 |
| 1:S:896:HIS:HB2 | 1:S:905:TRP:CG | 2.32 | 0.64 |
| 3:U:2961[A]:HIS:CE1 | 3:U:2980[A]:HIS:NE2 | 2.57 | 0.64 |
| 3:U:2969[B]:TYR:CZ | 3:d:2980[B]:HIS:CD2 | 2.86 | 0.64 |
| 3:U:3154[B]:PRO:CA | 3:d:3153[B]:LYS:H | 2.11 | 0.64 |
| 3:U:3240[B]:THR:HG22 | 3:U:3241[B]:PHE:N | 2.13 | 0.64 |
| 3:U:3254[B]:MET:HE1 | 3:d:3254[B]:MET:HE3 | 0.65 | 0.64 |
| 3:U:3258[B]:PHE:HA | 3:d:2969[B]:TYR:O | 1.98 | 0.64 |
| 1:V:450:LYS:HE3 | 1:V:505:ARG:HH21 | 1.61 | 0.64 |
| 2:W:2572:VAL:HG22 | 2:W:2768:LEU:HD22 | 1.80 | 0.64 |
| 3:X:2933[B]:SER:O | 3:X:2936[B]:GLU:HB3 | 1.96 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2951[B]:ASP:O | 3:X:2956[B]:LYS:CE | 2.45 | 0.64 |
| 3:X:2954[A]:TYR:HA | 3:X:2957[A]:ILE:HG22 | 1.80 | 0.64 |
| 3:X:2955[B]:GLN:OE1 | 3:X:3037[B]:TYR:CE1 | 2.50 | 0.64 |
| 3:X:2966[B]:SER:HB2 | 3:X:2977[B]:CYS:CB | 2.21 | 0.64 |
| 3:X:3200[A]:LEU:HD22 | 3:X:3204[A]:LEU:CD1 | 2.27 | 0.64 |
| 3:X:3217[B]:PHE:HE1 | 3:X:3230[B]:PHE:HZ | 0.80 | 0.64 |
| 3:X:3298[A]:ASN:HD21 | 3:X:3301[A]:PRO:HA | 1.60 | 0.64 |
| 1:Y:830:ASN:HA | 1:Y:831:VAL:C | 2.22 | 0.64 |
| 2:Z:2711:HIS:HA | 2:Z:2714:VAL:HG22 | 1.79 | 0.64 |
| 3:a:2948[A]:ASP:HB3 | 3:a:2953[A]:GLY:CA | 2.24 | 0.64 |
| 3:a:3014[A]:TRP:CG | 3:a:3092[A]:ILE:HD11 | 2.32 | 0.64 |
| 3:a:3217[A]:PHE:HB2 | 3:a:3219[A]:LEU:HD21 | 1.79 | 0.64 |
| 3:a:3298[B]:ASN:ND2 | 3:a:3301[B]:PRO:O | 2.30 | 0.64 |
| 3:d:3014[A]:TRP:CG | 3:d:3092[A]:ILE:HD11 | 2.32 | 0.64 |
| 3:d:3117[B]:TYR:O | 3:d:3120[B]:HIS:HB2 | 1.97 | 0.64 |
| 3:d:3228[A]:VAL:HG21 | 3:d:3245[A]:PHE:CE1 | 2.32 | 0.64 |
| 1:A:630:PHE:O | 1:A:633:HIS:HB3 | 1.98 | 0.64 |
| 2:B:2149:ALA:HA | 2:B:2260:GLU:HG2 | 1.77 | 0.64 |
| 3:C:2982[B]:MET:H | 3:L:2967[B]:CYS:HB3 | 1.62 | 0.64 |
| 3:C:3066[B]:TYR:HD1 | 3:C:3193[B]:HIS:CE1 | 2.16 | 0.64 |
| 3:C:3224[B]:GLN:HA | 3:L:3252[B]:TYR:OH | 1.97 | 0.64 |
| 1:D:1301:PRO:HB3 | 1:D:1308:VAL:HG12 | 1.79 | 0.64 |
| 3:F:3092[A]:ILE:HG23 | 3:F:3096[A]:VAL:CG2 | 2.28 | 0.64 |
| 3:F:3159[B]:SER:CB | 3:a:3150[B]:LYS:O | 2.45 | 0.64 |
| 3:F:3232[B]:VAL:CG2 | 3:F:3273[B]:LEU:HD11 | 2.27 | 0.64 |
| 1:G:166:GLU:OE2 | 1:G:297:ARG:NH1 | 2.31 | 0.64 |
| 3:I:2933[B]:SER:O | 3:I:2936[B]:GLU:HB3 | 1.96 | 0.64 |
| 3:I:2937[A]:ASN:HB3 | 3:I:3006[A]:LYS:HD3 | 1.79 | 0.64 |
| 3:I:2952[A]:ALA:H | 3:I:2953[A]:GLY:CA | 2.04 | 0.64 |
| 3:I:3156[B]:MET:HB3 | 3:R:2982[B]:MET:HB2 | 1.80 | 0.64 |
| 3:I:3159[B]:SER:N | 3:R:3150[B]:LYS:O | 2.31 | 0.64 |
| 3:L:2994[B]:LYS:O | 3:L:2995[B]:GLN:C | 2.38 | 0.64 |
| 1:M:1018:ILE:HA | 1:M:1021:LEU:HB2 | 1.78 | 0.64 |
| 2:N:2889:ALA:N | 2:N:2890:VAL:HA | 2.12 | 0.64 |
| 3:R:2937[A]:ASN:HB3 | 3:R:3006[A]:LYS:HD3 | 1.79 | 0.64 |
| 3:R:3279[A]:ASP:OD1 | 3:R:3279[A]:ASP:N | 2.25 | 0.64 |
| 3:U:2971[B]:ASP:OD1 | 3:U:2973[B]:THR:OG1 | 2.04 | 0.64 |
| 3:U:3117[B]:TYR:O | 3:U:3120[B]:HIS:HB2 | 1.98 | 0.64 |
| 3:U:3162[B]:ASP:CG | 3:d:3260[B]:ARG:NH1 | 2.54 | 0.64 |
| 3:X:3066[A]:TYR:HD1 | 3:X:3193[A]:HIS:CE1 | 2.16 | 0.64 |
| 3:a:2937[B]:ASN:ND2 | 3:a:3006[B]:LYS:HD3 | 2.11 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2954[A]:TYR:HA | 3:a:2957[A]:ILE:HG22 | 1.80 | 0.64 |
| 3:a:2966[A]:SER:HB2 | 3:a:2977[A]:CYS:CB | 2.21 | 0.64 |
| 3:a:3117[A]:TYR:O | 3:a:3120[A]:HIS:HB2 | 1.97 | 0.64 |
| 3:d:2951[A]:ASP:O | 3:d:2956[A]:LYS:CE | 2.45 | 0.64 |
| 3:d:3117[A]:TYR:O | 3:d:3120[A]:HIS:HB2 | 1.98 | 0.64 |
| 3:d:3273[A]:LEU:CB | 3:d:3275[A]:LEU:HD13 | 2.28 | 0.64 |
| 3:d:3298[B]:ASN:HD21 | 3:d:3301[B]:PRO:HA | 1.60 | 0.64 |
| 3:C:2937[A]:ASN:HB3 | 3:C:3006[A]:LYS:HD3 | 1.79 | 0.64 |
| 3:C:3200[A]:LEU:HD22 | 3:C:3204[A]:LEU:CD1 | 2.27 | 0.64 |
| 3:C:3200[B]:LEU:HD22 | 3:C:3204[B]:LEU:CD1 | 2.27 | 0.64 |
| 3:F:2965[B]:LEU:C | 3:a:3221[B]:ALA:CB | 2.71 | 0.64 |
| 3:F:2979[B]:GLN:C | 3:a:2967[B]:CYS:HB2 | 2.23 | 0.64 |
| 3:F:3152[B]:LYS:HD3 | 3:a:3170[B]:ALA:O | 1.89 | 0.64 |
| 3:F:3180[B]:TYR:CB | 3:F:3183[B]:LEU:HD22 | 2.27 | 0.64 |
| 3:F:3259[B]:ASP:CA | 3:a:3162[B]:ASP:HB3 | 2.26 | 0.64 |
| 1:G:729:VAL:HG11 | 1:G:785:LEU:HD12 | 1.80 | 0.64 |
| 3:I:2954[B]:TYR:HA | 3:I:2957[B]:ILE:HG22 | 1.80 | 0.64 |
| 3:I:2988[B]:TRP:NE1 | 3:I:3158[B]:PHE:HE2 | 1.96 | 0.64 |
| 3:I:2990[A]:ARG:CZ | 3:I:3180[A]:TYR:HB3 | 2.28 | 0.64 |
| 3:I:3116[B]:PHE:HE2 | 3:R:2969[B]:TYR:CG | 1.98 | 0.64 |
| 3:I:3254[B]:MET:O | 3:R:2966[B]:SER:OG | 2.15 | 0.64 |
| 3:I:3259[B]:ASP:HB3 | 3:R:3162[B]:ASP:CA | 2.27 | 0.64 |
| 3:L:2952[B]:ALA:H | 3:L:2953[B]:GLY:CA | 2.04 | 0.64 |
| 3:L:2966[A]:SER:HB3 | 3:L:2977[A]:CYS:HB2 | 1.78 | 0.64 |
| 3:L:3232[A]:VAL:CG2 | 3:L:3273[A]:LEU:HD11 | 2.27 | 0.64 |
| 1:M:567:LEU:HB3 | 1:M:570:GLN:O | 1.97 | 0.64 |
| 3:O:3066[A]:TYR:CE1 | 3:O:3193[A]:HIS:HE1 | 2.15 | 0.64 |
| 3:O:3066[B]:TYR:HD1 | 3:O:3193[B]:HIS:CE1 | 2.16 | 0.64 |
| 1:P:1348:TRP:HH2 | 1:P:1461:VAL:HG23 | 1.63 | 0.64 |
| 1:P:1492:PRO:HB2 | 1:P:1497:SER:HB3 | 1.78 | 0.64 |
| 3:R:3014[A]:TRP:CG | 3:R:3092[A]:ILE:HD11 | 2.32 | 0.64 |
| 2:T:2180:TRP:HB2 | 2:T:2243:LEU:HD22 | 1.79 | 0.64 |
| 2:T:2240:GLN:HE21 | 2:T:2241:THR:HG22 | 1.61 | 0.64 |
| 3:U:2966[B]:SER:HB3 | 3:U:2977[B]:CYS:HB2 | 1.78 | 0.64 |
| 3:U:2988[A]:TRP:NE1 | 3:U:3158[A]:PHE:HE2 | 1.96 | 0.64 |
| 3:U:3014[B]:TRP:CG | 3:U:3092[B]:ILE:HD11 | 2.32 | 0.64 |
| 3:U:3255[B]:PRO:CD | 3:d:3252[B]:TYR:O | 2.45 | 0.64 |
| 3:U:3285[B]:VAL:HG22 | 3:U:3286[B]:THR:H | 1.62 | 0.64 |
| 3:X:2948[A]:ASP:HB3 | 3:X:2953[A]:GLY:CA | 2.24 | 0.64 |
| 3:X:2954[B]:TYR:HA | 3:X:2957[B]:ILE:HG22 | 1.80 | 0.64 |
| 3:X:2969[A]:TYR:HD2 | 3:X:2971[A]:ASP:N | 1.84 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3228[A]:VAL:HG21 | 3:X:3245[A]:PHE:CE1 | 2.32 | 0.64 |
| 3:X:3284[B]:LYS:CD | 3:X:3285[B]:VAL:H | 2.10 | 0.64 |
| 1:Y:1620:LEU:C | 3:d:3189[B]:ASN:ND2 | 2.55 | 0.64 |
| 3:a:2990[B]:ARG:CZ | 3:a:3180[B]:TYR:HB3 | 2.28 | 0.64 |
| 3:d:3014[B]:TRP:CG | 3:d:3092[B]:ILE:HD11 | 2.32 | 0.64 |
| 3:C:2928[A]:ASN:OD1 | 3:C:2929[A]:SER:N | 2.31 | 0.64 |
| 3:C:2928[B]:ASN:OD1 | 3:C:2929[B]:SER:N | 2.31 | 0.64 |
| 3:C:2955[B]:GLN:OE1 | 3:C:3037[B]:TYR:CE1 | 2.51 | 0.64 |
| 3:C:3157[B]:PRO:N | 3:L:2982[B]:MET:SD | 2.71 | 0.64 |
| 3:F:3066[A]:TYR:CE1 | 3:F:3193[A]:HIS:HE1 | 2.15 | 0.64 |
| 1:G:567:LEU:HB3 | 1:G:570:GLN:O | 1.97 | 0.64 |
| 1:G:1031:ALA:O | 1:G:1154:SER:OG | 2.10 | 0.64 |
| 3:I:2981[B]:GLY:CA | 3:R:2968[B]:GLN:OE1 | 2.46 | 0.64 |
| 3:I:3090[B]:ASN:HB3 | 3:R:2972[B]:GLY:C | 2.23 | 0.64 |
| 3:I:3153[B]:LYS:C | 3:R:3155[B]:MET:N | 2.53 | 0.64 |
| 1:J:1358:LEU:HD23 | 1:J:1456:LEU:HD21 | 1.79 | 0.64 |
| 1:J:1565:SER:HB3 | 1:J:1594:GLY:H | 1.63 | 0.64 |
| 3:L:3014[B]:TRP:CG | 3:L:3092[B]:ILE:HD11 | 2.32 | 0.64 |
| 3:L:3298[B]:ASN:ND2 | 3:L:3301[B]:PRO:O | 2.30 | 0.64 |
| 2:N:2833:GLY:HA3 | 2:N:2854:MET:HE1 | 1.80 | 0.64 |
| 3:O:3120[A]:HIS:NE2 | 9:O:3401[A]:CUO:O1 | 2.30 | 0.64 |
| 3:O:3151[B]:LEU:O | 3:O:3174[B]:GLY:HA3 | 1.97 | 0.64 |
| 3:O:3240[B]:THR:HG22 | 3:O:3241[B]:PHE:N | 2.13 | 0.64 |
| 3:R:2951[A]:ASP:O | 3:R:2956[A]:LYS:CE | 2.45 | 0.64 |
| 3:R:3092[A]:ILE:HG23 | 3:R:3096[A]:VAL:CG2 | 2.28 | 0.64 |
| 3:R:3200[B]:LEU:HD22 | 3:R:3204[B]:LEU:CD1 | 2.27 | 0.64 |
| 3:R:3273[A]:LEU:CB | 3:R:3275[A]:LEU:HD13 | 2.28 | 0.64 |
| 1:S:749:VAL:HB | 1:S:754:GLU:HB3 | 1.80 | 0.64 |
| 3:U:2948[A]:ASP:CB | 3:U:2949[A]:LYS:HA | 2.15 | 0.64 |
| 3:U:3212[A]:ARG:HH11 | 3:U:3212[A]:ARG:CG | 2.11 | 0.64 |
| 3:U:3217[A]:PHE:CE2 | 3:U:3303[A]:PRO:HG3 | 2.33 | 0.64 |
| 3:U:3298[B]:ASN:HD21 | 3:U:3301[B]:PRO:HA | 1.60 | 0.64 |
| 2:W:2800:LYS:O | 3:X:3023[A]:ILE:HD11 | 1.97 | 0.64 |
| 3:X:2928[B]:ASN:OD1 | 3:X:2929[B]:SER:N | 2.31 | 0.64 |
| 3:X:2988[A]:TRP:NE1 | 3:X:3158[A]:PHE:HE2 | 1.96 | 0.64 |
| 3:X:2988[B]:TRP:NE1 | 3:X:3158[B]:PHE:HE2 | 1.96 | 0.64 |
| 3:X:3120[A]:HIS:NE2 | 9:X:3401[A]:CUO:O1 | 2.30 | 0.64 |
| 3:X:3217[B]:PHE:CE2 | 3:X:3303[B]:PRO:HG3 | 2.33 | 0.64 |
| 3:a:2965[B]:LEU:CD1 | 3:a:2975[B]:PHE:H | 2.08 | 0.64 |
| 3:a:2988[A]:TRP:NE1 | 3:a:3158[A]:PHE:HE2 | 1.96 | 0.64 |
| 3:a:3092[B]:ILE:HG23 | 3:a:3096[B]:VAL:CG2 | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3157[A]:PRO:O | 3:a:3160[A]:SER:N | 2.30 | 0.64 |
| 1:b:450:LYS:HE3 | 1:b:451:SER:H | 1.61 | 0.64 |
| 3:d:3066[A]:TYR:CE1 | 3:d:3193[A]:HIS:HE1 | 2.15 | 0.64 |
| 3:d:3092[B]:ILE:HG23 | 3:d:3096[B]:VAL:CG2 | 2.28 | 0.64 |
| 3:d:3200[B]:LEU:HD22 | 3:d:3204[B]:LEU:CD1 | 2.27 | 0.64 |
| 1:A:928:TYR:HB3 | 1:A:1047:SER:HB3 | 1.80 | 0.64 |
| 3:C:2982[B]:MET:SD | 3:L:3156[B]:MET:CA | 2.85 | 0.64 |
| 3:C:2990[A]:ARG:CZ | 3:C:3180[A]:TYR:HB3 | 2.28 | 0.64 |
| 3:C:3092[B]:ILE:HG23 | 3:C:3096[B]:VAL:CG2 | 2.28 | 0.64 |
| 3:C:3117[A]:TYR:O | 3:C:3120[A]:HIS:HB2 | 1.97 | 0.64 |
| 3:C:3223[B]:GLY:H | 3:L:2963[B]:MET:CE | 2.07 | 0.64 |
| 3:C:3228[B]:VAL:HG21 | 3:C:3245[B]:PHE:CE1 | 2.32 | 0.64 |
| 1:D:1585:ASN:OD1 | 1:G:329:ARG:NH2 | 2.32 | 0.64 |
| 3:F:2961[B]:HIS:HB3 | 3:F:3111[B]:SER:CB | 2.28 | 0.64 |
| 3:F:2966[B]:SER:CA | 3:a:3255[B]:PRO:O | 2.45 | 0.64 |
| 3:F:2982[B]:MET:SD | 3:a:3156[B]:MET:HB2 | 2.37 | 0.64 |
| 3:F:3155[B]:MET:CA | 3:a:3153[B]:LYS:HB3 | 2.28 | 0.64 |
| 3:F:3217[B]:PHE:CE2 | 3:F:3303[B]:PRO:HG3 | 2.33 | 0.64 |
| 3:F:3240[A]:THR:HG22 | 3:F:3241[A]:PHE:N | 2.13 | 0.64 |
| 3:F:3255[B]:PRO:O | 3:a:2966[B]:SER:CB | 2.46 | 0.64 |
| 1:G:911:LEU:HG | 1:G:915:ASN:HD21 | 1.63 | 0.64 |
| 1:G:1471:LEU:HD12 | 1:G:1537:ILE:HG23 | 1.79 | 0.64 |
| 3:I:3117[A]:TYR:O | 3:I:3120[A]:HIS:HB2 | 1.98 | 0.64 |
| 3:I:3255[B]:PRO:CD | 3:R:2962[B]:GLY:C | 2.64 | 0.64 |
| 2:K:2451:LEU:HD22 | 2:K:2456:LEU:HD11 | 1.78 | 0.64 |
| 3:O:2955[B]:GLN:OE1 | 3:O:3037[B]:TYR:CE1 | 2.51 | 0.64 |
| 3:O:2971[B]:ASP:O | 3:X:2988[B]:TRP:CE3 | 2.50 | 0.64 |
| 3:O:3014[B]:TRP:CG | 3:O:3092[B]:ILE:HD11 | 2.32 | 0.64 |
| 3:O:3089[A]:HIS:CE1 | 3:O:3119[A]:HIS:CE1 | 2.81 | 0.64 |
| 3:O:3254[B]:MET:SD | 3:X:3154[B]:PRO:HB2 | 2.37 | 0.64 |
| 1:P:1130:SER:O | 1:P:1134:ASN:ND2 | 2.31 | 0.64 |
| 1:P:1301:PRO:O | 1:P:1494:ARG:NH2 | 2.29 | 0.64 |
| 3:R:2937[B]:ASN:HB3 | 3:R:3006[B]:LYS:HD3 | 1.79 | 0.64 |
| 3:R:3066[A]:TYR:HD1 | 3:R:3193[A]:HIS:CE1 | 2.16 | 0.64 |
| 1:S:678:ASN:O | 1:S:684:ARG:NH1 | 2.31 | 0.64 |
| 3:U:2928[B]:ASN:OD1 | 3:U:2929[B]:SER:N | 2.31 | 0.64 |
| 3:U:2957[B]:ILE:CA | 3:U:2960[B]:PHE:HE1 | 2.11 | 0.64 |
| 3:U:3066[A]:TYR:CE1 | 3:U:3193[A]:HIS:HE1 | 2.15 | 0.64 |
| 3:U:3169[B]:LYS:HD3 | 3:d:3147[B]:GLU:HA | 1.77 | 0.64 |
| 3:U:3298[A]:ASN:HD21 | 3:U:3301[A]:PRO:HA | 1.60 | 0.64 |
| 3:X:2990[B]:ARG:CZ | 3:X:3180[B]:TYR:HB3 | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3117[B]:TYR:O | 3:X:3120[B]:HIS:HB2 | 1.98 | 0.64 |
| 3:X:3217[A]:PHE:HB2 | 3:X:3219[A]:LEU:HD21 | 1.78 | 0.64 |
| 3:a:3066[B]:TYR:HD1 | 3:a:3193[B]:HIS:CE1 | 2.16 | 0.64 |
| 3:d:2948[B]:ASP:HB3 | 3:d:2953[B]:GLY:CA | 2.24 | 0.64 |
| 3:d:2987[A]:HIS:NE2 | 3:d:3178[A]:PHE:HE1 | 1.95 | 0.64 |
| 3:C:2951[B]:ASP:O | 3:C:2956[B]:LYS:CE | 2.45 | 0.63 |
| 3:C:2965[B]:LEU:HD22 | 3:L:3253[B]:GLU:CD | 2.11 | 0.63 |
| 3:C:2985[B]:PHE:HE2 | 3:L:2970[B]:PRO:N | 1.81 | 0.63 |
| 3:C:3014[A]:TRP:CG | 3:C:3092[A]:ILE:HD11 | 2.32 | 0.63 |
| 3:C:3120[B]:HIS:NE2 | 3:L:2969[B]:TYR:OH | 2.26 | 0.63 |
| 3:C:3124[A]:ASP:OD2 | 3:C:3187[A]:TYR:OH | 2.15 | 0.63 |
| 3:C:3149[B]:ASN:C | 3:L:3172[B]:SER:HG | 2.05 | 0.63 |
| 3:C:3153[B]:LYS:HZ3 | 3:L:2988[B]:TRP:HE1 | 1.44 | 0.63 |
| 3:C:3162[B]:ASP:OD1 | 3:C:3162[B]:ASP:N | 2.31 | 0.63 |
| 3:C:3217[B]:PHE:CE2 | 3:C:3303[B]:PRO:HG3 | 2.33 | 0.63 |
| 3:C:3284[B]:LYS:CD | 3:C:3285[B]:VAL:H | 2.10 | 0.63 |
| 3:F:3176[B]:LYS:HB3 | 3:F:3176[B]:LYS:HZ2 | 1.60 | 0.63 |
| 3:F:3217[A]:PHE:CE2 | 3:F:3303[A]:PRO:HG3 | 2.33 | 0.63 |
| 1:G:468:CYS:SG | 1:G:669:LYS:HB3 | 2.39 | 0.63 |
| 2:H:2252:GLU:O | 2:H:2389:ARG:NH2 | 2.31 | 0.63 |
| 3:I:2962[B]:GLY:O | 3:R:3255[B]:PRO:HG3 | 1.98 | 0.63 |
| 3:I:2977[B]:CYS:HB2 | 3:R:2982[B]:MET:CE | 2.28 | 0.63 |
| 3:I:3173[B]:THR:C | 3:R:3154[B]:PRO:CB | 2.68 | 0.63 |
| 3:I:3211[A]:ASP:OD1 | 3:I:3211[A]:ASP:N | 2.27 | 0.63 |
| 3:I:3255[B]:PRO:CB | 3:R:2959[B]:SER:HB2 | 2.15 | 0.63 |
| 1:J:883:CYS:N | 1:J:894:CYS:SG | 2.70 | 0.63 |
| 1:J:1506:LEU:O | 1:J:1510:ASN:ND2 | 2.28 | 0.63 |
| 3:L:3162[A]:ASP:N | 3:L:3162[A]:ASP:OD1 | 2.31 | 0.63 |
| 3:L:3217[B]:PHE:CE2 | 3:L:3303[B]:PRO:HG3 | 2.33 | 0.63 |
| 3:O:2966[A]:SER:HB2 | 3:O:2977[A]:CYS:CB | 2.21 | 0.63 |
| 3:O:2970[B]:PRO:HD2 | 3:X:2991[B]:LEU:HD13 | 1.35 | 0.63 |
| 3:O:3092[A]:ILE:HG23 | 3:O:3096[A]:VAL:CG2 | 2.28 | 0.63 |
| 3:O:3157[A]:PRO:O | 3:O:3160[A]:SER:N | 2.30 | 0.63 |
| 3:O:3157[B]:PRO:O | 3:O:3160[B]:SER:N | 2.30 | 0.63 |
| 3:O:3180[B]:TYR:CB | 3:O:3183[B]:LEU:HD22 | 2.27 | 0.63 |
| 3:R:2937[A]:ASN:ND2 | 3:R:3006[A]:LYS:HD3 | 2.11 | 0.63 |
| 3:R:2954[A]:TYR:HA | 3:R:2957[A]:ILE:HG22 | 1.80 | 0.63 |
| 3:R:2965[B]:LEU:CD1 | 3:R:2975[B]:PHE:H | 2.08 | 0.63 |
| 3:R:2987[B]:HIS:NE2 | 3:R:3178[B]:PHE:HE1 | 1.96 | 0.63 |
| 3:R:3232[A]:VAL:CG2 | 3:R:3273[A]:LEU:HD11 | 2.27 | 0.63 |
| 1:S:806:ASN:OD1 | 4:9:1:NAG:N2 | 2.30 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2969[B]:TYR:CZ | 3:d:2980[B]:HIS:NE2 | 2.66 | 0.63 |
| 3:U:3066[A]:TYR:HD1 | 3:U:3193[A]:HIS:CE1 | 2.16 | 0.63 |
| 1:V:327:ASP:OD1 | 1:V:328:LYS:N | 2.31 | 0.63 |
| 3:X:2928[A]:ASN:OD1 | 3:X:2929[A]:SER:N | 2.31 | 0.63 |
| 3:X:2949[A]:LYS:HD3 | 3:X:2949[A]:LYS:C | 2.24 | 0.63 |
| 1:Y:534:ASP:HB2 | 1:Y:541:LYS:HE2 | 1.80 | 0.63 |
| 3:a:2930[A]:LEU:H | 3:a:2930[A]:LEU:CD2 | 1.97 | 0.63 |
| 3:a:2990[A]:ARG:CZ | 3:a:3180[A]:TYR:HB3 | 2.28 | 0.63 |
| 3:a:3240[A]:THR:HG22 | 3:a:3241[A]:PHE:N | 2.13 | 0.63 |
| 1:b:1536:SER:N | 1:b:1539:GLN:OE1 | 2.30 | 0.63 |
| 3:d:2949[A]:LYS:HD3 | 3:d:2949[A]:LYS:C | 2.24 | 0.63 |
| 8:0:1:NAG:H61 | 8:0:2:NAG:N2 | 2.11 | 0.63 |
| 6:GA:1:NAG:C4 | 6:GA:2:NAG:C7 | 2.75 | 0.63 |
| 3:C:2952[B]:ALA:H | 3:C:2953[B]:GLY:CA | 2.04 | 0.63 |
| 3:C:2954[B]:TYR:HA | 3:C:2957[B]:ILE:HG22 | 1.80 | 0.63 |
| 3:C:2957[A]:ILE:CA | 3:C:2960[A]:PHE:HE1 | 2.11 | 0.63 |
| 3:C:3090[B]:ASN:CB | 3:L:2972[B]:GLY:HA3 | 2.25 | 0.63 |
| 3:C:3217[A]:PHE:CE2 | 3:C:3303[A]:PRO:HG3 | 2.33 | 0.63 |
| 3:F:2928[B]:ASN:OD1 | 3:F:2929[B]:SER:N | 2.31 | 0.63 |
| 3:F:2965[B]:LEU:HA | 3:a:3253[B]:GLU:HG3 | 1.78 | 0.63 |
| 3:F:3273[B]:LEU:CB | 3:F:3275[B]:LEU:HD13 | 2.28 | 0.63 |
| 1:G:983:PRO:HG3 | 1:G:989:THR:HB | 1.81 | 0.63 |
| 3:I:2955[A]:GLN:OE1 | 3:I:3037[A]:TYR:CE1 | 2.51 | 0.63 |
| 3:I:3066[B]:TYR:HD1 | 3:I:3193[B]:HIS:CE1 | 2.16 | 0.63 |
| 3:I:3124[A]:ASP:OD2 | 3:I:3187[A]:TYR:OH | 2.15 | 0.63 |
| 3:L:2937[B]:ASN:HB3 | 3:L:3006[B]:LYS:HD3 | 1.79 | 0.63 |
| 3:L:2957[B]:ILE:CA | 3:L:2960[B]:PHE:HE1 | 2.11 | 0.63 |
| 3:L:3066[A]:TYR:HD1 | 3:L:3193[A]:HIS:CE1 | 2.16 | 0.63 |
| 3:L:3092[B]:ILE:HG23 | 3:L:3096[B]:VAL:CG2 | 2.28 | 0.63 |
| 3:L:3117[A]:TYR:O | 3:L:3120[A]:HIS:HB2 | 1.98 | 0.63 |
| 3:L:3117[B]:TYR:O | 3:L:3120[B]:HIS:HB2 | 1.97 | 0.63 |
| 3:L:3180[A]:TYR:CB | 3:L:3183[A]:LEU:HD22 | 2.27 | 0.63 |
| 3:L:3240[B]:THR:HG22 | 3:L:3241[B]:PHE:N | 2.13 | 0.63 |
| 2:N:2107:LEU:HD23 | 2:N:2208:PRO:HB2 | 1.80 | 0.63 |
| 3:O:2928[A]:ASN:OD1 | 3:O:2929[A]:SER:N | 2.31 | 0.63 |
| 3:O:2975[B]:PHE:CD1 | 3:X:3156[B]:MET:C | 2.77 | 0.63 |
| 3:O:2988[A]:TRP:NE1 | 3:O:3158[A]:PHE:HE2 | 1.96 | 0.63 |
| 3:O:2990[B]:ARG:CZ | 3:O:3180[B]:TYR:HB3 | 2.28 | 0.63 |
| 3:O:3228[A]:VAL:HG21 | 3:O:3245[A]:PHE:CE1 | 2.32 | 0.63 |
| 3:R:3092[B]:ILE:HG23 | 3:R:3096[B]:VAL:CG2 | 2.28 | 0.63 |
| 3:R:3117[B]:TYR:O | 3:R:3120[B]:HIS:HB2 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3240[B]:THR:HG22 | 3:R:3241[B]:PHE:N | 2.13 | 0.63 |
| 2:T:2117:ASP:OD2 | 2:T:2168:ARG:NH2 | 2.30 | 0.63 |
| 3:U:2951[B]:ASP:O | 3:U:2956[B]:LYS:CE | 2.45 | 0.63 |
| 3:U:3066[B]:TYR:HD1 | 3:U:3193[B]:HIS:CE1 | 2.16 | 0.63 |
| 3:U:3173[A]:THR:CG2 | 3:U:3174[A]:GLY:H | 2.12 | 0.63 |
| 3:U:3232[A]:VAL:CG2 | 3:U:3273[A]:LEU:HD11 | 2.27 | 0.63 |
| 3:U:3256[B]:TRP:CB | 3:d:2969[B]:TYR:CA | 2.52 | 0.63 |
| 1:V:1627:ARG:NH2 | 1:V:1629:GLU:OE1 | 2.30 | 0.63 |
| 3:X:3092[A]:ILE:HG23 | 3:X:3096[A]:VAL:CG2 | 2.28 | 0.63 |
| 3:X:3157[B]:PRO:O | 3:X:3160[B]:SER:N | 2.30 | 0.63 |
| 1:Y:465:PRO:HG2 | 1:Y:467:LYS:HG2 | 1.79 | 0.63 |
| 1:Y:563:ILE:HG23 | 1:Y:565:GLU:HB2 | 1.80 | 0.63 |
| 1:Y:622:HIS:HE1 | 1:Y:767:LYS:H | 1.46 | 0.63 |
| 3:a:2928[B]:ASN:OD1 | 3:a:2929[B]:SER:N | 2.31 | 0.63 |
| 3:a:3162[B]:ASP:N | 3:a:3162[B]:ASP:OD1 | 2.31 | 0.63 |
| 3:a:3173[B]:THR:CG2 | 3:a:3174[B]:GLY:H | 2.12 | 0.63 |
| 3:a:3285[B]:VAL:HG22 | 3:a:3286[B]:THR:H | 1.61 | 0.63 |
| 3:d:2954[B]:TYR:HA | 3:d:2957[B]:ILE:HG22 | 1.80 | 0.63 |
| 1:A:907:ARG:NH2 | 1:A:1057:GLN:OE1 | 2.31 | 0.63 |
| 1:A:1286:ARG:NH2 | 1:A:1333:GLU:OE2 | 2.30 | 0.63 |
| 3:C:3120[A]:HIS:NE2 | 9:L:3401[A]:CUO:O1 | 2.30 | 0.63 |
| 3:C:3149[B]:ASN:C | 3:L:3172[B]:SER:OG | 2.40 | 0.63 |
| 3:C:3157[A]:PRO:O | 3:C:3160[A]:SER:N | 2.30 | 0.63 |
| 3:C:3180[B]:TYR:CB | 3:C:3183[B]:LEU:HD22 | 2.27 | 0.63 |
| 3:C:3232[B]:VAL:CG2 | 3:C:3273[B]:LEU:HD11 | 2.27 | 0.63 |
| 3:F:3173[B]:THR:HB | 3:F:3176[B]:LYS:HG2 | 1.81 | 0.63 |
| 3:F:3211[A]:ASP:OD1 | 3:F:3211[A]:ASP:N | 2.28 | 0.63 |
| 9:F:3401[A]:CUO:O1 | 3:a:3120[A]:HIS:NE2 | 2.30 | 0.63 |
| 1:G:460:GLU:HB3 | 1:G:465:PRO:HG2 | 1.81 | 0.63 |
| 1:G:757:VAL:HG21 | 1:G:781:ILE:HG22 | 1.79 | 0.63 |
| 3:I:3180[B]:TYR:CB | 3:I:3183[B]:LEU:HD22 | 2.27 | 0.63 |
| 3:I:3232[B]:VAL:CG2 | 3:I:3273[B]:LEU:HD11 | 2.27 | 0.63 |
| 3:L:2949[A]:LYS:HD3 | 3:L:2949[A]:LYS:C | 2.24 | 0.63 |
| 3:L:2951[B]:ASP:O | 3:L:2956[B]:LYS:CE | 2.45 | 0.63 |
| 3:L:2954[A]:TYR:HA | 3:L:2957[A]:ILE:HG22 | 1.80 | 0.63 |
| 3:L:2955[B]:GLN:OE1 | 3:L:3037[B]:TYR:CE1 | 2.51 | 0.63 |
| 3:L:2987[A]:HIS:NE2 | 3:L:3178[A]:PHE:HE1 | 1.96 | 0.63 |
| 3:L:2988[A]:TRP:NE1 | 3:L:3158[A]:PHE:HE2 | 1.96 | 0.63 |
| 3:O:2954[A]:TYR:HA | 3:O:2957[A]:ILE:HG22 | 1.80 | 0.63 |
| 3:O:2961[B]:HIS:HB3 | 3:O:3111[B]:SER:CB | 2.28 | 0.63 |
| 3:O:3298[A]:ASN:HD21 | 3:O:3301[A]:PRO:HA | 1.60 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:843:VAL:HG13 | 1:P:927:PRO:HB2 | 1.81 | 0.63 |
| 3:R:3066[B]:TYR:HD1 | 3:R:3193[B]:HIS:CE1 | 2.16 | 0.63 |
| 3:R:3117[A]:TYR:O | 3:R:3120[A]:HIS:HB2 | 1.98 | 0.63 |
| 3:U:2955[A]:GLN:OE1 | 3:U:3037[A]:TYR:CE1 | 2.51 | 0.63 |
| 3:U:2961[B]:HIS:HB3 | 3:U:3111[B]:SER:CB | 2.28 | 0.63 |
| 3:U:3200[B]:LEU:HD22 | 3:U:3204[B]:LEU:CD1 | 2.27 | 0.63 |
| 3:U:3252[B]:TYR:CE2 | 3:d:3222[B]:ILE:HD12 | 2.22 | 0.63 |
| 1:V:972:SER:HA | 1:V:1028:VAL:HG22 | 1.80 | 0.63 |
| 3:X:2949[B]:LYS:HD3 | 3:X:2949[B]:LYS:C | 2.23 | 0.63 |
| 3:X:2961[B]:HIS:CE1 | 3:X:2980[B]:HIS:NE2 | 2.57 | 0.63 |
| 3:X:2961[B]:HIS:HB3 | 3:X:3111[B]:SER:CB | 2.29 | 0.63 |
| 3:X:2994[A]:LYS:O | 3:X:2995[A]:GLN:C | 2.38 | 0.63 |
| 3:X:3066[B]:TYR:CE1 | 3:X:3193[B]:HIS:HE1 | 2.15 | 0.63 |
| 3:X:3089[A]:HIS:CE1 | 3:X:3119[A]:HIS:CE1 | 2.81 | 0.63 |
| 1:Y:675:SER:O | 1:Y:679:ASN:ND2 | 2.31 | 0.63 |
| 3:a:3014[B]:TRP:CG | 3:a:3092[B]:ILE:HD11 | 2.32 | 0.63 |
| 3:a:3096[A]:VAL:HG11 | 3:a:3115[A]:LEU:HD13 | 1.81 | 0.63 |
| 3:a:3180[A]:TYR:CB | 3:a:3183[A]:LEU:HD22 | 2.27 | 0.63 |
| 1:b:43:GLU:HG3 | 1:b:44:PRO:HA | 1.81 | 0.63 |
| 3:d:2961[B]:HIS:HB3 | 3:d:3111[B]:SER:CB | 2.28 | 0.63 |
| 3:d:2988[A]:TRP:NE1 | 3:d:3158[A]:PHE:HE2 | 1.96 | 0.63 |
| 3:d:3173[B]:THR:HB | 3:d:3176[B]:LYS:HG2 | 1.81 | 0.63 |
| 3:d:3217[A]:PHE:CE2 | 3:d:3303[A]:PRO:HG3 | 2.33 | 0.63 |
| 3:d:3217[B]:PHE:HE1 | 3:d:3230[B]:PHE:HZ | 0.80 | 0.63 |
| 1:A:1210:LYS:HA | 1:A:1211:TYR:CD2 | 2.34 | 0.63 |
| 3:C:3096[B]:VAL:HG11 | 3:C:3115[B]:LEU:HD13 | 1.81 | 0.63 |
| 3:C:3298[B]:ASN:CB | 3:C:3300[B]:LEU:N | 2.60 | 0.63 |
| 3:F:3228[B]:VAL:HG21 | 3:F:3245[B]:PHE:CE1 | 2.32 | 0.63 |
| 1:G:1321:HIS:HD2 | 1:G:1465:TRP:CH2 | 2.17 | 0.63 |
| 3:I:3092[B]:ILE:HG23 | 3:I:3096[B]:VAL:CG2 | 2.28 | 0.63 |
| 3:I:3173[A]:THR:CG2 | 3:I:3174[A]:GLY:H | 2.12 | 0.63 |
| 3:I:3232[A]:VAL:CG2 | 3:I:3273[A]:LEU:HD11 | 2.27 | 0.63 |
| 3:L:2954[B]:TYR:HA | 3:L:2957[B]:ILE:HG22 | 1.80 | 0.63 |
| 1:M:167:ASP:OD1 | 1:M:167:ASP:N | 2.31 | 0.63 |
| 2:N:2166:LEU:HA | 2:N:2169:HIS:HB2 | 1.80 | 0.63 |
| 3:O:2949[A]:LYS:C | 3:O:2949[A]:LYS:HD3 | 2.24 | 0.63 |
| 3:O:2990[A]:ARG:CZ | 3:O:3180[A]:TYR:HB3 | 2.28 | 0.63 |
| 3:O:3155[B]:MET:HG3 | 3:O:3172[B]:SER:O | 1.99 | 0.63 |
| 1:P:757:VAL:HG21 | 1:P:781:ILE:HG23 | 1.80 | 0.63 |
| 3:R:2928[B]:ASN:OD1 | 3:R:2929[B]:SER:N | 2.31 | 0.63 |
| 3:R:2988[B]:TRP:NE1 | 3:R:3158[B]:PHE:HE2 | 1.96 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:566:ARG:HG3 | 1:S:567:LEU:HB2 | 1.79 | 0.63 |
| 3:U:2971[B]:ASP:C | 3:d:3090[B]:ASN:ND2 | 2.57 | 0.63 |
| 3:U:2988[B]:TRP:NE1 | 3:U:3158[B]:PHE:HE2 | 1.96 | 0.63 |
| 3:U:3092[A]:ILE:HG23 | 3:U:3096[A]:VAL:CG2 | 2.28 | 0.63 |
| 3:U:3155[B]:MET:HG3 | 3:U:3172[B]:SER:O | 1.99 | 0.63 |
| 2:W:2472:ASN:HD21 | 4:HA:1:NAG:C6 | 2.06 | 0.63 |
| 3:X:2957[A]:ILE:CA | 3:X:2960[A]:PHE:HE1 | 2.11 | 0.63 |
| 3:X:2966[A]:SER:HB2 | 3:X:2977[A]:CYS:CB | 2.21 | 0.63 |
| 3:X:3120[B]:HIS:NE2 | 9:X:3401[B]:CUO:O1 | 2.30 | 0.63 |
| 3:X:3124[B]:ASP:OD2 | 3:X:3187[B]:TYR:OH | 2.15 | 0.63 |
| 3:X:3169[B]:LYS:C | 3:X:3172[B]:SER:HG | 2.00 | 0.63 |
| 3:X:3217[A]:PHE:CE2 | 3:X:3303[A]:PRO:HG3 | 2.33 | 0.63 |
| 3:X:3285[B]:VAL:HG22 | 3:X:3286[B]:THR:H | 1.62 | 0.63 |
| 1:Y:1301:PRO:HB3 | 1:Y:1308:VAL:HG12 | 1.81 | 0.63 |
| 2:Z:2166:LEU:HA | 2:Z:2169:HIS:HB2 | 1.80 | 0.63 |
| 3:a:2928[A]:ASN:OD1 | 3:a:2929[A]:SER:N | 2.31 | 0.63 |
| 3:a:2957[B]:ILE:CA | 3:a:2960[B]:PHE:HE1 | 2.11 | 0.63 |
| 3:a:3066[A]:TYR:HD1 | 3:a:3193[A]:HIS:CE1 | 2.16 | 0.63 |
| 3:a:3066[A]:TYR:CE1 | 3:a:3193[A]:HIS:HE1 | 2.15 | 0.63 |
| 3:a:3217[B]:PHE:CE2 | 3:a:3303[B]:PRO:HG3 | 2.33 | 0.63 |
| 1:b:1046:HIS:HA | 1:b:1049:VAL:HB | 1.79 | 0.63 |
| 3:d:2966[B]:SER:HB2 | 3:d:2977[B]:CYS:CB | 2.21 | 0.63 |
| 3:C:2994[B]:LYS:O | 3:C:2995[B]:GLN:C | 2.38 | 0.63 |
| 3:C:3154[B]:PRO:HB2 | 3:L:3151[B]:LEU:C | 2.22 | 0.63 |
| 3:C:3162[A]:ASP:OD1 | 3:C:3162[A]:ASP:N | 2.31 | 0.63 |
| 1:D:1067:TYR:H | 1:D:1067:TYR:HD1 | 1.45 | 0.63 |
| 3:F:2928[A]:ASN:OD1 | 3:F:2929[A]:SER:N | 2.31 | 0.63 |
| 3:F:2961[A]:HIS:HB3 | 3:F:3111[A]:SER:CB | 2.29 | 0.63 |
| 3:F:2988[B]:TRP:NE1 | 3:F:3158[B]:PHE:HE2 | 1.96 | 0.63 |
| 3:F:3096[B]:VAL:HG11 | 3:F:3115[B]:LEU:HD13 | 1.81 | 0.63 |
| 3:F:3153[B]:LYS:C | 3:a:3155[B]:MET:CB | 2.69 | 0.63 |
| 1:G:437:TYR:HB3 | 1:G:985:PHE:HZ | 1.64 | 0.63 |
| 3:I:2961[A]:HIS:HB3 | 3:I:3111[A]:SER:CB | 2.29 | 0.63 |
| 3:I:2961[B]:HIS:HB3 | 3:I:3111[B]:SER:CB | 2.29 | 0.63 |
| 3:I:2969[B]:TYR:HD2 | 3:R:3093[B]:HIS:NE2 | 1.95 | 0.63 |
| 3:I:2994[B]:LYS:O | 3:I:2995[B]:GLN:C | 2.38 | 0.63 |
| 3:I:3066[A]:TYR:HD1 | 3:I:3193[A]:HIS:CE1 | 2.16 | 0.63 |
| 3:I:3252[B]:TYR:O | 3:R:2976[B]:ALA:CB | 2.47 | 0.63 |
| 3:I:3273[B]:LEU:CB | 3:I:3275[B]:LEU:HD13 | 2.28 | 0.63 |
| 3:I:3285[B]:VAL:HG22 | 3:I:3286[B]:THR:H | 1.61 | 0.63 |
| 1:J:1427:HIS:HE1 | 1:J:1458:HIS:NE2 | 1.95 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:2955[A]:GLN:OE1 | 3:L:3037[A]:TYR:CE1 | 2.51 | 0.63 |
| 3:L:3212[B]:ARG:HH11 | 3:L:3212[B]:ARG:CG | 2.12 | 0.63 |
| 3:L:3217[A]:PHE:HE1 | 3:L:3230[A]:PHE:HZ | 0.81 | 0.63 |
| 3:L:3284[A]:LYS:CD | 3:L:3285[A]:VAL:H | 2.10 | 0.63 |
| 1:M:961:SER:OG | 1:M:974:ALA:N | 2.31 | 0.63 |
| 3:O:2954[B]:TYR:HA | 3:O:2957[B]:ILE:HG22 | 1.80 | 0.63 |
| 3:O:2957[A]:ILE:CA | 3:O:2960[A]:PHE:HE1 | 2.11 | 0.63 |
| 3:O:3117[A]:TYR:O | 3:O:3120[A]:HIS:HB2 | 1.97 | 0.63 |
| 3:O:3155[A]:MET:HG3 | 3:O:3172[A]:SER:O | 1.99 | 0.63 |
| 3:O:3198[B]:PRO:HD3 | 1:P:1618:LEU:O | 1.97 | 0.63 |
| 3:O:3228[A]:VAL:HG12 | 3:O:3287[A]:ILE:CG1 | 2.29 | 0.63 |
| 3:O:3232[B]:VAL:CG2 | 3:O:3273[B]:LEU:HD11 | 2.27 | 0.63 |
| 3:O:3255[B]:PRO:HG2 | 3:X:3163[B]:ASN:CG | 2.24 | 0.63 |
| 3:O:3256[B]:TRP:HE1 | 3:X:3161[B]:GLU:CD | 2.07 | 0.63 |
| 3:O:3285[A]:VAL:HG22 | 3:O:3286[A]:THR:H | 1.62 | 0.63 |
| 3:R:3066[B]:TYR:CD1 | 3:R:3193[B]:HIS:HE1 | 2.17 | 0.63 |
| 2:T:2630:LYS:O | 2:T:2632:GLU:N | 2.30 | 0.63 |
| 3:U:2928[A]:ASN:OD1 | 3:U:2929[A]:SER:N | 2.31 | 0.63 |
| 3:U:3155[A]:MET:HG3 | 3:U:3172[A]:SER:O | 1.99 | 0.63 |
| 3:U:3162[B]:ASP:N | 3:U:3162[B]:ASP:OD1 | 2.31 | 0.63 |
| 3:U:3217[B]:PHE:CE2 | 3:U:3303[B]:PRO:HG3 | 2.33 | 0.63 |
| 3:U:3228[A]:VAL:HG12 | 3:U:3287[A]:ILE:CG1 | 2.29 | 0.63 |
| 3:U:3284[B]:LYS:CD | 3:U:3285[B]:VAL:H | 2.09 | 0.63 |
| 2:W:2684:HIS:NE2 | 2:W:2711:HIS:CE1 | 2.66 | 0.63 |
| 3:X:2965[B]:LEU:CD1 | 3:X:2975[B]:PHE:H | 2.08 | 0.63 |
| 3:X:3120[B]:HIS:C | 3:X:3122[B]:ASN:N | 2.55 | 0.63 |
| 3:X:3173[B]:THR:HB | 3:X:3176[B]:LYS:HG2 | 1.81 | 0.63 |
| 3:X:3285[A]:VAL:HG22 | 3:X:3286[A]:THR:H | 1.62 | 0.63 |
| 1:Y:932:THR:HG22 | 1:Y:995:ILE:HD12 | 1.80 | 0.63 |
| 3:a:2951[B]:ASP:O | 3:a:2956[B]:LYS:CE | 2.45 | 0.63 |
| 3:a:2988[B]:TRP:NE1 | 3:a:3158[B]:PHE:HE2 | 1.96 | 0.63 |
| 3:a:3092[A]:ILE:HG23 | 3:a:3096[A]:VAL:CG2 | 2.28 | 0.63 |
| 3:a:3173[B]:THR:HB | 3:a:3176[B]:LYS:HG2 | 1.81 | 0.63 |
| 3:a:3212[A]:ARG:HH11 | 3:a:3212[A]:ARG:CG | 2.12 | 0.63 |
| 1:b:533:VAL:HG12 | 1:b:540:THR:HG22 | 1.81 | 0.63 |
| 2:c:2800:LYS:HB3 | 3:d:3023[A]:ILE:CD1 | 2.29 | 0.63 |
| 3:d:3155[A]:MET:HG3 | 3:d:3172[A]:SER:O | 1.99 | 0.63 |
| 1:A:804:ASP:OD2 | 4:f:1:NAG:O6 | 2.16 | 0.63 |
| 2:B:2799:LYS:HB3 | 2:B:2907:LYS:HD3 | 1.79 | 0.63 |
| 3:C:2965[B]:LEU:CD1 | 3:C:2975[B]:PHE:H | 2.08 | 0.63 |
| 3:C:2971[B]:ASP:CG | 3:L:3248[B]:LEU:CD2 | 2.71 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2972[B]:GLY:C | 3:L:3090[B]:ASN:HB3 | 2.23 | 0.63 |
| 3:C:3149[B]:ASN:CB | 3:L:3169[B]:LYS:N | 2.34 | 0.63 |
| 3:C:3211[A]:ASP:OD1 | 3:C:3211[A]:ASP:N | 2.28 | 0.63 |
| 1:D:898:GLY:HA2 | 1:D:1186:TRP:HB2 | 1.80 | 0.63 |
| 1:D:1244:GLY:HA2 | 1:D:1476:LYS:HD3 | 1.79 | 0.63 |
| 3:F:3135[B]:LYS:HG3 | 3:F:3141[B]:TYR:CD1 | 2.33 | 0.63 |
| 1:G:931:TRP:CG | 1:G:1018:ILE:HD11 | 2.34 | 0.63 |
| 1:G:1396:GLU:OE2 | 1:G:1569:ARG:NH2 | 2.32 | 0.63 |
| 3:I:2988[A]:TRP:NE1 | 3:I:3158[A]:PHE:HE2 | 1.96 | 0.63 |
| 3:I:3092[A]:ILE:HG23 | 3:I:3096[A]:VAL:CG2 | 2.28 | 0.63 |
| 3:I:3161[B]:GLU:HG2 | 3:R:3079[B]:CYS:CB | 2.29 | 0.63 |
| 3:I:3217[B]:PHE:CE2 | 3:I:3303[B]:PRO:HG3 | 2.33 | 0.63 |
| 3:I:3240[A]:THR:HG22 | 3:I:3241[A]:PHE:N | 2.13 | 0.63 |
| 3:I:3284[B]:LYS:HA | 3:I:3284[B]:LYS:CE | 2.22 | 0.63 |
| 3:I:3285[A]:VAL:HG22 | 3:I:3286[A]:THR:H | 1.62 | 0.63 |
| 1:J:119:LYS:HB2 | 1:J:120:LYS:C | 2.24 | 0.63 |
| 1:J:838:ARG:NH2 | 1:J:915:ASN:OD1 | 2.31 | 0.63 |
| 3:L:2988[B]:TRP:NE1 | 3:L:3158[B]:PHE:HE2 | 1.96 | 0.63 |
| 3:L:3092[A]:ILE:HG23 | 3:L:3096[A]:VAL:CG2 | 2.28 | 0.63 |
| 3:L:3124[B]:ASP:OD2 | 3:L:3187[B]:TYR:OH | 2.15 | 0.63 |
| 3:L:3228[A]:VAL:HG21 | 3:L:3245[A]:PHE:CE1 | 2.32 | 0.63 |
| 3:L:3228[A]:VAL:HG12 | 3:L:3287[A]:ILE:CG1 | 2.29 | 0.63 |
| 3:O:2961[A]:HIS:HB3 | 3:O:3111[A]:SER:CB | 2.29 | 0.63 |
| 3:O:2988[B]:TRP:NE1 | 3:O:3158[B]:PHE:HE2 | 1.96 | 0.63 |
| 3:O:3066[A]:TYR:CD1 | 3:O:3193[A]:HIS:HE1 | 2.17 | 0.63 |
| 3:O:3109[B]:TYR:CZ | 3:X:2969[B]:TYR:O | 2.52 | 0.63 |
| 3:O:3284[B]:LYS:CD | 3:O:3285[B]:VAL:H | 2.10 | 0.63 |
| 1:P:401:VAL:HG22 | 1:P:662:SER:HB3 | 1.80 | 0.63 |
| 1:P:1170:MET:HB3 | 1:P:1203:MET:HE2 | 1.81 | 0.63 |
| 1:P:1470:GLU:HG3 | 1:P:1530:LEU:HD12 | 1.80 | 0.63 |
| 3:R:2949[B]:LYS:HD3 | 3:R:2949[B]:LYS:C | 2.24 | 0.63 |
| 3:R:2957[B]:ILE:CA | 3:R:2960[B]:PHE:HE1 | 2.11 | 0.63 |
| 3:R:3240[A]:THR:HG22 | 3:R:3241[A]:PHE:N | 2.13 | 0.63 |
| 3:U:2969[B]:TYR:N | 3:d:3256[B]:TRP:CD1 | 2.66 | 0.63 |
| 3:U:3200[A]:LEU:HD22 | 3:U:3204[A]:LEU:CD1 | 2.27 | 0.63 |
| 3:X:2937[A]:ASN:HD22 | 3:X:3006[A]:LYS:HD3 | 1.61 | 0.63 |
| 3:X:2961[A]:HIS:HB3 | 3:X:3111[A]:SER:CB | 2.29 | 0.63 |
| 1:Y:327:ASP:OD1 | 1:Y:328:LYS:N | 2.30 | 0.63 |
| 1:Y:622:HIS:CE1 | 1:Y:767:LYS:H | 2.16 | 0.63 |
| 3:a:2949[B]:LYS:C | 3:a:2949[B]:LYS:HD3 | 2.24 | 0.63 |
| 3:a:3180[B]:TYR:CB | 3:a:3183[B]:LEU:HD22 | 2.27 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:1462:ASP:OD2 | 1:b:1525:TYR:OH | 2.15 | 0.63 |
| 3:d:2955[B]:GLN:OE1 | 3:d:3037[B]:TYR:CE1 | 2.51 | 0.63 |
| 3:d:2988[B]:TRP:NE1 | 3:d:3158[B]:PHE:HE2 | 1.96 | 0.63 |
| 3:d:3228[A]:VAL:HG12 | 3:d:3287[A]:ILE:CG1 | 2.29 | 0.63 |
| 3:d:3285[A]:VAL:HG22 | 3:d:3286[A]:THR:H | 1.62 | 0.63 |
| 2:B:2851:ASN:HD21 | 1:D:1189:ASP:HB2 | 1.62 | 0.63 |
| 3:C:3086[B]:GLU:CG | 3:L:2968[B]:GLN:HE21 | 2.12 | 0.63 |
| 3:C:3153[B]:LYS:C | 3:L:3155[B]:MET:HG2 | 2.22 | 0.63 |
| 3:C:3228[B]:VAL:HG12 | 3:C:3287[B]:ILE:CG1 | 2.29 | 0.63 |
| 1:D:1290:ILE:HD13 | 1:D:1329:LEU:HG | 1.79 | 0.63 |
| 2:E:2868:GLU:CD | 2:E:2868:GLU:H | 2.07 | 0.63 |
| 3:F:2949[A]:LYS:HD3 | 3:F:2949[A]:LYS:C | 2.24 | 0.63 |
| 3:F:2954[B]:TYR:HA | 3:F:2957[B]:ILE:HG22 | 1.80 | 0.63 |
| 3:F:3092[B]:ILE:HG23 | 3:F:3096[B]:VAL:CG2 | 2.28 | 0.63 |
| 3:F:3163[B]:ASN:HB2 | 3:a:3150[B]:LYS:CE | 2.26 | 0.63 |
| 3:F:3252[B]:TYR:HA | 3:a:3108[B]:HIS:NE2 | 2.12 | 0.63 |
| 3:F:3255[B]:PRO:C | 3:a:2966[B]:SER:HA | 2.24 | 0.63 |
| 3:F:3273[A]:LEU:CB | 3:F:3275[A]:LEU:HD13 | 2.28 | 0.63 |
| 3:I:2990[B]:ARG:CZ | 3:I:3180[B]:TYR:HB3 | 2.28 | 0.63 |
| 3:I:3228[A]:VAL:HG12 | 3:I:3287[A]:ILE:CG1 | 2.29 | 0.63 |
| 1:J:590:ASP:O | 1:J:648:GLN:NE2 | 2.32 | 0.63 |
| 3:L:2961[B]:HIS:HB3 | 3:L:3111[B]:SER:CB | 2.28 | 0.63 |
| 1:M:965:ASP:OD2 | 1:M:969:ALA:N | 2.31 | 0.63 |
| 1:M:1212:HIS:H | 1:M:1212:HIS:CD2 | 2.15 | 0.63 |
| 1:M:1427:HIS:CE1 | 1:M:1458:HIS:NE2 | 2.66 | 0.63 |
| 3:O:3124[B]:ASP:OD2 | 3:O:3187[B]:TYR:OH | 2.15 | 0.63 |
| 3:O:3232[A]:VAL:CG2 | 3:O:3273[A]:LEU:HD11 | 2.27 | 0.63 |
| 3:R:2957[A]:ILE:HA | 3:R:2960[A]:PHE:HE1 | 1.64 | 0.63 |
| 2:T:2746:MET:HE3 | 2:T:2765:PRO:HG3 | 1.80 | 0.63 |
| 3:U:2975[B]:PHE:CE2 | 3:d:3254[B]:MET:CB | 2.79 | 0.63 |
| 3:U:2980[B]:HIS:CB | 3:d:2969[B]:TYR:CE1 | 2.69 | 0.63 |
| 3:U:3169[B]:LYS:CD | 3:d:3148[B]:ILE:H | 2.08 | 0.63 |
| 3:U:3173[A]:THR:HB | 3:U:3176[A]:LYS:HG2 | 1.81 | 0.63 |
| 3:U:3173[B]:THR:HB | 3:U:3176[B]:LYS:HG2 | 1.81 | 0.63 |
| 3:U:3240[A]:THR:HG22 | 3:U:3241[A]:PHE:N | 2.13 | 0.63 |
| 3:X:2990[A]:ARG:CZ | 3:X:3180[A]:TYR:HB3 | 2.28 | 0.63 |
| 3:X:3155[B]:MET:HG3 | 3:X:3172[B]:SER:O | 1.99 | 0.63 |
| 1:Y:1335:LEU:HD23 | 1:Y:1339:SER:HB3 | 1.80 | 0.63 |
| 3:a:2937[B]:ASN:HB3 | 3:a:3006[B]:LYS:HD3 | 1.79 | 0.63 |
| 3:a:3228[B]:VAL:HG12 | 3:a:3287[B]:ILE:CG1 | 2.29 | 0.63 |
| 1:b:898:GLY:N | 1:b:899:MET:HA | 2.12 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:1438:ASP:OD1 | 1:b:1439:VAL:N | 2.32 | 0.63 |
| 3:d:2961[A]:HIS:HB3 | 3:d:3111[A]:SER:CB | 2.29 | 0.63 |
| 3:d:2966[A]:SER:HB3 | 3:d:2977[A]:CYS:HB2 | 1.78 | 0.63 |
| 3:d:3151[A]:LEU:O | 3:d:3174[A]:GLY:HA3 | 1.97 | 0.63 |
| 3:d:3180[A]:TYR:CB | 3:d:3183[A]:LEU:HD22 | 2.27 | 0.63 |
| 3:d:3217[B]:PHE:CE2 | 3:d:3303[B]:PRO:HG3 | 2.34 | 0.63 |
| 1:A:460:GLU:OE2 | 1:A:1368:ARG:NH2 | 2.30 | 0.63 |
| 3:C:3092[A]:ILE:HG23 | 3:C:3096[A]:VAL:CG2 | 2.28 | 0.63 |
| 3:C:3146[B]:CYS:SG | 3:L:3161[B]:GLU:HG3 | 2.34 | 0.63 |
| 3:C:3159[B]:SER:CB | 3:L:3150[B]:LYS:O | 2.46 | 0.63 |
| 3:C:3173[A]:THR:CG2 | 3:C:3174[A]:GLY:H | 2.12 | 0.63 |
| 3:C:3240[B]:THR:HG22 | 3:C:3241[B]:PHE:N | 2.13 | 0.63 |
| 1:D:949:ASP:OD1 | 1:D:950:ALA:N | 2.26 | 0.63 |
| 3:F:2930[A]:LEU:HD22 | 3:F:2930[A]:LEU:N | 2.02 | 0.63 |
| 3:F:2988[B]:TRP:CH2 | 3:a:2975[B]:PHE:CE2 | 2.86 | 0.63 |
| 3:F:3066[B]:TYR:HD1 | 3:F:3193[B]:HIS:CE1 | 2.16 | 0.63 |
| 3:F:3160[B]:SER:CA | 3:a:3150[B]:LYS:HZ2 | 2.12 | 0.63 |
| 3:F:3169[B]:LYS:CD | 3:a:3148[B]:ILE:C | 2.30 | 0.63 |
| 3:F:3284[B]:LYS:CD | 3:F:3285[B]:VAL:H | 2.10 | 0.63 |
| 1:G:1576:THR:HG23 | 1:G:1581:GLU:HG2 | 1.80 | 0.63 |
| 3:I:2957[A]:ILE:CA | 3:I:2960[A]:PHE:HE1 | 2.11 | 0.63 |
| 3:I:3147[B]:GLU:HG3 | 3:R:3160[B]:SER:O | 1.97 | 0.63 |
| 1:J:730:PHE:HA | 1:J:780:GLU:HA | 1.79 | 0.63 |
| 1:J:804:ASP:OD1 | 1:J:805:VAL:N | 2.32 | 0.63 |
| 1:J:1472:GLN:OE1 | 1:J:1475:ARG:NH1 | 2.32 | 0.63 |
| 3:L:3124[A]:ASP:OD2 | 3:L:3187[A]:TYR:OH | 2.15 | 0.63 |
| 3:L:3217[A]:PHE:CE2 | 3:L:3303[A]:PRO:HG3 | 2.33 | 0.63 |
| 3:O:3240[A]:THR:HG22 | 3:O:3241[A]:PHE:N | 2.13 | 0.63 |
| 3:R:2957[A]:ILE:CA | 3:R:2960[A]:PHE:HE1 | 2.11 | 0.63 |
| 3:U:2957[A]:ILE:CA | 3:U:2960[A]:PHE:HE1 | 2.11 | 0.63 |
| 3:U:2965[A]:LEU:CD1 | 3:U:2975[A]:PHE:H | 2.08 | 0.63 |
| 3:U:3089[B]:HIS:CE1 | 3:U:3119[B]:HIS:CE1 | 2.81 | 0.63 |
| 3:U:3092[B]:ILE:HG23 | 3:U:3096[B]:VAL:CG2 | 2.28 | 0.63 |
| 3:U:3096[B]:VAL:HG11 | 3:U:3115[B]:LEU:HD13 | 1.81 | 0.63 |
| 3:U:3120[B]:HIS:NE2 | 9:U:3401[B]:CUO:O1 | 2.30 | 0.63 |
| 3:U:3173[B]:THR:CG2 | 3:U:3174[B]:GLY:H | 2.12 | 0.63 |
| 1:V:898:GLY:N | 1:V:899:MET:HA | 2.14 | 0.63 |
| 3:X:3155[A]:MET:HG3 | 3:X:3172[A]:SER:O | 1.99 | 0.63 |
| 3:X:3173[A]:THR:HB | 3:X:3176[A]:LYS:HG2 | 1.81 | 0.63 |
| 3:X:3173[A]:THR:CG2 | 3:X:3174[A]:GLY:H | 2.12 | 0.63 |
| 3:X:3240[A]:THR:HG22 | 3:X:3241[A]:PHE:N | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:1655:SER:C | 3:d:3006[B]:LYS:HZ3 | 2.05 | 0.63 |
| 2:Z:2345:ASN:HB3 | 2:Z:2348:THR:HB | 1.81 | 0.63 |
| 3:a:2961[B]:HIS:HB3 | 3:a:3111[B]:SER:CB | 2.29 | 0.63 |
| 3:a:3162[A]:ASP:OD1 | 3:a:3162[A]:ASP:N | 2.31 | 0.63 |
| 3:a:3173[A]:THR:CG2 | 3:a:3174[A]:GLY:H | 2.12 | 0.63 |
| 2:c:2133:PRO:HG2 | 2:c:2140:ARG:HA | 1.81 | 0.63 |
| 3:d:2957[A]:ILE:CA | 3:d:2960[A]:PHE:HE1 | 2.11 | 0.63 |
| 3:d:2957[B]:ILE:CA | 3:d:2960[B]:PHE:HE1 | 2.11 | 0.63 |
| 3:d:2990[A]:ARG:CZ | 3:d:3180[A]:TYR:HB3 | 2.28 | 0.63 |
| 3:d:3240[A]:THR:HG22 | 3:d:3241[A]:PHE:N | 2.13 | 0.63 |
| 1:A:639:ARG:NH2 | 1:A:707:PHE:O | 2.31 | 0.63 |
| 3:C:2965[A]:LEU:CD1 | 3:C:2975[A]:PHE:H | 2.08 | 0.63 |
| 3:C:3156[B]:MET:CG | 3:L:2982[B]:MET:CB | 2.77 | 0.63 |
| 3:C:3253[B]:GLU:HG3 | 3:L:2976[B]:ALA:HB2 | 1.79 | 0.63 |
| 1:D:1494:ARG:HG3 | 1:D:1494:ARG:NH1 | 2.05 | 0.63 |
| 3:F:2971[B]:ASP:C | 3:a:3093[B]:HIS:CD2 | 2.48 | 0.63 |
| 3:F:3212[A]:ARG:HH11 | 3:F:3212[A]:ARG:CG | 2.11 | 0.63 |
| 1:G:804:ASP:OD2 | 1:G:806:ASN:ND2 | 2.32 | 0.63 |
| 3:I:2982[B]:MET:HG3 | 3:R:3156[B]:MET:CB | 2.21 | 0.63 |
| 3:I:3117[B]:TYR:O | 3:I:3120[B]:HIS:HB2 | 1.98 | 0.63 |
| 3:I:3279[B]:ASP:OD1 | 3:I:3279[B]:ASP:N | 2.25 | 0.63 |
| 2:K:2128:LEU:HD23 | 2:K:2216:PHE:HZ | 1.62 | 0.63 |
| 3:L:2928[A]:ASN:OD1 | 3:L:2929[A]:SER:N | 2.31 | 0.63 |
| 3:L:2949[B]:LYS:HD3 | 3:L:2949[B]:LYS:C | 2.23 | 0.63 |
| 3:L:2961[A]:HIS:HB3 | 3:L:3111[A]:SER:CB | 2.29 | 0.63 |
| 2:N:2446:GLU:HG2 | 2:N:2448:THR:HG22 | 1.81 | 0.63 |
| 3:O:3066[B]:TYR:CD1 | 3:O:3193[B]:HIS:HE1 | 2.17 | 0.63 |
| 3:O:3135[B]:LYS:CB | 3:O:3141[B]:TYR:HD1 | 2.12 | 0.63 |
| 3:O:3162[A]:ASP:N | 3:O:3162[A]:ASP:OD1 | 2.31 | 0.63 |
| 3:O:3211[B]:ASP:OD1 | 3:O:3211[B]:ASP:N | 2.28 | 0.63 |
| 3:O:3212[B]:ARG:HH11 | 3:O:3212[B]:ARG:CG | 2.12 | 0.63 |
| 3:R:2988[A]:TRP:NE1 | 3:R:3158[A]:PHE:HE2 | 1.96 | 0.63 |
| 3:R:3114[A]:PRO:CD | 3:R:3115[A]:LEU:H | 2.12 | 0.63 |
| 3:R:3217[A]:PHE:CE2 | 3:R:3303[A]:PRO:HG3 | 2.33 | 0.63 |
| 3:R:3273[B]:LEU:CB | 3:R:3275[B]:LEU:HD13 | 2.28 | 0.63 |
| 3:U:2990[B]:ARG:CZ | 3:U:3180[B]:TYR:HB3 | 2.28 | 0.63 |
| 3:U:3066[A]:TYR:CD1 | 3:U:3193[A]:HIS:HE1 | 2.17 | 0.63 |
| 3:U:3066[B]:TYR:CD1 | 3:U:3193[B]:HIS:HE1 | 2.17 | 0.63 |
| 3:U:3120[A]:HIS:NE2 | 9:U:3401[A]:CUO:O1 | 2.30 | 0.63 |
| 3:U:3157[A]:PRO:O | 3:U:3160[A]:SER:N | 2.30 | 0.63 |
| 3:U:3307[B]:PHE:HE1 | 3:U:3309[B]:PRO:CG | 2.08 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:965:ASP:OD1 | 1:V:965:ASP:N | 2.28 | 0.63 |
| 1:Y:930:ASP:OD1 | 1:Y:1051:ARG:NH2 | 2.32 | 0.63 |
| 2:Z:2107:LEU:HD23 | 2:Z:2208:PRO:HB2 | 1.80 | 0.63 |
| 2:Z:2866:PRO:HG3 | 3:a:2933[A]:SER:OG | 1.99 | 0.63 |
| 3:a:2957[A]:ILE:CA | 3:a:2960[A]:PHE:HE1 | 2.11 | 0.63 |
| 3:a:3155[A]:MET:HG3 | 3:a:3172[A]:SER:O | 1.99 | 0.63 |
| 2:c:2235:PRO:HG3 | 2:c:2240:GLN:HE22 | 1.64 | 0.63 |
| 3:d:3066[A]:TYR:CD1 | 3:d:3193[A]:HIS:HE1 | 2.17 | 0.63 |
| 3:d:3114[B]:PRO:CD | 3:d:3115[B]:LEU:H | 2.12 | 0.63 |
| 3:d:3157[A]:PRO:O | 3:d:3160[A]:SER:N | 2.30 | 0.63 |
| 3:d:3173[A]:THR:CG2 | 3:d:3174[A]:GLY:H | 2.12 | 0.63 |
| 3:d:3212[A]:ARG:HH11 | 3:d:3212[A]:ARG:CG | 2.12 | 0.63 |
| 3:d:3240[B]:THR:HG22 | 3:d:3241[B]:PHE:N | 2.13 | 0.63 |
| 3:C:2960[B]:PHE:H | 3:C:2960[B]:PHE:HD1 | 1.41 | 0.62 |
| 3:C:2988[B]:TRP:NE1 | 3:C:3158[B]:PHE:HE2 | 1.96 | 0.62 |
| 3:C:2990[B]:ARG:CZ | 3:C:3180[B]:TYR:HB3 | 2.28 | 0.62 |
| 3:C:3066[B]:TYR:CD1 | 3:C:3193[B]:HIS:HE1 | 2.17 | 0.62 |
| 3:C:3173[B]:THR:CG2 | 3:C:3174[B]:GLY:H | 2.12 | 0.62 |
| 1:D:1636:ASN:OD1 | 1:D:1636:ASN:N | 2.29 | 0.62 |
| 3:F:2937[A]:ASN:HB3 | 3:F:3006[A]:LYS:HD3 | 1.78 | 0.62 |
| 3:F:2957[A]:ILE:N | 3:F:2960[A]:PHE:HE1 | 1.97 | 0.62 |
| 3:F:2990[A]:ARG:CZ | 3:F:3180[A]:TYR:HB3 | 2.28 | 0.62 |
| 1:G:104:LEU:HB3 | 1:G:123:PHE:HD2 | 1.64 | 0.62 |
| 1:G:1240:ILE:HG13 | 1:G:1247:ARG:HG3 | 1.80 | 0.62 |
| 1:G:1329:LEU:HB2 | 1:G:1507:THR:HG21 | 1.80 | 0.62 |
| 3:I:2928[A]:ASN:OD1 | 3:I:2929[A]:SER:N | 2.31 | 0.62 |
| 3:I:2957[B]:ILE:CA | 3:I:2960[B]:PHE:HE1 | 2.11 | 0.62 |
| 3:I:2965[B]:LEU:CB | 3:R:3253[B]:GLU:OE2 | 2.40 | 0.62 |
| 3:I:2987[A]:HIS:NE2 | 3:I:3178[A]:PHE:HE1 | 1.96 | 0.62 |
| 3:I:3066[B]:TYR:CD1 | 3:I:3193[B]:HIS:HE1 | 2.17 | 0.62 |
| 3:I:3162[B]:ASP:H | 3:R:2983[B]:VAL:CG2 | 2.12 | 0.62 |
| 3:I:3212[B]:ARG:HH11 | 3:I:3212[B]:ARG:CG | 2.12 | 0.62 |
| 3:I:3217[A]:PHE:CE2 | 3:I:3303[A]:PRO:HG3 | 2.33 | 0.62 |
| 1:J:392:PRO:HB2 | 1:J:394:GLN:HG2 | 1.79 | 0.62 |
| 1:J:1013:ILE:HD11 | 1:J:1175:PHE:CD2 | 2.33 | 0.62 |
| 1:M:1441:SER:OG | 1:M:1442:MET:N | 2.31 | 0.62 |
| 2:N:2728:ARG:NH1 | 2:N:2792:GLU:OE1 | 2.28 | 0.62 |
| 2:N:2825:ILE:HB | 2:N:2865:ILE:HD11 | 1.80 | 0.62 |
| 2:N:2890:VAL:N | 2:N:2891:LEU:HA | 2.12 | 0.62 |
| 3:O:2957[A]:ILE:HA | 3:O:2960[A]:PHE:HE1 | 1.64 | 0.62 |
| 3:O:2957[B]:ILE:HA | 3:O:2960[B]:PHE:HE1 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3169[B]:LYS:CG | 3:X:3148[B]:ILE:HG23 | 1.85 | 0.62 |
| 3:R:2966[B]:SER:HB3 | 3:R:2977[B]:CYS:HB2 | 1.78 | 0.62 |
| 3:R:2990[B]:ARG:CZ | 3:R:3180[B]:TYR:HB3 | 2.28 | 0.62 |
| 3:R:3066[A]:TYR:CD1 | 3:R:3193[A]:HIS:HE1 | 2.17 | 0.62 |
| 3:R:3135[B]:LYS:HG3 | 3:R:3141[B]:TYR:CD1 | 2.33 | 0.62 |
| 1:S:416:ASN:CG | 3:X:3196[A]:THR:CG2 | 2.32 | 0.62 |
| 3:U:2954[A]:TYR:HA | 3:U:2957[A]:ILE:HG22 | 1.80 | 0.62 |
| 3:X:3092[B]:ILE:HG23 | 3:X:3096[B]:VAL:CG2 | 2.28 | 0.62 |
| 3:X:3117[A]:TYR:O | 3:X:3120[A]:HIS:HB2 | 1.98 | 0.62 |
| 3:a:2949[A]:LYS:HD3 | 3:a:2949[A]:LYS:C | 2.24 | 0.62 |
| 3:a:2961[A]:HIS:HB3 | 3:a:3111[A]:SER:CB | 2.28 | 0.62 |
| 3:a:3027[A]:GLU:CD | 3:a:3028[A]:PRO:HD2 | 2.24 | 0.62 |
| 3:a:3228[A]:VAL:HG12 | 3:a:3287[A]:ILE:CG1 | 2.29 | 0.62 |
| 3:d:2928[B]:ASN:OD1 | 3:d:2929[B]:SER:N | 2.31 | 0.62 |
| 3:d:2949[B]:LYS:HD3 | 3:d:2949[B]:LYS:C | 2.24 | 0.62 |
| 3:d:3169[A]:LYS:C | 3:d:3172[A]:SER:HG | 2.00 | 0.62 |
| 3:d:3180[B]:TYR:CB | 3:d:3183[B]:LEU:HD22 | 2.27 | 0.62 |
| 3:C:2954[A]:TYR:HA | 3:C:2957[A]:ILE:HG22 | 1.80 | 0.62 |
| 3:C:3027[B]:GLU:CD | 3:C:3028[B]:PRO:HD2 | 2.25 | 0.62 |
| 3:C:3148[B]:ILE:O | 3:L:3170[B]:ALA:N | 2.30 | 0.62 |
| 3:C:3153[B]:LYS:NZ | 3:L:3156[B]:MET:O | 2.27 | 0.62 |
| 3:C:3155[B]:MET:SD | 3:L:3154[B]:PRO:O | 2.57 | 0.62 |
| 1:D:898:GLY:N | 1:D:899:MET:HA | 2.12 | 0.62 |
| 2:E:2507:ARG:HA | 2:E:2779:ASP:HB2 | 1.81 | 0.62 |
| 3:F:2988[A]:TRP:NE1 | 3:F:3158[A]:PHE:HE2 | 1.96 | 0.62 |
| 3:F:3027[B]:GLU:CD | 3:F:3028[B]:PRO:HD2 | 2.24 | 0.62 |
| 3:F:3093[B]:HIS:HD2 | 3:a:2973[B]:THR:OG1 | 1.83 | 0.62 |
| 3:F:3173[B]:THR:CG2 | 3:F:3174[B]:GLY:H | 2.12 | 0.62 |
| 3:F:3285[B]:VAL:HG22 | 3:F:3286[B]:THR:H | 1.62 | 0.62 |
| 1:G:1358:LEU:HD23 | 1:G:1456:LEU:HD21 | 1.80 | 0.62 |
| 3:I:3259[B]:ASP:H | 3:R:3162[B]:ASP:HB3 | 1.65 | 0.62 |
| 1:J:195:SER:HB2 | 1:J:386:ILE:HD11 | 1.81 | 0.62 |
| 3:L:2957[A]:ILE:CA | 3:L:2960[A]:PHE:HE1 | 2.11 | 0.62 |
| 3:L:3066[B]:TYR:CD1 | 3:L:3193[B]:HIS:HE1 | 2.17 | 0.62 |
| 3:L:3162[B]:ASP:OD1 | 3:L:3162[B]:ASP:N | 2.31 | 0.62 |
| 3:O:3027[A]:GLU:CD | 3:O:3028[A]:PRO:HD2 | 2.24 | 0.62 |
| 3:O:3092[B]:ILE:HG23 | 3:O:3096[B]:VAL:CG2 | 2.28 | 0.62 |
| 3:O:3217[B]:PHE:CE2 | 3:O:3303[B]:PRO:HG3 | 2.33 | 0.62 |
| 3:O:3228[B]:VAL:HG21 | 3:O:3245[B]:PHE:CE1 | 2.32 | 0.62 |
| 3:R:2928[A]:ASN:OD1 | 3:R:2929[A]:SER:N | 2.31 | 0.62 |
| 3:R:3217[A]:PHE:HE1 | 3:R:3230[A]:PHE:HZ | 0.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3228[A]:VAL:HG12 | 3:R:3287[A]:ILE:CG1 | 2.29 | 0.62 |
| 3:U:3135[A]:LYS:CB | 3:U:3141[A]:TYR:HD1 | 2.13 | 0.62 |
| 3:U:3154[B]:PRO:C | 3:d:3150[B]:LYS:CB | 2.61 | 0.62 |
| 3:U:3162[A]:ASP:OD1 | 3:U:3162[A]:ASP:N | 2.31 | 0.62 |
| 3:X:2957[B]:ILE:CA | 3:X:2960[B]:PHE:HE1 | 2.11 | 0.62 |
| 2:Z:2524:LEU:HA | 2:Z:2581:MET:HE1 | 1.81 | 0.62 |
| 3:a:2954[B]:TYR:HA | 3:a:2957[B]:ILE:HG22 | 1.80 | 0.62 |
| 3:a:3124[A]:ASP:OD2 | 3:a:3187[A]:TYR:OH | 2.16 | 0.62 |
| 3:a:3217[A]:PHE:CE2 | 3:a:3303[A]:PRO:HG3 | 2.33 | 0.62 |
| 1:b:277:ASP:OD1 | 1:b:278:ASP:N | 2.31 | 0.62 |
| 3:d:2990[B]:ARG:CZ | 3:d:3180[B]:TYR:HB3 | 2.28 | 0.62 |
| 3:d:2994[B]:LYS:O | 3:d:2995[B]:GLN:C | 2.38 | 0.62 |
| 3:d:3092[A]:ILE:HG23 | 3:d:3096[A]:VAL:CG2 | 2.28 | 0.62 |
| 1:A:804:ASP:OD1 | 1:A:805:VAL:N | 2.32 | 0.62 |
| 3:C:2957[B]:ILE:CA | 3:C:2960[B]:PHE:HE1 | 2.11 | 0.62 |
| 3:C:2961[A]:HIS:HB3 | 3:C:3111[A]:SER:CB | 2.29 | 0.62 |
| 3:C:3155[A]:MET:HG3 | 3:C:3172[A]:SER:O | 1.99 | 0.62 |
| 3:C:3160[B]:SER:O | 3:L:3149[B]:ASN:ND2 | 2.30 | 0.62 |
| 9:C:3401[A]:CUO:O1 | 3:L:3120[A]:HIS:NE2 | 2.30 | 0.62 |
| 1:D:1140:ASN:OD1 | 1:D:1239:GLY:N | 2.25 | 0.62 |
| 1:D:1639:LYS:HG3 | 4:m:1:NAG:O5 | 1.98 | 0.62 |
| 3:F:2957[B]:ILE:CA | 3:F:2960[B]:PHE:HE1 | 2.11 | 0.62 |
| 3:F:2990[B]:ARG:CZ | 3:F:3180[B]:TYR:HB3 | 2.28 | 0.62 |
| 3:F:3173[A]:THR:CG2 | 3:F:3174[A]:GLY:H | 2.12 | 0.62 |
| 1:G:104:LEU:HD23 | 1:G:123:PHE:HE2 | 1.64 | 0.62 |
| 2:H:2887:ASP:OD1 | 2:H:2887:ASP:N | 2.32 | 0.62 |
| 3:I:2957[B]:ILE:HA | 3:I:2960[B]:PHE:HE1 | 1.64 | 0.62 |
| 3:I:2962[B]:GLY:O | 3:R:3255[B]:PRO:CG | 2.47 | 0.62 |
| 3:I:3038[A]:ILE:HG22 | 3:I:3041[A]:ALA:H | 1.65 | 0.62 |
| 3:I:3124[B]:ASP:OD2 | 3:I:3187[B]:TYR:OH | 2.15 | 0.62 |
| 3:I:3155[B]:MET:HB2 | 3:R:3153[B]:LYS:HB3 | 1.80 | 0.62 |
| 3:I:3173[B]:THR:CG2 | 3:I:3174[B]:GLY:H | 2.12 | 0.62 |
| 3:I:3174[B]:GLY:CA | 3:R:3154[B]:PRO:CG | 2.47 | 0.62 |
| 1:J:240:PHE:HA | 1:J:263:ALA:HB3 | 1.81 | 0.62 |
| 1:J:806:ASN:OD1 | 4:u:1:NAG:H82 | 1.99 | 0.62 |
| 3:L:2957[A]:ILE:N | 3:L:2960[A]:PHE:HE1 | 1.97 | 0.62 |
| 3:L:2990[A]:ARG:CZ | 3:L:3180[A]:TYR:HB3 | 2.28 | 0.62 |
| 3:L:2990[B]:ARG:CZ | 3:L:3180[B]:TYR:HB3 | 2.28 | 0.62 |
| 3:L:3135[B]:LYS:HG3 | 3:L:3141[B]:TYR:CD1 | 2.33 | 0.62 |
| 3:L:3228[B]:VAL:HG12 | 3:L:3287[B]:ILE:CG1 | 2.29 | 0.62 |
| 1:M:450:LYS:HB3 | 1:M:454:GLY:HA3 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:2625:LEU:O | 2:N:2638:ARG:NH1 | 2.32 | 0.62 |
| 2:N:2643:GLU:O | 2:N:2647:LEU:N | 2.32 | 0.62 |
| 3:O:2949[B]:LYS:HD3 | 3:O:2949[B]:LYS:C | 2.24 | 0.62 |
| 3:O:3120[A]:HIS:C | 3:O:3122[A]:ASN:N | 2.55 | 0.62 |
| 3:O:3153[B]:LYS:HG3 | 3:X:3176[B]:LYS:NZ | 2.12 | 0.62 |
| 3:O:3228[B]:VAL:HG12 | 3:O:3287[B]:ILE:CG1 | 2.29 | 0.62 |
| 1:P:1582:ASN:HB3 | 1:P:1583:CYS:CB | 2.27 | 0.62 |
| 3:R:2949[A]:LYS:HD3 | 3:R:2949[A]:LYS:C | 2.24 | 0.62 |
| 3:R:2957[B]:ILE:N | 3:R:2960[B]:PHE:HE1 | 1.97 | 0.62 |
| 3:R:3162[B]:ASP:OD1 | 3:R:3162[B]:ASP:N | 2.31 | 0.62 |
| 3:R:3211[A]:ASP:OD1 | 3:R:3211[A]:ASP:N | 2.28 | 0.62 |
| 1:S:2:LEU:HD21 | 1:S:81:VAL:HG21 | 1.81 | 0.62 |
| 2:T:2191:LEU:O | 2:T:2225:ARG:NH2 | 2.31 | 0.62 |
| 3:U:2974[B]:ALA:CB | 3:d:3220[B]:ARG:CD | 2.77 | 0.62 |
| 3:U:3135[B]:LYS:CB | 3:U:3141[B]:TYR:HD1 | 2.12 | 0.62 |
| 3:U:3180[B]:TYR:CB | 3:U:3183[B]:LEU:HD22 | 2.27 | 0.62 |
| 1:V:127:GLU:HG3 | 1:V:133:LYS:HB3 | 1.80 | 0.62 |
| 3:X:3038[B]:ILE:HG22 | 3:X:3041[B]:ALA:H | 1.65 | 0.62 |
| 1:Y:932:THR:O | 1:Y:989:THR:OG1 | 2.17 | 0.62 |
| 2:Z:2142:ALA:HB2 | 2:Z:2433:THR:HG23 | 1.82 | 0.62 |
| 3:a:2955[B]:GLN:OE1 | 3:a:3037[B]:TYR:CE1 | 2.51 | 0.62 |
| 3:a:3038[B]:ILE:HG22 | 3:a:3041[B]:ALA:H | 1.65 | 0.62 |
| 3:a:3273[B]:LEU:CB | 3:a:3275[B]:LEU:HD13 | 2.29 | 0.62 |
| 1:b:979:LEU:HB2 | 1:b:980:TYR:CB | 2.29 | 0.62 |
| 3:d:2966[B]:SER:HB3 | 3:d:2977[B]:CYS:HB2 | 1.78 | 0.62 |
| 3:d:2969[A]:TYR:HD2 | 3:d:2971[A]:ASP:N | 1.84 | 0.62 |
| 3:d:3124[A]:ASP:OD2 | 3:d:3187[A]:TYR:OH | 2.15 | 0.62 |
| 3:d:3135[B]:LYS:HG3 | 3:d:3141[B]:TYR:CD1 | 2.33 | 0.62 |
| 3:d:3162[B]:ASP:OD1 | 3:d:3162[B]:ASP:N | 2.31 | 0.62 |
| 3:d:3300[A]:LEU:HD23 | 3:d:3300[A]:LEU:N | 2.14 | 0.62 |
| 6:5:1:NAG:O4 | 6:5:2:NAG:O7 | 2.16 | 0.62 |
| 2:B:2667:GLU:HB3 | 2:B:2730:LEU:HD22 | 1.81 | 0.62 |
| 3:C:2989[B]:HIS:NE2 | 3:L:2969[B]:TYR:HA | 2.15 | 0.62 |
| 3:C:3096[A]:VAL:HG11 | 3:C:3115[A]:LEU:HD13 | 1.81 | 0.62 |
| 3:C:3114[A]:PRO:CD | 3:C:3115[A]:LEU:H | 2.12 | 0.62 |
| 3:C:3151[B]:LEU:HA | 3:L:3154[B]:PRO:CB | 2.30 | 0.62 |
| 3:C:3252[B]:TYR:CD2 | 3:L:3223[B]:GLY:O | 2.53 | 0.62 |
| 2:E:2665:GLU:OE1 | 2:E:2798:GLN:NE2 | 2.31 | 0.62 |
| 3:F:2983[B]:VAL:HB | 3:a:3161[B]:GLU:N | 2.14 | 0.62 |
| 3:F:3153[B]:LYS:HG2 | 3:a:3155[B]:MET:SD | 2.38 | 0.62 |
| 1:G:11:THR:HG22 | 1:G:13:ASP:H | 1.63 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:64:THR:HG21 | 1:G:239:LEU:HB2 | 1.81 | 0.62 |
| 1:G:157:GLU:OE2 | 1:G:296:ARG:NH2 | 2.32 | 0.62 |
| 2:H:2426:PHE:HB3 | 2:H:2445:MET:HE1 | 1.80 | 0.62 |
| 3:I:2930[A]:LEU:H | 3:I:2930[A]:LEU:CD2 | 1.98 | 0.62 |
| 3:I:3066[A]:TYR:CD1 | 3:I:3193[A]:HIS:HE1 | 2.17 | 0.62 |
| 3:I:3096[A]:VAL:HG11 | 3:I:3115[A]:LEU:HD13 | 1.81 | 0.62 |
| 3:I:3107[B]:LEU:HD11 | 3:R:2975[B]:PHE:CG | 2.30 | 0.62 |
| 3:I:3155[B]:MET:O | 3:R:3153[B]:LYS:HB3 | 2.00 | 0.62 |
| 3:L:2928[B]:ASN:OD1 | 3:L:2929[B]:SER:N | 2.31 | 0.62 |
| 3:L:3027[A]:GLU:CD | 3:L:3028[A]:PRO:HD2 | 2.24 | 0.62 |
| 3:L:3135[B]:LYS:CB | 3:L:3141[B]:TYR:HD1 | 2.13 | 0.62 |
| 3:L:3155[A]:MET:HG3 | 3:L:3172[A]:SER:O | 1.99 | 0.62 |
| 2:N:2650:GLY:HA3 | 2:N:2653:GLU:H | 1.63 | 0.62 |
| 3:O:2928[B]:ASN:OD1 | 3:O:2929[B]:SER:N | 2.31 | 0.62 |
| 3:O:3066[A]:TYR:HD1 | 3:O:3193[A]:HIS:CE1 | 2.16 | 0.62 |
| 3:O:3273[A]:LEU:CB | 3:O:3275[A]:LEU:HD13 | 2.28 | 0.62 |
| 3:R:2961[A]:HIS:CE1 | 3:R:2980[A]:HIS:NE2 | 2.57 | 0.62 |
| 3:R:2961[B]:HIS:HB3 | 3:R:3111[B]:SER:HG | 1.63 | 0.62 |
| 3:R:2994[A]:LYS:O | 3:R:2995[A]:GLN:C | 2.38 | 0.62 |
| 3:R:3212[B]:ARG:HH11 | 3:R:3212[B]:ARG:CG | 2.11 | 0.62 |
| 3:U:3038[B]:ILE:HG22 | 3:U:3041[B]:ALA:H | 1.65 | 0.62 |
| 3:U:3162[B]:ASP:HB3 | 3:d:3260[B]:ARG:NH2 | 2.14 | 0.62 |
| 1:V:926:LEU:HD12 | 1:V:927:PRO:HD2 | 1.80 | 0.62 |
| 2:W:2090:LYS:NZ | 2:W:2099:GLU:OE2 | 2.32 | 0.62 |
| 3:X:2987[B]:HIS:NE2 | 3:X:3178[B]:PHE:HE1 | 1.95 | 0.62 |
| 3:X:3135[B]:LYS:CB | 3:X:3141[B]:TYR:HD1 | 2.13 | 0.62 |
| 3:X:3240[B]:THR:HG22 | 3:X:3241[B]:PHE:N | 2.13 | 0.62 |
| 1:Y:757:VAL:HG21 | 1:Y:781:ILE:HG22 | 1.81 | 0.62 |
| 3:a:3300[B]:LEU:HD23 | 3:a:3300[B]:LEU:N | 2.14 | 0.62 |
| 3:d:2952[B]:ALA:N | 3:d:2953[B]:GLY:HA2 | 2.06 | 0.62 |
| 3:d:3228[B]:VAL:HG12 | 3:d:3287[B]:ILE:CG1 | 2.29 | 0.62 |
| 1:A:883:CYS:HB2 | 1:A:891:LYS:HD3 | 1.81 | 0.62 |
| 2:B:2877:ILE:O | 1:D:1078:ARG:NH1 | 2.32 | 0.62 |
| 3:C:2949[A]:LYS:HD3 | 3:C:2949[A]:LYS:C | 2.23 | 0.62 |
| 3:F:3155[A]:MET:HG3 | 3:F:3172[A]:SER:O | 1.99 | 0.62 |
| 3:F:3169[B]:LYS:C | 3:a:3148[B]:ILE:O | 2.43 | 0.62 |
| 3:F:3228[B]:VAL:HG12 | 3:F:3287[B]:ILE:CG1 | 2.29 | 0.62 |
| 1:G:161:ASN:ND2 | 1:G:174:GLN:OE1 | 2.32 | 0.62 |
| 1:G:164:GLU:OE2 | 1:G:301:ARG:NH2 | 2.33 | 0.62 |
| 1:G:304:ALA:HB1 | 1:G:306:PHE:HE1 | 1.65 | 0.62 |
| 3:I:2928[B]:ASN:OD1 | 3:I:2929[B]:SER:N | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3162[A]:ASP:OD1 | 3:I:3162[A]:ASP:N | 2.31 | 0.62 |
| 3:I:3298[B]:ASN:CB | 3:I:3300[B]:LEU:N | 2.60 | 0.62 |
| 3:L:3114[B]:PRO:CD | 3:L:3115[B]:LEU:H | 2.12 | 0.62 |
| 3:L:3173[B]:THR:CG2 | 3:L:3174[B]:GLY:H | 2.12 | 0.62 |
| 1:M:527:LEU:HD13 | 1:M:629:MET:HG3 | 1.82 | 0.62 |
| 3:O:2957[A]:ILE:N | 3:O:2960[A]:PHE:HE1 | 1.97 | 0.62 |
| 3:O:3041[B]:ALA:CB | 3:X:2971[B]:ASP:OD2 | 2.48 | 0.62 |
| 1:P:500:ASN:O | 1:P:504:THR:OG1 | 2.18 | 0.62 |
| 1:P:1372:ILE:HD12 | 1:S:1438:ASP:HB2 | 1.80 | 0.62 |
| 3:R:3135[B]:LYS:CB | 3:R:3141[B]:TYR:HD1 | 2.12 | 0.62 |
| 3:U:2954[B]:TYR:HA | 3:U:2957[B]:ILE:HG22 | 1.80 | 0.62 |
| 3:U:2994[A]:LYS:HD2 | 3:U:2998[A]:ASP:OD2 | 2.00 | 0.62 |
| 3:U:3228[B]:VAL:HG12 | 3:U:3287[B]:ILE:CG1 | 2.29 | 0.62 |
| 3:U:3273[A]:LEU:CB | 3:U:3275[A]:LEU:HD13 | 2.28 | 0.62 |
| 3:U:3273[B]:LEU:CB | 3:U:3275[B]:LEU:HD13 | 2.28 | 0.62 |
| 3:X:3027[A]:GLU:CD | 3:X:3028[A]:PRO:HD2 | 2.24 | 0.62 |
| 3:X:3300[A]:LEU:HD23 | 3:X:3300[A]:LEU:N | 2.15 | 0.62 |
| 1:Y:157:GLU:OE2 | 1:Y:296:ARG:NH2 | 2.33 | 0.62 |
| 3:a:2955[A]:GLN:OE1 | 3:a:3037[A]:TYR:CE1 | 2.50 | 0.62 |
| 3:d:2928[A]:ASN:OD1 | 3:d:2929[A]:SER:N | 2.31 | 0.62 |
| 3:C:2959[B]:SER:O | 3:L:3255[B]:PRO:CG | 2.47 | 0.62 |
| 3:C:3117[B]:TYR:O | 3:C:3120[B]:HIS:HB2 | 1.98 | 0.62 |
| 3:C:3149[B]:ASN:HB2 | 3:L:3158[B]:PHE:O | 1.99 | 0.62 |
| 3:C:3156[B]:MET:CG | 3:L:2979[B]:GLN:HG3 | 2.30 | 0.62 |
| 3:C:3156[B]:MET:CG | 3:L:2982[B]:MET:HB2 | 2.30 | 0.62 |
| 3:C:3220[B]:ARG:HH11 | 3:C:3220[B]:ARG:CG | 2.12 | 0.62 |
| 3:C:3240[A]:THR:HG22 | 3:C:3241[A]:PHE:N | 2.13 | 0.62 |
| 3:C:3298[B]:ASN:HD21 | 3:C:3301[B]:PRO:HA | 1.60 | 0.62 |
| 3:F:2957[B]:ILE:N | 3:F:2960[B]:PHE:HE1 | 1.98 | 0.62 |
| 3:F:3114[A]:PRO:CD | 3:F:3115[A]:LEU:H | 2.12 | 0.62 |
| 3:F:3156[B]:MET:HB3 | 3:a:2982[B]:MET:CB | 2.29 | 0.62 |
| 3:F:3259[B]:ASP:HB3 | 3:a:3162[B]:ASP:CA | 2.30 | 0.62 |
| 3:F:3270[A]:LEU:O | 3:F:3274[A]:ARG:N | 2.33 | 0.62 |
| 3:I:2994[B]:LYS:HD2 | 3:I:2998[B]:ASP:OD2 | 2.00 | 0.62 |
| 3:I:3027[A]:GLU:CD | 3:I:3028[A]:PRO:HD2 | 2.24 | 0.62 |
| 3:I:3152[B]:LYS:HB2 | 3:R:3171[B]:HIS:N | 2.10 | 0.62 |
| 3:I:3240[B]:THR:HG22 | 3:I:3241[B]:PHE:N | 2.13 | 0.62 |
| 3:L:2948[A]:ASP:HB3 | 3:L:2953[A]:GLY:CA | 2.24 | 0.62 |
| 3:L:3173[B]:THR:HB | 3:L:3176[B]:LYS:HG2 | 1.81 | 0.62 |
| 1:M:1219:ASP:OD1 | 1:M:1223:ALA:N | 2.33 | 0.62 |
| 1:P:447:MET:HA | 1:P:455:TYR:HB2 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3027[A]:GLU:CD | 3:R:3028[A]:PRO:HD2 | 2.24 | 0.62 |
| 3:U:2957[A]:ILE:N | 3:U:2960[A]:PHE:HE1 | 1.97 | 0.62 |
| 3:U:3222[A]:ILE:HD11 | 3:U:3224[A]:GLN:OE1 | 2.00 | 0.62 |
| 1:V:484:MET:HE2 | 1:V:663:GLU:HG3 | 1.80 | 0.62 |
| 3:X:2994[A]:LYS:HD2 | 3:X:2998[A]:ASP:OD2 | 2.00 | 0.62 |
| 3:X:3162[A]:ASP:OD1 | 3:X:3162[A]:ASP:N | 2.32 | 0.62 |
| 3:X:3220[A]:ARG:HH11 | 3:X:3220[A]:ARG:CG | 2.12 | 0.62 |
| 3:a:2957[B]:ILE:HA | 3:a:2960[B]:PHE:HE1 | 1.64 | 0.62 |
| 3:a:3220[B]:ARG:HH11 | 3:a:3220[B]:ARG:CG | 2.12 | 0.62 |
| 3:a:3240[B]:THR:HG22 | 3:a:3241[B]:PHE:N | 2.13 | 0.62 |
| 3:a:3298[B]:ASN:HD21 | 3:a:3301[B]:PRO:HA | 1.60 | 0.62 |
| 3:a:3300[A]:LEU:HD23 | 3:a:3300[A]:LEU:N | 2.15 | 0.62 |
| 3:d:3038[A]:ILE:HG22 | 3:d:3041[A]:ALA:H | 1.65 | 0.62 |
| 3:d:3222[A]:ILE:HD11 | 3:d:3224[A]:GLN:OE1 | 2.00 | 0.62 |
| 3:d:3298[A]:ASN:CB | 3:d:3300[A]:LEU:N | 2.60 | 0.62 |
| 3:C:2961[B]:HIS:HB3 | 3:C:3111[B]:SER:CB | 2.28 | 0.62 |
| 3:C:2994[A]:LYS:O | 3:C:2995[A]:GLN:C | 2.38 | 0.62 |
| 3:C:2994[B]:LYS:HD2 | 3:C:2998[B]:ASP:OD2 | 2.00 | 0.62 |
| 3:C:3038[B]:ILE:HG12 | 3:C:3112[B]:TYR:CE2 | 2.35 | 0.62 |
| 3:C:3155[B]:MET:CG | 3:L:3154[B]:PRO:O | 2.47 | 0.62 |
| 3:C:3252[B]:TYR:CB | 3:L:3253[B]:GLU:CG | 2.77 | 0.62 |
| 3:C:3279[A]:ASP:OD1 | 3:C:3279[A]:ASP:N | 2.25 | 0.62 |
| 1:D:1499:SER:HA | 1:D:1508:PHE:HE2 | 1.65 | 0.62 |
| 3:F:2957[A]:ILE:CA | 3:F:2960[A]:PHE:HE1 | 2.11 | 0.62 |
| 3:F:3038[B]:ILE:HG22 | 3:F:3041[B]:ALA:H | 1.65 | 0.62 |
| 3:F:3090[B]:ASN:CB | 3:a:2971[B]:ASP:O | 2.48 | 0.62 |
| 3:F:3124[A]:ASP:OD2 | 3:F:3187[A]:TYR:OH | 2.15 | 0.62 |
| 3:F:3135[A]:LYS:CB | 3:F:3141[A]:TYR:HD1 | 2.12 | 0.62 |
| 3:F:3222[A]:ILE:HD11 | 3:F:3224[A]:GLN:OE1 | 2.00 | 0.62 |
| 3:F:3240[B]:THR:HG22 | 3:F:3241[B]:PHE:N | 2.13 | 0.62 |
| 3:F:3251[B]:ASP:HB2 | 3:a:3251[B]:ASP:CG | 2.24 | 0.62 |
| 3:F:3256[B]:TRP:CD1 | 3:a:2967[B]:CYS:N | 2.67 | 0.62 |
| 1:G:1286:ARG:NH2 | 1:G:1333:GLU:OE2 | 2.33 | 0.62 |
| 3:I:2949[A]:LYS:HD3 | 3:I:2949[A]:LYS:C | 2.23 | 0.62 |
| 3:I:3135[A]:LYS:CB | 3:I:3141[A]:TYR:HD1 | 2.13 | 0.62 |
| 3:I:3135[B]:LYS:CB | 3:I:3141[B]:TYR:HD1 | 2.12 | 0.62 |
| 3:I:3157[A]:PRO:O | 3:I:3160[A]:SER:N | 2.30 | 0.62 |
| 3:I:3222[A]:ILE:HD11 | 3:I:3224[A]:GLN:OE1 | 2.00 | 0.62 |
| 3:I:3270[A]:LEU:O | 3:I:3274[A]:ARG:N | 2.33 | 0.62 |
| 3:I:3298[B]:ASN:HD21 | 3:I:3301[B]:PRO:HA | 1.60 | 0.62 |
| 3:L:3066[A]:TYR:CD1 | 3:L:3193[A]:HIS:HE1 | 2.17 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3114[A]:PRO:CD | 3:L:3115[A]:LEU:H | 2.12 | 0.62 |
| 3:L:3120[B]:HIS:C | 3:L:3122[B]:ASN:N | 2.55 | 0.62 |
| 3:L:3270[A]:LEU:O | 3:L:3274[A]:ARG:N | 2.33 | 0.62 |
| 3:L:3270[B]:LEU:O | 3:L:3274[B]:ARG:N | 2.33 | 0.62 |
| 3:O:2968[B]:GLN:CB | 3:O:2972[B]:GLY:HA2 | 2.19 | 0.62 |
| 3:O:2994[B]:LYS:HD2 | 3:O:2998[B]:ASP:OD2 | 2.00 | 0.62 |
| 3:O:3038[B]:ILE:HG12 | 3:O:3112[B]:TYR:CE2 | 2.35 | 0.62 |
| 3:O:3217[A]:PHE:CE2 | 3:O:3303[A]:PRO:HG3 | 2.33 | 0.62 |
| 1:P:452:ILE:HD11 | 1:P:676:PRO:O | 2.00 | 0.62 |
| 1:P:909:ILE:HG12 | 1:P:1084:PHE:HZ | 1.64 | 0.62 |
| 3:R:2990[A]:ARG:CZ | 3:R:3180[A]:TYR:HB3 | 2.28 | 0.62 |
| 3:R:2994[A]:LYS:HD2 | 3:R:2998[A]:ASP:OD2 | 2.00 | 0.62 |
| 3:R:3155[A]:MET:HG3 | 3:R:3172[A]:SER:O | 1.99 | 0.62 |
| 3:R:3173[B]:THR:CG2 | 3:R:3174[B]:GLY:H | 2.12 | 0.62 |
| 3:R:3212[A]:ARG:HH11 | 3:R:3212[A]:ARG:CG | 2.12 | 0.62 |
| 3:R:3270[A]:LEU:O | 3:R:3274[A]:ARG:N | 2.33 | 0.62 |
| 3:R:3284[A]:LYS:CD | 3:R:3285[A]:VAL:H | 2.10 | 0.62 |
| 1:S:1140:ASN:OD1 | 1:S:1239:GLY:N | 2.22 | 0.62 |
| 2:T:2345:ASN:O | 2:T:2349:THR:OG1 | 2.16 | 0.62 |
| 2:T:2756:ASN:HD21 | 2:T:2759:THR:HG23 | 1.65 | 0.62 |
| 3:U:2949[A]:LYS:HD3 | 3:U:2949[A]:LYS:C | 2.24 | 0.62 |
| 3:U:3027[B]:GLU:CD | 3:U:3028[B]:PRO:HD2 | 2.25 | 0.62 |
| 3:U:3038[A]:ILE:HG22 | 3:U:3041[A]:ALA:H | 1.65 | 0.62 |
| 3:U:3038[B]:ILE:HG12 | 3:U:3112[B]:TYR:CE2 | 2.35 | 0.62 |
| 3:U:3270[A]:LEU:O | 3:U:3274[A]:ARG:N | 2.33 | 0.62 |
| 1:V:1195:ASP:O | 1:V:1196:ILE:HG12 | 1.99 | 0.62 |
| 1:V:1286:ARG:NH2 | 1:V:1333:GLU:OE2 | 2.33 | 0.62 |
| 2:W:2345:ASN:O | 2:W:2349:THR:OG1 | 2.18 | 0.62 |
| 3:X:2937[A]:ASN:HB3 | 3:X:3006[A]:LYS:HD3 | 1.79 | 0.62 |
| 3:X:3222[A]:ILE:HD11 | 3:X:3224[A]:GLN:OE1 | 2.00 | 0.62 |
| 3:X:3228[B]:VAL:HG12 | 3:X:3287[B]:ILE:CG1 | 2.29 | 0.62 |
| 1:Y:589:GLN:HG2 | 1:Y:594:ASP:HB3 | 1.82 | 0.62 |
| 1:Y:1317:PRO:HD2 | 1:Y:1488:LEU:HD12 | 1.82 | 0.62 |
| 1:Y:1613:ASP:OD2 | 3:d:3184[B]:ASN:OD1 | 2.16 | 0.62 |
| 3:a:2961[A]:HIS:CE1 | 3:a:2980[A]:HIS:NE2 | 2.57 | 0.62 |
| 3:a:3066[A]:TYR:CD1 | 3:a:3193[A]:HIS:HE1 | 2.17 | 0.62 |
| 3:a:3147[B]:GLU:HG3 | 3:a:3149[B]:ASN:HD21 | 1.65 | 0.62 |
| 1:b:1470:GLU:OE2 | 1:b:1473:ARG:NH1 | 2.33 | 0.62 |
| 3:d:2987[B]:HIS:NE2 | 3:d:3178[B]:PHE:HE1 | 1.95 | 0.62 |
| 3:d:3024[A]:LEU:CD1 | 3:d:3025[A]:VAL:H | 1.83 | 0.62 |
| 3:C:2948[B]:ASP:HB3 | 3:C:2953[B]:GLY:CA | 2.24 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3086[B]:GLU:HB3 | 3:L:2968[B]:GLN:HE21 | 1.63 | 0.62 |
| 3:C:3114[B]:PRO:CD | 3:C:3115[B]:LEU:H | 2.12 | 0.62 |
| 3:C:3135[B]:LYS:CB | 3:C:3141[B]:TYR:HD1 | 2.13 | 0.62 |
| 3:C:3173[B]:THR:HB | 3:C:3176[B]:LYS:HG2 | 1.81 | 0.62 |
| 3:F:2949[B]:LYS:C | 3:F:2949[B]:LYS:HD3 | 2.24 | 0.62 |
| 3:F:3066[B]:TYR:CD1 | 3:F:3193[B]:HIS:HE1 | 2.17 | 0.62 |
| 3:F:3162[A]:ASP:OD1 | 3:F:3162[A]:ASP:N | 2.31 | 0.62 |
| 3:F:3222[B]:ILE:HD11 | 3:F:3224[B]:GLN:OE1 | 2.00 | 0.62 |
| 1:G:1441:SER:OG | 1:G:1442:MET:N | 2.31 | 0.62 |
| 3:I:2957[A]:ILE:N | 3:I:2960[A]:PHE:HE1 | 1.97 | 0.62 |
| 3:I:3114[A]:PRO:CD | 3:I:3115[A]:LEU:H | 2.12 | 0.62 |
| 3:I:3155[B]:MET:SD | 3:R:3154[B]:PRO:CD | 2.88 | 0.62 |
| 3:I:3249[B]:GLY:N | 3:R:2974[B]:ALA:H | 1.96 | 0.62 |
| 3:L:3038[A]:ILE:HG12 | 3:L:3112[A]:TYR:CE2 | 2.35 | 0.62 |
| 3:L:3038[B]:ILE:HG22 | 3:L:3041[B]:ALA:H | 1.65 | 0.62 |
| 2:N:2882:GLU:OE1 | 2:N:2884:LYS:NZ | 2.32 | 0.62 |
| 3:O:2974[B]:ALA:HB2 | 3:X:2978[B]:CYS:N | 2.15 | 0.62 |
| 3:O:3135[A]:LYS:CB | 3:O:3141[A]:TYR:HD1 | 2.13 | 0.62 |
| 3:O:3270[B]:LEU:O | 3:O:3274[B]:ARG:N | 2.33 | 0.62 |
| 3:R:2954[B]:TYR:HA | 3:R:2957[B]:ILE:HG22 | 1.80 | 0.62 |
| 3:R:2961[B]:HIS:HB3 | 3:R:3111[B]:SER:CB | 2.29 | 0.62 |
| 3:U:3027[A]:GLU:CD | 3:U:3028[A]:PRO:HD2 | 2.24 | 0.62 |
| 3:U:3114[B]:PRO:CD | 3:U:3115[B]:LEU:H | 2.12 | 0.62 |
| 2:W:2500:ILE:HG12 | 2:W:2501:PRO:HD2 | 1.81 | 0.62 |
| 3:X:2957[A]:ILE:N | 3:X:2960[A]:PHE:HE1 | 1.98 | 0.62 |
| 3:X:2994[B]:LYS:O | 3:X:2995[B]:GLN:C | 2.38 | 0.62 |
| 3:X:3038[A]:ILE:HG22 | 3:X:3041[A]:ALA:H | 1.65 | 0.62 |
| 3:X:3066[B]:TYR:HD1 | 3:X:3193[B]:HIS:CE1 | 2.16 | 0.62 |
| 2:Z:2564:PRO:HA | 2:Z:2673:GLU:HG3 | 1.82 | 0.62 |
| 3:a:2948[B]:ASP:CB | 3:a:2949[B]:LYS:HA | 2.16 | 0.62 |
| 3:a:2949[A]:LYS:HZ2 | 3:a:2950[A]:THR:HA | 1.65 | 0.62 |
| 3:a:3270[B]:LEU:O | 3:a:3274[B]:ARG:N | 2.33 | 0.62 |
| 1:b:105:VAL:HG12 | 1:b:123:PHE:HB3 | 1.82 | 0.62 |
| 3:d:3038[B]:ILE:HG12 | 3:d:3112[B]:TYR:CE2 | 2.35 | 0.62 |
| 3:d:3114[A]:PRO:CD | 3:d:3115[A]:LEU:H | 2.12 | 0.62 |
| 1:A:492:ARG:HD2 | 1:A:692:VAL:HG22 | 1.82 | 0.62 |
| 3:C:3152[B]:LYS:HG3 | 3:L:3172[B]:SER:OG | 1.99 | 0.62 |
| 3:C:3154[B]:PRO:HB3 | 3:L:3174[B]:GLY:N | 2.14 | 0.62 |
| 3:C:3155[B]:MET:N | 3:L:3153[B]:LYS:C | 2.57 | 0.62 |
| 3:C:3212[B]:ARG:HH11 | 3:C:3212[B]:ARG:CG | 2.12 | 0.62 |
| 1:D:43:GLU:HG3 | 1:D:44:PRO:HA | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2966[B]:SER:HB3 | 3:F:2977[B]:CYS:HB2 | 1.78 | 0.62 |
| 3:F:2967[B]:CYS:SG | 3:a:2982[B]:MET:HG3 | 2.38 | 0.62 |
| 3:I:2965[B]:LEU:HB2 | 3:R:3253[B]:GLU:OE2 | 1.99 | 0.62 |
| 3:I:2975[B]:PHE:CE1 | 3:R:2961[B]:HIS:CE1 | 2.87 | 0.62 |
| 3:I:3155[A]:MET:HG3 | 3:I:3172[A]:SER:O | 1.99 | 0.62 |
| 3:I:3162[B]:ASP:OD1 | 3:I:3162[B]:ASP:N | 2.31 | 0.62 |
| 3:I:3228[B]:VAL:HG12 | 3:I:3287[B]:ILE:CG1 | 2.29 | 0.62 |
| 1:J:238:ASN:OD1 | 1:J:238:ASN:N | 2.33 | 0.62 |
| 1:J:325:THR:HG22 | 1:J:327:ASP:H | 1.62 | 0.62 |
| 3:L:3027[B]:GLU:CD | 3:L:3028[B]:PRO:HD2 | 2.24 | 0.62 |
| 3:L:3038[A]:ILE:HG22 | 3:L:3041[A]:ALA:H | 1.65 | 0.62 |
| 3:L:3273[A]:LEU:CB | 3:L:3275[A]:LEU:HD13 | 2.28 | 0.62 |
| 3:O:3027[B]:GLU:CD | 3:O:3028[B]:PRO:HD2 | 2.25 | 0.62 |
| 3:R:2994[B]:LYS:HD2 | 3:R:2998[B]:ASP:OD2 | 2.00 | 0.62 |
| 1:S:164:GLU:O | 1:S:297:ARG:NH2 | 2.32 | 0.62 |
| 3:U:3169[A]:LYS:C | 3:U:3172[A]:SER:HG | 1.99 | 0.62 |
| 1:V:329:ARG:HH22 | 1:Y:1574:VAL:H | 1.46 | 0.62 |
| 2:W:2128:LEU:HB2 | 2:W:2286:HIS:HB3 | 1.82 | 0.62 |
| 3:X:3066[A]:TYR:CD1 | 3:X:3193[A]:HIS:HE1 | 2.17 | 0.62 |
| 3:X:3066[B]:TYR:CD1 | 3:X:3193[B]:HIS:HE1 | 2.17 | 0.62 |
| 3:X:3270[B]:LEU:O | 3:X:3274[B]:ARG:N | 2.33 | 0.62 |
| 2:Z:2497:GLU:HB2 | 2:Z:2498:VAL:HA | 1.82 | 0.62 |
| 3:a:2994[B]:LYS:HD2 | 3:a:2998[B]:ASP:OD2 | 2.00 | 0.62 |
| 3:a:3027[B]:GLU:CD | 3:a:3028[B]:PRO:HD2 | 2.24 | 0.62 |
| 3:d:2954[A]:TYR:HA | 3:d:2957[A]:ILE:HG22 | 1.80 | 0.62 |
| 3:d:3135[A]:LYS:CB | 3:d:3141[A]:TYR:HD1 | 2.12 | 0.62 |
| 3:d:3220[B]:ARG:HH11 | 3:d:3220[B]:ARG:CG | 2.12 | 0.62 |
| 2:B:2109:ARG:NH1 | 2:B:2169:HIS:O | 2.33 | 0.62 |
| 3:C:2949[B]:LYS:HD3 | 3:C:2949[B]:LYS:C | 2.24 | 0.62 |
| 3:C:2957[B]:ILE:N | 3:C:2960[B]:PHE:HE1 | 1.97 | 0.62 |
| 3:C:3147[A]:GLU:HG3 | 3:C:3149[A]:ASN:HD21 | 1.65 | 0.62 |
| 3:C:3212[A]:ARG:HH11 | 3:C:3212[A]:ARG:CG | 2.12 | 0.62 |
| 3:C:3256[B]:TRP:HZ2 | 3:L:2965[B]:LEU:CG | 2.10 | 0.62 |
| 3:F:2979[B]:GLN:HA | 3:a:2977[B]:CYS:SG | 2.38 | 0.62 |
| 3:F:3228[A]:VAL:HG12 | 3:F:3287[A]:ILE:CG1 | 2.29 | 0.62 |
| 1:G:402:THR:HG23 | 1:G:659:CYS:HA | 1.81 | 0.62 |
| 3:I:2948[B]:ASP:HB3 | 3:I:2953[B]:GLY:CA | 2.24 | 0.62 |
| 3:I:3270[B]:LEU:O | 3:I:3274[B]:ARG:N | 2.33 | 0.62 |
| 3:L:3147[A]:GLU:HG3 | 3:L:3149[A]:ASN:HD21 | 1.65 | 0.62 |
| 3:L:3173[A]:THR:CG2 | 3:L:3174[A]:GLY:H | 2.12 | 0.62 |
| 3:L:3222[B]:ILE:HD11 | 3:L:3224[B]:GLN:OE1 | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3300[B]:LEU:HD23 | 3:L:3300[B]:LEU:N | 2.15 | 0.62 |
| 3:O:2964[A]:PRO:HG3 | 3:O:3040[A]:VAL:HG11 | 1.82 | 0.62 |
| 3:O:3173[A]:THR:CG2 | 3:O:3174[A]:GLY:H | 2.12 | 0.62 |
| 3:O:3298[A]:ASN:CB | 3:O:3300[A]:LEU:CD2 | 2.61 | 0.62 |
| 1:P:474:LEU:HD23 | 1:P:475:ASN:H | 1.65 | 0.62 |
| 2:Q:2889:ALA:N | 2:Q:2890:VAL:HA | 2.14 | 0.62 |
| 3:R:2961[A]:HIS:HB3 | 3:R:3111[A]:SER:CB | 2.29 | 0.62 |
| 3:R:3024[B]:LEU:CD1 | 3:R:3025[B]:VAL:H | 1.84 | 0.62 |
| 3:R:3147[A]:GLU:HG3 | 3:R:3149[A]:ASN:HD21 | 1.65 | 0.62 |
| 3:R:3173[A]:THR:HB | 3:R:3176[A]:LYS:HG2 | 1.81 | 0.62 |
| 3:R:3222[B]:ILE:HD11 | 3:R:3224[B]:GLN:OE1 | 2.00 | 0.62 |
| 3:R:3298[A]:ASN:CB | 3:R:3300[A]:LEU:N | 2.60 | 0.62 |
| 1:S:757:VAL:HG21 | 1:S:781:ILE:HG13 | 1.80 | 0.62 |
| 2:T:2800:LYS:HB3 | 3:U:3023[A]:ILE:HD13 | 1.76 | 0.62 |
| 3:U:2975[B]:PHE:CB | 3:d:3256[B]:TRP:CD1 | 2.81 | 0.62 |
| 3:U:2990[A]:ARG:CZ | 3:U:3180[A]:TYR:HB3 | 2.28 | 0.62 |
| 3:U:3170[B]:ALA:C | 3:d:3152[B]:LYS:NZ | 2.55 | 0.62 |
| 3:U:3259[B]:ASP:N | 3:d:2968[B]:GLN:HG3 | 2.14 | 0.62 |
| 2:W:2884:LYS:HG3 | 2:W:2889:ALA:O | 2.00 | 0.62 |
| 3:X:2957[A]:ILE:HA | 3:X:2960[A]:PHE:HE1 | 1.64 | 0.62 |
| 3:X:3228[A]:VAL:HG12 | 3:X:3287[A]:ILE:CG1 | 2.29 | 0.62 |
| 3:X:3270[A]:LEU:O | 3:X:3274[A]:ARG:N | 2.33 | 0.62 |
| 1:Y:673:PHE:HB3 | 1:Y:677:LEU:HB2 | 1.82 | 0.62 |
| 3:a:2964[B]:PRO:HG3 | 3:a:3040[B]:VAL:HG11 | 1.82 | 0.62 |
| 3:a:3120[A]:HIS:C | 3:a:3122[A]:ASN:N | 2.55 | 0.62 |
| 3:a:3285[A]:VAL:HG22 | 3:a:3286[A]:THR:H | 1.61 | 0.62 |
| 1:b:46:ASP:OD2 | 1:b:249:ARG:NH2 | 2.33 | 0.62 |
| 3:d:2994[A]:LYS:HD2 | 3:d:2998[A]:ASP:OD2 | 2.00 | 0.62 |
| 3:d:3270[A]:LEU:O | 3:d:3274[A]:ARG:N | 2.33 | 0.62 |
| 4:i:1:NAG:O3 | 4:i:2:NAG:N2 | 2.33 | 0.62 |
| 6:DA:1:NAG:H61 | 6:DA:2:NAG:C7 | 2.30 | 0.62 |
| 3:C:2976[B]:ALA:N | 3:L:3253[B]:GLU:CA | 2.61 | 0.61 |
| 3:C:3025[A]:VAL:HG22 | 3:C:3025[A]:VAL:O | 2.00 | 0.61 |
| 3:C:3273[A]:LEU:CB | 3:C:3275[A]:LEU:HD13 | 2.28 | 0.61 |
| 1:D:1317:PRO:HA | 1:D:1420:GLU:HG3 | 1.82 | 0.61 |
| 3:F:2962[B]:GLY:O | 3:a:3255[B]:PRO:CD | 2.48 | 0.61 |
| 3:F:2965[B]:LEU:C | 3:a:3256[B]:TRP:N | 2.58 | 0.61 |
| 3:F:3114[B]:PRO:CD | 3:F:3115[B]:LEU:H | 2.12 | 0.61 |
| 3:F:3150[B]:LYS:HG3 | 3:a:3163[B]:ASN:ND2 | 2.10 | 0.61 |
| 3:F:3155[B]:MET:HG3 | 3:F:3172[B]:SER:O | 1.99 | 0.61 |
| 3:F:3162[B]:ASP:CB | 3:a:3259[B]:ASP:N | 2.63 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1082:SER:O | 1:G:1086:LEU:HG | 2.00 | 0.61 |
| 1:G:1163:ALA:O | 1:G:1167:ASP:HB2 | 2.00 | 0.61 |
| 2:H:2226:GLU:HG2 | 2:H:2276:GLY:HA3 | 1.81 | 0.61 |
| 2:H:2725:GLN:OE1 | 2:H:2728:ARG:NH2 | 2.31 | 0.61 |
| 3:I:2964[B]:PRO:CB | 3:R:3255[B]:PRO:HB3 | 2.30 | 0.61 |
| 3:I:2966[A]:SER:HB3 | 3:I:2977[A]:CYS:HB2 | 1.78 | 0.61 |
| 3:I:3025[B]:VAL:HG22 | 3:I:3025[B]:VAL:O | 2.00 | 0.61 |
| 3:I:3171[B]:HIS:CA | 3:R:3152[B]:LYS:HB3 | 2.30 | 0.61 |
| 1:M:931:TRP:CG | 1:M:1018:ILE:HD11 | 2.34 | 0.61 |
| 3:O:2977[B]:CYS:N | 3:X:3153[B]:LYS:HG2 | 2.15 | 0.61 |
| 3:O:3173[B]:THR:CG2 | 3:O:3174[B]:GLY:H | 2.12 | 0.61 |
| 3:R:2994[B]:LYS:O | 3:R:2995[B]:GLN:C | 2.38 | 0.61 |
| 1:S:492:ARG:NH1 | 1:S:701:TYR:OH | 2.32 | 0.61 |
| 1:S:946:GLU:HG2 | 1:S:955:LYS:HD2 | 1.81 | 0.61 |
| 3:U:2961[A]:HIS:HB3 | 3:U:3111[A]:SER:CB | 2.29 | 0.61 |
| 3:U:3114[A]:PRO:CD | 3:U:3115[A]:LEU:H | 2.12 | 0.61 |
| 2:W:2625:LEU:HG | 2:W:2626:ARG:HG2 | 1.81 | 0.61 |
| 3:X:2987[A]:HIS:NE2 | 3:X:3178[A]:PHE:HE1 | 1.95 | 0.61 |
| 1:Y:946:GLU:HA | 1:Y:956:PRO:HB3 | 1.82 | 0.61 |
| 2:Z:2545:SER:CA | 2:Z:2546:LEU:HB2 | 2.30 | 0.61 |
| 3:a:3038[A]:ILE:HG12 | 3:a:3112[A]:TYR:CE2 | 2.35 | 0.61 |
| 3:a:3096[B]:VAL:HG11 | 3:a:3115[B]:LEU:HD13 | 1.81 | 0.61 |
| 3:d:3066[B]:TYR:CD1 | 3:d:3193[B]:HIS:HE1 | 2.17 | 0.61 |
| 3:d:3155[B]:MET:HG3 | 3:d:3172[B]:SER:O | 1.99 | 0.61 |
| 3:d:3173[B]:THR:CG2 | 3:d:3174[B]:GLY:H | 2.12 | 0.61 |
| 3:C:2957[A]:ILE:N | 3:C:2960[A]:PHE:HE1 | 1.97 | 0.61 |
| 3:C:2975[B]:PHE:HE1 | 3:L:3107[B]:LEU:CD1 | 2.03 | 0.61 |
| 3:C:3027[A]:GLU:CD | 3:C:3028[A]:PRO:HD2 | 2.24 | 0.61 |
| 3:C:3155[B]:MET:HG2 | 3:L:3154[B]:PRO:N | 2.07 | 0.61 |
| 3:C:3158[B]:PHE:HE2 | 3:L:3153[B]:LYS:NZ | 1.93 | 0.61 |
| 3:C:3300[A]:LEU:HD23 | 3:C:3300[A]:LEU:N | 2.15 | 0.61 |
| 2:E:2394:VAL:HG11 | 2:E:2451:LEU:HD12 | 1.82 | 0.61 |
| 3:F:2964[A]:PRO:HG3 | 3:F:3040[A]:VAL:HG11 | 1.82 | 0.61 |
| 3:F:2994[B]:LYS:HD2 | 3:F:2998[B]:ASP:OD2 | 2.00 | 0.61 |
| 3:F:3066[A]:TYR:CD1 | 3:F:3193[A]:HIS:HE1 | 2.17 | 0.61 |
| 3:F:3253[B]:GLU:CD | 3:a:2974[B]:ALA:HB1 | 2.21 | 0.61 |
| 3:I:2949[B]:LYS:HD3 | 3:I:2949[B]:LYS:C | 2.24 | 0.61 |
| 3:I:2964[B]:PRO:HD2 | 3:R:3255[B]:PRO:CG | 2.30 | 0.61 |
| 3:I:2994[A]:LYS:HD2 | 3:I:2998[A]:ASP:OD2 | 2.00 | 0.61 |
| 3:I:3169[B]:LYS:O | 3:R:3152[B]:LYS:N | 2.30 | 0.61 |
| 3:L:2994[A]:LYS:HD2 | 3:L:2998[A]:ASP:OD2 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3135[A]:LYS:CB | 3:L:3141[A]:TYR:HD1 | 2.13 | 0.61 |
| 1:M:293:LEU:HB3 | 1:M:297:ARG:HH21 | 1.65 | 0.61 |
| 3:O:3025[A]:VAL:HG22 | 3:O:3025[A]:VAL:O | 2.00 | 0.61 |
| 3:O:3038[A]:ILE:HG12 | 3:O:3112[A]:TYR:CE2 | 2.35 | 0.61 |
| 3:O:3038[A]:ILE:HG22 | 3:O:3041[A]:ALA:H | 1.65 | 0.61 |
| 3:O:3038[B]:ILE:HG22 | 3:O:3041[B]:ALA:H | 1.65 | 0.61 |
| 1:P:780:GLU:O | 1:P:782:THR:N | 2.33 | 0.61 |
| 3:R:3038[A]:ILE:HG12 | 3:R:3112[A]:TYR:CE2 | 2.35 | 0.61 |
| 3:R:3200[A]:LEU:HD22 | 3:R:3204[A]:LEU:HD13 | 1.82 | 0.61 |
| 3:R:3228[B]:VAL:HG12 | 3:R:3287[B]:ILE:CG1 | 2.29 | 0.61 |
| 1:V:957:ASN:HD22 | 1:V:960:PHE:HB2 | 1.64 | 0.61 |
| 3:X:3027[B]:GLU:CD | 3:X:3028[B]:PRO:HD2 | 2.24 | 0.61 |
| 3:X:3038[B]:ILE:HG12 | 3:X:3112[B]:TYR:CE2 | 2.35 | 0.61 |
| 3:a:3114[B]:PRO:CD | 3:a:3115[B]:LEU:H | 2.12 | 0.61 |
| 1:b:115:GLY:HA2 | 1:b:116:LYS:HB2 | 1.82 | 0.61 |
| 3:d:3300[B]:LEU:HD23 | 3:d:3300[B]:LEU:N | 2.15 | 0.61 |
| 3:C:3038[B]:ILE:HG22 | 3:C:3041[B]:ALA:H | 1.65 | 0.61 |
| 1:D:1304:ASP:N | 1:D:1305:GLY:HA2 | 2.15 | 0.61 |
| 2:E:2107:LEU:HD23 | 2:E:2208:PRO:HB2 | 1.80 | 0.61 |
| 3:F:2994[A]:LYS:O | 3:F:2995[A]:GLN:C | 2.38 | 0.61 |
| 3:F:3270[B]:LEU:O | 3:F:3274[B]:ARG:N | 2.33 | 0.61 |
| 3:I:2969[B]:TYR:O | 3:R:2980[B]:HIS:HD2 | 1.84 | 0.61 |
| 1:J:573:LYS:HB3 | 1:J:574:GLY:HA2 | 1.83 | 0.61 |
| 1:J:930:ASP:OD1 | 1:J:1051:ARG:NH2 | 2.34 | 0.61 |
| 1:J:1144:VAL:HG23 | 1:J:1234:VAL:HG22 | 1.82 | 0.61 |
| 3:L:3200[B]:LEU:HD22 | 3:L:3204[B]:LEU:HD13 | 1.83 | 0.61 |
| 1:M:1414:THR:HG23 | 1:M:1477:LEU:HD13 | 1.82 | 0.61 |
| 3:O:3256[B]:TRP:CE2 | 3:X:3161[B]:GLU:HG3 | 2.35 | 0.61 |
| 3:O:3276[B]:ASP:HB3 | 3:O:3278[B]:HIS:HB2 | 1.83 | 0.61 |
| 3:O:3298[B]:ASN:CB | 3:O:3300[B]:LEU:N | 2.60 | 0.61 |
| 1:P:1641:THR:HG21 | 1:P:1644:ILE:HD11 | 1.83 | 0.61 |
| 3:R:3124[B]:ASP:OD2 | 3:R:3187[B]:TYR:OH | 2.15 | 0.61 |
| 3:R:3217[B]:PHE:CE2 | 3:R:3303[B]:PRO:HG3 | 2.33 | 0.61 |
| 3:R:3300[B]:LEU:HD23 | 3:R:3300[B]:LEU:N | 2.15 | 0.61 |
| 1:S:221:GLN:NE2 | 1:S:267:PHE:O | 2.30 | 0.61 |
| 1:S:865:LYS:HE2 | 1:S:964:ILE:HD11 | 1.81 | 0.61 |
| 3:U:2930[A]:LEU:HD22 | 3:U:2930[A]:LEU:N | 2.02 | 0.61 |
| 3:U:2957[B]:ILE:N | 3:U:2960[B]:PHE:HE1 | 1.98 | 0.61 |
| 3:U:3025[A]:VAL:HG22 | 3:U:3025[A]:VAL:O | 2.00 | 0.61 |
| 3:U:3155[B]:MET:O | 3:d:3149[B]:ASN:CB | 2.48 | 0.61 |
| 3:U:3220[B]:ARG:HB2 | 3:d:2973[B]:THR:HA | 1.79 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:11:THR:HG22 | 1:V:13:ASP:H | 1.65 | 0.61 |
| 3:X:3024[A]:LEU:CD1 | 3:X:3025[A]:VAL:H | 1.83 | 0.61 |
| 3:X:3025[A]:VAL:HG22 | 3:X:3025[A]:VAL:O | 2.00 | 0.61 |
| 1:Y:1358:LEU:HD23 | 1:Y:1456:LEU:HD21 | 1.80 | 0.61 |
| 3:a:2957[A]:ILE:N | 3:a:2960[A]:PHE:HE1 | 1.97 | 0.61 |
| 3:a:2987[A]:HIS:NE2 | 3:a:3178[A]:PHE:HE1 | 1.95 | 0.61 |
| 3:a:3276[B]:ASP:HB3 | 3:a:3278[B]:HIS:HB2 | 1.83 | 0.61 |
| 3:d:3027[B]:GLU:CD | 3:d:3028[B]:PRO:HD2 | 2.24 | 0.61 |
| 3:d:3135[B]:LYS:CB | 3:d:3141[B]:TYR:HD1 | 2.13 | 0.61 |
| 3:d:3270[B]:LEU:O | 3:d:3274[B]:ARG:N | 2.33 | 0.61 |
| 3:d:3273[B]:LEU:CB | 3:d:3275[B]:LEU:HD13 | 2.28 | 0.61 |
| 3:d:3284[B]:LYS:CD | 3:d:3285[B]:VAL:H | 2.09 | 0.61 |
| 1:A:304:ALA:HB1 | 1:A:306:PHE:HE1 | 1.64 | 0.61 |
| 3:C:2961[A]:HIS:CE1 | 3:C:2980[A]:HIS:NE2 | 2.57 | 0.61 |
| 3:C:2988[A]:TRP:NE1 | 3:C:3158[A]:PHE:HE2 | 1.96 | 0.61 |
| 3:C:3154[B]:PRO:O | 3:L:3155[B]:MET:HE3 | 1.99 | 0.61 |
| 3:C:3270[A]:LEU:O | 3:C:3274[A]:ARG:N | 2.33 | 0.61 |
| 1:D:1462:ASP:OD2 | 1:D:1525:TYR:OH | 2.14 | 0.61 |
| 2:E:2344:LEU:HD23 | 2:E:2346:PRO:HA | 1.82 | 0.61 |
| 3:F:3027[A]:GLU:CD | 3:F:3028[A]:PRO:HD2 | 2.25 | 0.61 |
| 3:F:3160[B]:SER:CA | 3:a:3150[B]:LYS:NZ | 2.63 | 0.61 |
| 3:F:3276[A]:ASP:HB3 | 3:F:3278[A]:HIS:HB2 | 1.83 | 0.61 |
| 3:F:3276[B]:ASP:HB3 | 3:F:3278[B]:HIS:HB2 | 1.83 | 0.61 |
| 3:F:3300[A]:LEU:HD23 | 3:F:3300[A]:LEU:N | 2.14 | 0.61 |
| 1:G:456:GLN:HG2 | 1:G:551:GLU:HB2 | 1.81 | 0.61 |
| 1:G:1026:GLU:OE1 | 1:G:1029:SER:N | 2.32 | 0.61 |
| 3:I:2964[B]:PRO:C | 3:R:3221[B]:ALA:HB3 | 2.16 | 0.61 |
| 3:I:3027[B]:GLU:CD | 3:I:3028[B]:PRO:HD2 | 2.24 | 0.61 |
| 3:I:3038[B]:ILE:HG12 | 3:I:3112[B]:TYR:CE2 | 2.35 | 0.61 |
| 3:I:3150[B]:LYS:NZ | 3:R:3160[B]:SER:CB | 2.55 | 0.61 |
| 3:I:3152[B]:LYS:HB3 | 3:R:3172[B]:SER:N | 2.04 | 0.61 |
| 3:I:3155[B]:MET:HB3 | 3:R:3153[B]:LYS:HD2 | 1.74 | 0.61 |
| 3:I:3222[B]:ILE:HD11 | 3:I:3224[B]:GLN:OE1 | 2.00 | 0.61 |
| 3:I:3300[B]:LEU:HD23 | 3:I:3300[B]:LEU:N | 2.15 | 0.61 |
| 2:K:2122:ILE:O | 2:K:2125:PHE:HB2 | 1.99 | 0.61 |
| 2:K:2344:LEU:HA | 2:K:2345:ASN:C | 2.25 | 0.61 |
| 2:K:2472:ASN:N | 2:K:2473:GLY:HA2 | 2.16 | 0.61 |
| 3:O:2987[A]:HIS:NE2 | 3:O:3178[A]:PHE:HE1 | 1.95 | 0.61 |
| 3:O:2994[A]:LYS:HD2 | 3:O:2998[A]:ASP:OD2 | 2.00 | 0.61 |
| 3:O:3101[B]:PRO:CB | 3:X:2971[B]:ASP:C | 2.53 | 0.61 |
| 3:O:3114[B]:PRO:CD | 3:O:3115[B]:LEU:H | 2.12 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3147[A]:GLU:HG3 | 3:O:3149[A]:ASN:HD21 | 1.65 | 0.61 |
| 3:O:3273[B]:LEU:CB | 3:O:3275[B]:LEU:HD13 | 2.28 | 0.61 |
| 2:Q:2419:ASP:OD1 | 2:Q:2419:ASP:N | 2.33 | 0.61 |
| 3:R:3027[B]:GLU:CD | 3:R:3028[B]:PRO:HD2 | 2.24 | 0.61 |
| 3:R:3038[A]:ILE:HG22 | 3:R:3041[A]:ALA:H | 1.65 | 0.61 |
| 3:R:3120[B]:HIS:C | 3:R:3122[B]:ASN:N | 2.55 | 0.61 |
| 3:U:2970[B]:PRO:HB3 | 3:d:2980[B]:HIS:HB3 | 1.72 | 0.61 |
| 3:U:3300[A]:LEU:HD23 | 3:U:3300[A]:LEU:N | 2.15 | 0.61 |
| 3:X:3096[A]:VAL:HG11 | 3:X:3115[A]:LEU:HD13 | 1.81 | 0.61 |
| 3:X:3169[A]:LYS:C | 3:X:3172[A]:SER:HG | 2.00 | 0.61 |
| 3:X:3300[B]:LEU:HD23 | 3:X:3300[B]:LEU:N | 2.15 | 0.61 |
| 1:Y:1627:ARG:NH2 | 1:Y:1629:GLU:OE1 | 2.31 | 0.61 |
| 1:Y:1655:SER:C | 3:d:3006[B]:LYS:HD2 | 2.26 | 0.61 |
| 3:a:3135[B]:LYS:CB | 3:a:3141[B]:TYR:HD1 | 2.12 | 0.61 |
| 3:a:3222[A]:ILE:HD11 | 3:a:3224[A]:GLN:OE1 | 2.00 | 0.61 |
| 3:a:3270[A]:LEU:O | 3:a:3274[A]:ARG:N | 2.33 | 0.61 |
| 3:d:3162[A]:ASP:OD1 | 3:d:3162[A]:ASP:N | 2.31 | 0.61 |
| 3:d:3173[A]:THR:HB | 3:d:3176[A]:LYS:HG2 | 1.81 | 0.61 |
| 3:C:2974[B]:ALA:C | 3:L:3249[B]:GLY:HA2 | 2.25 | 0.61 |
| 3:C:2984[B]:THR:HB | 3:L:3154[B]:PRO:CG | 2.30 | 0.61 |
| 3:C:2994[A]:LYS:HD2 | 3:C:2998[A]:ASP:OD2 | 2.00 | 0.61 |
| 3:C:3200[B]:LEU:HD22 | 3:C:3204[B]:LEU:HD13 | 1.83 | 0.61 |
| 2:E:2567:MET:HE3 | 2:E:2718:TRP:HB2 | 1.82 | 0.61 |
| 3:F:2984[B]:THR:CG2 | 3:a:3159[B]:SER:OG | 2.15 | 0.61 |
| 3:F:3157[A]:PRO:O | 3:F:3160[A]:SER:N | 2.30 | 0.61 |
| 2:H:2820:HIS:HB3 | 2:H:2822:LYS:HE2 | 1.83 | 0.61 |
| 3:I:2957[B]:ILE:N | 3:I:2960[B]:PHE:HE1 | 1.98 | 0.61 |
| 3:I:2964[A]:PRO:HG3 | 3:I:3040[A]:VAL:HG11 | 1.82 | 0.61 |
| 3:I:2987[B]:HIS:NE2 | 3:I:3178[B]:PHE:HE1 | 1.96 | 0.61 |
| 3:I:3120[B]:HIS:C | 3:I:3122[B]:ASN:N | 2.55 | 0.61 |
| 3:I:3147[B]:GLU:HG3 | 3:I:3149[B]:ASN:HD21 | 1.65 | 0.61 |
| 3:I:3150[B]:LYS:CA | 3:R:3159[B]:SER:HA | 2.18 | 0.61 |
| 3:I:3194[A]:GLY:O | 3:I:3195[A]:MET:HG2 | 2.01 | 0.61 |
| 1:J:332:ASP:OD2 | 1:J:378:TYR:OH | 2.16 | 0.61 |
| 3:L:3194[B]:GLY:O | 3:L:3195[B]:MET:HG2 | 2.01 | 0.61 |
| 1:M:1140:ASN:ND2 | 1:M:1236:TYR:OH | 2.34 | 0.61 |
| 1:M:1210:LYS:HA | 1:M:1211:TYR:HB2 | 1.82 | 0.61 |
| 3:O:3173[A]:THR:HB | 3:O:3176[A]:LYS:HG2 | 1.81 | 0.61 |
| 3:O:3270[A]:LEU:O | 3:O:3274[A]:ARG:N | 2.33 | 0.61 |
| 3:O:3300[B]:LEU:HD23 | 3:O:3300[B]:LEU:N | 2.15 | 0.61 |
| 1:P:1639:LYS:HE3 | 1:S:473:ALA:HA | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3124[A]:ASP:OD2 | 3:R:3187[A]:TYR:OH | 2.16 | 0.61 |
| 3:R:3135[A]:LYS:CB | 3:R:3141[A]:TYR:HD1 | 2.13 | 0.61 |
| 3:R:3173[A]:THR:CG2 | 3:R:3174[A]:GLY:H | 2.12 | 0.61 |
| 3:R:3293[B]:LYS:CB | 3:R:3294[B]:SER:CB | 2.54 | 0.61 |
| 3:U:3252[B]:TYR:O | 3:d:3255[B]:PRO:HG3 | 2.00 | 0.61 |
| 3:U:3257[B]:ALA:CB | 3:d:2973[B]:THR:C | 2.52 | 0.61 |
| 3:U:3300[B]:LEU:HD23 | 3:U:3300[B]:LEU:N | 2.15 | 0.61 |
| 2:W:2263:PHE:HE1 | 2:W:2304:LEU:HB3 | 1.65 | 0.61 |
| 3:X:2994[B]:LYS:HD2 | 3:X:2998[B]:ASP:OD2 | 2.00 | 0.61 |
| 3:X:3124[A]:ASP:OD2 | 3:X:3187[A]:TYR:OH | 2.15 | 0.61 |
| 3:X:3139[A]:LEU:N | 3:X:3139[A]:LEU:HD22 | 2.16 | 0.61 |
| 2:Z:2876:LYS:HA | 1:b:1078:ARG:HH22 | 1.65 | 0.61 |
| 2:Z:2878:ARG:NH1 | 2:Z:2880:GLU:OE2 | 2.34 | 0.61 |
| 3:a:3066[B]:TYR:CD1 | 3:a:3193[B]:HIS:HE1 | 2.17 | 0.61 |
| 3:a:3173[A]:THR:HB | 3:a:3176[A]:LYS:HG2 | 1.81 | 0.61 |
| 2:c:2476:LEU:HB3 | 2:c:2480:LEU:HD21 | 1.81 | 0.61 |
| 3:d:3027[A]:GLU:CD | 3:d:3028[A]:PRO:HD2 | 2.24 | 0.61 |
| 3:d:3222[B]:ILE:HD11 | 3:d:3224[B]:GLN:OE1 | 2.00 | 0.61 |
| 3:d:3276[A]:ASP:HB3 | 3:d:3278[A]:HIS:HB2 | 1.83 | 0.61 |
| 1:A:126:GLY:HA3 | 1:A:202:TYR:O | 2.00 | 0.61 |
| 1:A:1486:LEU:HB2 | 2:E:2486:ILE:HB | 1.81 | 0.61 |
| 3:C:3147[B]:GLU:HG3 | 3:C:3149[B]:ASN:HD21 | 1.65 | 0.61 |
| 3:C:3200[A]:LEU:HD22 | 3:C:3204[A]:LEU:HD13 | 1.83 | 0.61 |
| 3:C:3228[A]:VAL:HG12 | 3:C:3287[A]:ILE:CG1 | 2.29 | 0.61 |
| 1:G:1492:PRO:HB2 | 1:G:1497:SER:HB3 | 1.82 | 0.61 |
| 3:I:3173[B]:THR:HB | 3:I:3176[B]:LYS:HG2 | 1.81 | 0.61 |
| 3:I:3200[B]:LEU:HD22 | 3:I:3204[B]:LEU:HD13 | 1.83 | 0.61 |
| 3:I:3254[B]:MET:CA | 3:R:2966[B]:SER:OG | 2.48 | 0.61 |
| 3:I:3273[A]:LEU:CB | 3:I:3275[A]:LEU:HD13 | 2.28 | 0.61 |
| 3:L:2957[B]:ILE:N | 3:L:2960[B]:PHE:HE1 | 1.97 | 0.61 |
| 3:L:2994[B]:LYS:HD2 | 3:L:2998[B]:ASP:OD2 | 2.00 | 0.61 |
| 3:L:3120[A]:HIS:C | 3:L:3122[A]:ASN:N | 2.55 | 0.61 |
| 3:O:2968[B]:GLN:HB2 | 3:X:2988[B]:TRP:CA | 2.29 | 0.61 |
| 1:P:1321:HIS:HD2 | 1:P:1465:TRP:CH2 | 2.18 | 0.61 |
| 1:P:1562:ILE:HD13 | 1:P:1644:ILE:HD12 | 1.81 | 0.61 |
| 2:Q:2181:THR:HB | 2:Q:2374:ASN:H | 1.66 | 0.61 |
| 3:R:3147[B]:GLU:HG3 | 3:R:3149[B]:ASN:HD21 | 1.65 | 0.61 |
| 3:R:3194[A]:GLY:O | 3:R:3195[A]:MET:HG2 | 2.01 | 0.61 |
| 3:R:3200[B]:LEU:HD22 | 3:R:3204[B]:LEU:HD13 | 1.83 | 0.61 |
| 3:R:3300[A]:LEU:HD23 | 3:R:3300[A]:LEU:N | 2.15 | 0.61 |
| 1:S:505:ARG:NE | 1:S:1339:SER:OG | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:2128:LEU:HD23 | 2:T:2216:PHE:HZ | 1.65 | 0.61 |
| 3:U:2949[B]:LYS:HD3 | 3:U:2949[B]:LYS:C | 2.24 | 0.61 |
| 3:U:2973[B]:THR:OG1 | 3:d:3248[B]:LEU:C | 2.43 | 0.61 |
| 3:U:3270[B]:LEU:O | 3:U:3274[B]:ARG:N | 2.33 | 0.61 |
| 1:V:1018:ILE:HA | 1:V:1021:LEU:HB2 | 1.81 | 0.61 |
| 1:V:1143:ALA:HB3 | 1:V:1235:ILE:HG13 | 1.83 | 0.61 |
| 2:W:2849:ASP:OD2 | 2:W:2850:ARG:NH2 | 2.33 | 0.61 |
| 3:X:3096[B]:VAL:HG11 | 3:X:3115[B]:LEU:HD13 | 1.81 | 0.61 |
| 3:X:3114[B]:PRO:CD | 3:X:3115[B]:LEU:H | 2.12 | 0.61 |
| 3:X:3135[A]:LYS:CB | 3:X:3141[A]:TYR:HD1 | 2.13 | 0.61 |
| 2:Z:2394:VAL:HG11 | 2:Z:2451:LEU:HD12 | 1.82 | 0.61 |
| 3:a:2930[B]:LEU:HD22 | 3:a:2930[B]:LEU:N | 2.02 | 0.61 |
| 3:a:2994[A]:LYS:HD2 | 3:a:2998[A]:ASP:OD2 | 2.00 | 0.61 |
| 3:a:3222[B]:ILE:HD11 | 3:a:3224[B]:GLN:OE1 | 2.00 | 0.61 |
| 3:a:3307[A]:PHE:HE1 | 3:a:3309[A]:PRO:CG | 2.08 | 0.61 |
| 1:b:22:LEU:HD12 | 1:b:25:MET:HG2 | 1.83 | 0.61 |
| 2:c:2567:MET:HE3 | 2:c:2718:TRP:HB2 | 1.83 | 0.61 |
| 3:d:3038[B]:ILE:HG22 | 3:d:3041[B]:ALA:H | 1.65 | 0.61 |
| 3:C:3152[B]:LYS:N | 3:L:3172[B]:SER:CB | 2.62 | 0.61 |
| 3:C:3173[A]:THR:HB | 3:C:3176[A]:LYS:HG2 | 1.81 | 0.61 |
| 3:C:3300[B]:LEU:HD23 | 3:C:3300[B]:LEU:N | 2.15 | 0.61 |
| 3:F:2948[A]:ASP:HB3 | 3:F:2953[A]:GLY:CA | 2.24 | 0.61 |
| 3:F:3025[A]:VAL:HG22 | 3:F:3025[A]:VAL:O | 2.00 | 0.61 |
| 3:F:3194[A]:GLY:O | 3:F:3195[A]:MET:HG2 | 2.01 | 0.61 |
| 2:K:2819:VAL:HB | 2:K:2835:ILE:HG23 | 1.82 | 0.61 |
| 3:L:3025[A]:VAL:HG22 | 3:L:3025[A]:VAL:O | 2.00 | 0.61 |
| 3:L:3194[A]:GLY:O | 3:L:3195[A]:MET:HG2 | 2.01 | 0.61 |
| 3:O:3120[B]:HIS:C | 3:O:3122[B]:ASN:N | 2.55 | 0.61 |
| 1:P:439:LEU:HD23 | 1:P:509:ILE:HD12 | 1.82 | 0.61 |
| 1:P:488:PRO:HB2 | 1:P:641:TRP:CE3 | 2.36 | 0.61 |
| 1:P:935:ILE:HD11 | 1:P:980:TYR:HE2 | 1.65 | 0.61 |
| 3:R:3038[B]:ILE:HG12 | 3:R:3112[B]:TYR:CE2 | 2.35 | 0.61 |
| 3:R:3114[B]:PRO:CD | 3:R:3115[B]:LEU:H | 2.13 | 0.61 |
| 1:S:1429:THR:HG23 | 1:S:1433:TRP:CZ2 | 2.36 | 0.61 |
| 3:U:3254[B]:MET:HA | 3:d:3253[B]:GLU:O | 2.00 | 0.61 |
| 3:U:3274[A]:ARG:NE | 3:U:3274[A]:ARG:HA | 2.16 | 0.61 |
| 1:V:906:HIS:CD2 | 9:V:5003:CUO:O1 | 2.53 | 0.61 |
| 1:V:1441:SER:OG | 1:V:1442:MET:N | 2.30 | 0.61 |
| 1:Y:1656:ASP:N | 3:d:3006[B]:LYS:CB | 2.63 | 0.61 |
| 3:a:3135[A]:LYS:CB | 3:a:3141[A]:TYR:HD1 | 2.13 | 0.61 |
| 1:b:622:HIS:CE1 | 1:b:767:LYS:H | 2.18 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2957[B]:ILE:N | 3:d:2960[B]:PHE:HE1 | 1.97 | 0.61 |
| 3:d:2994[B]:LYS:HD2 | 3:d:2998[B]:ASP:OD2 | 2.00 | 0.61 |
| 3:d:3096[B]:VAL:HG11 | 3:d:3115[B]:LEU:HD13 | 1.81 | 0.61 |
| 3:d:3307[A]:PHE:HE1 | 3:d:3309[A]:PRO:CG | 2.08 | 0.61 |
| 3:C:3276[B]:ASP:HB3 | 3:C:3278[B]:HIS:HB2 | 1.83 | 0.61 |
| 1:D:909:ILE:HG12 | 1:D:1084:PHE:HZ | 1.64 | 0.61 |
| 2:E:2356:ASP:O | 2:E:2363:ASN:ND2 | 2.33 | 0.61 |
| 3:F:2964[B]:PRO:CB | 3:a:3221[B]:ALA:HB3 | 2.31 | 0.61 |
| 3:F:3038[A]:ILE:HG12 | 3:F:3112[A]:TYR:CE2 | 2.35 | 0.61 |
| 3:F:3162[B]:ASP:N | 3:F:3162[B]:ASP:OD1 | 2.31 | 0.61 |
| 1:G:684:ARG:O | 1:G:687:SER:OG | 2.18 | 0.61 |
| 3:I:2949[B]:LYS:HZ2 | 3:I:2950[B]:THR:HA | 1.66 | 0.61 |
| 3:I:2967[B]:CYS:SG | 3:R:2982[B]:MET:HE3 | 2.40 | 0.61 |
| 3:I:3120[A]:HIS:C | 3:I:3122[A]:ASN:N | 2.55 | 0.61 |
| 3:I:3156[B]:MET:HB3 | 3:R:2982[B]:MET:CB | 2.31 | 0.61 |
| 3:I:3220[B]:ARG:HH11 | 3:I:3220[B]:ARG:CG | 2.12 | 0.61 |
| 2:K:2109:ARG:NH1 | 2:K:2169:HIS:O | 2.34 | 0.61 |
| 3:L:3222[A]:ILE:HD11 | 3:L:3224[A]:GLN:OE1 | 2.00 | 0.61 |
| 1:M:946:GLU:HA | 1:M:955:LYS:HB3 | 1.82 | 0.61 |
| 3:O:3194[B]:GLY:O | 3:O:3195[B]:MET:HG2 | 2.01 | 0.61 |
| 3:O:3254[B]:MET:HB3 | 3:X:3159[B]:SER:OG | 2.00 | 0.61 |
| 1:P:1498:ASN:ND2 | 1:P:1500:THR:O | 2.33 | 0.61 |
| 3:R:3270[B]:LEU:O | 3:R:3274[B]:ARG:N | 2.33 | 0.61 |
| 3:R:3276[B]:ASP:HB3 | 3:R:3278[B]:HIS:HB2 | 1.83 | 0.61 |
| 1:S:1162:ALA:HB2 | 1:S:1169:LYS:HG2 | 1.83 | 0.61 |
| 1:S:1394:GLN:HB2 | 1:S:1433:TRP:HB2 | 1.83 | 0.61 |
| 3:U:3200[A]:LEU:HD22 | 3:U:3204[A]:LEU:HD13 | 1.83 | 0.61 |
| 1:V:133:LYS:HB2 | 1:V:134:VAL:HG22 | 1.82 | 0.61 |
| 3:X:2957[B]:ILE:HA | 3:X:2960[B]:PHE:HE1 | 1.64 | 0.61 |
| 1:Y:594:ASP:OD1 | 1:Y:775:ARG:NH1 | 2.34 | 0.61 |
| 1:Y:639:ARG:NH2 | 1:Y:707:PHE:O | 2.33 | 0.61 |
| 2:Z:2243:LEU:HD11 | 2:Z:2273:TRP:HZ3 | 1.64 | 0.61 |
| 3:a:3194[A]:GLY:O | 3:a:3195[A]:MET:HG2 | 2.01 | 0.61 |
| 3:a:3200[B]:LEU:HD22 | 3:a:3204[B]:LEU:HD13 | 1.83 | 0.61 |
| 2:c:2885:SER:HB3 | 2:c:2890:VAL:HG22 | 1.83 | 0.61 |
| 3:d:2930[A]:LEU:HD22 | 3:d:2930[A]:LEU:N | 2.02 | 0.61 |
| 3:d:3298[A]:ASN:HD21 | 3:d:3301[A]:PRO:HA | 1.60 | 0.61 |
| 3:d:3307[B]:PHE:HE1 | 3:d:3309[B]:PRO:CG | 2.08 | 0.61 |
| 2:B:2619:VAL:HG23 | 1:b:190:PHE:HD2 | 1.66 | 0.61 |
| 3:C:2985[B]:PHE:HE2 | 3:L:2969[B]:TYR:CA | 2.12 | 0.61 |
| 3:C:3222[B]:ILE:HD11 | 3:C:3224[B]:GLN:OE1 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3270[B]:LEU:O | 3:C:3274[B]:ARG:N | 2.33 | 0.61 |
| 3:C:3272[A]:HIS:CD2 | 1:D:1543:ILE:HD11 | 2.36 | 0.61 |
| 3:C:3281[A]:PHE:CE1 | 3:C:3305[A]:ILE:HG21 | 2.36 | 0.61 |
| 9:C:3401[B]:CUO:O1 | 3:L:3120[B]:HIS:NE2 | 2.30 | 0.61 |
| 1:D:465:PRO:HD2 | 1:D:467:LYS:NZ | 2.16 | 0.61 |
| 1:D:619:SER:HB2 | 1:D:805:VAL:HG11 | 1.81 | 0.61 |
| 1:D:804:ASP:OD1 | 1:D:805:VAL:N | 2.33 | 0.61 |
| 3:F:3038[B]:ILE:HG12 | 3:F:3112[B]:TYR:CE2 | 2.35 | 0.61 |
| 3:F:3173[A]:THR:HB | 3:F:3176[A]:LYS:HG2 | 1.81 | 0.61 |
| 2:H:2472:ASN:N | 2:H:2473:GLY:HA2 | 2.16 | 0.61 |
| 3:I:2964[B]:PRO:HG3 | 3:I:3040[B]:VAL:HG11 | 1.82 | 0.61 |
| 3:I:2969[B]:TYR:CD2 | 3:R:3093[B]:HIS:NE2 | 2.68 | 0.61 |
| 3:I:3114[B]:PRO:CD | 3:I:3115[B]:LEU:H | 2.12 | 0.61 |
| 3:I:3139[A]:LEU:N | 3:I:3139[A]:LEU:HD22 | 2.16 | 0.61 |
| 3:I:3147[A]:GLU:HG3 | 3:I:3149[A]:ASN:HD21 | 1.65 | 0.61 |
| 3:I:3163[B]:ASN:HB3 | 3:R:3150[B]:LYS:NZ | 2.16 | 0.61 |
| 1:J:517:THR:HG21 | 1:J:708:PHE:HE1 | 1.65 | 0.61 |
| 1:J:926:LEU:HD11 | 1:J:1043:MET:HB3 | 1.83 | 0.61 |
| 3:O:2967[B]:CYS:H | 3:X:2979[B]:GLN:NE2 | 1.98 | 0.61 |
| 3:O:3038[B]:ILE:CD1 | 3:X:2969[B]:TYR:HE2 | 2.05 | 0.61 |
| 3:O:3157[B]:PRO:CA | 3:X:3153[B]:LYS:H | 2.11 | 0.61 |
| 3:O:3300[A]:LEU:HD23 | 3:O:3300[A]:LEU:N | 2.14 | 0.61 |
| 2:Q:2130:PRO:O | 2:Q:2140:ARG:HD2 | 2.01 | 0.61 |
| 3:R:2948[A]:ASP:CB | 3:R:2949[A]:LYS:CA | 2.78 | 0.61 |
| 3:R:2987[A]:HIS:NE2 | 3:R:3178[A]:PHE:HE1 | 1.96 | 0.61 |
| 3:R:3173[B]:THR:HB | 3:R:3176[B]:LYS:HG2 | 1.81 | 0.61 |
| 3:R:3194[B]:GLY:O | 3:R:3195[B]:MET:HG2 | 2.01 | 0.61 |
| 2:T:2201:THR:O | 2:T:2203:ILE:N | 2.32 | 0.61 |
| 3:U:2965[B]:LEU:H | 3:d:3220[B]:ARG:NH2 | 1.98 | 0.61 |
| 3:U:2979[B]:GLN:NE2 | 3:d:3153[B]:LYS:CE | 2.64 | 0.61 |
| 3:U:2994[B]:LYS:HD2 | 3:U:2998[B]:ASP:OD2 | 2.00 | 0.61 |
| 3:U:3194[B]:GLY:O | 3:U:3195[B]:MET:HG2 | 2.01 | 0.61 |
| 3:U:3252[B]:TYR:C | 3:d:3255[B]:PRO:CG | 2.73 | 0.61 |
| 3:U:3256[B]:TRP:CG | 3:d:2969[B]:TYR:CG | 2.86 | 0.61 |
| 3:X:2957[B]:ILE:N | 3:X:2960[B]:PHE:HE1 | 1.98 | 0.61 |
| 3:X:2964[A]:PRO:HG3 | 3:X:3040[A]:VAL:HG11 | 1.82 | 0.61 |
| 3:X:3156[B]:MET:HA | 3:X:3157[B]:PRO:C | 2.26 | 0.61 |
| 3:X:3222[B]:ILE:HD11 | 3:X:3224[B]:GLN:OE1 | 2.00 | 0.61 |
| 3:X:3298[B]:ASN:CA | 3:X:3300[B]:LEU:HD23 | 2.31 | 0.61 |
| 1:Y:1551:ASP:OD1 | 3:d:3007[B]:ILE:CD1 | 2.49 | 0.61 |
| 3:a:3200[A]:LEU:HD22 | 3:a:3204[A]:LEU:HD13 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:c:2128:LEU:HD13 | 2:c:2286:HIS:CG | 2.35 | 0.61 |
| 2:c:2800:LYS:O | 3:d:3023[A]:ILE:HD11 | 2.00 | 0.61 |
| 3:d:3025[A]:VAL:HG22 | 3:d:3025[A]:VAL:O | 2.00 | 0.61 |
| 1:A:562:GLN:HG2 | 1:A:614:GLU:HG3 | 1.81 | 0.61 |
| 3:C:2963[B]:MET:HE1 | 3:L:3222[B]:ILE:CD1 | 2.24 | 0.61 |
| 3:C:2964[A]:PRO:HG3 | 3:C:3040[A]:VAL:HG11 | 1.82 | 0.61 |
| 3:C:3038[A]:ILE:HG22 | 3:C:3041[A]:ALA:H | 1.65 | 0.61 |
| 3:F:2977[B]:CYS:HB2 | 3:a:2982[B]:MET:CE | 2.31 | 0.61 |
| 3:F:3135[B]:LYS:CB | 3:F:3141[B]:TYR:HD1 | 2.13 | 0.61 |
| 3:F:3149[B]:ASN:ND2 | 3:a:3163[B]:ASN:O | 2.32 | 0.61 |
| 3:F:3300[B]:LEU:HD23 | 3:F:3300[B]:LEU:N | 2.15 | 0.61 |
| 3:I:2998[B]:ASP:O | 3:I:3001[B]:LYS:HB2 | 2.01 | 0.61 |
| 3:I:3171[B]:HIS:CA | 3:R:3152[B]:LYS:HB2 | 2.30 | 0.61 |
| 2:K:2421:TYR:HB2 | 2:K:2454:MET:HE3 | 1.83 | 0.61 |
| 3:L:3157[A]:PRO:O | 3:L:3160[A]:SER:N | 2.30 | 0.61 |
| 3:L:3200[A]:LEU:HD22 | 3:L:3204[A]:LEU:HD13 | 1.83 | 0.61 |
| 2:N:2851:ASN:OD1 | 2:N:2851:ASN:N | 2.34 | 0.61 |
| 3:O:3139[B]:LEU:N | 3:O:3139[B]:LEU:HD22 | 2.16 | 0.61 |
| 2:Q:2795:ILE:O | 2:Q:2798:GLN:HG2 | 2.00 | 0.61 |
| 3:R:2948[A]:ASP:HB3 | 3:R:2953[A]:GLY:CA | 2.24 | 0.61 |
| 1:S:240:PHE:HA | 1:S:263:ALA:HB3 | 1.82 | 0.61 |
| 1:S:1301:PRO:HB3 | 1:S:1308:VAL:HG12 | 1.83 | 0.61 |
| 3:U:2939[A]:ARG:HH11 | 3:U:2939[A]:ARG:HG3 | 1.66 | 0.61 |
| 3:X:2948[A]:ASP:CB | 3:X:2949[A]:LYS:CA | 2.78 | 0.61 |
| 3:X:3120[A]:HIS:C | 3:X:3122[A]:ASN:N | 2.55 | 0.61 |
| 3:X:3194[A]:GLY:O | 3:X:3195[A]:MET:HG2 | 2.01 | 0.61 |
| 3:X:3274[B]:ARG:NE | 3:X:3274[B]:ARG:HA | 2.16 | 0.61 |
| 3:X:3276[A]:ASP:HB3 | 3:X:3278[A]:HIS:HB2 | 1.83 | 0.61 |
| 2:Z:2889:ALA:N | 2:Z:2890:VAL:HA | 2.15 | 0.61 |
| 3:a:2957[B]:ILE:N | 3:a:2960[B]:PHE:HE1 | 1.97 | 0.61 |
| 3:a:3194[B]:GLY:O | 3:a:3195[B]:MET:HG2 | 2.01 | 0.61 |
| 3:a:3273[A]:LEU:CB | 3:a:3275[A]:LEU:HD13 | 2.28 | 0.61 |
| 3:d:3038[A]:ILE:HG12 | 3:d:3112[A]:TYR:CE2 | 2.35 | 0.61 |
| 3:d:3139[A]:LEU:N | 3:d:3139[A]:LEU:HD22 | 2.16 | 0.61 |
| 3:d:3218[B]:LEU:O | 3:d:3219[B]:LEU:HD13 | 2.01 | 0.61 |
| 2:B:2094:ARG:HH21 | 2:E:2094:ARG:HH21 | 1.49 | 0.60 |
| 3:C:2985[B]:PHE:CE2 | 3:L:2968[B]:GLN:O | 2.54 | 0.60 |
| 3:C:3066[A]:TYR:CD1 | 3:C:3193[A]:HIS:HE1 | 2.17 | 0.60 |
| 3:C:3276[A]:ASP:HB3 | 3:C:3278[A]:HIS:HB2 | 1.83 | 0.60 |
| 1:D:135:THR:HG21 | 1:D:192:HIS:HB3 | 1.83 | 0.60 |
| 3:F:2964[B]:PRO:HG3 | 3:F:3040[B]:VAL:HG11 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2975[B]:PHE:HD1 | 3:a:3107[B]:LEU:CD2 | 2.13 | 0.60 |
| 3:F:3147[A]:GLU:HG3 | 3:F:3149[A]:ASN:HD21 | 1.65 | 0.60 |
| 3:F:3170[B]:ALA:O | 3:a:3152[B]:LYS:CG | 2.48 | 0.60 |
| 1:G:1242:ASN:HB3 | 1:G:1479:TYR:OH | 2.02 | 0.60 |
| 3:I:2965[B]:LEU:HA | 3:R:3253[B]:GLU:CG | 2.31 | 0.60 |
| 3:I:3191[A]:ASN:ND2 | 3:I:3191[A]:ASN:H | 1.99 | 0.60 |
| 3:I:3281[B]:PHE:CE1 | 3:I:3305[B]:ILE:HG21 | 2.36 | 0.60 |
| 3:I:3298[B]:ASN:CA | 3:I:3300[B]:LEU:HD23 | 2.31 | 0.60 |
| 2:K:2166:LEU:HA | 2:K:2169:HIS:HB2 | 1.83 | 0.60 |
| 3:L:2939[A]:ARG:HG3 | 3:L:2939[A]:ARG:HH11 | 1.66 | 0.60 |
| 3:L:2945[A]:VAL:HG22 | 3:L:2945[A]:VAL:O | 2.01 | 0.60 |
| 3:L:2964[A]:PRO:HG3 | 3:L:3040[A]:VAL:HG11 | 1.82 | 0.60 |
| 3:L:3025[B]:VAL:HG22 | 3:L:3025[B]:VAL:O | 2.00 | 0.60 |
| 3:L:3211[B]:ASP:OD1 | 3:L:3211[B]:ASP:N | 2.28 | 0.60 |
| 3:L:3212[A]:ARG:HH11 | 3:L:3212[A]:ARG:CG | 2.12 | 0.60 |
| 3:O:3025[B]:VAL:HG22 | 3:O:3025[B]:VAL:O | 2.00 | 0.60 |
| 3:O:3114[A]:PRO:CD | 3:O:3115[A]:LEU:H | 2.12 | 0.60 |
| 3:O:3218[A]:LEU:O | 3:O:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 3:R:3025[B]:VAL:HG22 | 3:R:3025[B]:VAL:O | 2.00 | 0.60 |
| 3:R:3134[B]:GLN:O | 3:R:3135[B]:LYS:C | 2.44 | 0.60 |
| 1:S:452:ILE:HD12 | 1:S:1367:SER:HB2 | 1.83 | 0.60 |
| 1:S:881:GLN:OE1 | 1:S:888:ALA:HB3 | 2.01 | 0.60 |
| 3:U:2949[B]:LYS:HZ2 | 3:U:2950[B]:THR:HA | 1.66 | 0.60 |
| 3:U:2969[B]:TYR:HE2 | 3:d:3248[B]:LEU:HD23 | 1.66 | 0.60 |
| 3:U:3169[B]:LYS:CD | 3:d:3146[B]:CYS:HA | 2.31 | 0.60 |
| 1:V:1019:HIS:HE2 | 1:V:1046:HIS:CE1 | 2.19 | 0.60 |
| 1:V:1582:ASN:HB3 | 1:V:1583:CYS:CB | 2.26 | 0.60 |
| 3:X:2964[B]:PRO:HG3 | 3:X:3040[B]:VAL:HG11 | 1.82 | 0.60 |
| 3:X:3114[A]:PRO:CD | 3:X:3115[A]:LEU:H | 2.12 | 0.60 |
| 3:X:3218[A]:LEU:O | 3:X:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 3:a:3038[B]:ILE:HG12 | 3:a:3112[B]:TYR:CE2 | 2.35 | 0.60 |
| 1:b:1067:TYR:H | 1:b:1067:TYR:HD1 | 1.48 | 0.60 |
| 1:b:1595:GLY:O | 1:b:1598:GLU:HG2 | 2.01 | 0.60 |
| 3:d:3274[A]:ARG:NE | 3:d:3274[A]:ARG:HA | 2.16 | 0.60 |
| 3:d:3281[B]:PHE:CE1 | 3:d:3305[B]:ILE:HG21 | 2.36 | 0.60 |
| 3:d:3298[B]:ASN:CB | 3:d:3300[B]:LEU:N | 2.60 | 0.60 |
| 3:C:2998[B]:ASP:O | 3:C:3001[B]:LYS:HB2 | 2.01 | 0.60 |
| 3:C:3135[A]:LYS:CB | 3:C:3141[A]:TYR:HD1 | 2.12 | 0.60 |
| 3:C:3218[A]:LEU:O | 3:C:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 3:C:3222[A]:ILE:HD11 | 3:C:3224[A]:GLN:OE1 | 2.00 | 0.60 |
| 3:C:3281[B]:PHE:CE1 | 3:C:3305[B]:ILE:HG21 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3155[B]:MET:HB3 | 3:a:3153[B]:LYS:HD3 | 1.71 | 0.60 |
| 3:F:3157[B]:PRO:HD3 | 3:a:3254[B]:MET:HE2 | 1.83 | 0.60 |
| 3:F:3212[B]:ARG:HH11 | 3:F:3212[B]:ARG:CG | 2.12 | 0.60 |
| 3:F:3281[A]:PHE:CE1 | 3:F:3305[A]:ILE:HG21 | 2.36 | 0.60 |
| 1:G:488:PRO:HB2 | 1:G:641:TRP:CE3 | 2.36 | 0.60 |
| 2:H:2670:CYS:N | 2:H:2737:CYS:SG | 2.74 | 0.60 |
| 3:I:2945[A]:VAL:HG22 | 3:I:2945[A]:VAL:O | 2.02 | 0.60 |
| 3:I:2948[A]:ASP:HB3 | 3:I:2953[A]:GLY:CA | 2.24 | 0.60 |
| 3:I:2948[A]:ASP:CB | 3:I:2949[A]:LYS:CA | 2.78 | 0.60 |
| 3:I:2975[B]:PHE:CZ | 3:R:2961[B]:HIS:C | 2.79 | 0.60 |
| 3:I:3156[A]:MET:HA | 3:I:3157[A]:PRO:C | 2.26 | 0.60 |
| 3:I:3194[B]:GLY:O | 3:I:3195[B]:MET:HG2 | 2.01 | 0.60 |
| 3:I:3300[A]:LEU:HD23 | 3:I:3300[A]:LEU:N | 2.15 | 0.60 |
| 3:L:3298[A]:ASN:CA | 3:L:3300[A]:LEU:HD23 | 2.31 | 0.60 |
| 3:O:3222[A]:ILE:HD11 | 3:O:3224[A]:GLN:OE1 | 2.00 | 0.60 |
| 3:O:3222[B]:ILE:HD11 | 3:O:3224[B]:GLN:OE1 | 2.00 | 0.60 |
| 3:O:3274[B]:ARG:NE | 3:O:3274[B]:ARG:HA | 2.16 | 0.60 |
| 3:O:3307[A]:PHE:HE1 | 3:O:3309[A]:PRO:CG | 2.08 | 0.60 |
| 2:Q:2225:ARG:HD2 | 2:Q:2274:LEU:HD22 | 1.83 | 0.60 |
| 3:R:2949[A]:LYS:HZ2 | 3:R:2950[A]:THR:HA | 1.65 | 0.60 |
| 3:R:2957[A]:ILE:N | 3:R:2960[A]:PHE:HE1 | 1.97 | 0.60 |
| 3:R:2964[A]:PRO:HG3 | 3:R:3040[A]:VAL:HG11 | 1.82 | 0.60 |
| 3:R:3218[A]:LEU:O | 3:R:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 3:R:3281[B]:PHE:CE1 | 3:R:3305[B]:ILE:HG21 | 2.36 | 0.60 |
| 1:S:1195:ASP:HA | 1:S:1196:ILE:HB | 1.82 | 0.60 |
| 1:S:1304:ASP:N | 1:S:1305:GLY:HA2 | 2.15 | 0.60 |
| 3:U:2949[A]:LYS:HZ2 | 3:U:2950[A]:THR:HA | 1.66 | 0.60 |
| 3:U:3038[A]:ILE:HG12 | 3:U:3112[A]:TYR:CE2 | 2.35 | 0.60 |
| 3:U:3139[A]:LEU:N | 3:U:3139[A]:LEU:HD22 | 2.16 | 0.60 |
| 3:U:3176[B]:LYS:HB3 | 3:U:3176[B]:LYS:HZ2 | 1.66 | 0.60 |
| 3:U:3194[A]:GLY:O | 3:U:3195[A]:MET:HG2 | 2.01 | 0.60 |
| 3:U:3222[B]:ILE:HD11 | 3:U:3224[B]:GLN:OE1 | 2.00 | 0.60 |
| 3:X:2939[B]:ARG:HH11 | 3:X:2939[B]:ARG:HG3 | 1.66 | 0.60 |
| 3:X:3200[B]:LEU:HD22 | 3:X:3204[B]:LEU:HD13 | 1.83 | 0.60 |
| 2:Z:2849:ASP:OD2 | 2:Z:2850:ARG:NH2 | 2.34 | 0.60 |
| 3:a:3114[A]:PRO:CD | 3:a:3115[A]:LEU:H | 2.12 | 0.60 |
| 3:a:3134[B]:GLN:O | 3:a:3135[B]:LYS:C | 2.44 | 0.60 |
| 3:a:3218[A]:LEU:O | 3:a:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 3:a:3281[A]:PHE:CE1 | 3:a:3305[A]:ILE:HG21 | 2.36 | 0.60 |
| 2:c:2903:TYR:OH | 3:d:2932[A]:PRO:HD2 | 2.00 | 0.60 |
| 3:d:3298[B]:ASN:CA | 3:d:3300[B]:LEU:HD23 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2830:GLN:HB2 | 2:B:2863:ARG:HH12 | 1.66 | 0.60 |
| 3:C:2945[B]:VAL:HG22 | 3:C:2945[B]:VAL:O | 2.02 | 0.60 |
| 3:C:3124[B]:ASP:OD2 | 3:C:3187[B]:TYR:OH | 2.15 | 0.60 |
| 3:C:3134[B]:GLN:O | 3:C:3135[B]:LYS:C | 2.44 | 0.60 |
| 3:C:3154[B]:PRO:CB | 3:L:3174[B]:GLY:N | 2.65 | 0.60 |
| 3:C:3273[B]:LEU:CB | 3:C:3275[B]:LEU:HD13 | 2.28 | 0.60 |
| 3:C:3284[A]:LYS:CD | 3:C:3285[A]:VAL:H | 2.09 | 0.60 |
| 1:D:325:THR:HG21 | 1:D:329:ARG:O | 2.00 | 0.60 |
| 2:E:2210:ASN:O | 2:E:2225:ARG:NH2 | 2.34 | 0.60 |
| 3:F:2939[A]:ARG:HH11 | 3:F:2939[A]:ARG:HG3 | 1.66 | 0.60 |
| 3:F:2939[B]:ARG:HG3 | 3:F:2939[B]:ARG:HH11 | 1.66 | 0.60 |
| 3:F:2994[A]:LYS:HD2 | 3:F:2998[A]:ASP:OD2 | 2.00 | 0.60 |
| 3:F:3038[A]:ILE:HG22 | 3:F:3041[A]:ALA:H | 1.65 | 0.60 |
| 3:F:3135[A]:LYS:HG3 | 3:F:3141[A]:TYR:CD1 | 2.33 | 0.60 |
| 3:F:3139[B]:LEU:N | 3:F:3139[B]:LEU:HD22 | 2.16 | 0.60 |
| 1:G:71:LEU:HD22 | 1:G:266:LEU:HD21 | 1.82 | 0.60 |
| 3:I:2965[B]:LEU:HD21 | 3:R:3250[B]:GLY:H | 1.65 | 0.60 |
| 3:I:3221[B]:ALA:CB | 3:R:2964[B]:PRO:CB | 2.62 | 0.60 |
| 2:K:2300:ASN:OD1 | 2:K:2303:ARG:NH1 | 2.34 | 0.60 |
| 3:L:3038[B]:ILE:HG12 | 3:L:3112[B]:TYR:CE2 | 2.35 | 0.60 |
| 1:M:898:GLY:N | 1:M:899:MET:HA | 2.16 | 0.60 |
| 3:O:2973[B]:THR:CB | 3:X:3158[B]:PHE:CZ | 2.82 | 0.60 |
| 3:O:2998[B]:ASP:O | 3:O:3001[B]:LYS:HB2 | 2.01 | 0.60 |
| 3:O:3272[A]:HIS:CD2 | 1:P:1542:ARG:HH22 | 2.19 | 0.60 |
| 1:P:622:HIS:CE1 | 1:P:767:LYS:H | 2.19 | 0.60 |
| 3:R:3096[B]:VAL:HG11 | 3:R:3115[B]:LEU:HD13 | 1.81 | 0.60 |
| 3:R:3120[A]:HIS:C | 3:R:3122[A]:ASN:N | 2.55 | 0.60 |
| 3:R:3139[B]:LEU:N | 3:R:3139[B]:LEU:HD22 | 2.16 | 0.60 |
| 3:R:3156[B]:MET:HA | 3:R:3157[B]:PRO:C | 2.26 | 0.60 |
| 3:R:3191[B]:ASN:ND2 | 3:R:3191[B]:ASN:H | 1.99 | 0.60 |
| 3:R:3274[B]:ARG:HA | 3:R:3274[B]:ARG:NE | 2.16 | 0.60 |
| 3:R:3307[A]:PHE:HE1 | 3:R:3309[A]:PRO:CG | 2.08 | 0.60 |
| 1:S:494:VAL:HG23 | 1:S:671:PHE:HZ | 1.67 | 0.60 |
| 1:S:1639:LYS:HE3 | 4:BA:2:NAG:H82 | 1.83 | 0.60 |
| 2:T:2830:GLN:HE22 | 2:T:2863:ARG:HH11 | 1.49 | 0.60 |
| 2:T:2879:LEU:HD21 | 2:T:2901:LEU:HD11 | 1.83 | 0.60 |
| 3:U:2987[B]:HIS:NE2 | 3:U:3178[B]:PHE:HE1 | 1.95 | 0.60 |
| 3:U:3218[B]:LEU:O | 3:U:3219[B]:LEU:HD13 | 2.01 | 0.60 |
| 1:V:555:ALA:HB3 | 1:V:557:VAL:HG12 | 1.83 | 0.60 |
| 3:X:3212[B]:ARG:HH11 | 3:X:3212[B]:ARG:CG | 2.12 | 0.60 |
| 3:X:3276[B]:ASP:HB3 | 3:X:3278[B]:HIS:HB2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:545:PHE:O | 1:Y:561:ARG:NH2 | 2.34 | 0.60 |
| 1:Y:606:ILE:O | 1:Y:610:THR:OG1 | 2.18 | 0.60 |
| 1:Y:729:VAL:HG11 | 1:Y:785:LEU:HD12 | 1.84 | 0.60 |
| 2:Z:2745:PRO:HB2 | 2:Z:2750:ILE:HD11 | 1.82 | 0.60 |
| 3:a:2998[A]:ASP:O | 3:a:3001[A]:LYS:HB2 | 2.01 | 0.60 |
| 3:a:3139[B]:LEU:N | 3:a:3139[B]:LEU:HD22 | 2.16 | 0.60 |
| 3:a:3156[B]:MET:HA | 3:a:3157[B]:PRO:C | 2.26 | 0.60 |
| 3:a:3218[B]:LEU:O | 3:a:3219[B]:LEU:HD13 | 2.02 | 0.60 |
| 3:a:3298[A]:ASN:CA | 3:a:3300[A]:LEU:HD23 | 2.31 | 0.60 |
| 3:a:3298[B]:ASN:ND2 | 3:a:3301[B]:PRO:C | 2.60 | 0.60 |
| 3:d:2949[A]:LYS:HZ2 | 3:d:2950[A]:THR:HA | 1.66 | 0.60 |
| 3:d:2957[A]:ILE:N | 3:d:2960[A]:PHE:HE1 | 1.98 | 0.60 |
| 3:d:3139[B]:LEU:HD22 | 3:d:3139[B]:LEU:N | 2.16 | 0.60 |
| 3:d:3218[A]:LEU:O | 3:d:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 6:LA:1:NAG:O4 | 6:LA:2:NAG:C7 | 2.49 | 0.60 |
| 3:C:3139[A]:LEU:HD22 | 3:C:3139[A]:LEU:N | 2.16 | 0.60 |
| 3:C:3154[B]:PRO:N | 3:L:3173[B]:THR:C | 2.59 | 0.60 |
| 3:C:3194[A]:GLY:O | 3:C:3195[A]:MET:HG2 | 2.01 | 0.60 |
| 1:D:262:LYS:NZ | 1:D:795:GLU:OE1 | 2.35 | 0.60 |
| 1:D:411:ASP:OD1 | 1:D:658:TYR:OH | 2.16 | 0.60 |
| 3:F:2994[B]:LYS:O | 3:F:2995[B]:GLN:C | 2.38 | 0.60 |
| 3:F:3155[B]:MET:CB | 3:a:3153[B]:LYS:CB | 2.76 | 0.60 |
| 3:F:3255[B]:PRO:CG | 3:a:2964[B]:PRO:CD | 2.80 | 0.60 |
| 3:F:3255[B]:PRO:C | 3:a:2965[B]:LEU:C | 2.67 | 0.60 |
| 1:G:238:ASN:OD1 | 1:G:238:ASN:N | 2.33 | 0.60 |
| 3:I:2964[B]:PRO:CA | 3:R:3221[B]:ALA:HB3 | 2.30 | 0.60 |
| 3:I:2977[B]:CYS:SG | 3:R:2982[B]:MET:HE3 | 2.41 | 0.60 |
| 3:I:3025[A]:VAL:HG22 | 3:I:3025[A]:VAL:O | 2.00 | 0.60 |
| 3:I:3222[A]:ILE:HG13 | 3:I:3224[A]:GLN:HG2 | 1.84 | 0.60 |
| 1:J:444:GLU:HG3 | 1:J:544:PRO:HG3 | 1.84 | 0.60 |
| 1:J:456:GLN:HG2 | 1:J:551:GLU:HB2 | 1.84 | 0.60 |
| 3:L:2998[B]:ASP:O | 3:L:3001[B]:LYS:HB2 | 2.01 | 0.60 |
| 3:L:3134[B]:GLN:O | 3:L:3135[B]:LYS:C | 2.44 | 0.60 |
| 3:L:3139[A]:LEU:N | 3:L:3139[A]:LEU:HD22 | 2.16 | 0.60 |
| 3:L:3274[A]:ARG:HA | 3:L:3274[A]:ARG:NE | 2.16 | 0.60 |
| 3:L:3300[A]:LEU:HD23 | 3:L:3300[A]:LEU:N | 2.15 | 0.60 |
| 3:O:3102[B]:TYR:CA | 3:X:2971[B]:ASP:CA | 2.78 | 0.60 |
| 3:O:3139[A]:LEU:N | 3:O:3139[A]:LEU:HD22 | 2.16 | 0.60 |
| 3:O:3298[B]:ASN:ND2 | 3:O:3301[B]:PRO:C | 2.60 | 0.60 |
| 3:R:2939[A]:ARG:HH11 | 3:R:2939[A]:ARG:HG3 | 1.66 | 0.60 |
| 3:R:3038[B]:ILE:HG22 | 3:R:3041[B]:ALA:H | 1.65 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3222[A]:ILE:HD11 | 3:R:3224[A]:GLN:OE1 | 2.00 | 0.60 |
| 3:R:3222[B]:ILE:HG13 | 3:R:3224[B]:GLN:HG2 | 1.84 | 0.60 |
| 3:R:3298[B]:ASN:CB | 3:R:3300[B]:LEU:CD2 | 2.61 | 0.60 |
| 1:S:575:ASP:N | 1:S:576:HIS:HA | 2.16 | 0.60 |
| 3:U:3298[A]:ASN:ND2 | 3:U:3301[A]:PRO:C | 2.60 | 0.60 |
| 1:V:533:VAL:HG12 | 1:V:540:THR:HG22 | 1.82 | 0.60 |
| 1:V:1143:ALA:HA | 1:V:1195:ASP:O | 2.01 | 0.60 |
| 3:X:3025[B]:VAL:HG22 | 3:X:3025[B]:VAL:O | 2.00 | 0.60 |
| 1:Y:1296:VAL:HB | 1:Y:1446:ASP:HB3 | 1.82 | 0.60 |
| 3:a:2952[A]:ALA:N | 3:a:2953[A]:GLY:HA2 | 2.06 | 0.60 |
| 3:a:3038[A]:ILE:HG22 | 3:a:3041[A]:ALA:H | 1.65 | 0.60 |
| 3:a:3155[B]:MET:HG3 | 3:a:3172[B]:SER:O | 1.99 | 0.60 |
| 1:b:589:GLN:O | 1:b:651:ARG:NH1 | 2.34 | 0.60 |
| 3:d:3096[A]:VAL:HG11 | 3:d:3115[A]:LEU:HD13 | 1.81 | 0.60 |
| 3:d:3200[A]:LEU:HD22 | 3:d:3204[A]:LEU:HD13 | 1.83 | 0.60 |
| 1:A:1242:ASN:OD1 | 1:A:1243:PHE:N | 2.35 | 0.60 |
| 2:B:2133:PRO:HG2 | 2:B:2140:ARG:HA | 1.82 | 0.60 |
| 3:C:2978[B]:CYS:H | 3:L:3254[B]:MET:CB | 1.76 | 0.60 |
| 3:C:3154[B]:PRO:N | 3:L:3155[B]:MET:CG | 2.64 | 0.60 |
| 3:C:3194[B]:GLY:O | 3:C:3195[B]:MET:HG2 | 2.01 | 0.60 |
| 1:D:979:LEU:HB3 | 1:D:980:TYR:CD2 | 2.36 | 0.60 |
| 3:F:2948[B]:ASP:CB | 3:F:2949[B]:LYS:CA | 2.78 | 0.60 |
| 3:F:3220[A]:ARG:HH11 | 3:F:3220[A]:ARG:CG | 2.12 | 0.60 |
| 3:F:3298[B]:ASN:ND2 | 3:F:3301[B]:PRO:C | 2.60 | 0.60 |
| 1:G:221:GLN:NE2 | 1:G:267:PHE:O | 2.32 | 0.60 |
| 1:G:1427:HIS:HD2 | 1:G:1457:HIS:HE1 | 1.49 | 0.60 |
| 3:I:2966[B]:SER:CB | 3:R:2982[B]:MET:HE2 | 2.27 | 0.60 |
| 3:I:3160[B]:SER:CB | 3:R:2982[B]:MET:CA | 2.79 | 0.60 |
| 3:I:3298[B]:ASN:ND2 | 3:I:3301[B]:PRO:C | 2.60 | 0.60 |
| 3:L:3218[B]:LEU:O | 3:L:3219[B]:LEU:HD13 | 2.01 | 0.60 |
| 3:L:3274[B]:ARG:NE | 3:L:3274[B]:ARG:HA | 2.16 | 0.60 |
| 3:O:2957[B]:ILE:N | 3:O:2960[B]:PHE:HE1 | 1.97 | 0.60 |
| 3:O:3101[B]:PRO:CG | 3:X:2971[B]:ASP:O | 2.48 | 0.60 |
| 3:O:3173[B]:THR:HB | 3:O:3176[B]:LYS:HG2 | 1.81 | 0.60 |
| 3:O:3274[A]:ARG:HA | 3:O:3274[A]:ARG:NE | 2.16 | 0.60 |
| 3:O:3276[A]:ASP:HB3 | 3:O:3278[A]:HIS:HB2 | 1.83 | 0.60 |
| 3:O:3281[B]:PHE:CE1 | 3:O:3305[B]:ILE:HG21 | 2.36 | 0.60 |
| 1:P:23:ARG:HD3 | 1:P:120:LYS:HD3 | 1.83 | 0.60 |
| 1:P:1417:CYS:N | 1:P:1484:CYS:SG | 2.73 | 0.60 |
| 1:P:1639:LYS:HG2 | 4:6:1:NAG:HN2 | 1.66 | 0.60 |
| 2:Q:2684:HIS:HA | 2:Q:2695:MET:HG3 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2964[B]:PRO:HG3 | 3:R:3040[B]:VAL:HG11 | 1.82 | 0.60 |
| 3:R:3025[A]:VAL:HG22 | 3:R:3025[A]:VAL:O | 2.00 | 0.60 |
| 3:R:3134[A]:GLN:O | 3:R:3135[A]:LYS:C | 2.44 | 0.60 |
| 3:R:3191[A]:ASN:ND2 | 3:R:3191[A]:ASN:H | 2.00 | 0.60 |
| 1:S:975:PRO:HG3 | 1:S:1026:GLU:HG3 | 1.83 | 0.60 |
| 1:S:1296:VAL:HB | 1:S:1446:ASP:HB3 | 1.83 | 0.60 |
| 3:U:3025[B]:VAL:HG22 | 3:U:3025[B]:VAL:O | 2.00 | 0.60 |
| 3:U:3154[B]:PRO:CG | 3:d:2984[B]:THR:HG23 | 2.26 | 0.60 |
| 3:U:3220[A]:ARG:HH11 | 3:U:3220[A]:ARG:CG | 2.12 | 0.60 |
| 3:U:3259[B]:ASP:N | 3:d:2968[B]:GLN:HE21 | 1.98 | 0.60 |
| 3:U:3298[A]:ASN:CA | 3:U:3300[A]:LEU:HD23 | 2.31 | 0.60 |
| 3:X:2949[A]:LYS:HZ2 | 3:X:2950[A]:THR:HA | 1.65 | 0.60 |
| 3:X:3273[B]:LEU:CB | 3:X:3275[B]:LEU:HD13 | 2.28 | 0.60 |
| 3:X:3298[B]:ASN:ND2 | 3:X:3301[B]:PRO:C | 2.60 | 0.60 |
| 3:a:3025[B]:VAL:HG22 | 3:a:3025[B]:VAL:O | 2.00 | 0.60 |
| 3:a:3139[A]:LEU:N | 3:a:3139[A]:LEU:HD22 | 2.16 | 0.60 |
| 3:a:3147[A]:GLU:HG3 | 3:a:3149[A]:ASN:HD21 | 1.65 | 0.60 |
| 2:c:2406:SER:HB3 | 2:c:2429:LEU:HA | 1.83 | 0.60 |
| 2:c:2509:ILE:HD11 | 2:c:2605:LEU:HD23 | 1.83 | 0.60 |
| 1:A:717:GLN:O | 1:A:721:GLU:HG2 | 2.02 | 0.60 |
| 2:B:2863:ARG:HB2 | 2:B:2865:ILE:HG13 | 1.83 | 0.60 |
| 3:C:2949[A]:LYS:C | 3:C:2949[A]:LYS:HZ3 | 2.09 | 0.60 |
| 3:C:3134[A]:GLN:O | 3:C:3135[A]:LYS:C | 2.44 | 0.60 |
| 3:C:3147[B]:GLU:CD | 3:L:3163[B]:ASN:N | 2.46 | 0.60 |
| 3:C:3222[A]:ILE:HG13 | 3:C:3224[A]:GLN:HG2 | 1.84 | 0.60 |
| 3:C:3253[B]:GLU:OE1 | 3:L:2974[B]:ALA:HB1 | 2.01 | 0.60 |
| 1:D:177:VAL:HA | 1:D:180:ASN:HD22 | 1.65 | 0.60 |
| 1:D:931:TRP:CG | 1:D:1018:ILE:HD11 | 2.36 | 0.60 |
| 3:F:2961[B]:HIS:HB3 | 3:F:3111[B]:SER:HG | 1.67 | 0.60 |
| 3:F:2966[A]:SER:HB3 | 3:F:2977[A]:CYS:HB2 | 1.78 | 0.60 |
| 3:F:2966[B]:SER:HB3 | 3:a:2982[B]:MET:CE | 2.30 | 0.60 |
| 3:F:3025[B]:VAL:HG22 | 3:F:3025[B]:VAL:O | 2.00 | 0.60 |
| 3:F:3281[B]:PHE:CE1 | 3:F:3305[B]:ILE:HG21 | 2.36 | 0.60 |
| 3:F:3298[A]:ASN:CB | 3:F:3300[A]:LEU:N | 2.60 | 0.60 |
| 3:F:3298[A]:ASN:HD21 | 3:F:3301[A]:PRO:HA | 1.60 | 0.60 |
| 1:G:829:ALA:HA | 1:G:830:ASN:C | 2.27 | 0.60 |
| 3:I:3158[B]:PHE:H | 3:R:3153[B]:LYS:CE | 2.13 | 0.60 |
| 3:I:3281[A]:PHE:CE1 | 3:I:3305[A]:ILE:HG21 | 2.36 | 0.60 |
| 3:I:3284[B]:LYS:CD | 3:I:3285[B]:VAL:H | 2.10 | 0.60 |
| 3:I:3298[A]:ASN:CB | 3:I:3300[A]:LEU:N | 2.60 | 0.60 |
| 3:L:3169[B]:LYS:C | 3:L:3172[B]:SER:HG | 2.03 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:392:PRO:O | 1:M:395:THR:OG1 | 2.18 | 0.60 |
| 1:M:896:HIS:HB2 | 1:M:905:TRP:CG | 2.36 | 0.60 |
| 3:O:2963[B]:MET:CE | 3:X:2975[B]:PHE:CB | 2.56 | 0.60 |
| 3:O:3156[B]:MET:HA | 3:O:3157[B]:PRO:C | 2.26 | 0.60 |
| 3:O:3194[A]:GLY:O | 3:O:3195[A]:MET:HG2 | 2.01 | 0.60 |
| 3:O:3298[A]:ASN:ND2 | 3:O:3301[A]:PRO:C | 2.60 | 0.60 |
| 3:O:3298[B]:ASN:HD21 | 3:O:3301[B]:PRO:HA | 1.60 | 0.60 |
| 3:R:2939[B]:ARG:HG3 | 3:R:2939[B]:ARG:HH11 | 1.66 | 0.60 |
| 3:R:3139[A]:LEU:HD22 | 3:R:3139[A]:LEU:N | 2.16 | 0.60 |
| 3:U:2964[A]:PRO:HG3 | 3:U:3040[A]:VAL:HG11 | 1.83 | 0.60 |
| 3:U:2964[B]:PRO:HG3 | 3:U:3040[B]:VAL:HG11 | 1.82 | 0.60 |
| 3:U:3200[B]:LEU:HD22 | 3:U:3204[B]:LEU:HD13 | 1.82 | 0.60 |
| 3:U:3276[A]:ASP:HB3 | 3:U:3278[A]:HIS:HB2 | 1.83 | 0.60 |
| 3:U:3281[A]:PHE:CE1 | 3:U:3305[A]:ILE:HG21 | 2.36 | 0.60 |
| 3:U:3281[B]:PHE:CE1 | 3:U:3305[B]:ILE:HG21 | 2.36 | 0.60 |
| 3:X:3281[B]:PHE:CE1 | 3:X:3305[B]:ILE:HG21 | 2.36 | 0.60 |
| 1:Y:1411:PHE:O | 1:Y:1475:ARG:NH2 | 2.29 | 0.60 |
| 1:Y:1655:SER:HB3 | 3:d:3007[B]:ILE:CG2 | 2.30 | 0.60 |
| 3:a:2998[B]:ASP:O | 3:a:3001[B]:LYS:HB2 | 2.02 | 0.60 |
| 2:c:2891:LEU:H | 2:c:2891:LEU:HD12 | 1.66 | 0.60 |
| 3:d:2948[B]:ASP:CB | 3:d:2949[B]:LYS:HA | 2.16 | 0.60 |
| 2:B:2166:LEU:HA | 2:B:2169:HIS:HB2 | 1.82 | 0.60 |
| 3:C:2972[B]:GLY:CA | 3:L:3090[B]:ASN:HB3 | 2.31 | 0.60 |
| 3:C:3139[B]:LEU:N | 3:C:3139[B]:LEU:HD22 | 2.16 | 0.60 |
| 3:C:3274[B]:ARG:HA | 3:C:3274[B]:ARG:NE | 2.16 | 0.60 |
| 3:C:3307[A]:PHE:HE1 | 3:C:3309[A]:PRO:CG | 2.08 | 0.60 |
| 2:E:2141:HIS:ND1 | 2:E:2141:HIS:O | 2.35 | 0.60 |
| 3:F:2979[B]:GLN:OE1 | 3:a:2977[B]:CYS:SG | 2.60 | 0.60 |
| 3:F:3191[A]:ASN:ND2 | 3:F:3191[A]:ASN:H | 1.99 | 0.60 |
| 3:F:3200[B]:LEU:HD22 | 3:F:3204[B]:LEU:HD13 | 1.83 | 0.60 |
| 3:F:3218[A]:LEU:O | 3:F:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 1:G:1138:ALA:HA | 1:G:1240:ILE:HG22 | 1.84 | 0.60 |
| 3:I:3139[B]:LEU:HD22 | 3:I:3139[B]:LEU:N | 2.16 | 0.60 |
| 1:J:133:LYS:HA | 1:J:133:LYS:HE3 | 1.82 | 0.60 |
| 3:L:2964[B]:PRO:HG3 | 3:L:3040[B]:VAL:HG11 | 1.82 | 0.60 |
| 3:L:3014[A]:TRP:CE3 | 3:L:3092[A]:ILE:HD12 | 2.37 | 0.60 |
| 3:O:2970[B]:PRO:CG | 3:X:2991[B]:LEU:CD1 | 2.80 | 0.60 |
| 3:O:3298[A]:ASN:CA | 3:O:3300[A]:LEU:HD23 | 2.31 | 0.60 |
| 2:Q:2303:ARG:NH2 | 2:Q:2372:GLU:O | 2.34 | 0.60 |
| 2:Q:2830:GLN:HB2 | 2:Q:2863:ARG:HH12 | 1.67 | 0.60 |
| 3:R:2998[A]:ASP:O | 3:R:3001[A]:LYS:HB2 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3182[B]:GLN:O | 3:R:3183[B]:LEU:HD12 | 2.02 | 0.60 |
| 1:S:871:GLN:NE2 | 1:S:964:ILE:HG13 | 2.13 | 0.60 |
| 1:S:1157:VAL:HB | 1:S:1217:ILE:HD13 | 1.84 | 0.60 |
| 2:T:2180:TRP:HB3 | 2:T:2184:MET:HE1 | 1.84 | 0.60 |
| 2:T:2800:LYS:C | 3:U:3023[A]:ILE:CD1 | 2.75 | 0.60 |
| 3:U:3218[A]:LEU:O | 3:U:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 3:U:3274[B]:ARG:HA | 3:U:3274[B]:ARG:NE | 2.16 | 0.60 |
| 3:X:2998[A]:ASP:O | 3:X:3001[A]:LYS:HB2 | 2.01 | 0.60 |
| 3:X:3104[A]:MET:SD | 3:X:3110[A]:THR:HG22 | 2.42 | 0.60 |
| 3:a:3025[A]:VAL:HG22 | 3:a:3025[A]:VAL:O | 2.00 | 0.60 |
| 3:a:3104[B]:MET:SD | 3:a:3110[B]:THR:HG22 | 2.42 | 0.60 |
| 3:a:3281[B]:PHE:CE1 | 3:a:3305[B]:ILE:HG21 | 2.36 | 0.60 |
| 3:a:3298[B]:ASN:CA | 3:a:3300[B]:LEU:HD23 | 2.31 | 0.60 |
| 1:b:324:PRO:HG2 | 1:b:376:ASN:ND2 | 2.16 | 0.60 |
| 2:c:2644:LEU:HD22 | 2:c:2687:ILE:HG22 | 1.84 | 0.60 |
| 2:c:2874:ASP:OD1 | 2:c:2874:ASP:N | 2.18 | 0.60 |
| 3:d:3147[A]:GLU:HG3 | 3:d:3149[A]:ASN:HD21 | 1.65 | 0.60 |
| 3:d:3194[A]:GLY:O | 3:d:3195[A]:MET:HG2 | 2.01 | 0.60 |
| 1:A:1156:LEU:HD13 | 1:A:1176:TYR:CZ | 2.36 | 0.60 |
| 3:C:2949[B]:LYS:HZ2 | 3:C:2950[B]:THR:HA | 1.66 | 0.60 |
| 3:C:2952[A]:ALA:N | 3:C:2953[A]:GLY:HA2 | 2.06 | 0.60 |
| 3:C:2998[A]:ASP:O | 3:C:3001[A]:LYS:HB2 | 2.01 | 0.60 |
| 3:C:3224[B]:GLN:HA | 3:L:3252[B]:TYR:CZ | 2.36 | 0.60 |
| 1:D:1304:ASP:OD2 | 1:D:1306:THR:OG1 | 2.20 | 0.60 |
| 2:E:2828:ASP:OD2 | 2:E:2830:GLN:NE2 | 2.35 | 0.60 |
| 3:F:2981[B]:GLY:N | 3:a:2968[B]:GLN:CD | 2.56 | 0.60 |
| 3:F:3182[B]:GLN:O | 3:F:3183[B]:LEU:HD12 | 2.02 | 0.60 |
| 3:F:3218[B]:LEU:O | 3:F:3219[B]:LEU:HD13 | 2.01 | 0.60 |
| 1:G:327:ASP:OD1 | 1:G:328:LYS:N | 2.32 | 0.60 |
| 3:I:2975[B]:PHE:HE2 | 3:R:2988[B]:TRP:CH2 | 2.19 | 0.60 |
| 3:I:3158[B]:PHE:H | 3:R:3153[B]:LYS:HE3 | 1.67 | 0.60 |
| 3:I:3200[A]:LEU:HD22 | 3:I:3204[A]:LEU:HD13 | 1.83 | 0.60 |
| 1:J:898:GLY:HA2 | 1:J:1186:TRP:HB2 | 1.84 | 0.60 |
| 3:L:3096[B]:VAL:HG11 | 3:L:3115[B]:LEU:HD13 | 1.81 | 0.60 |
| 3:L:3222[A]:ILE:HG13 | 3:L:3224[A]:GLN:HG2 | 1.84 | 0.60 |
| 1:M:126:GLY:CA | 1:M:127:GLU:HB3 | 2.31 | 0.60 |
| 1:M:757:VAL:HG21 | 1:M:781:ILE:HG22 | 1.83 | 0.60 |
| 1:M:881:GLN:HE21 | 1:M:888:ALA:HB3 | 1.65 | 0.60 |
| 3:O:2939[A]:ARG:HG3 | 3:O:2939[A]:ARG:HH11 | 1.67 | 0.60 |
| 3:O:2945[B]:VAL:HG22 | 3:O:2945[B]:VAL:O | 2.01 | 0.60 |
| 3:O:2964[B]:PRO:HG3 | 3:O:3040[B]:VAL:HG11 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3218[B]:LEU:O | 3:O:3219[B]:LEU:HD13 | 2.01 | 0.60 |
| 3:R:3182[A]:GLN:O | 3:R:3183[A]:LEU:HD12 | 2.02 | 0.60 |
| 2:T:2901:LEU:HB2 | 1:V:1074:ILE:HB | 1.84 | 0.60 |
| 3:U:2971[B]:ASP:N | 3:d:3090[B]:ASN:HD22 | 2.00 | 0.60 |
| 3:U:2975[B]:PHE:CZ | 3:d:3254[B]:MET:N | 2.69 | 0.60 |
| 3:U:2998[B]:ASP:O | 3:U:3001[B]:LYS:HB2 | 2.01 | 0.60 |
| 3:U:3124[A]:ASP:OD2 | 3:U:3187[A]:TYR:OH | 2.15 | 0.60 |
| 3:U:3147[B]:GLU:HG3 | 3:U:3149[B]:ASN:HD21 | 1.65 | 0.60 |
| 3:U:3222[A]:ILE:HG13 | 3:U:3224[A]:GLN:HG2 | 1.84 | 0.60 |
| 1:V:317:VAL:HG22 | 1:V:383:VAL:HG22 | 1.82 | 0.60 |
| 2:W:2394:VAL:H | 2:W:2448:THR:HG22 | 1.67 | 0.60 |
| 3:X:2998[B]:ASP:O | 3:X:3001[B]:LYS:HB2 | 2.01 | 0.60 |
| 3:X:3156[A]:MET:HA | 3:X:3157[A]:PRO:C | 2.26 | 0.60 |
| 3:X:3194[B]:GLY:O | 3:X:3195[B]:MET:HG2 | 2.01 | 0.60 |
| 3:a:3104[A]:MET:SD | 3:a:3110[A]:THR:HG22 | 2.42 | 0.60 |
| 1:b:736:MET:HG3 | 1:b:772:ARG:HD2 | 1.84 | 0.60 |
| 3:d:3135[A]:LYS:HG3 | 3:d:3141[A]:TYR:CD1 | 2.33 | 0.60 |
| 3:d:3156[B]:MET:HA | 3:d:3157[B]:PRO:C | 2.26 | 0.60 |
| 3:d:3276[B]:ASP:HB3 | 3:d:3278[B]:HIS:HB2 | 1.83 | 0.60 |
| 3:d:3281[A]:PHE:CE1 | 3:d:3305[A]:ILE:HG21 | 2.36 | 0.60 |
| 3:C:3025[B]:VAL:HG22 | 3:C:3025[B]:VAL:O | 2.00 | 0.60 |
| 3:C:3182[B]:GLN:O | 3:C:3183[B]:LEU:HD12 | 2.02 | 0.60 |
| 3:F:2948[B]:ASP:HB3 | 3:F:2953[B]:GLY:CA | 2.24 | 0.60 |
| 3:F:3023[A]:ILE:O | 3:F:3024[A]:LEU:C | 2.45 | 0.60 |
| 3:F:3104[B]:MET:SD | 3:F:3110[B]:THR:HG22 | 2.42 | 0.60 |
| 3:F:3156[A]:MET:HA | 3:F:3157[A]:PRO:C | 2.26 | 0.60 |
| 3:F:3169[B]:LYS:HD3 | 3:a:3148[B]:ILE:C | 2.24 | 0.60 |
| 3:F:3200[A]:LEU:HD22 | 3:F:3204[A]:LEU:HD13 | 1.83 | 0.60 |
| 3:F:3284[A]:LYS:CD | 3:F:3285[A]:VAL:H | 2.09 | 0.60 |
| 3:F:3298[A]:ASN:ND2 | 3:F:3301[A]:PRO:C | 2.60 | 0.60 |
| 1:G:448:SER:O | 1:G:450:LYS:NZ | 2.35 | 0.60 |
| 1:G:1414:THR:HG23 | 1:G:1477:LEU:HD13 | 1.84 | 0.60 |
| 2:H:2373:MET:HB3 | 2:H:2381:LEU:HD11 | 1.84 | 0.60 |
| 3:I:2945[B]:VAL:HG22 | 3:I:2945[B]:VAL:O | 2.01 | 0.60 |
| 3:I:3134[A]:GLN:O | 3:I:3135[A]:LYS:C | 2.44 | 0.60 |
| 3:I:3134[B]:GLN:O | 3:I:3135[B]:LYS:C | 2.44 | 0.60 |
| 3:I:3218[A]:LEU:O | 3:I:3219[A]:LEU:HD13 | 2.01 | 0.60 |
| 3:L:3023[B]:ILE:O | 3:L:3024[B]:LEU:C | 2.45 | 0.60 |
| 3:L:3288[A]:MET:CG | 3:L:3295[A]:LEU:HD21 | 2.32 | 0.60 |
| 3:L:3298[A]:ASN:ND2 | 3:L:3301[A]:PRO:C | 2.60 | 0.60 |
| 3:L:3298[B]:ASN:ND2 | 3:L:3301[B]:PRO:C | 2.60 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2939[B]:ARG:HH11 | 3:O:2939[B]:ARG:HG3 | 1.66 | 0.60 |
| 3:O:3135[B]:LYS:CB | 3:O:3141[B]:TYR:CD1 | 2.85 | 0.60 |
| 3:O:3147[B]:GLU:HG3 | 3:O:3149[B]:ASN:HD21 | 1.65 | 0.60 |
| 3:O:3197[B]:ILE:HD12 | 1:P:1617:LYS:O | 2.02 | 0.60 |
| 3:O:3212[A]:ARG:HH11 | 3:O:3212[A]:ARG:CG | 2.12 | 0.60 |
| 3:O:3222[A]:ILE:HG13 | 3:O:3224[A]:GLN:HG2 | 1.84 | 0.60 |
| 1:P:149:GLU:OE1 | 1:P:152:LYS:NZ | 2.28 | 0.60 |
| 2:Q:2722:GLN:NE2 | 2:Q:2769:PHE:O | 2.31 | 0.60 |
| 1:S:1074:ILE:HB | 2:W:2901:LEU:HB2 | 1.83 | 0.60 |
| 3:U:3104[B]:MET:SD | 3:U:3110[B]:THR:HG22 | 2.42 | 0.60 |
| 3:U:3139[B]:LEU:HD22 | 3:U:3139[B]:LEU:N | 2.16 | 0.60 |
| 3:U:3307[A]:PHE:HE1 | 3:U:3309[A]:PRO:CG | 2.08 | 0.60 |
| 2:W:2506:ARG:NE | 2:W:2578:GLU:OE2 | 2.29 | 0.60 |
| 2:W:2603:PRO:HG2 | 2:W:2606:LEU:HD12 | 1.84 | 0.60 |
| 3:X:2942[B]:LEU:CD1 | 3:X:3033[B]:PHE:CE1 | 2.85 | 0.60 |
| 3:X:3200[A]:LEU:HD22 | 3:X:3204[A]:LEU:HD13 | 1.83 | 0.60 |
| 3:X:3288[A]:MET:CG | 3:X:3295[A]:LEU:HD21 | 2.32 | 0.60 |
| 3:X:3298[A]:ASN:CB | 3:X:3300[A]:LEU:N | 2.60 | 0.60 |
| 1:Y:1063:ARG:HB3 | 1:Y:1065:LYS:HD2 | 1.84 | 0.60 |
| 3:a:2939[B]:ARG:HG3 | 3:a:2939[B]:ARG:HH11 | 1.66 | 0.60 |
| 3:a:2942[B]:LEU:CD1 | 3:a:3033[B]:PHE:CE1 | 2.85 | 0.60 |
| 3:a:3023[A]:ILE:O | 3:a:3024[A]:LEU:C | 2.45 | 0.60 |
| 3:a:3120[B]:HIS:C | 3:a:3122[B]:ASN:N | 2.55 | 0.60 |
| 3:a:3173[B]:THR:HG22 | 3:a:3174[B]:GLY:H | 1.67 | 0.60 |
| 3:d:2942[A]:LEU:CD1 | 3:d:3033[A]:PHE:CE1 | 2.85 | 0.60 |
| 3:d:2965[A]:LEU:CD1 | 3:d:2975[A]:PHE:H | 2.08 | 0.60 |
| 3:d:2998[A]:ASP:O | 3:d:3001[A]:LYS:HB2 | 2.01 | 0.60 |
| 3:d:3014[B]:TRP:CE3 | 3:d:3092[B]:ILE:HD12 | 2.37 | 0.60 |
| 3:d:3025[B]:VAL:HG22 | 3:d:3025[B]:VAL:O | 2.00 | 0.60 |
| 3:d:3104[A]:MET:SD | 3:d:3110[A]:THR:HG22 | 2.42 | 0.60 |
| 3:d:3182[A]:GLN:O | 3:d:3183[A]:LEU:HD12 | 2.02 | 0.60 |
| 3:d:3222[A]:ILE:HG13 | 3:d:3224[A]:GLN:HG2 | 1.84 | 0.60 |
| 3:d:3274[B]:ARG:HA | 3:d:3274[B]:ARG:NE | 2.16 | 0.60 |
| 3:C:3014[A]:TRP:CE3 | 3:C:3092[A]:ILE:HD12 | 2.37 | 0.60 |
| 3:C:3104[B]:MET:SD | 3:C:3110[B]:THR:HG22 | 2.42 | 0.60 |
| 3:C:3135[A]:LYS:CB | 3:C:3141[A]:TYR:CD1 | 2.85 | 0.60 |
| 3:C:3191[A]:ASN:ND2 | 3:C:3191[A]:ASN:H | 1.99 | 0.60 |
| 3:C:3274[A]:ARG:HA | 3:C:3274[A]:ARG:NE | 2.16 | 0.60 |
| 2:E:2564:PRO:HA | 2:E:2673:GLU:HG3 | 1.84 | 0.60 |
| 3:F:3090[B]:ASN:HB3 | 3:a:2972[B]:GLY:CA | 2.31 | 0.60 |
| 3:F:3104[A]:MET:SD | 3:F:3110[A]:THR:HG22 | 2.42 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3194[B]:GLY:O | 3:F:3195[B]:MET:HG2 | 2.01 | 0.60 |
| 3:I:2942[B]:LEU:CD1 | 3:I:3033[B]:PHE:CE1 | 2.85 | 0.60 |
| 3:I:3014[B]:TRP:CE3 | 3:I:3092[B]:ILE:HD12 | 2.37 | 0.60 |
| 3:I:3071[B]:PHE:O | 3:I:3074[B]:GLU:HB2 | 2.02 | 0.60 |
| 3:I:3104[B]:MET:SD | 3:I:3110[B]:THR:HG22 | 2.42 | 0.60 |
| 3:I:3196[A]:THR:OG1 | 1:J:416:ASN:ND2 | 2.34 | 0.60 |
| 3:L:2957[A]:ILE:HA | 3:L:2960[A]:PHE:HE1 | 1.64 | 0.60 |
| 1:P:1442:MET:HE1 | 1:P:1454:PHE:HA | 1.82 | 0.60 |
| 3:R:2942[B]:LEU:CD1 | 3:R:3033[B]:PHE:CE1 | 2.85 | 0.60 |
| 3:R:3096[A]:VAL:HG11 | 3:R:3115[A]:LEU:HD13 | 1.81 | 0.60 |
| 3:R:3281[A]:PHE:CE1 | 3:R:3305[A]:ILE:HG21 | 2.36 | 0.60 |
| 3:R:3298[B]:ASN:CB | 3:R:3300[B]:LEU:N | 2.60 | 0.60 |
| 1:S:212:ASN:OD1 | 1:S:215:ARG:NH1 | 2.35 | 0.60 |
| 1:S:832:LYS:HB2 | 1:S:834:ASP:OD1 | 2.02 | 0.60 |
| 3:U:2932[A]:PRO:CA | 3:U:2935[A]:ILE:HD12 | 2.31 | 0.60 |
| 3:U:2969[A]:TYR:CD2 | 3:U:2970[A]:PRO:CD | 2.85 | 0.60 |
| 3:U:3023[A]:ILE:O | 3:U:3024[A]:LEU:C | 2.45 | 0.60 |
| 3:U:3135[A]:LYS:CB | 3:U:3141[A]:TYR:CD1 | 2.85 | 0.60 |
| 3:U:3182[A]:GLN:O | 3:U:3183[A]:LEU:HD12 | 2.02 | 0.60 |
| 3:U:3222[B]:ILE:HG13 | 3:U:3224[B]:GLN:HG2 | 1.84 | 0.60 |
| 3:U:3254[B]:MET:C | 3:d:2975[B]:PHE:CE1 | 2.79 | 0.60 |
| 3:X:2930[A]:LEU:HD22 | 3:X:2930[A]:LEU:N | 2.02 | 0.60 |
| 3:X:2942[A]:LEU:CD1 | 3:X:3033[A]:PHE:CE1 | 2.85 | 0.60 |
| 3:X:3014[A]:TRP:CE3 | 3:X:3092[A]:ILE:HD12 | 2.37 | 0.60 |
| 3:X:3139[B]:LEU:N | 3:X:3139[B]:LEU:HD22 | 2.16 | 0.60 |
| 3:X:3162[B]:ASP:OD1 | 3:X:3162[B]:ASP:N | 2.31 | 0.60 |
| 3:X:3284[A]:LYS:HE2 | 3:X:3284[A]:LYS:CA | 2.30 | 0.60 |
| 3:a:3014[B]:TRP:CE3 | 3:a:3092[B]:ILE:HD12 | 2.37 | 0.60 |
| 3:a:3023[B]:ILE:O | 3:a:3024[B]:LEU:C | 2.45 | 0.60 |
| 3:a:3134[A]:GLN:O | 3:a:3135[A]:LYS:C | 2.44 | 0.60 |
| 3:a:3182[B]:GLN:O | 3:a:3183[B]:LEU:HD12 | 2.02 | 0.60 |
| 3:a:3298[B]:ASN:CB | 3:a:3300[B]:LEU:N | 2.60 | 0.60 |
| 3:d:2964[A]:PRO:HG3 | 3:d:3040[A]:VAL:HG11 | 1.82 | 0.60 |
| 3:d:2964[B]:PRO:HG3 | 3:d:3040[B]:VAL:HG11 | 1.82 | 0.60 |
| 3:d:3156[A]:MET:HA | 3:d:3157[A]:PRO:C | 2.26 | 0.60 |
| 3:d:3173[A]:THR:HG22 | 3:d:3174[A]:GLY:H | 1.67 | 0.60 |
| 3:d:3191[B]:ASN:ND2 | 3:d:3191[B]:ASN:H | 1.99 | 0.60 |
| 3:d:3288[A]:MET:CG | 3:d:3295[A]:LEU:HD21 | 2.32 | 0.60 |
| 3:d:3298[A]:ASN:ND2 | 3:d:3301[A]:PRO:C | 2.60 | 0.60 |
| 3:d:3298[B]:ASN:ND2 | 3:d:3301[B]:PRO:C | 2.60 | 0.60 |
| 1:A:7:VAL:HG13 | 1:A:104:LEU:HD22 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:483:GLY:HA3 | 1:A:771:TRP:CE3 | 2.37 | 0.59 |
| 3:C:3155[B]:MET:HE2 | 3:L:3153[B]:LYS:CD | 2.32 | 0.59 |
| 3:C:3218[B]:LEU:O | 3:C:3219[B]:LEU:HD13 | 2.01 | 0.59 |
| 3:C:3298[A]:ASN:ND2 | 3:C:3301[A]:PRO:C | 2.60 | 0.59 |
| 3:C:3298[B]:ASN:ND2 | 3:C:3301[B]:PRO:C | 2.60 | 0.59 |
| 1:D:81:VAL:HA | 1:D:85:SER:HB3 | 1.84 | 0.59 |
| 1:D:321:LEU:HB2 | 1:D:338:ALA:HB2 | 1.83 | 0.59 |
| 3:F:2942[A]:LEU:CD1 | 3:F:3033[A]:PHE:CE1 | 2.85 | 0.59 |
| 3:F:2998[B]:ASP:O | 3:F:3001[B]:LYS:HB2 | 2.01 | 0.59 |
| 3:F:3134[A]:GLN:O | 3:F:3135[A]:LYS:C | 2.44 | 0.59 |
| 3:F:3150[B]:LYS:HE2 | 3:a:3157[B]:PRO:HB2 | 1.84 | 0.59 |
| 1:G:128:ILE:HG22 | 1:G:202:TYR:CG | 2.37 | 0.59 |
| 1:G:567:LEU:HD22 | 1:G:568:PHE:H | 1.67 | 0.59 |
| 3:I:2932[B]:PRO:CA | 3:I:2935[B]:ILE:HD12 | 2.30 | 0.59 |
| 3:I:3014[A]:TRP:CE3 | 3:I:3092[A]:ILE:HD12 | 2.37 | 0.59 |
| 3:I:3023[A]:ILE:O | 3:I:3024[A]:LEU:C | 2.45 | 0.59 |
| 3:I:3038[A]:ILE:HG12 | 3:I:3112[A]:TYR:CE2 | 2.35 | 0.59 |
| 3:I:3071[A]:PHE:O | 3:I:3074[A]:GLU:HB2 | 2.02 | 0.59 |
| 3:I:3096[B]:VAL:HG11 | 3:I:3115[B]:LEU:HD13 | 1.81 | 0.59 |
| 3:I:3172[B]:SER:HB3 | 3:R:3150[B]:LYS:HA | 1.82 | 0.59 |
| 1:J:450:LYS:NZ | 1:J:505:ARG:HH21 | 2.00 | 0.59 |
| 2:K:2545:SER:HB3 | 2:K:2547:MET:N | 2.17 | 0.59 |
| 3:L:3173[A]:THR:HB | 3:L:3176[A]:LYS:HG2 | 1.81 | 0.59 |
| 3:L:3276[B]:ASP:HB3 | 3:L:3278[B]:HIS:HB2 | 1.83 | 0.59 |
| 3:L:3281[B]:PHE:CE1 | 3:L:3305[B]:ILE:HG21 | 2.36 | 0.59 |
| 3:L:3293[B]:LYS:CB | 3:L:3294[B]:SER:CB | 2.54 | 0.59 |
| 3:O:2965[B]:LEU:CD2 | 3:X:3156[B]:MET:HE3 | 2.32 | 0.59 |
| 3:O:3135[A]:LYS:CB | 3:O:3141[A]:TYR:CD1 | 2.85 | 0.59 |
| 3:O:3200[A]:LEU:HD22 | 3:O:3204[A]:LEU:HD13 | 1.83 | 0.59 |
| 3:O:3200[B]:LEU:HD22 | 3:O:3204[B]:LEU:HD13 | 1.83 | 0.59 |
| 3:O:3222[B]:ILE:HG13 | 3:O:3224[B]:GLN:HG2 | 1.84 | 0.59 |
| 1:P:1372:ILE:HD11 | 1:S:1392:ASP:HB2 | 1.84 | 0.59 |
| 3:R:2998[B]:ASP:O | 3:R:3001[B]:LYS:HB2 | 2.02 | 0.59 |
| 3:R:3162[A]:ASP:OD1 | 3:R:3162[A]:ASP:N | 2.31 | 0.59 |
| 3:R:3288[A]:MET:CG | 3:R:3295[A]:LEU:HD21 | 2.32 | 0.59 |
| 2:T:2889:ALA:N | 2:T:2890:VAL:HA | 2.16 | 0.59 |
| 3:U:3071[B]:PHE:O | 3:U:3074[B]:GLU:HB2 | 2.02 | 0.59 |
| 3:U:3147[A]:GLU:HG3 | 3:U:3149[A]:ASN:HD21 | 1.65 | 0.59 |
| 3:U:3153[B]:LYS:CG | 3:d:2979[B]:GLN:NE2 | 2.65 | 0.59 |
| 3:U:3182[B]:GLN:O | 3:U:3183[B]:LEU:HD12 | 2.02 | 0.59 |
| 3:U:3254[B]:MET:HG2 | 3:d:3255[B]:PRO:HD2 | 1.82 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:567:LEU:HA | 1:V:571:PRO:HD2 | 1.84 | 0.59 |
| 2:W:2344:LEU:HA | 2:W:2345:ASN:C | 2.26 | 0.59 |
| 3:X:3182[A]:GLN:O | 3:X:3183[A]:LEU:HD12 | 2.02 | 0.59 |
| 1:Y:462:HIS:HA | 1:Y:490:TRP:HH2 | 1.67 | 0.59 |
| 1:Y:1348:TRP:CD1 | 1:Y:1403:LEU:HD13 | 2.37 | 0.59 |
| 3:a:2945[B]:VAL:HG22 | 3:a:2945[B]:VAL:O | 2.01 | 0.59 |
| 3:a:3135[B]:LYS:CB | 3:a:3141[B]:TYR:CD1 | 2.85 | 0.59 |
| 3:a:3274[B]:ARG:HA | 3:a:3274[B]:ARG:NE | 2.16 | 0.59 |
| 3:a:3288[B]:MET:CG | 3:a:3295[B]:LEU:HD21 | 2.32 | 0.59 |
| 3:a:3293[B]:LYS:CB | 3:a:3294[B]:SER:CB | 2.54 | 0.59 |
| 1:b:330:GLN:O | 1:b:332:ASP:N | 2.31 | 0.59 |
| 2:c:2800:LYS:O | 3:d:3023[A]:ILE:HD13 | 2.00 | 0.59 |
| 3:d:2939[B]:ARG:HH11 | 3:d:2939[B]:ARG:HG3 | 1.66 | 0.59 |
| 3:d:3104[B]:MET:SD | 3:d:3110[B]:THR:HG22 | 2.42 | 0.59 |
| 3:d:3183[B]:LEU:N | 3:d:3184[B]:ASN:HA | 2.11 | 0.59 |
| 3:d:3200[B]:LEU:HD22 | 3:d:3204[B]:LEU:HD13 | 1.82 | 0.59 |
| 1:A:69:HIS:NE2 | 9:A:5001:CUO:O1 | 2.35 | 0.59 |
| 1:A:1210:LYS:HG3 | 2:E:2743:ALA:HB3 | 1.84 | 0.59 |
| 3:C:3071[A]:PHE:O | 3:C:3074[A]:GLU:HB2 | 2.02 | 0.59 |
| 3:C:3222[B]:ILE:HG13 | 3:C:3224[B]:GLN:HG2 | 1.84 | 0.59 |
| 3:C:3293[A]:LYS:CB | 3:C:3294[A]:SER:CB | 2.54 | 0.59 |
| 3:F:2975[B]:PHE:CZ | 3:a:2961[B]:HIS:CA | 2.73 | 0.59 |
| 3:F:3014[B]:TRP:CE3 | 3:F:3092[B]:ILE:HD12 | 2.37 | 0.59 |
| 3:F:3182[A]:GLN:O | 3:F:3183[A]:LEU:HD12 | 2.02 | 0.59 |
| 3:I:2942[A]:LEU:CD1 | 3:I:3033[A]:PHE:CE1 | 2.85 | 0.59 |
| 3:I:3038[B]:ILE:HG22 | 3:I:3041[B]:ALA:H | 1.65 | 0.59 |
| 3:I:3156[B]:MET:HA | 3:I:3157[B]:PRO:C | 2.26 | 0.59 |
| 3:I:3276[B]:ASP:HB3 | 3:I:3278[B]:HIS:HB2 | 1.83 | 0.59 |
| 2:K:2545:SER:HA | 2:K:2546:LEU:CG | 2.31 | 0.59 |
| 3:L:2939[B]:ARG:HH11 | 3:L:2939[B]:ARG:HG3 | 1.66 | 0.59 |
| 3:L:3014[B]:TRP:CE3 | 3:L:3092[B]:ILE:HD12 | 2.37 | 0.59 |
| 3:L:3023[A]:ILE:O | 3:L:3024[A]:LEU:C | 2.45 | 0.59 |
| 3:L:3135[B]:LYS:CB | 3:L:3141[B]:TYR:CD1 | 2.85 | 0.59 |
| 2:N:2644:LEU:HD22 | 2:N:2687:ILE:HG22 | 1.82 | 0.59 |
| 3:O:2949[A]:LYS:HZ2 | 3:O:2950[A]:THR:HA | 1.67 | 0.59 |
| 3:R:3274[A]:ARG:HA | 3:R:3274[A]:ARG:NE | 2.16 | 0.59 |
| 3:R:3298[A]:ASN:ND2 | 3:R:3301[A]:PRO:C | 2.60 | 0.59 |
| 3:R:3298[A]:ASN:CA | 3:R:3300[A]:LEU:HD23 | 2.31 | 0.59 |
| 3:R:3298[B]:ASN:CA | 3:R:3300[B]:LEU:HD23 | 2.31 | 0.59 |
| 3:U:3096[A]:VAL:HG11 | 3:U:3115[A]:LEU:HD13 | 1.81 | 0.59 |
| 3:U:3254[B]:MET:HG3 | 3:d:2975[B]:PHE:CZ | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3298[B]:ASN:CA | 3:U:3300[B]:LEU:HD23 | 2.31 | 0.59 |
| 3:X:2939[A]:ARG:HH11 | 3:X:2939[A]:ARG:HG3 | 1.67 | 0.59 |
| 3:X:3071[B]:PHE:O | 3:X:3074[B]:GLU:HB2 | 2.02 | 0.59 |
| 1:Y:416:ASN:ND2 | 3:d:3196[A]:THR:HG21 | 2.16 | 0.59 |
| 3:a:2969[A]:TYR:CD2 | 3:a:2970[A]:PRO:CD | 2.85 | 0.59 |
| 1:b:447:MET:HA | 1:b:455:TYR:CB | 2.32 | 0.59 |
| 3:d:2930[B]:LEU:H | 3:d:2930[B]:LEU:CD2 | 1.98 | 0.59 |
| 3:d:3134[A]:GLN:O | 3:d:3135[A]:LYS:C | 2.44 | 0.59 |
| 3:d:3194[B]:GLY:O | 3:d:3195[B]:MET:HG2 | 2.01 | 0.59 |
| 2:B:2722:GLN:NE2 | 2:B:2769:PHE:O | 2.32 | 0.59 |
| 3:C:2969[B]:TYR:CZ | 3:L:3120[B]:HIS:CD2 | 2.71 | 0.59 |
| 3:C:3173[B]:THR:HG22 | 3:C:3174[B]:GLY:H | 1.67 | 0.59 |
| 3:C:3249[B]:GLY:HA2 | 3:L:2974[B]:ALA:O | 1.90 | 0.59 |
| 1:D:942:VAL:HG21 | 1:D:1041:ILE:HD11 | 1.84 | 0.59 |
| 3:F:2980[B]:HIS:N | 3:a:2968[B]:GLN:O | 2.33 | 0.59 |
| 3:F:3132[B]:ALA:CB | 3:F:3197[B]:ILE:HD13 | 2.33 | 0.59 |
| 3:F:3135[A]:LYS:CB | 3:F:3141[A]:TYR:CD1 | 2.85 | 0.59 |
| 3:F:3135[B]:LYS:CB | 3:F:3141[B]:TYR:CD1 | 2.85 | 0.59 |
| 3:F:3155[B]:MET:SD | 3:a:3154[B]:PRO:CG | 2.88 | 0.59 |
| 3:F:3160[B]:SER:CB | 3:a:3150[B]:LYS:HZ2 | 1.91 | 0.59 |
| 3:F:3274[B]:ARG:HA | 3:F:3274[B]:ARG:NE | 2.16 | 0.59 |
| 3:F:3298[B]:ASN:CA | 3:F:3300[B]:LEU:HD23 | 2.31 | 0.59 |
| 3:I:2972[B]:GLY:C | 3:R:3090[B]:ASN:HB3 | 2.26 | 0.59 |
| 3:I:2989[B]:HIS:CE1 | 3:R:2970[B]:PRO:CD | 2.84 | 0.59 |
| 3:I:3135[A]:LYS:CB | 3:I:3141[A]:TYR:CD1 | 2.85 | 0.59 |
| 3:I:3153[B]:LYS:C | 3:R:3155[B]:MET:CB | 2.74 | 0.59 |
| 3:I:3153[B]:LYS:HB3 | 3:R:3155[B]:MET:C | 2.27 | 0.59 |
| 3:I:3169[B]:LYS:CD | 3:R:3148[B]:ILE:C | 2.64 | 0.59 |
| 3:I:3191[B]:ASN:ND2 | 3:I:3191[B]:ASN:H | 1.99 | 0.59 |
| 3:I:3222[B]:ILE:HG13 | 3:I:3224[B]:GLN:HG2 | 1.84 | 0.59 |
| 3:I:3251[B]:ASP:HB2 | 3:R:3251[B]:ASP:CB | 2.09 | 0.59 |
| 1:J:602:THR:O | 1:J:605:SER:OG | 2.20 | 0.59 |
| 3:L:2949[A]:LYS:HZ2 | 3:L:2950[A]:THR:HA | 1.66 | 0.59 |
| 3:L:3104[B]:MET:SD | 3:L:3110[B]:THR:HG22 | 2.42 | 0.59 |
| 3:L:3139[B]:LEU:N | 3:L:3139[B]:LEU:HD22 | 2.16 | 0.59 |
| 3:L:3217[B]:PHE:HE1 | 3:L:3230[B]:PHE:HZ | 0.80 | 0.59 |
| 3:L:3298[A]:ASN:CB | 3:L:3300[A]:LEU:N | 2.60 | 0.59 |
| 3:O:2970[B]:PRO:O | 3:X:2989[B]:HIS:CA | 2.35 | 0.59 |
| 3:O:3156[A]:MET:HA | 3:O:3157[A]:PRO:C | 2.26 | 0.59 |
| 3:O:3157[B]:PRO:HA | 3:X:3152[B]:LYS:N | 2.16 | 0.59 |
| 3:R:2969[A]:TYR:CD2 | 3:R:2970[A]:PRO:CD | 2.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3071[A]:PHE:O | 3:R:3074[A]:GLU:HB2 | 2.02 | 0.59 |
| 3:R:3156[A]:MET:HA | 3:R:3157[A]:PRO:C | 2.26 | 0.59 |
| 3:R:3188[A]:ASP:N | 3:R:3188[A]:ASP:OD2 | 2.36 | 0.59 |
| 3:R:3217[B]:PHE:HE1 | 3:R:3230[B]:PHE:HZ | 0.80 | 0.59 |
| 3:R:3276[A]:ASP:HB3 | 3:R:3278[A]:HIS:HB2 | 1.83 | 0.59 |
| 3:U:2970[B]:PRO:HB3 | 3:d:2985[B]:PHE:CD2 | 2.37 | 0.59 |
| 3:U:3276[B]:ASP:HB3 | 3:U:3278[B]:HIS:HB2 | 1.83 | 0.59 |
| 1:V:760:ILE:HG21 | 1:V:777:TYR:HE2 | 1.67 | 0.59 |
| 1:V:830:ASN:OD1 | 1:V:830:ASN:N | 2.34 | 0.59 |
| 3:X:2928[A]:ASN:N | 3:X:2930[A]:LEU:HD21 | 2.18 | 0.59 |
| 3:X:3024[B]:LEU:O | 3:X:3031[B]:ASN:ND2 | 2.36 | 0.59 |
| 3:X:3104[B]:MET:SD | 3:X:3110[B]:THR:HG22 | 2.42 | 0.59 |
| 3:X:3134[A]:GLN:O | 3:X:3135[A]:LYS:C | 2.44 | 0.59 |
| 3:X:3218[B]:LEU:O | 3:X:3219[B]:LEU:HD13 | 2.01 | 0.59 |
| 2:Z:2806:ALA:HB2 | 2:Z:2856:ILE:HD11 | 1.84 | 0.59 |
| 3:a:2964[A]:PRO:HG3 | 3:a:3040[A]:VAL:HG11 | 1.82 | 0.59 |
| 3:a:3014[A]:TRP:CE3 | 3:a:3092[A]:ILE:HD12 | 2.37 | 0.59 |
| 3:a:3276[A]:ASP:HB3 | 3:a:3278[A]:HIS:HB2 | 1.83 | 0.59 |
| 3:d:2945[B]:VAL:HG22 | 3:d:2945[B]:VAL:O | 2.01 | 0.59 |
| 3:d:2969[A]:TYR:CD2 | 3:d:2970[A]:PRO:HG2 | 2.38 | 0.59 |
| 3:d:2998[B]:ASP:O | 3:d:3001[B]:LYS:HB2 | 2.01 | 0.59 |
| 3:d:3071[B]:PHE:O | 3:d:3074[B]:GLU:HB2 | 2.02 | 0.59 |
| 1:A:558:HIS:ND1 | 1:A:558:HIS:O | 2.35 | 0.59 |
| 3:C:3071[B]:PHE:O | 3:C:3074[B]:GLU:HB2 | 2.02 | 0.59 |
| 3:C:3104[A]:MET:SD | 3:C:3110[A]:THR:HG22 | 2.42 | 0.59 |
| 3:C:3135[B]:LYS:CB | 3:C:3141[B]:TYR:CD1 | 2.85 | 0.59 |
| 3:C:3152[B]:LYS:CG | 3:L:3169[B]:LYS:O | 2.40 | 0.59 |
| 3:C:3174[B]:GLY:N | 3:L:3154[B]:PRO:CD | 2.62 | 0.59 |
| 3:C:3191[B]:ASN:ND2 | 3:C:3191[B]:ASN:H | 1.99 | 0.59 |
| 3:F:2928[A]:ASN:N | 3:F:2930[A]:LEU:HD21 | 2.18 | 0.59 |
| 3:F:2969[A]:TYR:CD2 | 3:F:2970[A]:PRO:CD | 2.85 | 0.59 |
| 3:F:2983[B]:VAL:CB | 3:a:3160[B]:SER:HA | 2.33 | 0.59 |
| 1:G:330:GLN:O | 1:G:332:ASP:N | 2.35 | 0.59 |
| 1:G:898:GLY:N | 1:G:899:MET:HA | 2.18 | 0.59 |
| 3:I:2985[B]:PHE:CE2 | 3:R:2968[B]:GLN:O | 2.54 | 0.59 |
| 3:I:3024[A]:LEU:O | 3:I:3031[A]:ASN:ND2 | 2.36 | 0.59 |
| 3:I:3155[B]:MET:C | 3:R:3153[B]:LYS:HD2 | 2.26 | 0.59 |
| 3:I:3218[B]:LEU:O | 3:I:3219[B]:LEU:HD13 | 2.01 | 0.59 |
| 3:I:3255[B]:PRO:HB2 | 3:R:2959[B]:SER:HB3 | 1.74 | 0.59 |
| 3:I:3255[B]:PRO:CG | 3:R:2959[B]:SER:CA | 2.80 | 0.59 |
| 3:L:3134[A]:GLN:O | 3:L:3135[A]:LYS:C | 2.44 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3222[B]:ILE:HG13 | 3:L:3224[B]:GLN:HG2 | 1.84 | 0.59 |
| 3:L:3276[A]:ASP:HB3 | 3:L:3278[A]:HIS:HB2 | 1.83 | 0.59 |
| 1:M:67:MET:HE1 | 1:M:233:PRO:HG2 | 1.84 | 0.59 |
| 2:N:2556:TYR:CE1 | 2:N:2845:PRO:HD2 | 2.30 | 0.59 |
| 3:O:2928[B]:ASN:N | 3:O:2930[B]:LEU:HD21 | 2.17 | 0.59 |
| 3:O:2945[A]:VAL:HG22 | 3:O:2945[A]:VAL:O | 2.01 | 0.59 |
| 3:O:3024[A]:LEU:O | 3:O:3031[A]:ASN:ND2 | 2.36 | 0.59 |
| 3:O:3071[A]:PHE:O | 3:O:3074[A]:GLU:HB2 | 2.02 | 0.59 |
| 3:O:3182[A]:GLN:O | 3:O:3183[A]:LEU:HD12 | 2.02 | 0.59 |
| 3:O:3281[A]:PHE:CE1 | 3:O:3305[A]:ILE:HG21 | 2.36 | 0.59 |
| 3:R:2935[A]:ILE:HD13 | 3:R:2935[A]:ILE:N | 2.18 | 0.59 |
| 3:R:2945[A]:VAL:HG22 | 3:R:2945[A]:VAL:O | 2.01 | 0.59 |
| 3:R:2945[B]:VAL:HG22 | 3:R:2945[B]:VAL:O | 2.01 | 0.59 |
| 3:R:3024[A]:LEU:O | 3:R:3031[A]:ASN:ND2 | 2.36 | 0.59 |
| 3:R:3104[A]:MET:SD | 3:R:3110[A]:THR:HG22 | 2.42 | 0.59 |
| 3:R:3284[B]:LYS:CD | 3:R:3285[B]:VAL:H | 2.10 | 0.59 |
| 1:S:1358:LEU:HD23 | 1:S:1456:LEU:HD21 | 1.83 | 0.59 |
| 2:T:2094:ARG:HH21 | 2:W:2094:ARG:HH21 | 1.49 | 0.59 |
| 3:U:2968[B]:GLN:N | 3:d:3256[B]:TRP:CB | 2.46 | 0.59 |
| 3:U:3134[A]:GLN:O | 3:U:3135[A]:LYS:C | 2.44 | 0.59 |
| 3:U:3154[B]:PRO:HD2 | 3:d:2984[B]:THR:HG21 | 1.81 | 0.59 |
| 3:U:3162[B]:ASP:CB | 3:d:3260[B]:ARG:CZ | 2.81 | 0.59 |
| 3:U:3188[B]:ASP:N | 3:U:3188[B]:ASP:OD2 | 2.36 | 0.59 |
| 3:U:3191[A]:ASN:ND2 | 3:U:3191[A]:ASN:H | 1.99 | 0.59 |
| 3:U:3298[B]:ASN:ND2 | 3:U:3301[B]:PRO:C | 2.60 | 0.59 |
| 3:X:3001[A]:LYS:HE3 | 3:X:3002[A]:ALA:HB2 | 1.85 | 0.59 |
| 3:X:3157[A]:PRO:O | 3:X:3160[A]:SER:N | 2.30 | 0.59 |
| 3:X:3222[A]:ILE:HG13 | 3:X:3224[A]:GLN:HG2 | 1.84 | 0.59 |
| 3:X:3222[B]:ILE:HG13 | 3:X:3224[B]:GLN:HG2 | 1.84 | 0.59 |
| 3:X:3281[A]:PHE:CE1 | 3:X:3305[A]:ILE:HG21 | 2.36 | 0.59 |
| 3:a:2928[A]:ASN:N | 3:a:2930[A]:LEU:HD21 | 2.17 | 0.59 |
| 3:a:3001[A]:LYS:HE3 | 3:a:3002[A]:ALA:HB2 | 1.85 | 0.59 |
| 3:a:3222[B]:ILE:HG13 | 3:a:3224[B]:GLN:HG2 | 1.84 | 0.59 |
| 3:a:3298[A]:ASN:ND2 | 3:a:3301[A]:PRO:C | 2.60 | 0.59 |
| 3:a:3298[A]:ASN:HD21 | 3:a:3301[A]:PRO:HA | 1.60 | 0.59 |
| 3:d:2961[A]:HIS:CE1 | 3:d:2980[A]:HIS:NE2 | 2.57 | 0.59 |
| 2:B:2571:ARG:NH1 | 2:B:2771:TYR:HB3 | 2.18 | 0.59 |
| 3:C:2939[A]:ARG:HG3 | 3:C:2939[A]:ARG:HH11 | 1.66 | 0.59 |
| 3:C:3182[A]:GLN:O | 3:C:3183[A]:LEU:HD12 | 2.02 | 0.59 |
| 3:C:3255[B]:PRO:HB3 | 3:L:2964[B]:PRO:C | 2.25 | 0.59 |
| 1:D:142:ARG:NH1 | 1:D:340:GLN:HE22 | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:899:MET:HE2 | 1:D:1012:GLU:CD | 2.26 | 0.59 |
| 2:E:2218:SER:HB3 | 2:E:2221:THR:HG23 | 1.84 | 0.59 |
| 3:F:3096[A]:VAL:HG11 | 3:F:3115[A]:LEU:HD13 | 1.81 | 0.59 |
| 3:F:3147[B]:GLU:HG3 | 3:F:3149[B]:ASN:HD21 | 1.65 | 0.59 |
| 3:F:3149[B]:ASN:ND2 | 3:a:3163[B]:ASN:ND2 | 2.49 | 0.59 |
| 3:F:3156[B]:MET:HB3 | 3:a:2982[B]:MET:CG | 2.31 | 0.59 |
| 1:G:1207:TYR:O | 1:G:1211:TYR:OH | 2.16 | 0.59 |
| 3:I:2928[A]:ASN:N | 3:I:2930[A]:LEU:HD21 | 2.17 | 0.59 |
| 3:I:3182[B]:GLN:O | 3:I:3183[B]:LEU:HD12 | 2.02 | 0.59 |
| 3:I:3274[B]:ARG:HA | 3:I:3274[B]:ARG:NE | 2.16 | 0.59 |
| 2:K:2252:GLU:O | 2:K:2389:ARG:NH2 | 2.35 | 0.59 |
| 3:L:2945[B]:VAL:HG22 | 3:L:2945[B]:VAL:O | 2.01 | 0.59 |
| 3:L:2998[A]:ASP:O | 3:L:3001[A]:LYS:HB2 | 2.01 | 0.59 |
| 3:L:3182[B]:GLN:O | 3:L:3183[B]:LEU:HD12 | 2.02 | 0.59 |
| 3:L:3191[B]:ASN:ND2 | 3:L:3191[B]:ASN:H | 2.00 | 0.59 |
| 1:M:492:ARG:HD2 | 1:M:692:VAL:HG13 | 1.85 | 0.59 |
| 3:O:3134[B]:GLN:O | 3:O:3135[B]:LYS:C | 2.44 | 0.59 |
| 3:O:3135[B]:LYS:HG3 | 3:O:3141[B]:TYR:CD1 | 2.33 | 0.59 |
| 3:O:3279[B]:ASP:OD1 | 3:O:3279[B]:ASP:N | 2.25 | 0.59 |
| 3:R:2942[A]:LEU:CD1 | 3:R:3033[A]:PHE:CE1 | 2.85 | 0.59 |
| 3:U:2935[A]:ILE:HD13 | 3:U:2935[A]:ILE:N | 2.18 | 0.59 |
| 3:U:3257[B]:ALA:HB2 | 3:d:2974[B]:ALA:N | 2.17 | 0.59 |
| 1:V:402:THR:HG23 | 1:V:659:CYS:HA | 1.84 | 0.59 |
| 1:V:673:PHE:HB3 | 1:V:677:LEU:HB2 | 1.84 | 0.59 |
| 2:W:2856:ILE:HG22 | 2:W:2859:VAL:HB | 1.85 | 0.59 |
| 3:X:2969[A]:TYR:CD2 | 3:X:2970[A]:PRO:CD | 2.85 | 0.59 |
| 1:Y:898:GLY:N | 1:Y:899:MET:HA | 2.16 | 0.59 |
| 1:Y:1286:ARG:NH2 | 1:Y:1333:GLU:OE2 | 2.35 | 0.59 |
| 3:a:2948[A]:ASP:CB | 3:a:2949[A]:LYS:HA | 2.16 | 0.59 |
| 3:a:2969[A]:TYR:CD2 | 3:a:2970[A]:PRO:HG2 | 2.38 | 0.59 |
| 1:b:1492:PRO:HB2 | 1:b:1497:SER:HB3 | 1.83 | 0.59 |
| 2:c:2124:SER:HB2 | 2:c:2129:PRO:HG2 | 1.83 | 0.59 |
| 2:c:2141:HIS:ND1 | 2:c:2141:HIS:O | 2.35 | 0.59 |
| 3:d:3023[B]:ILE:O | 3:d:3024[B]:LEU:C | 2.45 | 0.59 |
| 3:d:3288[B]:MET:CG | 3:d:3295[B]:LEU:HD21 | 2.32 | 0.59 |
| 3:C:2964[B]:PRO:HG3 | 3:C:3040[B]:VAL:HG11 | 1.82 | 0.59 |
| 3:C:3038[A]:ILE:HG12 | 3:C:3112[A]:TYR:CE2 | 2.35 | 0.59 |
| 3:C:3120[A]:HIS:C | 3:C:3122[A]:ASN:N | 2.55 | 0.59 |
| 3:F:2945[B]:VAL:HG22 | 3:F:2945[B]:VAL:O | 2.01 | 0.59 |
| 3:F:2949[B]:LYS:HZ2 | 3:F:2950[B]:THR:HA | 1.67 | 0.59 |
| 3:F:3024[A]:LEU:O | 3:F:3031[A]:ASN:ND2 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3139[A]:LEU:N | 3:F:3139[A]:LEU:HD22 | 2.16 | 0.59 |
| 3:F:3155[B]:MET:CG | 3:a:3154[B]:PRO:CD | 2.78 | 0.59 |
| 3:F:3155[B]:MET:HE3 | 3:a:3156[B]:MET:HG2 | 1.84 | 0.59 |
| 3:F:3157[B]:PRO:N | 3:a:2982[B]:MET:SD | 2.74 | 0.59 |
| 3:F:3160[B]:SER:HA | 3:a:2983[B]:VAL:N | 2.09 | 0.59 |
| 3:F:3160[B]:SER:O | 3:a:3147[B]:GLU:HG3 | 2.01 | 0.59 |
| 3:F:3284[A]:LYS:HE2 | 3:F:3284[A]:LYS:CA | 2.30 | 0.59 |
| 3:F:3307[A]:PHE:HE1 | 3:F:3309[A]:PRO:CG | 2.08 | 0.59 |
| 3:I:2969[A]:TYR:CD2 | 3:I:2970[A]:PRO:HG2 | 2.38 | 0.59 |
| 3:I:2998[A]:ASP:O | 3:I:3001[A]:LYS:HB2 | 2.02 | 0.59 |
| 3:I:3023[B]:ILE:O | 3:I:3024[B]:LEU:C | 2.45 | 0.59 |
| 3:I:3147[B]:GLU:H | 3:R:3161[B]:GLU:HA | 1.66 | 0.59 |
| 3:I:3150[B]:LYS:O | 3:R:3159[B]:SER:CB | 2.48 | 0.59 |
| 3:I:3169[B]:LYS:HG2 | 3:R:3151[B]:LEU:N | 2.06 | 0.59 |
| 3:I:3255[B]:PRO:CG | 3:R:2959[B]:SER:HA | 2.31 | 0.59 |
| 3:I:3274[A]:ARG:NE | 3:I:3274[A]:ARG:HA | 2.16 | 0.59 |
| 3:I:3288[B]:MET:CG | 3:I:3295[B]:LEU:HD21 | 2.32 | 0.59 |
| 3:I:3298[A]:ASN:CA | 3:I:3300[A]:LEU:HD23 | 2.31 | 0.59 |
| 2:K:2509:ILE:HD11 | 2:K:2605:LEU:HD23 | 1.84 | 0.59 |
| 3:L:3024[A]:LEU:O | 3:L:3031[A]:ASN:ND2 | 2.36 | 0.59 |
| 3:L:3071[A]:PHE:O | 3:L:3074[A]:GLU:HB2 | 2.02 | 0.59 |
| 3:L:3071[B]:PHE:O | 3:L:3074[B]:GLU:HB2 | 2.02 | 0.59 |
| 3:O:3104[B]:MET:SD | 3:O:3110[B]:THR:HG22 | 2.42 | 0.59 |
| 3:R:2928[A]:ASN:N | 3:R:2930[A]:LEU:HD21 | 2.17 | 0.59 |
| 3:R:3001[A]:LYS:HE3 | 3:R:3002[A]:ALA:HB2 | 1.85 | 0.59 |
| 3:R:3024[B]:LEU:O | 3:R:3031[B]:ASN:ND2 | 2.36 | 0.59 |
| 3:R:3135[A]:LYS:CB | 3:R:3141[A]:TYR:CD1 | 2.85 | 0.59 |
| 3:R:3218[B]:LEU:O | 3:R:3219[B]:LEU:HD13 | 2.01 | 0.59 |
| 3:R:3222[A]:ILE:HG13 | 3:R:3224[A]:GLN:HG2 | 1.84 | 0.59 |
| 1:S:1324:ARG:NH1 | 1:S:1516:VAL:O | 2.35 | 0.59 |
| 3:U:3071[A]:PHE:O | 3:U:3074[A]:GLU:HB2 | 2.02 | 0.59 |
| 3:U:3120[B]:HIS:C | 3:U:3122[B]:ASN:N | 2.55 | 0.59 |
| 3:U:3156[A]:MET:HA | 3:U:3157[A]:PRO:C | 2.26 | 0.59 |
| 2:W:2252:GLU:HG2 | 2:W:2385:ILE:HG23 | 1.83 | 0.59 |
| 3:X:2932[A]:PRO:CA | 3:X:2935[A]:ILE:HD12 | 2.30 | 0.59 |
| 3:X:2945[A]:VAL:HG22 | 3:X:2945[A]:VAL:O | 2.01 | 0.59 |
| 1:Y:553:LEU:HB2 | 1:Y:557:VAL:HG11 | 1.84 | 0.59 |
| 2:Z:2851:ASN:OD1 | 2:Z:2851:ASN:N | 2.32 | 0.59 |
| 3:a:2935[A]:ILE:HD13 | 3:a:2935[A]:ILE:N | 2.18 | 0.59 |
| 3:a:3071[B]:PHE:O | 3:a:3074[B]:GLU:HB2 | 2.03 | 0.59 |
| 3:a:3182[A]:GLN:O | 3:a:3183[A]:LEU:HD12 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3191[B]:ASN:ND2 | 3:a:3191[B]:ASN:H | 1.99 | 0.59 |
| 1:b:355:ALA:HB1 | 1:b:776:VAL:HB | 1.85 | 0.59 |
| 1:b:673:PHE:HB3 | 1:b:677:LEU:HB2 | 1.83 | 0.59 |
| 3:d:2935[B]:ILE:HD13 | 3:d:2935[B]:ILE:N | 2.18 | 0.59 |
| 3:d:3132[B]:ALA:CB | 3:d:3197[B]:ILE:HD13 | 2.33 | 0.59 |
| 3:d:3134[B]:GLN:O | 3:d:3135[B]:LYS:C | 2.44 | 0.59 |
| 3:d:3135[A]:LYS:CB | 3:d:3141[A]:TYR:CD1 | 2.85 | 0.59 |
| 3:d:3135[B]:LYS:CB | 3:d:3141[B]:TYR:CD1 | 2.85 | 0.59 |
| 2:B:2141:HIS:ND1 | 2:B:2141:HIS:O | 2.36 | 0.59 |
| 3:C:2981[B]:GLY:O | 3:L:2966[B]:SER:O | 2.21 | 0.59 |
| 3:C:3023[A]:ILE:O | 3:C:3024[A]:LEU:C | 2.45 | 0.59 |
| 3:C:3132[B]:ALA:CB | 3:C:3197[B]:ILE:HD13 | 2.33 | 0.59 |
| 1:D:240:PHE:HA | 1:D:263:ALA:HB3 | 1.83 | 0.59 |
| 3:F:2928[B]:ASN:N | 3:F:2930[B]:LEU:HD21 | 2.18 | 0.59 |
| 3:F:2935[A]:ILE:HD13 | 3:F:2935[A]:ILE:N | 2.18 | 0.59 |
| 3:F:2979[B]:GLN:NE2 | 3:a:3156[B]:MET:CG | 2.52 | 0.59 |
| 3:F:3014[A]:TRP:CE3 | 3:F:3092[A]:ILE:HD12 | 2.37 | 0.59 |
| 3:F:3156[B]:MET:HA | 3:F:3157[B]:PRO:C | 2.26 | 0.59 |
| 1:G:105:VAL:HG12 | 1:G:123:PHE:HB3 | 1.85 | 0.59 |
| 1:G:957:ASN:HB3 | 1:G:960:PHE:H | 1.67 | 0.59 |
| 2:H:2090:LYS:NZ | 2:H:2099:GLU:OE2 | 2.34 | 0.59 |
| 2:H:2868:GLU:OE2 | 3:I:2933[A]:SER:N | 2.32 | 0.59 |
| 3:I:2935[A]:ILE:HD13 | 3:I:2935[A]:ILE:N | 2.18 | 0.59 |
| 3:I:2939[B]:ARG:HH11 | 3:I:2939[B]:ARG:HG3 | 1.67 | 0.59 |
| 3:I:2961[B]:HIS:ND1 | 3:R:2975[B]:PHE:HE1 | 1.98 | 0.59 |
| 3:I:3276[A]:ASP:HB3 | 3:I:3278[A]:HIS:HB2 | 1.83 | 0.59 |
| 2:K:2731:PRO:HB3 | 2:K:2734:LYS:HG3 | 1.82 | 0.59 |
| 3:L:2942[B]:LEU:CD1 | 3:L:3033[B]:PHE:CE1 | 2.85 | 0.59 |
| 3:L:3014[A]:TRP:CD2 | 3:L:3092[A]:ILE:HD12 | 2.38 | 0.59 |
| 3:L:3281[A]:PHE:CE1 | 3:L:3305[A]:ILE:HG21 | 2.36 | 0.59 |
| 3:O:2974[B]:ALA:HA | 3:X:2979[B]:GLN:CD | 2.27 | 0.59 |
| 3:O:2987[B]:HIS:NE2 | 3:O:3178[B]:PHE:HE1 | 1.95 | 0.59 |
| 3:O:3071[B]:PHE:O | 3:O:3074[B]:GLU:HB2 | 2.02 | 0.59 |
| 3:U:3024[A]:LEU:O | 3:U:3031[A]:ASN:ND2 | 2.36 | 0.59 |
| 3:U:3104[A]:MET:SD | 3:U:3110[A]:THR:HG22 | 2.42 | 0.59 |
| 3:U:3120[A]:HIS:C | 3:U:3122[A]:ASN:N | 2.55 | 0.59 |
| 3:U:3134[B]:GLN:O | 3:U:3135[B]:LYS:C | 2.44 | 0.59 |
| 3:X:3014[B]:TRP:CE3 | 3:X:3092[B]:ILE:HD12 | 2.37 | 0.59 |
| 3:a:3212[B]:ARG:HH11 | 3:a:3212[B]:ARG:CG | 2.12 | 0.59 |
| 1:b:710:GLY:O | 1:b:841:LYS:NZ | 2.33 | 0.59 |
| 1:b:1348:TRP:HD1 | 1:b:1403:LEU:HD13 | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:1441:SER:OG | 1:b:1442:MET:N | 2.34 | 0.59 |
| 3:d:2969[B]:TYR:CD2 | 3:d:2970[B]:PRO:HG2 | 2.38 | 0.59 |
| 3:d:3132[A]:ALA:CB | 3:d:3197[A]:ILE:HD13 | 2.33 | 0.59 |
| 2:B:2550:THR:H | 2:B:2553:ALA:HB3 | 1.66 | 0.59 |
| 3:C:2945[A]:VAL:HG22 | 3:C:2945[A]:VAL:O | 2.01 | 0.59 |
| 3:C:2961[B]:HIS:CE1 | 3:C:2980[B]:HIS:NE2 | 2.57 | 0.59 |
| 3:C:3093[B]:HIS:ND1 | 3:L:2971[B]:ASP:CB | 2.25 | 0.59 |
| 3:C:3253[B]:GLU:OE1 | 3:L:2974[B]:ALA:C | 2.46 | 0.59 |
| 3:F:2969[A]:TYR:CD2 | 3:F:2970[A]:PRO:HG2 | 2.38 | 0.59 |
| 3:F:3071[B]:PHE:O | 3:F:3074[B]:GLU:HB2 | 2.02 | 0.59 |
| 3:F:3274[A]:ARG:NE | 3:F:3274[A]:ARG:HA | 2.16 | 0.59 |
| 3:I:3152[B]:LYS:CB | 3:R:3171[B]:HIS:CA | 2.81 | 0.59 |
| 3:I:3298[A]:ASN:ND2 | 3:I:3301[A]:PRO:C | 2.60 | 0.59 |
| 2:K:2497:GLU:HB2 | 2:K:2498:VAL:HA | 1.84 | 0.59 |
| 2:K:2507:ARG:HA | 2:K:2779:ASP:HB2 | 1.85 | 0.59 |
| 3:L:3000[B]:LEU:N | 3:L:3000[B]:LEU:HD23 | 2.18 | 0.59 |
| 3:O:2942[A]:LEU:CD1 | 3:O:3033[A]:PHE:CE1 | 2.85 | 0.59 |
| 3:O:3038[B]:ILE:HG23 | 3:X:2969[B]:TYR:OH | 2.02 | 0.59 |
| 3:O:3104[A]:MET:SD | 3:O:3110[A]:THR:HG22 | 2.42 | 0.59 |
| 3:O:3191[A]:ASN:ND2 | 3:O:3191[A]:ASN:H | 1.99 | 0.59 |
| 1:P:871:GLN:NE2 | 1:P:964:ILE:O | 2.33 | 0.59 |
| 1:P:898:GLY:N | 1:P:899:MET:HA | 2.17 | 0.59 |
| 2:Q:2128:LEU:HD23 | 2:Q:2216:PHE:HZ | 1.68 | 0.59 |
| 2:Q:2133:PRO:HG2 | 2:Q:2140:ARG:HA | 1.83 | 0.59 |
| 3:R:3288[B]:MET:CG | 3:R:3295[B]:LEU:HD21 | 2.32 | 0.59 |
| 1:S:804:ASP:OD1 | 1:S:805:VAL:N | 2.36 | 0.59 |
| 2:T:2386:ARG:HB3 | 2:T:2496:LEU:HD21 | 1.82 | 0.59 |
| 3:U:2928[B]:ASN:N | 3:U:2930[B]:LEU:HD21 | 2.17 | 0.59 |
| 3:U:2942[B]:LEU:CD1 | 3:U:3033[B]:PHE:CE1 | 2.85 | 0.59 |
| 3:U:2967[B]:CYS:SG | 3:d:3257[B]:ALA:O | 2.61 | 0.59 |
| 3:U:3014[B]:TRP:CE3 | 3:U:3092[B]:ILE:HD12 | 2.37 | 0.59 |
| 3:U:3132[B]:ALA:CB | 3:U:3197[B]:ILE:HD13 | 2.33 | 0.59 |
| 3:X:2948[B]:ASP:CB | 3:X:2949[B]:LYS:CA | 2.78 | 0.59 |
| 3:X:3014[B]:TRP:CD2 | 3:X:3092[B]:ILE:HD12 | 2.38 | 0.59 |
| 3:X:3071[A]:PHE:O | 3:X:3074[A]:GLU:HB2 | 2.03 | 0.59 |
| 3:X:3135[A]:LYS:CB | 3:X:3141[A]:TYR:CD1 | 2.85 | 0.59 |
| 3:X:3135[B]:LYS:CB | 3:X:3141[B]:TYR:CD1 | 2.85 | 0.59 |
| 3:X:3288[B]:MET:CG | 3:X:3295[B]:LEU:HD21 | 2.32 | 0.59 |
| 3:X:3298[A]:ASN:ND2 | 3:X:3301[A]:PRO:C | 2.60 | 0.59 |
| 3:X:3298[B]:ASN:CB | 3:X:3300[B]:LEU:N | 2.60 | 0.59 |
| 1:Y:1323:HIS:CD2 | 9:Y:2105:CUO:O2 | 2.54 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2939[A]:ARG:HH11 | 3:a:2939[A]:ARG:HG3 | 1.66 | 0.59 |
| 3:d:2928[A]:ASN:N | 3:d:2930[A]:LEU:HD21 | 2.17 | 0.59 |
| 3:d:2928[B]:ASN:N | 3:d:2930[B]:LEU:HD21 | 2.17 | 0.59 |
| 3:d:3071[A]:PHE:O | 3:d:3074[A]:GLU:HB2 | 2.02 | 0.59 |
| 3:d:3298[A]:ASN:CA | 3:d:3300[A]:LEU:HD23 | 2.31 | 0.59 |
| 2:B:2128:LEU:HD13 | 2:B:2286:HIS:CG | 2.38 | 0.59 |
| 3:C:2942[A]:LEU:CD1 | 3:C:3033[A]:PHE:CE1 | 2.85 | 0.59 |
| 3:C:2942[B]:LEU:CD1 | 3:C:3033[B]:PHE:CE1 | 2.85 | 0.59 |
| 3:C:2969[A]:TYR:CD2 | 3:C:2970[A]:PRO:HG2 | 2.38 | 0.59 |
| 3:C:2987[A]:HIS:NE2 | 3:C:3178[A]:PHE:HE1 | 1.95 | 0.59 |
| 3:C:3014[B]:TRP:CE3 | 3:C:3092[B]:ILE:HD12 | 2.37 | 0.59 |
| 2:E:2816:SER:HB2 | 2:E:2886:VAL:HG21 | 1.85 | 0.59 |
| 3:F:2942[B]:LEU:CD1 | 3:F:3033[B]:PHE:CE1 | 2.85 | 0.59 |
| 3:F:2949[A]:LYS:HZ2 | 3:F:2950[A]:THR:HA | 1.68 | 0.59 |
| 3:F:2966[B]:SER:OG | 3:a:3255[B]:PRO:C | 2.45 | 0.59 |
| 3:F:2966[B]:SER:HB3 | 3:a:2982[B]:MET:HE2 | 1.84 | 0.59 |
| 3:F:3000[B]:LEU:HD23 | 3:F:3000[B]:LEU:N | 2.18 | 0.59 |
| 3:F:3134[B]:GLN:O | 3:F:3135[B]:LYS:C | 2.44 | 0.59 |
| 3:F:3153[B]:LYS:CD | 3:a:3155[B]:MET:C | 2.74 | 0.59 |
| 3:I:3001[A]:LYS:HE3 | 3:I:3002[A]:ALA:HB2 | 1.85 | 0.59 |
| 1:J:109:LEU:HD12 | 1:J:119:LYS:HB3 | 1.84 | 0.59 |
| 1:J:546:PHE:O | 1:J:561:ARG:NH1 | 2.29 | 0.59 |
| 3:L:2965[B]:LEU:HD11 | 3:L:2974[B]:ALA:C | 2.28 | 0.59 |
| 3:L:2969[A]:TYR:CD2 | 3:L:2970[A]:PRO:CD | 2.85 | 0.59 |
| 3:L:3104[A]:MET:SD | 3:L:3110[A]:THR:HG22 | 2.42 | 0.59 |
| 3:L:3156[A]:MET:HA | 3:L:3157[A]:PRO:C | 2.26 | 0.59 |
| 1:M:1492:PRO:HB2 | 1:M:1497:SER:HB3 | 1.85 | 0.59 |
| 2:N:2856:ILE:HG22 | 2:N:2859:VAL:HB | 1.83 | 0.59 |
| 3:O:2935[B]:ILE:HD13 | 3:O:2935[B]:ILE:N | 2.18 | 0.59 |
| 3:O:2969[B]:TYR:CB | 3:X:3158[B]:PHE:CD1 | 2.78 | 0.59 |
| 3:O:3014[B]:TRP:CE3 | 3:O:3092[B]:ILE:HD12 | 2.37 | 0.59 |
| 3:O:3288[A]:MET:CG | 3:O:3295[A]:LEU:HD21 | 2.32 | 0.59 |
| 2:Q:2128:LEU:HD13 | 2:Q:2286:HIS:CG | 2.38 | 0.59 |
| 3:R:3014[A]:TRP:CE3 | 3:R:3092[A]:ILE:HD12 | 2.37 | 0.59 |
| 3:R:3071[B]:PHE:O | 3:R:3074[B]:GLU:HB2 | 2.02 | 0.59 |
| 3:R:3157[A]:PRO:O | 3:R:3160[A]:SER:N | 2.30 | 0.59 |
| 3:R:3220[A]:ARG:HH11 | 3:R:3220[A]:ARG:CG | 2.12 | 0.59 |
| 3:R:3284[A]:LYS:HE2 | 3:R:3284[A]:LYS:CA | 2.30 | 0.59 |
| 1:S:1627:ARG:NH2 | 1:S:1629:GLU:OE1 | 2.35 | 0.59 |
| 3:U:2939[B]:ARG:HG3 | 3:U:2939[B]:ARG:HH11 | 1.67 | 0.59 |
| 3:U:2945[A]:VAL:HG22 | 3:U:2945[A]:VAL:O | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2969[B]:TYR:CD2 | 3:U:2970[B]:PRO:CD | 2.86 | 0.59 |
| 3:U:2969[B]:TYR:CD2 | 3:U:2970[B]:PRO:HG2 | 2.38 | 0.59 |
| 3:U:2998[A]:ASP:O | 3:U:3001[A]:LYS:HB2 | 2.01 | 0.59 |
| 3:U:3023[B]:ILE:O | 3:U:3024[B]:LEU:C | 2.45 | 0.59 |
| 3:U:3113[B]:ASP:O | 3:U:3115[B]:LEU:N | 2.36 | 0.59 |
| 3:U:3161[B]:GLU:C | 3:d:3260[B]:ARG:HH12 | 2.07 | 0.59 |
| 3:U:3191[B]:ASN:ND2 | 3:U:3191[B]:ASN:H | 1.99 | 0.59 |
| 3:U:3288[A]:MET:CG | 3:U:3295[A]:LEU:HD21 | 2.32 | 0.59 |
| 1:V:1000:GLU:OE1 | 1:V:1141:ARG:NH2 | 2.36 | 0.59 |
| 1:V:1505:ARG:O | 1:V:1509:THR:OG1 | 2.21 | 0.59 |
| 3:X:3000[B]:LEU:HD23 | 3:X:3000[B]:LEU:N | 2.18 | 0.59 |
| 3:X:3134[B]:GLN:O | 3:X:3135[B]:LYS:C | 2.44 | 0.59 |
| 3:X:3274[A]:ARG:HA | 3:X:3274[A]:ARG:NE | 2.16 | 0.59 |
| 3:a:3000[B]:LEU:HD23 | 3:a:3000[B]:LEU:N | 2.18 | 0.59 |
| 3:a:3156[A]:MET:HA | 3:a:3157[A]:PRO:C | 2.26 | 0.59 |
| 3:a:3222[A]:ILE:HG13 | 3:a:3224[A]:GLN:HG2 | 1.84 | 0.59 |
| 3:d:2942[B]:LEU:CD1 | 3:d:3033[B]:PHE:CE1 | 2.85 | 0.59 |
| 3:d:3001[A]:LYS:HE3 | 3:d:3002[A]:ALA:HB2 | 1.85 | 0.59 |
| 3:d:3023[A]:ILE:O | 3:d:3024[A]:LEU:C | 2.45 | 0.59 |
| 3:d:3284[B]:LYS:HE2 | 3:d:3284[B]:LYS:CA | 2.30 | 0.59 |
| 1:A:1210:LYS:HD3 | 2:E:2744:PHE:CE1 | 2.37 | 0.59 |
| 2:B:2541:GLY:O | 2:B:2545:SER:OG | 2.13 | 0.59 |
| 3:C:2935[A]:ILE:HD13 | 3:C:2935[A]:ILE:N | 2.18 | 0.59 |
| 3:C:2965[B]:LEU:HD11 | 3:C:2974[B]:ALA:C | 2.28 | 0.59 |
| 3:C:3000[B]:LEU:N | 3:C:3000[B]:LEU:HD23 | 2.18 | 0.59 |
| 3:C:3113[B]:ASP:O | 3:C:3115[B]:LEU:N | 2.36 | 0.59 |
| 3:C:3146[B]:CYS:O | 3:L:3161[B]:GLU:HG3 | 2.03 | 0.59 |
| 3:C:3288[B]:MET:CG | 3:C:3295[B]:LEU:HD21 | 2.32 | 0.59 |
| 1:D:490:TRP:CZ3 | 1:D:494:VAL:HG21 | 2.38 | 0.59 |
| 1:D:896:HIS:HB2 | 1:D:905:TRP:CD1 | 2.38 | 0.59 |
| 2:E:2833:GLY:HA3 | 2:E:2854:MET:HE1 | 1.84 | 0.59 |
| 3:F:2991[B]:LEU:O | 3:F:2994[B]:LYS:HB3 | 2.03 | 0.59 |
| 3:F:3023[B]:ILE:O | 3:F:3024[B]:LEU:C | 2.45 | 0.59 |
| 3:F:3103[A]:GLY:O | 3:F:3106[A]:THR:HG22 | 2.03 | 0.59 |
| 3:F:3155[B]:MET:CE | 3:a:3156[B]:MET:HG2 | 2.32 | 0.59 |
| 3:F:3158[B]:PHE:HB2 | 3:a:3153[B]:LYS:HB2 | 1.84 | 0.59 |
| 3:F:3222[A]:ILE:HG13 | 3:F:3224[A]:GLN:HG2 | 1.84 | 0.59 |
| 1:G:898:GLY:N | 1:G:899:MET:SD | 2.68 | 0.59 |
| 3:I:2930[B]:LEU:H | 3:I:2930[B]:LEU:CD2 | 1.98 | 0.59 |
| 3:I:2969[A]:TYR:CD2 | 3:I:2970[A]:PRO:CD | 2.85 | 0.59 |
| 3:I:3153[B]:LYS:HD3 | 3:R:2988[B]:TRP:HD1 | 1.68 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3156[B]:MET:HG2 | 3:R:3155[B]:MET:HE1 | 1.83 | 0.59 |
| 3:I:3288[A]:MET:CG | 3:I:3295[A]:LEU:HD21 | 2.32 | 0.59 |
| 1:J:1302:SER:HB2 | 1:J:1303:GLU:HB2 | 1.85 | 0.59 |
| 3:L:3014[B]:TRP:CD2 | 3:L:3092[B]:ILE:HD12 | 2.38 | 0.59 |
| 1:M:1013:ILE:HD11 | 1:M:1175:PHE:CD2 | 2.37 | 0.59 |
| 3:O:2942[B]:LEU:CD1 | 3:O:3033[B]:PHE:CE1 | 2.85 | 0.59 |
| 3:O:2969[A]:TYR:CD2 | 3:O:2970[A]:PRO:CD | 2.86 | 0.59 |
| 3:O:3288[B]:MET:CG | 3:O:3295[B]:LEU:HD21 | 2.32 | 0.59 |
| 3:R:3014[A]:TRP:CD2 | 3:R:3092[A]:ILE:HD12 | 2.38 | 0.59 |
| 3:R:3298[B]:ASN:ND2 | 3:R:3301[B]:PRO:C | 2.60 | 0.59 |
| 2:T:2166:LEU:HA | 2:T:2169:HIS:HB2 | 1.83 | 0.59 |
| 3:U:2945[B]:VAL:HG22 | 3:U:2945[B]:VAL:O | 2.02 | 0.59 |
| 3:U:2995[B]:GLN:HG2 | 3:U:3168[B]:THR:HG21 | 1.85 | 0.59 |
| 3:U:3161[B]:GLU:CA | 3:d:3146[B]:CYS:HB2 | 2.27 | 0.59 |
| 3:U:3176[B]:LYS:HD3 | 3:d:3152[B]:LYS:CD | 2.32 | 0.59 |
| 1:V:79:ALA:O | 1:V:83:HIS:ND1 | 2.27 | 0.59 |
| 1:V:566:ARG:HB2 | 1:V:609:TRP:NE1 | 2.18 | 0.59 |
| 1:V:864:ASP:HB3 | 1:V:869:GLY:HA3 | 1.85 | 0.59 |
| 3:X:3000[A]:LEU:N | 3:X:3000[A]:LEU:HD23 | 2.18 | 0.59 |
| 3:X:3038[A]:ILE:HG12 | 3:X:3112[A]:TYR:CE2 | 2.35 | 0.59 |
| 3:X:3113[A]:ASP:O | 3:X:3115[A]:LEU:N | 2.36 | 0.59 |
| 3:X:3113[B]:ASP:O | 3:X:3115[B]:LEU:N | 2.36 | 0.59 |
| 3:X:3147[A]:GLU:HG3 | 3:X:3149[A]:ASN:HD21 | 1.65 | 0.59 |
| 3:a:2935[B]:ILE:HD13 | 3:a:2935[B]:ILE:N | 2.18 | 0.59 |
| 3:a:2948[A]:ASP:CB | 3:a:2949[A]:LYS:CA | 2.78 | 0.59 |
| 3:a:3135[A]:LYS:CB | 3:a:3141[A]:TYR:CD1 | 2.85 | 0.59 |
| 3:a:3274[A]:ARG:NE | 3:a:3274[A]:ARG:HA | 2.16 | 0.59 |
| 3:a:3288[A]:MET:CG | 3:a:3295[A]:LEU:HD21 | 2.32 | 0.59 |
| 3:d:2969[A]:TYR:CD2 | 3:d:2970[A]:PRO:CD | 2.85 | 0.59 |
| 3:d:3000[B]:LEU:HD23 | 3:d:3000[B]:LEU:N | 2.18 | 0.59 |
| 3:d:3014[B]:TRP:CD2 | 3:d:3092[B]:ILE:HD12 | 2.38 | 0.59 |
| 3:d:3024[A]:LEU:O | 3:d:3031[A]:ASN:ND2 | 2.36 | 0.59 |
| 3:d:3113[B]:ASP:O | 3:d:3115[B]:LEU:N | 2.36 | 0.59 |
| 3:d:3191[A]:ASN:ND2 | 3:d:3191[A]:ASN:H | 1.99 | 0.59 |
| 2:B:2361:LYS:HD2 | 2:B:2362:GLN:HG3 | 1.84 | 0.58 |
| 3:C:2928[B]:ASN:N | 3:C:2930[B]:LEU:HD21 | 2.17 | 0.58 |
| 3:C:2939[B]:ARG:HH11 | 3:C:2939[B]:ARG:HG3 | 1.66 | 0.58 |
| 3:C:3001[B]:LYS:HE3 | 3:C:3002[B]:ALA:HB2 | 1.85 | 0.58 |
| 3:C:3014[A]:TRP:CD2 | 3:C:3092[A]:ILE:HD12 | 2.38 | 0.58 |
| 3:C:3132[A]:ALA:CB | 3:C:3197[A]:ILE:HD13 | 2.33 | 0.58 |
| 3:C:3293[B]:LYS:CB | 3:C:3294[B]:SER:CB | 2.54 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2986[A]:PRO:HB3 | 3:F:3127[A]:TRP:CE3 | 2.38 | 0.58 |
| 3:I:2968[B]:GLN:HG2 | 3:R:2981[B]:GLY:H | 1.67 | 0.58 |
| 3:I:2981[B]:GLY:HA3 | 3:R:2966[B]:SER:O | 2.02 | 0.58 |
| 3:I:3014[B]:TRP:CD2 | 3:I:3092[B]:ILE:HD12 | 2.38 | 0.58 |
| 3:I:3024[B]:LEU:O | 3:I:3031[B]:ASN:ND2 | 2.36 | 0.58 |
| 3:I:3104[A]:MET:SD | 3:I:3110[A]:THR:HG22 | 2.42 | 0.58 |
| 1:J:11:THR:HG22 | 1:J:13:ASP:H | 1.68 | 0.58 |
| 2:K:2179:ASP:HA | 2:K:2300:ASN:ND2 | 2.17 | 0.58 |
| 3:L:2928[A]:ASN:N | 3:L:2930[A]:LEU:HD21 | 2.18 | 0.58 |
| 3:L:2935[B]:ILE:HD13 | 3:L:2935[B]:ILE:N | 2.18 | 0.58 |
| 3:L:2942[A]:LEU:CD1 | 3:L:3033[A]:PHE:CE1 | 2.85 | 0.58 |
| 3:L:2991[A]:LEU:O | 3:L:2994[A]:LYS:HB3 | 2.03 | 0.58 |
| 3:L:3000[A]:LEU:N | 3:L:3000[A]:LEU:HD23 | 2.18 | 0.58 |
| 3:L:3001[B]:LYS:HE3 | 3:L:3002[B]:ALA:HB2 | 1.85 | 0.58 |
| 3:L:3113[A]:ASP:O | 3:L:3115[A]:LEU:N | 2.36 | 0.58 |
| 3:L:3156[B]:MET:HA | 3:L:3157[B]:PRO:C | 2.26 | 0.58 |
| 3:L:3182[A]:GLN:O | 3:L:3183[A]:LEU:HD12 | 2.02 | 0.58 |
| 2:N:2265:ILE:HD12 | 2:N:2443:TYR:CD1 | 2.38 | 0.58 |
| 2:N:2303:ARG:NH2 | 2:N:2372:GLU:O | 2.36 | 0.58 |
| 3:O:2998[A]:ASP:O | 3:O:3001[A]:LYS:HB2 | 2.02 | 0.58 |
| 3:O:3014[A]:TRP:CE3 | 3:O:3092[A]:ILE:HD12 | 2.37 | 0.58 |
| 3:R:3113[B]:ASP:O | 3:R:3115[B]:LEU:N | 2.36 | 0.58 |
| 3:R:3132[B]:ALA:CB | 3:R:3197[B]:ILE:HD13 | 2.33 | 0.58 |
| 1:S:51:ASP:OD2 | 1:S:813:THR:OG1 | 2.21 | 0.58 |
| 2:T:2625:LEU:HA | 2:T:2638:ARG:HH22 | 1.65 | 0.58 |
| 3:U:2942[A]:LEU:CD1 | 3:U:3033[A]:PHE:CE1 | 2.85 | 0.58 |
| 3:U:2987[A]:HIS:NE2 | 3:U:3178[A]:PHE:HE1 | 1.95 | 0.58 |
| 3:U:3161[B]:GLU:HB2 | 3:d:3260[B]:ARG:HH11 | 1.67 | 0.58 |
| 3:U:3212[B]:ARG:HH11 | 3:U:3212[B]:ARG:CG | 2.12 | 0.58 |
| 3:U:3298[B]:ASN:CB | 3:U:3300[B]:LEU:N | 2.60 | 0.58 |
| 2:W:2254:THR:HG23 | 2:W:2317:LEU:HD13 | 1.85 | 0.58 |
| 2:W:2830:GLN:HG2 | 2:W:2863:ARG:NE | 2.18 | 0.58 |
| 3:X:2948[B]:ASP:HB3 | 3:X:2953[B]:GLY:CA | 2.24 | 0.58 |
| 3:X:2986[A]:PRO:HB3 | 3:X:3127[A]:TRP:CE3 | 2.38 | 0.58 |
| 3:X:3001[B]:LYS:HE3 | 3:X:3002[B]:ALA:HB2 | 1.85 | 0.58 |
| 3:a:2945[A]:VAL:HG22 | 3:a:2945[A]:VAL:O | 2.02 | 0.58 |
| 3:a:3113[A]:ASP:O | 3:a:3115[A]:LEU:N | 2.36 | 0.58 |
| 3:a:3113[B]:ASP:O | 3:a:3115[B]:LEU:N | 2.36 | 0.58 |
| 2:c:2849:ASP:HB3 | 2:c:2850:ARG:NE | 2.18 | 0.58 |
| 3:d:2945[A]:VAL:HG22 | 3:d:2945[A]:VAL:O | 2.02 | 0.58 |
| 3:d:3014[A]:TRP:CE3 | 3:d:3092[A]:ILE:HD12 | 2.37 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3103[A]:GLY:O | 3:d:3106[A]:THR:HG22 | 2.03 | 0.58 |
| 3:d:3120[A]:HIS:C | 3:d:3122[A]:ASN:N | 2.55 | 0.58 |
| 3:d:3176[B]:LYS:HB3 | 3:d:3176[B]:LYS:HZ2 | 1.68 | 0.58 |
| 1:A:71:LEU:HD21 | 1:A:261:SER:HA | 1.84 | 0.58 |
| 1:A:619:SER:HB2 | 1:A:805:VAL:HG11 | 1.85 | 0.58 |
| 1:A:1148:LEU:HB2 | 1:A:1188:PHE:HD2 | 1.67 | 0.58 |
| 3:C:2960[B]:PHE:O | 3:L:3255[B]:PRO:HD2 | 2.03 | 0.58 |
| 3:C:2969[A]:TYR:CD2 | 3:C:2970[A]:PRO:CD | 2.86 | 0.58 |
| 3:C:3156[A]:MET:HA | 3:C:3157[A]:PRO:C | 2.26 | 0.58 |
| 3:F:2962[B]:GLY:C | 3:a:3255[B]:PRO:CG | 2.76 | 0.58 |
| 3:F:3001[B]:LYS:HE3 | 3:F:3002[B]:ALA:HB2 | 1.85 | 0.58 |
| 3:F:3014[A]:TRP:CD2 | 3:F:3092[A]:ILE:HD12 | 2.38 | 0.58 |
| 3:F:3183[B]:LEU:N | 3:F:3184[B]:ASN:HA | 2.11 | 0.58 |
| 3:F:3188[A]:ASP:N | 3:F:3188[A]:ASP:OD2 | 2.36 | 0.58 |
| 3:F:3251[B]:ASP:OD1 | 3:a:3108[B]:HIS:HE1 | 1.83 | 0.58 |
| 2:H:2109:ARG:NH1 | 2:H:2169:HIS:O | 2.36 | 0.58 |
| 3:I:2928[B]:ASN:N | 3:I:2930[B]:LEU:HD21 | 2.18 | 0.58 |
| 3:I:3154[B]:PRO:HD3 | 3:R:3173[B]:THR:C | 2.28 | 0.58 |
| 3:I:3173[A]:THR:HB | 3:I:3176[A]:LYS:HG2 | 1.81 | 0.58 |
| 3:I:3182[A]:GLN:O | 3:I:3183[A]:LEU:HD12 | 2.02 | 0.58 |
| 3:I:3258[B]:PHE:HA | 3:R:3162[B]:ASP:OD2 | 2.02 | 0.58 |
| 1:J:285:THR:HB | 1:J:288:GLU:H | 1.68 | 0.58 |
| 3:L:2995[A]:GLN:HG2 | 3:L:3168[A]:THR:HG21 | 1.85 | 0.58 |
| 3:L:3024[B]:LEU:O | 3:L:3031[B]:ASN:ND2 | 2.36 | 0.58 |
| 3:L:3273[B]:LEU:CB | 3:L:3275[B]:LEU:HD13 | 2.28 | 0.58 |
| 3:L:3298[B]:ASN:CA | 3:L:3300[B]:LEU:HD23 | 2.31 | 0.58 |
| 3:O:2968[B]:GLN:HE22 | 3:X:2985[B]:PHE:HA | 1.51 | 0.58 |
| 3:O:2995[B]:GLN:HG2 | 3:O:3168[B]:THR:HG21 | 1.85 | 0.58 |
| 3:O:3096[A]:VAL:HG11 | 3:O:3115[A]:LEU:HD13 | 1.81 | 0.58 |
| 3:O:3096[B]:VAL:HG11 | 3:O:3115[B]:LEU:HD13 | 1.81 | 0.58 |
| 3:O:3182[B]:GLN:O | 3:O:3183[B]:LEU:HD12 | 2.02 | 0.58 |
| 3:O:3298[B]:ASN:CA | 3:O:3300[B]:LEU:HD23 | 2.31 | 0.58 |
| 3:R:3014[B]:TRP:CE3 | 3:R:3092[B]:ILE:HD12 | 2.37 | 0.58 |
| 3:R:3183[A]:LEU:N | 3:R:3184[A]:ASN:HA | 2.12 | 0.58 |
| 1:S:984:ASP:OD1 | 1:S:985:PHE:N | 2.29 | 0.58 |
| 1:S:1348:TRP:CG | 1:S:1430:ILE:HD11 | 2.38 | 0.58 |
| 3:U:2935[B]:ILE:HD13 | 3:U:2935[B]:ILE:N | 2.18 | 0.58 |
| 3:U:2969[A]:TYR:CD2 | 3:U:2970[A]:PRO:HG2 | 2.38 | 0.58 |
| 3:U:2969[B]:TYR:CE1 | 3:d:2980[B]:HIS:CE1 | 2.91 | 0.58 |
| 3:U:3113[A]:ASP:O | 3:U:3115[A]:LEU:N | 2.36 | 0.58 |
| 3:U:3132[A]:ALA:CB | 3:U:3197[A]:ILE:HD13 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3156[B]:MET:HA | 3:U:3157[B]:PRO:C | 2.26 | 0.58 |
| 1:V:121:ASN:HD21 | 1:V:124:TYR:CB | 2.17 | 0.58 |
| 3:X:2991[B]:LEU:O | 3:X:2994[B]:LYS:HB3 | 2.03 | 0.58 |
| 3:X:3191[B]:ASN:ND2 | 3:X:3191[B]:ASN:H | 1.99 | 0.58 |
| 1:Y:166:GLU:OE2 | 1:Y:297:ARG:NH1 | 2.37 | 0.58 |
| 1:Y:1302:SER:OG | 1:Y:1494:ARG:NH1 | 2.31 | 0.58 |
| 3:a:2948[B]:ASP:HB3 | 3:a:2953[B]:GLY:CA | 2.24 | 0.58 |
| 3:a:3024[B]:LEU:O | 3:a:3031[B]:ASN:ND2 | 2.36 | 0.58 |
| 3:a:3103[B]:GLY:O | 3:a:3106[B]:THR:HG22 | 2.03 | 0.58 |
| 3:a:3132[B]:ALA:CB | 3:a:3197[B]:ILE:HD13 | 2.33 | 0.58 |
| 1:b:905:TRP:HE1 | 1:b:1083:PRO:HD2 | 1.68 | 0.58 |
| 3:d:2935[A]:ILE:HD13 | 3:d:2935[A]:ILE:N | 2.18 | 0.58 |
| 3:d:3222[B]:ILE:HG13 | 3:d:3224[B]:GLN:HG2 | 1.84 | 0.58 |
| 3:C:3023[B]:ILE:O | 3:C:3024[B]:LEU:C | 2.45 | 0.58 |
| 3:C:3108[B]:HIS:CE1 | 3:L:3251[B]:ASP:OD1 | 2.47 | 0.58 |
| 3:C:3288[A]:MET:CG | 3:C:3295[A]:LEU:HD21 | 2.32 | 0.58 |
| 2:E:2866:PRO:HB2 | 2:E:2868:GLU:OE1 | 2.02 | 0.58 |
| 3:F:2998[A]:ASP:O | 3:F:3001[A]:LYS:HB2 | 2.02 | 0.58 |
| 3:F:3014[B]:TRP:CD2 | 3:F:3092[B]:ILE:HD12 | 2.38 | 0.58 |
| 3:F:3024[B]:LEU:O | 3:F:3031[B]:ASN:ND2 | 2.36 | 0.58 |
| 3:F:3113[A]:ASP:O | 3:F:3115[A]:LEU:N | 2.36 | 0.58 |
| 3:F:3113[B]:ASP:O | 3:F:3115[B]:LEU:N | 2.36 | 0.58 |
| 3:F:3152[B]:LYS:CG | 3:a:3172[B]:SER:OG | 2.28 | 0.58 |
| 1:G:573:LYS:HB3 | 1:G:574:GLY:HA2 | 1.85 | 0.58 |
| 3:I:2969[B]:TYR:HE2 | 3:R:3120[B]:HIS:CD2 | 2.21 | 0.58 |
| 3:I:3000[A]:LEU:N | 3:I:3000[A]:LEU:HD23 | 2.18 | 0.58 |
| 3:I:3103[A]:GLY:O | 3:I:3106[A]:THR:HG22 | 2.03 | 0.58 |
| 3:I:3113[A]:ASP:O | 3:I:3115[A]:LEU:N | 2.36 | 0.58 |
| 3:I:3132[B]:ALA:CB | 3:I:3197[B]:ILE:HD13 | 2.33 | 0.58 |
| 3:I:3156[B]:MET:HG2 | 3:R:3155[B]:MET:CE | 2.32 | 0.58 |
| 3:I:3279[A]:ASP:OD1 | 3:I:3279[A]:ASP:N | 2.25 | 0.58 |
| 1:J:567:LEU:HD23 | 1:J:571:PRO:HG2 | 1.85 | 0.58 |
| 3:L:2969[A]:TYR:CD2 | 3:L:2970[A]:PRO:HG2 | 2.38 | 0.58 |
| 3:L:3001[A]:LYS:HE3 | 3:L:3002[A]:ALA:HB2 | 1.85 | 0.58 |
| 3:L:3096[A]:VAL:HG11 | 3:L:3115[A]:LEU:HD13 | 1.81 | 0.58 |
| 3:L:3132[B]:ALA:CB | 3:L:3197[B]:ILE:HD13 | 2.33 | 0.58 |
| 3:L:3135[A]:LYS:CB | 3:L:3141[A]:TYR:CD1 | 2.85 | 0.58 |
| 3:L:3218[A]:LEU:O | 3:L:3219[A]:LEU:HD13 | 2.01 | 0.58 |
| 1:M:361:GLU:HG2 | 1:M:363:THR:HG22 | 1.84 | 0.58 |
| 1:M:527:LEU:O | 1:M:561:ARG:NH1 | 2.36 | 0.58 |
| 1:M:1321:HIS:HD2 | 1:M:1465:TRP:CH2 | 2.21 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2928[A]:ASN:N | 3:O:2930[A]:LEU:HD21 | 2.17 | 0.58 |
| 3:O:2969[A]:TYR:CD2 | 3:O:2970[A]:PRO:HG2 | 2.38 | 0.58 |
| 3:O:3014[A]:TRP:CD2 | 3:O:3092[A]:ILE:HD12 | 2.38 | 0.58 |
| 3:O:3023[A]:ILE:O | 3:O:3024[A]:LEU:C | 2.45 | 0.58 |
| 3:O:3191[B]:ASN:ND2 | 3:O:3191[B]:ASN:H | 1.99 | 0.58 |
| 1:P:110:PHE:N | 1:P:119:LYS:O | 2.35 | 0.58 |
| 1:P:972:SER:HA | 1:P:1028:VAL:HG22 | 1.84 | 0.58 |
| 3:R:2935[B]:ILE:HD13 | 3:R:2935[B]:ILE:N | 2.18 | 0.58 |
| 3:R:2952[A]:ALA:H | 3:R:2953[A]:GLY:CA | 2.04 | 0.58 |
| 3:R:3176[B]:LYS:HB3 | 3:R:3176[B]:LYS:HZ2 | 1.66 | 0.58 |
| 1:S:1407:THR:HG22 | 1:S:1426:LEU:HD21 | 1.86 | 0.58 |
| 3:U:2991[B]:LEU:O | 3:U:2994[B]:LYS:HB3 | 2.03 | 0.58 |
| 3:U:3014[A]:TRP:CD2 | 3:U:3092[A]:ILE:HD12 | 2.38 | 0.58 |
| 3:U:3014[B]:TRP:CD2 | 3:U:3092[B]:ILE:HD12 | 2.38 | 0.58 |
| 3:U:3103[A]:GLY:O | 3:U:3106[A]:THR:HG22 | 2.03 | 0.58 |
| 1:V:527:LEU:HD23 | 1:V:632:LEU:HD12 | 1.86 | 0.58 |
| 1:V:941:LEU:HD22 | 1:V:941:LEU:H | 1.69 | 0.58 |
| 3:X:2965[B]:LEU:HD11 | 3:X:2974[B]:ALA:C | 2.28 | 0.58 |
| 3:X:3188[B]:ASP:N | 3:X:3188[B]:ASP:OD2 | 2.36 | 0.58 |
| 1:Y:456:GLN:NE2 | 1:Y:549:PRO:O | 2.30 | 0.58 |
| 3:a:3293[A]:LYS:CB | 3:a:3294[A]:SER:CB | 2.54 | 0.58 |
| 1:b:705:THR:HG22 | 1:b:1118:THR:HG23 | 1.85 | 0.58 |
| 3:d:2995[B]:GLN:HG2 | 3:d:3168[B]:THR:HG21 | 1.85 | 0.58 |
| 3:d:3182[B]:GLN:O | 3:d:3183[B]:LEU:HD12 | 2.02 | 0.58 |
| 1:A:573:LYS:HB3 | 1:A:574:GLY:HA2 | 1.86 | 0.58 |
| 3:C:2928[A]:ASN:N | 3:C:2930[A]:LEU:HD21 | 2.18 | 0.58 |
| 3:C:2966[B]:SER:CB | 3:L:2982[B]:MET:HE2 | 2.31 | 0.58 |
| 3:C:3129[B]:ILE:HD13 | 3:C:3190[B]:LEU:O | 2.04 | 0.58 |
| 2:E:2890:VAL:N | 2:E:2891:LEU:HA | 2.19 | 0.58 |
| 3:F:2945[A]:VAL:HG22 | 3:F:2945[A]:VAL:O | 2.01 | 0.58 |
| 3:F:3298[B]:ASN:CB | 3:F:3300[B]:LEU:CD2 | 2.61 | 0.58 |
| 1:G:1078:ARG:NH2 | 2:K:2876:LYS:O | 2.36 | 0.58 |
| 1:G:1199:VAL:O | 1:G:1203:MET:HG2 | 2.03 | 0.58 |
| 3:I:2949[A]:LYS:HZ2 | 3:I:2950[A]:THR:HA | 1.67 | 0.58 |
| 3:I:2995[A]:GLN:HG2 | 3:I:3168[A]:THR:HG21 | 1.85 | 0.58 |
| 3:I:3001[B]:LYS:HE3 | 3:I:3002[B]:ALA:HB2 | 1.85 | 0.58 |
| 3:I:3129[B]:ILE:HD13 | 3:I:3190[B]:LEU:O | 2.04 | 0.58 |
| 1:J:167:ASP:OD1 | 1:J:168:PHE:N | 2.37 | 0.58 |
| 3:L:3298[B]:ASN:CB | 3:L:3300[B]:LEU:N | 2.60 | 0.58 |
| 3:O:2948[A]:ASP:CB | 3:O:2949[A]:LYS:CA | 2.78 | 0.58 |
| 3:O:2978[B]:CYS:O | 3:X:3154[B]:PRO:HG3 | 2.01 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3113[A]:ASP:O | 3:O:3115[A]:LEU:N | 2.36 | 0.58 |
| 3:O:3132[A]:ALA:CB | 3:O:3197[A]:ILE:HD13 | 2.33 | 0.58 |
| 3:O:3298[A]:ASN:CB | 3:O:3300[A]:LEU:N | 2.60 | 0.58 |
| 2:Q:2107:LEU:HD23 | 2:Q:2208:PRO:HB2 | 1.85 | 0.58 |
| 1:S:128:ILE:HG22 | 1:S:130:PHE:O | 2.02 | 0.58 |
| 1:S:997:SER:O | 1:S:1001:GLN:NE2 | 2.34 | 0.58 |
| 2:T:2800:LYS:C | 3:U:3023[A]:ILE:HD11 | 2.29 | 0.58 |
| 3:U:2957[A]:ILE:HA | 3:U:2960[A]:PHE:HE1 | 1.64 | 0.58 |
| 3:U:2966[A]:SER:HB3 | 3:U:2977[A]:CYS:HB2 | 1.78 | 0.58 |
| 3:U:3103[B]:GLY:O | 3:U:3106[B]:THR:HG22 | 2.03 | 0.58 |
| 3:U:3288[B]:MET:CG | 3:U:3295[B]:LEU:HD21 | 2.32 | 0.58 |
| 3:X:3014[A]:TRP:CD2 | 3:X:3092[A]:ILE:HD12 | 2.38 | 0.58 |
| 3:X:3182[B]:GLN:O | 3:X:3183[B]:LEU:HD12 | 2.02 | 0.58 |
| 3:X:3211[A]:ASP:OD1 | 3:X:3211[A]:ASP:N | 2.27 | 0.58 |
| 1:Y:899:MET:HE2 | 1:Y:1186:TRP:CD2 | 2.38 | 0.58 |
| 1:Y:1304:ASP:N | 1:Y:1305:GLY:HA2 | 2.19 | 0.58 |
| 3:a:2942[A]:LEU:CD1 | 3:a:3033[A]:PHE:CE1 | 2.85 | 0.58 |
| 3:a:2949[B]:LYS:HZ2 | 3:a:2950[B]:THR:HA | 1.67 | 0.58 |
| 1:b:684:ARG:O | 1:b:687:SER:OG | 2.20 | 0.58 |
| 1:b:750:ALA:HA | 1:b:796:TYR:HB3 | 1.85 | 0.58 |
| 1:b:1138:ALA:HA | 1:b:1240:ILE:HG22 | 1.86 | 0.58 |
| 3:d:3113[A]:ASP:O | 3:d:3115[A]:LEU:N | 2.36 | 0.58 |
| 6:GA:1:NAG:O3 | 6:GA:2:NAG:C7 | 2.51 | 0.58 |
| 3:C:2991[A]:LEU:O | 3:C:2994[A]:LYS:HB3 | 2.03 | 0.58 |
| 3:C:2995[B]:GLN:HG2 | 3:C:3168[B]:THR:HG21 | 1.85 | 0.58 |
| 3:C:3024[A]:LEU:O | 3:C:3031[A]:ASN:ND2 | 2.36 | 0.58 |
| 3:C:3113[A]:ASP:O | 3:C:3115[A]:LEU:N | 2.36 | 0.58 |
| 1:D:105:VAL:HG12 | 1:D:123:PHE:HB3 | 1.86 | 0.58 |
| 2:E:2680:HIS:NE2 | 2:E:2684:HIS:CD2 | 2.70 | 0.58 |
| 3:F:2965[B]:LEU:HD13 | 3:a:3256[B]:TRP:NE1 | 2.06 | 0.58 |
| 3:F:2966[B]:SER:HA | 3:a:3255[B]:PRO:O | 2.02 | 0.58 |
| 3:F:2986[B]:PRO:HB3 | 3:F:3127[B]:TRP:CE3 | 2.38 | 0.58 |
| 3:F:3129[B]:ILE:HD13 | 3:F:3190[B]:LEU:O | 2.04 | 0.58 |
| 3:F:3153[B]:LYS:NZ | 3:a:3158[B]:PHE:H | 2.00 | 0.58 |
| 3:F:3188[B]:ASP:N | 3:F:3188[B]:ASP:OD2 | 2.36 | 0.58 |
| 3:F:3225[A]:SER:OG | 3:F:3290[A]:ILE:HD13 | 2.04 | 0.58 |
| 3:F:3255[B]:PRO:O | 3:a:2966[B]:SER:CA | 2.52 | 0.58 |
| 2:H:2252:GLU:HG3 | 2:H:2389:ARG:HE | 1.69 | 0.58 |
| 3:I:2967[B]:CYS:CB | 3:R:2979[B]:GLN:C | 2.65 | 0.58 |
| 3:I:3173[B]:THR:CA | 3:R:3154[B]:PRO:N | 2.67 | 0.58 |
| 1:J:61:GLY:HA2 | 1:J:354:PHE:HE1 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:474:LEU:H | 1:J:474:LEU:HD13 | 1.68 | 0.58 |
| 3:L:2965[A]:LEU:HD11 | 3:L:2974[A]:ALA:C | 2.28 | 0.58 |
| 3:L:3188[B]:ASP:N | 3:L:3188[B]:ASP:OD2 | 2.36 | 0.58 |
| 3:L:3191[A]:ASN:ND2 | 3:L:3191[A]:ASN:H | 1.99 | 0.58 |
| 3:O:2932[B]:PRO:CA | 3:O:2935[B]:ILE:HD12 | 2.30 | 0.58 |
| 3:O:2948[B]:ASP:HB3 | 3:O:2953[B]:GLY:CA | 2.24 | 0.58 |
| 3:O:2969[B]:TYR:CG | 3:X:3158[B]:PHE:CD1 | 2.70 | 0.58 |
| 3:O:2974[B]:ALA:HB3 | 3:X:2977[B]:CYS:O | 2.02 | 0.58 |
| 3:O:2991[A]:LEU:O | 3:O:2994[A]:LYS:HB3 | 2.03 | 0.58 |
| 3:O:3108[B]:HIS:HE2 | 3:X:2967[B]:CYS:HB3 | 1.67 | 0.58 |
| 3:O:3134[A]:GLN:O | 3:O:3135[A]:LYS:C | 2.44 | 0.58 |
| 3:O:3188[A]:ASP:N | 3:O:3188[A]:ASP:OD2 | 2.36 | 0.58 |
| 1:P:472:ASP:HB3 | 1:S:1638:SER:HB2 | 1.85 | 0.58 |
| 3:R:3014[B]:TRP:CD2 | 3:R:3092[B]:ILE:HD12 | 2.38 | 0.58 |
| 3:R:3104[B]:MET:SD | 3:R:3110[B]:THR:HG22 | 2.42 | 0.58 |
| 3:R:3188[B]:ASP:OD2 | 3:R:3188[B]:ASP:N | 2.36 | 0.58 |
| 2:T:2598:PRO:HD3 | 2:T:2651:GLN:HB3 | 1.85 | 0.58 |
| 2:T:2643:GLU:O | 2:T:2647:LEU:N | 2.37 | 0.58 |
| 3:U:2928[A]:ASN:N | 3:U:2930[A]:LEU:HD21 | 2.18 | 0.58 |
| 3:U:3135[B]:LYS:CB | 3:U:3141[B]:TYR:CD1 | 2.85 | 0.58 |
| 1:V:444:GLU:HG3 | 1:V:544:PRO:HG3 | 1.85 | 0.58 |
| 1:V:754:GLU:OE2 | 1:V:799:ARG:NH2 | 2.33 | 0.58 |
| 3:X:3103[B]:GLY:O | 3:X:3106[B]:THR:HG22 | 2.03 | 0.58 |
| 3:X:3132[A]:ALA:CB | 3:X:3197[A]:ILE:HD13 | 2.33 | 0.58 |
| 3:X:3132[B]:ALA:CB | 3:X:3197[B]:ILE:HD13 | 2.33 | 0.58 |
| 3:X:3176[A]:LYS:HB3 | 3:X:3176[A]:LYS:HZ2 | 1.68 | 0.58 |
| 3:X:3191[A]:ASN:ND2 | 3:X:3191[A]:ASN:H | 1.99 | 0.58 |
| 1:Y:456:GLN:HG2 | 1:Y:551:GLU:HB2 | 1.83 | 0.58 |
| 3:a:3071[A]:PHE:O | 3:a:3074[A]:GLU:HB2 | 2.03 | 0.58 |
| 3:a:3103[A]:GLY:O | 3:a:3106[A]:THR:HG22 | 2.03 | 0.58 |
| 3:a:3225[A]:SER:OG | 3:a:3290[A]:ILE:HD13 | 2.04 | 0.58 |
| 1:b:545:PHE:O | 1:b:561:ARG:NH2 | 2.37 | 0.58 |
| 3:d:2939[A]:ARG:HH11 | 3:d:2939[A]:ARG:HG3 | 1.66 | 0.58 |
| 3:d:2986[B]:PRO:HB3 | 3:d:3127[B]:TRP:CE3 | 2.39 | 0.58 |
| 3:d:3129[A]:ILE:HD13 | 3:d:3190[A]:LEU:O | 2.04 | 0.58 |
| 3:d:3225[A]:SER:OG | 3:d:3290[A]:ILE:HD13 | 2.04 | 0.58 |
| 3:C:2960[A]:PHE:CD1 | 3:C:2960[A]:PHE:N | 2.72 | 0.58 |
| 3:C:2986[A]:PRO:HB3 | 3:C:3127[A]:TRP:CE3 | 2.38 | 0.58 |
| 3:C:2987[B]:HIS:NE2 | 3:C:3178[B]:PHE:HE1 | 1.95 | 0.58 |
| 3:C:3103[B]:GLY:O | 3:C:3106[B]:THR:HG22 | 2.03 | 0.58 |
| 3:C:3253[B]:GLU:OE1 | 3:L:2975[B]:PHE:N | 2.37 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3298[A]:ASN:CB | 3:C:3300[A]:LEU:N | 2.60 | 0.58 |
| 1:D:946:GLU:HG2 | 1:D:955:LYS:HB3 | 1.85 | 0.58 |
| 3:F:2930[B]:LEU:HD22 | 3:F:2930[B]:LEU:N | 2.02 | 0.58 |
| 3:F:2935[B]:ILE:HD13 | 3:F:2935[B]:ILE:N | 2.18 | 0.58 |
| 3:F:2961[A]:HIS:HB3 | 3:F:3111[A]:SER:HG | 1.65 | 0.58 |
| 3:F:2965[B]:LEU:HD11 | 3:F:2974[B]:ALA:C | 2.28 | 0.58 |
| 3:F:3120[A]:HIS:C | 3:F:3122[A]:ASN:N | 2.55 | 0.58 |
| 3:F:3132[A]:ALA:CB | 3:F:3197[A]:ILE:HD13 | 2.33 | 0.58 |
| 3:F:3222[B]:ILE:HG13 | 3:F:3224[B]:GLN:HG2 | 1.84 | 0.58 |
| 1:G:105:VAL:HB | 1:G:137:ARG:HH12 | 1.68 | 0.58 |
| 2:H:2309:GLN:HE21 | 2:H:2320:TYR:HD1 | 1.52 | 0.58 |
| 3:I:2961[B]:HIS:O | 3:R:2975[B]:PHE:CE1 | 2.57 | 0.58 |
| 3:I:2983[B]:VAL:CA | 3:R:3160[B]:SER:HA | 2.26 | 0.58 |
| 3:I:2986[A]:PRO:HB3 | 3:I:3127[A]:TRP:CE3 | 2.38 | 0.58 |
| 3:I:3158[B]:PHE:CB | 3:R:3153[B]:LYS:HB2 | 2.32 | 0.58 |
| 3:I:3173[B]:THR:CB | 3:R:3173[B]:THR:HG23 | 2.28 | 0.58 |
| 1:J:806:ASN:ND2 | 4:u:1:NAG:H82 | 2.18 | 0.58 |
| 2:K:2426:PHE:HB3 | 2:K:2445:MET:HE1 | 1.86 | 0.58 |
| 3:L:2935[A]:ILE:HD13 | 3:L:2935[A]:ILE:N | 2.18 | 0.58 |
| 3:L:2986[B]:PRO:HB3 | 3:L:3127[B]:TRP:CE3 | 2.38 | 0.58 |
| 3:L:3103[A]:GLY:O | 3:L:3106[A]:THR:HG22 | 2.03 | 0.58 |
| 3:L:3129[A]:ILE:HD13 | 3:L:3190[A]:LEU:O | 2.04 | 0.58 |
| 3:L:3132[A]:ALA:CB | 3:L:3197[A]:ILE:HD13 | 2.33 | 0.58 |
| 1:M:931:TRP:CD1 | 1:M:1048:ASN:HD22 | 2.22 | 0.58 |
| 3:O:3001[B]:LYS:HE3 | 3:O:3002[B]:ALA:HB2 | 1.85 | 0.58 |
| 3:O:3129[A]:ILE:HD13 | 3:O:3190[A]:LEU:O | 2.04 | 0.58 |
| 3:O:3132[B]:ALA:CB | 3:O:3197[B]:ILE:HD13 | 2.33 | 0.58 |
| 3:O:3293[B]:LYS:CB | 3:O:3294[B]:SER:CB | 2.54 | 0.58 |
| 1:P:1472:GLN:OE1 | 1:P:1475:ARG:NH1 | 2.36 | 0.58 |
| 2:Q:2128:LEU:HD23 | 2:Q:2216:PHE:CZ | 2.39 | 0.58 |
| 2:Q:2825:ILE:HG23 | 2:Q:2826:GLU:H | 1.67 | 0.58 |
| 3:R:2986[B]:PRO:HB3 | 3:R:3127[B]:TRP:CE3 | 2.38 | 0.58 |
| 3:R:3135[B]:LYS:CB | 3:R:3141[B]:TYR:CD1 | 2.85 | 0.58 |
| 2:T:2533:ASP:HB3 | 2:T:2755:PRO:HG3 | 1.84 | 0.58 |
| 3:U:2986[B]:PRO:HB3 | 3:U:3127[B]:TRP:CE3 | 2.38 | 0.58 |
| 3:U:2995[A]:GLN:HG2 | 3:U:3168[A]:THR:HG21 | 1.85 | 0.58 |
| 3:U:3258[B]:PHE:O | 3:d:2968[B]:GLN:NE2 | 2.37 | 0.58 |
| 1:V:105:VAL:HB | 1:V:137:ARG:NH2 | 2.18 | 0.58 |
| 3:X:2928[B]:ASN:N | 3:X:2930[B]:LEU:HD21 | 2.18 | 0.58 |
| 3:X:2995[A]:GLN:HG2 | 3:X:3168[A]:THR:HG21 | 1.85 | 0.58 |
| 3:X:3225[A]:SER:OG | 3:X:3290[A]:ILE:HD13 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3273[A]:LEU:CB | 3:X:3275[A]:LEU:HD13 | 2.28 | 0.58 |
| 1:Y:588:GLU:OE2 | 1:Y:728:ARG:NH2 | 2.33 | 0.58 |
| 3:a:3024[A]:LEU:O | 3:a:3031[A]:ASN:ND2 | 2.36 | 0.58 |
| 3:a:3191[A]:ASN:ND2 | 3:a:3191[A]:ASN:H | 1.99 | 0.58 |
| 3:d:2948[A]:ASP:CB | 3:d:2949[A]:LYS:CA | 2.78 | 0.58 |
| 3:d:3024[B]:LEU:O | 3:d:3031[B]:ASN:ND2 | 2.36 | 0.58 |
| 1:A:140:ASP:OD2 | 1:A:142:ARG:NE | 2.27 | 0.58 |
| 1:A:219:LEU:HG | 1:A:279:LEU:O | 2.04 | 0.58 |
| 3:C:2991[B]:LEU:O | 3:C:2994[B]:LYS:HB3 | 2.03 | 0.58 |
| 3:C:2995[A]:GLN:HG2 | 3:C:3168[A]:THR:HG21 | 1.85 | 0.58 |
| 3:C:3001[A]:LYS:HE3 | 3:C:3002[A]:ALA:HB2 | 1.85 | 0.58 |
| 3:C:3156[B]:MET:C | 3:L:2982[B]:MET:SD | 2.87 | 0.58 |
| 1:D:10:LEU:HD12 | 1:D:104:LEU:HD21 | 1.86 | 0.58 |
| 1:D:499:GLU:HG3 | 1:D:511:VAL:HG12 | 1.85 | 0.58 |
| 3:F:3155[B]:MET:SD | 3:a:3154[B]:PRO:HD2 | 2.43 | 0.58 |
| 3:F:3248[B]:LEU:C | 3:a:2974[B]:ALA:H | 2.10 | 0.58 |
| 3:F:3288[A]:MET:CG | 3:F:3295[A]:LEU:HD21 | 2.32 | 0.58 |
| 3:I:2935[B]:ILE:HD13 | 3:I:2935[B]:ILE:N | 2.18 | 0.58 |
| 3:I:2939[A]:ARG:HH11 | 3:I:2939[A]:ARG:HG3 | 1.66 | 0.58 |
| 3:I:3113[B]:ASP:O | 3:I:3115[B]:LEU:N | 2.36 | 0.58 |
| 3:I:3135[B]:LYS:CB | 3:I:3141[B]:TYR:CD1 | 2.85 | 0.58 |
| 3:I:3160[B]:SER:CB | 3:R:2982[B]:MET:HA | 2.33 | 0.58 |
| 3:I:3217[A]:PHE:HE1 | 3:I:3230[A]:PHE:HZ | 0.80 | 0.58 |
| 3:I:3225[B]:SER:OG | 3:I:3290[B]:ILE:HD13 | 2.04 | 0.58 |
| 1:J:714:ARG:NH1 | 1:J:1115:GLU:OE1 | 2.37 | 0.58 |
| 1:J:907:ARG:NH2 | 1:J:1057:GLN:OE1 | 2.37 | 0.58 |
| 3:L:2995[B]:GLN:HG2 | 3:L:3168[B]:THR:HG21 | 1.85 | 0.58 |
| 3:L:3188[A]:ASP:N | 3:L:3188[A]:ASP:OD2 | 2.36 | 0.58 |
| 2:N:2667:GLU:HB3 | 2:N:2730:LEU:HD22 | 1.85 | 0.58 |
| 3:O:3000[B]:LEU:N | 3:O:3000[B]:LEU:HD23 | 2.18 | 0.58 |
| 3:R:2965[A]:LEU:HD11 | 3:R:2974[A]:ALA:C | 2.28 | 0.58 |
| 3:R:3000[A]:LEU:HD23 | 3:R:3000[A]:LEU:N | 2.18 | 0.58 |
| 3:R:3103[B]:GLY:O | 3:R:3106[B]:THR:HG22 | 2.03 | 0.58 |
| 1:S:854:LEU:HD23 | 1:S:941:LEU:HD21 | 1.85 | 0.58 |
| 1:S:1152:LYS:HB3 | 1:S:1181:GLU:HA | 1.85 | 0.58 |
| 3:U:3024[B]:LEU:O | 3:U:3031[B]:ASN:ND2 | 2.36 | 0.58 |
| 3:U:3170[B]:ALA:C | 3:d:3148[B]:ILE:HG21 | 2.28 | 0.58 |
| 3:U:3217[B]:PHE:HE1 | 3:U:3230[B]:PHE:HZ | 0.80 | 0.58 |
| 1:V:488:PRO:HB2 | 1:V:641:TRP:CE3 | 2.39 | 0.58 |
| 2:W:2802:ASP:OD2 | 3:X:2932[A]:PRO:HD3 | 2.03 | 0.58 |
| 3:X:2935[A]:ILE:HD13 | 3:X:2935[A]:ILE:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3023[B]:ILE:O | 3:X:3024[B]:LEU:C | 2.45 | 0.58 |
| 2:Z:2560:LEU:HD23 | 2:Z:2565:THR:HB | 1.85 | 0.58 |
| 2:Z:2690:HIS:HA | 2:Z:2886:VAL:O | 2.03 | 0.58 |
| 3:a:2928[B]:ASN:N | 3:a:2930[B]:LEU:HD21 | 2.18 | 0.58 |
| 3:a:2960[A]:PHE:CD1 | 3:a:2960[A]:PHE:N | 2.72 | 0.58 |
| 3:a:2965[A]:LEU:HD11 | 3:a:2974[A]:ALA:C | 2.28 | 0.58 |
| 3:a:2986[B]:PRO:HB3 | 3:a:3127[B]:TRP:CE3 | 2.38 | 0.58 |
| 3:a:3014[B]:TRP:CD2 | 3:a:3092[B]:ILE:HD12 | 2.38 | 0.58 |
| 3:a:3132[A]:ALA:CB | 3:a:3197[A]:ILE:HD13 | 2.33 | 0.58 |
| 3:a:3225[B]:SER:OG | 3:a:3290[B]:ILE:HD13 | 2.04 | 0.58 |
| 1:b:931:TRP:CG | 1:b:1018:ILE:HD11 | 2.38 | 0.58 |
| 3:d:2995[A]:GLN:HG2 | 3:d:3168[A]:THR:HG21 | 1.85 | 0.58 |
| 3:d:3293[B]:LYS:CB | 3:d:3294[B]:SER:CB | 2.54 | 0.58 |
| 1:A:942:VAL:HG11 | 1:A:1041:ILE:HD11 | 1.85 | 0.58 |
| 3:C:2968[B]:GLN:NE2 | 3:L:3086[B]:GLU:CG | 2.66 | 0.58 |
| 3:C:3103[A]:GLY:O | 3:C:3106[A]:THR:HG22 | 2.03 | 0.58 |
| 3:C:3225[B]:SER:OG | 3:C:3290[B]:ILE:HD13 | 2.04 | 0.58 |
| 1:D:1154:SER:HB2 | 1:D:1220:MET:HE2 | 1.86 | 0.58 |
| 1:D:1397:LEU:HB2 | 1:D:1433:TRP:HB3 | 1.86 | 0.58 |
| 1:D:1472:GLN:OE1 | 1:D:1475:ARG:NH1 | 2.37 | 0.58 |
| 3:F:2982[B]:MET:HE2 | 3:a:2966[B]:SER:C | 2.28 | 0.58 |
| 3:F:3000[A]:LEU:N | 3:F:3000[A]:LEU:HD23 | 2.18 | 0.58 |
| 3:F:3071[A]:PHE:O | 3:F:3074[A]:GLU:HB2 | 2.02 | 0.58 |
| 3:F:3191[B]:ASN:ND2 | 3:F:3191[B]:ASN:H | 1.99 | 0.58 |
| 3:I:2976[B]:ALA:H | 3:R:2976[B]:ALA:HB3 | 1.67 | 0.58 |
| 3:I:2991[B]:LEU:O | 3:I:2994[B]:LYS:HB3 | 2.03 | 0.58 |
| 1:J:1138:ALA:HA | 1:J:1240:ILE:HG22 | 1.84 | 0.58 |
| 3:L:2928[B]:ASN:N | 3:L:2930[B]:LEU:HD21 | 2.18 | 0.58 |
| 3:L:2991[A]:LEU:O | 3:L:2994[A]:LYS:N | 2.37 | 0.58 |
| 2:N:2711:HIS:HA | 2:N:2714:VAL:HG22 | 1.86 | 0.58 |
| 2:N:2803:ARG:HH21 | 2:N:2805:PHE:HZ | 1.52 | 0.58 |
| 3:O:2935[A]:ILE:HD13 | 3:O:2935[A]:ILE:N | 2.18 | 0.58 |
| 3:O:2965[A]:LEU:HD11 | 3:O:2974[A]:ALA:C | 2.28 | 0.58 |
| 3:O:3103[B]:GLY:O | 3:O:3106[B]:THR:HG22 | 2.03 | 0.58 |
| 1:P:935:ILE:HD11 | 1:P:980:TYR:CE2 | 2.39 | 0.58 |
| 3:R:2960[B]:PHE:CD1 | 3:R:2960[B]:PHE:N | 2.72 | 0.58 |
| 3:R:2995[B]:GLN:HG2 | 3:R:3168[B]:THR:HG21 | 1.85 | 0.58 |
| 3:U:2932[B]:PRO:CA | 3:U:2935[B]:ILE:HD12 | 2.30 | 0.58 |
| 3:U:3014[A]:TRP:CE3 | 3:U:3092[A]:ILE:HD12 | 2.37 | 0.58 |
| 3:U:3298[A]:ASN:CB | 3:U:3300[A]:LEU:N | 2.60 | 0.58 |
| 3:X:2986[B]:PRO:HB3 | 3:X:3127[B]:TRP:CE3 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2991[A]:LEU:O | 3:X:2994[A]:LYS:HB3 | 2.03 | 0.58 |
| 3:a:3298[A]:ASN:CB | 3:a:3300[A]:LEU:N | 2.60 | 0.58 |
| 1:b:1632:LEU:HB3 | 1:b:1641:THR:HB | 1.86 | 0.58 |
| 2:c:2890:VAL:N | 2:c:2891:LEU:HA | 2.18 | 0.58 |
| 3:C:2935[B]:ILE:HD13 | 3:C:2935[B]:ILE:N | 2.18 | 0.58 |
| 3:C:3024[B]:LEU:O | 3:C:3031[B]:ASN:ND2 | 2.36 | 0.58 |
| 3:C:3129[A]:ILE:HD13 | 3:C:3190[A]:LEU:O | 2.04 | 0.58 |
| 3:C:3156[B]:MET:C | 3:L:3153[B]:LYS:HZ2 | 2.04 | 0.58 |
| 3:C:3293[A]:LYS:CD | 3:C:3294[A]:SER:N | 2.63 | 0.58 |
| 1:D:104:LEU:HD23 | 1:D:123:PHE:HE2 | 1.69 | 0.58 |
| 1:D:317:VAL:HG22 | 1:D:383:VAL:HG22 | 1.85 | 0.58 |
| 1:D:462:HIS:HA | 1:D:490:TRP:HH2 | 1.68 | 0.58 |
| 1:D:1315:GLY:HA3 | 1:D:1601:TRP:HB2 | 1.85 | 0.58 |
| 1:D:1397:LEU:HA | 1:D:1433:TRP:HD1 | 1.68 | 0.58 |
| 3:F:2970[B]:PRO:HA | 3:a:2985[B]:PHE:CE2 | 2.37 | 0.58 |
| 3:F:2995[B]:GLN:HG2 | 3:F:3168[B]:THR:HG21 | 1.85 | 0.58 |
| 1:G:1162:ALA:HB1 | 1:G:1167:ASP:OD2 | 2.04 | 0.58 |
| 3:I:2991[A]:LEU:O | 3:I:2994[A]:LYS:HB3 | 2.03 | 0.58 |
| 3:I:2991[A]:LEU:O | 3:I:2994[A]:LYS:N | 2.37 | 0.58 |
| 3:I:3000[B]:LEU:HD23 | 3:I:3000[B]:LEU:N | 2.18 | 0.58 |
| 3:I:3014[A]:TRP:CD2 | 3:I:3092[A]:ILE:HD12 | 2.38 | 0.58 |
| 3:I:3129[A]:ILE:HD13 | 3:I:3190[A]:LEU:O | 2.04 | 0.58 |
| 3:L:2932[A]:PRO:CA | 3:L:2935[A]:ILE:HD12 | 2.30 | 0.58 |
| 3:L:3113[B]:ASP:O | 3:L:3115[B]:LEU:N | 2.36 | 0.58 |
| 3:L:3225[A]:SER:OG | 3:L:3290[A]:ILE:HD13 | 2.04 | 0.58 |
| 1:M:105:VAL:HG12 | 1:M:123:PHE:HB3 | 1.84 | 0.58 |
| 3:O:3129[B]:ILE:HD13 | 3:O:3190[B]:LEU:O | 2.04 | 0.58 |
| 3:O:3293[A]:LYS:CD | 3:O:3294[A]:SER:N | 2.64 | 0.58 |
| 1:P:1421:VAL:HG23 | 1:P:1422:HIS:HD1 | 1.68 | 0.58 |
| 3:R:2928[B]:ASN:N | 3:R:2930[B]:LEU:HD21 | 2.17 | 0.58 |
| 3:R:2965[B]:LEU:HD11 | 3:R:2974[B]:ALA:C | 2.28 | 0.58 |
| 3:R:2969[A]:TYR:CD2 | 3:R:2970[A]:PRO:HG2 | 2.38 | 0.58 |
| 3:R:2995[A]:GLN:HG2 | 3:R:3168[A]:THR:HG21 | 1.85 | 0.58 |
| 3:R:3113[A]:ASP:O | 3:R:3115[A]:LEU:N | 2.36 | 0.58 |
| 3:R:3132[A]:ALA:CB | 3:R:3197[A]:ILE:HD13 | 2.33 | 0.58 |
| 3:R:3225[A]:SER:OG | 3:R:3290[A]:ILE:HD13 | 2.04 | 0.58 |
| 1:S:574:GLY:C | 1:S:576:HIS:HA | 2.28 | 0.58 |
| 1:S:1018:ILE:HA | 1:S:1021:LEU:HG | 1.85 | 0.58 |
| 3:U:2965[A]:LEU:HD11 | 3:U:2974[A]:ALA:C | 2.28 | 0.58 |
| 3:U:3129[B]:ILE:HD13 | 3:U:3190[B]:LEU:O | 2.04 | 0.58 |
| 1:V:472:ASP:OD1 | 1:V:472:ASP:N | 2.37 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W:2089:ARG:HD2 | 2:W:2175:VAL:O | 2.04 | 0.58 |
| 3:X:2945[B]:VAL:HG22 | 3:X:2945[B]:VAL:O | 2.01 | 0.58 |
| 3:a:3129[B]:ILE:HD13 | 3:a:3190[B]:LEU:O | 2.04 | 0.58 |
| 3:a:3188[A]:ASP:N | 3:a:3188[A]:ASP:OD2 | 2.36 | 0.58 |
| 3:d:2991[B]:LEU:O | 3:d:2994[B]:LYS:HB3 | 2.03 | 0.58 |
| 1:A:781:ILE:HG23 | 1:A:784:ALA:HB3 | 1.85 | 0.58 |
| 1:A:1372:ILE:HD13 | 1:b:1390:ASP:HB3 | 1.84 | 0.58 |
| 1:A:1642:GLN:NE2 | 1:A:1642:GLN:O | 2.36 | 0.58 |
| 3:C:3014[B]:TRP:CD2 | 3:C:3092[B]:ILE:HD12 | 2.38 | 0.58 |
| 3:C:3135[A]:LYS:HG3 | 3:C:3141[A]:TYR:CD1 | 2.33 | 0.58 |
| 1:D:744:VAL:HG12 | 1:D:802:ILE:HG23 | 1.85 | 0.58 |
| 1:D:1029:SER:OG | 1:D:1030:MET:N | 2.34 | 0.58 |
| 3:F:2991[A]:LEU:O | 3:F:2994[A]:LYS:HB3 | 2.03 | 0.58 |
| 3:F:3019[B]:HIS:CD2 | 3:F:3019[B]:HIS:H | 2.22 | 0.58 |
| 3:F:3103[B]:GLY:O | 3:F:3106[B]:THR:HG22 | 2.03 | 0.58 |
| 1:G:949:ASP:OD1 | 1:G:950:ALA:N | 2.37 | 0.58 |
| 1:G:1467:ILE:HD13 | 1:G:1532:PHE:HB2 | 1.85 | 0.58 |
| 2:H:2181:THR:HB | 2:H:2374:ASN:H | 1.69 | 0.58 |
| 2:H:2851:ASN:OD1 | 2:H:2851:ASN:N | 2.36 | 0.58 |
| 3:I:2960[B]:PHE:CD2 | 3:I:3157[B]:PRO:CG | 2.74 | 0.58 |
| 3:I:2965[B]:LEU:HG | 3:R:3249[B]:GLY:CA | 2.33 | 0.58 |
| 3:I:3154[B]:PRO:HB3 | 3:R:3174[B]:GLY:H | 1.60 | 0.58 |
| 3:I:3255[B]:PRO:CG | 3:R:2964[B]:PRO:N | 2.65 | 0.58 |
| 3:I:3293[B]:LYS:CD | 3:I:3294[B]:SER:N | 2.64 | 0.58 |
| 3:L:2986[A]:PRO:HB3 | 3:L:3127[A]:TRP:CE3 | 2.38 | 0.58 |
| 3:O:3019[B]:HIS:H | 3:O:3019[B]:HIS:CD2 | 2.22 | 0.58 |
| 3:O:3024[B]:LEU:O | 3:O:3031[B]:ASN:ND2 | 2.36 | 0.58 |
| 3:O:3169[B]:LYS:HZ1 | 3:X:3148[B]:ILE:H | 1.51 | 0.58 |
| 1:P:1171:LYS:NZ | 1:P:1174:GLU:OE2 | 2.29 | 0.58 |
| 3:R:3001[B]:LYS:HE3 | 3:R:3002[B]:ALA:HB2 | 1.85 | 0.58 |
| 3:R:3293[B]:LYS:CD | 3:R:3294[B]:SER:N | 2.64 | 0.58 |
| 1:S:979:LEU:HB2 | 1:S:980:TYR:CD2 | 2.38 | 0.58 |
| 2:T:2687:ILE:HD11 | 2:T:2695:MET:HG2 | 1.84 | 0.58 |
| 3:U:3001[A]:LYS:HE3 | 3:U:3002[A]:ALA:HB2 | 1.85 | 0.58 |
| 1:V:1013:ILE:HD11 | 1:V:1148:LEU:HD11 | 1.85 | 0.58 |
| 3:X:2991[B]:LEU:O | 3:X:2994[B]:LYS:N | 2.37 | 0.58 |
| 3:X:3225[B]:SER:OG | 3:X:3290[B]:ILE:HD13 | 2.04 | 0.58 |
| 2:Z:2544:GLY:HA3 | 2:Z:2699:MET:O | 2.04 | 0.58 |
| 3:a:2995[A]:GLN:HG2 | 3:a:3168[A]:THR:HG21 | 1.85 | 0.58 |
| 3:a:3014[A]:TRP:CD2 | 3:a:3092[A]:ILE:HD12 | 2.38 | 0.58 |
| 1:b:308:LEU:O | 1:b:772:ARG:NH2 | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:c:2638:ARG:HH11 | 2:c:2706:ILE:HG13 | 1.68 | 0.58 |
| 3:d:2991[A]:LEU:O | 3:d:2994[A]:LYS:HB3 | 2.03 | 0.58 |
| 1:A:926:LEU:HD11 | 1:A:1043:MET:HB3 | 1.85 | 0.57 |
| 1:D:639:ARG:NH2 | 1:D:707:PHE:O | 2.37 | 0.57 |
| 1:D:900:ALA:HB3 | 1:D:1076:ILE:HD12 | 1.85 | 0.57 |
| 3:F:3157[B]:PRO:HD2 | 3:a:3153[B]:LYS:NZ | 2.18 | 0.57 |
| 3:I:3019[B]:HIS:CD2 | 3:I:3019[B]:HIS:H | 2.22 | 0.57 |
| 3:I:3103[B]:GLY:O | 3:I:3106[B]:THR:HG22 | 2.03 | 0.57 |
| 3:I:3132[A]:ALA:CB | 3:I:3197[A]:ILE:HD13 | 2.33 | 0.57 |
| 3:I:3293[A]:LYS:CB | 3:I:3294[A]:SER:CB | 2.54 | 0.57 |
| 1:J:425:ARG:NE | 1:J:499:GLU:OE2 | 2.35 | 0.57 |
| 1:J:460:GLU:HB3 | 1:J:465:PRO:HG2 | 1.85 | 0.57 |
| 1:J:1492:PRO:HB2 | 1:J:1497:SER:HB3 | 1.86 | 0.57 |
| 2:K:2601:ASN:OD1 | 2:K:2601:ASN:N | 2.36 | 0.57 |
| 2:K:2606:LEU:HD13 | 2:K:2706:ILE:HG13 | 1.85 | 0.57 |
| 3:L:3284[B]:LYS:CD | 3:L:3285[B]:VAL:H | 2.10 | 0.57 |
| 2:N:2722:GLN:NE2 | 2:N:2769:PHE:O | 2.34 | 0.57 |
| 3:O:2991[A]:LEU:O | 3:O:2994[A]:LYS:N | 2.37 | 0.57 |
| 3:O:2991[B]:LEU:O | 3:O:2994[B]:LYS:N | 2.37 | 0.57 |
| 3:O:3113[B]:ASP:O | 3:O:3115[B]:LEU:N | 2.36 | 0.57 |
| 3:O:3176[B]:LYS:HB3 | 3:O:3176[B]:LYS:HZ2 | 1.68 | 0.57 |
| 1:P:567:LEU:HD13 | 1:P:571:PRO:HA | 1.86 | 0.57 |
| 2:Q:2117:ASP:OD2 | 2:Q:2168:ARG:NH1 | 2.36 | 0.57 |
| 2:Q:2142:ALA:HB1 | 2:Q:2143:CYS:HB2 | 1.86 | 0.57 |
| 3:R:2960[B]:PHE:CD2 | 3:R:3157[B]:PRO:CG | 2.74 | 0.57 |
| 3:R:2991[A]:LEU:O | 3:R:2994[A]:LYS:HB3 | 2.03 | 0.57 |
| 1:S:187:GLY:HA3 | 1:S:195:SER:HB3 | 1.85 | 0.57 |
| 1:S:565:GLU:HG3 | 1:S:566:ARG:H | 1.69 | 0.57 |
| 3:U:2965[B]:LEU:HD23 | 3:d:3220[B]:ARG:HH11 | 1.67 | 0.57 |
| 3:U:2969[B]:TYR:C | 3:d:3086[B]:GLU:OE1 | 2.47 | 0.57 |
| 3:U:2991[B]:LEU:O | 3:U:2994[B]:LYS:N | 2.37 | 0.57 |
| 3:U:3001[B]:LYS:HE3 | 3:U:3002[B]:ALA:HB2 | 1.85 | 0.57 |
| 3:U:3129[A]:ILE:HD13 | 3:U:3190[A]:LEU:O | 2.04 | 0.57 |
| 3:U:3225[B]:SER:OG | 3:U:3290[B]:ILE:HD13 | 2.04 | 0.57 |
| 1:V:984:ASP:OD1 | 1:V:984:ASP:N | 2.36 | 0.57 |
| 3:X:3023[A]:ILE:O | 3:X:3024[A]:LEU:C | 2.45 | 0.57 |
| 1:Y:372:ALA:O | 1:Y:375:SER:OG | 2.21 | 0.57 |
| 1:Y:1348:TRP:CG | 1:Y:1430:ILE:HD11 | 2.39 | 0.57 |
| 3:a:2960[B]:PHE:CD1 | 3:a:2960[B]:PHE:N | 2.72 | 0.57 |
| 3:a:2965[B]:LEU:HD11 | 3:a:2974[B]:ALA:C | 2.28 | 0.57 |
| 3:a:2986[A]:PRO:HB3 | 3:a:3127[A]:TRP:CE3 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:980:TYR:CE2 | 1:b:1021:LEU:HD13 | 2.39 | 0.57 |
| 2:c:2265:ILE:HD12 | 2:c:2443:TYR:CG | 2.39 | 0.57 |
| 3:d:2986[A]:PRO:HB3 | 3:d:3127[A]:TRP:CE3 | 2.39 | 0.57 |
| 3:d:2991[B]:LEU:O | 3:d:2994[B]:LYS:N | 2.37 | 0.57 |
| 1:A:124:TYR:O | 1:A:137:ARG:NH2 | 2.37 | 0.57 |
| 1:A:979:LEU:HD22 | 1:A:979:LEU:H | 1.69 | 0.57 |
| 1:A:1144:VAL:HG22 | 1:A:1196:ILE:HD12 | 1.86 | 0.57 |
| 2:B:2544:GLY:HA3 | 2:B:2699:MET:O | 2.05 | 0.57 |
| 3:C:2948[A]:ASP:HB3 | 3:C:2953[A]:GLY:CA | 2.24 | 0.57 |
| 3:C:2991[A]:LEU:O | 3:C:2994[A]:LYS:N | 2.37 | 0.57 |
| 3:C:3135[B]:LYS:HG3 | 3:C:3141[B]:TYR:CD1 | 2.33 | 0.57 |
| 3:C:3225[A]:SER:OG | 3:C:3290[A]:ILE:HD13 | 2.04 | 0.57 |
| 3:C:3298[B]:ASN:CA | 3:C:3300[B]:LEU:HD23 | 2.31 | 0.57 |
| 3:F:2965[A]:LEU:HD11 | 3:F:2974[A]:ALA:C | 2.28 | 0.57 |
| 3:F:2967[B]:CYS:CB | 3:a:2980[B]:HIS:N | 2.66 | 0.57 |
| 3:F:3163[B]:ASN:HD21 | 3:a:3149[B]:ASN:CB | 2.05 | 0.57 |
| 1:G:1018:ILE:HB | 1:G:1045:HIS:CD2 | 2.39 | 0.57 |
| 2:H:2756:ASN:HD21 | 2:H:2759:THR:HG23 | 1.69 | 0.57 |
| 3:I:3130[B]:TRP:CE2 | 3:I:3134[B]:GLN:NE2 | 2.72 | 0.57 |
| 3:I:3160[B]:SER:HB2 | 3:R:2982[B]:MET:CB | 2.28 | 0.57 |
| 3:I:3169[B]:LYS:HE3 | 3:R:3150[B]:LYS:HB2 | 1.86 | 0.57 |
| 2:K:2394:VAL:HG11 | 2:K:2451:LEU:HD12 | 1.85 | 0.57 |
| 1:M:704:ASP:OD1 | 1:M:704:ASP:N | 2.37 | 0.57 |
| 2:N:2506:ARG:NE | 2:N:2578:GLU:OE2 | 2.27 | 0.57 |
| 3:O:3130[B]:TRP:CE2 | 3:O:3134[B]:GLN:NE2 | 2.72 | 0.57 |
| 3:R:2932[A]:PRO:CA | 3:R:2935[A]:ILE:HD12 | 2.31 | 0.57 |
| 3:R:2952[B]:ALA:N | 3:R:2953[B]:GLY:HA2 | 2.06 | 0.57 |
| 3:R:3023[A]:ILE:O | 3:R:3024[A]:LEU:C | 2.45 | 0.57 |
| 3:U:2967[B]:CYS:CB | 3:d:3256[B]:TRP:CA | 2.79 | 0.57 |
| 3:U:2991[A]:LEU:O | 3:U:2994[A]:LYS:N | 2.37 | 0.57 |
| 3:U:3019[A]:HIS:CD2 | 3:U:3019[A]:HIS:H | 2.22 | 0.57 |
| 3:U:3255[B]:PRO:C | 3:d:2975[B]:PHE:HA | 2.28 | 0.57 |
| 1:V:157:GLU:OE2 | 1:V:296:ARG:NH2 | 2.37 | 0.57 |
| 1:V:262:LYS:NZ | 1:V:795:GLU:OE1 | 2.37 | 0.57 |
| 3:X:2995[B]:GLN:HG2 | 3:X:3168[B]:THR:HG21 | 1.85 | 0.57 |
| 3:X:3024[A]:LEU:O | 3:X:3031[A]:ASN:ND2 | 2.36 | 0.57 |
| 3:X:3103[A]:GLY:O | 3:X:3106[A]:THR:HG22 | 2.03 | 0.57 |
| 1:Y:1550:ARG:HE | 3:d:3008[B]:GLY:C | 2.11 | 0.57 |
| 1:Y:1616:LYS:NZ | 3:d:3188[B]:ASP:HA | 2.19 | 0.57 |
| 1:Y:1656:ASP:H | 3:d:3006[B]:LYS:CB | 2.15 | 0.57 |
| 3:a:2991[B]:LEU:O | 3:a:2994[B]:LYS:HB3 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2995[B]:GLN:HG2 | 3:a:3168[B]:THR:HG21 | 1.85 | 0.57 |
| 3:a:3001[B]:LYS:HE3 | 3:a:3002[B]:ALA:HB2 | 1.85 | 0.57 |
| 1:b:105:VAL:HB | 1:b:137:ARG:HH22 | 1.67 | 0.57 |
| 1:b:977:GLU:HG3 | 1:b:978:ALA:H | 1.69 | 0.57 |
| 3:d:3103[B]:GLY:O | 3:d:3106[B]:THR:HG22 | 2.03 | 0.57 |
| 1:A:447:MET:HA | 1:A:455:TYR:HB2 | 1.86 | 0.57 |
| 2:B:2179:ASP:HA | 2:B:2300:ASN:ND2 | 2.18 | 0.57 |
| 2:B:2226:GLU:OE2 | 2:B:2278:GLU:N | 2.37 | 0.57 |
| 2:B:2830:GLN:HB2 | 2:B:2863:ARG:HH22 | 1.69 | 0.57 |
| 2:B:2833:GLY:HA3 | 2:B:2854:MET:HE1 | 1.86 | 0.57 |
| 3:C:2985[B]:PHE:HD2 | 3:L:2968[B]:GLN:O | 1.87 | 0.57 |
| 3:C:3019[A]:HIS:CD2 | 3:C:3019[A]:HIS:H | 2.22 | 0.57 |
| 3:C:3130[A]:TRP:CE2 | 3:C:3134[A]:GLN:NE2 | 2.72 | 0.57 |
| 1:D:518:LYS:HD2 | 1:D:519:PRO:HD2 | 1.86 | 0.57 |
| 1:D:757:VAL:HG21 | 1:D:781:ILE:HG13 | 1.86 | 0.57 |
| 1:D:1627:ARG:NH2 | 1:D:1629:GLU:OE1 | 2.37 | 0.57 |
| 2:E:2242:TRP:O | 2:E:2246:ASN:ND2 | 2.34 | 0.57 |
| 3:F:2952[B]:ALA:H | 3:F:2953[B]:GLY:CA | 2.04 | 0.57 |
| 3:F:2956[B]:LYS:HD2 | 3:a:3257[B]:ALA:HB3 | 1.85 | 0.57 |
| 3:F:2967[B]:CYS:SG | 3:a:2982[B]:MET:SD | 3.03 | 0.57 |
| 3:F:2969[B]:TYR:CA | 3:a:2989[B]:HIS:NE2 | 2.68 | 0.57 |
| 3:F:2991[B]:LEU:O | 3:F:2994[B]:LYS:N | 2.37 | 0.57 |
| 3:F:3001[A]:LYS:HE3 | 3:F:3002[A]:ALA:HB2 | 1.85 | 0.57 |
| 1:G:439:LEU:HD23 | 1:G:509:ILE:HD12 | 1.86 | 0.57 |
| 1:G:1486:LEU:HB2 | 2:K:2486:ILE:HB | 1.85 | 0.57 |
| 3:I:2981[B]:GLY:N | 3:R:2968[B]:GLN:HG2 | 2.19 | 0.57 |
| 3:I:3188[A]:ASP:N | 3:I:3188[A]:ASP:OD2 | 2.36 | 0.57 |
| 1:J:469:PRO:O | 1:J:669:LYS:HD2 | 2.04 | 0.57 |
| 1:J:1150:GLY:N | 1:J:1186:TRP:O | 2.36 | 0.57 |
| 1:J:1324:ARG:NE | 1:J:1462:ASP:OD1 | 2.37 | 0.57 |
| 2:K:2090:LYS:NZ | 2:K:2099:GLU:OE2 | 2.32 | 0.57 |
| 3:L:2991[B]:LEU:O | 3:L:2994[B]:LYS:HB3 | 2.03 | 0.57 |
| 3:L:2991[B]:LEU:O | 3:L:2994[B]:LYS:N | 2.37 | 0.57 |
| 3:L:3019[A]:HIS:CD2 | 3:L:3019[A]:HIS:H | 2.22 | 0.57 |
| 3:L:3120[A]:HIS:HA | 3:L:3123[A]:THR:HG1 | 1.68 | 0.57 |
| 3:L:3129[B]:ILE:HD13 | 3:L:3190[B]:LEU:O | 2.04 | 0.57 |
| 3:O:2960[B]:PHE:CD1 | 3:O:2960[B]:PHE:N | 2.72 | 0.57 |
| 3:O:2986[A]:PRO:HB3 | 3:O:3127[A]:TRP:CE3 | 2.38 | 0.57 |
| 3:O:3284[A]:LYS:HE2 | 3:O:3284[A]:LYS:CA | 2.29 | 0.57 |
| 1:P:1171:LYS:HG2 | 1:P:1173:GLY:H | 1.69 | 0.57 |
| 3:R:3000[B]:LEU:HD23 | 3:R:3000[B]:LEU:N | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3103[A]:GLY:O | 3:R:3106[A]:THR:HG22 | 2.03 | 0.57 |
| 3:R:3284[B]:LYS:HE2 | 3:R:3284[B]:LYS:CA | 2.30 | 0.57 |
| 3:U:2948[B]:ASP:CB | 3:U:2949[B]:LYS:CA | 2.78 | 0.57 |
| 3:U:2972[B]:GLY:CA | 3:d:3247[B]:VAL:HG13 | 2.34 | 0.57 |
| 3:U:3225[A]:SER:OG | 3:U:3290[A]:ILE:HD13 | 2.04 | 0.57 |
| 3:U:3256[B]:TRP:CB | 3:d:2969[B]:TYR:H | 2.12 | 0.57 |
| 1:V:545:PHE:O | 1:V:561:ARG:NH2 | 2.36 | 0.57 |
| 3:X:3129[B]:ILE:HD13 | 3:X:3190[B]:LEU:O | 2.04 | 0.57 |
| 3:X:3307[A]:PHE:HE1 | 3:X:3309[A]:PRO:CG | 2.08 | 0.57 |
| 3:a:3293[A]:LYS:CD | 3:a:3294[A]:SER:N | 2.64 | 0.57 |
| 1:b:227:ARG:CZ | 1:b:227:ARG:HA | 2.34 | 0.57 |
| 1:b:583:LEU:HG | 1:b:602:THR:HG21 | 1.85 | 0.57 |
| 1:b:1493:MET:HG2 | 1:b:1511:SER:O | 2.04 | 0.57 |
| 3:d:2965[A]:LEU:HD11 | 3:d:2974[A]:ALA:C | 2.28 | 0.57 |
| 3:d:3014[A]:TRP:CD2 | 3:d:3092[A]:ILE:HD12 | 2.38 | 0.57 |
| 3:d:3019[A]:HIS:H | 3:d:3019[A]:HIS:CD2 | 2.22 | 0.57 |
| 1:A:460:GLU:CD | 1:A:1368:ARG:HH22 | 2.12 | 0.57 |
| 1:A:801:ASP:N | 1:A:801:ASP:OD1 | 2.35 | 0.57 |
| 2:B:2345:ASN:N | 2:E:2515:ARG:HD3 | 2.16 | 0.57 |
| 2:B:2515:ARG:HD3 | 2:E:2345:ASN:H | 1.70 | 0.57 |
| 3:C:3000[A]:LEU:HD23 | 3:C:3000[A]:LEU:N | 2.18 | 0.57 |
| 3:C:3079[B]:CYS:HB3 | 3:L:3161[B]:GLU:CG | 2.30 | 0.57 |
| 3:C:3120[B]:HIS:C | 3:C:3122[B]:ASN:N | 2.55 | 0.57 |
| 3:C:3156[B]:MET:HE2 | 3:L:2979[B]:GLN:HG3 | 0.78 | 0.57 |
| 1:D:329:ARG:HB2 | 1:G:1583:CYS:N | 2.18 | 0.57 |
| 3:F:3172[B]:SER:HB3 | 3:a:3150[B]:LYS:CA | 2.34 | 0.57 |
| 2:H:2158:TYR:O | 2:H:2161:GLN:HB3 | 2.04 | 0.57 |
| 3:I:2965[A]:LEU:HD11 | 3:I:2974[A]:ALA:C | 2.28 | 0.57 |
| 3:I:2966[B]:SER:CB | 3:R:3254[B]:MET:CB | 2.81 | 0.57 |
| 3:I:3225[A]:SER:OG | 3:I:3290[A]:ILE:HD13 | 2.04 | 0.57 |
| 1:J:979:LEU:HB3 | 1:J:980:TYR:CD1 | 2.39 | 0.57 |
| 3:L:2987[B]:HIS:NE2 | 3:L:3178[B]:PHE:HE1 | 1.95 | 0.57 |
| 3:L:3130[A]:TRP:CE2 | 3:L:3134[A]:GLN:NE2 | 2.72 | 0.57 |
| 3:L:3225[B]:SER:OG | 3:L:3290[B]:ILE:HD13 | 2.04 | 0.57 |
| 3:O:3014[B]:TRP:CD2 | 3:O:3092[B]:ILE:HD12 | 2.38 | 0.57 |
| 3:O:3225[A]:SER:OG | 3:O:3290[A]:ILE:HD13 | 2.04 | 0.57 |
| 1:P:1458:HIS:HA | 1:P:1461:VAL:HB | 1.86 | 0.57 |
| 2:Q:2180:TRP:HB3 | 2:Q:2184:MET:HE2 | 1.85 | 0.57 |
| 3:R:3130[B]:TRP:CE2 | 3:R:3134[B]:GLN:NE2 | 2.73 | 0.57 |
| 3:R:3135[B]:LYS:HG3 | 3:R:3141[B]:TYR:HE1 | 1.29 | 0.57 |
| 1:S:618:MET:HE1 | 1:S:633:HIS:HD2 | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3162[B]:ASP:HB3 | 3:d:3260[B]:ARG:CZ | 2.35 | 0.57 |
| 3:U:3252[B]:TYR:CD2 | 3:d:3222[B]:ILE:HA | 2.40 | 0.57 |
| 1:V:51:ASP:CG | 1:V:52:GLY:HA2 | 2.29 | 0.57 |
| 1:V:450:LYS:NZ | 1:V:451:SER:H | 2.01 | 0.57 |
| 1:V:899:MET:HE2 | 1:V:1012:GLU:OE2 | 2.05 | 0.57 |
| 1:V:949:ASP:OD1 | 1:V:950:ALA:N | 2.36 | 0.57 |
| 3:X:2932[B]:PRO:CA | 3:X:2935[B]:ILE:HD12 | 2.30 | 0.57 |
| 1:Y:804:ASP:OD1 | 1:Y:805:VAL:N | 2.37 | 0.57 |
| 1:Y:928:TYR:HB2 | 1:Y:1048:ASN:HB2 | 1.86 | 0.57 |
| 1:Y:947:TYR:HE1 | 1:Y:957:ASN:H | 1.51 | 0.57 |
| 1:Y:1137:LYS:HA | 1:Y:1141:ARG:HH12 | 1.69 | 0.57 |
| 3:a:3176[A]:LYS:H | 3:a:3176[A]:LYS:CE | 2.17 | 0.57 |
| 2:c:2114:ARG:HH12 | 2:c:2120:GLU:HG3 | 1.69 | 0.57 |
| 3:d:3212[B]:ARG:HH11 | 3:d:3212[B]:ARG:CG | 2.12 | 0.57 |
| 1:A:959:PHE:HA | 1:A:1040:PRO:HG2 | 1.86 | 0.57 |
| 3:C:3150[B]:LYS:N | 3:L:3169[B]:LYS:HG2 | 2.10 | 0.57 |
| 3:C:3160[B]:SER:OG | 3:L:2983[B]:VAL:HG22 | 2.00 | 0.57 |
| 1:D:460:GLU:O | 1:D:467:LYS:NZ | 2.33 | 0.57 |
| 3:F:2948[A]:ASP:CB | 3:F:2949[A]:LYS:CA | 2.78 | 0.57 |
| 3:F:2995[A]:GLN:HG2 | 3:F:3168[A]:THR:HG21 | 1.86 | 0.57 |
| 3:F:3158[B]:PHE:N | 3:a:3153[B]:LYS:CE | 2.62 | 0.57 |
| 3:F:3160[B]:SER:CB | 3:a:3150[B]:LYS:CE | 2.78 | 0.57 |
| 3:F:3174[B]:GLY:N | 3:a:3154[B]:PRO:CA | 2.65 | 0.57 |
| 3:F:3255[B]:PRO:HG2 | 3:a:2964[B]:PRO:HD2 | 1.85 | 0.57 |
| 3:F:3283[A]:ILE:CB | 3:F:3305[A]:ILE:HD11 | 2.35 | 0.57 |
| 3:F:3298[A]:ASN:CA | 3:F:3300[A]:LEU:HD23 | 2.31 | 0.57 |
| 1:G:493:LEU:HD12 | 1:G:668:MET:HG3 | 1.86 | 0.57 |
| 1:G:1361:GLU:HG3 | 1:G:1363:THR:H | 1.69 | 0.57 |
| 3:I:2965[B]:LEU:HD11 | 3:I:2974[B]:ALA:C | 2.29 | 0.57 |
| 3:I:2965[B]:LEU:HD13 | 3:R:3256[B]:TRP:HE1 | 1.66 | 0.57 |
| 3:I:2989[B]:HIS:ND1 | 3:R:2970[B]:PRO:HD3 | 2.08 | 0.57 |
| 3:L:2960[A]:PHE:CD2 | 3:L:3157[A]:PRO:CG | 2.74 | 0.57 |
| 3:L:3019[B]:HIS:CD2 | 3:L:3019[B]:HIS:H | 2.22 | 0.57 |
| 3:L:3103[B]:GLY:O | 3:L:3106[B]:THR:HG22 | 2.03 | 0.57 |
| 3:L:3176[A]:LYS:HB3 | 3:L:3176[A]:LYS:HZ2 | 1.68 | 0.57 |
| 3:O:2965[B]:LEU:HD11 | 3:O:2974[B]:ALA:C | 2.28 | 0.57 |
| 3:O:2968[B]:GLN:CG | 3:X:2984[B]:THR:CB | 2.79 | 0.57 |
| 3:O:2969[B]:TYR:N | 3:X:2988[B]:TRP:CB | 2.55 | 0.57 |
| 3:O:2975[B]:PHE:C | 3:X:3155[B]:MET:HA | 2.09 | 0.57 |
| 3:O:3001[A]:LYS:HE3 | 3:O:3002[A]:ALA:HB2 | 1.85 | 0.57 |
| 3:O:3130[A]:TRP:CE2 | 3:O:3134[A]:GLN:NE2 | 2.72 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2991[B]:LEU:O | 3:R:2994[B]:LYS:N | 2.37 | 0.57 |
| 3:R:3089[A]:HIS:CE1 | 3:R:3119[A]:HIS:CE1 | 2.81 | 0.57 |
| 2:T:2872:GLU:OE1 | 2:T:2874:ASP:N | 2.36 | 0.57 |
| 3:U:2948[B]:ASP:HB3 | 3:U:2953[B]:GLY:CA | 2.24 | 0.57 |
| 3:U:2991[A]:LEU:O | 3:U:2994[A]:LYS:HB3 | 2.03 | 0.57 |
| 3:U:3130[B]:TRP:CE2 | 3:U:3134[B]:GLN:NE2 | 2.72 | 0.57 |
| 3:U:3217[A]:PHE:HE1 | 3:U:3230[A]:PHE:HZ | 0.80 | 0.57 |
| 3:X:2935[B]:ILE:HD13 | 3:X:2935[B]:ILE:N | 2.18 | 0.57 |
| 3:X:3130[A]:TRP:CE2 | 3:X:3134[A]:GLN:NE2 | 2.72 | 0.57 |
| 3:X:3130[B]:TRP:CE2 | 3:X:3134[B]:GLN:NE2 | 2.72 | 0.57 |
| 3:X:3284[A]:LYS:CD | 3:X:3285[A]:VAL:H | 2.10 | 0.57 |
| 3:X:3298[A]:ASN:CA | 3:X:3300[A]:LEU:HD23 | 2.31 | 0.57 |
| 1:Y:931:TRP:CD1 | 1:Y:1048:ASN:HD22 | 2.23 | 0.57 |
| 3:a:2987[B]:HIS:NE2 | 3:a:3178[B]:PHE:HE1 | 1.95 | 0.57 |
| 3:a:2991[B]:LEU:O | 3:a:2994[B]:LYS:N | 2.37 | 0.57 |
| 1:b:19:GLN:NE2 | 1:b:121:ASN:OD1 | 2.37 | 0.57 |
| 1:b:549:PRO:HA | 1:b:557:VAL:HB | 1.87 | 0.57 |
| 1:b:931:TRP:CD1 | 1:b:1048:ASN:HD22 | 2.23 | 0.57 |
| 1:b:975:PRO:HG2 | 1:b:1024:GLY:HA3 | 1.86 | 0.57 |
| 3:d:3293[B]:LYS:CD | 3:d:3294[B]:SER:N | 2.64 | 0.57 |
| 3:C:3130[B]:TRP:CE2 | 3:C:3134[B]:GLN:NE2 | 2.72 | 0.57 |
| 3:C:3156[B]:MET:HE2 | 3:L:2979[B]:GLN:HB3 | 1.77 | 0.57 |
| 3:C:3169[B]:LYS:HG2 | 3:L:3150[B]:LYS:H | 1.69 | 0.57 |
| 3:C:3298[A]:ASN:CA | 3:C:3300[A]:LEU:HD23 | 2.31 | 0.57 |
| 1:D:488:PRO:HB2 | 1:D:641:TRP:CE3 | 2.39 | 0.57 |
| 1:D:1372:ILE:HD11 | 1:G:1392:ASP:HB2 | 1.85 | 0.57 |
| 3:F:2960[A]:PHE:CD1 | 3:F:2960[A]:PHE:N | 2.72 | 0.57 |
| 3:F:2961[A]:HIS:CE1 | 3:F:2980[A]:HIS:NE2 | 2.57 | 0.57 |
| 3:F:3130[B]:TRP:CZ2 | 3:F:3134[B]:GLN:NE2 | 2.73 | 0.57 |
| 1:G:760:ILE:HG21 | 1:G:777:TYR:HE2 | 1.68 | 0.57 |
| 1:G:1101:VAL:HG21 | 2:K:2873:HIS:ND1 | 2.19 | 0.57 |
| 2:H:2086:ASN:N | 2:H:2086:ASN:OD1 | 2.37 | 0.57 |
| 2:H:2597:MET:HE2 | 2:H:2598:PRO:HD2 | 1.86 | 0.57 |
| 3:I:2986[B]:PRO:HB3 | 3:I:3127[B]:TRP:CE3 | 2.38 | 0.57 |
| 3:I:2989[B]:HIS:HE1 | 3:R:2969[B]:TYR:HA | 1.56 | 0.57 |
| 3:I:2991[B]:LEU:O | 3:I:2994[B]:LYS:N | 2.37 | 0.57 |
| 3:I:3130[A]:TRP:CZ2 | 3:I:3134[A]:GLN:NE2 | 2.73 | 0.57 |
| 3:I:3162[B]:ASP:CG | 3:R:3259[B]:ASP:H | 2.12 | 0.57 |
| 3:I:3162[B]:ASP:O | 3:R:3150[B]:LYS:NZ | 2.36 | 0.57 |
| 3:I:3169[B]:LYS:CB | 3:R:3149[B]:ASN:OD1 | 2.44 | 0.57 |
| 3:I:3256[B]:TRP:CA | 3:R:2966[B]:SER:HA | 2.33 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2795:ILE:O | 2:K:2798:GLN:HG2 | 2.05 | 0.57 |
| 1:M:240:PHE:HA | 1:M:263:ALA:HB3 | 1.87 | 0.57 |
| 3:O:2932[A]:PRO:CA | 3:O:2935[A]:ILE:HD12 | 2.31 | 0.57 |
| 3:O:2948[A]:ASP:HB3 | 3:O:2953[A]:GLY:CA | 2.24 | 0.57 |
| 3:O:2963[B]:MET:CE | 3:X:2975[B]:PHE:HB2 | 2.30 | 0.57 |
| 3:O:3000[A]:LEU:HD23 | 3:O:3000[A]:LEU:N | 2.18 | 0.57 |
| 1:P:1394:GLN:HG2 | 1:P:1395:PRO:HD2 | 1.86 | 0.57 |
| 3:R:2961[A]:HIS:NE2 | 3:R:2980[A]:HIS:CE1 | 2.73 | 0.57 |
| 3:R:3019[B]:HIS:CD2 | 3:R:3019[B]:HIS:H | 2.22 | 0.57 |
| 3:R:3023[B]:ILE:O | 3:R:3024[B]:LEU:C | 2.45 | 0.57 |
| 3:R:3129[B]:ILE:HD13 | 3:R:3190[B]:LEU:O | 2.04 | 0.57 |
| 3:R:3130[A]:TRP:CE2 | 3:R:3134[A]:GLN:NE2 | 2.72 | 0.57 |
| 3:R:3130[B]:TRP:CZ2 | 3:R:3134[B]:GLN:NE2 | 2.73 | 0.57 |
| 1:S:946:GLU:HG2 | 1:S:955:LYS:HB3 | 1.85 | 0.57 |
| 1:S:1140:ASN:ND2 | 1:S:1236:TYR:OH | 2.37 | 0.57 |
| 2:T:2833:GLY:HA3 | 2:T:2854:MET:HE1 | 1.85 | 0.57 |
| 3:U:2965[B]:LEU:HD11 | 3:U:2974[B]:ALA:C | 2.28 | 0.57 |
| 3:U:2965[B]:LEU:HA | 3:d:3220[B]:ARG:HH11 | 1.59 | 0.57 |
| 3:U:2986[A]:PRO:HB3 | 3:U:3127[A]:TRP:CE3 | 2.38 | 0.57 |
| 3:U:3000[B]:LEU:HD23 | 3:U:3000[B]:LEU:N | 2.18 | 0.57 |
| 3:U:3130[B]:TRP:CZ2 | 3:U:3134[B]:GLN:NE2 | 2.73 | 0.57 |
| 3:U:3180[A]:TYR:C | 3:U:3183[A]:LEU:HD22 | 2.30 | 0.57 |
| 3:X:3183[A]:LEU:N | 3:X:3184[A]:ASN:HA | 2.11 | 0.57 |
| 1:Y:688:VAL:HG12 | 1:Y:690:THR:HG23 | 1.87 | 0.57 |
| 2:Z:2128:LEU:HD13 | 2:Z:2286:HIS:CG | 2.40 | 0.57 |
| 2:Z:2866:PRO:CG | 3:a:2933[A]:SER:HB2 | 2.34 | 0.57 |
| 1:b:35:GLN:HE21 | 1:b:129:LYS:HB2 | 1.69 | 0.57 |
| 1:b:1143:ALA:HA | 1:b:1195:ASP:O | 2.03 | 0.57 |
| 3:d:2969[B]:TYR:CE2 | 3:d:2970[B]:PRO:CG | 2.86 | 0.57 |
| 3:d:3130[B]:TRP:CZ2 | 3:d:3134[B]:GLN:NE2 | 2.73 | 0.57 |
| 3:d:3225[B]:SER:OG | 3:d:3290[B]:ILE:HD13 | 2.04 | 0.57 |
| 2:B:2344:LEU:HA | 2:B:2345:ASN:C | 2.29 | 0.57 |
| 3:C:2972[B]:GLY:C | 3:L:3090[B]:ASN:CG | 2.71 | 0.57 |
| 3:C:2991[B]:LEU:O | 3:C:2994[B]:LYS:N | 2.37 | 0.57 |
| 3:C:3293[B]:LYS:CD | 3:C:3294[B]:SER:N | 2.63 | 0.57 |
| 3:C:3298[A]:ASN:HD21 | 3:C:3301[A]:PRO:HA | 1.60 | 0.57 |
| 1:D:908:LEU:HD22 | 1:D:1096:THR:HG23 | 1.85 | 0.57 |
| 1:G:639:ARG:NH2 | 1:G:707:PHE:O | 2.37 | 0.57 |
| 1:G:943:LEU:HD13 | 1:G:944:GLU:HG3 | 1.86 | 0.57 |
| 3:I:3173[B]:THR:C | 3:R:3154[B]:PRO:CA | 2.77 | 0.57 |
| 3:I:3180[B]:TYR:C | 3:I:3183[B]:LEU:HD22 | 2.30 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3220[A]:ARG:HH11 | 3:I:3220[A]:ARG:CG | 2.12 | 0.57 |
| 1:J:572:SER:OG | 1:J:573:LYS:N | 2.35 | 0.57 |
| 1:J:619:SER:HB2 | 1:J:805:VAL:HG11 | 1.86 | 0.57 |
| 1:J:1639:LYS:HD3 | 6:w:1:NAG:O5 | 2.04 | 0.57 |
| 3:L:2961[B]:HIS:NE2 | 3:L:2980[B]:HIS:CE1 | 2.73 | 0.57 |
| 3:L:3173[A]:THR:HG22 | 3:L:3174[A]:GLY:H | 1.67 | 0.57 |
| 3:O:2986[B]:PRO:HB3 | 3:O:3127[B]:TRP:CE3 | 2.38 | 0.57 |
| 3:O:3023[B]:ILE:O | 3:O:3024[B]:LEU:C | 2.45 | 0.57 |
| 3:O:3103[A]:GLY:O | 3:O:3106[A]:THR:HG22 | 2.03 | 0.57 |
| 3:O:3217[B]:PHE:HE1 | 3:O:3230[B]:PHE:HZ | 0.81 | 0.57 |
| 3:O:3255[B]:PRO:N | 3:X:3160[B]:SER:C | 2.44 | 0.57 |
| 3:O:3283[B]:ILE:CB | 3:O:3305[B]:ILE:HD11 | 2.35 | 0.57 |
| 1:P:163:LEU:HB3 | 1:P:293:LEU:HD21 | 1.86 | 0.57 |
| 3:R:2971[B]:ASP:CG | 3:R:2973[B]:THR:HG1 | 2.10 | 0.57 |
| 3:R:3283[B]:ILE:CB | 3:R:3305[B]:ILE:HD11 | 2.35 | 0.57 |
| 1:S:622:HIS:CE1 | 1:S:767:LYS:H | 2.23 | 0.57 |
| 1:S:879:SER:HB2 | 1:S:1182:ASN:ND2 | 2.18 | 0.57 |
| 3:X:2949[B]:LYS:HZ2 | 3:X:2950[B]:THR:HA | 1.69 | 0.57 |
| 3:X:3129[A]:ILE:HD13 | 3:X:3190[A]:LEU:O | 2.04 | 0.57 |
| 1:Y:533:VAL:HG12 | 1:Y:540:THR:HG22 | 1.87 | 0.57 |
| 3:a:3180[A]:TYR:C | 3:a:3183[A]:LEU:HD22 | 2.30 | 0.57 |
| 3:a:3180[B]:TYR:C | 3:a:3183[B]:LEU:HD22 | 2.30 | 0.57 |
| 1:b:639:ARG:NH2 | 1:b:707:PHE:O | 2.36 | 0.57 |
| 1:b:961:SER:OG | 1:b:972:SER:O | 2.17 | 0.57 |
| 3:d:2942[B]:LEU:HD13 | 3:d:3033[B]:PHE:CZ | 2.40 | 0.57 |
| 3:d:3000[A]:LEU:N | 3:d:3000[A]:LEU:HD23 | 2.18 | 0.57 |
| 1:A:1263:LEU:HD11 | 1:A:1358:LEU:HD22 | 1.86 | 0.57 |
| 2:B:2879:LEU:HD13 | 2:B:2901:LEU:HD11 | 1.85 | 0.57 |
| 3:C:2942[B]:LEU:HD13 | 3:C:3033[B]:PHE:CZ | 2.40 | 0.57 |
| 3:C:2986[B]:PRO:HB3 | 3:C:3127[B]:TRP:CE3 | 2.38 | 0.57 |
| 3:C:3130[A]:TRP:CZ2 | 3:C:3134[A]:GLN:NE2 | 2.73 | 0.57 |
| 3:C:3152[B]:LYS:HB2 | 3:L:3172[B]:SER:CA | 2.32 | 0.57 |
| 3:C:3180[B]:TYR:C | 3:C:3183[B]:LEU:HD22 | 2.30 | 0.57 |
| 1:D:929:TRP:O | 1:D:1048:ASN:ND2 | 2.37 | 0.57 |
| 1:D:1155:LEU:HD13 | 1:D:1217:ILE:HG21 | 1.87 | 0.57 |
| 1:D:1166:THR:HB | 1:D:1168:GLN:N | 2.20 | 0.57 |
| 3:F:3013[B]:ASP:OD1 | 3:F:3015[B]:THR:OG1 | 2.23 | 0.57 |
| 3:F:3093[A]:HIS:CE1 | 3:F:3119[A]:HIS:CD2 | 2.92 | 0.57 |
| 2:H:2598:PRO:HG3 | 2:H:2651:GLN:HB2 | 1.85 | 0.57 |
| 3:I:2942[B]:LEU:HD13 | 3:I:3033[B]:PHE:CZ | 2.40 | 0.57 |
| 3:I:3130[A]:TRP:CE2 | 3:I:3134[A]:GLN:NE2 | 2.72 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3293[B]:LYS:CB | 3:I:3294[B]:SER:CB | 2.54 | 0.57 |
| 1:J:566:ARG:H | 1:J:567:LEU:HD13 | 1.69 | 0.57 |
| 1:J:1462:ASP:OD2 | 1:J:1525:TYR:OH | 2.17 | 0.57 |
| 1:M:11:THR:HG22 | 1:M:13:ASP:H | 1.68 | 0.57 |
| 1:M:1472:GLN:OE1 | 1:M:1475:ARG:NH1 | 2.38 | 0.57 |
| 3:O:2969[B]:TYR:CE1 | 3:X:3168[B]:THR:HG22 | 2.38 | 0.57 |
| 3:O:3013[B]:ASP:OD1 | 3:O:3015[B]:THR:OG1 | 2.23 | 0.57 |
| 1:P:832:LYS:HD3 | 1:P:833:PHE:H | 1.69 | 0.57 |
| 3:R:2952[B]:ALA:HB3 | 3:R:2954[B]:TYR:N | 2.18 | 0.57 |
| 3:R:3225[B]:SER:OG | 3:R:3290[B]:ILE:HD13 | 2.04 | 0.57 |
| 1:S:1493:MET:HG2 | 1:S:1511:SER:O | 2.04 | 0.57 |
| 2:T:2803:ARG:HE | 2:T:2805:PHE:HZ | 1.53 | 0.57 |
| 3:U:2969[A]:TYR:CE2 | 3:U:2970[A]:PRO:CG | 2.86 | 0.57 |
| 1:V:126:GLY:HA3 | 1:V:202:TYR:O | 2.04 | 0.57 |
| 1:V:897:HIS:HB3 | 1:V:899:MET:HE1 | 1.86 | 0.57 |
| 3:X:3019[B]:HIS:CD2 | 3:X:3019[B]:HIS:H | 2.22 | 0.57 |
| 3:X:3220[B]:ARG:HG2 | 3:X:3221[B]:ALA:H | 1.70 | 0.57 |
| 3:X:3283[B]:ILE:CB | 3:X:3305[B]:ILE:HD11 | 2.35 | 0.57 |
| 1:Y:1019:HIS:NE2 | 1:Y:1046:HIS:CE1 | 2.73 | 0.57 |
| 3:a:3130[A]:TRP:CE2 | 3:a:3134[A]:GLN:NE2 | 2.72 | 0.57 |
| 3:a:3130[B]:TRP:CE2 | 3:a:3134[B]:GLN:NE2 | 2.72 | 0.57 |
| 3:a:3284[B]:LYS:CD | 3:a:3285[B]:VAL:H | 2.09 | 0.57 |
| 3:d:2960[B]:PHE:CD1 | 3:d:2960[B]:PHE:N | 2.72 | 0.57 |
| 3:d:3013[B]:ASP:OD1 | 3:d:3015[B]:THR:OG1 | 2.23 | 0.57 |
| 3:d:3129[B]:ILE:HD13 | 3:d:3190[B]:LEU:O | 2.04 | 0.57 |
| 2:B:2500:ILE:HG13 | 2:B:2501:PRO:HD2 | 1.87 | 0.57 |
| 3:C:2971[B]:ASP:CB | 3:L:3093[B]:HIS:ND1 | 2.56 | 0.57 |
| 3:C:3019[B]:HIS:H | 3:C:3019[B]:HIS:CD2 | 2.22 | 0.57 |
| 3:C:3130[B]:TRP:CZ2 | 3:C:3134[B]:GLN:NE2 | 2.73 | 0.57 |
| 2:E:2687:ILE:HD11 | 2:E:2695:MET:HG2 | 1.87 | 0.57 |
| 3:F:2942[B]:LEU:HD13 | 3:F:3033[B]:PHE:CZ | 2.40 | 0.57 |
| 3:F:2971[B]:ASP:C | 3:a:3090[B]:ASN:HB3 | 2.30 | 0.57 |
| 3:F:3129[A]:ILE:HD13 | 3:F:3190[A]:LEU:O | 2.04 | 0.57 |
| 3:F:3288[B]:MET:CG | 3:F:3295[B]:LEU:HD21 | 2.32 | 0.57 |
| 1:G:1427:HIS:CD2 | 1:G:1457:HIS:HE1 | 2.23 | 0.57 |
| 3:I:2942[A]:LEU:HD13 | 3:I:3033[A]:PHE:CZ | 2.40 | 0.57 |
| 3:I:2979[B]:GLN:NE2 | 3:R:3156[B]:MET:H | 2.02 | 0.57 |
| 3:I:2995[B]:GLN:HG2 | 3:I:3168[B]:THR:HG21 | 1.86 | 0.57 |
| 3:I:3130[B]:TRP:CZ2 | 3:I:3134[B]:GLN:NE2 | 2.73 | 0.57 |
| 3:I:3255[B]:PRO:CB | 3:R:2964[B]:PRO:CD | 2.83 | 0.57 |
| 1:J:179:HIS:HB2 | 1:J:213:VAL:HG11 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:2942[B]:LEU:HD13 | 3:L:3033[B]:PHE:CZ | 2.40 | 0.57 |
| 3:L:3130[B]:TRP:CE2 | 3:L:3134[B]:GLN:NE2 | 2.72 | 0.57 |
| 3:L:3130[B]:TRP:CZ2 | 3:L:3134[B]:GLN:NE2 | 2.73 | 0.57 |
| 3:L:3288[B]:MET:CG | 3:L:3295[B]:LEU:HD21 | 2.32 | 0.57 |
| 3:L:3293[A]:LYS:CB | 3:L:3294[A]:SER:CB | 2.54 | 0.57 |
| 2:N:2133:PRO:HG2 | 2:N:2140:ARG:HA | 1.84 | 0.57 |
| 3:O:2971[A]:ASP:CG | 3:O:2973[A]:THR:HG1 | 2.13 | 0.57 |
| 3:O:2991[B]:LEU:O | 3:O:2994[B]:LYS:HB3 | 2.03 | 0.57 |
| 3:O:3108[B]:HIS:HB2 | 3:X:2970[B]:PRO:CA | 2.33 | 0.57 |
| 3:O:3130[A]:TRP:CZ2 | 3:O:3134[A]:GLN:NE2 | 2.73 | 0.57 |
| 3:O:3225[B]:SER:OG | 3:O:3290[B]:ILE:HD13 | 2.04 | 0.57 |
| 3:O:3284[B]:LYS:HE2 | 3:O:3284[B]:LYS:CA | 2.29 | 0.57 |
| 3:R:2942[A]:LEU:HD13 | 3:R:3033[A]:PHE:CZ | 2.40 | 0.57 |
| 3:R:2961[B]:HIS:NE2 | 3:R:2980[B]:HIS:CE1 | 2.73 | 0.57 |
| 3:R:3019[A]:HIS:CD2 | 3:R:3019[A]:HIS:H | 2.22 | 0.57 |
| 3:R:3129[A]:ILE:HD13 | 3:R:3190[A]:LEU:O | 2.04 | 0.57 |
| 1:S:124:TYR:O | 1:S:137:ARG:NH2 | 2.38 | 0.57 |
| 1:S:837:HIS:HA | 1:S:1113:HIS:O | 2.04 | 0.57 |
| 1:S:898:GLY:N | 1:S:899:MET:HA | 2.20 | 0.57 |
| 2:T:2177:TYR:HB2 | 2:T:2300:ASN:HB2 | 1.87 | 0.57 |
| 3:U:3000[A]:LEU:N | 3:U:3000[A]:LEU:HD23 | 2.18 | 0.57 |
| 3:U:3130[A]:TRP:CZ2 | 3:U:3134[A]:GLN:NE2 | 2.73 | 0.57 |
| 3:U:3173[B]:THR:CG2 | 3:d:3152[B]:LYS:O | 2.50 | 0.57 |
| 3:U:3253[B]:GLU:N | 3:d:3255[B]:PRO:HG3 | 2.19 | 0.57 |
| 1:V:1358:LEU:HD23 | 1:V:1456:LEU:HD21 | 1.86 | 0.57 |
| 3:X:2965[A]:LEU:HD11 | 3:X:2974[A]:ALA:C | 2.28 | 0.57 |
| 1:Y:187:GLY:HA3 | 1:Y:195:SER:HB3 | 1.87 | 0.57 |
| 2:Z:2832:ALA:HB1 | 2:Z:2856:ILE:HG21 | 1.86 | 0.57 |
| 3:a:2961[A]:HIS:NE2 | 3:a:2980[A]:HIS:CE1 | 2.73 | 0.57 |
| 3:a:2991[A]:LEU:O | 3:a:2994[A]:LYS:HB3 | 2.03 | 0.57 |
| 3:a:3220[A]:ARG:HG2 | 3:a:3221[A]:ALA:H | 1.70 | 0.57 |
| 1:b:717:GLN:O | 1:b:721:GLU:HG3 | 2.05 | 0.57 |
| 1:b:977:GLU:HB3 | 1:b:979:LEU:HD21 | 1.86 | 0.57 |
| 3:d:3130[A]:TRP:CZ2 | 3:d:3134[A]:GLN:NE2 | 2.73 | 0.57 |
| 1:A:904:HIS:O | 1:A:907:ARG:HB3 | 2.05 | 0.57 |
| 1:A:941:LEU:HD11 | 1:A:959:PHE:CD2 | 2.40 | 0.57 |
| 2:B:2142:ALA:HB1 | 2:B:2143:CYS:HB2 | 1.85 | 0.57 |
| 3:C:2942[A]:LEU:HD13 | 3:C:3033[A]:PHE:CZ | 2.40 | 0.57 |
| 3:C:3147[B]:GLU:CD | 3:L:3169[B]:LYS:HZ2 | 1.91 | 0.57 |
| 3:C:3248[B]:LEU:CB | 3:L:2972[B]:GLY:C | 2.54 | 0.57 |
| 3:F:3180[B]:TYR:C | 3:F:3183[B]:LEU:HD22 | 2.30 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:883:CYS:N | 1:G:894:CYS:SG | 2.78 | 0.57 |
| 3:I:3150[B]:LYS:CA | 3:R:3172[B]:SER:HB3 | 2.35 | 0.57 |
| 3:I:3180[A]:TYR:C | 3:I:3183[A]:LEU:HD22 | 2.30 | 0.57 |
| 3:I:3284[B]:LYS:HE2 | 3:I:3284[B]:LYS:CA | 2.29 | 0.57 |
| 1:J:1241:GLY:HA2 | 1:J:1252:PRO:HB3 | 1.87 | 0.57 |
| 1:M:43:GLU:HG3 | 1:M:44:PRO:HA | 1.87 | 0.57 |
| 1:M:127:GLU:HG3 | 1:M:135:THR:HG23 | 1.86 | 0.57 |
| 1:M:589:GLN:HG2 | 1:M:594:ASP:HB3 | 1.87 | 0.57 |
| 1:M:602:THR:O | 1:M:605:SER:OG | 2.19 | 0.57 |
| 3:O:3160[B]:SER:CB | 3:X:3151[B]:LEU:HG | 2.35 | 0.57 |
| 3:O:3251[B]:ASP:O | 3:X:2967[B]:CYS:HB3 | 2.04 | 0.57 |
| 2:Q:2799:LYS:HA | 2:Q:2803:ARG:HH12 | 1.69 | 0.57 |
| 3:R:2986[A]:PRO:HB3 | 3:R:3127[A]:TRP:CE3 | 2.38 | 0.57 |
| 3:R:3251[B]:ASP:HB3 | 3:R:3252[B]:TYR:CD1 | 2.40 | 0.57 |
| 1:S:1498:ASN:ND2 | 1:S:1500:THR:O | 2.37 | 0.57 |
| 3:U:3130[A]:TRP:CE2 | 3:U:3134[A]:GLN:NE2 | 2.72 | 0.57 |
| 3:U:3161[B]:GLU:HB2 | 3:d:3260[B]:ARG:HD2 | 1.85 | 0.57 |
| 3:U:3176[B]:LYS:H | 3:U:3176[B]:LYS:CE | 2.17 | 0.57 |
| 3:U:3251[A]:ASP:HB3 | 3:U:3252[A]:TYR:CD1 | 2.40 | 0.57 |
| 1:V:329:ARG:HA | 1:Y:1583:CYS:O | 2.04 | 0.57 |
| 3:X:2942[B]:LEU:HD13 | 3:X:3033[B]:PHE:CZ | 2.40 | 0.57 |
| 3:X:3307[B]:PHE:HE1 | 3:X:3309[B]:PRO:CG | 2.08 | 0.57 |
| 1:Y:859:ALA:O | 1:Y:863:ALA:N | 2.38 | 0.57 |
| 1:Y:1618:LEU:HA | 3:d:3190[B]:LEU:HB2 | 1.87 | 0.57 |
| 3:a:2991[A]:LEU:O | 3:a:2994[A]:LYS:N | 2.37 | 0.57 |
| 1:b:838:ARG:NH1 | 1:b:915:ASN:OD1 | 2.38 | 0.57 |
| 3:d:3251[A]:ASP:HB3 | 3:d:3252[A]:TYR:CD1 | 2.40 | 0.57 |
| 2:B:2516:ASP:OD1 | 2:E:2168:ARG:NH2 | 2.35 | 0.56 |
| 3:C:3013[B]:ASP:OD1 | 3:C:3015[B]:THR:OG1 | 2.23 | 0.56 |
| 3:C:3153[B]:LYS:HD3 | 3:L:3155[B]:MET:CE | 2.30 | 0.56 |
| 3:C:3155[B]:MET:HG2 | 3:L:3154[B]:PRO:C | 2.30 | 0.56 |
| 3:F:2942[A]:LEU:HD13 | 3:F:3033[A]:PHE:CZ | 2.40 | 0.56 |
| 3:F:3130[B]:TRP:CE2 | 3:F:3134[B]:GLN:NE2 | 2.72 | 0.56 |
| 3:F:3152[B]:LYS:HB2 | 3:a:3172[B]:SER:H | 0.64 | 0.56 |
| 3:F:3173[A]:THR:HG22 | 3:F:3174[A]:GLY:H | 1.67 | 0.56 |
| 3:F:3284[B]:LYS:HE2 | 3:F:3284[B]:LYS:CA | 2.30 | 0.56 |
| 1:G:262:LYS:NZ | 1:G:795:GLU:OE1 | 2.36 | 0.56 |
| 2:H:2128:LEU:HD13 | 2:H:2286:HIS:CG | 2.40 | 0.56 |
| 3:I:3093[B]:HIS:CE1 | 3:I:3119[B]:HIS:CD2 | 2.92 | 0.56 |
| 3:I:3169[B]:LYS:NZ | 3:R:3149[B]:ASN:CG | 2.62 | 0.56 |
| 1:J:903:PRO:HG2 | 1:J:904:HIS:HD2 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2800:LYS:O | 3:L:3023[A]:ILE:CD1 | 2.53 | 0.56 |
| 3:L:2949[B]:LYS:HZ2 | 3:L:2950[B]:THR:HA | 1.69 | 0.56 |
| 3:L:3220[B]:ARG:HG2 | 3:L:3221[B]:ALA:H | 1.70 | 0.56 |
| 1:M:136:ALA:H | 1:M:190:PHE:HE2 | 1.51 | 0.56 |
| 3:O:2942[B]:LEU:HD13 | 3:O:3033[B]:PHE:CZ | 2.40 | 0.56 |
| 3:O:3153[B]:LYS:HG3 | 3:X:3176[B]:LYS:HD3 | 1.76 | 0.56 |
| 3:R:2960[A]:PHE:CD1 | 3:R:2960[A]:PHE:N | 2.72 | 0.56 |
| 3:R:2991[A]:LEU:O | 3:R:2994[A]:LYS:N | 2.37 | 0.56 |
| 3:R:3251[A]:ASP:HB3 | 3:R:3252[A]:TYR:CD1 | 2.40 | 0.56 |
| 3:R:3283[A]:ILE:CB | 3:R:3305[A]:ILE:HD11 | 2.35 | 0.56 |
| 1:S:879:SER:HB2 | 1:S:1182:ASN:HD22 | 1.70 | 0.56 |
| 3:U:3150[B]:LYS:CG | 3:d:3156[B]:MET:CG | 2.83 | 0.56 |
| 2:W:2808:PHE:CZ | 2:W:2821:LEU:HD13 | 2.33 | 0.56 |
| 3:X:2991[A]:LEU:O | 3:X:2994[A]:LYS:N | 2.37 | 0.56 |
| 3:X:3283[A]:ILE:CB | 3:X:3305[A]:ILE:HD11 | 2.35 | 0.56 |
| 1:Y:151:GLN:N | 1:Y:151:GLN:OE1 | 2.38 | 0.56 |
| 1:Y:1485:ALA:HB3 | 1:Y:1489:MET:HE2 | 1.85 | 0.56 |
| 3:a:3130[A]:TRP:CZ2 | 3:a:3134[A]:GLN:NE2 | 2.73 | 0.56 |
| 3:a:3130[B]:TRP:CZ2 | 3:a:3134[B]:GLN:NE2 | 2.73 | 0.56 |
| 1:b:35:GLN:OE1 | 1:b:35:GLN:HA | 2.05 | 0.56 |
| 3:d:3093[B]:HIS:CE1 | 3:d:3119[B]:HIS:CD2 | 2.92 | 0.56 |
| 3:d:3130[B]:TRP:CE2 | 3:d:3134[B]:GLN:NE2 | 2.72 | 0.56 |
| 2:B:2627:GLY:HA3 | 2:B:2703:PHE:O | 2.05 | 0.56 |
| 3:F:2987[B]:HIS:NE2 | 3:F:3178[B]:PHE:HE1 | 1.95 | 0.56 |
| 3:F:2991[A]:LEU:O | 3:F:2994[A]:LYS:N | 2.37 | 0.56 |
| 3:F:3120[B]:HIS:C | 3:F:3122[B]:ASN:N | 2.55 | 0.56 |
| 3:F:3163[B]:ASN:H | 3:a:3147[B]:GLU:CD | 2.13 | 0.56 |
| 1:G:1543:ILE:HD11 | 3:L:3272[A]:HIS:CD2 | 2.40 | 0.56 |
| 2:H:2863:ARG:HB3 | 2:H:2865:ILE:HG13 | 1.87 | 0.56 |
| 3:I:2932[A]:PRO:CA | 3:I:2935[A]:ILE:HD12 | 2.30 | 0.56 |
| 3:I:2966[B]:SER:HA | 3:R:3256[B]:TRP:CA | 2.34 | 0.56 |
| 3:I:3255[B]:PRO:HB3 | 3:R:2964[B]:PRO:HD2 | 1.86 | 0.56 |
| 3:I:3293[A]:LYS:CD | 3:I:3294[A]:SER:N | 2.64 | 0.56 |
| 1:J:361:GLU:HG2 | 1:J:363:THR:HG22 | 1.87 | 0.56 |
| 3:L:2942[A]:LEU:HD13 | 3:L:3033[A]:PHE:CZ | 2.40 | 0.56 |
| 3:O:2949[B]:LYS:HZ2 | 3:O:2950[B]:THR:HA | 1.70 | 0.56 |
| 3:O:3130[B]:TRP:CZ2 | 3:O:3134[B]:GLN:NE2 | 2.73 | 0.56 |
| 1:P:105:VAL:HB | 1:P:137:ARG:NH2 | 2.20 | 0.56 |
| 3:U:3135[B]:LYS:HG3 | 3:U:3141[B]:TYR:CD1 | 2.33 | 0.56 |
| 3:U:3257[B]:ALA:H | 3:d:2969[B]:TYR:N | 1.96 | 0.56 |
| 3:U:3284[A]:LYS:HE2 | 3:U:3284[A]:LYS:CA | 2.29 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2969[A]:TYR:CD2 | 3:X:2970[A]:PRO:HG2 | 2.38 | 0.56 |
| 3:X:3180[B]:TYR:C | 3:X:3183[B]:LEU:HD22 | 2.30 | 0.56 |
| 3:X:3251[A]:ASP:HB3 | 3:X:3252[A]:TYR:CD1 | 2.40 | 0.56 |
| 3:X:3293[A]:LYS:CD | 3:X:3294[A]:SER:N | 2.64 | 0.56 |
| 3:a:2942[B]:LEU:HD13 | 3:a:3033[B]:PHE:CZ | 2.40 | 0.56 |
| 3:a:3284[A]:LYS:HE2 | 3:a:3284[A]:LYS:CA | 2.30 | 0.56 |
| 1:b:1013:ILE:HD11 | 1:b:1175:PHE:CD2 | 2.40 | 0.56 |
| 3:d:3019[B]:HIS:CD2 | 3:d:3019[B]:HIS:H | 2.22 | 0.56 |
| 3:d:3130[A]:TRP:CE2 | 3:d:3134[A]:GLN:NE2 | 2.72 | 0.56 |
| 3:d:3283[B]:ILE:CB | 3:d:3305[B]:ILE:HD11 | 2.35 | 0.56 |
| 1:A:128:ILE:HG22 | 1:A:130:PHE:O | 2.05 | 0.56 |
| 1:A:1195:ASP:HA | 1:A:1196:ILE:HG22 | 1.86 | 0.56 |
| 2:B:2161:GLN:HE22 | 2:B:2348:THR:HG21 | 1.71 | 0.56 |
| 2:B:2300:ASN:OD1 | 2:B:2303:ARG:NH1 | 2.38 | 0.56 |
| 2:B:2344:LEU:HA | 2:B:2345:ASN:O | 2.05 | 0.56 |
| 3:C:2983[B]:VAL:HB | 3:L:3160[B]:SER:HA | 1.86 | 0.56 |
| 3:C:3154[B]:PRO:CB | 3:L:3151[B]:LEU:CA | 2.79 | 0.56 |
| 3:C:3180[A]:TYR:C | 3:C:3183[A]:LEU:HD22 | 2.30 | 0.56 |
| 3:C:3220[B]:ARG:HG2 | 3:C:3221[B]:ALA:H | 1.70 | 0.56 |
| 3:C:3255[B]:PRO:HG2 | 3:L:2962[B]:GLY:N | 2.05 | 0.56 |
| 3:C:3283[B]:ILE:CB | 3:C:3305[B]:ILE:HD11 | 2.35 | 0.56 |
| 1:D:885:SER:HB3 | 1:D:886:PRO:HA | 1.86 | 0.56 |
| 2:E:2568:HIS:ND1 | 2:E:2765:PRO:HB3 | 2.20 | 0.56 |
| 3:F:3130[A]:TRP:CE2 | 3:F:3134[A]:GLN:NE2 | 2.72 | 0.56 |
| 3:F:3180[A]:TYR:C | 3:F:3183[A]:LEU:HD22 | 2.30 | 0.56 |
| 3:F:3225[B]:SER:OG | 3:F:3290[B]:ILE:HD13 | 2.04 | 0.56 |
| 3:F:3255[B]:PRO:N | 3:a:2966[B]:SER:OG | 2.38 | 0.56 |
| 1:G:480:CYS:SG | 1:G:621:LEU:HD11 | 2.45 | 0.56 |
| 2:H:2180:TRP:HD1 | 2:H:2247:ILE:HD11 | 1.69 | 0.56 |
| 3:I:2931[B]:THR:HG1 | 3:I:2934[B]:GLU:CD | 2.03 | 0.56 |
| 3:I:2965[B]:LEU:CD1 | 3:R:3256[B]:TRP:NE1 | 2.66 | 0.56 |
| 3:I:2965[B]:LEU:HA | 3:R:3253[B]:GLU:CD | 2.30 | 0.56 |
| 3:I:2973[B]:THR:OG1 | 3:R:3093[B]:HIS:HD2 | 1.88 | 0.56 |
| 3:I:2981[B]:GLY:N | 3:R:2968[B]:GLN:OE1 | 2.38 | 0.56 |
| 3:I:3013[A]:ASP:OD1 | 3:I:3015[A]:THR:OG1 | 2.23 | 0.56 |
| 3:I:3152[B]:LYS:HB3 | 3:R:3171[B]:HIS:C | 2.28 | 0.56 |
| 3:I:3259[B]:ASP:H | 3:R:3162[B]:ASP:CB | 2.18 | 0.56 |
| 3:I:3283[B]:ILE:CB | 3:I:3305[B]:ILE:HD11 | 2.35 | 0.56 |
| 1:J:353:ASN:HD22 | 1:J:772:ARG:HH22 | 1.51 | 0.56 |
| 1:J:729:VAL:HG12 | 1:J:782:THR:HG23 | 1.86 | 0.56 |
| 1:J:836:GLN:HG3 | 1:J:838:ARG:NH2 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:841:LYS:HA | 1:J:1117:ASP:HB2 | 1.86 | 0.56 |
| 1:J:871:GLN:NE2 | 1:J:966:SER:OG | 2.36 | 0.56 |
| 1:J:1013:ILE:HG21 | 1:J:1192:TYR:CD1 | 2.40 | 0.56 |
| 1:J:1034:GLU:HB2 | 1:J:1182:ASN:HD21 | 1.71 | 0.56 |
| 1:J:1439:VAL:HG22 | 1:J:1440:HIS:HD2 | 1.71 | 0.56 |
| 1:J:1587:ALA:HA | 1:J:1614:GLU:HG2 | 1.88 | 0.56 |
| 3:L:2960[A]:PHE:CD1 | 3:L:2960[A]:PHE:N | 2.72 | 0.56 |
| 3:L:3093[A]:HIS:CE1 | 3:L:3119[A]:HIS:CD2 | 2.92 | 0.56 |
| 3:L:3180[A]:TYR:C | 3:L:3183[A]:LEU:HD22 | 2.30 | 0.56 |
| 3:L:3298[A]:ASN:HA | 3:L:3299[A]:LEU:HB3 | 1.88 | 0.56 |
| 1:M:479:CYS:HB3 | 1:M:670:PRO:HD3 | 1.87 | 0.56 |
| 3:O:2971[B]:ASP:CG | 3:O:2973[B]:THR:HG1 | 2.12 | 0.56 |
| 3:O:2995[A]:GLN:HG2 | 3:O:3168[A]:THR:HG21 | 1.85 | 0.56 |
| 3:O:3180[A]:TYR:C | 3:O:3183[A]:LEU:HD22 | 2.30 | 0.56 |
| 3:O:3252[B]:TYR:HA | 3:X:3157[B]:PRO:HA | 1.86 | 0.56 |
| 3:O:3256[B]:TRP:NE1 | 3:X:3161[B]:GLU:CG | 2.68 | 0.56 |
| 3:O:3256[B]:TRP:NE1 | 3:X:3161[B]:GLU:HG3 | 2.21 | 0.56 |
| 3:O:3283[A]:ILE:CB | 3:O:3305[A]:ILE:HD11 | 2.35 | 0.56 |
| 3:O:3293[B]:LYS:CD | 3:O:3294[B]:SER:N | 2.64 | 0.56 |
| 1:P:931:TRP:CG | 1:P:1018:ILE:HD11 | 2.39 | 0.56 |
| 3:R:2948[B]:ASP:HB3 | 3:R:2953[B]:GLY:CA | 2.24 | 0.56 |
| 3:R:2991[B]:LEU:O | 3:R:2994[B]:LYS:HB3 | 2.03 | 0.56 |
| 3:R:3130[A]:TRP:CZ2 | 3:R:3134[A]:GLN:NE2 | 2.73 | 0.56 |
| 3:R:3220[A]:ARG:HG2 | 3:R:3221[A]:ALA:H | 1.70 | 0.56 |
| 3:R:3268[A]:LYS:O | 3:R:3271[A]:VAL:HG23 | 2.06 | 0.56 |
| 3:U:2965[B]:LEU:CG | 3:d:3221[B]:ALA:N | 2.66 | 0.56 |
| 3:U:2969[B]:TYR:CD1 | 3:d:3107[B]:LEU:HD13 | 2.38 | 0.56 |
| 3:U:3151[B]:LEU:C | 3:d:3153[B]:LYS:HA | 2.31 | 0.56 |
| 3:U:3188[A]:ASP:N | 3:U:3188[A]:ASP:OD2 | 2.36 | 0.56 |
| 3:U:3268[A]:LYS:O | 3:U:3271[A]:VAL:HG23 | 2.06 | 0.56 |
| 3:U:3283[A]:ILE:CB | 3:U:3305[A]:ILE:HD11 | 2.35 | 0.56 |
| 3:U:3283[B]:ILE:CB | 3:U:3305[B]:ILE:HD11 | 2.35 | 0.56 |
| 3:U:3293[B]:LYS:CB | 3:U:3294[B]:SER:CB | 2.54 | 0.56 |
| 1:V:392:PRO:O | 1:V:395:THR:OG1 | 2.23 | 0.56 |
| 1:V:1296:VAL:HB | 1:V:1446:ASP:HB3 | 1.88 | 0.56 |
| 2:W:2234:GLN:HG3 | 2:W:2235:PRO:HD2 | 1.86 | 0.56 |
| 2:W:2235:PRO:HG3 | 2:W:2240:GLN:NE2 | 2.20 | 0.56 |
| 3:X:3130[A]:TRP:CZ2 | 3:X:3134[A]:GLN:NE2 | 2.73 | 0.56 |
| 3:X:3130[B]:TRP:CZ2 | 3:X:3134[B]:GLN:NE2 | 2.73 | 0.56 |
| 1:Y:190:PHE:HB3 | 1:Y:193:SER:HB2 | 1.87 | 0.56 |
| 2:Z:2121:THR:HG23 | 2:c:2615:TRP:CH2 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:2542:TYR:HB2 | 2:Z:2573:TYR:HE1 | 1.70 | 0.56 |
| 2:Z:2764:THR:HB | 2:Z:2767:LYS:HG3 | 1.87 | 0.56 |
| 3:a:3000[A]:LEU:N | 3:a:3000[A]:LEU:HD23 | 2.18 | 0.56 |
| 3:a:3173[A]:THR:HG22 | 3:a:3174[A]:GLY:H | 1.67 | 0.56 |
| 3:a:3283[B]:ILE:CB | 3:a:3305[B]:ILE:HD11 | 2.35 | 0.56 |
| 1:b:372:ALA:O | 1:b:375:SER:OG | 2.22 | 0.56 |
| 1:b:517:THR:HG21 | 1:b:708:PHE:HE1 | 1.70 | 0.56 |
| 1:b:749:VAL:HB | 1:b:754:GLU:HB3 | 1.87 | 0.56 |
| 3:d:2965[B]:LEU:HD11 | 3:d:2974[B]:ALA:C | 2.28 | 0.56 |
| 3:d:2991[A]:LEU:O | 3:d:2994[A]:LYS:N | 2.37 | 0.56 |
| 3:d:3220[A]:ARG:HH11 | 3:d:3220[A]:ARG:CG | 2.12 | 0.56 |
| 3:C:3156[B]:MET:HA | 3:C:3157[B]:PRO:C | 2.26 | 0.56 |
| 3:C:3284[A]:LYS:HE2 | 3:C:3284[A]:LYS:CA | 2.30 | 0.56 |
| 1:D:137:ARG:NH1 | 1:D:203:ASP:OD1 | 2.39 | 0.56 |
| 1:D:883:CYS:N | 1:D:894:CYS:SG | 2.78 | 0.56 |
| 3:F:2975[B]:PHE:CE1 | 3:a:2961[B]:HIS:O | 2.58 | 0.56 |
| 3:F:3298[A]:ASN:HA | 3:F:3299[A]:LEU:HB3 | 1.88 | 0.56 |
| 3:I:3212[A]:ARG:HH11 | 3:I:3212[A]:ARG:CG | 2.12 | 0.56 |
| 3:I:3268[A]:LYS:O | 3:I:3271[A]:VAL:HG23 | 2.06 | 0.56 |
| 3:I:3284[A]:LYS:CD | 3:I:3285[A]:VAL:H | 2.09 | 0.56 |
| 2:K:2092:VAL:HG11 | 2:K:2188:PRO:HB3 | 1.87 | 0.56 |
| 3:L:3180[B]:TYR:C | 3:L:3183[B]:LEU:HD22 | 2.30 | 0.56 |
| 3:L:3183[A]:LEU:N | 3:L:3184[A]:ASN:HA | 2.12 | 0.56 |
| 3:L:3251[A]:ASP:HB3 | 3:L:3252[A]:TYR:CD1 | 2.40 | 0.56 |
| 3:L:3268[A]:LYS:O | 3:L:3271[A]:VAL:HG23 | 2.06 | 0.56 |
| 2:N:2128:LEU:HD23 | 2:N:2216:PHE:HZ | 1.70 | 0.56 |
| 3:O:3157[B]:PRO:CB | 3:X:3150[B]:LYS:HA | 2.36 | 0.56 |
| 3:O:3162[B]:ASP:N | 3:O:3162[B]:ASP:OD1 | 2.31 | 0.56 |
| 3:O:3281[A]:PHE:HE1 | 3:O:3305[A]:ILE:HD13 | 1.71 | 0.56 |
| 1:P:157:GLU:OE2 | 1:P:296:ARG:NH2 | 2.39 | 0.56 |
| 2:Q:2596:THR:HG21 | 2:Q:2783:PHE:HZ | 1.71 | 0.56 |
| 3:R:2942[B]:LEU:HD13 | 3:R:3033[B]:PHE:CZ | 2.40 | 0.56 |
| 3:U:2975[B]:PHE:CE1 | 3:d:3256[B]:TRP:NE1 | 2.71 | 0.56 |
| 2:Z:2568:HIS:ND1 | 2:Z:2765:PRO:HB3 | 2.20 | 0.56 |
| 1:b:864:ASP:HB3 | 1:b:869:GLY:HA3 | 1.86 | 0.56 |
| 2:c:2826:GLU:HG2 | 2:c:2876:LYS:HD3 | 1.86 | 0.56 |
| 3:d:3251[B]:ASP:HB3 | 3:d:3252[B]:TYR:CD1 | 2.40 | 0.56 |
| 1:A:1195:ASP:HA | 1:A:1196:ILE:CB | 2.36 | 0.56 |
| 3:C:2971[B]:ASP:HB2 | 3:L:3090[B]:ASN:HA | 1.88 | 0.56 |
| 3:C:3255[B]:PRO:CD | 3:L:2961[B]:HIS:C | 2.78 | 0.56 |
| 1:D:1209:ASP:O | 1:D:1211:TYR:HB3 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:2641:GLN:HB3 | 2:E:2643:GLU:OE1 | 2.05 | 0.56 |
| 3:F:3019[A]:HIS:CD2 | 3:F:3019[A]:HIS:H | 2.22 | 0.56 |
| 3:F:3256[B]:TRP:N | 3:a:2966[B]:SER:HA | 2.20 | 0.56 |
| 3:F:3293[A]:LYS:CB | 3:F:3294[A]:SER:CB | 2.54 | 0.56 |
| 3:I:3153[B]:LYS:HD2 | 3:R:3155[B]:MET:C | 2.31 | 0.56 |
| 3:I:3255[B]:PRO:HG3 | 3:R:2964[B]:PRO:CD | 2.36 | 0.56 |
| 1:J:533:VAL:HG12 | 1:J:540:THR:HG22 | 1.87 | 0.56 |
| 1:J:1028:VAL:HA | 1:J:1035:TYR:CD2 | 2.40 | 0.56 |
| 2:K:2799:LYS:HA | 2:K:2803:ARG:HH12 | 1.70 | 0.56 |
| 3:L:3130[A]:TRP:CZ2 | 3:L:3134[A]:GLN:NE2 | 2.73 | 0.56 |
| 3:L:3283[A]:ILE:CB | 3:L:3305[A]:ILE:HD11 | 2.35 | 0.56 |
| 3:L:3283[B]:ILE:CB | 3:L:3305[B]:ILE:HD11 | 2.35 | 0.56 |
| 3:O:3013[A]:ASP:OD1 | 3:O:3015[A]:THR:OG1 | 2.23 | 0.56 |
| 2:Q:2830:GLN:O | 2:Q:2863:ARG:NH2 | 2.38 | 0.56 |
| 3:R:3093[B]:HIS:CE1 | 3:R:3119[B]:HIS:CD2 | 2.92 | 0.56 |
| 2:T:2799:LYS:HA | 2:T:2803:ARG:HH12 | 1.70 | 0.56 |
| 3:U:2948[A]:ASP:HB3 | 3:U:2953[A]:GLY:CA | 2.24 | 0.56 |
| 3:U:2961[A]:HIS:NE2 | 3:U:2980[A]:HIS:CE1 | 2.73 | 0.56 |
| 3:U:3220[A]:ARG:HG2 | 3:U:3221[A]:ALA:H | 1.70 | 0.56 |
| 3:U:3255[B]:PRO:HG3 | 3:d:3252[B]:TYR:CA | 1.99 | 0.56 |
| 1:V:109:LEU:HG | 1:V:118:ALA:HB1 | 1.87 | 0.56 |
| 2:W:2833:GLY:HA3 | 2:W:2854:MET:HE1 | 1.88 | 0.56 |
| 3:X:3019[A]:HIS:H | 3:X:3019[A]:HIS:CD2 | 2.22 | 0.56 |
| 3:X:3188[A]:ASP:N | 3:X:3188[A]:ASP:OD2 | 2.36 | 0.56 |
| 1:Y:1075:GLU:HG2 | 2:c:2900:SER:HA | 1.88 | 0.56 |
| 1:Y:1542:ARG:O | 3:d:3002[B]:ALA:HB2 | 2.05 | 0.56 |
| 2:Z:2651:GLN:CD | 2:Z:2651:GLN:H | 2.13 | 0.56 |
| 3:a:3129[A]:ILE:HD13 | 3:a:3190[A]:LEU:O | 2.04 | 0.56 |
| 3:a:3251[A]:ASP:HB3 | 3:a:3252[A]:TYR:CD1 | 2.40 | 0.56 |
| 3:a:3268[A]:LYS:O | 3:a:3271[A]:VAL:HG23 | 2.06 | 0.56 |
| 2:c:2698:LEU:HD12 | 2:c:2838:LEU:HB3 | 1.86 | 0.56 |
| 2:c:2879:LEU:HD12 | 2:c:2899:PRO:HB2 | 1.88 | 0.56 |
| 3:C:2949[A]:LYS:NZ | 3:C:2950[A]:THR:HA | 2.21 | 0.56 |
| 3:C:2965[A]:LEU:HD11 | 3:C:2974[A]:ALA:C | 2.28 | 0.56 |
| 3:C:3153[B]:LYS:HA | 3:L:3173[B]:THR:C | 2.30 | 0.56 |
| 3:C:3255[B]:PRO:HD3 | 3:L:2961[B]:HIS:O | 2.05 | 0.56 |
| 1:D:1242:ASN:ND2 | 1:D:1479:TYR:OH | 2.38 | 0.56 |
| 2:E:2122:ILE:O | 2:E:2125:PHE:HB2 | 2.05 | 0.56 |
| 3:F:2965[B]:LEU:CA | 3:a:3255[B]:PRO:HA | 2.34 | 0.56 |
| 3:F:3130[A]:TRP:CZ2 | 3:F:3134[A]:GLN:NE2 | 2.73 | 0.56 |
| 3:F:3200[B]:LEU:O | 3:F:3204[B]:LEU:HD13 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2956[B]:LYS:CD | 3:R:3257[B]:ALA:HB3 | 2.22 | 0.56 |
| 3:I:2969[B]:TYR:HA | 3:R:2989[B]:HIS:NE2 | 2.19 | 0.56 |
| 3:I:3093[A]:HIS:CE1 | 3:I:3119[A]:HIS:CD2 | 2.92 | 0.56 |
| 3:I:3154[B]:PRO:HA | 3:R:3153[B]:LYS:O | 2.05 | 0.56 |
| 3:L:2960[B]:PHE:CD1 | 3:L:2960[B]:PHE:N | 2.72 | 0.56 |
| 3:L:3268[B]:LYS:O | 3:L:3271[B]:VAL:HG23 | 2.06 | 0.56 |
| 3:L:3281[B]:PHE:HE1 | 3:L:3305[B]:ILE:HD13 | 1.71 | 0.56 |
| 1:M:684:ARG:O | 1:M:687:SER:OG | 2.23 | 0.56 |
| 1:M:1164:ASP:OD1 | 1:M:1164:ASP:N | 2.37 | 0.56 |
| 1:M:1182:ASN:OD1 | 1:M:1182:ASN:N | 2.34 | 0.56 |
| 1:M:1604:ASP:OD1 | 1:M:1605:ARG:NH1 | 2.39 | 0.56 |
| 3:O:2966[B]:SER:HB2 | 3:O:2977[B]:CYS:CB | 2.21 | 0.56 |
| 3:O:2974[B]:ALA:CB | 3:X:2977[B]:CYS:HA | 2.36 | 0.56 |
| 3:O:3173[B]:THR:HG22 | 3:O:3174[B]:GLY:H | 1.67 | 0.56 |
| 3:O:3200[A]:LEU:O | 3:O:3204[A]:LEU:HD13 | 2.06 | 0.56 |
| 3:O:3220[A]:ARG:HG2 | 3:O:3221[A]:ALA:H | 1.70 | 0.56 |
| 1:P:302:ALA:H | 1:P:363:THR:HB | 1.70 | 0.56 |
| 2:Q:2426:PHE:HB3 | 2:Q:2445:MET:HE1 | 1.88 | 0.56 |
| 3:R:3180[A]:TYR:C | 3:R:3183[A]:LEU:HD22 | 2.30 | 0.56 |
| 3:R:3268[B]:LYS:O | 3:R:3271[B]:VAL:HG23 | 2.06 | 0.56 |
| 2:T:2142:ALA:HB1 | 2:T:2143:CYS:HB2 | 1.88 | 0.56 |
| 2:T:2757:PRO:HB3 | 2:T:2760:ARG:HH21 | 1.70 | 0.56 |
| 3:U:2942[B]:LEU:HD13 | 3:U:3033[B]:PHE:CZ | 2.40 | 0.56 |
| 3:U:2979[B]:GLN:HE21 | 3:d:3153[B]:LYS:HE2 | 1.69 | 0.56 |
| 3:U:3180[B]:TYR:C | 3:U:3183[B]:LEU:HD22 | 2.30 | 0.56 |
| 3:U:3251[B]:ASP:HB3 | 3:U:3252[B]:TYR:CD1 | 2.40 | 0.56 |
| 3:U:3257[B]:ALA:N | 3:d:2968[B]:GLN:C | 2.61 | 0.56 |
| 2:W:2161:GLN:OE1 | 2:W:2345:ASN:ND2 | 2.38 | 0.56 |
| 3:X:3220[B]:ARG:HH11 | 3:X:3220[B]:ARG:CG | 2.12 | 0.56 |
| 2:Z:2476:LEU:HD22 | 4:MA:2:NAG:H82 | 1.86 | 0.56 |
| 2:Z:2644:LEU:HB2 | 2:Z:2686:LEU:HB3 | 1.88 | 0.56 |
| 3:a:2942[A]:LEU:HD13 | 3:a:3033[A]:PHE:CZ | 2.40 | 0.56 |
| 3:a:3200[B]:LEU:O | 3:a:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 3:a:3281[B]:PHE:HE1 | 3:a:3305[B]:ILE:HD13 | 1.71 | 0.56 |
| 3:d:3180[A]:TYR:C | 3:d:3183[A]:LEU:HD22 | 2.30 | 0.56 |
| 3:C:3090[B]:ASN:CG | 3:L:2972[B]:GLY:C | 2.67 | 0.56 |
| 3:C:3281[A]:PHE:HE1 | 3:C:3305[A]:ILE:HD13 | 1.71 | 0.56 |
| 1:D:389:THR:OG1 | 4:j:1:NAG:O7 | 2.21 | 0.56 |
| 1:D:830:ASN:N | 1:D:830:ASN:OD1 | 2.30 | 0.56 |
| 3:F:3153[B]:LYS:HD3 | 3:a:3155[B]:MET:HB3 | 1.83 | 0.56 |
| 3:F:3155[B]:MET:O | 3:a:3153[B]:LYS:CE | 2.53 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3251[A]:ASP:HB3 | 3:F:3252[A]:TYR:CD1 | 2.40 | 0.56 |
| 1:G:460:GLU:OE2 | 1:G:1368:ARG:NH2 | 2.38 | 0.56 |
| 1:G:668:MET:HE2 | 1:G:668:MET:HA | 1.86 | 0.56 |
| 1:G:1281:MET:HE1 | 1:G:1330:VAL:HG23 | 1.88 | 0.56 |
| 2:H:2179:ASP:HA | 2:H:2300:ASN:ND2 | 2.21 | 0.56 |
| 3:I:3172[B]:SER:HB3 | 3:R:3150[B]:LYS:O | 2.00 | 0.56 |
| 3:I:3220[A]:ARG:HG2 | 3:I:3221[A]:ALA:H | 1.70 | 0.56 |
| 3:I:3255[B]:PRO:O | 3:R:2966[B]:SER:OG | 2.21 | 0.56 |
| 3:I:3268[B]:LYS:O | 3:I:3271[B]:VAL:HG23 | 2.06 | 0.56 |
| 1:J:873:VAL:CG2 | 1:J:912:ASN:HB3 | 2.35 | 0.56 |
| 2:K:2128:LEU:HD13 | 2:K:2286:HIS:CG | 2.41 | 0.56 |
| 2:K:2680:HIS:CE1 | 2:K:2711:HIS:NE2 | 2.73 | 0.56 |
| 3:L:3083[B]:ILE:HD12 | 3:L:3260[B]:ARG:HB2 | 1.88 | 0.56 |
| 1:M:1553:ILE:HD11 | 1:M:1622:GLN:HG3 | 1.88 | 0.56 |
| 2:N:2795:ILE:O | 2:N:2799:LYS:HG3 | 2.06 | 0.56 |
| 3:O:2969[B]:TYR:HE1 | 3:X:3168[B]:THR:CG2 | 2.18 | 0.56 |
| 3:O:3251[A]:ASP:HB3 | 3:O:3252[A]:TYR:CD1 | 2.40 | 0.56 |
| 3:O:3298[B]:ASN:CB | 3:O:3300[B]:LEU:CD2 | 2.61 | 0.56 |
| 1:P:372:ALA:O | 1:P:375:SER:OG | 2.21 | 0.56 |
| 1:P:946:GLU:HG2 | 1:P:955:LYS:HB3 | 1.88 | 0.56 |
| 2:T:2089:ARG:HD2 | 2:T:2175:VAL:O | 2.06 | 0.56 |
| 2:T:2554:PRO:HA | 2:T:2555:GLU:HB2 | 1.87 | 0.56 |
| 3:U:2961[B]:HIS:NE2 | 3:U:2980[B]:HIS:CE1 | 2.73 | 0.56 |
| 3:U:2969[B]:TYR:HB2 | 3:d:3256[B]:TRP:NE1 | 2.21 | 0.56 |
| 3:U:3157[B]:PRO:O | 3:d:3147[B]:GLU:CD | 2.48 | 0.56 |
| 2:W:2218:SER:HG | 2:W:2221:THR:HG1 | 1.53 | 0.56 |
| 1:Y:912:ASN:ND2 | 1:Y:1091:ASN:OD1 | 2.38 | 0.56 |
| 3:a:3083[A]:ILE:HD12 | 3:a:3260[A]:ARG:HB2 | 1.88 | 0.56 |
| 3:a:3307[B]:PHE:HE1 | 3:a:3309[B]:PRO:CG | 2.08 | 0.56 |
| 1:b:24:ALA:HB3 | 1:b:83:HIS:HB3 | 1.87 | 0.56 |
| 3:d:2942[A]:LEU:HD13 | 3:d:3033[A]:PHE:CZ | 2.40 | 0.56 |
| 3:C:2969[B]:TYR:CA | 3:L:2985[B]:PHE:CE2 | 2.61 | 0.56 |
| 3:C:3200[A]:LEU:O | 3:C:3204[A]:LEU:HD13 | 2.06 | 0.56 |
| 3:C:3251[A]:ASP:HB3 | 3:C:3252[A]:TYR:CD1 | 2.40 | 0.56 |
| 3:C:3283[A]:ILE:CB | 3:C:3305[A]:ILE:HD11 | 2.35 | 0.56 |
| 2:E:2398:PHE:HE1 | 2:E:2466:THR:HG21 | 1.70 | 0.56 |
| 3:F:2961[A]:HIS:NE2 | 3:F:2980[A]:HIS:CE1 | 2.73 | 0.56 |
| 3:F:2966[B]:SER:CB | 3:a:3255[B]:PRO:C | 2.78 | 0.56 |
| 3:F:3093[B]:HIS:CE1 | 3:F:3119[B]:HIS:CD2 | 2.92 | 0.56 |
| 1:G:1636:ASN:CB | 1:G:1639:LYS:HD3 | 2.36 | 0.56 |
| 3:I:3154[B]:PRO:CD | 3:R:3155[B]:MET:CG | 2.67 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3281[A]:PHE:HE1 | 3:I:3305[A]:ILE:HD13 | 1.71 | 0.56 |
| 2:K:2133:PRO:HG2 | 2:K:2140:ARG:HA | 1.87 | 0.56 |
| 3:L:3220[A]:ARG:HG2 | 3:L:3221[A]:ALA:H | 1.70 | 0.56 |
| 1:M:148:GLN:C | 1:M:150:GLY:H | 2.13 | 0.56 |
| 1:M:452:ILE:HG21 | 1:M:1367:SER:HB2 | 1.88 | 0.56 |
| 1:M:673:PHE:HB3 | 1:M:677:LEU:HB2 | 1.88 | 0.56 |
| 1:M:1328:SER:HB2 | 1:M:1523:LEU:HD13 | 1.88 | 0.56 |
| 2:N:2867:PRO:O | 2:N:2870:LEU:HB2 | 2.06 | 0.56 |
| 3:O:2963[B]:MET:HB2 | 3:X:2970[B]:PRO:HD2 | 1.88 | 0.56 |
| 3:O:2964[B]:PRO:HA | 3:X:2975[B]:PHE:CE2 | 2.29 | 0.56 |
| 3:O:2977[B]:CYS:CA | 3:X:3153[B]:LYS:HG2 | 2.05 | 0.56 |
| 3:O:3169[B]:LYS:CE | 3:X:3148[B]:ILE:N | 2.67 | 0.56 |
| 1:P:905:TRP:HE1 | 1:P:1083:PRO:HD2 | 1.70 | 0.56 |
| 1:P:1339:SER:CB | 1:P:1340:GLY:HA2 | 2.36 | 0.56 |
| 2:Q:2711:HIS:HA | 2:Q:2714:VAL:HG22 | 1.86 | 0.56 |
| 3:R:3180[B]:TYR:C | 3:R:3183[B]:LEU:HD22 | 2.30 | 0.56 |
| 3:R:3200[B]:LEU:O | 3:R:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 1:S:516:TRP:HB2 | 1:S:579:LEU:HD13 | 1.87 | 0.56 |
| 1:S:564:ASP:OD1 | 1:S:564:ASP:N | 2.39 | 0.56 |
| 3:U:3228[B]:VAL:CG2 | 3:U:3245[B]:PHE:CE2 | 2.89 | 0.56 |
| 3:U:3268[B]:LYS:O | 3:U:3271[B]:VAL:HG23 | 2.06 | 0.56 |
| 1:V:492:ARG:HD2 | 1:V:692:VAL:HG13 | 1.87 | 0.56 |
| 2:W:2680:HIS:NE2 | 2:W:2684:HIS:CD2 | 2.74 | 0.56 |
| 3:X:3013[B]:ASP:OD1 | 3:X:3015[B]:THR:OG1 | 2.23 | 0.56 |
| 3:X:3083[B]:ILE:HD12 | 3:X:3260[B]:ARG:HB2 | 1.88 | 0.56 |
| 3:X:3135[A]:LYS:HG3 | 3:X:3141[A]:TYR:CD1 | 2.33 | 0.56 |
| 1:Y:148:GLN:HG3 | 1:Y:150:GLY:O | 2.06 | 0.56 |
| 1:Y:215:ARG:HE | 1:Y:279:LEU:HA | 1.70 | 0.56 |
| 3:a:3293[B]:LYS:CD | 3:a:3294[B]:SER:N | 2.64 | 0.56 |
| 1:b:648:GLN:OE1 | 1:b:651:ARG:NH1 | 2.38 | 0.56 |
| 1:b:1209:ASP:OD1 | 1:b:1209:ASP:N | 2.22 | 0.56 |
| 2:c:2373:MET:HB3 | 2:c:2381:LEU:HD11 | 1.87 | 0.56 |
| 2:c:2742:MET:HA | 2:c:2765:PRO:HB2 | 1.87 | 0.56 |
| 1:A:326:GLU:CD | 1:A:326:GLU:H | 2.13 | 0.56 |
| 1:A:516:TRP:CD2 | 1:A:606:ILE:HD11 | 2.41 | 0.56 |
| 1:A:1573:CYS:HB2 | 1:A:1627:ARG:HG2 | 1.87 | 0.56 |
| 3:C:2969[B]:TYR:CG | 3:C:2970[B]:PRO:HD2 | 2.41 | 0.56 |
| 3:C:3083[A]:ILE:HD12 | 3:C:3260[A]:ARG:HB2 | 1.88 | 0.56 |
| 3:C:3173[B]:THR:C | 3:L:3154[B]:PRO:HD3 | 2.30 | 0.56 |
| 2:E:2263:PHE:HE1 | 2:E:2304:LEU:HB3 | 1.71 | 0.56 |
| 3:F:2987[A]:HIS:NE2 | 3:F:3178[A]:PHE:HE1 | 1.95 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3150[B]:LYS:CG | 3:a:3158[B]:PHE:CA | 2.50 | 0.56 |
| 3:F:3256[B]:TRP:HE1 | 3:a:2965[B]:LEU:HD12 | 1.41 | 0.56 |
| 1:G:906:HIS:CD2 | 9:G:2104:CUO:O1 | 2.59 | 0.56 |
| 1:G:1415:ASP:OD1 | 1:G:1416:PHE:N | 2.38 | 0.56 |
| 1:G:1494:ARG:HG3 | 1:G:1494:ARG:HH11 | 1.70 | 0.56 |
| 3:I:2948[B]:ASP:CB | 3:I:2949[B]:LYS:CA | 2.78 | 0.56 |
| 3:I:2961[A]:HIS:NE2 | 3:I:2980[A]:HIS:CE1 | 2.73 | 0.56 |
| 3:I:2966[B]:SER:OG | 3:R:3255[B]:PRO:O | 2.24 | 0.56 |
| 3:I:3078[B]:PHE:CE2 | 3:R:3161[B]:GLU:OE1 | 2.58 | 0.56 |
| 1:J:157:GLU:OE2 | 1:J:296:ARG:NH2 | 2.39 | 0.56 |
| 2:K:2887:ASP:O | 2:K:2890:VAL:N | 2.38 | 0.56 |
| 3:L:3176[B]:LYS:H | 3:L:3176[B]:LYS:CE | 2.17 | 0.56 |
| 3:L:3200[A]:LEU:O | 3:L:3204[A]:LEU:HD13 | 2.06 | 0.56 |
| 1:M:19:GLN:NE2 | 1:M:121:ASN:OD1 | 2.39 | 0.56 |
| 1:M:1261:LYS:HG3 | 1:M:1266:PHE:HE1 | 1.71 | 0.56 |
| 3:O:2965[B]:LEU:O | 3:X:3153[B]:LYS:NZ | 2.24 | 0.56 |
| 3:O:2968[B]:GLN:HB3 | 3:X:2988[B]:TRP:CB | 2.16 | 0.56 |
| 3:O:3180[B]:TYR:C | 3:O:3183[B]:LEU:HD22 | 2.30 | 0.56 |
| 3:O:3228[A]:VAL:CG2 | 3:O:3245[A]:PHE:CE2 | 2.89 | 0.56 |
| 1:P:494:VAL:HG23 | 1:P:671:PHE:HZ | 1.71 | 0.56 |
| 1:P:1348:TRP:CD1 | 1:P:1403:LEU:HD13 | 2.41 | 0.56 |
| 2:Q:2643:GLU:O | 2:Q:2647:LEU:N | 2.39 | 0.56 |
| 3:R:2969[A]:TYR:CE2 | 3:R:2970[A]:PRO:CG | 2.86 | 0.56 |
| 3:U:3013[A]:ASP:OD1 | 3:U:3015[A]:THR:OG1 | 2.23 | 0.56 |
| 3:U:3083[B]:ILE:HD12 | 3:U:3260[B]:ARG:HB2 | 1.88 | 0.56 |
| 3:U:3153[B]:LYS:HB2 | 3:d:3154[B]:PRO:C | 2.24 | 0.56 |
| 3:U:3154[B]:PRO:O | 3:d:3153[B]:LYS:HE3 | 2.05 | 0.56 |
| 3:U:3211[A]:ASP:OD1 | 3:U:3211[A]:ASP:N | 2.27 | 0.56 |
| 3:U:3255[B]:PRO:HB2 | 3:d:2974[B]:ALA:O | 2.05 | 0.56 |
| 3:U:3298[B]:ASN:CB | 3:U:3300[B]:LEU:CD2 | 2.61 | 0.56 |
| 1:V:566:ARG:NH1 | 1:V:745:ASP:OD1 | 2.39 | 0.56 |
| 3:X:3200[B]:LEU:O | 3:X:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 3:X:3251[B]:ASP:HB3 | 3:X:3252[B]:TYR:CD1 | 2.40 | 0.56 |
| 3:X:3268[A]:LYS:O | 3:X:3271[A]:VAL:HG23 | 2.06 | 0.56 |
| 3:a:3013[A]:ASP:OD1 | 3:a:3015[A]:THR:OG1 | 2.23 | 0.56 |
| 2:c:2643:GLU:O | 2:c:2647:LEU:N | 2.38 | 0.56 |
| 2:c:2760:ARG:O | 2:c:2763:SER:OG | 2.22 | 0.56 |
| 3:d:3083[B]:ILE:HD12 | 3:d:3260[B]:ARG:HB2 | 1.88 | 0.56 |
| 3:d:3200[B]:LEU:O | 3:d:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 1:A:606:ILE:O | 1:A:610:THR:OG1 | 2.23 | 0.56 |
| 1:A:897:HIS:HB3 | 1:A:899:MET:SD | 2.45 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:990:HIS:O | 1:A:992:ALA:N | 2.38 | 0.56 |
| 2:B:2406:SER:HB3 | 2:B:2429:LEU:HA | 1.87 | 0.56 |
| 3:C:2969[B]:TYR:OH | 3:L:3120[B]:HIS:HD2 | 1.75 | 0.56 |
| 3:C:3083[B]:ILE:HD12 | 3:C:3260[B]:ARG:HB2 | 1.88 | 0.56 |
| 3:C:3154[B]:PRO:O | 3:L:3155[B]:MET:SD | 2.64 | 0.56 |
| 3:C:3200[B]:LEU:O | 3:C:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 2:E:2823:ILE:HG12 | 2:E:2832:ALA:HB2 | 1.86 | 0.56 |
| 3:F:3228[B]:VAL:CG2 | 3:F:3245[B]:PHE:CE2 | 2.89 | 0.56 |
| 1:G:1104:ASP:O | 1:G:1111:ASN:ND2 | 2.39 | 0.56 |
| 2:H:2711:HIS:HA | 2:H:2714:VAL:HG22 | 1.88 | 0.56 |
| 3:I:2949[A]:LYS:NZ | 3:I:2950[A]:THR:HA | 2.21 | 0.56 |
| 3:I:3019[A]:HIS:H | 3:I:3019[A]:HIS:CD2 | 2.22 | 0.56 |
| 3:I:3163[B]:ASN:CG | 3:R:3150[B]:LYS:HE3 | 2.19 | 0.56 |
| 3:I:3200[A]:LEU:O | 3:I:3204[A]:LEU:HD13 | 2.06 | 0.56 |
| 3:I:3200[B]:LEU:O | 3:I:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 3:I:3250[B]:GLY:HA2 | 3:R:3252[B]:TYR:CZ | 2.41 | 0.56 |
| 1:J:944:GLU:O | 1:J:957:ASN:ND2 | 2.39 | 0.56 |
| 3:L:3033[B]:PHE:HD1 | 3:L:3114[B]:PRO:HB2 | 1.72 | 0.56 |
| 3:L:3183[B]:LEU:N | 3:L:3184[B]:ASN:HA | 2.11 | 0.56 |
| 3:L:3200[B]:LEU:O | 3:L:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 2:N:2394:VAL:HA | 2:N:2488:ARG:HA | 1.86 | 0.56 |
| 2:N:2800:LYS:O | 3:O:3023[A]:ILE:HD13 | 2.00 | 0.56 |
| 3:O:2942[A]:LEU:HD13 | 3:O:3033[A]:PHE:CZ | 2.40 | 0.56 |
| 3:O:3019[A]:HIS:CD2 | 3:O:3019[A]:HIS:H | 2.22 | 0.56 |
| 3:O:3093[A]:HIS:CE1 | 3:O:3119[A]:HIS:CD2 | 2.92 | 0.56 |
| 3:O:3200[B]:LEU:O | 3:O:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 1:P:895:CYS:O | 1:P:897:HIS:ND1 | 2.37 | 0.56 |
| 3:R:3083[A]:ILE:HD12 | 3:R:3260[A]:ARG:HB2 | 1.88 | 0.56 |
| 2:T:2276:GLY:O | 2:T:2283:ASN:ND2 | 2.39 | 0.56 |
| 3:U:2942[A]:LEU:HD13 | 3:U:3033[A]:PHE:CZ | 2.40 | 0.56 |
| 3:U:2952[A]:ALA:HB3 | 3:U:2954[A]:TYR:N | 2.17 | 0.56 |
| 3:U:3200[B]:LEU:O | 3:U:3204[B]:LEU:HD13 | 2.06 | 0.56 |
| 1:V:1161:ILE:HB | 1:V:1203:MET:HE3 | 1.88 | 0.56 |
| 1:V:1206:HIS:CE1 | 1:V:1209:ASP:HB2 | 2.41 | 0.56 |
| 1:V:1414:THR:HG23 | 1:V:1477:LEU:HD13 | 1.87 | 0.56 |
| 3:X:2949[B]:LYS:NZ | 3:X:2950[B]:THR:HA | 2.21 | 0.56 |
| 3:X:2969[A]:TYR:CG | 3:X:2970[A]:PRO:HD2 | 2.41 | 0.56 |
| 3:X:3033[A]:PHE:HD1 | 3:X:3114[A]:PRO:HB2 | 1.71 | 0.56 |
| 3:X:3228[B]:VAL:CG2 | 3:X:3245[B]:PHE:CE2 | 2.89 | 0.56 |
| 2:Z:2503:ASN:HB3 | 2:c:2168:ARG:O | 2.06 | 0.56 |
| 3:a:3200[A]:LEU:O | 3:a:3204[A]:LEU:HD13 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:1358:LEU:O | 1:b:1375:ASN:ND2 | 2.36 | 0.56 |
| 2:c:2472:ASN:N | 2:c:2473:GLY:HA2 | 2.21 | 0.56 |
| 2:c:2568:HIS:ND1 | 2:c:2765:PRO:HB3 | 2.21 | 0.56 |
| 3:d:3093[A]:HIS:CE1 | 3:d:3119[A]:HIS:CD2 | 2.92 | 0.56 |
| 3:d:3120[B]:HIS:C | 3:d:3122[B]:ASN:N | 2.55 | 0.56 |
| 3:d:3180[B]:TYR:C | 3:d:3183[B]:LEU:HD22 | 2.30 | 0.56 |
| 3:d:3281[A]:PHE:HE1 | 3:d:3305[A]:ILE:HD13 | 1.71 | 0.56 |
| 3:C:3220[A]:ARG:HG2 | 3:C:3221[A]:ALA:H | 1.70 | 0.55 |
| 3:C:3268[B]:LYS:O | 3:C:3271[B]:VAL:HG23 | 2.06 | 0.55 |
| 3:C:3307[B]:PHE:HE1 | 3:C:3309[B]:PRO:CG | 2.08 | 0.55 |
| 1:D:215:ARG:HE | 1:D:279:LEU:HA | 1.71 | 0.55 |
| 2:E:2272:SER:HA | 2:E:2283:ASN:HD22 | 1.71 | 0.55 |
| 3:F:3159[B]:SER:CB | 3:a:2984[B]:THR:CB | 2.82 | 0.55 |
| 1:G:215:ARG:HE | 1:G:279:LEU:HA | 1.70 | 0.55 |
| 1:G:490:TRP:HE1 | 1:G:670:PRO:HD3 | 1.70 | 0.55 |
| 1:G:893:ALA:HB2 | 1:G:1182:ASN:HB2 | 1.88 | 0.55 |
| 1:G:979:LEU:HD12 | 1:G:980:TYR:HA | 1.87 | 0.55 |
| 3:I:3155[B]:MET:HE3 | 3:R:3156[B]:MET:HG2 | 1.86 | 0.55 |
| 3:I:3251[A]:ASP:HB3 | 3:I:3252[A]:TYR:CD1 | 2.40 | 0.55 |
| 3:I:3251[B]:ASP:OD1 | 3:R:3108[B]:HIS:HE1 | 1.83 | 0.55 |
| 3:I:3283[A]:ILE:CB | 3:I:3305[A]:ILE:HD11 | 2.35 | 0.55 |
| 1:J:219:LEU:HG | 1:J:279:LEU:O | 2.06 | 0.55 |
| 2:K:2554:PRO:HA | 2:K:2555:GLU:HB3 | 1.89 | 0.55 |
| 2:K:2627:GLY:HA3 | 2:K:2703:PHE:O | 2.06 | 0.55 |
| 1:M:238:ASN:OD1 | 1:M:238:ASN:N | 2.36 | 0.55 |
| 3:O:3033[A]:PHE:HD1 | 3:O:3114[A]:PRO:HB2 | 1.71 | 0.55 |
| 3:O:3281[B]:PHE:HE1 | 3:O:3305[B]:ILE:HD13 | 1.71 | 0.55 |
| 2:Q:2185:THR:HG23 | 2:Q:2186:GLU:HG2 | 1.87 | 0.55 |
| 3:R:3033[B]:PHE:HD1 | 3:R:3114[B]:PRO:HB2 | 1.72 | 0.55 |
| 1:S:802:ILE:O | 1:S:810:LEU:N | 2.37 | 0.55 |
| 3:U:2952[A]:ALA:N | 3:U:2953[A]:GLY:HA2 | 2.06 | 0.55 |
| 1:V:866:GLU:C | 1:V:868:THR:H | 2.13 | 0.55 |
| 1:V:895:CYS:SG | 1:V:896:HIS:N | 2.80 | 0.55 |
| 3:X:2942[A]:LEU:HD13 | 3:X:3033[A]:PHE:CZ | 2.40 | 0.55 |
| 3:X:3083[A]:ILE:HD12 | 3:X:3260[A]:ARG:HB2 | 1.88 | 0.55 |
| 3:X:3212[A]:ARG:HH11 | 3:X:3212[A]:ARG:CG | 2.12 | 0.55 |
| 1:Y:80:LEU:O | 1:Y:84:GLY:HA2 | 2.05 | 0.55 |
| 1:Y:1616:LYS:C | 3:d:3187[B]:TYR:N | 2.37 | 0.55 |
| 3:a:3183[A]:LEU:N | 3:a:3184[A]:ASN:HA | 2.12 | 0.55 |
| 1:b:35:GLN:NE2 | 1:b:129:LYS:HB2 | 2.21 | 0.55 |
| 1:b:447:MET:HA | 1:b:455:TYR:HB2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:1407:THR:HG22 | 1:b:1426:LEU:HD21 | 1.88 | 0.55 |
| 3:d:2948[A]:ASP:HB3 | 3:d:2953[A]:GLY:CA | 2.24 | 0.55 |
| 3:d:3200[A]:LEU:O | 3:d:3204[A]:LEU:HD13 | 2.06 | 0.55 |
| 3:d:3283[A]:ILE:CB | 3:d:3305[A]:ILE:HD11 | 2.35 | 0.55 |
| 1:A:1567:ASP:OD1 | 1:A:1591:SER:OG | 2.21 | 0.55 |
| 3:C:2961[B]:HIS:NE2 | 3:C:2980[B]:HIS:CE1 | 2.73 | 0.55 |
| 3:C:3268[A]:LYS:O | 3:C:3271[A]:VAL:HG23 | 2.06 | 0.55 |
| 2:E:2107:LEU:O | 2:E:2111:GLN:HB2 | 2.06 | 0.55 |
| 3:F:2969[A]:TYR:CG | 3:F:2970[A]:PRO:HD2 | 2.41 | 0.55 |
| 3:F:3155[B]:MET:SD | 3:a:3154[B]:PRO:CD | 2.95 | 0.55 |
| 3:F:3268[B]:LYS:O | 3:F:3271[B]:VAL:HG23 | 2.06 | 0.55 |
| 3:F:3281[B]:PHE:HE1 | 3:F:3305[B]:ILE:HD13 | 1.71 | 0.55 |
| 3:F:3298[B]:ASN:CB | 3:F:3300[B]:LEU:N | 2.60 | 0.55 |
| 2:H:2885:SER:OG | 2:H:2886:VAL:N | 2.37 | 0.55 |
| 3:I:3162[B]:ASP:N | 3:R:2983[B]:VAL:CG2 | 2.65 | 0.55 |
| 3:L:2952[A]:ALA:HB3 | 3:L:2954[A]:TYR:N | 2.18 | 0.55 |
| 3:L:2969[A]:TYR:CG | 3:L:2970[A]:PRO:HD2 | 2.41 | 0.55 |
| 3:L:3083[A]:ILE:HD12 | 3:L:3260[A]:ARG:HB2 | 1.88 | 0.55 |
| 1:M:49:ALA:HB3 | 1:M:55:ILE:HD12 | 1.88 | 0.55 |
| 2:N:2130:PRO:CB | 2:N:2142:ALA:HB3 | 2.35 | 0.55 |
| 3:O:2971[B]:ASP:CG | 3:X:3158[B]:PHE:HZ | 2.13 | 0.55 |
| 3:O:3268[A]:LYS:O | 3:O:3271[A]:VAL:HG23 | 2.06 | 0.55 |
| 3:O:3268[B]:LYS:O | 3:O:3271[B]:VAL:HG23 | 2.06 | 0.55 |
| 3:R:2971[A]:ASP:CG | 3:R:2973[A]:THR:HG1 | 2.12 | 0.55 |
| 1:S:931:TRP:CG | 1:S:1018:ILE:HD11 | 2.41 | 0.55 |
| 2:T:2509:ILE:HD11 | 2:T:2605:LEU:HD23 | 1.88 | 0.55 |
| 3:U:3019[B]:HIS:CD2 | 3:U:3019[B]:HIS:H | 2.22 | 0.55 |
| 3:U:3158[B]:PHE:CB | 3:d:3149[B]:ASN:HB3 | 2.35 | 0.55 |
| 3:U:3176[B]:LYS:HG3 | 3:d:3152[B]:LYS:NZ | 2.18 | 0.55 |
| 3:U:3281[A]:PHE:HE1 | 3:U:3305[A]:ILE:HD13 | 1.71 | 0.55 |
| 3:U:3281[B]:PHE:HE1 | 3:U:3305[B]:ILE:HD13 | 1.71 | 0.55 |
| 2:W:2571:ARG:NH1 | 2:W:2776:TYR:OH | 2.33 | 0.55 |
| 2:W:2723:GLU:HG2 | 2:W:2788:ILE:HD13 | 1.88 | 0.55 |
| 3:X:3298[B]:ASN:HA | 3:X:3299[B]:LEU:HB3 | 1.88 | 0.55 |
| 1:Y:1136:ARG:O | 1:Y:1141:ARG:NH1 | 2.40 | 0.55 |
| 2:Z:2534:PHE:CD1 | 2:Z:2755:PRO:HB3 | 2.41 | 0.55 |
| 3:a:3014[B]:TRP:CZ3 | 3:a:3119[B]:HIS:CE1 | 2.94 | 0.55 |
| 3:a:3188[B]:ASP:N | 3:a:3188[B]:ASP:OD2 | 2.36 | 0.55 |
| 1:b:327:ASP:OD1 | 1:b:328:LYS:N | 2.39 | 0.55 |
| 1:b:527:LEU:HD22 | 1:b:629:MET:HG3 | 1.89 | 0.55 |
| 1:b:893:ALA:HB2 | 1:b:1182:ASN:HD22 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:965:ASP:OD1 | 1:b:965:ASP:N | 2.36 | 0.55 |
| 3:d:2949[B]:LYS:NZ | 3:d:2950[B]:THR:HA | 2.21 | 0.55 |
| 3:d:2961[A]:HIS:NE2 | 3:d:2980[A]:HIS:CE1 | 2.73 | 0.55 |
| 3:d:3220[A]:ARG:HG2 | 3:d:3221[A]:ALA:H | 1.70 | 0.55 |
| 1:A:195:SER:HB2 | 1:A:386:ILE:HG13 | 1.89 | 0.55 |
| 1:A:270:GLU:N | 1:A:270:GLU:OE1 | 2.35 | 0.55 |
| 2:B:2715:ASP:O | 2:B:2718:TRP:HB3 | 2.07 | 0.55 |
| 3:C:3153[B]:LYS:CA | 3:L:3173[B]:THR:C | 2.78 | 0.55 |
| 3:C:3253[B]:GLU:HG2 | 3:L:3252[B]:TYR:HB2 | 1.89 | 0.55 |
| 3:F:2949[A]:LYS:NZ | 3:F:2950[A]:THR:HA | 2.21 | 0.55 |
| 3:F:3014[A]:TRP:CZ3 | 3:F:3119[A]:HIS:CE1 | 2.95 | 0.55 |
| 3:F:3083[B]:ILE:HD12 | 3:F:3260[B]:ARG:HB2 | 1.88 | 0.55 |
| 3:F:3156[B]:MET:HG3 | 3:a:2979[B]:GLN:OE1 | 1.60 | 0.55 |
| 3:F:3281[A]:PHE:HE1 | 3:F:3305[A]:ILE:HD13 | 1.71 | 0.55 |
| 3:F:3283[B]:ILE:CB | 3:F:3305[B]:ILE:HD11 | 2.35 | 0.55 |
| 1:G:792:MET:O | 1:G:796:TYR:OH | 2.25 | 0.55 |
| 1:G:931:TRP:CD2 | 1:G:1018:ILE:HD11 | 2.41 | 0.55 |
| 2:H:2294:PHE:O | 2:H:2297:HIS:HB3 | 2.05 | 0.55 |
| 3:I:3156[B]:MET:HB2 | 3:R:2982[B]:MET:SD | 2.45 | 0.55 |
| 1:J:516:TRP:HH2 | 1:J:637:VAL:HG22 | 1.71 | 0.55 |
| 1:J:1017:HIS:O | 1:J:1021:LEU:HG | 2.06 | 0.55 |
| 2:K:2153:GLN:NE2 | 2:K:2329:MET:HE1 | 2.20 | 0.55 |
| 2:K:2562:GLY:H | 2:K:2846:TRP:HB2 | 1.71 | 0.55 |
| 2:K:2885:SER:OG | 2:K:2886:VAL:N | 2.32 | 0.55 |
| 1:M:494:VAL:HG23 | 1:M:671:PHE:HZ | 1.71 | 0.55 |
| 3:O:2969[A]:TYR:CG | 3:O:2970[A]:PRO:HD2 | 2.42 | 0.55 |
| 3:O:2974[B]:ALA:CB | 3:X:2977[B]:CYS:O | 2.53 | 0.55 |
| 3:O:3157[B]:PRO:HA | 3:X:3153[B]:LYS:H | 1.70 | 0.55 |
| 1:S:549:PRO:HA | 1:S:557:VAL:HG12 | 1.87 | 0.55 |
| 2:T:2218:SER:O | 2:T:2221:THR:OG1 | 2.21 | 0.55 |
| 2:T:2849:ASP:OD2 | 2:T:2850:ARG:NH2 | 2.39 | 0.55 |
| 3:U:2952[B]:ALA:N | 3:U:2953[B]:GLY:HA2 | 2.06 | 0.55 |
| 3:U:3156[B]:MET:SD | 3:d:2982[B]:MET:CA | 2.93 | 0.55 |
| 1:V:473:ALA:HB3 | 1:V:476:ARG:HB3 | 1.88 | 0.55 |
| 1:V:1019:HIS:NE2 | 1:V:1046:HIS:CE1 | 2.74 | 0.55 |
| 1:V:1397:LEU:HB2 | 1:V:1433:TRP:HB3 | 1.88 | 0.55 |
| 2:W:2823:ILE:CG1 | 2:W:2830:GLN:HE22 | 2.16 | 0.55 |
| 3:X:3014[A]:TRP:CZ3 | 3:X:3119[A]:HIS:CE1 | 2.95 | 0.55 |
| 2:Z:2470:ALA:HB2 | 2:Z:2476:LEU:HD11 | 1.87 | 0.55 |
| 1:b:729:VAL:HG11 | 1:b:785:LEU:HD12 | 1.86 | 0.55 |
| 3:d:2961[B]:HIS:NE2 | 3:d:2980[B]:HIS:CE1 | 2.73 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3014[A]:TRP:CZ3 | 3:d:3119[A]:HIS:CE1 | 2.95 | 0.55 |
| 3:d:3176[A]:LYS:H | 3:d:3176[A]:LYS:CE | 2.17 | 0.55 |
| 3:d:3298[B]:ASN:HA | 3:d:3299[B]:LEU:HB3 | 1.88 | 0.55 |
| 1:A:357:PRO:HB3 | 1:A:774:ASP:HB2 | 1.88 | 0.55 |
| 1:A:439:LEU:HD23 | 1:A:509:ILE:HD12 | 1.88 | 0.55 |
| 2:B:2553:ALA:N | 2:B:2554:PRO:HD3 | 2.21 | 0.55 |
| 3:C:2965[B]:LEU:HA | 3:L:3255[B]:PRO:HA | 1.89 | 0.55 |
| 3:C:3013[A]:ASP:OD1 | 3:C:3015[A]:THR:OG1 | 2.23 | 0.55 |
| 3:C:3155[B]:MET:CE | 3:L:3153[B]:LYS:HD3 | 2.33 | 0.55 |
| 3:C:3156[B]:MET:HB3 | 3:L:2982[B]:MET:HB2 | 1.86 | 0.55 |
| 3:C:3176[A]:LYS:H | 3:C:3176[A]:LYS:CE | 2.17 | 0.55 |
| 1:D:926:LEU:HD12 | 1:D:927:PRO:HD2 | 1.88 | 0.55 |
| 1:D:1324:ARG:NH1 | 1:D:1519:TYR:HB3 | 2.22 | 0.55 |
| 2:E:2180:TRP:HD1 | 2:E:2247:ILE:HD11 | 1.71 | 0.55 |
| 3:F:2932[A]:PRO:CA | 3:F:2935[A]:ILE:HD12 | 2.30 | 0.55 |
| 3:F:2985[B]:PHE:HZ | 3:a:2970[B]:PRO:CA | 2.11 | 0.55 |
| 3:F:3254[B]:MET:HB2 | 3:a:2966[B]:SER:CB | 2.36 | 0.55 |
| 3:F:3298[B]:ASN:HA | 3:F:3299[B]:LEU:HB3 | 1.88 | 0.55 |
| 1:G:418:ASP:OD1 | 1:G:419:THR:N | 2.40 | 0.55 |
| 1:G:904:HIS:HB3 | 1:G:1105:VAL:HG21 | 1.88 | 0.55 |
| 1:G:944:GLU:O | 1:G:957:ASN:ND2 | 2.40 | 0.55 |
| 3:I:2961[B]:HIS:NE2 | 3:I:2980[B]:HIS:CE1 | 2.73 | 0.55 |
| 3:I:2969[A]:TYR:CG | 3:I:2970[A]:PRO:HD2 | 2.41 | 0.55 |
| 3:I:3033[B]:PHE:HD1 | 3:I:3114[B]:PRO:HB2 | 1.71 | 0.55 |
| 1:J:462:HIS:HA | 1:J:490:TRP:HH2 | 1.71 | 0.55 |
| 1:J:566:ARG:HH22 | 1:J:803:LYS:HZ1 | 1.53 | 0.55 |
| 2:K:2180:TRP:HB3 | 2:K:2184:MET:HE2 | 1.87 | 0.55 |
| 2:K:2346:PRO:O | 2:K:2349:THR:OG1 | 2.20 | 0.55 |
| 3:L:2949[A]:LYS:NZ | 3:L:2950[A]:THR:HA | 2.21 | 0.55 |
| 3:L:3013[A]:ASP:OD1 | 3:L:3015[A]:THR:OG1 | 2.23 | 0.55 |
| 1:M:488:PRO:HB2 | 1:M:641:TRP:CE3 | 2.42 | 0.55 |
| 2:N:2548:CYS:O | 2:N:2556:TYR:HB3 | 2.06 | 0.55 |
| 3:O:2947[A]:ALA:HA | 3:O:2949[A]:LYS:HB3 | 1.89 | 0.55 |
| 3:O:3083[A]:ILE:HD12 | 3:O:3260[A]:ARG:HB2 | 1.88 | 0.55 |
| 3:O:3160[B]:SER:OG | 3:X:3151[B]:LEU:N | 2.39 | 0.55 |
| 3:O:3251[B]:ASP:CG | 3:X:2968[B]:GLN:OE1 | 2.49 | 0.55 |
| 3:U:2969[B]:TYR:CZ | 3:d:3107[B]:LEU:HD11 | 2.05 | 0.55 |
| 3:U:2969[B]:TYR:CG | 3:U:2970[B]:PRO:HD2 | 2.41 | 0.55 |
| 1:V:1125:SER:O | 1:V:1129:LEU:HB2 | 2.06 | 0.55 |
| 1:Y:565:GLU:C | 1:Y:567:LEU:HA | 2.32 | 0.55 |
| 3:a:2932[B]:PRO:CA | 3:a:2935[B]:ILE:HD12 | 2.30 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2947[B]:ALA:HA | 3:d:2949[B]:LYS:HB3 | 1.89 | 0.55 |
| 3:d:3151[B]:LEU:HB2 | 3:d:3175[B]:TYR:HE2 | 1.67 | 0.55 |
| 3:d:3268[A]:LYS:O | 3:d:3271[A]:VAL:HG23 | 2.06 | 0.55 |
| 1:A:142:ARG:O | 1:A:145:GLN:NE2 | 2.40 | 0.55 |
| 1:A:1166:THR:N | 1:A:1167:ASP:HA | 2.22 | 0.55 |
| 3:C:2947[B]:ALA:HA | 3:C:2949[B]:LYS:HB3 | 1.89 | 0.55 |
| 3:C:2982[B]:MET:N | 3:L:2967[B]:CYS:CB | 2.67 | 0.55 |
| 3:C:3153[B]:LYS:CB | 3:L:3155[B]:MET:H | 2.13 | 0.55 |
| 3:C:3188[B]:ASP:N | 3:C:3188[B]:ASP:OD2 | 2.36 | 0.55 |
| 3:C:3228[B]:VAL:CG2 | 3:C:3245[B]:PHE:CE2 | 2.89 | 0.55 |
| 3:F:2949[B]:LYS:NZ | 3:F:2950[B]:THR:HA | 2.21 | 0.55 |
| 3:F:3183[A]:LEU:N | 3:F:3184[A]:ASN:HA | 2.11 | 0.55 |
| 3:F:3255[B]:PRO:HB3 | 3:a:2964[B]:PRO:CD | 2.36 | 0.55 |
| 1:G:164:GLU:O | 1:G:297:ARG:NH2 | 2.39 | 0.55 |
| 2:H:2890:VAL:N | 2:H:2891:LEU:HA | 2.22 | 0.55 |
| 1:J:447:MET:HA | 1:J:455:TYR:HB2 | 1.88 | 0.55 |
| 1:J:494:VAL:HG13 | 1:J:631:TRP:HZ3 | 1.72 | 0.55 |
| 3:L:3014[A]:TRP:CZ3 | 3:L:3119[A]:HIS:CE1 | 2.94 | 0.55 |
| 3:L:3033[A]:PHE:HD1 | 3:L:3114[A]:PRO:HB2 | 1.72 | 0.55 |
| 3:O:3083[B]:ILE:HD12 | 3:O:3260[B]:ARG:HB2 | 1.88 | 0.55 |
| 1:P:1493:MET:HG2 | 1:P:1511:SER:O | 2.06 | 0.55 |
| 2:Q:2851:ASN:OD1 | 2:Q:2851:ASN:N | 2.38 | 0.55 |
| 3:R:3281[B]:PHE:HE1 | 3:R:3305[B]:ILE:HD13 | 1.71 | 0.55 |
| 2:T:2680:HIS:NE2 | 2:T:2684:HIS:CD2 | 2.74 | 0.55 |
| 3:U:2947[A]:ALA:HA | 3:U:2949[A]:LYS:HB3 | 1.89 | 0.55 |
| 3:U:3033[A]:PHE:HD1 | 3:U:3114[A]:PRO:HB2 | 1.72 | 0.55 |
| 3:U:3159[B]:SER:HB3 | 3:d:3147[B]:GLU:HG3 | 1.88 | 0.55 |
| 3:U:3273[A]:LEU:HB2 | 3:U:3275[A]:LEU:CD1 | 2.34 | 0.55 |
| 1:V:17:ASN:HD21 | 1:V:86:THR:H | 1.55 | 0.55 |
| 2:W:2562:GLY:H | 2:W:2846:TRP:CB | 2.19 | 0.55 |
| 3:X:2969[A]:TYR:CE2 | 3:X:2970[A]:PRO:CG | 2.86 | 0.55 |
| 3:X:3293[B]:LYS:CB | 3:X:3294[B]:SER:CB | 2.54 | 0.55 |
| 3:a:2969[A]:TYR:CE2 | 3:a:2970[A]:PRO:CG | 2.86 | 0.55 |
| 3:a:3014[A]:TRP:CZ3 | 3:a:3119[A]:HIS:CE1 | 2.94 | 0.55 |
| 3:a:3083[B]:ILE:HD12 | 3:a:3260[B]:ARG:HB2 | 1.88 | 0.55 |
| 3:a:3268[B]:LYS:O | 3:a:3271[B]:VAL:HG23 | 2.06 | 0.55 |
| 1:b:1573:CYS:HB2 | 1:b:1627:ARG:HG2 | 1.89 | 0.55 |
| 3:d:3228[B]:VAL:CG2 | 3:d:3245[B]:PHE:CE2 | 2.89 | 0.55 |
| 1:A:723:ALA:O | 1:A:728:ARG:NH1 | 2.40 | 0.55 |
| 1:A:1493:MET:HG2 | 1:A:1511:SER:O | 2.06 | 0.55 |
| 3:C:2949[A]:LYS:HZ2 | 3:C:2950[A]:THR:HA | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2963[B]:MET:C | 3:L:3255[B]:PRO:HB3 | 2.32 | 0.55 |
| 3:C:2969[A]:TYR:CG | 3:C:2970[A]:PRO:HD2 | 2.42 | 0.55 |
| 3:C:3014[A]:TRP:CZ3 | 3:C:3119[A]:HIS:CE1 | 2.94 | 0.55 |
| 3:C:3014[B]:TRP:CZ3 | 3:C:3119[B]:HIS:CE1 | 2.94 | 0.55 |
| 3:F:2960[B]:PHE:CD1 | 3:F:2960[B]:PHE:N | 2.72 | 0.55 |
| 3:F:2983[B]:VAL:HG23 | 3:a:3160[B]:SER:C | 2.27 | 0.55 |
| 1:G:559:THR:HG21 | 1:G:627:ASP:HA | 1.88 | 0.55 |
| 1:G:664:VAL:HG12 | 1:G:690:THR:HG22 | 1.89 | 0.55 |
| 1:G:1576:THR:H | 1:G:1581:GLU:HB3 | 1.71 | 0.55 |
| 3:I:3281[B]:PHE:HE1 | 3:I:3305[B]:ILE:HD13 | 1.71 | 0.55 |
| 1:J:307:ARG:NH1 | 1:J:772:ARG:O | 2.40 | 0.55 |
| 3:L:3014[B]:TRP:CZ3 | 3:L:3119[B]:HIS:CE1 | 2.94 | 0.55 |
| 3:L:3284[A]:LYS:HE2 | 3:L:3284[A]:LYS:CA | 2.30 | 0.55 |
| 1:M:883:CYS:N | 1:M:894:CYS:SG | 2.80 | 0.55 |
| 2:N:2128:LEU:HD23 | 2:N:2216:PHE:CZ | 2.42 | 0.55 |
| 3:O:2949[B]:LYS:NZ | 3:O:2950[B]:THR:HA | 2.21 | 0.55 |
| 3:O:3014[A]:TRP:CZ3 | 3:O:3119[A]:HIS:CE1 | 2.95 | 0.55 |
| 3:O:3154[B]:PRO:HD2 | 3:X:3176[B]:LYS:HZ1 | 1.66 | 0.55 |
| 3:O:3254[B]:MET:HE3 | 3:X:3172[B]:SER:HB2 | 1.87 | 0.55 |
| 1:P:1002:GLU:HB2 | 1:P:1065:LYS:HD3 | 1.87 | 0.55 |
| 3:R:3120[B]:HIS:HA | 3:R:3123[B]:THR:HG1 | 1.71 | 0.55 |
| 3:R:3220[B]:ARG:HG2 | 3:R:3221[B]:ALA:H | 1.70 | 0.55 |
| 3:R:3281[A]:PHE:HE1 | 3:R:3305[A]:ILE:HD13 | 1.71 | 0.55 |
| 3:U:2952[B]:ALA:HB3 | 3:U:2954[B]:TYR:N | 2.17 | 0.55 |
| 3:U:3013[B]:ASP:OD1 | 3:U:3015[B]:THR:OG1 | 2.23 | 0.55 |
| 3:U:3014[A]:TRP:CZ3 | 3:U:3119[A]:HIS:CE1 | 2.95 | 0.55 |
| 3:U:3014[B]:TRP:CZ3 | 3:U:3119[B]:HIS:CE1 | 2.95 | 0.55 |
| 3:U:3033[B]:PHE:HD1 | 3:U:3114[B]:PRO:HB2 | 1.72 | 0.55 |
| 3:U:3093[B]:HIS:CE1 | 3:U:3119[B]:HIS:CD2 | 2.92 | 0.55 |
| 1:V:741:SER:HB2 | 1:V:764:GLY:H | 1.71 | 0.55 |
| 1:V:1271:MET:HE1 | 1:V:1357:ARG:HH11 | 1.72 | 0.55 |
| 1:V:1301:PRO:HB3 | 1:V:1308:VAL:HG12 | 1.88 | 0.55 |
| 3:X:3176[B]:LYS:CE | 3:X:3176[B]:LYS:H | 2.17 | 0.55 |
| 3:X:3180[A]:TYR:C | 3:X:3183[A]:LEU:HD22 | 2.30 | 0.55 |
| 3:X:3268[B]:LYS:O | 3:X:3271[B]:VAL:HG23 | 2.06 | 0.55 |
| 1:Y:164:GLU:HG3 | 1:Y:297:ARG:HE | 1.72 | 0.55 |
| 2:Z:2480:LEU:HD22 | 4:MA:2:NAG:H81 | 1.87 | 0.55 |
| 3:a:3019[A]:HIS:CD2 | 3:a:3019[A]:HIS:H | 2.22 | 0.55 |
| 3:a:3228[B]:VAL:CG2 | 3:a:3245[B]:PHE:CE2 | 2.89 | 0.55 |
| 3:a:3283[A]:ILE:CB | 3:a:3305[A]:ILE:HD11 | 2.35 | 0.55 |
| 3:d:2969[A]:TYR:CG | 3:d:2970[A]:PRO:HD2 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3151[A]:LEU:HB2 | 3:d:3175[A]:TYR:HE2 | 1.67 | 0.55 |
| 3:d:3281[B]:PHE:HE1 | 3:d:3305[B]:ILE:HD13 | 1.71 | 0.55 |
| 1:A:2:LEU:HD21 | 1:A:81:VAL:HG21 | 1.87 | 0.55 |
| 1:A:573:LYS:HD3 | 1:A:757:VAL:O | 2.06 | 0.55 |
| 1:A:1160:PHE:CD1 | 1:A:1169:LYS:HD3 | 2.41 | 0.55 |
| 1:A:1296:VAL:HB | 1:A:1446:ASP:HB3 | 1.87 | 0.55 |
| 1:A:1358:LEU:HD23 | 1:A:1456:LEU:HD21 | 1.89 | 0.55 |
| 3:C:3253[B]:GLU:HA | 3:L:3253[B]:GLU:CA | 2.33 | 0.55 |
| 3:F:2983[B]:VAL:HG21 | 3:a:3161[B]:GLU:HB2 | 1.85 | 0.55 |
| 3:F:3014[B]:TRP:CZ3 | 3:F:3119[B]:HIS:CE1 | 2.95 | 0.55 |
| 3:I:3033[A]:PHE:HD1 | 3:I:3114[A]:PRO:HB2 | 1.72 | 0.55 |
| 1:J:630:PHE:O | 1:J:633:HIS:HB3 | 2.07 | 0.55 |
| 3:L:2948[B]:ASP:HB3 | 3:L:2953[B]:GLY:CA | 2.24 | 0.55 |
| 1:M:77:GLU:O | 1:M:81:VAL:HG23 | 2.07 | 0.55 |
| 1:M:954:ALA:O | 1:M:956:PRO:HD3 | 2.07 | 0.55 |
| 1:M:1074:ILE:HB | 2:Q:2901:LEU:HB2 | 1.88 | 0.55 |
| 2:N:2265:ILE:HD12 | 2:N:2443:TYR:CG | 2.42 | 0.55 |
| 3:O:2961[B]:HIS:NE2 | 3:O:2980[B]:HIS:CE1 | 2.73 | 0.55 |
| 3:O:3135[A]:LYS:HG3 | 3:O:3141[A]:TYR:CD1 | 2.33 | 0.55 |
| 3:O:3251[B]:ASP:HB3 | 3:O:3252[B]:TYR:CD1 | 2.40 | 0.55 |
| 3:R:2949[B]:LYS:NZ | 3:R:2950[B]:THR:HA | 2.21 | 0.55 |
| 3:R:2949[B]:LYS:C | 3:R:2949[B]:LYS:HZ3 | 2.10 | 0.55 |
| 3:R:3176[A]:LYS:H | 3:R:3176[A]:LYS:CE | 2.17 | 0.55 |
| 3:R:3183[B]:LEU:N | 3:R:3184[B]:ASN:HA | 2.12 | 0.55 |
| 3:R:3200[A]:LEU:O | 3:R:3204[A]:LEU:HD13 | 2.06 | 0.55 |
| 1:S:1315:GLY:HA3 | 1:S:1601:TRP:CB | 2.37 | 0.55 |
| 2:T:2114:ARG:HG3 | 2:W:2526:ARG:HE | 1.72 | 0.55 |
| 2:T:2115:SER:OG | 2:T:2116:SER:N | 2.39 | 0.55 |
| 2:T:2237:LEU:H | 2:T:2237:LEU:HD13 | 1.71 | 0.55 |
| 3:U:3093[A]:HIS:CE1 | 3:U:3119[A]:HIS:CD2 | 2.92 | 0.55 |
| 3:U:3169[B]:LYS:HD3 | 3:d:3146[B]:CYS:HA | 1.88 | 0.55 |
| 1:V:1136:ARG:O | 1:V:1141:ARG:NH1 | 2.39 | 0.55 |
| 3:X:2960[B]:PHE:CD1 | 3:X:2960[B]:PHE:N | 2.72 | 0.55 |
| 1:Y:11:THR:HG22 | 1:Y:13:ASP:H | 1.71 | 0.55 |
| 3:a:3019[A]:HIS:CD2 | 3:a:3019[A]:HIS:N | 2.75 | 0.55 |
| 3:d:2949[B]:LYS:HZ2 | 3:d:2950[B]:THR:HA | 1.71 | 0.55 |
| 1:A:875:ALA:C | 1:A:877:HIS:H | 2.15 | 0.55 |
| 3:C:3153[B]:LYS:HD3 | 3:L:3155[B]:MET:HE2 | 1.87 | 0.55 |
| 1:D:140:ASP:OD2 | 1:D:142:ARG:NE | 2.40 | 0.55 |
| 1:D:1206:HIS:N | 1:D:1206:HIS:ND1 | 2.54 | 0.55 |
| 3:F:2947[B]:ALA:HA | 3:F:2949[B]:LYS:HB3 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2952[A]:ALA:HB3 | 3:F:2954[A]:TYR:N | 2.17 | 0.55 |
| 3:F:3156[B]:MET:H | 3:a:2979[B]:GLN:NE2 | 2.04 | 0.55 |
| 3:F:3200[A]:LEU:O | 3:F:3204[A]:LEU:HD13 | 2.06 | 0.55 |
| 1:G:21:SER:HB2 | 1:G:83:HIS:O | 2.07 | 0.55 |
| 3:I:2947[B]:ALA:HA | 3:I:2949[B]:LYS:HB3 | 1.89 | 0.55 |
| 3:I:2966[B]:SER:HA | 3:R:3256[B]:TRP:N | 2.22 | 0.55 |
| 3:I:3259[B]:ASP:HB3 | 3:R:3162[B]:ASP:HA | 1.87 | 0.55 |
| 2:K:2786:MET:HE1 | 2:K:2794:LEU:HB2 | 1.89 | 0.55 |
| 3:L:2932[B]:PRO:CA | 3:L:2935[B]:ILE:HD12 | 2.30 | 0.55 |
| 3:O:3220[B]:ARG:HG2 | 3:O:3221[B]:ALA:H | 1.70 | 0.55 |
| 3:R:2969[A]:TYR:CG | 3:R:2970[A]:PRO:HD2 | 2.41 | 0.55 |
| 3:R:3273[B]:LEU:HB2 | 3:R:3275[B]:LEU:CD1 | 2.34 | 0.55 |
| 1:S:902:PHE:CE2 | 1:S:1012:GLU:HB2 | 2.41 | 0.55 |
| 3:U:3096[B]:VAL:HG11 | 3:U:3115[B]:LEU:HD12 | 1.89 | 0.55 |
| 1:V:714:ARG:HH11 | 1:V:837:HIS:CD2 | 2.24 | 0.55 |
| 3:X:2960[B]:PHE:CD2 | 3:X:3157[B]:PRO:CG | 2.74 | 0.55 |
| 3:X:3013[A]:ASP:OD1 | 3:X:3015[A]:THR:OG1 | 2.23 | 0.55 |
| 3:X:3093[A]:HIS:CE1 | 3:X:3119[A]:HIS:CD2 | 2.92 | 0.55 |
| 3:X:3220[A]:ARG:HG2 | 3:X:3221[A]:ALA:H | 1.70 | 0.55 |
| 3:X:3228[A]:VAL:CG2 | 3:X:3245[A]:PHE:CE2 | 2.89 | 0.55 |
| 1:Y:905:TRP:HZ2 | 1:Y:1083:PRO:HG2 | 1.70 | 0.55 |
| 1:Y:1618:LEU:CA | 3:d:3190[B]:LEU:HB2 | 2.36 | 0.55 |
| 3:a:2969[A]:TYR:CG | 3:a:2970[A]:PRO:HD2 | 2.41 | 0.55 |
| 3:a:3014[A]:TRP:C | 3:a:3014[A]:TRP:CD1 | 2.85 | 0.55 |
| 3:a:3298[B]:ASN:HA | 3:a:3299[B]:LEU:HB3 | 1.88 | 0.55 |
| 1:b:1180:SER:H | 1:b:1183:GLU:HG2 | 1.72 | 0.55 |
| 1:b:1564:ALA:HB1 | 4:QA:1:NAG:H83 | 1.89 | 0.55 |
| 2:c:2811:HIS:HB3 | 2:c:2847:HIS:CD2 | 2.42 | 0.55 |
| 3:d:2932[B]:PRO:CA | 3:d:2935[B]:ILE:HD12 | 2.30 | 0.55 |
| 3:d:2957[B]:ILE:HA | 3:d:2960[B]:PHE:HE1 | 1.64 | 0.55 |
| 3:d:3033[B]:PHE:HD1 | 3:d:3114[B]:PRO:HB2 | 1.72 | 0.55 |
| 1:A:71:LEU:HD22 | 1:A:266:LEU:HD21 | 1.88 | 0.55 |
| 1:A:877:HIS:HD2 | 1:A:1033:LEU:HD13 | 1.72 | 0.55 |
| 1:A:979:LEU:CB | 1:A:980:TYR:HA | 2.36 | 0.55 |
| 1:A:1135:ARG:O | 1:A:1139:LYS:NZ | 2.31 | 0.55 |
| 2:B:2606:LEU:HD22 | 2:B:2706:ILE:HG12 | 1.87 | 0.55 |
| 2:B:2635:TYR:HB2 | 1:b:109:LEU:HD21 | 1.89 | 0.55 |
| 3:C:2985[B]:PHE:CE2 | 3:L:2969[B]:TYR:O | 2.59 | 0.55 |
| 1:D:1304:ASP:H | 1:D:1305:GLY:HA2 | 1.72 | 0.55 |
| 2:E:2089:ARG:HD2 | 2:E:2175:VAL:O | 2.07 | 0.55 |
| 3:F:2983[B]:VAL:CG2 | 3:a:3160[B]:SER:OG | 2.46 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2983[B]:VAL:CG2 | 3:a:3160[B]:SER:CA | 2.82 | 0.55 |
| 3:F:3014[A]:TRP:C | 3:F:3014[A]:TRP:CD1 | 2.85 | 0.55 |
| 3:F:3019[B]:HIS:CD2 | 3:F:3019[B]:HIS:N | 2.75 | 0.55 |
| 3:F:3033[B]:PHE:HD1 | 3:F:3114[B]:PRO:HB2 | 1.72 | 0.55 |
| 3:F:3157[B]:PRO:C | 3:a:3150[B]:LYS:HD3 | 2.17 | 0.55 |
| 3:F:3162[B]:ASP:HA | 3:a:3147[B]:GLU:OE1 | 2.07 | 0.55 |
| 3:F:3255[B]:PRO:HB2 | 3:a:2959[B]:SER:C | 2.32 | 0.55 |
| 1:G:1576:THR:H | 1:G:1581:GLU:HG2 | 1.72 | 0.55 |
| 2:H:2698:LEU:HD12 | 2:H:2838:LEU:HB3 | 1.89 | 0.55 |
| 3:I:3083[B]:ILE:HD12 | 3:I:3260[B]:ARG:HB2 | 1.88 | 0.55 |
| 3:I:3150[B]:LYS:CG | 3:R:3158[B]:PHE:HA | 2.20 | 0.55 |
| 3:I:3220[B]:ARG:HG2 | 3:I:3221[B]:ALA:H | 1.70 | 0.55 |
| 1:J:328:LYS:NZ | 1:M:1631:GLU:OE1 | 2.30 | 0.55 |
| 3:L:3135[A]:LYS:HG3 | 3:L:3141[A]:TYR:CD1 | 2.33 | 0.55 |
| 1:M:1471:LEU:HD23 | 1:M:1541:GLU:HG2 | 1.89 | 0.55 |
| 1:M:1650:ILE:H | 2:Q:2327:GLU:HG2 | 1.72 | 0.55 |
| 2:N:2795:ILE:O | 2:N:2798:GLN:HG2 | 2.07 | 0.55 |
| 3:O:3157[B]:PRO:HD3 | 3:X:3153[B]:LYS:CA | 2.37 | 0.55 |
| 1:P:957:ASN:N | 1:P:958:PRO:HA | 2.22 | 0.55 |
| 1:P:1627:ARG:NH2 | 1:P:1629:GLU:OE1 | 2.38 | 0.55 |
| 1:P:1639:LYS:NZ | 1:S:471:PRO:O | 2.32 | 0.55 |
| 3:R:2949[A]:LYS:NZ | 3:R:2950[A]:THR:HA | 2.21 | 0.55 |
| 3:R:3019[A]:HIS:CD2 | 3:R:3019[A]:HIS:N | 2.75 | 0.55 |
| 1:S:81:VAL:HA | 1:S:85:SER:HB3 | 1.88 | 0.55 |
| 3:U:2949[B]:LYS:NZ | 3:U:2950[B]:THR:HA | 2.21 | 0.55 |
| 3:U:2974[B]:ALA:HB1 | 3:d:3220[B]:ARG:HD3 | 1.89 | 0.55 |
| 3:U:2980[B]:HIS:HB2 | 3:d:2969[B]:TYR:CZ | 2.42 | 0.55 |
| 3:U:3082[B]:GLU:CD | 3:d:2970[B]:PRO:CB | 2.77 | 0.55 |
| 3:U:3155[B]:MET:CE | 3:d:3153[B]:LYS:HE2 | 2.29 | 0.55 |
| 3:U:3258[B]:PHE:CA | 3:d:2969[B]:TYR:O | 2.54 | 0.55 |
| 3:U:3284[B]:LYS:HE2 | 3:U:3284[B]:LYS:CA | 2.30 | 0.55 |
| 2:W:2472:ASN:N | 2:W:2473:GLY:HA2 | 2.21 | 0.55 |
| 3:X:2949[A]:LYS:NZ | 3:X:2950[A]:THR:HA | 2.21 | 0.55 |
| 3:X:2961[A]:HIS:NE2 | 3:X:2980[A]:HIS:CE1 | 2.73 | 0.55 |
| 3:X:3135[B]:LYS:HG3 | 3:X:3141[B]:TYR:CD1 | 2.33 | 0.55 |
| 3:X:3200[A]:LEU:O | 3:X:3204[A]:LEU:HD13 | 2.06 | 0.55 |
| 3:X:3284[A]:LYS:HD3 | 3:X:3284[A]:LYS:C | 2.32 | 0.55 |
| 2:Z:2132:CYS:O | 2:Z:2334:LYS:HD3 | 2.07 | 0.55 |
| 3:a:2947[A]:ALA:HA | 3:a:2949[A]:LYS:HB3 | 1.89 | 0.55 |
| 3:a:2949[B]:LYS:NZ | 3:a:2950[B]:THR:HA | 2.21 | 0.55 |
| 3:a:3019[B]:HIS:CD2 | 3:a:3019[B]:HIS:N | 2.75 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:163:LEU:HB3 | 1:b:293:LEU:HD21 | 1.89 | 0.55 |
| 2:c:2476:LEU:HD12 | 2:c:2480:LEU:HD21 | 1.89 | 0.55 |
| 3:d:2949[A]:LYS:NZ | 3:d:2950[A]:THR:HA | 2.21 | 0.55 |
| 3:d:3019[B]:HIS:CD2 | 3:d:3019[B]:HIS:N | 2.75 | 0.55 |
| 1:A:931:TRP:CZ3 | 1:A:995:ILE:HD11 | 2.42 | 0.55 |
| 1:A:983:PRO:HB3 | 1:A:989:THR:HG22 | 1.88 | 0.55 |
| 2:B:2870:LEU:HD21 | 2:B:2901:LEU:HD23 | 1.89 | 0.55 |
| 3:C:2947[A]:ALA:HA | 3:C:2949[A]:LYS:HB3 | 1.89 | 0.55 |
| 3:C:2961[B]:HIS:O | 3:L:3255[B]:PRO:HD3 | 2.07 | 0.55 |
| 3:C:2965[B]:LEU:CD2 | 3:L:3253[B]:GLU:OE2 | 2.14 | 0.55 |
| 3:C:2972[B]:GLY:C | 3:L:3090[B]:ASN:CB | 2.80 | 0.55 |
| 3:C:3298[A]:ASN:HA | 3:C:3299[A]:LEU:HB3 | 1.88 | 0.55 |
| 1:D:105:VAL:HB | 1:D:137:ARG:HH22 | 1.72 | 0.55 |
| 2:E:2265:ILE:HD12 | 2:E:2443:TYR:CG | 2.42 | 0.55 |
| 2:E:2606:LEU:HD21 | 2:E:2709:VAL:HG21 | 1.88 | 0.55 |
| 2:E:2635:TYR:HB2 | 1:G:109:LEU:HD21 | 1.88 | 0.55 |
| 3:F:2932[B]:PRO:CA | 3:F:2935[B]:ILE:HD12 | 2.30 | 0.55 |
| 3:F:2966[B]:SER:CA | 3:a:3256[B]:TRP:N | 2.61 | 0.55 |
| 3:F:3082[B]:GLU:OE2 | 3:F:3086[B]:GLU:HB2 | 2.07 | 0.55 |
| 3:F:3176[B]:LYS:H | 3:F:3176[B]:LYS:CE | 2.17 | 0.55 |
| 3:F:3228[A]:VAL:CG2 | 3:F:3245[A]:PHE:CE2 | 2.89 | 0.55 |
| 3:F:3256[B]:TRP:CD1 | 3:a:2965[B]:LEU:HD13 | 2.41 | 0.55 |
| 3:F:3307[B]:PHE:HE1 | 3:F:3309[B]:PRO:CG | 2.08 | 0.55 |
| 3:F:3307[B]:PHE:C | 3:F:3307[B]:PHE:CD1 | 2.85 | 0.55 |
| 1:G:235:CYS:HA | 1:G:820:VAL:O | 2.07 | 0.55 |
| 2:H:2107:LEU:HD23 | 2:H:2208:PRO:HB2 | 1.88 | 0.55 |
| 3:I:2947[A]:ALA:HA | 3:I:2949[A]:LYS:HB3 | 1.89 | 0.55 |
| 3:I:2949[B]:LYS:NZ | 3:I:2950[B]:THR:HA | 2.21 | 0.55 |
| 3:I:2979[B]:GLN:C | 3:R:2967[B]:CYS:HB2 | 2.10 | 0.55 |
| 3:I:3293[A]:LYS:CG | 3:I:3294[A]:SER:HB2 | 2.36 | 0.55 |
| 1:J:928:TYR:HB3 | 1:J:1047:SER:HB3 | 1.89 | 0.55 |
| 2:K:2132:CYS:O | 2:K:2334:LYS:HD3 | 2.07 | 0.55 |
| 2:K:2550:THR:O | 2:K:2553:ALA:N | 2.28 | 0.55 |
| 3:L:2960[B]:PHE:CD2 | 3:L:3157[B]:PRO:CG | 2.74 | 0.55 |
| 3:L:3082[B]:GLU:OE2 | 3:L:3086[B]:GLU:HB2 | 2.07 | 0.55 |
| 3:L:3307[A]:PHE:HE1 | 3:L:3309[A]:PRO:CG | 2.08 | 0.55 |
| 2:N:2094:ARG:HH21 | 2:Q:2094:ARG:HH21 | 1.53 | 0.55 |
| 3:O:2969[A]:TYR:CE2 | 3:O:2970[A]:PRO:CG | 2.86 | 0.55 |
| 3:O:3033[B]:PHE:HD1 | 3:O:3114[B]:PRO:HB2 | 1.72 | 0.55 |
| 3:O:3307[A]:PHE:C | 3:O:3307[A]:PHE:CD1 | 2.85 | 0.55 |
| 1:P:1441:SER:OG | 1:P:1442:MET:N | 2.34 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2932[B]:PRO:CA | 3:R:2935[B]:ILE:HD12 | 2.30 | 0.55 |
| 3:R:3307[B]:PHE:C | 3:R:3307[B]:PHE:CD1 | 2.85 | 0.55 |
| 1:S:1195:ASP:HA | 1:S:1196:ILE:CB | 2.37 | 0.55 |
| 3:U:2969[A]:TYR:CG | 3:U:2970[A]:PRO:HD2 | 2.41 | 0.55 |
| 3:U:3284[B]:LYS:HD3 | 3:U:3284[B]:LYS:C | 2.31 | 0.55 |
| 1:V:979:LEU:HB3 | 1:V:980:TYR:CD2 | 2.42 | 0.55 |
| 2:W:2890:VAL:H | 2:W:2891:LEU:HA | 1.70 | 0.55 |
| 3:X:3281[A]:PHE:HE1 | 3:X:3305[A]:ILE:HD13 | 1.71 | 0.55 |
| 1:Y:416:ASN:OD1 | 3:d:3196[A]:THR:HG21 | 2.08 | 0.55 |
| 1:Y:747:PHE:HB2 | 1:Y:799:ARG:HB3 | 1.89 | 0.55 |
| 3:a:2932[A]:PRO:CA | 3:a:2935[A]:ILE:HD12 | 2.30 | 0.55 |
| 3:a:2969[B]:TYR:CE2 | 3:a:2970[B]:PRO:CG | 2.86 | 0.55 |
| 3:d:2947[A]:ALA:HA | 3:d:2949[A]:LYS:HB3 | 1.89 | 0.55 |
| 3:d:3211[A]:ASP:OD1 | 3:d:3211[A]:ASP:N | 2.28 | 0.55 |
| 3:d:3268[B]:LYS:O | 3:d:3271[B]:VAL:HG23 | 2.06 | 0.55 |
| 1:A:1257:SER:O | 1:A:1525:TYR:HA | 2.07 | 0.54 |
| 3:C:2933[B]:SER:C | 3:C:2936[B]:GLU:H | 2.16 | 0.54 |
| 3:C:3033[B]:PHE:HD1 | 3:C:3114[B]:PRO:HB2 | 1.71 | 0.54 |
| 3:C:3185[B]:TYR:C | 3:C:3185[B]:TYR:CD2 | 2.86 | 0.54 |
| 2:E:2294:PHE:O | 2:E:2297:HIS:HB3 | 2.06 | 0.54 |
| 3:F:2937[B]:ASN:CB | 3:F:3006[B]:LYS:CD | 2.86 | 0.54 |
| 1:G:10:LEU:HD12 | 1:G:104:LEU:HD21 | 1.88 | 0.54 |
| 3:I:2981[B]:GLY:H | 3:R:2968[B]:GLN:CG | 2.19 | 0.54 |
| 3:I:3013[B]:ASP:OD1 | 3:I:3015[B]:THR:OG1 | 2.23 | 0.54 |
| 3:I:3083[A]:ILE:HD12 | 3:I:3260[A]:ARG:HB2 | 1.88 | 0.54 |
| 3:I:3096[B]:VAL:HG11 | 3:I:3115[B]:LEU:HD12 | 1.89 | 0.54 |
| 3:I:3172[B]:SER:OG | 3:R:3151[B]:LEU:N | 2.41 | 0.54 |
| 3:I:3173[B]:THR:HG22 | 3:I:3174[B]:GLY:H | 1.68 | 0.54 |
| 3:I:3176[B]:LYS:H | 3:I:3176[B]:LYS:CE | 2.17 | 0.54 |
| 3:I:3251[B]:ASP:C | 3:R:3251[B]:ASP:HB3 | 2.32 | 0.54 |
| 3:I:3284[A]:LYS:HE2 | 3:I:3284[A]:LYS:CA | 2.30 | 0.54 |
| 1:J:415:VAL:HG21 | 1:J:697:ALA:CB | 2.36 | 0.54 |
| 1:J:899:MET:HB3 | 1:J:1012:GLU:OE1 | 2.07 | 0.54 |
| 1:J:1328:SER:HB2 | 1:J:1523:LEU:HD13 | 1.88 | 0.54 |
| 3:L:2933[A]:SER:C | 3:L:2936[A]:GLU:H | 2.15 | 0.54 |
| 3:L:2969[B]:TYR:CG | 3:L:2970[B]:PRO:HD2 | 2.41 | 0.54 |
| 3:L:3273[A]:LEU:CB | 3:L:3275[A]:LEU:CD1 | 2.85 | 0.54 |
| 1:M:1296:VAL:HB | 1:M:1446:ASP:HB3 | 1.89 | 0.54 |
| 3:O:3173[A]:THR:HG22 | 3:O:3174[A]:GLY:H | 1.67 | 0.54 |
| 1:P:329:ARG:HA | 1:S:1583:CYS:O | 2.06 | 0.54 |
| 3:R:3013[B]:ASP:OD1 | 3:R:3015[B]:THR:OG1 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3014[A]:TRP:CZ3 | 3:R:3119[A]:HIS:CE1 | 2.94 | 0.54 |
| 3:R:3014[B]:TRP:CZ3 | 3:R:3119[B]:HIS:CE1 | 2.94 | 0.54 |
| 3:R:3096[B]:VAL:HG11 | 3:R:3115[B]:LEU:HD12 | 1.89 | 0.54 |
| 3:R:3132[A]:ALA:HB1 | 3:R:3197[A]:ILE:HD13 | 1.89 | 0.54 |
| 3:R:3293[A]:LYS:CG | 3:R:3294[A]:SER:HB2 | 2.36 | 0.54 |
| 3:U:2933[B]:SER:HA | 3:U:2935[B]:ILE:CD1 | 2.38 | 0.54 |
| 3:U:2970[B]:PRO:C | 3:d:3090[B]:ASN:HD22 | 2.14 | 0.54 |
| 3:U:2973[B]:THR:HA | 3:d:3247[B]:VAL:HG11 | 1.89 | 0.54 |
| 3:U:3132[B]:ALA:HB1 | 3:U:3197[B]:ILE:HD13 | 1.89 | 0.54 |
| 3:U:3255[B]:PRO:HG2 | 3:d:3252[B]:TYR:HB3 | 1.89 | 0.54 |
| 1:V:1470:GLU:HB3 | 1:V:1537:ILE:HD13 | 1.89 | 0.54 |
| 3:X:2933[A]:SER:HA | 3:X:2935[A]:ILE:CD1 | 2.38 | 0.54 |
| 3:X:2952[B]:ALA:HB3 | 3:X:2954[B]:TYR:N | 2.17 | 0.54 |
| 3:X:3033[B]:PHE:HD1 | 3:X:3114[B]:PRO:HB2 | 1.71 | 0.54 |
| 3:X:3211[B]:ASP:OD1 | 3:X:3211[B]:ASP:N | 2.28 | 0.54 |
| 3:X:3293[B]:LYS:CG | 3:X:3294[B]:SER:HB2 | 2.36 | 0.54 |
| 3:a:3014[B]:TRP:C | 3:a:3014[B]:TRP:CD1 | 2.85 | 0.54 |
| 3:a:3019[B]:HIS:CD2 | 3:a:3019[B]:HIS:H | 2.22 | 0.54 |
| 3:a:3082[B]:GLU:OE2 | 3:a:3086[B]:GLU:HB2 | 2.07 | 0.54 |
| 3:a:3307[A]:PHE:CD1 | 3:a:3307[A]:PHE:C | 2.85 | 0.54 |
| 1:b:7:VAL:HG13 | 1:b:104:LEU:HD12 | 1.89 | 0.54 |
| 1:b:597:VAL:O | 1:b:601:VAL:HG12 | 2.07 | 0.54 |
| 1:b:926:LEU:HD11 | 1:b:1043:MET:HB3 | 1.88 | 0.54 |
| 1:b:1627:ARG:NH2 | 1:b:1629:GLU:OE1 | 2.38 | 0.54 |
| 3:d:2969[B]:TYR:CD2 | 3:d:2970[B]:PRO:CD | 2.86 | 0.54 |
| 1:A:483:GLY:HA3 | 1:A:771:TRP:HE3 | 1.73 | 0.54 |
| 3:C:2949[B]:LYS:NZ | 3:C:2950[B]:THR:HA | 2.21 | 0.54 |
| 3:C:3079[B]:CYS:HA | 3:L:3161[B]:GLU:OE1 | 2.07 | 0.54 |
| 3:C:3157[B]:PRO:CA | 3:L:2982[B]:MET:SD | 2.94 | 0.54 |
| 1:D:132:ASN:OD1 | 1:D:132:ASN:N | 2.34 | 0.54 |
| 1:D:449:ASP:HB2 | 1:D:1280:GLN:NE2 | 2.22 | 0.54 |
| 1:D:1034:GLU:HG3 | 1:D:1182:ASN:HD21 | 1.72 | 0.54 |
| 1:D:1310:THR:HG23 | 1:D:1597:THR:HG23 | 1.89 | 0.54 |
| 3:F:2933[A]:SER:HA | 3:F:2935[A]:ILE:CD1 | 2.37 | 0.54 |
| 3:F:2952[B]:ALA:HB3 | 3:F:2954[B]:TYR:N | 2.17 | 0.54 |
| 3:F:3185[A]:TYR:C | 3:F:3185[A]:TYR:CD2 | 2.86 | 0.54 |
| 3:F:3220[B]:ARG:HG2 | 3:F:3221[B]:ALA:H | 1.70 | 0.54 |
| 3:F:3252[B]:TYR:C | 3:a:3252[B]:TYR:C | 2.75 | 0.54 |
| 3:I:2937[A]:ASN:CB | 3:I:3006[A]:LYS:CD | 2.86 | 0.54 |
| 3:I:2983[B]:VAL:CG2 | 3:R:3160[B]:SER:OG | 2.52 | 0.54 |
| 3:I:3014[A]:TRP:CZ3 | 3:I:3119[A]:HIS:CE1 | 2.94 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1203:MET:HB2 | 1:J:1205:LEU:HB2 | 1.90 | 0.54 |
| 3:L:3196[A]:THR:OG1 | 3:L:3199[A]:GLN:CB | 2.56 | 0.54 |
| 3:L:3307[B]:PHE:CD1 | 3:L:3307[B]:PHE:C | 2.85 | 0.54 |
| 2:N:2180:TRP:CD1 | 2:N:2247:ILE:HD11 | 2.43 | 0.54 |
| 3:O:2933[B]:SER:HA | 3:O:2935[B]:ILE:CD1 | 2.37 | 0.54 |
| 3:O:2969[B]:TYR:H | 3:X:2988[B]:TRP:CG | 2.24 | 0.54 |
| 3:O:3014[B]:TRP:CZ3 | 3:O:3119[B]:HIS:CE1 | 2.95 | 0.54 |
| 3:O:3019[A]:HIS:CD2 | 3:O:3019[A]:HIS:N | 2.75 | 0.54 |
| 3:O:3093[B]:HIS:CE1 | 3:O:3119[B]:HIS:CD2 | 2.92 | 0.54 |
| 3:O:3183[A]:LEU:N | 3:O:3184[A]:ASN:HA | 2.12 | 0.54 |
| 3:R:3014[B]:TRP:C | 3:R:3014[B]:TRP:CD1 | 2.85 | 0.54 |
| 3:R:3019[B]:HIS:CD2 | 3:R:3019[B]:HIS:N | 2.75 | 0.54 |
| 3:R:3082[B]:GLU:OE2 | 3:R:3086[B]:GLU:HB2 | 2.07 | 0.54 |
| 1:S:873:VAL:HA | 1:S:876:PHE:CD2 | 2.42 | 0.54 |
| 1:S:1260:ARG:HD3 | 1:S:1331:GLU:OE1 | 2.07 | 0.54 |
| 2:T:2506:ARG:NE | 2:T:2578:GLU:OE2 | 2.27 | 0.54 |
| 3:U:3083[A]:ILE:HD12 | 3:U:3260[A]:ARG:HB2 | 1.88 | 0.54 |
| 3:U:3089[A]:HIS:CE1 | 3:U:3119[A]:HIS:CE1 | 2.81 | 0.54 |
| 3:U:3298[B]:ASN:HA | 3:U:3299[B]:LEU:HB3 | 1.88 | 0.54 |
| 1:V:51:ASP:OD1 | 1:V:51:ASP:N | 2.37 | 0.54 |
| 2:W:2556:TYR:CE1 | 2:W:2845:PRO:HD2 | 2.35 | 0.54 |
| 3:X:2960[A]:PHE:CD1 | 3:X:2960[A]:PHE:N | 2.72 | 0.54 |
| 3:X:3082[A]:GLU:OE2 | 3:X:3086[A]:GLU:HB2 | 2.08 | 0.54 |
| 1:Y:402:THR:HG23 | 1:Y:659:CYS:HA | 1.87 | 0.54 |
| 1:Y:1070:ALA:HB3 | 1:Y:1077:LEU:HD21 | 1.90 | 0.54 |
| 2:Z:2446:GLU:HG2 | 2:Z:2448:THR:HG22 | 1.89 | 0.54 |
| 3:a:2933[A]:SER:HA | 3:a:2935[A]:ILE:CD1 | 2.38 | 0.54 |
| 3:a:3033[B]:PHE:HD1 | 3:a:3114[B]:PRO:HB2 | 1.71 | 0.54 |
| 3:a:3211[A]:ASP:OD1 | 3:a:3211[A]:ASP:N | 2.28 | 0.54 |
| 3:a:3281[A]:PHE:HE1 | 3:a:3305[A]:ILE:HD13 | 1.71 | 0.54 |
| 3:a:3298[A]:ASN:HA | 3:a:3299[A]:LEU:HB3 | 1.88 | 0.54 |
| 1:b:103:GLU:OE2 | 1:b:106:GLN:NE2 | 2.40 | 0.54 |
| 3:d:2937[A]:ASN:CB | 3:d:3006[A]:LYS:CD | 2.86 | 0.54 |
| 3:d:3014[B]:TRP:CZ3 | 3:d:3119[B]:HIS:CE1 | 2.95 | 0.54 |
| 2:B:2313:LYS:HD3 | 2:B:2320:TYR:HE2 | 1.72 | 0.54 |
| 3:C:2933[A]:SER:HA | 3:C:2935[A]:ILE:CD1 | 2.37 | 0.54 |
| 3:C:2960[B]:PHE:CD2 | 3:C:3157[B]:PRO:CG | 2.74 | 0.54 |
| 3:C:2988[B]:TRP:CD1 | 3:L:3153[B]:LYS:CD | 2.81 | 0.54 |
| 3:C:3014[A]:TRP:C | 3:C:3014[A]:TRP:CD1 | 2.85 | 0.54 |
| 3:C:3149[B]:ASN:HB2 | 3:L:3163[B]:ASN:HD21 | 1.54 | 0.54 |
| 3:C:3169[B]:LYS:CG | 3:L:3150[B]:LYS:N | 2.64 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3252[B]:TYR:CG | 3:L:3223[B]:GLY:O | 2.60 | 0.54 |
| 3:C:3273[A]:LEU:CB | 3:C:3275[A]:LEU:CD1 | 2.86 | 0.54 |
| 1:D:983:PRO:HB3 | 1:D:989:THR:OG1 | 2.08 | 0.54 |
| 1:D:1315:GLY:HA3 | 1:D:1601:TRP:CB | 2.37 | 0.54 |
| 2:E:2768:LEU:HD23 | 2:E:2774:LEU:HD21 | 1.88 | 0.54 |
| 3:F:2952[B]:ALA:N | 3:F:2953[B]:GLY:HA2 | 2.06 | 0.54 |
| 3:F:2969[B]:TYR:CE2 | 3:a:3120[B]:HIS:CD2 | 2.95 | 0.54 |
| 3:F:2976[B]:ALA:O | 3:a:2976[B]:ALA:O | 2.26 | 0.54 |
| 3:F:3154[B]:PRO:HD2 | 3:a:3155[B]:MET:CG | 2.21 | 0.54 |
| 3:I:3014[B]:TRP:C | 3:I:3014[B]:TRP:CD1 | 2.85 | 0.54 |
| 3:I:3153[B]:LYS:HG2 | 3:R:3155[B]:MET:CB | 2.32 | 0.54 |
| 3:I:3196[A]:THR:OG1 | 3:I:3199[A]:GLN:CB | 2.56 | 0.54 |
| 3:I:3253[B]:GLU:HG3 | 3:R:2965[B]:LEU:HA | 1.89 | 0.54 |
| 3:I:3273[B]:LEU:HB2 | 3:I:3275[B]:LEU:CD1 | 2.34 | 0.54 |
| 3:I:3307[B]:PHE:CD1 | 3:I:3307[B]:PHE:C | 2.85 | 0.54 |
| 1:J:673:PHE:HB3 | 1:J:677:LEU:HB2 | 1.89 | 0.54 |
| 3:L:2937[A]:ASN:CB | 3:L:3006[A]:LYS:CD | 2.85 | 0.54 |
| 3:L:3013[B]:ASP:OD1 | 3:L:3015[B]:THR:OG1 | 2.23 | 0.54 |
| 3:L:3082[A]:GLU:OE2 | 3:L:3086[A]:GLU:HB2 | 2.08 | 0.54 |
| 3:L:3240[A]:THR:CG2 | 3:L:3241[A]:PHE:N | 2.71 | 0.54 |
| 1:M:744:VAL:HG22 | 1:M:760:ILE:HG12 | 1.89 | 0.54 |
| 1:M:1438:ASP:HB3 | 1:M:1441:SER:HB2 | 1.88 | 0.54 |
| 3:O:2968[B]:GLN:CB | 3:X:2979[B]:GLN:HG2 | 2.36 | 0.54 |
| 3:O:3162[B]:ASP:OD2 | 3:X:3150[B]:LYS:NZ | 2.39 | 0.54 |
| 3:O:3196[B]:THR:OG1 | 3:O:3199[B]:GLN:CB | 2.56 | 0.54 |
| 3:R:2933[B]:SER:HA | 3:R:2935[B]:ILE:CD1 | 2.37 | 0.54 |
| 3:R:2949[B]:LYS:HZ2 | 3:R:2950[B]:THR:HA | 1.71 | 0.54 |
| 3:R:3082[A]:GLU:OE2 | 3:R:3086[A]:GLU:HB2 | 2.08 | 0.54 |
| 3:U:3019[B]:HIS:CD2 | 3:U:3019[B]:HIS:N | 2.75 | 0.54 |
| 3:U:3151[A]:LEU:HB2 | 3:U:3175[A]:TYR:HE2 | 1.68 | 0.54 |
| 3:U:3151[B]:LEU:HB2 | 3:U:3175[B]:TYR:HE2 | 1.68 | 0.54 |
| 3:U:3151[B]:LEU:O | 3:d:3153[B]:LYS:HA | 2.08 | 0.54 |
| 3:U:3200[A]:LEU:O | 3:U:3204[A]:LEU:HD13 | 2.06 | 0.54 |
| 1:V:664:VAL:O | 1:V:689:PRO:HD2 | 2.06 | 0.54 |
| 3:X:2947[A]:ALA:HA | 3:X:2949[A]:LYS:HB3 | 1.89 | 0.54 |
| 3:X:3196[B]:THR:OG1 | 3:X:3199[B]:GLN:CB | 2.56 | 0.54 |
| 1:Y:1170:MET:HB2 | 1:Y:1203:MET:HE2 | 1.88 | 0.54 |
| 3:a:3093[B]:HIS:CE1 | 3:a:3119[B]:HIS:CD2 | 2.92 | 0.54 |
| 3:a:3185[B]:TYR:C | 3:a:3185[B]:TYR:CD2 | 2.86 | 0.54 |
| 3:a:3273[B]:LEU:CB | 3:a:3275[B]:LEU:CD1 | 2.86 | 0.54 |
| 3:a:3284[B]:LYS:HD3 | 3:a:3284[B]:LYS:C | 2.32 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:806:ASN:N | 1:b:807:GLY:HA2 | 2.22 | 0.54 |
| 2:c:2780:HIS:HD2 | 2:c:2782:ASN:OD1 | 1.90 | 0.54 |
| 2:c:2883:ILE:HD12 | 2:c:2894:ASN:HA | 1.89 | 0.54 |
| 1:A:864:ASP:HB3 | 1:A:869:GLY:HA3 | 1.89 | 0.54 |
| 1:A:1641:THR:HG21 | 6:h:2:NAG:H81 | 1.88 | 0.54 |
| 3:C:2969[A]:TYR:CE2 | 3:C:2970[A]:PRO:CG | 2.86 | 0.54 |
| 3:C:3042[A]:ASP:N | 3:C:3042[A]:ASP:OD2 | 2.41 | 0.54 |
| 3:C:3273[B]:LEU:CB | 3:C:3275[B]:LEU:CD1 | 2.86 | 0.54 |
| 3:C:3307[B]:PHE:C | 3:C:3307[B]:PHE:CD1 | 2.85 | 0.54 |
| 1:D:1638:SER:O | 1:G:472:ASP:HB3 | 2.08 | 0.54 |
| 2:E:2573:TYR:HE2 | 2:E:2707:PHE:HE2 | 1.54 | 0.54 |
| 2:E:2863:ARG:HB2 | 2:E:2865:ILE:HG13 | 1.90 | 0.54 |
| 3:F:2947[A]:ALA:HA | 3:F:2949[A]:LYS:HB3 | 1.89 | 0.54 |
| 3:F:3196[B]:THR:OG1 | 3:F:3199[B]:GLN:CB | 2.56 | 0.54 |
| 3:F:3252[B]:TYR:O | 3:a:3253[B]:GLU:CA | 2.56 | 0.54 |
| 1:G:898:GLY:HA2 | 1:G:1186:TRP:HB2 | 1.90 | 0.54 |
| 2:H:2406:SER:HG | 2:H:2430:GLY:H | 1.53 | 0.54 |
| 3:I:2933[A]:SER:HA | 3:I:2935[A]:ILE:CD1 | 2.38 | 0.54 |
| 3:I:3014[B]:TRP:CZ3 | 3:I:3119[B]:HIS:CE1 | 2.95 | 0.54 |
| 3:I:3082[B]:GLU:OE2 | 3:I:3086[B]:GLU:HB2 | 2.07 | 0.54 |
| 1:J:145:GLN:HG2 | 1:J:151:GLN:CD | 2.31 | 0.54 |
| 1:J:402:THR:HG23 | 1:J:659:CYS:HA | 1.88 | 0.54 |
| 2:K:2569:TRP:O | 2:K:2572:VAL:HG23 | 2.08 | 0.54 |
| 2:K:2828:ASP:HB2 | 2:K:2830:GLN:OE1 | 2.07 | 0.54 |
| 3:L:3014[B]:TRP:CD1 | 3:L:3014[B]:TRP:C | 2.85 | 0.54 |
| 1:M:499:GLU:HG3 | 1:M:511:VAL:H | 1.72 | 0.54 |
| 1:M:1209:ASP:O | 1:M:1211:TYR:HB2 | 2.06 | 0.54 |
| 3:O:2937[B]:ASN:CB | 3:O:3006[B]:LYS:CD | 2.86 | 0.54 |
| 3:O:2949[A]:LYS:NZ | 3:O:2950[A]:THR:HA | 2.21 | 0.54 |
| 3:O:3185[B]:TYR:C | 3:O:3185[B]:TYR:CD2 | 2.86 | 0.54 |
| 3:O:3228[B]:VAL:CG2 | 3:O:3245[B]:PHE:CE2 | 2.89 | 0.54 |
| 3:O:3256[B]:TRP:CE2 | 3:X:3161[B]:GLU:CG | 2.90 | 0.54 |
| 1:P:22:LEU:HD12 | 1:P:25:MET:HG2 | 1.90 | 0.54 |
| 2:Q:2179:ASP:HA | 2:Q:2300:ASN:ND2 | 2.23 | 0.54 |
| 3:R:3013[A]:ASP:OD1 | 3:R:3015[A]:THR:OG1 | 2.23 | 0.54 |
| 3:R:3196[B]:THR:OG1 | 3:R:3199[B]:GLN:CB | 2.56 | 0.54 |
| 1:S:105:VAL:HG12 | 1:S:123:PHE:HB3 | 1.89 | 0.54 |
| 1:S:484:MET:HE3 | 1:S:663:GLU:HG3 | 1.90 | 0.54 |
| 2:T:2570:HIS:CD2 | 9:T:3002:CUO:O1 | 2.60 | 0.54 |
| 3:U:2937[A]:ASN:CB | 3:U:3006[A]:LYS:CD | 2.86 | 0.54 |
| 3:U:2947[B]:ALA:HA | 3:U:2949[B]:LYS:HB3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3240[B]:THR:CG2 | 3:U:3241[B]:PHE:N | 2.71 | 0.54 |
| 3:U:3273[B]:LEU:CB | 3:U:3275[B]:LEU:CD1 | 2.85 | 0.54 |
| 1:V:1390:ASP:CB | 1:Y:1372:ILE:HD11 | 2.36 | 0.54 |
| 3:X:3281[B]:PHE:HE1 | 3:X:3305[B]:ILE:HD13 | 1.71 | 0.54 |
| 3:X:3293[A]:LYS:CG | 3:X:3294[A]:SER:HB2 | 2.36 | 0.54 |
| 3:a:2933[B]:SER:C | 3:a:2936[B]:GLU:H | 2.15 | 0.54 |
| 3:a:3093[A]:HIS:CE1 | 3:a:3119[A]:HIS:CD2 | 2.92 | 0.54 |
| 1:b:524:PRO:HD2 | 1:b:527:LEU:HD11 | 1.89 | 0.54 |
| 3:d:3014[A]:TRP:CD1 | 3:d:3014[A]:TRP:C | 2.85 | 0.54 |
| 3:d:3083[A]:ILE:HD12 | 3:d:3260[A]:ARG:HB2 | 1.88 | 0.54 |
| 1:A:1328:SER:HB2 | 1:A:1523:LEU:HD13 | 1.89 | 0.54 |
| 2:B:2122:ILE:O | 2:B:2125:PHE:HB2 | 2.07 | 0.54 |
| 3:C:3033[A]:PHE:HD1 | 3:C:3114[A]:PRO:HB2 | 1.72 | 0.54 |
| 3:C:3082[A]:GLU:OE2 | 3:C:3086[A]:GLU:HB2 | 2.08 | 0.54 |
| 3:C:3188[A]:ASP:N | 3:C:3188[A]:ASP:OD2 | 2.36 | 0.54 |
| 1:D:105:VAL:HB | 1:D:137:ARG:NH2 | 2.22 | 0.54 |
| 1:D:899:MET:HE2 | 1:D:1012:GLU:OE2 | 2.07 | 0.54 |
| 2:E:2275:GLY:HA3 | 2:E:2283:ASN:HB2 | 1.90 | 0.54 |
| 3:F:2933[A]:SER:C | 3:F:2936[A]:GLU:H | 2.16 | 0.54 |
| 3:F:3013[B]:ASP:OD1 | 3:F:3015[B]:THR:HG23 | 2.08 | 0.54 |
| 3:F:3083[A]:ILE:HD12 | 3:F:3260[A]:ARG:HB2 | 1.88 | 0.54 |
| 3:F:3268[A]:LYS:O | 3:F:3271[A]:VAL:HG23 | 2.06 | 0.54 |
| 1:G:740:THR:OG1 | 1:G:741:SER:N | 2.39 | 0.54 |
| 1:G:1034:GLU:HB2 | 1:G:1182:ASN:HD21 | 1.72 | 0.54 |
| 2:H:2446:GLU:HG2 | 2:H:2448:THR:HG22 | 1.90 | 0.54 |
| 3:I:2975[B]:PHE:CD1 | 3:R:3107[B]:LEU:HD21 | 2.42 | 0.54 |
| 3:I:3132[B]:ALA:HB1 | 3:I:3197[B]:ILE:HD13 | 1.89 | 0.54 |
| 3:I:3172[B]:SER:OG | 3:R:3150[B]:LYS:C | 2.49 | 0.54 |
| 3:I:3185[A]:TYR:C | 3:I:3185[A]:TYR:CD2 | 2.85 | 0.54 |
| 3:I:3307[A]:PHE:HE1 | 3:I:3309[A]:PRO:CG | 2.08 | 0.54 |
| 3:L:2933[B]:SER:C | 3:L:2936[B]:GLU:H | 2.16 | 0.54 |
| 3:L:2949[B]:LYS:NZ | 3:L:2950[B]:THR:HA | 2.21 | 0.54 |
| 3:L:3014[A]:TRP:C | 3:L:3014[A]:TRP:CD1 | 2.85 | 0.54 |
| 3:L:3196[B]:THR:OG1 | 3:L:3199[B]:GLN:CB | 2.56 | 0.54 |
| 3:L:3240[B]:THR:CG2 | 3:L:3241[B]:PHE:N | 2.71 | 0.54 |
| 3:L:3281[A]:PHE:HE1 | 3:L:3305[A]:ILE:HD13 | 1.71 | 0.54 |
| 3:L:3293[B]:LYS:CD | 3:L:3294[B]:SER:N | 2.64 | 0.54 |
| 1:M:633:HIS:C | 1:M:633:HIS:HD1 | 2.15 | 0.54 |
| 1:M:1210:LYS:HA | 1:M:1211:TYR:HB3 | 1.89 | 0.54 |
| 2:N:2768:LEU:HA | 2:N:2774:LEU:HD11 | 1.89 | 0.54 |
| 3:O:3014[A]:TRP:C | 3:O:3014[A]:TRP:CD1 | 2.85 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3163[B]:ASN:ND2 | 3:X:3148[B]:ILE:HG22 | 2.22 | 0.54 |
| 3:O:3185[A]:TYR:C | 3:O:3185[A]:TYR:CD2 | 2.86 | 0.54 |
| 1:P:128:ILE:HG22 | 1:P:130:PHE:O | 2.07 | 0.54 |
| 3:R:2937[A]:ASN:CB | 3:R:3006[A]:LYS:CD | 2.86 | 0.54 |
| 3:R:2937[B]:ASN:CB | 3:R:3006[B]:LYS:CD | 2.86 | 0.54 |
| 3:R:3093[A]:HIS:CE1 | 3:R:3119[A]:HIS:CD2 | 2.92 | 0.54 |
| 3:R:3196[A]:THR:OG1 | 3:R:3199[A]:GLN:CB | 2.56 | 0.54 |
| 1:S:1549:GLY:HA2 | 1:S:1656:ASP:HB3 | 1.89 | 0.54 |
| 3:U:2960[A]:PHE:CD1 | 3:U:2960[A]:PHE:N | 2.72 | 0.54 |
| 3:U:2967[B]:CYS:CB | 3:d:3257[B]:ALA:O | 2.49 | 0.54 |
| 3:U:3170[B]:ALA:O | 3:d:3148[B]:ILE:CG2 | 2.56 | 0.54 |
| 1:V:419:THR:HG22 | 1:V:1062:PHE:HA | 1.89 | 0.54 |
| 1:V:525:SER:HA | 1:V:528:ALA:HB3 | 1.88 | 0.54 |
| 2:W:2180:TRP:HD1 | 2:W:2247:ILE:HD11 | 1.71 | 0.54 |
| 2:W:2757:PRO:HA | 2:W:2760:ARG:HE | 1.73 | 0.54 |
| 3:X:3240[A]:THR:CG2 | 3:X:3241[A]:PHE:N | 2.71 | 0.54 |
| 3:X:3307[B]:PHE:CD1 | 3:X:3307[B]:PHE:C | 2.85 | 0.54 |
| 2:Z:2179:ASP:HA | 2:Z:2300:ASN:ND2 | 2.22 | 0.54 |
| 3:a:2933[B]:SER:HA | 3:a:2935[B]:ILE:CD1 | 2.37 | 0.54 |
| 3:a:3033[A]:PHE:HD1 | 3:a:3114[A]:PRO:HB2 | 1.72 | 0.54 |
| 3:a:3196[A]:THR:OG1 | 3:a:3199[A]:GLN:CB | 2.56 | 0.54 |
| 1:b:450:LYS:HD3 | 1:b:1338:GLY:O | 2.07 | 0.54 |
| 1:b:956:PRO:HB2 | 1:b:957:ASN:C | 2.32 | 0.54 |
| 3:d:2933[B]:SER:HA | 3:d:2935[B]:ILE:CD1 | 2.38 | 0.54 |
| 3:d:2969[A]:TYR:CE2 | 3:d:2970[A]:PRO:CG | 2.86 | 0.54 |
| 3:d:3019[A]:HIS:CD2 | 3:d:3019[A]:HIS:N | 2.75 | 0.54 |
| 3:d:3033[A]:PHE:HD1 | 3:d:3114[A]:PRO:HB2 | 1.72 | 0.54 |
| 3:d:3082[B]:GLU:OE2 | 3:d:3086[B]:GLU:HB2 | 2.07 | 0.54 |
| 2:B:2271:HIS:O | 2:B:2283:ASN:HB3 | 2.08 | 0.54 |
| 3:C:2932[A]:PRO:CA | 3:C:2935[A]:ILE:HD12 | 2.30 | 0.54 |
| 3:C:3086[B]:GLU:CB | 3:L:2968[B]:GLN:HE21 | 2.21 | 0.54 |
| 3:C:3153[B]:LYS:CE | 3:L:3158[B]:PHE:CG | 2.79 | 0.54 |
| 3:C:3255[B]:PRO:CD | 3:L:2960[B]:PHE:O | 2.46 | 0.54 |
| 3:C:3284[B]:LYS:HE2 | 3:C:3284[B]:LYS:CA | 2.29 | 0.54 |
| 1:D:210:HIS:HA | 1:D:213:VAL:HG22 | 1.90 | 0.54 |
| 3:F:3170[B]:ALA:C | 3:a:3152[B]:LYS:HB2 | 2.31 | 0.54 |
| 3:F:3220[A]:ARG:HG2 | 3:F:3221[A]:ALA:H | 1.70 | 0.54 |
| 3:F:3240[B]:THR:CG2 | 3:F:3241[B]:PHE:N | 2.71 | 0.54 |
| 3:I:3150[B]:LYS:HB2 | 3:R:3159[B]:SER:C | 2.23 | 0.54 |
| 3:I:3155[B]:MET:HG3 | 3:R:3154[B]:PRO:CD | 2.33 | 0.54 |
| 1:J:840:ARG:NH2 | 1:J:914:GLU:OE2 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1108:TYR:HB2 | 1:J:1114:TYR:CE1 | 2.43 | 0.54 |
| 1:J:1470:GLU:HB3 | 1:J:1537:ILE:HD11 | 1.90 | 0.54 |
| 3:O:2968[B]:GLN:CG | 3:X:2984[B]:THR:OG1 | 2.55 | 0.54 |
| 3:O:3096[A]:VAL:HG11 | 3:O:3115[A]:LEU:HD12 | 1.89 | 0.54 |
| 3:O:3254[B]:MET:SD | 3:X:3154[B]:PRO:CB | 2.96 | 0.54 |
| 1:P:567:LEU:N | 1:P:571:PRO:HB3 | 2.23 | 0.54 |
| 1:P:1396:GLU:OE2 | 1:P:1569:ARG:NH2 | 2.41 | 0.54 |
| 1:P:1639:LYS:HD2 | 1:S:472:ASP:HA | 1.88 | 0.54 |
| 2:Q:2252:GLU:CD | 2:Q:2393:ARG:HH12 | 2.16 | 0.54 |
| 3:R:3220[B]:ARG:HH11 | 3:R:3220[B]:ARG:CG | 2.12 | 0.54 |
| 3:U:2949[A]:LYS:NZ | 3:U:2950[A]:THR:HA | 2.21 | 0.54 |
| 3:U:2969[B]:TYR:CE2 | 3:U:2970[B]:PRO:CG | 2.86 | 0.54 |
| 3:U:3156[B]:MET:HE3 | 3:d:2982[B]:MET:CE | 2.26 | 0.54 |
| 3:U:3293[A]:LYS:CD | 3:U:3294[A]:SER:N | 2.64 | 0.54 |
| 2:W:2179:ASP:HA | 2:W:2300:ASN:ND2 | 2.22 | 0.54 |
| 2:W:2336:PHE:O | 2:W:2343:ASN:ND2 | 2.40 | 0.54 |
| 3:X:2931[A]:THR:HG1 | 3:X:2934[A]:GLU:CD | 2.00 | 0.54 |
| 3:X:3042[A]:ASP:N | 3:X:3042[A]:ASP:OD2 | 2.41 | 0.54 |
| 3:X:3047[B]:ARG:HH21 | 3:X:3113[B]:ASP:CG | 2.16 | 0.54 |
| 3:X:3093[B]:HIS:CE1 | 3:X:3119[B]:HIS:CD2 | 2.92 | 0.54 |
| 3:X:3284[B]:LYS:HE2 | 3:X:3284[B]:LYS:CA | 2.30 | 0.54 |
| 1:Y:712:SER:O | 1:Y:716:LEU:N | 2.35 | 0.54 |
| 3:a:3173[B]:THR:HG22 | 3:a:3175[B]:TYR:H | 1.73 | 0.54 |
| 3:a:3240[B]:THR:CG2 | 3:a:3241[B]:PHE:N | 2.71 | 0.54 |
| 3:a:3273[B]:LEU:HB2 | 3:a:3275[B]:LEU:CD1 | 2.34 | 0.54 |
| 1:b:150:GLY:HA2 | 1:b:151:GLN:C | 2.33 | 0.54 |
| 1:b:287:GLU:N | 1:b:287:GLU:OE1 | 2.40 | 0.54 |
| 1:b:325:THR:N | 1:b:332:ASP:OD1 | 2.40 | 0.54 |
| 1:b:452:ILE:HD12 | 1:b:1367:SER:HB2 | 1.90 | 0.54 |
| 1:b:1258:ARG:NH2 | 1:b:1332:ASP:OD1 | 2.41 | 0.54 |
| 1:b:1470:GLU:HG3 | 1:b:1530:LEU:HD12 | 1.88 | 0.54 |
| 2:c:2606:LEU:HD22 | 2:c:2706:ILE:HG12 | 1.90 | 0.54 |
| 3:d:3013[B]:ASP:OD1 | 3:d:3015[B]:THR:HG23 | 2.08 | 0.54 |
| 3:d:3014[B]:TRP:C | 3:d:3014[B]:TRP:CD1 | 2.85 | 0.54 |
| 3:d:3240[A]:THR:CG2 | 3:d:3241[A]:PHE:N | 2.71 | 0.54 |
| 1:A:494:VAL:HG23 | 1:A:671:PHE:HZ | 1.72 | 0.54 |
| 1:A:915:ASN:ND2 | 1:A:1093:ASP:OD2 | 2.38 | 0.54 |
| 1:A:1028:VAL:HA | 1:A:1035:TYR:CE2 | 2.43 | 0.54 |
| 3:C:2952[A]:ALA:HB3 | 3:C:2954[A]:TYR:N | 2.18 | 0.54 |
| 3:C:3013[A]:ASP:OD1 | 3:C:3015[A]:THR:HG23 | 2.08 | 0.54 |
| 3:C:3079[B]:CYS:CB | 3:L:3161[B]:GLU:CB | 2.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3293[A]:LYS:CG | 3:C:3294[A]:SER:HB2 | 2.36 | 0.54 |
| 1:D:241:HIS:CE1 | 1:D:795:GLU:HA | 2.43 | 0.54 |
| 1:D:277:ASP:OD1 | 1:D:278:ASP:N | 2.41 | 0.54 |
| 1:D:1414:THR:HG23 | 1:D:1477:LEU:HD13 | 1.89 | 0.54 |
| 3:F:3019[A]:HIS:CD2 | 3:F:3019[A]:HIS:N | 2.75 | 0.54 |
| 3:F:3154[B]:PRO:CD | 3:a:3173[B]:THR:C | 2.78 | 0.54 |
| 1:G:567:LEU:HD13 | 1:G:569:LYS:H | 1.73 | 0.54 |
| 3:I:2933[B]:SER:C | 3:I:2936[B]:GLU:H | 2.16 | 0.54 |
| 3:I:2989[B]:HIS:CB | 3:R:2970[B]:PRO:HD3 | 2.24 | 0.54 |
| 3:I:3132[A]:ALA:HB1 | 3:I:3197[A]:ILE:HD13 | 1.89 | 0.54 |
| 3:I:3185[B]:TYR:C | 3:I:3185[B]:TYR:CD2 | 2.86 | 0.54 |
| 3:I:3240[A]:THR:CG2 | 3:I:3241[A]:PHE:N | 2.71 | 0.54 |
| 3:I:3240[B]:THR:CG2 | 3:I:3241[B]:PHE:N | 2.71 | 0.54 |
| 3:I:3264[A]:TYR:C | 3:I:3264[A]:TYR:HD1 | 2.16 | 0.54 |
| 3:I:3273[A]:LEU:CB | 3:I:3275[A]:LEU:CD1 | 2.86 | 0.54 |
| 1:J:92:TRP:O | 1:J:212:ASN:ND2 | 2.37 | 0.54 |
| 1:J:675:SER:O | 1:J:679:ASN:ND2 | 2.41 | 0.54 |
| 1:J:1490:ASN:O | 1:J:1512:ARG:NE | 2.41 | 0.54 |
| 1:J:1604:ASP:OD1 | 1:J:1605:ARG:NH1 | 2.40 | 0.54 |
| 3:L:2947[B]:ALA:HA | 3:L:2949[B]:LYS:HB3 | 1.89 | 0.54 |
| 3:L:3013[B]:ASP:OD1 | 3:L:3015[B]:THR:HG23 | 2.08 | 0.54 |
| 3:L:3185[B]:TYR:C | 3:L:3185[B]:TYR:CD2 | 2.85 | 0.54 |
| 2:N:2336:PHE:HB3 | 2:N:2348:THR:HG22 | 1.89 | 0.54 |
| 3:O:2952[B]:ALA:HB3 | 3:O:2954[B]:TYR:N | 2.18 | 0.54 |
| 3:O:3082[A]:GLU:OE2 | 3:O:3086[A]:GLU:HB2 | 2.07 | 0.54 |
| 3:O:3153[B]:LYS:HG3 | 3:X:3176[B]:LYS:HZ2 | 1.73 | 0.54 |
| 3:O:3173[A]:THR:HG22 | 3:O:3175[A]:TYR:H | 1.73 | 0.54 |
| 1:P:84:GLY:HA2 | 1:P:85:SER:HB3 | 1.88 | 0.54 |
| 1:P:705:THR:HG22 | 1:P:1118:THR:HG23 | 1.90 | 0.54 |
| 1:P:1317:PRO:HA | 1:P:1420:GLU:HG3 | 1.88 | 0.54 |
| 3:R:3185[A]:TYR:C | 3:R:3185[A]:TYR:CD2 | 2.86 | 0.54 |
| 3:R:3273[A]:LEU:HB2 | 3:R:3275[A]:LEU:CD1 | 2.34 | 0.54 |
| 1:S:84:GLY:HA2 | 1:S:85:SER:HB3 | 1.90 | 0.54 |
| 2:T:2823:ILE:HG22 | 2:T:2879:LEU:HD22 | 1.90 | 0.54 |
| 3:U:2970[B]:PRO:C | 3:d:3090[B]:ASN:ND2 | 2.62 | 0.54 |
| 3:U:3014[B]:TRP:C | 3:U:3014[B]:TRP:CD1 | 2.85 | 0.54 |
| 3:U:3019[A]:HIS:CD2 | 3:U:3019[A]:HIS:N | 2.75 | 0.54 |
| 3:U:3082[B]:GLU:OE2 | 3:U:3086[B]:GLU:HB2 | 2.08 | 0.54 |
| 3:U:3173[A]:THR:HG22 | 3:U:3175[A]:TYR:H | 1.73 | 0.54 |
| 3:U:3254[B]:MET:CA | 3:d:3254[B]:MET:CA | 2.54 | 0.54 |
| 3:X:2933[B]:SER:HA | 3:X:2935[B]:ILE:CD1 | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2937[A]:ASN:CB | 3:X:3006[A]:LYS:CD | 2.86 | 0.54 |
| 3:X:3014[B]:TRP:CZ3 | 3:X:3119[B]:HIS:CE1 | 2.95 | 0.54 |
| 1:Y:1556:GLY:HA3 | 1:Y:1606:LEU:HD13 | 1.90 | 0.54 |
| 2:Z:2528:LYS:NZ | 2:Z:2626:ARG:O | 2.40 | 0.54 |
| 3:a:2933[A]:SER:C | 3:a:2936[A]:GLU:H | 2.16 | 0.54 |
| 3:a:2937[A]:ASN:CB | 3:a:3006[A]:LYS:CD | 2.86 | 0.54 |
| 3:a:3047[A]:ARG:HH21 | 3:a:3113[A]:ASP:CG | 2.16 | 0.54 |
| 3:a:3176[B]:LYS:H | 3:a:3176[B]:LYS:CE | 2.17 | 0.54 |
| 1:b:1271:MET:HG2 | 1:b:1358:LEU:HD13 | 1.90 | 0.54 |
| 3:d:3284[A]:LYS:HD3 | 3:d:3284[A]:LYS:C | 2.31 | 0.54 |
| 3:d:3307[A]:PHE:C | 3:d:3307[A]:PHE:CD1 | 2.85 | 0.54 |
| 1:A:838:ARG:NH1 | 1:A:914:GLU:OE2 | 2.41 | 0.54 |
| 2:B:2883:ILE:HG22 | 2:B:2894:ASN:HD22 | 1.72 | 0.54 |
| 3:C:2978[B]:CYS:CA | 3:L:3254[B]:MET:HB3 | 2.26 | 0.54 |
| 3:C:3170[B]:ALA:HA | 3:L:3148[B]:ILE:HG22 | 1.90 | 0.54 |
| 3:C:3196[B]:THR:OG1 | 3:C:3199[B]:GLN:CB | 2.56 | 0.54 |
| 1:D:17:ASN:ND2 | 1:D:86:THR:H | 2.06 | 0.54 |
| 2:E:2320:TYR:HA | 2:E:2358:PHE:HB3 | 1.90 | 0.54 |
| 3:F:3307[A]:PHE:CD1 | 3:F:3307[A]:PHE:C | 2.85 | 0.54 |
| 1:G:287:GLU:OE1 | 1:G:287:GLU:N | 2.37 | 0.54 |
| 2:H:2651:GLN:HG2 | 2:H:2652:LYS:HD2 | 1.90 | 0.54 |
| 3:I:2937[B]:ASN:CB | 3:I:3006[B]:LYS:CD | 2.86 | 0.54 |
| 3:I:3196[B]:THR:OG1 | 3:I:3199[B]:GLN:CB | 2.56 | 0.54 |
| 3:I:3259[B]:ASP:CG | 3:R:3162[B]:ASP:HB3 | 2.30 | 0.54 |
| 3:I:3264[B]:TYR:C | 3:I:3264[B]:TYR:HD1 | 2.16 | 0.54 |
| 1:J:491:HIS:CD2 | 9:J:5002:CUO:O1 | 2.59 | 0.54 |
| 3:L:3019[B]:HIS:CD2 | 3:L:3019[B]:HIS:N | 2.75 | 0.54 |
| 3:L:3273[B]:LEU:CB | 3:L:3275[B]:LEU:CD1 | 2.86 | 0.54 |
| 3:L:3307[A]:PHE:C | 3:L:3307[A]:PHE:CD1 | 2.85 | 0.54 |
| 1:M:603:HIS:NE2 | 1:M:607:HIS:CD2 | 2.76 | 0.54 |
| 2:N:2526:ARG:HE | 2:Q:2114:ARG:HG3 | 1.73 | 0.54 |
| 3:O:2961[A]:HIS:NE2 | 3:O:2980[A]:HIS:CE1 | 2.73 | 0.54 |
| 3:O:3159[B]:SER:O | 3:X:3151[B]:LEU:HD12 | 2.08 | 0.54 |
| 3:O:3293[B]:LYS:CG | 3:O:3294[B]:SER:HB2 | 2.36 | 0.54 |
| 1:P:1011:TYR:OH | 1:P:1049:VAL:O | 2.22 | 0.54 |
| 3:R:2947[A]:ALA:HA | 3:R:2949[A]:LYS:HB3 | 1.89 | 0.54 |
| 3:R:2960[A]:PHE:CD2 | 3:R:3157[A]:PRO:CG | 2.74 | 0.54 |
| 3:R:3185[B]:TYR:C | 3:R:3185[B]:TYR:CD2 | 2.86 | 0.54 |
| 3:R:3264[A]:TYR:C | 3:R:3264[A]:TYR:HD1 | 2.16 | 0.54 |
| 2:T:2419:ASP:N | 2:T:2419:ASP:OD1 | 2.41 | 0.54 |
| 2:T:2476:LEU:HD13 | 6:CA:2:NAG:H81 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:2723:GLU:HG2 | 2:T:2788:ILE:HD12 | 1.89 | 0.54 |
| 3:U:2933[A]:SER:HA | 3:U:2935[A]:ILE:CD1 | 2.38 | 0.54 |
| 3:U:3173[B]:THR:HG22 | 3:U:3174[B]:GLY:H | 1.67 | 0.54 |
| 3:U:3220[B]:ARG:CG | 3:d:2973[B]:THR:CG2 | 2.82 | 0.54 |
| 3:U:3307[A]:PHE:C | 3:U:3307[A]:PHE:CD1 | 2.85 | 0.54 |
| 1:V:1055:THR:HA | 1:V:1119:LEU:HD13 | 1.89 | 0.54 |
| 3:X:2952[B]:ALA:CA | 3:X:2956[B]:LYS:HB3 | 2.38 | 0.54 |
| 3:X:2954[B]:TYR:CD2 | 3:X:2954[B]:TYR:C | 2.86 | 0.54 |
| 3:X:2961[B]:HIS:NE2 | 3:X:2980[B]:HIS:CE1 | 2.73 | 0.54 |
| 3:X:3273[A]:LEU:CB | 3:X:3275[A]:LEU:CD1 | 2.86 | 0.54 |
| 3:X:3307[A]:PHE:C | 3:X:3307[A]:PHE:CD1 | 2.85 | 0.54 |
| 1:Y:949:ASP:HB3 | 1:Y:955:LYS:HE3 | 1.89 | 0.54 |
| 3:a:2949[A]:LYS:NZ | 3:a:2950[A]:THR:HA | 2.21 | 0.54 |
| 3:a:3096[B]:VAL:HG11 | 3:a:3115[B]:LEU:HD12 | 1.89 | 0.54 |
| 3:a:3220[B]:ARG:HG2 | 3:a:3221[B]:ALA:H | 1.70 | 0.54 |
| 3:a:3264[B]:TYR:HD1 | 3:a:3264[B]:TYR:C | 2.16 | 0.54 |
| 2:c:2394:VAL:HG11 | 2:c:2451:LEU:HD12 | 1.88 | 0.54 |
| 2:c:2570:HIS:CD2 | 2:c:2711:HIS:CE1 | 2.93 | 0.54 |
| 3:d:2948[B]:ASP:CB | 3:d:2949[B]:LYS:CA | 2.78 | 0.54 |
| 3:d:3264[B]:TYR:C | 3:d:3264[B]:TYR:HD1 | 2.16 | 0.54 |
| 3:d:3273[B]:LEU:CB | 3:d:3275[B]:LEU:CD1 | 2.86 | 0.54 |
| 3:d:3307[B]:PHE:CD1 | 3:d:3307[B]:PHE:C | 2.85 | 0.54 |
| 6:5:2:NAG:H61 | 6:5:3:BMA:H2 | 1.90 | 0.54 |
| 1:A:1206:HIS:CE1 | 1:A:1209:ASP:HB2 | 2.43 | 0.54 |
| 1:A:1206:HIS:HE1 | 1:A:1209:ASP:HB2 | 1.72 | 0.54 |
| 2:B:2180:TRP:HB3 | 2:B:2184:MET:HE2 | 1.90 | 0.54 |
| 2:B:2506:ARG:NE | 2:B:2578:GLU:OE2 | 2.27 | 0.54 |
| 2:B:2690:HIS:ND1 | 2:B:2886:VAL:O | 2.41 | 0.54 |
| 3:C:2937[B]:ASN:CB | 3:C:3006[B]:LYS:CD | 2.86 | 0.54 |
| 3:C:3013[B]:ASP:OD1 | 3:C:3015[B]:THR:HG23 | 2.08 | 0.54 |
| 3:C:3014[B]:TRP:CD1 | 3:C:3014[B]:TRP:C | 2.85 | 0.54 |
| 3:C:3082[B]:GLU:OE2 | 3:C:3086[B]:GLU:HB2 | 2.07 | 0.54 |
| 3:C:3173[B]:THR:HG22 | 3:C:3175[B]:TYR:H | 1.73 | 0.54 |
| 3:C:3185[A]:TYR:C | 3:C:3185[A]:TYR:CD2 | 2.86 | 0.54 |
| 3:C:3264[A]:TYR:C | 3:C:3264[A]:TYR:HD1 | 2.16 | 0.54 |
| 1:D:673:PHE:HB3 | 1:D:677:LEU:HB2 | 1.87 | 0.54 |
| 1:D:1492:PRO:HB2 | 1:D:1497:SER:HB3 | 1.90 | 0.54 |
| 3:F:2983[B]:VAL:H | 3:a:3160[B]:SER:HA | 1.73 | 0.54 |
| 3:F:3253[B]:GLU:CB | 3:a:2976[B]:ALA:N | 2.70 | 0.54 |
| 3:F:3264[B]:TYR:CD1 | 3:F:3264[B]:TYR:C | 2.86 | 0.54 |
| 1:G:1016:ASN:HD22 | 1:G:1177:VAL:HA | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3082[A]:GLU:OE2 | 3:I:3086[A]:GLU:HB2 | 2.08 | 0.54 |
| 3:I:3157[B]:PRO:CD | 3:R:2982[B]:MET:HE1 | 2.37 | 0.54 |
| 1:J:1195:ASP:OD1 | 1:J:1196:ILE:N | 2.40 | 0.54 |
| 2:K:2635:TYR:HB2 | 1:M:109:LEU:HD21 | 1.89 | 0.54 |
| 3:L:2933[A]:SER:HA | 3:L:2935[A]:ILE:CD1 | 2.38 | 0.54 |
| 3:L:3173[B]:THR:HG22 | 3:L:3174[B]:GLY:H | 1.67 | 0.54 |
| 1:M:489:HIS:HB3 | 1:M:689:PRO:HB3 | 1.88 | 0.54 |
| 3:O:2933[A]:SER:C | 3:O:2936[A]:GLU:H | 2.16 | 0.54 |
| 3:O:2933[A]:SER:HA | 3:O:2935[A]:ILE:CD1 | 2.38 | 0.54 |
| 3:O:2937[A]:ASN:CB | 3:O:3006[A]:LYS:CD | 2.86 | 0.54 |
| 3:O:3196[A]:THR:OG1 | 3:O:3199[A]:GLN:CB | 2.56 | 0.54 |
| 3:O:3264[B]:TYR:C | 3:O:3264[B]:TYR:HD1 | 2.16 | 0.54 |
| 3:O:3273[A]:LEU:CB | 3:O:3275[A]:LEU:CD1 | 2.86 | 0.54 |
| 3:O:3307[B]:PHE:C | 3:O:3307[B]:PHE:CD1 | 2.85 | 0.54 |
| 3:R:3273[B]:LEU:CB | 3:R:3275[B]:LEU:CD1 | 2.85 | 0.54 |
| 1:S:843:VAL:HG13 | 1:S:927:PRO:HB2 | 1.90 | 0.54 |
| 1:S:1089:ASP:N | 1:S:1089:ASP:OD1 | 2.40 | 0.54 |
| 2:T:2243:LEU:HD11 | 2:T:2273:TRP:HZ3 | 1.72 | 0.54 |
| 2:T:2359:ASN:OD1 | 2:T:2359:ASN:N | 2.39 | 0.54 |
| 3:U:2979[B]:GLN:HE21 | 3:d:3153[B]:LYS:CE | 2.20 | 0.54 |
| 3:X:2933[B]:SER:C | 3:X:2936[B]:GLU:H | 2.15 | 0.54 |
| 3:X:3014[B]:TRP:C | 3:X:3014[B]:TRP:CD1 | 2.85 | 0.54 |
| 3:X:3082[B]:GLU:OE2 | 3:X:3086[B]:GLU:HB2 | 2.08 | 0.54 |
| 3:X:3284[B]:LYS:HD3 | 3:X:3284[B]:LYS:C | 2.32 | 0.54 |
| 2:Z:2265:ILE:HD12 | 2:Z:2443:TYR:CD1 | 2.42 | 0.54 |
| 2:Z:2867:PRO:HD2 | 3:a:2932[A]:PRO:CB | 2.38 | 0.54 |
| 3:a:3264[A]:TYR:C | 3:a:3264[A]:TYR:CD1 | 2.86 | 0.54 |
| 3:a:3264[A]:TYR:C | 3:a:3264[A]:TYR:HD1 | 2.16 | 0.54 |
| 2:c:2625:LEU:HB2 | 2:c:2638:ARG:HH22 | 1.72 | 0.54 |
| 3:d:3047[A]:ARG:HH21 | 3:d:3113[A]:ASP:CG | 2.16 | 0.54 |
| 3:d:3132[B]:ALA:CB | 3:d:3197[B]:ILE:CD1 | 2.86 | 0.54 |
| 3:d:3240[B]:THR:CG2 | 3:d:3241[B]:PHE:N | 2.71 | 0.54 |
| 3:d:3273[A]:LEU:CB | 3:d:3275[A]:LEU:CD1 | 2.85 | 0.54 |
| 1:A:448:SER:OG | 1:A:450:LYS:NZ | 2.41 | 0.54 |
| 2:B:2603:PRO:HG2 | 2:B:2606:LEU:HD12 | 1.90 | 0.54 |
| 3:C:3132[A]:ALA:CB | 3:C:3197[A]:ILE:CD1 | 2.86 | 0.54 |
| 3:C:3157[B]:PRO:HD2 | 3:L:3153[B]:LYS:HZ1 | 1.72 | 0.54 |
| 3:C:3240[A]:THR:CG2 | 3:C:3241[A]:PHE:N | 2.71 | 0.54 |
| 1:D:1394:GLN:HG2 | 1:D:1395:PRO:HD2 | 1.89 | 0.54 |
| 2:E:2115:SER:OG | 2:E:2116:SER:N | 2.41 | 0.54 |
| 3:F:2930[B]:LEU:H | 3:F:2930[B]:LEU:CD2 | 1.98 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2933[B]:SER:HA | 3:F:2935[B]:ILE:CD1 | 2.38 | 0.54 |
| 3:F:2954[B]:TYR:CD2 | 3:F:2954[B]:TYR:C | 2.86 | 0.54 |
| 3:F:2962[B]:GLY:C | 3:a:3255[B]:PRO:HG3 | 2.32 | 0.54 |
| 3:F:2975[B]:PHE:CZ | 3:a:2961[B]:HIS:O | 2.61 | 0.54 |
| 3:F:3042[B]:ASP:N | 3:F:3042[B]:ASP:OD2 | 2.41 | 0.54 |
| 3:F:3047[A]:ARG:HH21 | 3:F:3113[A]:ASP:CG | 2.16 | 0.54 |
| 3:F:3150[B]:LYS:CE | 3:a:3160[B]:SER:CB | 2.75 | 0.54 |
| 3:F:3173[B]:THR:HG22 | 3:F:3175[B]:TYR:H | 1.73 | 0.54 |
| 3:F:3196[A]:THR:OG1 | 3:F:3199[A]:GLN:CB | 2.56 | 0.54 |
| 3:F:3273[B]:LEU:CB | 3:F:3275[B]:LEU:CD1 | 2.86 | 0.54 |
| 1:G:1273:SER:HB3 | 1:G:1340:GLY:H | 1.72 | 0.54 |
| 3:I:3307[A]:PHE:C | 3:I:3307[A]:PHE:CD1 | 2.85 | 0.54 |
| 1:J:325:THR:HG21 | 1:J:329:ARG:O | 2.08 | 0.54 |
| 3:L:2961[A]:HIS:NE2 | 3:L:2980[A]:HIS:CE1 | 2.73 | 0.54 |
| 3:L:3104[B]:MET:HA | 3:L:3110[B]:THR:CG2 | 2.17 | 0.54 |
| 3:L:3228[A]:VAL:CG2 | 3:L:3245[A]:PHE:CE2 | 2.89 | 0.54 |
| 3:L:3228[B]:VAL:CG2 | 3:L:3245[B]:PHE:CE2 | 2.89 | 0.54 |
| 3:L:3284[B]:LYS:HD3 | 3:L:3284[B]:LYS:C | 2.32 | 0.54 |
| 1:M:1582:ASN:HB3 | 1:M:1583:CYS:CB | 2.33 | 0.54 |
| 3:O:2933[B]:SER:C | 3:O:2936[B]:GLU:H | 2.15 | 0.54 |
| 3:O:3153[B]:LYS:CD | 3:X:3176[B]:LYS:HD2 | 2.07 | 0.54 |
| 3:O:3284[B]:LYS:HD3 | 3:O:3284[B]:LYS:C | 2.31 | 0.54 |
| 1:P:1163:ALA:HA | 1:P:1211:TYR:H | 1.73 | 0.54 |
| 2:Q:2300:ASN:OD1 | 2:Q:2303:ARG:NH1 | 2.41 | 0.54 |
| 3:R:3264[B]:TYR:HD1 | 3:R:3264[B]:TYR:C | 2.16 | 0.54 |
| 1:S:1328:SER:HB2 | 1:S:1523:LEU:HD13 | 1.90 | 0.54 |
| 1:S:1352:PHE:O | 1:S:1398:PHE:HB3 | 2.08 | 0.54 |
| 3:U:2933[A]:SER:C | 3:U:2936[A]:GLU:H | 2.16 | 0.54 |
| 3:U:3042[B]:ASP:OD2 | 3:U:3042[B]:ASP:N | 2.41 | 0.54 |
| 3:U:3120[A]:HIS:HA | 3:U:3123[A]:THR:HG1 | 1.72 | 0.54 |
| 3:U:3135[A]:LYS:HG3 | 3:U:3141[A]:TYR:CD1 | 2.33 | 0.54 |
| 3:U:3240[A]:THR:CG2 | 3:U:3241[A]:PHE:N | 2.71 | 0.54 |
| 3:U:3264[B]:TYR:CD1 | 3:U:3264[B]:TYR:C | 2.86 | 0.54 |
| 3:U:3273[A]:LEU:CB | 3:U:3275[A]:LEU:CD1 | 2.86 | 0.54 |
| 1:V:426:LYS:NZ | 1:V:1123:GLY:O | 2.21 | 0.54 |
| 3:X:3014[A]:TRP:CD1 | 3:X:3014[A]:TRP:C | 2.85 | 0.54 |
| 3:X:3132[A]:ALA:CB | 3:X:3197[A]:ILE:CD1 | 2.87 | 0.54 |
| 3:X:3176[A]:LYS:H | 3:X:3176[A]:LYS:CE | 2.17 | 0.54 |
| 2:Z:2825:ILE:HA | 2:Z:2877:ILE:HG22 | 1.90 | 0.54 |
| 3:a:3120[A]:HIS:HA | 3:a:3123[A]:THR:HG1 | 1.73 | 0.54 |
| 1:b:1400:ASN:HD22 | 1:b:1403:LEU:HG | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2952[B]:ALA:CA | 3:d:2956[B]:LYS:HB3 | 2.38 | 0.54 |
| 1:A:238:ASN:HD21 | 1:A:820:VAL:HG23 | 1.72 | 0.53 |
| 3:C:2933[B]:SER:HA | 3:C:2935[B]:ILE:CD1 | 2.38 | 0.53 |
| 3:C:3093[A]:HIS:CE1 | 3:C:3119[A]:HIS:CD2 | 2.92 | 0.53 |
| 3:C:3307[A]:PHE:CD1 | 3:C:3307[A]:PHE:C | 2.85 | 0.53 |
| 3:F:2969[B]:TYR:CD2 | 3:a:3093[B]:HIS:NE2 | 2.77 | 0.53 |
| 3:F:3033[A]:PHE:HD1 | 3:F:3114[A]:PRO:HB2 | 1.72 | 0.53 |
| 3:F:3185[B]:TYR:C | 3:F:3185[B]:TYR:CD2 | 2.86 | 0.53 |
| 3:F:3255[B]:PRO:HA | 3:a:2965[B]:LEU:C | 2.33 | 0.53 |
| 2:H:2884:LYS:HB2 | 2:H:2889:ALA:O | 2.09 | 0.53 |
| 3:I:2975[B]:PHE:CD1 | 3:R:3107[B]:LEU:CD2 | 2.91 | 0.53 |
| 1:J:450:LYS:HZ3 | 1:J:505:ARG:HH21 | 1.56 | 0.53 |
| 1:J:873:VAL:HG21 | 1:J:912:ASN:HB3 | 1.90 | 0.53 |
| 1:J:1093:ASP:OD1 | 1:J:1096:THR:OG1 | 2.20 | 0.53 |
| 3:L:2954[A]:TYR:CD2 | 3:L:2954[A]:TYR:C | 2.86 | 0.53 |
| 3:L:3042[B]:ASP:N | 3:L:3042[B]:ASP:OD2 | 2.41 | 0.53 |
| 1:M:135:THR:HB | 1:M:192:HIS:O | 2.07 | 0.53 |
| 1:M:613:SER:HA | 1:M:805:VAL:HG12 | 1.90 | 0.53 |
| 1:M:1019:HIS:HE2 | 1:M:1046:HIS:CE1 | 2.26 | 0.53 |
| 3:O:3014[B]:TRP:CD1 | 3:O:3014[B]:TRP:C | 2.85 | 0.53 |
| 3:O:3273[B]:LEU:CB | 3:O:3275[B]:LEU:CD1 | 2.86 | 0.53 |
| 1:P:1573:CYS:HB2 | 1:P:1627:ARG:HG2 | 1.90 | 0.53 |
| 2:Q:2824:CYS:SG | 2:Q:2878:ARG:NH1 | 2.81 | 0.53 |
| 2:Q:2849:ASP:OD2 | 2:Q:2850:ARG:NH1 | 2.40 | 0.53 |
| 3:R:2954[B]:TYR:CD2 | 3:R:2954[B]:TYR:C | 2.86 | 0.53 |
| 3:R:3240[B]:THR:CG2 | 3:R:3241[B]:PHE:N | 2.71 | 0.53 |
| 3:R:3273[A]:LEU:CB | 3:R:3275[A]:LEU:CD1 | 2.85 | 0.53 |
| 1:S:1348:TRP:HD1 | 1:S:1403:LEU:HD13 | 1.73 | 0.53 |
| 2:T:2545:SER:CA | 2:T:2546:LEU:HB2 | 2.35 | 0.53 |
| 3:U:2933[B]:SER:C | 3:U:2936[B]:GLU:H | 2.15 | 0.53 |
| 3:U:2954[B]:TYR:CD2 | 3:U:2954[B]:TYR:C | 2.86 | 0.53 |
| 3:U:3013[B]:ASP:OD1 | 3:U:3015[B]:THR:HG23 | 2.08 | 0.53 |
| 3:U:3047[B]:ARG:HH21 | 3:U:3113[B]:ASP:CG | 2.16 | 0.53 |
| 3:U:3162[B]:ASP:CG | 3:d:3260[B]:ARG:CZ | 2.81 | 0.53 |
| 3:U:3196[B]:THR:OG1 | 3:U:3199[B]:GLN:CB | 2.56 | 0.53 |
| 3:X:3019[A]:HIS:CD2 | 3:X:3019[A]:HIS:N | 2.75 | 0.53 |
| 3:X:3019[B]:HIS:CD2 | 3:X:3019[B]:HIS:N | 2.75 | 0.53 |
| 3:X:3185[A]:TYR:C | 3:X:3185[A]:TYR:CD2 | 2.86 | 0.53 |
| 1:Y:28:ASP:OD2 | 1:Y:83:HIS:NE2 | 2.34 | 0.53 |
| 3:a:3132[B]:ALA:CB | 3:a:3197[B]:ILE:CD1 | 2.86 | 0.53 |
| 1:b:778:LYS:HG2 | 1:b:821:ILE:HD11 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:1427:HIS:CD2 | 1:b:1457:HIS:HE1 | 2.26 | 0.53 |
| 2:c:2650:GLY:N | 2:c:2651:GLN:HA | 2.22 | 0.53 |
| 3:d:2933[B]:SER:C | 3:d:2936[B]:GLU:H | 2.15 | 0.53 |
| 3:d:3185[A]:TYR:C | 3:d:3185[A]:TYR:CD2 | 2.86 | 0.53 |
| 3:d:3273[A]:LEU:HB2 | 3:d:3275[A]:LEU:CD1 | 2.34 | 0.53 |
| 3:C:2937[A]:ASN:CB | 3:C:3006[A]:LYS:CD | 2.86 | 0.53 |
| 3:C:3281[B]:PHE:HE1 | 3:C:3305[B]:ILE:HD13 | 1.71 | 0.53 |
| 1:D:1595:GLY:O | 1:D:1598:GLU:HG2 | 2.08 | 0.53 |
| 3:F:2933[B]:SER:C | 3:F:2936[B]:GLU:H | 2.16 | 0.53 |
| 3:F:2975[B]:PHE:HA | 3:a:3107[B]:LEU:HD22 | 1.88 | 0.53 |
| 3:F:3082[A]:GLU:OE2 | 3:F:3086[A]:GLU:HB2 | 2.08 | 0.53 |
| 3:F:3132[B]:ALA:CB | 3:F:3197[B]:ILE:CD1 | 2.86 | 0.53 |
| 3:F:3173[A]:THR:HG22 | 3:F:3175[A]:TYR:H | 1.73 | 0.53 |
| 1:G:142:ARG:NH1 | 1:G:340:GLN:OE1 | 2.41 | 0.53 |
| 2:H:2739:LEU:HD13 | 1:J:1207:TYR:HD2 | 1.73 | 0.53 |
| 2:H:2856:ILE:HG22 | 2:H:2859:VAL:HB | 1.90 | 0.53 |
| 3:I:2933[A]:SER:C | 3:I:2936[A]:GLU:H | 2.16 | 0.53 |
| 3:I:3132[B]:ALA:CB | 3:I:3197[B]:ILE:CD1 | 2.86 | 0.53 |
| 3:I:3151[A]:LEU:HB2 | 3:I:3175[A]:TYR:HE2 | 1.68 | 0.53 |
| 3:I:3153[B]:LYS:NZ | 3:R:3158[B]:PHE:H | 2.05 | 0.53 |
| 1:M:741:SER:HB3 | 1:M:764:GLY:H | 1.73 | 0.53 |
| 1:M:1348:TRP:HD1 | 1:M:1403:LEU:HD13 | 1.74 | 0.53 |
| 2:N:2132:CYS:O | 2:N:2334:LYS:HD3 | 2.07 | 0.53 |
| 2:N:2738:ALA:HB1 | 2:N:2741:GLN:HB2 | 1.90 | 0.53 |
| 3:O:2975[B]:PHE:CD1 | 3:X:3156[B]:MET:CA | 2.89 | 0.53 |
| 3:O:3082[B]:GLU:OE2 | 3:O:3086[B]:GLU:HB2 | 2.08 | 0.53 |
| 3:O:3240[B]:THR:CG2 | 3:O:3241[B]:PHE:N | 2.71 | 0.53 |
| 3:O:3264[A]:TYR:C | 3:O:3264[A]:TYR:HD1 | 2.16 | 0.53 |
| 3:O:3293[A]:LYS:CB | 3:O:3294[A]:SER:CB | 2.54 | 0.53 |
| 1:P:931:TRP:CD1 | 1:P:1048:ASN:HD22 | 2.26 | 0.53 |
| 2:Q:2578:GLU:HG3 | 2:Q:2590:VAL:HG23 | 1.90 | 0.53 |
| 2:Q:2724:LEU:HA | 2:Q:2788:ILE:HD11 | 1.89 | 0.53 |
| 3:R:3173[A]:THR:HG22 | 3:R:3175[A]:TYR:H | 1.73 | 0.53 |
| 3:U:3082[A]:GLU:OE2 | 3:U:3086[A]:GLU:HB2 | 2.08 | 0.53 |
| 3:U:3173[B]:THR:HG22 | 3:U:3175[B]:TYR:H | 1.73 | 0.53 |
| 3:U:3185[B]:TYR:C | 3:U:3185[B]:TYR:CD2 | 2.86 | 0.53 |
| 3:U:3220[B]:ARG:NH1 | 3:d:2974[B]:ALA:HB2 | 2.24 | 0.53 |
| 3:U:3255[B]:PRO:HD3 | 3:d:3253[B]:GLU:CA | 2.36 | 0.53 |
| 1:V:563:ILE:O | 1:V:612:GLY:HA3 | 2.08 | 0.53 |
| 1:V:1102:PRO:HA | 1:V:1105:VAL:HG22 | 1.91 | 0.53 |
| 3:X:3013[A]:ASP:OD1 | 3:X:3015[A]:THR:HG23 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3185[B]:TYR:C | 3:X:3185[B]:TYR:CD2 | 2.86 | 0.53 |
| 3:a:2948[B]:ASP:CB | 3:a:2949[B]:LYS:CA | 2.78 | 0.53 |
| 3:a:2952[A]:ALA:HB3 | 3:a:2954[A]:TYR:N | 2.17 | 0.53 |
| 3:a:2954[B]:TYR:CD2 | 3:a:2954[B]:TYR:C | 2.86 | 0.53 |
| 3:a:3013[A]:ASP:OD1 | 3:a:3015[A]:THR:HG23 | 2.08 | 0.53 |
| 3:a:3196[B]:THR:OG1 | 3:a:3199[B]:GLN:CB | 2.56 | 0.53 |
| 3:a:3273[A]:LEU:CB | 3:a:3275[A]:LEU:CD1 | 2.86 | 0.53 |
| 1:b:664:VAL:O | 1:b:689:PRO:HD2 | 2.08 | 0.53 |
| 3:d:2960[B]:PHE:CD2 | 3:d:3157[B]:PRO:CG | 2.74 | 0.53 |
| 3:d:3013[A]:ASP:OD1 | 3:d:3015[A]:THR:HG23 | 2.08 | 0.53 |
| 3:d:3082[A]:GLU:OE2 | 3:d:3086[A]:GLU:HB2 | 2.07 | 0.53 |
| 1:A:416:ASN:ND2 | 3:F:3196[A]:THR:HG21 | 2.23 | 0.53 |
| 2:B:2090:LYS:NZ | 2:B:2099:GLU:OE2 | 2.37 | 0.53 |
| 2:B:2212:GLY:HA3 | 2:B:2290:TYR:O | 2.08 | 0.53 |
| 2:B:2509:ILE:HD11 | 2:B:2605:LEU:HD23 | 1.89 | 0.53 |
| 2:B:2859:VAL:O | 2:B:2863:ARG:HG2 | 2.07 | 0.53 |
| 3:C:3047[B]:ARG:HH21 | 3:C:3113[B]:ASP:CG | 2.16 | 0.53 |
| 3:C:3153[B]:LYS:HE3 | 3:L:3155[B]:MET:O | 2.09 | 0.53 |
| 3:C:3264[B]:TYR:C | 3:C:3264[B]:TYR:HD1 | 2.16 | 0.53 |
| 1:D:451:SER:OG | 1:D:452:ILE:N | 2.40 | 0.53 |
| 3:F:2933[B]:SER:CB | 3:F:2936[B]:GLU:CB | 2.85 | 0.53 |
| 3:F:3155[B]:MET:O | 3:a:3153[B]:LYS:CD | 2.56 | 0.53 |
| 3:F:3273[B]:LEU:HB2 | 3:F:3275[B]:LEU:CD1 | 2.34 | 0.53 |
| 1:G:704:ASP:HB2 | 1:G:1118:THR:HG21 | 1.90 | 0.53 |
| 1:G:931:TRP:NE1 | 1:G:1048:ASN:HD22 | 2.06 | 0.53 |
| 2:H:2504:ARG:HD3 | 2:H:2775:GLY:O | 2.08 | 0.53 |
| 3:I:2954[B]:TYR:CD2 | 3:I:2954[B]:TYR:C | 2.86 | 0.53 |
| 3:I:3014[A]:TRP:CD1 | 3:I:3014[A]:TRP:C | 2.85 | 0.53 |
| 3:I:3042[A]:ASP:N | 3:I:3042[A]:ASP:OD2 | 2.41 | 0.53 |
| 3:I:3163[B]:ASN:O | 3:R:3147[B]:GLU:CD | 2.52 | 0.53 |
| 3:I:3264[B]:TYR:C | 3:I:3264[B]:TYR:CD1 | 2.86 | 0.53 |
| 3:I:3273[B]:LEU:CB | 3:I:3275[B]:LEU:CD1 | 2.85 | 0.53 |
| 3:I:3307[B]:PHE:HE1 | 3:I:3309[B]:PRO:CG | 2.08 | 0.53 |
| 1:J:372:ALA:O | 1:J:375:SER:OG | 2.23 | 0.53 |
| 1:J:566:ARG:HH12 | 1:J:803:LYS:HZ3 | 1.57 | 0.53 |
| 2:K:2567:MET:HE3 | 2:K:2718:TRP:HB2 | 1.89 | 0.53 |
| 3:L:3093[B]:HIS:CE1 | 3:L:3119[B]:HIS:CD2 | 2.92 | 0.53 |
| 1:M:843:VAL:HG13 | 1:M:927:PRO:HB2 | 1.90 | 0.53 |
| 3:O:2975[B]:PHE:H | 3:X:2979[B]:GLN:NE2 | 2.07 | 0.53 |
| 3:O:3240[A]:THR:CG2 | 3:O:3241[A]:PHE:N | 2.71 | 0.53 |
| 3:O:3284[A]:LYS:CE | 3:O:3284[A]:LYS:CA | 2.85 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3013[B]:ASP:OD1 | 3:R:3015[B]:THR:HG23 | 2.08 | 0.53 |
| 3:R:3014[A]:TRP:C | 3:R:3014[A]:TRP:CD1 | 2.85 | 0.53 |
| 3:R:3042[A]:ASP:N | 3:R:3042[A]:ASP:OD2 | 2.41 | 0.53 |
| 3:R:3083[B]:ILE:HD12 | 3:R:3260[B]:ARG:HB2 | 1.88 | 0.53 |
| 3:R:3228[A]:VAL:CG2 | 3:R:3245[A]:PHE:CE2 | 2.89 | 0.53 |
| 3:R:3240[A]:THR:CG2 | 3:R:3241[A]:PHE:N | 2.71 | 0.53 |
| 3:R:3307[A]:PHE:CD1 | 3:R:3307[A]:PHE:C | 2.85 | 0.53 |
| 1:S:1161:ILE:HB | 1:S:1203:MET:HE1 | 1.89 | 0.53 |
| 1:S:1166:THR:OG1 | 1:S:1168:GLN:OE1 | 2.25 | 0.53 |
| 2:T:2265:ILE:HD12 | 2:T:2443:TYR:CG | 2.43 | 0.53 |
| 3:U:3185[A]:TYR:C | 3:U:3185[A]:TYR:CD2 | 2.86 | 0.53 |
| 3:U:3264[A]:TYR:C | 3:U:3264[A]:TYR:HD1 | 2.16 | 0.53 |
| 2:W:2344:LEU:HA | 2:W:2345:ASN:O | 2.08 | 0.53 |
| 2:W:2470:ALA:HB2 | 2:W:2476:LEU:HD11 | 1.91 | 0.53 |
| 2:W:2571:ARG:HG3 | 2:W:2715:ASP:OD1 | 2.08 | 0.53 |
| 3:X:2952[A]:ALA:HB3 | 3:X:2954[A]:TYR:N | 2.17 | 0.53 |
| 3:X:3047[A]:ARG:HH21 | 3:X:3113[A]:ASP:CG | 2.16 | 0.53 |
| 3:X:3264[A]:TYR:C | 3:X:3264[A]:TYR:HD1 | 2.16 | 0.53 |
| 1:Y:210:HIS:HA | 1:Y:213:VAL:HG22 | 1.89 | 0.53 |
| 2:Z:2419:ASP:OD1 | 2:Z:2419:ASP:N | 2.41 | 0.53 |
| 3:a:2937[B]:ASN:CB | 3:a:3006[B]:LYS:CD | 2.86 | 0.53 |
| 3:a:3042[B]:ASP:N | 3:a:3042[B]:ASP:OD2 | 2.41 | 0.53 |
| 3:a:3135[B]:LYS:HG3 | 3:a:3141[B]:TYR:CD1 | 2.33 | 0.53 |
| 3:a:3228[A]:VAL:CG2 | 3:a:3245[A]:PHE:CE2 | 2.89 | 0.53 |
| 2:c:2235:PRO:HG3 | 2:c:2240:GLN:NE2 | 2.22 | 0.53 |
| 3:d:2937[B]:ASN:CB | 3:d:3006[B]:LYS:CD | 2.85 | 0.53 |
| 3:d:3173[A]:THR:HG22 | 3:d:3175[A]:TYR:H | 1.73 | 0.53 |
| 3:d:3196[B]:THR:OG1 | 3:d:3199[B]:GLN:CB | 2.56 | 0.53 |
| 3:d:3264[A]:TYR:C | 3:d:3264[A]:TYR:HD1 | 2.16 | 0.53 |
| 3:d:3284[B]:LYS:HD3 | 3:d:3284[B]:LYS:C | 2.31 | 0.53 |
| 3:d:3293[A]:LYS:CD | 3:d:3294[A]:SER:N | 2.64 | 0.53 |
| 3:C:3047[A]:ARG:HH21 | 3:C:3113[A]:ASP:CG | 2.16 | 0.53 |
| 3:C:3169[B]:LYS:CD | 3:L:3149[B]:ASN:OD1 | 2.56 | 0.53 |
| 1:D:194:MET:HA | 1:D:200:THR:HA | 1.90 | 0.53 |
| 3:F:2937[A]:ASN:CB | 3:F:3006[A]:LYS:CD | 2.85 | 0.53 |
| 3:F:3014[B]:TRP:C | 3:F:3014[B]:TRP:CD1 | 2.85 | 0.53 |
| 3:F:3047[B]:ARG:HH21 | 3:F:3113[B]:ASP:CG | 2.16 | 0.53 |
| 3:F:3157[B]:PRO:N | 3:a:3153[B]:LYS:NZ | 2.56 | 0.53 |
| 3:F:3293[B]:LYS:CB | 3:F:3294[B]:SER:CB | 2.54 | 0.53 |
| 1:G:59:LEU:HD13 | 1:G:68:TRP:CD1 | 2.44 | 0.53 |
| 3:I:2952[B]:ALA:H | 3:I:2953[B]:GLY:CA | 2.04 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3019[A]:HIS:CD2 | 3:I:3019[A]:HIS:N | 2.75 | 0.53 |
| 3:I:3047[B]:ARG:HH21 | 3:I:3113[B]:ASP:CG | 2.16 | 0.53 |
| 3:I:3173[A]:THR:HG22 | 3:I:3175[A]:TYR:H | 1.73 | 0.53 |
| 1:J:561:ARG:HH11 | 1:J:561:ARG:HG2 | 1.74 | 0.53 |
| 1:J:1210:LYS:HA | 1:J:1211:TYR:HB3 | 1.91 | 0.53 |
| 1:J:1470:GLU:HG3 | 1:J:1530:LEU:HD12 | 1.91 | 0.53 |
| 3:L:2937[B]:ASN:CB | 3:L:3006[B]:LYS:CD | 2.86 | 0.53 |
| 3:L:3185[A]:TYR:C | 3:L:3185[A]:TYR:CD2 | 2.86 | 0.53 |
| 1:M:914:GLU:OE1 | 1:M:926:LEU:N | 2.34 | 0.53 |
| 3:O:3132[A]:ALA:HB1 | 3:O:3197[A]:ILE:HD13 | 1.89 | 0.53 |
| 3:O:3132[B]:ALA:HB1 | 3:O:3197[B]:ILE:HD13 | 1.89 | 0.53 |
| 3:O:3151[B]:LEU:HB2 | 3:O:3175[B]:TYR:HE2 | 1.68 | 0.53 |
| 2:Q:2161:GLN:NE2 | 2:Q:2348:THR:HG21 | 2.24 | 0.53 |
| 2:Q:2528:LYS:HA | 2:Q:2536:PHE:HB3 | 1.90 | 0.53 |
| 3:R:2933[A]:SER:C | 3:R:2936[A]:GLU:H | 2.15 | 0.53 |
| 3:R:2933[B]:SER:C | 3:R:2936[B]:GLU:H | 2.16 | 0.53 |
| 3:R:3132[A]:ALA:CB | 3:R:3197[A]:ILE:CD1 | 2.86 | 0.53 |
| 3:R:3293[A]:LYS:CD | 3:R:3294[A]:SER:N | 2.64 | 0.53 |
| 1:S:494:VAL:HG23 | 1:S:671:PHE:CZ | 2.43 | 0.53 |
| 1:S:1470:GLU:OE1 | 1:S:1473:ARG:NH1 | 2.42 | 0.53 |
| 3:U:2954[A]:TYR:C | 3:U:2954[A]:TYR:CD2 | 2.86 | 0.53 |
| 3:U:3047[A]:ARG:HH21 | 3:U:3113[A]:ASP:CG | 2.16 | 0.53 |
| 3:U:3132[B]:ALA:CB | 3:U:3197[B]:ILE:CD1 | 2.86 | 0.53 |
| 3:U:3264[B]:TYR:C | 3:U:3264[B]:TYR:HD1 | 2.16 | 0.53 |
| 3:U:3293[A]:LYS:CB | 3:U:3294[A]:SER:CB | 2.54 | 0.53 |
| 3:U:3307[B]:PHE:C | 3:U:3307[B]:PHE:CD1 | 2.85 | 0.53 |
| 1:V:195:SER:HB2 | 1:V:386:ILE:HD11 | 1.91 | 0.53 |
| 1:V:294:LYS:HA | 1:V:297:ARG:HD2 | 1.90 | 0.53 |
| 2:W:2121:THR:O | 2:W:2124:SER:OG | 2.24 | 0.53 |
| 3:X:3173[A]:THR:HG22 | 3:X:3175[A]:TYR:H | 1.73 | 0.53 |
| 1:Y:1482:ALA:HB3 | 1:Y:1489:MET:HE3 | 1.90 | 0.53 |
| 1:Y:1655:SER:C | 3:d:3006[B]:LYS:CD | 2.81 | 0.53 |
| 3:a:2933[A]:SER:CB | 3:a:2936[A]:GLU:CB | 2.86 | 0.53 |
| 3:a:3042[A]:ASP:N | 3:a:3042[A]:ASP:OD2 | 2.41 | 0.53 |
| 3:a:3307[B]:PHE:C | 3:a:3307[B]:PHE:CD1 | 2.85 | 0.53 |
| 1:b:655:TYR:HE1 | 1:b:693:TYR:HB3 | 1.73 | 0.53 |
| 1:b:1304:ASP:H | 1:b:1305:GLY:HA2 | 1.73 | 0.53 |
| 3:d:2954[B]:TYR:CD2 | 3:d:2954[B]:TYR:C | 2.86 | 0.53 |
| 3:d:3013[A]:ASP:OD1 | 3:d:3015[A]:THR:OG1 | 2.23 | 0.53 |
| 1:A:906:HIS:HA | 1:A:909:ILE:HB | 1.91 | 0.53 |
| 1:A:1195:ASP:HA | 1:A:1196:ILE:HB | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3019[B]:HIS:CD2 | 3:C:3019[B]:HIS:N | 2.75 | 0.53 |
| 3:C:3042[B]:ASP:N | 3:C:3042[B]:ASP:OD2 | 2.41 | 0.53 |
| 3:C:3132[B]:ALA:HB1 | 3:C:3197[B]:ILE:HD13 | 1.89 | 0.53 |
| 3:C:3132[B]:ALA:CB | 3:C:3197[B]:ILE:CD1 | 2.86 | 0.53 |
| 3:C:3154[B]:PRO:HG2 | 3:L:2984[B]:THR:HB | 1.90 | 0.53 |
| 3:C:3249[B]:GLY:O | 3:L:3252[B]:TYR:CE2 | 2.60 | 0.53 |
| 3:C:3298[B]:ASN:HA | 3:C:3299[B]:LEU:HB3 | 1.88 | 0.53 |
| 3:F:2988[B]:TRP:CZ2 | 3:a:2975[B]:PHE:HE2 | 2.26 | 0.53 |
| 3:F:3240[A]:THR:CG2 | 3:F:3241[A]:PHE:N | 2.71 | 0.53 |
| 3:F:3293[A]:LYS:CD | 3:F:3294[A]:SER:N | 2.64 | 0.53 |
| 1:G:308:LEU:O | 1:G:772:ARG:NH2 | 2.41 | 0.53 |
| 1:G:1543:ILE:HD11 | 3:L:3272[A]:HIS:HD2 | 1.73 | 0.53 |
| 3:I:3014[A]:TRP:CZ3 | 3:I:3119[A]:HIS:ND1 | 2.77 | 0.53 |
| 3:I:3147[A]:GLU:CD | 3:I:3149[A]:ASN:HD21 | 2.17 | 0.53 |
| 3:L:3132[B]:ALA:HB1 | 3:L:3197[B]:ILE:HD13 | 1.89 | 0.53 |
| 1:M:415:VAL:HB | 1:M:697:ALA:HB2 | 1.90 | 0.53 |
| 1:M:545:PHE:O | 1:M:561:ARG:NH2 | 2.38 | 0.53 |
| 1:M:907:ARG:NH1 | 1:M:1050:ASP:OD1 | 2.42 | 0.53 |
| 3:O:3109[B]:TYR:CG | 3:X:2969[B]:TYR:C | 2.82 | 0.53 |
| 3:O:3255[B]:PRO:HD3 | 3:X:3158[B]:PHE:C | 2.33 | 0.53 |
| 3:O:3284[A]:LYS:HD3 | 3:O:3284[A]:LYS:C | 2.32 | 0.53 |
| 1:P:61:GLY:HA3 | 1:P:352:TRP:CB | 2.37 | 0.53 |
| 1:P:1196:ILE:O | 1:P:1199:VAL:HG12 | 2.09 | 0.53 |
| 2:Q:2795:ILE:O | 2:Q:2799:LYS:HG3 | 2.08 | 0.53 |
| 3:R:2933[A]:SER:HA | 3:R:2935[A]:ILE:CD1 | 2.38 | 0.53 |
| 3:R:2947[B]:ALA:HA | 3:R:2949[B]:LYS:HB3 | 1.89 | 0.53 |
| 3:R:3013[A]:ASP:OD1 | 3:R:3015[A]:THR:HG23 | 2.08 | 0.53 |
| 3:R:3033[A]:PHE:HD1 | 3:R:3114[A]:PRO:HB2 | 1.72 | 0.53 |
| 3:R:3047[A]:ARG:HH21 | 3:R:3113[A]:ASP:CG | 2.16 | 0.53 |
| 3:R:3132[B]:ALA:HB1 | 3:R:3197[B]:ILE:HD13 | 1.89 | 0.53 |
| 3:R:3264[B]:TYR:C | 3:R:3264[B]:TYR:CD1 | 2.86 | 0.53 |
| 1:S:410:LYS:HE2 | 1:S:652:GLY:HA2 | 1.90 | 0.53 |
| 1:S:747:PHE:HB2 | 1:S:799:ARG:HB3 | 1.91 | 0.53 |
| 1:S:792:MET:O | 1:S:796:TYR:OH | 2.16 | 0.53 |
| 3:U:2971[B]:ASP:O | 3:d:3247[B]:VAL:CB | 2.56 | 0.53 |
| 3:U:3293[B]:LYS:CD | 3:U:3294[B]:SER:N | 2.64 | 0.53 |
| 1:V:474:LEU:HD23 | 1:V:474:LEU:H | 1.74 | 0.53 |
| 3:X:2933[A]:SER:C | 3:X:2936[A]:GLU:H | 2.16 | 0.53 |
| 3:X:2937[B]:ASN:CB | 3:X:3006[B]:LYS:CD | 2.86 | 0.53 |
| 3:X:3081[B]:PHE:C | 3:X:3081[B]:PHE:CD1 | 2.87 | 0.53 |
| 3:X:3151[A]:LEU:HB2 | 3:X:3175[A]:TYR:HE2 | 1.67 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3196[A]:THR:OG1 | 3:X:3199[A]:GLN:CB | 2.56 | 0.53 |
| 3:X:3273[B]:LEU:CB | 3:X:3275[B]:LEU:CD1 | 2.86 | 0.53 |
| 1:Y:124:TYR:O | 1:Y:137:ARG:NH2 | 2.41 | 0.53 |
| 1:Y:1576:THR:OG1 | 1:Y:1581:GLU:HB2 | 2.09 | 0.53 |
| 3:a:3081[B]:PHE:CD1 | 3:a:3081[B]:PHE:C | 2.87 | 0.53 |
| 3:a:3293[A]:LYS:CG | 3:a:3294[A]:SER:HB2 | 2.36 | 0.53 |
| 1:b:127:GLU:OE1 | 1:b:202:TYR:HB3 | 2.09 | 0.53 |
| 1:b:949:ASP:HB2 | 1:b:953:GLU:CB | 2.38 | 0.53 |
| 1:b:1140:ASN:OD1 | 1:b:1239:GLY:N | 2.36 | 0.53 |
| 1:b:1304:ASP:N | 1:b:1305:GLY:HA2 | 2.23 | 0.53 |
| 1:b:1639:LYS:HE2 | 4:QA:1:NAG:H61 | 1.91 | 0.53 |
| 2:c:2680:HIS:NE2 | 2:c:2684:HIS:CD2 | 2.75 | 0.53 |
| 1:A:1082:SER:OG | 1:A:1083:PRO:HD3 | 2.08 | 0.53 |
| 3:C:2933[B]:SER:CB | 3:C:2936[B]:GLU:CB | 2.86 | 0.53 |
| 3:C:2954[B]:TYR:CD2 | 3:C:2954[B]:TYR:C | 2.86 | 0.53 |
| 3:C:3153[B]:LYS:HE3 | 3:L:3158[B]:PHE:HD2 | 1.52 | 0.53 |
| 3:C:3183[A]:LEU:N | 3:C:3184[A]:ASN:HA | 2.11 | 0.53 |
| 3:C:3228[A]:VAL:CG2 | 3:C:3245[A]:PHE:CE2 | 2.89 | 0.53 |
| 1:D:704:ASP:OD1 | 1:D:705:THR:N | 2.41 | 0.53 |
| 3:F:3013[A]:ASP:OD1 | 3:F:3015[A]:THR:HG23 | 2.08 | 0.53 |
| 3:F:3132[A]:ALA:CB | 3:F:3197[A]:ILE:CD1 | 2.86 | 0.53 |
| 1:G:177:VAL:HG11 | 1:G:358:TYR:CZ | 2.44 | 0.53 |
| 3:I:2954[A]:TYR:C | 3:I:2954[A]:TYR:CD2 | 2.86 | 0.53 |
| 3:I:3013[A]:ASP:OD1 | 3:I:3015[A]:THR:HG23 | 2.08 | 0.53 |
| 3:I:3019[B]:HIS:CD2 | 3:I:3019[B]:HIS:N | 2.75 | 0.53 |
| 3:I:3107[B]:LEU:CG | 3:R:2975[B]:PHE:CD1 | 2.88 | 0.53 |
| 3:I:3153[B]:LYS:O | 3:R:3154[B]:PRO:C | 2.45 | 0.53 |
| 1:J:830:ASN:OD1 | 1:J:831:VAL:N | 2.41 | 0.53 |
| 1:J:949:ASP:OD1 | 1:J:950:ALA:N | 2.40 | 0.53 |
| 1:J:993:ASN:OD1 | 1:J:1136:ARG:NH2 | 2.42 | 0.53 |
| 3:L:3132[A]:ALA:HB1 | 3:L:3197[A]:ILE:HD13 | 1.89 | 0.53 |
| 3:L:3132[B]:ALA:CB | 3:L:3197[B]:ILE:CD1 | 2.86 | 0.53 |
| 3:L:3151[B]:LEU:HB2 | 3:L:3175[B]:TYR:HE2 | 1.67 | 0.53 |
| 3:L:3293[A]:LYS:CD | 3:L:3294[A]:SER:N | 2.64 | 0.53 |
| 1:M:1170:MET:HB3 | 1:M:1203:MET:HE2 | 1.91 | 0.53 |
| 1:M:1587:ALA:HA | 1:M:1614:GLU:HG2 | 1.91 | 0.53 |
| 3:O:2947[B]:ALA:HA | 3:O:2949[B]:LYS:HB3 | 1.89 | 0.53 |
| 3:O:2968[B]:GLN:HG2 | 3:X:2984[B]:THR:OG1 | 2.07 | 0.53 |
| 3:O:3013[B]:ASP:OD1 | 3:O:3015[B]:THR:HG23 | 2.08 | 0.53 |
| 3:O:3264[B]:TYR:C | 3:O:3264[B]:TYR:CD1 | 2.86 | 0.53 |
| 1:P:494:VAL:HG13 | 1:P:631:TRP:HZ3 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3284[A]:LYS:HD3 | 3:R:3284[A]:LYS:C | 2.31 | 0.53 |
| 2:T:2795:ILE:O | 2:T:2798:GLN:HG2 | 2.08 | 0.53 |
| 3:U:3162[B]:ASP:OD1 | 3:d:3260[B]:ARG:CZ | 2.55 | 0.53 |
| 3:U:3255[B]:PRO:HD3 | 3:d:3253[B]:GLU:N | 2.23 | 0.53 |
| 3:U:3257[B]:ALA:N | 3:d:2968[B]:GLN:CA | 2.16 | 0.53 |
| 3:U:3269[A]:SER:O | 3:U:3272[A]:HIS:HB2 | 2.09 | 0.53 |
| 1:V:449:ASP:OD1 | 1:V:1280:GLN:NE2 | 2.42 | 0.53 |
| 1:V:483:GLY:HA2 | 1:V:773:PHE:CZ | 2.44 | 0.53 |
| 1:V:732:GLY:N | 1:V:819:ILE:O | 2.30 | 0.53 |
| 3:X:3013[B]:ASP:OD1 | 3:X:3015[B]:THR:HG23 | 2.08 | 0.53 |
| 3:X:3173[B]:THR:HG22 | 3:X:3175[B]:TYR:H | 1.73 | 0.53 |
| 1:Y:17:ASN:OD1 | 1:Y:85:SER:HB3 | 2.09 | 0.53 |
| 1:Y:1472:GLN:OE1 | 1:Y:1475:ARG:NH1 | 2.42 | 0.53 |
| 3:a:2947[B]:ALA:HA | 3:a:2949[B]:LYS:HB3 | 1.89 | 0.53 |
| 3:a:3132[B]:ALA:HB1 | 3:a:3197[B]:ILE:HD13 | 1.89 | 0.53 |
| 3:a:3185[A]:TYR:C | 3:a:3185[A]:TYR:CD2 | 2.86 | 0.53 |
| 3:a:3240[A]:THR:CG2 | 3:a:3241[A]:PHE:N | 2.71 | 0.53 |
| 3:a:3269[B]:SER:O | 3:a:3272[B]:HIS:HB2 | 2.09 | 0.53 |
| 1:b:127:GLU:CD | 1:b:128:ILE:HA | 2.33 | 0.53 |
| 1:b:262:LYS:NZ | 1:b:795:GLU:OE1 | 2.42 | 0.53 |
| 3:d:2932[A]:PRO:CA | 3:d:2935[A]:ILE:HD12 | 2.30 | 0.53 |
| 3:d:2933[A]:SER:HA | 3:d:2935[A]:ILE:CD1 | 2.38 | 0.53 |
| 3:d:3176[B]:LYS:H | 3:d:3176[B]:LYS:CE | 2.17 | 0.53 |
| 1:A:1171:LYS:HG2 | 1:A:1173:GLY:H | 1.73 | 0.53 |
| 3:C:2952[B]:ALA:HB3 | 3:C:2954[B]:TYR:N | 2.17 | 0.53 |
| 3:C:2954[A]:TYR:CD2 | 3:C:2954[A]:TYR:C | 2.86 | 0.53 |
| 3:C:3014[B]:TRP:CZ3 | 3:C:3119[B]:HIS:ND1 | 2.77 | 0.53 |
| 3:C:3196[A]:THR:OG1 | 3:C:3199[A]:GLN:CB | 2.56 | 0.53 |
| 3:C:3273[B]:LEU:HB2 | 3:C:3275[B]:LEU:CD1 | 2.34 | 0.53 |
| 1:D:535:PRO:HG3 | 1:D:985:PHE:CZ | 2.44 | 0.53 |
| 1:D:603:HIS:O | 1:D:606:ILE:HG22 | 2.08 | 0.53 |
| 2:E:2746:MET:HE2 | 2:E:2765:PRO:HG3 | 1.91 | 0.53 |
| 3:F:3264[A]:TYR:C | 3:F:3264[A]:TYR:HD1 | 2.16 | 0.53 |
| 3:I:3135[A]:LYS:HG3 | 3:I:3141[A]:TYR:CD1 | 2.33 | 0.53 |
| 3:I:3173[B]:THR:HG23 | 3:R:3173[B]:THR:CB | 2.37 | 0.53 |
| 3:L:3014[B]:TRP:CZ3 | 3:L:3119[B]:HIS:ND1 | 2.77 | 0.53 |
| 3:L:3047[A]:ARG:HH21 | 3:L:3113[A]:ASP:CG | 2.16 | 0.53 |
| 1:M:308:LEU:O | 1:M:772:ARG:NH2 | 2.42 | 0.53 |
| 1:P:956:PRO:HB2 | 1:P:957:ASN:C | 2.34 | 0.53 |
| 1:P:1315:GLY:HA3 | 1:P:1601:TRP:CB | 2.39 | 0.53 |
| 1:S:831:VAL:HG12 | 1:S:832:LYS:H | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1638:SER:OG | 1:S:1639:LYS:N | 2.41 | 0.53 |
| 2:T:2571:ARG:NH1 | 2:T:2776:TYR:OH | 2.39 | 0.53 |
| 3:U:3014[A]:TRP:CD1 | 3:U:3014[A]:TRP:C | 2.85 | 0.53 |
| 3:U:3014[B]:TRP:CZ3 | 3:U:3119[B]:HIS:ND1 | 2.77 | 0.53 |
| 3:U:3269[B]:SER:O | 3:U:3272[B]:HIS:HB2 | 2.09 | 0.53 |
| 1:V:568:PHE:N | 1:V:568:PHE:HD1 | 2.07 | 0.53 |
| 1:V:570:GLN:HB3 | 1:V:571:PRO:HD3 | 1.91 | 0.53 |
| 1:V:1166:THR:N | 1:V:1167:ASP:HA | 2.24 | 0.53 |
| 2:W:2635:TYR:HB2 | 1:Y:109:LEU:HD21 | 1.89 | 0.53 |
| 3:X:3081[A]:PHE:CD1 | 3:X:3081[A]:PHE:C | 2.87 | 0.53 |
| 3:X:3132[B]:ALA:HB1 | 3:X:3197[B]:ILE:HD13 | 1.89 | 0.53 |
| 3:X:3132[B]:ALA:CB | 3:X:3197[B]:ILE:CD1 | 2.86 | 0.53 |
| 3:X:3147[A]:GLU:CD | 3:X:3149[A]:ASN:HD21 | 2.17 | 0.53 |
| 3:X:3240[B]:THR:CG2 | 3:X:3241[B]:PHE:N | 2.71 | 0.53 |
| 1:Y:1013:ILE:HD11 | 1:Y:1175:PHE:CD2 | 2.44 | 0.53 |
| 2:Z:2822:LYS:HG2 | 2:Z:2831:GLU:HA | 1.90 | 0.53 |
| 2:Z:2877:ILE:H | 1:b:1078:ARG:NH2 | 2.07 | 0.53 |
| 3:a:2952[B]:ALA:HB3 | 3:a:2954[B]:TYR:N | 2.18 | 0.53 |
| 3:a:3269[A]:SER:O | 3:a:3272[A]:HIS:HB2 | 2.09 | 0.53 |
| 3:d:3081[B]:PHE:C | 3:d:3081[B]:PHE:CD1 | 2.87 | 0.53 |
| 1:A:398:ARG:HH21 | 1:A:663:GLU:CD | 2.16 | 0.53 |
| 2:B:2553:ALA:H | 2:B:2554:PRO:HD3 | 1.74 | 0.53 |
| 2:B:2624:PHE:O | 2:B:2638:ARG:NH2 | 2.34 | 0.53 |
| 3:C:2933[A]:SER:C | 3:C:2936[A]:GLU:H | 2.16 | 0.53 |
| 3:C:2945[B]:VAL:HG22 | 3:C:2954[B]:TYR:HB2 | 1.91 | 0.53 |
| 3:C:3081[B]:PHE:CD1 | 3:C:3081[B]:PHE:C | 2.87 | 0.53 |
| 3:C:3149[B]:ASN:CB | 3:L:3163[B]:ASN:HD22 | 2.01 | 0.53 |
| 3:C:3253[B]:GLU:HB3 | 3:L:3252[B]:TYR:HB3 | 1.91 | 0.53 |
| 2:E:2545:SER:CA | 2:E:2546:LEU:HB2 | 2.34 | 0.53 |
| 3:F:2949[B]:LYS:C | 3:F:2953[B]:GLY:H | 2.17 | 0.53 |
| 3:F:3081[B]:PHE:CD1 | 3:F:3081[B]:PHE:C | 2.87 | 0.53 |
| 3:F:3155[B]:MET:C | 3:a:3153[B]:LYS:HB3 | 2.33 | 0.53 |
| 1:G:1171:LYS:HG2 | 1:G:1173:GLY:H | 1.73 | 0.53 |
| 2:H:2394:VAL:HG11 | 2:H:2451:LEU:HD12 | 1.90 | 0.53 |
| 2:H:2506:ARG:NE | 2:H:2578:GLU:OE2 | 2.39 | 0.53 |
| 3:I:3252[B]:TYR:O | 3:R:2976[B]:ALA:HB3 | 2.08 | 0.53 |
| 1:J:93:ASP:HA | 1:J:212:ASN:HD21 | 1.73 | 0.53 |
| 1:J:929:TRP:O | 1:J:1048:ASN:ND2 | 2.41 | 0.53 |
| 2:K:2568:HIS:HD2 | 2:K:2718:TRP:HH2 | 1.56 | 0.53 |
| 3:L:2933[B]:SER:HA | 3:L:2935[B]:ILE:CD1 | 2.38 | 0.53 |
| 3:L:3042[A]:ASP:N | 3:L:3042[A]:ASP:OD2 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3173[A]:THR:HG22 | 3:L:3175[A]:TYR:H | 1.73 | 0.53 |
| 3:L:3264[A]:TYR:HD1 | 3:L:3264[A]:TYR:C | 2.16 | 0.53 |
| 1:M:245:GLU:HG2 | 1:M:249:ARG:HH11 | 1.73 | 0.53 |
| 1:M:372:ALA:O | 1:M:375:SER:OG | 2.26 | 0.53 |
| 1:M:956:PRO:HB2 | 1:M:958:PRO:HD3 | 1.91 | 0.53 |
| 3:R:2951[A]:ASP:O | 3:R:2956[A]:LYS:HE2 | 2.09 | 0.53 |
| 3:R:3173[A]:THR:HG22 | 3:R:3174[A]:GLY:H | 1.67 | 0.53 |
| 3:R:3176[B]:LYS:H | 3:R:3176[B]:LYS:CE | 2.17 | 0.53 |
| 3:R:3284[B]:LYS:CE | 3:R:3284[B]:LYS:CA | 2.85 | 0.53 |
| 1:S:119:LYS:HD3 | 1:S:120:LYS:HD3 | 1.91 | 0.53 |
| 3:U:3081[A]:PHE:C | 3:U:3081[A]:PHE:CD1 | 2.87 | 0.53 |
| 3:U:3230[B]:PHE:H | 3:U:3243[B]:GLY:CA | 2.22 | 0.53 |
| 2:W:2107:LEU:O | 2:W:2111:GLN:HB2 | 2.09 | 0.53 |
| 2:W:2570:HIS:CD2 | 9:W:3002:CUO:O1 | 2.62 | 0.53 |
| 3:X:2947[B]:ALA:HA | 3:X:2949[B]:LYS:HB3 | 1.89 | 0.53 |
| 3:X:2949[A]:LYS:C | 3:X:2953[A]:GLY:H | 2.17 | 0.53 |
| 3:X:3120[B]:HIS:HA | 3:X:3123[B]:THR:HG1 | 1.72 | 0.53 |
| 3:X:3264[A]:TYR:C | 3:X:3264[A]:TYR:CD1 | 2.86 | 0.53 |
| 3:X:3298[A]:ASN:HA | 3:X:3299[A]:LEU:HB3 | 1.88 | 0.53 |
| 3:a:3081[A]:PHE:C | 3:a:3081[A]:PHE:CD1 | 2.87 | 0.53 |
| 3:a:3082[A]:GLU:OE2 | 3:a:3086[A]:GLU:HB2 | 2.07 | 0.53 |
| 3:a:3284[A]:LYS:HD3 | 3:a:3284[A]:LYS:C | 2.32 | 0.53 |
| 2:c:2602:LEU:HG | 2:c:2603:PRO:HD2 | 1.91 | 0.53 |
| 3:d:2945[A]:VAL:HG22 | 3:d:2954[A]:TYR:HB2 | 1.91 | 0.53 |
| 3:d:2949[B]:LYS:C | 3:d:2953[B]:GLY:H | 2.17 | 0.53 |
| 3:d:3185[B]:TYR:C | 3:d:3185[B]:TYR:CD2 | 2.86 | 0.53 |
| 3:d:3196[A]:THR:OG1 | 3:d:3199[A]:GLN:CB | 2.56 | 0.53 |
| 1:A:892:TYR:CE2 | 1:A:1184:MET:HG3 | 2.44 | 0.53 |
| 2:B:2326:ILE:HG13 | 1:D:1650:ILE:HG23 | 1.91 | 0.53 |
| 3:C:2961[A]:HIS:NE2 | 3:C:2980[A]:HIS:CE1 | 2.73 | 0.53 |
| 3:C:3132[A]:ALA:HB1 | 3:C:3197[A]:ILE:HD13 | 1.89 | 0.53 |
| 3:C:3150[B]:LYS:H | 3:L:3169[B]:LYS:CG | 2.12 | 0.53 |
| 3:C:3248[B]:LEU:CD2 | 3:L:2971[B]:ASP:OD2 | 2.54 | 0.53 |
| 1:D:301:ARG:HD2 | 1:D:361:GLU:OE2 | 2.09 | 0.53 |
| 1:D:589:GLN:O | 1:D:651:ARG:NH1 | 2.42 | 0.53 |
| 1:D:675:SER:O | 1:D:679:ASN:ND2 | 2.42 | 0.53 |
| 1:D:1470:GLU:HG3 | 1:D:1530:LEU:HD12 | 1.91 | 0.53 |
| 3:F:3160[B]:SER:HB2 | 3:a:2982[B]:MET:HB3 | 1.90 | 0.53 |
| 3:F:3264[B]:TYR:C | 3:F:3264[B]:TYR:HD1 | 2.16 | 0.53 |
| 3:F:3269[A]:SER:O | 3:F:3272[A]:HIS:HB2 | 2.09 | 0.53 |
| 3:F:3273[A]:LEU:CB | 3:F:3275[A]:LEU:CD1 | 2.86 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:167:ASP:OD1 | 1:G:168:PHE:N | 2.42 | 0.53 |
| 1:G:1315:GLY:HA3 | 1:G:1601:TRP:CB | 2.39 | 0.53 |
| 3:I:2951[B]:ASP:O | 3:I:2956[B]:LYS:HE2 | 2.09 | 0.53 |
| 3:I:3013[B]:ASP:OD1 | 3:I:3015[B]:THR:HG23 | 2.08 | 0.53 |
| 3:I:3230[B]:PHE:H | 3:I:3243[B]:GLY:CA | 2.22 | 0.53 |
| 1:J:465:PRO:HG2 | 1:J:467:LYS:HE2 | 1.89 | 0.53 |
| 1:J:926:LEU:HD12 | 1:J:927:PRO:HD2 | 1.91 | 0.53 |
| 2:K:2157:LEU:O | 2:K:2160:VAL:HG22 | 2.09 | 0.53 |
| 3:L:2945[B]:VAL:HG22 | 3:L:2954[B]:TYR:HB2 | 1.91 | 0.53 |
| 3:L:3013[A]:ASP:OD1 | 3:L:3015[A]:THR:HG23 | 2.08 | 0.53 |
| 3:L:3264[B]:TYR:C | 3:L:3264[B]:TYR:HD1 | 2.16 | 0.53 |
| 1:M:1075:GLU:HG2 | 2:Q:2900:SER:HA | 1.90 | 0.53 |
| 1:M:1215:LEU:HD23 | 1:M:1231:VAL:HG11 | 1.91 | 0.53 |
| 3:O:2960[A]:PHE:CD2 | 3:O:3157[A]:PRO:CG | 2.74 | 0.53 |
| 3:O:3264[A]:TYR:C | 3:O:3264[A]:TYR:CD1 | 2.86 | 0.53 |
| 1:P:804:ASP:OD1 | 1:P:805:VAL:N | 2.42 | 0.53 |
| 3:R:3147[A]:GLU:CD | 3:R:3149[A]:ASN:HD21 | 2.17 | 0.53 |
| 1:S:686:HIS:CE1 | 1:S:698:GLU:HB3 | 2.44 | 0.53 |
| 3:U:2945[A]:VAL:HG22 | 3:U:2954[A]:TYR:HB2 | 1.91 | 0.53 |
| 3:U:3013[A]:ASP:OD1 | 3:U:3015[A]:THR:HG23 | 2.08 | 0.53 |
| 3:U:3014[A]:TRP:CZ3 | 3:U:3119[A]:HIS:ND1 | 2.77 | 0.53 |
| 3:U:3132[A]:ALA:CB | 3:U:3197[A]:ILE:CD1 | 2.86 | 0.53 |
| 3:U:3196[A]:THR:OG1 | 3:U:3199[A]:GLN:CB | 2.56 | 0.53 |
| 1:V:579:LEU:H | 1:V:579:LEU:HD12 | 1.74 | 0.53 |
| 2:W:2115:SER:OG | 2:W:2116:SER:N | 2.42 | 0.53 |
| 3:X:2945[A]:VAL:HG22 | 3:X:2954[A]:TYR:HB2 | 1.91 | 0.53 |
| 3:X:3230[A]:PHE:H | 3:X:3243[A]:GLY:CA | 2.22 | 0.53 |
| 2:Z:2382:GLU:O | 2:Z:2386:ARG:HG3 | 2.09 | 0.53 |
| 3:a:2945[B]:VAL:HG22 | 3:a:2954[B]:TYR:HB2 | 1.91 | 0.53 |
| 3:a:3013[B]:ASP:OD1 | 3:a:3015[B]:THR:HG23 | 2.08 | 0.53 |
| 3:a:3147[A]:GLU:CD | 3:a:3149[A]:ASN:HD21 | 2.17 | 0.53 |
| 3:a:3230[B]:PHE:H | 3:a:3243[B]:GLY:CA | 2.22 | 0.53 |
| 1:b:570:GLN:HB3 | 1:b:571:PRO:HA | 1.91 | 0.53 |
| 3:d:2949[A]:LYS:C | 3:d:2953[A]:GLY:H | 2.17 | 0.53 |
| 3:d:3176[B]:LYS:C | 3:d:3177[B]:SER:HG | 2.07 | 0.53 |
| 3:d:3264[A]:TYR:C | 3:d:3264[A]:TYR:CD1 | 2.86 | 0.53 |
| 1:A:304:ALA:HB3 | 1:A:360:HIS:HB3 | 1.91 | 0.53 |
| 1:A:1138:ALA:HA | 1:A:1240:ILE:HG22 | 1.91 | 0.53 |
| 3:C:3019[A]:HIS:CD2 | 3:C:3019[A]:HIS:N | 2.75 | 0.53 |
| 3:C:3081[A]:PHE:C | 3:C:3081[A]:PHE:CD1 | 2.87 | 0.53 |
| 3:C:3169[B]:LYS:CG | 3:L:3150[B]:LYS:H | 2.22 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3264[A]:TYR:C | 3:C:3264[A]:TYR:CD1 | 2.86 | 0.53 |
| 3:F:2945[A]:VAL:HG22 | 3:F:2954[A]:TYR:HB2 | 1.91 | 0.53 |
| 3:F:2945[B]:VAL:HG22 | 3:F:2954[B]:TYR:HB2 | 1.91 | 0.53 |
| 3:F:3013[A]:ASP:OD1 | 3:F:3015[A]:THR:OG1 | 2.23 | 0.53 |
| 3:F:3014[B]:TRP:CZ3 | 3:F:3119[B]:HIS:ND1 | 2.77 | 0.53 |
| 3:F:3081[A]:PHE:C | 3:F:3081[A]:PHE:CD1 | 2.87 | 0.53 |
| 3:F:3132[A]:ALA:HB1 | 3:F:3197[A]:ILE:HD13 | 1.89 | 0.53 |
| 1:G:1498:ASN:ND2 | 1:G:1500:THR:O | 2.42 | 0.53 |
| 2:H:2094:ARG:HH21 | 2:K:2094:ARG:HH21 | 1.57 | 0.53 |
| 3:I:3042[B]:ASP:N | 3:I:3042[B]:ASP:OD2 | 2.41 | 0.53 |
| 3:I:3173[B]:THR:HG22 | 3:I:3175[B]:TYR:H | 1.73 | 0.53 |
| 3:I:3298[A]:ASN:HA | 3:I:3299[A]:LEU:HB3 | 1.88 | 0.53 |
| 1:J:902:PHE:CD2 | 1:J:1012:GLU:HG3 | 2.44 | 0.53 |
| 1:J:956:PRO:HB2 | 1:J:957:ASN:C | 2.33 | 0.53 |
| 2:K:2643:GLU:O | 2:K:2647:LEU:HB2 | 2.09 | 0.53 |
| 3:L:2954[B]:TYR:C | 3:L:2954[B]:TYR:CD2 | 2.86 | 0.53 |
| 3:L:3147[B]:GLU:CD | 3:L:3149[B]:ASN:HD21 | 2.17 | 0.53 |
| 1:M:664:VAL:O | 1:M:689:PRO:HD2 | 2.09 | 0.53 |
| 3:O:2945[B]:VAL:HG22 | 3:O:2954[B]:TYR:HB2 | 1.91 | 0.53 |
| 3:O:2949[B]:LYS:C | 3:O:2953[B]:GLY:H | 2.17 | 0.53 |
| 3:O:3013[A]:ASP:OD1 | 3:O:3015[A]:THR:HG23 | 2.08 | 0.53 |
| 1:P:483:GLY:HA3 | 1:P:771:TRP:CE3 | 2.44 | 0.53 |
| 1:P:1152:LYS:NZ | 1:P:1183:GLU:HG2 | 2.23 | 0.53 |
| 1:P:1348:TRP:HD1 | 1:P:1403:LEU:HD13 | 1.72 | 0.53 |
| 3:R:3047[B]:ARG:HH21 | 3:R:3113[B]:ASP:CG | 2.16 | 0.53 |
| 3:R:3173[B]:THR:HG22 | 3:R:3175[B]:TYR:H | 1.73 | 0.53 |
| 3:R:3230[A]:PHE:H | 3:R:3243[A]:GLY:CA | 2.22 | 0.53 |
| 3:R:3287[B]:ILE:O | 3:R:3287[B]:ILE:HG23 | 2.09 | 0.53 |
| 3:U:2937[B]:ASN:CB | 3:U:3006[B]:LYS:CD | 2.86 | 0.53 |
| 3:U:3150[B]:LYS:HG2 | 3:d:3156[B]:MET:CG | 2.38 | 0.53 |
| 3:U:3230[A]:PHE:H | 3:U:3243[A]:GLY:CA | 2.22 | 0.53 |
| 3:U:3255[B]:PRO:C | 3:d:2974[B]:ALA:O | 2.52 | 0.53 |
| 3:U:3293[B]:LYS:CG | 3:U:3294[B]:SER:HB2 | 2.36 | 0.53 |
| 1:V:1170:MET:HB3 | 1:V:1203:MET:HE2 | 1.90 | 0.53 |
| 3:X:2945[B]:VAL:HG22 | 3:X:2954[B]:TYR:HB2 | 1.91 | 0.53 |
| 3:X:3132[A]:ALA:HB1 | 3:X:3197[A]:ILE:HD13 | 1.89 | 0.53 |
| 3:X:3264[B]:TYR:C | 3:X:3264[B]:TYR:HD1 | 2.16 | 0.53 |
| 3:X:3269[A]:SER:O | 3:X:3272[A]:HIS:HB2 | 2.09 | 0.53 |
| 3:a:3014[A]:TRP:CZ3 | 3:a:3119[A]:HIS:ND1 | 2.77 | 0.53 |
| 1:b:534:ASP:HB2 | 1:b:541:LYS:HE2 | 1.91 | 0.53 |
| 1:b:675:SER:HB3 | 1:b:676:PRO:CD | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:979:LEU:H | 1:b:979:LEU:HD13 | 1.73 | 0.53 |
| 2:c:2851:ASN:OD1 | 2:c:2851:ASN:N | 2.39 | 0.53 |
| 3:d:2954[A]:TYR:C | 3:d:2954[A]:TYR:CD2 | 2.86 | 0.53 |
| 3:d:3042[B]:ASP:N | 3:d:3042[B]:ASP:OD2 | 2.41 | 0.53 |
| 3:d:3047[B]:ARG:HH21 | 3:d:3113[B]:ASP:CG | 2.16 | 0.53 |
| 1:A:121:ASN:HD22 | 1:A:124:TYR:H | 1.57 | 0.52 |
| 1:A:857:ALA:HB1 | 1:A:920:ASN:O | 2.09 | 0.52 |
| 1:A:1086:LEU:HB3 | 1:A:1090:ILE:CD1 | 2.39 | 0.52 |
| 3:C:3172[B]:SER:HG | 3:L:3149[B]:ASN:C | 2.17 | 0.52 |
| 3:C:3176[B]:LYS:H | 3:C:3176[B]:LYS:CE | 2.17 | 0.52 |
| 3:C:3240[B]:THR:CG2 | 3:C:3241[B]:PHE:N | 2.71 | 0.52 |
| 2:E:2166:LEU:HA | 2:E:2169:HIS:HB2 | 1.91 | 0.52 |
| 2:E:2539:ILE:O | 2:E:2573:TYR:OH | 2.17 | 0.52 |
| 3:F:2965[B]:LEU:H | 3:a:3221[B]:ALA:CB | 1.82 | 0.52 |
| 3:F:2975[B]:PHE:CE1 | 3:a:3107[B]:LEU:CG | 2.90 | 0.52 |
| 3:F:3107[B]:LEU:HD12 | 3:a:2973[B]:THR:C | 2.34 | 0.52 |
| 3:F:3157[B]:PRO:HD3 | 3:a:3254[B]:MET:CE | 2.39 | 0.52 |
| 3:F:3230[A]:PHE:H | 3:F:3243[A]:GLY:CA | 2.22 | 0.52 |
| 3:F:3284[B]:LYS:CE | 3:F:3284[B]:LYS:CA | 2.85 | 0.52 |
| 1:G:564:ASP:HA | 1:G:609:TRP:O | 2.09 | 0.52 |
| 2:H:2359:ASN:OD1 | 2:H:2359:ASN:N | 2.42 | 0.52 |
| 3:I:2933[B]:SER:HA | 3:I:2935[B]:ILE:CD1 | 2.38 | 0.52 |
| 3:I:2960[B]:PHE:CD1 | 3:I:2960[B]:PHE:N | 2.72 | 0.52 |
| 3:I:3120[B]:HIS:CD2 | 3:R:2969[B]:TYR:CZ | 2.97 | 0.52 |
| 3:I:3287[B]:ILE:O | 3:I:3287[B]:ILE:HG23 | 2.10 | 0.52 |
| 1:J:43:GLU:HG3 | 1:J:44:PRO:HA | 1.92 | 0.52 |
| 2:K:2539:ILE:O | 2:K:2573:TYR:OH | 2.11 | 0.52 |
| 3:L:3081[B]:PHE:C | 3:L:3081[B]:PHE:CD1 | 2.87 | 0.52 |
| 1:M:103:GLU:OE2 | 1:M:106:GLN:NE2 | 2.42 | 0.52 |
| 1:M:972:SER:HA | 1:M:1028:VAL:HG22 | 1.90 | 0.52 |
| 2:N:2648:ALA:HA | 2:N:2654:SER:HB3 | 1.90 | 0.52 |
| 2:N:2716:ARG:NH2 | 2:N:2780:HIS:O | 2.39 | 0.52 |
| 3:O:3042[A]:ASP:N | 3:O:3042[A]:ASP:OD2 | 2.41 | 0.52 |
| 3:O:3132[B]:ALA:CB | 3:O:3197[B]:ILE:CD1 | 2.87 | 0.52 |
| 3:O:3157[B]:PRO:HA | 3:X:3150[B]:LYS:C | 2.33 | 0.52 |
| 3:O:3169[B]:LYS:NZ | 3:X:3148[B]:ILE:N | 2.56 | 0.52 |
| 3:O:3176[A]:LYS:H | 3:O:3176[A]:LYS:CE | 2.17 | 0.52 |
| 3:O:3273[A]:LEU:HB2 | 3:O:3275[A]:LEU:CD1 | 2.34 | 0.52 |
| 2:Q:2403:PHE:CZ | 2:Q:2480:LEU:HD11 | 2.44 | 0.52 |
| 3:R:2945[A]:VAL:HG22 | 3:R:2954[A]:TYR:HB2 | 1.91 | 0.52 |
| 3:R:2945[B]:VAL:HG22 | 3:R:2954[B]:TYR:HB2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2949[A]:LYS:C | 3:R:2953[A]:GLY:H | 2.17 | 0.52 |
| 3:R:2952[A]:ALA:CA | 3:R:2956[A]:LYS:HB3 | 2.38 | 0.52 |
| 3:R:2954[A]:TYR:CD2 | 3:R:2954[A]:TYR:C | 2.86 | 0.52 |
| 3:R:3014[B]:TRP:CZ3 | 3:R:3119[B]:HIS:ND1 | 2.77 | 0.52 |
| 3:R:3269[B]:SER:O | 3:R:3272[B]:HIS:HB2 | 2.09 | 0.52 |
| 3:U:2951[B]:ASP:O | 3:U:2956[B]:LYS:HE2 | 2.09 | 0.52 |
| 3:U:2975[B]:PHE:CB | 3:d:3256[B]:TRP:CG | 2.70 | 0.52 |
| 3:U:3081[B]:PHE:C | 3:U:3081[B]:PHE:CD1 | 2.87 | 0.52 |
| 3:U:3132[A]:ALA:HB1 | 3:U:3197[A]:ILE:HD13 | 1.89 | 0.52 |
| 1:V:980:TYR:HE2 | 1:V:1021:LEU:HB3 | 1.73 | 0.52 |
| 2:W:2684:HIS:NE2 | 2:W:2711:HIS:HE1 | 2.07 | 0.52 |
| 1:Y:915:ASN:ND2 | 1:Y:1093:ASP:OD1 | 2.40 | 0.52 |
| 2:Z:2237:LEU:H | 2:Z:2237:LEU:HD22 | 1.74 | 0.52 |
| 3:a:2931[A]:THR:HG1 | 3:a:2934[A]:GLU:CD | 2.01 | 0.52 |
| 3:a:3115[A]:LEU:O | 3:a:3115[A]:LEU:HD22 | 2.10 | 0.52 |
| 3:a:3132[A]:ALA:CB | 3:a:3197[A]:ILE:CD1 | 2.86 | 0.52 |
| 3:a:3173[A]:THR:HG22 | 3:a:3175[A]:TYR:H | 1.73 | 0.52 |
| 1:b:931:TRP:CZ3 | 1:b:995:ILE:HD11 | 2.44 | 0.52 |
| 2:c:2768:LEU:HA | 2:c:2774:LEU:HD11 | 1.91 | 0.52 |
| 2:c:2869:ALA:O | 2:c:2875:SER:OG | 2.24 | 0.52 |
| 3:d:2933[A]:SER:CB | 3:d:2936[A]:GLU:CB | 2.85 | 0.52 |
| 3:d:2933[A]:SER:C | 3:d:2936[A]:GLU:H | 2.15 | 0.52 |
| 3:d:2945[B]:VAL:HG22 | 3:d:2954[B]:TYR:HB2 | 1.91 | 0.52 |
| 3:d:3014[B]:TRP:CZ3 | 3:d:3119[B]:HIS:ND1 | 2.77 | 0.52 |
| 3:d:3132[A]:ALA:CB | 3:d:3197[A]:ILE:CD1 | 2.86 | 0.52 |
| 3:d:3188[A]:ASP:N | 3:d:3188[A]:ASP:OD2 | 2.36 | 0.52 |
| 3:C:2932[B]:PRO:CA | 3:C:2935[B]:ILE:HD12 | 2.31 | 0.52 |
| 3:C:2933[A]:SER:CB | 3:C:2936[A]:GLU:CB | 2.86 | 0.52 |
| 3:C:2949[B]:LYS:C | 3:C:2953[B]:GLY:H | 2.17 | 0.52 |
| 3:C:2969[B]:TYR:HA | 3:L:2989[B]:HIS:CE1 | 2.44 | 0.52 |
| 3:C:3272[A]:HIS:HD2 | 1:D:1543:ILE:HD11 | 1.74 | 0.52 |
| 1:D:104:LEU:HD23 | 1:D:123:PHE:CE2 | 2.43 | 0.52 |
| 2:E:2795:ILE:O | 2:E:2799:LYS:HG3 | 2.08 | 0.52 |
| 3:F:3269[B]:SER:O | 3:F:3272[B]:HIS:HB2 | 2.09 | 0.52 |
| 1:G:871:GLN:NE2 | 1:G:964:ILE:HG13 | 2.24 | 0.52 |
| 1:G:891:LYS:HB2 | 1:G:892:TYR:CD2 | 2.44 | 0.52 |
| 1:G:1324:ARG:NH1 | 1:G:1519:TYR:HB3 | 2.24 | 0.52 |
| 1:G:1404:TYR:O | 1:G:1407:THR:OG1 | 2.28 | 0.52 |
| 1:G:1528:ASP:N | 1:G:1528:ASP:OD1 | 2.42 | 0.52 |
| 3:I:2975[B]:PHE:CE1 | 3:R:3107[B]:LEU:HG | 2.43 | 0.52 |
| 3:I:3081[A]:PHE:C | 3:I:3081[A]:PHE:CD1 | 2.87 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3092[A]:ILE:CG2 | 3:I:3096[A]:VAL:CG2 | 2.87 | 0.52 |
| 3:I:3230[A]:PHE:H | 3:I:3243[A]:GLY:CA | 2.22 | 0.52 |
| 3:I:3293[B]:LYS:CG | 3:I:3294[B]:SER:HB2 | 2.36 | 0.52 |
| 1:J:914:GLU:OE1 | 1:J:926:LEU:N | 2.40 | 0.52 |
| 1:J:1432:SER:OG | 1:J:1567:ASP:OD2 | 2.27 | 0.52 |
| 2:K:2740:ASP:OD1 | 2:K:2740:ASP:N | 2.41 | 0.52 |
| 3:L:3092[B]:ILE:CG2 | 3:L:3096[B]:VAL:CG2 | 2.88 | 0.52 |
| 3:L:3173[B]:THR:HG22 | 3:L:3175[B]:TYR:H | 1.73 | 0.52 |
| 3:O:3014[A]:TRP:CZ3 | 3:O:3119[A]:HIS:ND1 | 2.77 | 0.52 |
| 3:O:3081[A]:PHE:CD1 | 3:O:3081[A]:PHE:C | 2.87 | 0.52 |
| 3:O:3269[A]:SER:O | 3:O:3272[A]:HIS:HB2 | 2.09 | 0.52 |
| 1:P:566:ARG:N | 1:P:567:LEU:HA | 2.25 | 0.52 |
| 1:P:597:VAL:HG12 | 1:P:773:PHE:CD1 | 2.45 | 0.52 |
| 1:P:899:MET:HE2 | 1:P:1012:GLU:CD | 2.34 | 0.52 |
| 1:P:1339:SER:HB2 | 1:P:1340:GLY:HA2 | 1.90 | 0.52 |
| 1:P:1551:ASP:HB3 | 1:P:1652:PHE:HE1 | 1.73 | 0.52 |
| 3:R:3092[B]:ILE:CG2 | 3:R:3096[B]:VAL:CG2 | 2.88 | 0.52 |
| 3:R:3269[A]:SER:O | 3:R:3272[A]:HIS:HB2 | 2.09 | 0.52 |
| 3:R:3298[A]:ASN:HA | 3:R:3299[A]:LEU:HB3 | 1.88 | 0.52 |
| 1:S:785:LEU:HD13 | 1:S:792:MET:HA | 1.90 | 0.52 |
| 1:S:1301:PRO:HA | 1:S:1308:VAL:HA | 1.90 | 0.52 |
| 3:U:2933[B]:SER:CB | 3:U:2936[B]:GLU:CB | 2.85 | 0.52 |
| 3:U:2935[B]:ILE:CD1 | 3:U:2935[B]:ILE:N | 2.73 | 0.52 |
| 3:U:3264[A]:TYR:C | 3:U:3264[A]:TYR:CD1 | 2.86 | 0.52 |
| 1:V:306:PHE:HB3 | 1:V:308:LEU:HD13 | 1.91 | 0.52 |
| 1:V:1542:ARG:O | 1:V:1546:LYS:HG2 | 2.09 | 0.52 |
| 2:W:2533:ASP:OD1 | 2:W:2533:ASP:N | 2.41 | 0.52 |
| 3:X:2954[A]:TYR:C | 3:X:2954[A]:TYR:CD2 | 2.86 | 0.52 |
| 3:X:3114[A]:PRO:CD | 3:X:3115[A]:LEU:N | 2.72 | 0.52 |
| 3:X:3293[B]:LYS:CD | 3:X:3294[B]:SER:N | 2.64 | 0.52 |
| 1:Y:897:HIS:HB3 | 1:Y:899:MET:SD | 2.50 | 0.52 |
| 3:a:3120[B]:HIS:HA | 3:a:3123[B]:THR:HG1 | 1.71 | 0.52 |
| 3:a:3230[A]:PHE:H | 3:a:3243[A]:GLY:CA | 2.22 | 0.52 |
| 1:b:1059:LEU:O | 1:b:1063:ARG:N | 2.40 | 0.52 |
| 3:d:3230[A]:PHE:H | 3:d:3243[A]:GLY:CA | 2.22 | 0.52 |
| 3:d:3269[B]:SER:O | 3:d:3272[B]:HIS:HB2 | 2.09 | 0.52 |
| 3:d:3298[A]:ASN:CB | 3:d:3300[A]:LEU:CD2 | 2.61 | 0.52 |
| 4:7:1:NAG:C6 | 4:7:2:NAG:HN2 | 2.22 | 0.52 |
| 1:A:1075:GLU:HG2 | 2:E:2900:SER:HA | 1.91 | 0.52 |
| 3:C:3066[A]:TYR:CE1 | 3:C:3193[A]:HIS:CE1 | 2.98 | 0.52 |
| 3:C:3147[A]:GLU:CD | 3:C:3149[A]:ASN:HD21 | 2.17 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3147[B]:GLU:CD | 3:C:3149[B]:ASN:HD21 | 2.17 | 0.52 |
| 3:C:3147[B]:GLU:OE2 | 3:L:3169[B]:LYS:NZ | 2.40 | 0.52 |
| 3:C:3148[B]:ILE:HG22 | 3:L:3170[B]:ALA:CA | 2.38 | 0.52 |
| 1:D:482:HIS:CE1 | 1:D:621:LEU:HD11 | 2.44 | 0.52 |
| 2:E:2822:LYS:HG2 | 2:E:2829:CYS:HB3 | 1.91 | 0.52 |
| 3:F:2949[A]:LYS:C | 3:F:2953[A]:GLY:H | 2.17 | 0.52 |
| 3:F:2951[B]:ASP:O | 3:F:2956[B]:LYS:HE2 | 2.09 | 0.52 |
| 3:F:3114[A]:PRO:CD | 3:F:3115[A]:LEU:N | 2.72 | 0.52 |
| 3:F:3174[B]:GLY:HA2 | 3:a:3154[B]:PRO:CD | 2.37 | 0.52 |
| 3:F:3264[A]:TYR:C | 3:F:3264[A]:TYR:CD1 | 2.86 | 0.52 |
| 3:F:3300[A]:LEU:N | 3:F:3300[A]:LEU:CD2 | 2.73 | 0.52 |
| 1:G:957:ASN:N | 1:G:958:PRO:HA | 2.24 | 0.52 |
| 2:H:2539:ILE:O | 2:H:2573:TYR:OH | 2.15 | 0.52 |
| 3:I:2935[A]:ILE:CD1 | 3:I:2935[A]:ILE:N | 2.73 | 0.52 |
| 3:I:2945[A]:VAL:HG22 | 3:I:2954[A]:TYR:HB2 | 1.91 | 0.52 |
| 3:I:2973[B]:THR:CG2 | 3:R:3106[B]:THR:C | 2.82 | 0.52 |
| 3:I:3159[B]:SER:CA | 3:R:3150[B]:LYS:CA | 2.87 | 0.52 |
| 3:I:3228[A]:VAL:CG2 | 3:I:3245[A]:PHE:CE2 | 2.89 | 0.52 |
| 3:I:3269[B]:SER:O | 3:I:3272[B]:HIS:HB2 | 2.09 | 0.52 |
| 3:I:3284[B]:LYS:HD3 | 3:I:3284[B]:LYS:C | 2.32 | 0.52 |
| 3:I:3287[A]:ILE:O | 3:I:3287[A]:ILE:HG23 | 2.10 | 0.52 |
| 3:I:3298[B]:ASN:HA | 3:I:3299[B]:LEU:HB3 | 1.88 | 0.52 |
| 2:K:2823:ILE:HG12 | 2:K:2832:ALA:HB2 | 1.91 | 0.52 |
| 3:L:2961[A]:HIS:HB3 | 3:L:3111[A]:SER:HB3 | 1.92 | 0.52 |
| 3:L:3264[B]:TYR:C | 3:L:3264[B]:TYR:CD1 | 2.86 | 0.52 |
| 3:L:3275[A]:LEU:N | 3:L:3275[A]:LEU:CD1 | 2.73 | 0.52 |
| 3:L:3284[B]:LYS:HE2 | 3:L:3284[B]:LYS:CA | 2.29 | 0.52 |
| 2:N:2252:GLU:HG3 | 2:N:2385:ILE:HG23 | 1.91 | 0.52 |
| 2:N:2361:LYS:HD2 | 2:N:2362:GLN:HG3 | 1.92 | 0.52 |
| 3:O:2935[A]:ILE:CD1 | 3:O:2935[A]:ILE:N | 2.73 | 0.52 |
| 3:O:2951[A]:ASP:O | 3:O:2956[A]:LYS:HE2 | 2.09 | 0.52 |
| 3:O:3092[A]:ILE:CG2 | 3:O:3096[A]:VAL:CG2 | 2.88 | 0.52 |
| 3:O:3230[A]:PHE:H | 3:O:3243[A]:GLY:CA | 2.22 | 0.52 |
| 3:O:3252[B]:TYR:CG | 3:X:2966[B]:SER:O | 2.49 | 0.52 |
| 3:O:3300[A]:LEU:N | 3:O:3300[A]:LEU:CD2 | 2.73 | 0.52 |
| 3:R:2949[B]:LYS:C | 3:R:2953[B]:GLY:H | 2.17 | 0.52 |
| 3:R:3132[B]:ALA:CB | 3:R:3197[B]:ILE:CD1 | 2.86 | 0.52 |
| 3:R:3147[B]:GLU:CD | 3:R:3149[B]:ASN:HD21 | 2.17 | 0.52 |
| 3:R:3230[B]:PHE:H | 3:R:3243[B]:GLY:CA | 2.22 | 0.52 |
| 1:S:483:GLY:HA2 | 1:S:773:PHE:CZ | 2.45 | 0.52 |
| 1:S:897:HIS:HB3 | 1:S:899:MET:SD | 2.50 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:2684:HIS:NE2 | 2:T:2711:HIS:CE1 | 2.77 | 0.52 |
| 3:U:2975[B]:PHE:CD1 | 3:d:3256[B]:TRP:HD1 | 1.85 | 0.52 |
| 3:U:3254[B]:MET:HG2 | 3:d:3255[B]:PRO:CD | 2.39 | 0.52 |
| 1:V:1081:MET:HG2 | 1:V:1100:SER:O | 2.09 | 0.52 |
| 1:V:1163:ALA:HB2 | 1:V:1205:LEU:HD21 | 1.90 | 0.52 |
| 2:W:2373:MET:HG3 | 2:W:2376:MET:HE3 | 1.91 | 0.52 |
| 3:X:2935[A]:ILE:CD1 | 3:X:2936[A]:GLU:N | 2.73 | 0.52 |
| 3:X:2951[A]:ASP:O | 3:X:2956[A]:LYS:HE2 | 2.09 | 0.52 |
| 3:X:3139[A]:LEU:CD2 | 3:X:3139[A]:LEU:N | 2.73 | 0.52 |
| 3:X:3230[B]:PHE:H | 3:X:3243[B]:GLY:CA | 2.22 | 0.52 |
| 3:X:3284[B]:LYS:CE | 3:X:3284[B]:LYS:CA | 2.85 | 0.52 |
| 1:Y:142:ARG:NH1 | 1:Y:340:GLN:OE1 | 2.40 | 0.52 |
| 3:a:2935[A]:ILE:CD1 | 3:a:2935[A]:ILE:N | 2.73 | 0.52 |
| 3:a:2951[B]:ASP:O | 3:a:2956[B]:LYS:HE2 | 2.09 | 0.52 |
| 3:a:2952[B]:ALA:N | 3:a:2953[B]:GLY:HA2 | 2.06 | 0.52 |
| 3:a:3014[B]:TRP:CZ3 | 3:a:3119[B]:HIS:ND1 | 2.77 | 0.52 |
| 3:a:3047[B]:ARG:HH21 | 3:a:3113[B]:ASP:CG | 2.16 | 0.52 |
| 1:b:1470:GLU:HB3 | 1:b:1537:ILE:CD1 | 2.39 | 0.52 |
| 3:d:2948[A]:ASP:CB | 3:d:2949[A]:LYS:HA | 2.15 | 0.52 |
| 3:d:3110[B]:THR:O | 3:d:3111[B]:SER:C | 2.53 | 0.52 |
| 3:d:3230[B]:PHE:H | 3:d:3243[B]:GLY:CA | 2.22 | 0.52 |
| 3:d:3269[A]:SER:O | 3:d:3272[A]:HIS:HB2 | 2.09 | 0.52 |
| 3:d:3287[A]:ILE:O | 3:d:3287[A]:ILE:HG23 | 2.10 | 0.52 |
| 1:A:164:GLU:OE1 | 1:A:296:ARG:NH1 | 2.42 | 0.52 |
| 1:A:905:TRP:HE1 | 1:A:1083:PRO:CD | 2.22 | 0.52 |
| 3:C:2949[A]:LYS:C | 3:C:2953[A]:GLY:H | 2.17 | 0.52 |
| 3:C:2976[B]:ALA:HB2 | 3:L:3253[B]:GLU:CG | 2.39 | 0.52 |
| 3:C:3269[A]:SER:O | 3:C:3272[A]:HIS:HB2 | 2.09 | 0.52 |
| 1:D:1248:ARG:HG3 | 1:D:1249:TRP:N | 2.24 | 0.52 |
| 1:D:1574:VAL:H | 1:G:329:ARG:NH1 | 2.01 | 0.52 |
| 1:D:1582:ASN:HD21 | 1:D:1627:ARG:HE | 1.57 | 0.52 |
| 2:E:2393:ARG:HH21 | 2:E:2489:ILE:HD11 | 1.75 | 0.52 |
| 2:E:2670:CYS:N | 2:E:2737:CYS:SG | 2.82 | 0.52 |
| 3:F:2951[A]:ASP:O | 3:F:2956[A]:LYS:HE2 | 2.09 | 0.52 |
| 3:F:2960[B]:PHE:CD2 | 3:F:3157[B]:PRO:CG | 2.74 | 0.52 |
| 3:F:3115[B]:LEU:HD22 | 3:F:3115[B]:LEU:O | 2.10 | 0.52 |
| 3:F:3139[A]:LEU:CD2 | 3:F:3139[A]:LEU:N | 2.73 | 0.52 |
| 1:G:1070:ALA:HB3 | 1:G:1077:LEU:HD21 | 1.92 | 0.52 |
| 2:H:2554:PRO:HA | 2:H:2555:GLU:HB2 | 1.90 | 0.52 |
| 3:I:3157[B]:PRO:CD | 3:R:3153[B]:LYS:NZ | 2.73 | 0.52 |
| 3:I:3162[B]:ASP:CA | 3:R:3147[B]:GLU:OE1 | 2.58 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3253[B]:GLU:CB | 3:R:2976[B]:ALA:N | 2.70 | 0.52 |
| 1:J:1631:GLU:OE1 | 1:M:328:LYS:NZ | 2.35 | 0.52 |
| 3:L:2947[A]:ALA:HA | 3:L:2949[A]:LYS:HB3 | 1.89 | 0.52 |
| 3:L:3047[B]:ARG:HH21 | 3:L:3113[B]:ASP:CG | 2.16 | 0.52 |
| 3:L:3081[A]:PHE:CD1 | 3:L:3081[A]:PHE:C | 2.87 | 0.52 |
| 3:L:3230[B]:PHE:H | 3:L:3243[B]:GLY:CA | 2.22 | 0.52 |
| 1:M:630:PHE:O | 1:M:633:HIS:HB3 | 2.09 | 0.52 |
| 3:O:3014[B]:TRP:CZ3 | 3:O:3119[B]:HIS:ND1 | 2.77 | 0.52 |
| 3:O:3047[B]:ARG:HH21 | 3:O:3113[B]:ASP:CG | 2.16 | 0.52 |
| 3:O:3132[A]:ALA:CB | 3:O:3197[A]:ILE:CD1 | 2.86 | 0.52 |
| 3:O:3139[A]:LEU:CD2 | 3:O:3139[A]:LEU:N | 2.73 | 0.52 |
| 3:O:3173[B]:THR:HG22 | 3:O:3175[B]:TYR:H | 1.73 | 0.52 |
| 3:O:3255[B]:PRO:CA | 3:X:3161[B]:GLU:CA | 2.79 | 0.52 |
| 1:P:1036:SER:OG | 1:P:1037:ALA:N | 2.41 | 0.52 |
| 3:R:2935[A]:ILE:CD1 | 3:R:2935[A]:ILE:N | 2.73 | 0.52 |
| 3:R:3028[B]:PRO:HG2 | 3:R:3029[B]:LYS:CG | 2.40 | 0.52 |
| 3:R:3092[A]:ILE:CG2 | 3:R:3096[A]:VAL:CG2 | 2.88 | 0.52 |
| 3:R:3147[A]:GLU:CB | 3:R:3149[A]:ASN:ND2 | 2.73 | 0.52 |
| 1:S:69:HIS:NE2 | 9:S:2102:CUO:O2 | 2.43 | 0.52 |
| 3:U:2951[A]:ASP:O | 3:U:2956[A]:LYS:HE2 | 2.09 | 0.52 |
| 1:V:329:ARG:NH1 | 1:Y:1582:ASN:O | 2.42 | 0.52 |
| 1:V:1260:ARG:HD3 | 1:V:1331:GLU:OE1 | 2.10 | 0.52 |
| 3:X:2935[A]:ILE:CD1 | 3:X:2935[A]:ILE:N | 2.73 | 0.52 |
| 3:X:3014[B]:TRP:CZ3 | 3:X:3119[B]:HIS:ND1 | 2.77 | 0.52 |
| 1:Y:17:ASN:HA | 1:Y:20:VAL:HG12 | 1.90 | 0.52 |
| 1:Y:1617:LYS:HE2 | 3:d:3180[B]:TYR:CZ | 2.44 | 0.52 |
| 2:Z:2603:PRO:HG2 | 2:Z:2606:LEU:HD12 | 1.91 | 0.52 |
| 3:a:3300[A]:LEU:N | 3:a:3300[A]:LEU:CD2 | 2.73 | 0.52 |
| 1:b:132:ASN:HB2 | 1:b:133:LYS:HG2 | 1.91 | 0.52 |
| 1:b:957:ASN:N | 1:b:958:PRO:HA | 2.24 | 0.52 |
| 1:b:1029:SER:OG | 1:b:1030:MET:N | 2.43 | 0.52 |
| 3:d:3173[B]:THR:HG22 | 3:d:3175[B]:TYR:H | 1.73 | 0.52 |
| 8:0:1:NAG:H62 | 8:0:2:NAG:N2 | 2.24 | 0.52 |
| 4:7:1:NAG:H61 | 4:7:2:NAG:HN2 | 1.74 | 0.52 |
| 6:CA:1:NAG:H61 | 6:CA:2:NAG:C8 | 2.39 | 0.52 |
| 3:C:2952[B]:ALA:CB | 3:C:2956[B]:LYS:HB3 | 2.40 | 0.52 |
| 3:C:2965[B]:LEU:C | 3:L:3256[B]:TRP:O | 2.45 | 0.52 |
| 3:C:3014[A]:TRP:CZ3 | 3:C:3119[A]:HIS:ND1 | 2.77 | 0.52 |
| 1:D:137:ARG:HB2 | 1:D:186:VAL:O | 2.10 | 0.52 |
| 3:F:2961[B]:HIS:HB3 | 3:F:3111[B]:SER:HB3 | 1.92 | 0.52 |
| 3:F:3248[B]:LEU:CD1 | 3:a:2973[B]:THR:HG23 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3287[B]:ILE:O | 3:F:3287[B]:ILE:HG23 | 2.10 | 0.52 |
| 1:G:1234:VAL:H | 2:K:2738:ALA:HA | 1.74 | 0.52 |
| 2:H:2336:PHE:HB3 | 2:H:2348:THR:HG22 | 1.92 | 0.52 |
| 3:I:2970[B]:PRO:CD | 3:R:2989[B]:HIS:CE1 | 2.93 | 0.52 |
| 3:I:3300[B]:LEU:N | 3:I:3300[B]:LEU:CD2 | 2.73 | 0.52 |
| 1:J:227:ARG:NH2 | 1:J:297:ARG:HH22 | 2.07 | 0.52 |
| 1:J:439:LEU:HD23 | 1:J:509:ILE:HD12 | 1.91 | 0.52 |
| 1:J:810:LEU:HD11 | 4:u:1:NAG:H62 | 1.90 | 0.52 |
| 1:J:1136:ARG:O | 1:J:1141:ARG:NH1 | 2.43 | 0.52 |
| 3:L:2935[B]:ILE:CD1 | 3:L:2935[B]:ILE:N | 2.73 | 0.52 |
| 3:L:3014[A]:TRP:CZ3 | 3:L:3119[A]:HIS:ND1 | 2.77 | 0.52 |
| 3:L:3038[A]:ILE:HG23 | 3:L:3040[A]:VAL:HG22 | 1.90 | 0.52 |
| 3:L:3132[A]:ALA:CB | 3:L:3197[A]:ILE:CD1 | 2.87 | 0.52 |
| 3:L:3147[B]:GLU:CB | 3:L:3149[B]:ASN:ND2 | 2.73 | 0.52 |
| 3:L:3151[A]:LEU:HB2 | 3:L:3175[A]:TYR:HE2 | 1.68 | 0.52 |
| 3:L:3269[A]:SER:O | 3:L:3272[A]:HIS:HB2 | 2.09 | 0.52 |
| 3:L:3285[A]:VAL:CG2 | 3:L:3286[A]:THR:N | 2.73 | 0.52 |
| 3:O:2977[B]:CYS:H | 3:X:3153[B]:LYS:HG2 | 1.74 | 0.52 |
| 3:O:3115[B]:LEU:HD22 | 3:O:3115[B]:LEU:O | 2.10 | 0.52 |
| 3:O:3230[B]:PHE:H | 3:O:3243[B]:GLY:CA | 2.22 | 0.52 |
| 3:O:3287[B]:ILE:O | 3:O:3287[B]:ILE:HG23 | 2.10 | 0.52 |
| 3:O:3300[B]:LEU:N | 3:O:3300[B]:LEU:CD2 | 2.73 | 0.52 |
| 1:P:1013:ILE:HD11 | 1:P:1175:PHE:CD2 | 2.45 | 0.52 |
| 2:Q:2392:ASP:HB2 | 2:Q:2491:PRO:HG3 | 1.90 | 0.52 |
| 2:Q:2821:LEU:HD11 | 2:Q:2879:LEU:HG | 1.92 | 0.52 |
| 3:R:2951[B]:ASP:O | 3:R:2956[B]:LYS:HE2 | 2.09 | 0.52 |
| 3:R:3028[A]:PRO:HG2 | 3:R:3029[A]:LYS:CG | 2.40 | 0.52 |
| 3:R:3285[A]:VAL:CG2 | 3:R:3286[A]:THR:N | 2.73 | 0.52 |
| 3:R:3293[A]:LYS:CB | 3:R:3294[A]:SER:CB | 2.54 | 0.52 |
| 3:R:3293[B]:LYS:CG | 3:R:3294[B]:SER:HB2 | 2.36 | 0.52 |
| 3:U:3135[A]:LYS:HG3 | 3:U:3141[A]:TYR:HE1 | 1.29 | 0.52 |
| 3:U:3147[A]:GLU:CD | 3:U:3149[A]:ASN:HD21 | 2.17 | 0.52 |
| 3:U:3170[B]:ALA:C | 3:d:3152[B]:LYS:HZ1 | 2.17 | 0.52 |
| 1:V:22:LEU:HB3 | 1:V:122:VAL:HG21 | 1.92 | 0.52 |
| 1:V:730:PHE:CD1 | 1:V:780:GLU:HA | 2.44 | 0.52 |
| 3:a:2935[B]:ILE:CD1 | 3:a:2935[B]:ILE:N | 2.73 | 0.52 |
| 3:a:2954[A]:TYR:CD2 | 3:a:2954[A]:TYR:C | 2.86 | 0.52 |
| 2:c:2244:PHE:HE2 | 2:c:2374:ASN:HD22 | 1.57 | 0.52 |
| 2:c:2849:ASP:HB3 | 2:c:2850:ARG:HE | 1.73 | 0.52 |
| 3:d:2935[A]:ILE:CD1 | 3:d:2936[A]:GLU:N | 2.73 | 0.52 |
| 3:d:2937[A]:ASN:ND2 | 3:d:3006[A]:LYS:CD | 2.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3092[B]:ILE:CG2 | 3:d:3096[B]:VAL:CG2 | 2.88 | 0.52 |
| 3:d:3132[A]:ALA:HB1 | 3:d:3197[A]:ILE:HD13 | 1.89 | 0.52 |
| 3:d:3139[A]:LEU:CD2 | 3:d:3139[A]:LEU:N | 2.73 | 0.52 |
| 3:d:3139[B]:LEU:CD2 | 3:d:3139[B]:LEU:N | 2.73 | 0.52 |
| 3:d:3228[A]:VAL:CG2 | 3:d:3245[A]:PHE:CE2 | 2.89 | 0.52 |
| 3:d:3287[B]:ILE:O | 3:d:3287[B]:ILE:HG23 | 2.09 | 0.52 |
| 1:A:1144:VAL:HG23 | 1:A:1194:SER:O | 2.09 | 0.52 |
| 1:A:1195:ASP:HA | 1:A:1196:ILE:CG2 | 2.40 | 0.52 |
| 3:C:2961[A]:HIS:HB3 | 3:C:3111[A]:SER:HB3 | 1.92 | 0.52 |
| 3:C:3107[B]:LEU:CD1 | 3:L:2974[B]:ALA:O | 2.41 | 0.52 |
| 3:C:3110[A]:THR:O | 3:C:3111[A]:SER:C | 2.53 | 0.52 |
| 3:C:3173[A]:THR:HG22 | 3:C:3175[A]:TYR:H | 1.73 | 0.52 |
| 3:C:3176[B]:LYS:NZ | 3:C:3176[B]:LYS:CB | 2.73 | 0.52 |
| 3:C:3293[B]:LYS:CG | 3:C:3294[B]:SER:HB2 | 2.36 | 0.52 |
| 1:D:855:ARG:HD3 | 1:D:959:PHE:HD2 | 1.75 | 0.52 |
| 3:F:3115[A]:LEU:O | 3:F:3115[A]:LEU:HD22 | 2.10 | 0.52 |
| 3:F:3139[B]:LEU:CD2 | 3:F:3139[B]:LEU:N | 2.73 | 0.52 |
| 3:F:3147[B]:GLU:CD | 3:F:3149[B]:ASN:HD21 | 2.17 | 0.52 |
| 3:F:3153[B]:LYS:HB2 | 3:a:3158[B]:PHE:CB | 2.27 | 0.52 |
| 3:F:3255[B]:PRO:CB | 3:a:2964[B]:PRO:N | 2.73 | 0.52 |
| 3:F:3287[A]:ILE:O | 3:F:3287[A]:ILE:HG23 | 2.09 | 0.52 |
| 3:I:2937[B]:ASN:ND2 | 3:I:3006[B]:LYS:CD | 2.73 | 0.52 |
| 3:I:2952[A]:ALA:CA | 3:I:2956[A]:LYS:HB3 | 2.38 | 0.52 |
| 3:I:2952[B]:ALA:CB | 3:I:2956[B]:LYS:HB3 | 2.40 | 0.52 |
| 3:I:2961[B]:HIS:HA | 3:R:2975[B]:PHE:CE2 | 2.33 | 0.52 |
| 3:I:2966[B]:SER:HA | 3:R:3255[B]:PRO:C | 2.35 | 0.52 |
| 3:I:2970[B]:PRO:HD3 | 3:R:2989[B]:HIS:CE1 | 2.45 | 0.52 |
| 3:I:2983[B]:VAL:CG2 | 3:R:3162[B]:ASP:OD1 | 2.57 | 0.52 |
| 3:I:3089[A]:HIS:CE1 | 3:I:3119[A]:HIS:CE1 | 2.81 | 0.52 |
| 3:I:3115[A]:LEU:HD22 | 3:I:3115[A]:LEU:O | 2.10 | 0.52 |
| 3:I:3135[B]:LYS:HG3 | 3:I:3141[B]:TYR:CD1 | 2.33 | 0.52 |
| 3:I:3154[B]:PRO:CD | 3:R:3173[B]:THR:C | 2.83 | 0.52 |
| 3:I:3255[B]:PRO:HG3 | 3:R:2962[B]:GLY:O | 2.05 | 0.52 |
| 1:J:960:PHE:HD1 | 1:J:962:GLY:H | 1.58 | 0.52 |
| 2:K:2121:THR:O | 2:K:2124:SER:OG | 2.13 | 0.52 |
| 3:L:3038[B]:ILE:HG23 | 3:L:3040[B]:VAL:HG22 | 1.90 | 0.52 |
| 3:L:3110[B]:THR:C | 3:L:3112[B]:TYR:N | 2.68 | 0.52 |
| 3:L:3115[A]:LEU:HD22 | 3:L:3115[A]:LEU:O | 2.10 | 0.52 |
| 3:L:3300[A]:LEU:N | 3:L:3300[A]:LEU:CD2 | 2.73 | 0.52 |
| 1:M:892:TYR:CE1 | 1:M:1184:MET:HG3 | 2.45 | 0.52 |
| 2:N:2270:ILE:HB | 2:N:2297:HIS:CD2 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2954[B]:TYR:C | 3:O:2954[B]:TYR:CD2 | 2.86 | 0.52 |
| 3:O:3101[B]:PRO:C | 3:X:2971[B]:ASP:C | 2.78 | 0.52 |
| 3:O:3176[B]:LYS:NZ | 3:O:3176[B]:LYS:CB | 2.73 | 0.52 |
| 3:O:3183[B]:LEU:N | 3:O:3184[B]:ASN:HA | 2.11 | 0.52 |
| 2:Q:2822:LYS:HD3 | 2:Q:2829:CYS:HB2 | 1.91 | 0.52 |
| 2:Q:2884:LYS:HG2 | 2:Q:2891:LEU:HD23 | 1.92 | 0.52 |
| 3:R:2935[B]:ILE:CD1 | 3:R:2935[B]:ILE:N | 2.73 | 0.52 |
| 3:R:3081[A]:PHE:C | 3:R:3081[A]:PHE:CD1 | 2.87 | 0.52 |
| 3:R:3287[A]:ILE:O | 3:R:3287[A]:ILE:HG23 | 2.09 | 0.52 |
| 3:U:3092[A]:ILE:CG2 | 3:U:3096[A]:VAL:CG2 | 2.88 | 0.52 |
| 3:U:3139[A]:LEU:CD2 | 3:U:3139[A]:LEU:N | 2.73 | 0.52 |
| 3:U:3147[B]:GLU:CD | 3:U:3149[B]:ASN:HD21 | 2.17 | 0.52 |
| 3:U:3219[A]:LEU:N | 3:U:3219[A]:LEU:CD2 | 2.73 | 0.52 |
| 3:U:3287[A]:ILE:O | 3:U:3287[A]:ILE:HG23 | 2.09 | 0.52 |
| 2:W:2107:LEU:HD23 | 2:W:2208:PRO:HB2 | 1.90 | 0.52 |
| 3:X:2951[B]:ASP:O | 3:X:2956[B]:LYS:HE2 | 2.09 | 0.52 |
| 3:X:3273[A]:LEU:HB2 | 3:X:3275[A]:LEU:CD1 | 2.34 | 0.52 |
| 3:X:3287[A]:ILE:O | 3:X:3287[A]:ILE:HG23 | 2.10 | 0.52 |
| 1:Y:71:LEU:HD22 | 1:Y:266:LEU:HD21 | 1.91 | 0.52 |
| 1:Y:516:TRP:HH2 | 1:Y:637:VAL:HG22 | 1.75 | 0.52 |
| 3:a:2945[A]:VAL:HG22 | 3:a:2954[A]:TYR:HB2 | 1.91 | 0.52 |
| 3:a:2951[A]:ASP:O | 3:a:2956[A]:LYS:HE2 | 2.09 | 0.52 |
| 3:a:3139[B]:LEU:CD2 | 3:a:3139[B]:LEU:N | 2.73 | 0.52 |
| 3:a:3147[B]:GLU:CD | 3:a:3149[B]:ASN:HD21 | 2.17 | 0.52 |
| 1:b:488:PRO:HB2 | 1:b:641:TRP:CE3 | 2.45 | 0.52 |
| 1:b:926:LEU:HD12 | 1:b:927:PRO:HD2 | 1.92 | 0.52 |
| 1:b:1228:LEU:HD22 | 1:b:1229:LYS:HA | 1.91 | 0.52 |
| 2:c:2191:LEU:HD13 | 2:c:2296:LEU:HD22 | 1.91 | 0.52 |
| 2:c:2476:LEU:HB3 | 2:c:2480:LEU:CD2 | 2.39 | 0.52 |
| 3:d:3115[A]:LEU:HD22 | 3:d:3115[A]:LEU:O | 2.10 | 0.52 |
| 3:d:3176[B]:LYS:NZ | 3:d:3176[B]:LYS:CB | 2.73 | 0.52 |
| 3:d:3183[A]:LEU:N | 3:d:3184[A]:ASN:HA | 2.12 | 0.52 |
| 3:d:3285[A]:VAL:CG2 | 3:d:3286[A]:THR:N | 2.73 | 0.52 |
| 1:A:1028:VAL:HA | 1:A:1035:TYR:CD2 | 2.43 | 0.52 |
| 2:B:2332:PRO:HB2 | 2:B:2337:SER:HB2 | 1.91 | 0.52 |
| 3:C:2937[B]:ASN:ND2 | 3:C:3006[B]:LYS:CD | 2.73 | 0.52 |
| 3:C:2960[B]:PHE:CD1 | 3:C:2960[B]:PHE:N | 2.72 | 0.52 |
| 3:C:2968[B]:GLN:NE2 | 3:L:3086[B]:GLU:HB3 | 2.18 | 0.52 |
| 3:C:2972[B]:GLY:CA | 3:L:3090[B]:ASN:CB | 2.88 | 0.52 |
| 3:C:3264[B]:TYR:C | 3:C:3264[B]:TYR:CD1 | 2.86 | 0.52 |
| 3:C:3273[A]:LEU:HB2 | 3:C:3275[A]:LEU:CD1 | 2.34 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:2344:LEU:HA | 2:E:2345:ASN:C | 2.34 | 0.52 |
| 3:F:2948[A]:ASP:CB | 3:F:2949[A]:LYS:HA | 2.16 | 0.52 |
| 3:F:2961[A]:HIS:HB3 | 3:F:3111[A]:SER:HB3 | 1.92 | 0.52 |
| 3:F:3014[A]:TRP:CZ3 | 3:F:3119[A]:HIS:ND1 | 2.77 | 0.52 |
| 3:F:3092[A]:ILE:CG2 | 3:F:3096[A]:VAL:CG2 | 2.87 | 0.52 |
| 3:F:3151[B]:LEU:O | 3:a:3154[B]:PRO:HB3 | 2.09 | 0.52 |
| 3:F:3153[B]:LYS:CB | 3:a:3155[B]:MET:CA | 2.73 | 0.52 |
| 3:F:3157[B]:PRO:C | 3:a:3150[B]:LYS:HE2 | 2.29 | 0.52 |
| 3:F:3158[B]:PHE:HB2 | 3:a:3153[B]:LYS:CB | 2.39 | 0.52 |
| 3:F:3228[B]:VAL:HG23 | 3:F:3228[B]:VAL:O | 2.10 | 0.52 |
| 1:G:387:ASN:OD1 | 1:G:387:ASN:N | 2.40 | 0.52 |
| 1:G:1286:ARG:HG3 | 1:G:1337:ARG:NH2 | 2.25 | 0.52 |
| 2:H:2811:HIS:HB3 | 2:H:2847:HIS:HD2 | 1.75 | 0.52 |
| 3:I:3028[A]:PRO:HG2 | 3:I:3029[A]:LYS:CG | 2.40 | 0.52 |
| 3:I:3047[A]:ARG:HH21 | 3:I:3113[A]:ASP:CG | 2.16 | 0.52 |
| 3:I:3110[B]:THR:C | 3:I:3112[B]:TYR:N | 2.68 | 0.52 |
| 1:J:95:THR:O | 1:J:153:ASN:ND2 | 2.43 | 0.52 |
| 1:J:217:PHE:O | 1:J:220:TRP:HB3 | 2.10 | 0.52 |
| 1:J:695:TYR:H | 1:J:695:TYR:HD1 | 1.56 | 0.52 |
| 1:J:729:VAL:HG11 | 1:J:785:LEU:HD12 | 1.92 | 0.52 |
| 1:J:1018:ILE:HA | 1:J:1021:LEU:HB2 | 1.91 | 0.52 |
| 1:J:1182:ASN:O | 1:J:1182:ASN:ND2 | 2.43 | 0.52 |
| 2:K:2413:VAL:O | 2:K:2454:MET:HE1 | 2.09 | 0.52 |
| 2:K:2571:ARG:NH1 | 2:K:2771:TYR:HB3 | 2.25 | 0.52 |
| 3:L:2945[A]:VAL:HG22 | 3:L:2954[A]:TYR:HB2 | 1.91 | 0.52 |
| 3:L:2949[A]:LYS:C | 3:L:2953[A]:GLY:H | 2.17 | 0.52 |
| 3:L:2961[B]:HIS:HB3 | 3:L:3111[B]:SER:HB3 | 1.91 | 0.52 |
| 3:L:3096[B]:VAL:HG11 | 3:L:3115[B]:LEU:HD12 | 1.89 | 0.52 |
| 2:N:2394:VAL:HG11 | 2:N:2451:LEU:HD12 | 1.90 | 0.52 |
| 3:O:2945[A]:VAL:HG22 | 3:O:2954[A]:TYR:HB2 | 1.91 | 0.52 |
| 3:O:2954[A]:TYR:CD2 | 3:O:2954[A]:TYR:C | 2.86 | 0.52 |
| 3:O:2970[B]:PRO:O | 3:X:2989[B]:HIS:HB2 | 2.10 | 0.52 |
| 3:O:3110[A]:THR:C | 3:O:3112[A]:TYR:N | 2.68 | 0.52 |
| 3:O:3307[B]:PHE:HE1 | 3:O:3309[B]:PRO:CG | 2.08 | 0.52 |
| 1:P:724:LYS:HA | 1:P:728:ARG:NH1 | 2.25 | 0.52 |
| 1:P:1166:THR:HB | 1:P:1167:ASP:C | 2.35 | 0.52 |
| 2:Q:2692:LYS:HE2 | 2:Q:2700:PHE:HE2 | 1.74 | 0.52 |
| 2:Q:2800:LYS:O | 3:R:3023[A]:ILE:HD13 | 2.02 | 0.52 |
| 3:R:2933[A]:SER:CB | 3:R:2936[A]:GLU:CB | 2.86 | 0.52 |
| 3:R:3081[B]:PHE:CD1 | 3:R:3081[B]:PHE:C | 2.87 | 0.52 |
| 3:R:3110[B]:THR:O | 3:R:3111[B]:SER:C | 2.52 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3139[B]:LEU:CD2 | 3:R:3139[B]:LEU:N | 2.73 | 0.52 |
| 3:R:3300[B]:LEU:N | 3:R:3300[B]:LEU:CD2 | 2.73 | 0.52 |
| 1:S:142:ARG:O | 1:S:145:GLN:NE2 | 2.42 | 0.52 |
| 3:U:3066[B]:TYR:CE1 | 3:U:3193[B]:HIS:CE1 | 2.98 | 0.52 |
| 3:X:2933[A]:SER:CB | 3:X:2936[A]:GLU:CB | 2.85 | 0.52 |
| 3:X:3014[A]:TRP:CZ3 | 3:X:3119[A]:HIS:ND1 | 2.77 | 0.52 |
| 3:X:3038[A]:ILE:HG23 | 3:X:3040[A]:VAL:HG22 | 1.90 | 0.52 |
| 3:X:3110[A]:THR:O | 3:X:3111[A]:SER:C | 2.53 | 0.52 |
| 3:X:3115[A]:LEU:HD22 | 3:X:3115[A]:LEU:O | 2.10 | 0.52 |
| 3:X:3115[B]:LEU:O | 3:X:3115[B]:LEU:HD22 | 2.10 | 0.52 |
| 1:Y:865:LYS:HG3 | 1:Y:871:GLN:HG3 | 1.92 | 0.52 |
| 3:a:2937[B]:ASN:ND2 | 3:a:3006[B]:LYS:CD | 2.73 | 0.52 |
| 3:a:3013[B]:ASP:OD1 | 3:a:3015[B]:THR:OG1 | 2.23 | 0.52 |
| 3:a:3115[B]:LEU:HD22 | 3:a:3115[B]:LEU:O | 2.10 | 0.52 |
| 3:a:3135[A]:LYS:HG3 | 3:a:3141[A]:TYR:CD1 | 2.33 | 0.52 |
| 3:a:3176[A]:LYS:NZ | 3:a:3176[A]:LYS:CB | 2.73 | 0.52 |
| 3:a:3287[B]:ILE:O | 3:a:3287[B]:ILE:HG23 | 2.10 | 0.52 |
| 2:c:2496:LEU:HB3 | 2:c:2498:VAL:HG22 | 1.91 | 0.52 |
| 3:d:2935[B]:ILE:CD1 | 3:d:2936[B]:GLU:N | 2.73 | 0.52 |
| 3:d:3014[A]:TRP:CZ3 | 3:d:3119[A]:HIS:ND1 | 2.77 | 0.52 |
| 3:d:3115[B]:LEU:HD22 | 3:d:3115[B]:LEU:O | 2.10 | 0.52 |
| 3:d:3228[A]:VAL:O | 3:d:3228[A]:VAL:HG23 | 2.10 | 0.52 |
| 1:A:1017:HIS:O | 1:A:1021:LEU:HG | 2.08 | 0.52 |
| 3:C:2935[A]:ILE:CD1 | 3:C:2936[A]:GLU:N | 2.73 | 0.52 |
| 3:C:2966[B]:SER:O | 3:L:2981[B]:GLY:C | 2.53 | 0.52 |
| 3:C:3092[B]:ILE:CG2 | 3:C:3096[B]:VAL:CG2 | 2.88 | 0.52 |
| 3:C:3139[A]:LEU:CD2 | 3:C:3139[A]:LEU:N | 2.73 | 0.52 |
| 3:C:3230[B]:PHE:H | 3:C:3243[B]:GLY:CA | 2.22 | 0.52 |
| 3:C:3269[B]:SER:O | 3:C:3272[B]:HIS:HB2 | 2.09 | 0.52 |
| 3:C:3287[B]:ILE:O | 3:C:3287[B]:ILE:HG23 | 2.10 | 0.52 |
| 1:D:109:LEU:HD21 | 2:H:2635:TYR:HB2 | 1.91 | 0.52 |
| 1:D:972:SER:HA | 1:D:1028:VAL:HG22 | 1.92 | 0.52 |
| 3:F:2935[B]:ILE:CD1 | 3:F:2935[B]:ILE:N | 2.73 | 0.52 |
| 3:F:2969[A]:TYR:CE2 | 3:F:2970[A]:PRO:CG | 2.86 | 0.52 |
| 1:G:125:SER:OG | 1:G:127:GLU:OE2 | 2.27 | 0.52 |
| 1:G:481:ILE:HD12 | 1:G:668:MET:HE1 | 1.92 | 0.52 |
| 1:G:1299:GLN:HB2 | 1:G:1311:CYS:SG | 2.50 | 0.52 |
| 3:I:3115[B]:LEU:HD22 | 3:I:3115[B]:LEU:O | 2.10 | 0.52 |
| 3:I:3132[A]:ALA:CB | 3:I:3197[A]:ILE:CD1 | 2.86 | 0.52 |
| 3:I:3160[B]:SER:CB | 3:R:2982[B]:MET:CB | 2.88 | 0.52 |
| 3:I:3176[B]:LYS:NZ | 3:I:3176[B]:LYS:CB | 2.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3269[A]:SER:O | 3:I:3272[A]:HIS:HB2 | 2.09 | 0.52 |
| 3:I:3275[B]:LEU:N | 3:I:3275[B]:LEU:CD1 | 2.73 | 0.52 |
| 1:J:980:TYR:HE1 | 1:J:1021:LEU:HD13 | 1.74 | 0.52 |
| 2:K:2172:ILE:HG13 | 2:K:2173:VAL:HG13 | 1.92 | 0.52 |
| 3:L:2949[B]:LYS:C | 3:L:2953[B]:GLY:H | 2.17 | 0.52 |
| 3:L:2952[A]:ALA:CB | 3:L:2956[A]:LYS:HB3 | 2.40 | 0.52 |
| 3:L:3028[A]:PRO:HG2 | 3:L:3029[A]:LYS:CG | 2.40 | 0.52 |
| 3:L:3028[B]:PRO:HG2 | 3:L:3029[B]:LYS:CG | 2.40 | 0.52 |
| 3:L:3269[B]:SER:O | 3:L:3272[B]:HIS:HB2 | 2.09 | 0.52 |
| 3:L:3293[B]:LYS:CG | 3:L:3294[B]:SER:HB2 | 2.36 | 0.52 |
| 1:M:1583:CYS:SG | 1:M:1584:GLY:N | 2.80 | 0.52 |
| 3:O:2935[B]:ILE:CD1 | 3:O:2936[B]:GLU:N | 2.73 | 0.52 |
| 3:O:3047[A]:ARG:HH21 | 3:O:3113[A]:ASP:CG | 2.16 | 0.52 |
| 3:O:3081[B]:PHE:C | 3:O:3081[B]:PHE:CD1 | 2.87 | 0.52 |
| 3:O:3113[A]:ASP:O | 3:O:3114[A]:PRO:C | 2.53 | 0.52 |
| 1:P:468:CYS:SG | 1:P:669:LYS:HB3 | 2.50 | 0.52 |
| 3:R:2937[A]:ASN:ND2 | 3:R:3006[A]:LYS:CD | 2.73 | 0.52 |
| 3:R:3014[A]:TRP:CZ3 | 3:R:3119[A]:HIS:ND1 | 2.77 | 0.52 |
| 3:R:3139[A]:LEU:CD2 | 3:R:3139[A]:LEU:N | 2.73 | 0.52 |
| 3:R:3147[B]:GLU:CB | 3:R:3149[B]:ASN:ND2 | 2.73 | 0.52 |
| 3:R:3176[B]:LYS:NZ | 3:R:3176[B]:LYS:CB | 2.73 | 0.52 |
| 3:R:3228[B]:VAL:CG2 | 3:R:3245[B]:PHE:CE2 | 2.89 | 0.52 |
| 3:R:3300[A]:LEU:N | 3:R:3300[A]:LEU:CD2 | 2.73 | 0.52 |
| 2:T:2403:PHE:CZ | 2:T:2480:LEU:HD21 | 2.45 | 0.52 |
| 3:U:2949[A]:LYS:C | 3:U:2953[A]:GLY:H | 2.17 | 0.52 |
| 3:U:2969[B]:TYR:HB2 | 3:d:3256[B]:TRP:HE1 | 1.74 | 0.52 |
| 3:U:3275[A]:LEU:N | 3:U:3275[A]:LEU:CD1 | 2.73 | 0.52 |
| 1:V:563:ILE:HG22 | 1:V:565:GLU:HG3 | 1.91 | 0.52 |
| 2:W:2627:GLY:HA3 | 2:W:2703:PHE:O | 2.09 | 0.52 |
| 3:X:2935[B]:ILE:CD1 | 3:X:2936[B]:GLU:N | 2.73 | 0.52 |
| 3:X:2952[A]:ALA:CA | 3:X:2956[A]:LYS:HB3 | 2.38 | 0.52 |
| 3:X:3028[A]:PRO:HG2 | 3:X:3029[A]:LYS:CG | 2.40 | 0.52 |
| 3:X:3096[A]:VAL:HG11 | 3:X:3115[A]:LEU:HD12 | 1.89 | 0.52 |
| 3:X:3287[B]:ILE:O | 3:X:3287[B]:ILE:HG23 | 2.10 | 0.52 |
| 3:X:3300[B]:LEU:N | 3:X:3300[B]:LEU:CD2 | 2.73 | 0.52 |
| 1:Y:904:HIS:HB3 | 1:Y:1105:VAL:HG21 | 1.91 | 0.52 |
| 1:Y:904:HIS:O | 1:Y:907:ARG:HB3 | 2.10 | 0.52 |
| 1:Y:914:GLU:OE1 | 1:Y:926:LEU:N | 2.39 | 0.52 |
| 1:Y:1000:GLU:HG2 | 1:Y:1133:ILE:HG23 | 1.91 | 0.52 |
| 1:Y:1301:PRO:HA | 1:Y:1308:VAL:HA | 1.92 | 0.52 |
| 2:Z:2595:TRP:HE1 | 2:Z:2710:HIS:HD2 | 1.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:450:LYS:NZ | 1:b:1273:SER:OG | 2.43 | 0.52 |
| 1:b:745:ASP:OD1 | 1:b:759:SER:OG | 2.25 | 0.52 |
| 1:b:1310:THR:HG23 | 1:b:1597:THR:HG23 | 1.90 | 0.52 |
| 3:d:2937[B]:ASN:ND2 | 3:d:3006[B]:LYS:CD | 2.73 | 0.52 |
| 3:d:2952[A]:ALA:HB3 | 3:d:2954[A]:TYR:N | 2.17 | 0.52 |
| 3:d:2952[A]:ALA:CB | 3:d:2956[A]:LYS:HB3 | 2.40 | 0.52 |
| 3:d:3196[B]:THR:CA | 3:d:3199[B]:GLN:OE1 | 2.58 | 0.52 |
| 4:RA:1:NAG:O3 | 4:RA:2:NAG:O5 | 2.23 | 0.52 |
| 1:A:198:GLU:OE1 | 1:A:198:GLU:N | 2.36 | 0.52 |
| 1:A:996:ILE:HG23 | 1:A:1133:ILE:HG22 | 1.90 | 0.52 |
| 1:A:1414:THR:HG23 | 1:A:1477:LEU:HD13 | 1.91 | 0.52 |
| 2:B:2521:MET:HE3 | 2:B:2605:LEU:HD12 | 1.91 | 0.52 |
| 3:C:2935[B]:ILE:CD1 | 3:C:2936[B]:GLU:N | 2.73 | 0.52 |
| 3:C:2965[B]:LEU:CD2 | 3:L:3253[B]:GLU:CG | 2.79 | 0.52 |
| 3:C:3028[B]:PRO:HG2 | 3:C:3029[B]:LYS:CG | 2.40 | 0.52 |
| 3:C:3256[B]:TRP:CE2 | 3:L:2965[B]:LEU:CA | 2.93 | 0.52 |
| 3:C:3275[B]:LEU:N | 3:C:3275[B]:LEU:CD1 | 2.73 | 0.52 |
| 3:C:3284[B]:LYS:CE | 3:C:3284[B]:LYS:CA | 2.85 | 0.52 |
| 3:C:3285[B]:VAL:CG2 | 3:C:3286[B]:THR:N | 2.73 | 0.52 |
| 3:C:3287[A]:ILE:O | 3:C:3287[A]:ILE:HG23 | 2.09 | 0.52 |
| 3:C:3300[A]:LEU:N | 3:C:3300[A]:LEU:CD2 | 2.73 | 0.52 |
| 3:C:3300[B]:LEU:N | 3:C:3300[B]:LEU:CD2 | 2.73 | 0.52 |
| 1:D:439:LEU:HD23 | 1:D:509:ILE:HD12 | 1.91 | 0.52 |
| 1:D:1582:ASN:ND2 | 1:D:1627:ARG:HE | 2.07 | 0.52 |
| 2:E:2181:THR:HB | 2:E:2374:ASN:H | 1.73 | 0.52 |
| 3:F:2952[A]:ALA:CA | 3:F:2956[A]:LYS:HB3 | 2.38 | 0.52 |
| 3:F:3147[A]:GLU:CB | 3:F:3149[A]:ASN:ND2 | 2.73 | 0.52 |
| 3:F:3162[B]:ASP:CB | 3:a:3259[B]:ASP:H | 2.22 | 0.52 |
| 3:F:3196[A]:THR:CA | 3:F:3199[A]:GLN:OE1 | 2.58 | 0.52 |
| 3:F:3228[A]:VAL:O | 3:F:3228[A]:VAL:HG23 | 2.10 | 0.52 |
| 3:F:3230[B]:PHE:H | 3:F:3243[B]:GLY:CA | 2.22 | 0.52 |
| 3:F:3253[B]:GLU:N | 3:a:3252[B]:TYR:HB2 | 2.24 | 0.52 |
| 1:G:237:LEU:HB2 | 1:G:820:VAL:HB | 1.92 | 0.52 |
| 3:I:2989[B]:HIS:CD2 | 3:R:2970[B]:PRO:CB | 2.92 | 0.52 |
| 3:I:3081[B]:PHE:C | 3:I:3081[B]:PHE:CD1 | 2.87 | 0.52 |
| 3:I:3110[A]:THR:C | 3:I:3112[A]:TYR:N | 2.68 | 0.52 |
| 3:I:3139[A]:LEU:CD2 | 3:I:3139[A]:LEU:N | 2.73 | 0.52 |
| 3:I:3147[B]:GLU:CB | 3:I:3149[B]:ASN:ND2 | 2.73 | 0.52 |
| 3:I:3284[A]:LYS:CE | 3:I:3284[A]:LYS:CA | 2.85 | 0.52 |
| 1:J:121:ASN:HD22 | 1:J:124:TYR:H | 1.57 | 0.52 |
| 1:J:1441:SER:OG | 1:J:1442:MET:N | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3092[A]:ILE:CG2 | 3:L:3096[A]:VAL:CG2 | 2.88 | 0.52 |
| 3:L:3114[A]:PRO:CD | 3:L:3115[A]:LEU:N | 2.72 | 0.52 |
| 3:L:3147[A]:GLU:CD | 3:L:3149[A]:ASN:HD21 | 2.17 | 0.52 |
| 3:L:3219[B]:LEU:N | 3:L:3219[B]:LEU:CD2 | 2.73 | 0.52 |
| 3:L:3228[B]:VAL:O | 3:L:3228[B]:VAL:HG23 | 2.10 | 0.52 |
| 1:M:873:VAL:HA | 1:M:876:PHE:CD1 | 2.45 | 0.52 |
| 1:M:965:ASP:N | 1:M:966:SER:HA | 2.24 | 0.52 |
| 2:N:2179:ASP:HA | 2:N:2300:ASN:ND2 | 2.24 | 0.52 |
| 2:N:2180:TRP:HB3 | 2:N:2184:MET:HE2 | 1.90 | 0.52 |
| 3:O:2933[B]:SER:CB | 3:O:2936[B]:GLU:CB | 2.85 | 0.52 |
| 3:O:2952[A]:ALA:CB | 3:O:2956[A]:LYS:HB3 | 2.40 | 0.52 |
| 3:O:2961[A]:HIS:HB3 | 3:O:3111[A]:SER:HB3 | 1.92 | 0.52 |
| 3:O:3147[A]:GLU:CD | 3:O:3149[A]:ASN:HD21 | 2.17 | 0.52 |
| 3:O:3153[B]:LYS:CG | 3:X:3176[B]:LYS:HZ1 | 2.22 | 0.52 |
| 3:O:3176[A]:LYS:NZ | 3:O:3176[A]:LYS:CB | 2.73 | 0.52 |
| 3:O:3285[A]:VAL:CG2 | 3:O:3286[A]:THR:N | 2.73 | 0.52 |
| 1:S:110:PHE:N | 1:S:119:LYS:O | 2.37 | 0.52 |
| 1:S:972:SER:HA | 1:S:1028:VAL:HG22 | 1.92 | 0.52 |
| 1:S:1181:GLU:CD | 1:S:1181:GLU:H | 2.17 | 0.52 |
| 2:T:2394:VAL:HG11 | 2:T:2451:LEU:HD12 | 1.91 | 0.52 |
| 2:T:2825:ILE:HG22 | 2:T:2863:ARG:NH2 | 2.24 | 0.52 |
| 3:U:2952[B]:ALA:CB | 3:U:2956[B]:LYS:HB3 | 2.40 | 0.52 |
| 3:U:2961[A]:HIS:HB3 | 3:U:3111[A]:SER:HB3 | 1.92 | 0.52 |
| 3:U:3170[B]:ALA:O | 3:d:3148[B]:ILE:HG22 | 2.09 | 0.52 |
| 3:U:3183[B]:LEU:N | 3:U:3184[B]:ASN:HA | 2.12 | 0.52 |
| 1:V:22:LEU:HD12 | 1:V:25:MET:HG2 | 1.92 | 0.52 |
| 1:V:945:ALA:O | 1:V:957:ASN:ND2 | 2.43 | 0.52 |
| 1:V:993:ASN:OD1 | 1:V:1136:ARG:NH2 | 2.23 | 0.52 |
| 3:X:2952[B]:ALA:CB | 3:X:2956[B]:LYS:HB3 | 2.40 | 0.52 |
| 1:Y:1470:GLU:OE2 | 1:Y:1473:ARG:NH1 | 2.43 | 0.52 |
| 3:a:2961[B]:HIS:HB3 | 3:a:3111[B]:SER:HB3 | 1.92 | 0.52 |
| 2:c:2579:GLU:HG2 | 2:c:2758:THR:HG21 | 1.91 | 0.52 |
| 3:d:2949[B]:LYS:C | 3:d:2949[B]:LYS:HZ3 | 2.10 | 0.52 |
| 3:d:2951[A]:ASP:O | 3:d:2956[A]:LYS:HE2 | 2.09 | 0.52 |
| 3:d:2957[A]:ILE:HA | 3:d:2960[A]:PHE:HE1 | 1.64 | 0.52 |
| 3:d:3028[A]:PRO:HG2 | 3:d:3029[A]:LYS:CG | 2.40 | 0.52 |
| 3:d:3081[A]:PHE:C | 3:d:3081[A]:PHE:CD1 | 2.87 | 0.52 |
| 3:d:3092[A]:ILE:CG2 | 3:d:3096[A]:VAL:CG2 | 2.88 | 0.52 |
| 3:d:3264[B]:TYR:C | 3:d:3264[B]:TYR:CD1 | 2.86 | 0.52 |
| 1:A:885:SER:HB2 | 1:A:886:PRO:HA | 1.91 | 0.52 |
| 1:A:973:ARG:O | 1:A:1028:VAL:HG13 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2935[A]:ILE:CD1 | 3:C:2935[A]:ILE:N | 2.73 | 0.52 |
| 3:C:3113[B]:ASP:O | 3:C:3114[B]:PRO:C | 2.53 | 0.52 |
| 3:C:3115[B]:LEU:HD22 | 3:C:3115[B]:LEU:O | 2.10 | 0.52 |
| 3:C:3147[B]:GLU:CB | 3:C:3149[B]:ASN:ND2 | 2.73 | 0.52 |
| 1:D:1470:GLU:HB3 | 1:D:1537:ILE:CD1 | 2.40 | 0.52 |
| 1:D:1604:ASP:OD1 | 1:D:1605:ARG:NH1 | 2.43 | 0.52 |
| 2:E:2156:ARG:HD2 | 2:E:2357:VAL:HG12 | 1.91 | 0.52 |
| 2:E:2509:ILE:HD11 | 2:E:2605:LEU:HD23 | 1.92 | 0.52 |
| 2:E:2568:HIS:HD2 | 2:E:2718:TRP:CH2 | 2.28 | 0.52 |
| 3:F:3028[A]:PRO:HG2 | 3:F:3029[A]:LYS:CG | 2.40 | 0.52 |
| 3:F:3042[A]:ASP:N | 3:F:3042[A]:ASP:OD2 | 2.41 | 0.52 |
| 3:F:3291[A]:ASP:OD2 | 3:F:3293[A]:LYS:NZ | 2.43 | 0.52 |
| 1:G:564:ASP:HB3 | 1:G:610:THR:HA | 1.92 | 0.52 |
| 3:I:2949[A]:LYS:C | 3:I:2953[A]:GLY:H | 2.17 | 0.52 |
| 3:I:2952[A]:ALA:HB3 | 3:I:2954[A]:TYR:N | 2.17 | 0.52 |
| 3:I:3014[B]:TRP:CZ3 | 3:I:3119[B]:HIS:ND1 | 2.77 | 0.52 |
| 3:I:3028[B]:PRO:HG2 | 3:I:3029[B]:LYS:CG | 2.40 | 0.52 |
| 3:I:3110[B]:THR:O | 3:I:3111[B]:SER:C | 2.53 | 0.52 |
| 3:I:3254[B]:MET:HE2 | 3:R:3157[B]:PRO:HD3 | 1.92 | 0.52 |
| 2:K:2800:LYS:HB3 | 3:L:3023[A]:ILE:CD1 | 2.39 | 0.52 |
| 3:L:2952[B]:ALA:N | 3:L:2953[B]:GLY:HA2 | 2.06 | 0.52 |
| 3:L:2952[B]:ALA:CA | 3:L:2956[B]:LYS:HB3 | 2.38 | 0.52 |
| 3:L:3019[A]:HIS:CD2 | 3:L:3019[A]:HIS:N | 2.75 | 0.52 |
| 3:L:3139[A]:LEU:CD2 | 3:L:3139[A]:LEU:N | 2.73 | 0.52 |
| 3:L:3147[A]:GLU:CB | 3:L:3149[A]:ASN:ND2 | 2.73 | 0.52 |
| 1:M:293:LEU:O | 1:M:296:ARG:HG2 | 2.10 | 0.52 |
| 1:M:480:CYS:SG | 1:M:621:LEU:HD11 | 2.49 | 0.52 |
| 1:M:885:SER:HB3 | 1:M:886:PRO:HA | 1.92 | 0.52 |
| 3:O:2935[B]:ILE:CD1 | 3:O:2935[B]:ILE:N | 2.73 | 0.52 |
| 3:O:2952[A]:ALA:HB3 | 3:O:2954[A]:TYR:N | 2.17 | 0.52 |
| 3:O:2975[B]:PHE:CD1 | 3:X:3158[B]:PHE:N | 2.60 | 0.52 |
| 3:O:3102[B]:TYR:HA | 3:X:2971[B]:ASP:HA | 1.86 | 0.52 |
| 1:P:11:THR:HG22 | 1:P:13:ASP:H | 1.75 | 0.52 |
| 1:P:517:THR:HG21 | 1:P:708:PHE:HE1 | 1.74 | 0.52 |
| 3:R:3115[A]:LEU:O | 3:R:3115[A]:LEU:HD22 | 2.10 | 0.52 |
| 3:R:3147[A]:GLU:CG | 3:R:3149[A]:ASN:ND2 | 2.73 | 0.52 |
| 3:R:3307[B]:PHE:HE1 | 3:R:3309[B]:PRO:CG | 2.08 | 0.52 |
| 1:S:954:ALA:O | 1:S:956:PRO:HD3 | 2.09 | 0.52 |
| 2:T:2606:LEU:HD21 | 2:T:2709:VAL:HG21 | 1.92 | 0.52 |
| 3:U:3028[A]:PRO:HG2 | 3:U:3029[A]:LYS:CG | 2.40 | 0.52 |
| 3:U:3028[B]:PRO:HG2 | 3:U:3029[B]:LYS:CG | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3220[B]:ARG:HG3 | 3:d:2974[B]:ALA:H | 1.73 | 0.52 |
| 1:V:929:TRP:O | 1:V:1048:ASN:ND2 | 2.43 | 0.52 |
| 3:X:3176[A]:LYS:N | 3:X:3176[A]:LYS:CE | 2.73 | 0.52 |
| 3:X:3176[B]:LYS:NZ | 3:X:3176[B]:LYS:CB | 2.73 | 0.52 |
| 3:X:3219[B]:LEU:N | 3:X:3219[B]:LEU:CD2 | 2.73 | 0.52 |
| 3:X:3269[B]:SER:O | 3:X:3272[B]:HIS:HB2 | 2.09 | 0.52 |
| 1:Y:1621:ASN:HA | 3:d:3188[B]:ASP:HB2 | 1.90 | 0.52 |
| 2:Z:2359:ASN:OD1 | 2:Z:2359:ASN:N | 2.43 | 0.52 |
| 3:a:2952[A]:ALA:CB | 3:a:2956[A]:LYS:HB3 | 2.40 | 0.52 |
| 3:a:3132[A]:ALA:HB1 | 3:a:3197[A]:ILE:HD13 | 1.89 | 0.52 |
| 3:a:3220[A]:ARG:HH11 | 3:a:3220[A]:ARG:CG | 2.12 | 0.52 |
| 3:a:3264[B]:TYR:C | 3:a:3264[B]:TYR:CD1 | 2.86 | 0.52 |
| 2:c:2394:VAL:HA | 2:c:2488:ARG:HA | 1.92 | 0.52 |
| 3:d:2960[A]:PHE:CD2 | 3:d:3157[A]:PRO:CG | 2.74 | 0.52 |
| 3:d:3300[B]:LEU:N | 3:d:3300[B]:LEU:CD2 | 2.73 | 0.52 |
| 1:A:941:LEU:HD11 | 1:A:959:PHE:HD2 | 1.75 | 0.51 |
| 3:C:3092[A]:ILE:CG2 | 3:C:3096[A]:VAL:CG2 | 2.88 | 0.51 |
| 3:C:3114[B]:PRO:CD | 3:C:3115[B]:LEU:N | 2.72 | 0.51 |
| 3:C:3147[B]:GLU:OE2 | 3:L:3163[B]:ASN:O | 2.27 | 0.51 |
| 3:C:3154[B]:PRO:N | 3:L:3155[B]:MET:HG3 | 2.17 | 0.51 |
| 2:E:2808:PHE:CE2 | 2:E:2899:PRO:HG3 | 2.45 | 0.51 |
| 3:F:2935[A]:ILE:CD1 | 3:F:2935[A]:ILE:N | 2.73 | 0.51 |
| 3:F:2954[A]:TYR:CD2 | 3:F:2954[A]:TYR:C | 2.86 | 0.51 |
| 3:F:2971[B]:ASP:O | 3:a:3248[B]:LEU:HD22 | 2.10 | 0.51 |
| 3:F:3066[B]:TYR:CE1 | 3:F:3193[B]:HIS:CE1 | 2.98 | 0.51 |
| 3:F:3147[A]:GLU:CD | 3:F:3149[A]:ASN:HD21 | 2.17 | 0.51 |
| 3:F:3147[B]:GLU:CB | 3:F:3149[B]:ASN:ND2 | 2.73 | 0.51 |
| 3:F:3153[B]:LYS:HZ1 | 3:a:3158[B]:PHE:H | 1.58 | 0.51 |
| 3:F:3162[B]:ASP:HB3 | 3:a:3259[B]:ASP:H | 1.75 | 0.51 |
| 3:F:3176[B]:LYS:N | 3:F:3176[B]:LYS:CE | 2.73 | 0.51 |
| 3:F:3252[B]:TYR:CE1 | 3:a:3251[B]:ASP:CG | 2.67 | 0.51 |
| 1:G:22:LEU:HD12 | 1:G:25:MET:HG2 | 1.92 | 0.51 |
| 1:G:1072:CYS:HA | 2:K:2902:ILE:HG22 | 1.92 | 0.51 |
| 2:H:2161:GLN:NE2 | 2:H:2345:ASN:OD1 | 2.43 | 0.51 |
| 3:I:3139[B]:LEU:CD2 | 3:I:3139[B]:LEU:N | 2.73 | 0.51 |
| 3:I:3147[A]:GLU:CB | 3:I:3149[A]:ASN:ND2 | 2.73 | 0.51 |
| 3:I:3147[B]:GLU:CG | 3:I:3149[B]:ASN:ND2 | 2.73 | 0.51 |
| 3:I:3196[A]:THR:HG1 | 1:J:416:ASN:ND2 | 2.07 | 0.51 |
| 3:I:3196[B]:THR:CA | 3:I:3199[B]:GLN:OE1 | 2.58 | 0.51 |
| 3:I:3275[A]:LEU:N | 3:I:3275[A]:LEU:CD1 | 2.73 | 0.51 |
| 1:J:61:GLY:HA2 | 1:J:354:PHE:CE1 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:473:ALA:HB3 | 1:M:1639:LYS:HE3 | 1.92 | 0.51 |
| 1:J:1046:HIS:HA | 1:J:1049:VAL:HB | 1.92 | 0.51 |
| 2:K:2512:LEU:HD11 | 2:K:2591:PRO:HG3 | 1.91 | 0.51 |
| 2:K:2551:PRO:HD3 | 2:K:2751:TRP:CH2 | 2.45 | 0.51 |
| 3:L:2951[B]:ASP:O | 3:L:2956[B]:LYS:HE2 | 2.10 | 0.51 |
| 3:L:2988[B]:TRP:HE3 | 3:L:2989[B]:HIS:CE1 | 2.25 | 0.51 |
| 3:L:3101[A]:PRO:HG2 | 3:L:3102[A]:TYR:CD1 | 2.46 | 0.51 |
| 3:L:3176[A]:LYS:H | 3:L:3176[A]:LYS:CE | 2.17 | 0.51 |
| 3:L:3230[A]:PHE:H | 3:L:3243[A]:GLY:CA | 2.22 | 0.51 |
| 1:M:1262:ASN:OD1 | 1:M:1263:LEU:N | 2.43 | 0.51 |
| 1:M:1315:GLY:HA3 | 1:M:1601:TRP:CB | 2.40 | 0.51 |
| 1:M:1427:HIS:CE1 | 1:M:1457:HIS:CE1 | 2.98 | 0.51 |
| 1:M:1458:HIS:NE2 | 9:M:2105:CUO:O1 | 2.43 | 0.51 |
| 1:M:1493:MET:HG2 | 1:M:1511:SER:O | 2.10 | 0.51 |
| 2:N:2128:LEU:HD13 | 2:N:2286:HIS:CG | 2.45 | 0.51 |
| 3:O:3092[B]:ILE:CG2 | 3:O:3096[B]:VAL:CG2 | 2.88 | 0.51 |
| 3:O:3101[A]:PRO:HG2 | 3:O:3102[A]:TYR:CD1 | 2.46 | 0.51 |
| 3:O:3147[B]:GLU:CB | 3:O:3149[B]:ASN:ND2 | 2.73 | 0.51 |
| 1:P:37:ILE:HD13 | 1:P:75:GLN:HG3 | 1.91 | 0.51 |
| 3:R:2935[A]:ILE:CD1 | 3:R:2936[A]:GLU:N | 2.73 | 0.51 |
| 3:R:3219[B]:LEU:N | 3:R:3219[B]:LEU:CD2 | 2.73 | 0.51 |
| 1:S:419:THR:O | 1:S:1062:PHE:HE1 | 1.93 | 0.51 |
| 1:S:928:TYR:HB2 | 1:S:1048:ASN:HB2 | 1.91 | 0.51 |
| 3:U:2935[B]:ILE:CD1 | 3:U:2936[B]:GLU:N | 2.73 | 0.51 |
| 3:U:2969[B]:TYR:OH | 3:d:2980[B]:HIS:CE1 | 2.63 | 0.51 |
| 3:U:2980[B]:HIS:CB | 3:d:2969[B]:TYR:CZ | 2.92 | 0.51 |
| 3:U:3254[B]:MET:HE2 | 3:d:2975[B]:PHE:CE2 | 2.46 | 0.51 |
| 3:U:3285[A]:VAL:CG2 | 3:U:3286[A]:THR:N | 2.73 | 0.51 |
| 1:V:1411:PHE:O | 1:V:1475:ARG:NH2 | 2.41 | 0.51 |
| 1:V:1421:VAL:HG23 | 1:V:1422:HIS:HD1 | 1.75 | 0.51 |
| 2:W:2567:MET:HE3 | 2:W:2718:TRP:HB2 | 1.92 | 0.51 |
| 3:X:3101[B]:PRO:HG2 | 3:X:3102[B]:TYR:CD1 | 2.46 | 0.51 |
| 3:X:3139[B]:LEU:CD2 | 3:X:3139[B]:LEU:N | 2.73 | 0.51 |
| 1:Y:422:LEU:HD13 | 1:Y:696:GLN:HG2 | 1.90 | 0.51 |
| 1:Y:1613:ASP:OD1 | 3:d:3185[B]:TYR:HA | 2.09 | 0.51 |
| 2:Z:2605:LEU:O | 2:Z:2622:ASN:ND2 | 2.40 | 0.51 |
| 3:a:2949[A]:LYS:C | 3:a:2953[A]:GLY:H | 2.17 | 0.51 |
| 3:a:3028[B]:PRO:HG2 | 3:a:3029[B]:LYS:CG | 2.40 | 0.51 |
| 3:a:3101[A]:PRO:HG2 | 3:a:3102[A]:TYR:CD1 | 2.45 | 0.51 |
| 3:a:3287[A]:ILE:O | 3:a:3287[A]:ILE:HG23 | 2.09 | 0.51 |
| 1:b:346:GLY:O | 1:b:349:GLU:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:1166:THR:HB | 1:b:1168:GLN:N | 2.25 | 0.51 |
| 4:7:1:NAG:C6 | 4:7:2:NAG:N2 | 2.73 | 0.51 |
| 4:MA:1:NAG:C6 | 4:MA:2:NAG:C1 | 2.86 | 0.51 |
| 1:A:329:ARG:O | 1:b:1583:CYS:N | 2.43 | 0.51 |
| 2:B:2168:ARG:NH2 | 2:E:2515:ARG:HD2 | 2.26 | 0.51 |
| 3:C:2952[A]:ALA:CB | 3:C:2956[A]:LYS:HB3 | 2.40 | 0.51 |
| 3:C:3096[A]:VAL:HG11 | 3:C:3115[A]:LEU:HD12 | 1.89 | 0.51 |
| 2:E:2234:GLN:HG3 | 2:E:2235:PRO:HD2 | 1.91 | 0.51 |
| 2:E:2265:ILE:HD11 | 2:E:2400:LEU:CD1 | 2.40 | 0.51 |
| 3:F:2937[B]:ASN:ND2 | 3:F:3006[B]:LYS:CD | 2.73 | 0.51 |
| 3:F:3092[B]:ILE:CG2 | 3:F:3096[B]:VAL:CG2 | 2.88 | 0.51 |
| 3:F:3159[B]:SER:CB | 3:a:2984[B]:THR:OG1 | 2.58 | 0.51 |
| 3:F:3176[A]:LYS:N | 3:F:3176[A]:LYS:CE | 2.73 | 0.51 |
| 1:G:979:LEU:HB3 | 1:G:980:TYR:CD2 | 2.44 | 0.51 |
| 2:H:2800:LYS:C | 3:I:3023[A]:ILE:CD1 | 2.78 | 0.51 |
| 3:I:2952[A]:ALA:CB | 3:I:2956[A]:LYS:HB3 | 2.40 | 0.51 |
| 3:I:3147[B]:GLU:CD | 3:I:3149[B]:ASN:HD21 | 2.17 | 0.51 |
| 3:I:3150[B]:LYS:HD2 | 3:R:3160[B]:SER:CB | 2.39 | 0.51 |
| 3:I:3188[B]:ASP:N | 3:I:3188[B]:ASP:OD2 | 2.36 | 0.51 |
| 1:J:1171:LYS:HG2 | 1:J:1173:GLY:H | 1.75 | 0.51 |
| 3:L:2935[A]:ILE:CD1 | 3:L:2935[A]:ILE:N | 2.73 | 0.51 |
| 3:L:3176[A]:LYS:NZ | 3:L:3176[A]:LYS:CB | 2.73 | 0.51 |
| 3:L:3284[A]:LYS:HD3 | 3:L:3284[A]:LYS:C | 2.32 | 0.51 |
| 3:L:3291[B]:ASP:OD2 | 3:L:3293[B]:LYS:NZ | 2.43 | 0.51 |
| 1:M:1335:LEU:HD23 | 1:M:1339:SER:HA | 1.92 | 0.51 |
| 2:N:2094:ARG:CZ | 2:Q:2370:MET:HE1 | 2.40 | 0.51 |
| 2:N:2172:ILE:HG13 | 2:N:2173:VAL:HG13 | 1.92 | 0.51 |
| 3:O:2928[B]:ASN:C | 3:O:2930[B]:LEU:HD22 | 2.36 | 0.51 |
| 3:O:2949[A]:LYS:C | 3:O:2953[A]:GLY:H | 2.17 | 0.51 |
| 3:O:2968[B]:GLN:HB3 | 3:X:2979[B]:GLN:CB | 2.39 | 0.51 |
| 3:O:3019[B]:HIS:CD2 | 3:O:3019[B]:HIS:N | 2.75 | 0.51 |
| 3:O:3101[B]:PRO:HG2 | 3:O:3102[B]:TYR:CD1 | 2.45 | 0.51 |
| 3:O:3110[B]:THR:O | 3:O:3111[B]:SER:C | 2.53 | 0.51 |
| 3:O:3147[B]:GLU:CD | 3:O:3149[B]:ASN:HD21 | 2.17 | 0.51 |
| 3:O:3273[A]:LEU:O | 3:O:3275[A]:LEU:HD12 | 2.11 | 0.51 |
| 3:O:3293[A]:LYS:CG | 3:O:3294[A]:SER:HB2 | 2.36 | 0.51 |
| 1:P:1400:ASN:ND2 | 1:P:1433:TRP:HZ3 | 2.07 | 0.51 |
| 3:R:2952[B]:ALA:CA | 3:R:2956[B]:LYS:HB3 | 2.38 | 0.51 |
| 3:R:3120[A]:HIS:HA | 3:R:3123[A]:THR:HG1 | 1.73 | 0.51 |
| 2:T:2622:ASN:HB3 | 2:T:2625:LEU:HD12 | 1.93 | 0.51 |
| 3:U:2969[B]:TYR:CE2 | 3:d:3248[B]:LEU:HD23 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3110[A]:THR:O | 3:U:3111[A]:SER:C | 2.53 | 0.51 |
| 3:U:3110[A]:THR:C | 3:U:3112[A]:TYR:N | 2.68 | 0.51 |
| 3:U:3115[A]:LEU:HD22 | 3:U:3115[A]:LEU:O | 2.10 | 0.51 |
| 3:U:3139[B]:LEU:CD2 | 3:U:3139[B]:LEU:N | 2.73 | 0.51 |
| 3:U:3176[A]:LYS:H | 3:U:3176[A]:LYS:CE | 2.17 | 0.51 |
| 3:U:3228[A]:VAL:CG2 | 3:U:3245[A]:PHE:CE2 | 2.89 | 0.51 |
| 3:U:3275[B]:LEU:N | 3:U:3275[B]:LEU:CD1 | 2.73 | 0.51 |
| 3:U:3284[A]:LYS:CE | 3:U:3284[A]:LYS:CA | 2.85 | 0.51 |
| 3:U:3287[B]:ILE:O | 3:U:3287[B]:ILE:HG23 | 2.09 | 0.51 |
| 3:U:3298[A]:ASN:HA | 3:U:3299[A]:LEU:HB3 | 1.87 | 0.51 |
| 3:U:3300[A]:LEU:N | 3:U:3300[A]:LEU:CD2 | 2.73 | 0.51 |
| 2:W:2476:LEU:HD22 | 4:HA:2:NAG:H81 | 1.92 | 0.51 |
| 2:W:2823:ILE:HD13 | 2:W:2856:ILE:HG21 | 1.91 | 0.51 |
| 3:X:2949[B]:LYS:C | 3:X:2953[B]:GLY:H | 2.17 | 0.51 |
| 3:X:3147[A]:GLU:CB | 3:X:3149[A]:ASN:ND2 | 2.73 | 0.51 |
| 3:X:3176[A]:LYS:NZ | 3:X:3176[A]:LYS:CB | 2.73 | 0.51 |
| 3:X:3273[B]:LEU:O | 3:X:3275[B]:LEU:HD12 | 2.11 | 0.51 |
| 3:X:3300[A]:LEU:N | 3:X:3300[A]:LEU:CD2 | 2.73 | 0.51 |
| 1:Y:7:VAL:HG23 | 1:Y:91:TYR:O | 2.10 | 0.51 |
| 1:Y:1620:LEU:CD1 | 3:d:3189[B]:ASN:HB2 | 2.31 | 0.51 |
| 3:a:2949[B]:LYS:C | 3:a:2953[B]:GLY:H | 2.17 | 0.51 |
| 3:a:3110[A]:THR:C | 3:a:3112[A]:TYR:N | 2.68 | 0.51 |
| 3:a:3176[B]:LYS:N | 3:a:3176[B]:LYS:CE | 2.73 | 0.51 |
| 3:a:3275[A]:LEU:N | 3:a:3275[A]:LEU:CD1 | 2.73 | 0.51 |
| 3:a:3293[B]:LYS:CG | 3:a:3294[B]:SER:HB2 | 2.36 | 0.51 |
| 1:b:1195:ASP:OD1 | 1:b:1196:ILE:N | 2.44 | 0.51 |
| 1:A:300:ALA:HB2 | 1:A:406:PRO:HD3 | 1.92 | 0.51 |
| 1:A:1245:GLU:OE1 | 1:A:1246:GLY:N | 2.28 | 0.51 |
| 2:B:2569:TRP:O | 2:B:2572:VAL:HG23 | 2.10 | 0.51 |
| 3:C:2945[A]:VAL:HG22 | 3:C:2954[A]:TYR:HB2 | 1.91 | 0.51 |
| 3:C:3157[B]:PRO:HA | 3:L:2982[B]:MET:SD | 2.50 | 0.51 |
| 3:C:3230[A]:PHE:H | 3:C:3243[A]:GLY:CA | 2.22 | 0.51 |
| 1:D:157:GLU:OE2 | 1:D:296:ARG:NH2 | 2.43 | 0.51 |
| 1:D:329:ARG:HD3 | 1:G:1583:CYS:H | 1.76 | 0.51 |
| 1:D:1018:ILE:HD12 | 1:D:1045:HIS:CD2 | 2.45 | 0.51 |
| 1:D:1129:LEU:O | 1:D:1133:ILE:HG12 | 2.11 | 0.51 |
| 1:D:1421:VAL:HG23 | 1:D:1422:HIS:HD1 | 1.75 | 0.51 |
| 2:E:2179:ASP:HA | 2:E:2300:ASN:ND2 | 2.26 | 0.51 |
| 2:E:2798:GLN:O | 2:E:2803:ARG:NH1 | 2.44 | 0.51 |
| 3:F:2952[B]:ALA:CB | 3:F:2956[B]:LYS:HB3 | 2.40 | 0.51 |
| 3:F:2960[A]:PHE:CD2 | 3:F:3157[A]:PRO:CG | 2.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2966[B]:SER:C | 3:F:2967[B]:CYS:SG | 2.94 | 0.51 |
| 3:F:2968[B]:GLN:HG2 | 3:a:2980[B]:HIS:C | 2.32 | 0.51 |
| 3:F:3275[A]:LEU:N | 3:F:3275[A]:LEU:CD1 | 2.73 | 0.51 |
| 3:F:3285[A]:VAL:CG2 | 3:F:3286[A]:THR:N | 2.73 | 0.51 |
| 3:F:3300[B]:LEU:N | 3:F:3300[B]:LEU:CD2 | 2.73 | 0.51 |
| 1:G:1102:PRO:HA | 1:G:1105:VAL:HG22 | 1.91 | 0.51 |
| 1:G:1558:LEU:HD13 | 2:K:2440:ASP:HA | 1.92 | 0.51 |
| 2:H:2275:GLY:HA3 | 2:H:2283:ASN:HB2 | 1.93 | 0.51 |
| 2:H:2568:HIS:ND1 | 2:H:2765:PRO:HB3 | 2.24 | 0.51 |
| 2:H:2738:ALA:HB2 | 1:J:1233:SER:HA | 1.92 | 0.51 |
| 3:I:2945[B]:VAL:HG22 | 3:I:2954[B]:TYR:HB2 | 1.91 | 0.51 |
| 3:I:2961[B]:HIS:HB3 | 3:I:3111[B]:SER:HB3 | 1.92 | 0.51 |
| 3:I:2972[B]:GLY:N | 3:R:3089[B]:HIS:CD2 | 2.78 | 0.51 |
| 3:I:2973[B]:THR:OG1 | 3:R:3093[B]:HIS:CD2 | 2.64 | 0.51 |
| 3:I:3101[B]:PRO:HG2 | 3:I:3102[B]:TYR:CD1 | 2.46 | 0.51 |
| 3:I:3176[A]:LYS:NZ | 3:I:3176[A]:LYS:CB | 2.73 | 0.51 |
| 3:I:3254[B]:MET:CB | 3:R:2966[B]:SER:CB | 2.88 | 0.51 |
| 3:I:3285[A]:VAL:CG2 | 3:I:3286[A]:THR:N | 2.73 | 0.51 |
| 1:J:424:PHE:HB2 | 1:J:1128:GLN:HE22 | 1.75 | 0.51 |
| 1:J:493:LEU:HD12 | 1:J:668:MET:HG3 | 1.92 | 0.51 |
| 1:J:550:ILE:N | 1:J:557:VAL:O | 2.30 | 0.51 |
| 3:L:3115[B]:LEU:HD22 | 3:L:3115[B]:LEU:O | 2.10 | 0.51 |
| 3:L:3287[B]:ILE:O | 3:L:3287[B]:ILE:HG23 | 2.10 | 0.51 |
| 1:M:1229:LYS:HD2 | 1:M:1229:LYS:H | 1.76 | 0.51 |
| 1:M:1242:ASN:OD1 | 1:M:1244:GLY:N | 2.40 | 0.51 |
| 2:N:2901:LEU:HB2 | 1:P:1074:ILE:HB | 1.91 | 0.51 |
| 3:O:2968[B]:GLN:C | 3:X:2988[B]:TRP:HB2 | 2.35 | 0.51 |
| 3:O:3028[A]:PRO:HG2 | 3:O:3029[A]:LYS:CG | 2.40 | 0.51 |
| 3:O:3269[B]:SER:O | 3:O:3272[B]:HIS:HB2 | 2.09 | 0.51 |
| 2:Q:2411:PHE:HE2 | 2:Q:2445:MET:HE3 | 1.75 | 0.51 |
| 2:Q:2830:GLN:HB2 | 2:Q:2863:ARG:NH1 | 2.25 | 0.51 |
| 3:R:3264[A]:TYR:C | 3:R:3264[A]:TYR:CD1 | 2.86 | 0.51 |
| 3:U:2933[A]:SER:CB | 3:U:2936[A]:GLU:CB | 2.86 | 0.51 |
| 3:U:2935[A]:ILE:CD1 | 3:U:2935[A]:ILE:N | 2.73 | 0.51 |
| 3:U:2937[A]:ASN:ND2 | 3:U:3006[A]:LYS:CD | 2.73 | 0.51 |
| 3:U:2937[B]:ASN:ND2 | 3:U:3006[B]:LYS:CD | 2.73 | 0.51 |
| 3:U:2949[B]:LYS:C | 3:U:2953[B]:GLY:H | 2.17 | 0.51 |
| 3:U:2966[A]:SER:C | 3:U:2967[A]:CYS:SG | 2.94 | 0.51 |
| 3:U:2971[B]:ASP:O | 3:d:3247[B]:VAL:HG12 | 2.05 | 0.51 |
| 3:U:3114[A]:PRO:CD | 3:U:3115[A]:LEU:N | 2.72 | 0.51 |
| 3:U:3115[B]:LEU:HD22 | 3:U:3115[B]:LEU:O | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3293[A]:LYS:CG | 3:U:3294[A]:SER:HB2 | 2.36 | 0.51 |
| 1:V:210:HIS:HA | 1:V:213:VAL:HG22 | 1.92 | 0.51 |
| 1:V:1582:ASN:CB | 1:V:1583:CYS:HB2 | 2.28 | 0.51 |
| 1:Y:639:ARG:HB2 | 1:Y:703:TYR:CE1 | 2.46 | 0.51 |
| 2:Z:2415:PRO:HD3 | 2:Z:2454:MET:HE1 | 1.90 | 0.51 |
| 3:a:2928[B]:ASN:C | 3:a:2930[B]:LEU:HD22 | 2.36 | 0.51 |
| 3:a:3196[A]:THR:CA | 3:a:3199[A]:GLN:OE1 | 2.58 | 0.51 |
| 3:a:3196[B]:THR:CA | 3:a:3199[B]:GLN:OE1 | 2.58 | 0.51 |
| 1:b:59:LEU:HD13 | 1:b:68:TRP:CD1 | 2.45 | 0.51 |
| 1:b:247:PHE:O | 1:b:252:ASN:ND2 | 2.43 | 0.51 |
| 2:c:2506:ARG:NE | 2:c:2578:GLU:OE2 | 2.41 | 0.51 |
| 3:d:2951[B]:ASP:O | 3:d:2956[B]:LYS:HE2 | 2.09 | 0.51 |
| 3:d:2971[A]:ASP:CG | 3:d:2973[A]:THR:HG1 | 2.14 | 0.51 |
| 3:d:3176[A]:LYS:NZ | 3:d:3176[A]:LYS:CB | 2.73 | 0.51 |
| 3:d:3293[B]:LYS:CG | 3:d:3294[B]:SER:HB2 | 2.36 | 0.51 |
| 1:A:473:ALA:H | 1:A:474:LEU:HD23 | 1.76 | 0.51 |
| 1:A:571:PRO:O | 1:A:573:LYS:NZ | 2.44 | 0.51 |
| 1:A:946:GLU:HA | 1:A:955:LYS:HB3 | 1.93 | 0.51 |
| 3:C:2975[B]:PHE:CE1 | 3:L:3107[B]:LEU:HD12 | 2.39 | 0.51 |
| 3:C:2984[B]:THR:CB | 3:L:3154[B]:PRO:HG2 | 2.40 | 0.51 |
| 3:C:3028[A]:PRO:HG2 | 3:C:3029[A]:LYS:CG | 2.40 | 0.51 |
| 3:C:3110[B]:THR:C | 3:C:3112[B]:TYR:N | 2.68 | 0.51 |
| 3:C:3273[A]:LEU:O | 3:C:3275[A]:LEU:HD12 | 2.11 | 0.51 |
| 1:D:1055:THR:HG21 | 1:D:1121:LEU:HD13 | 1.91 | 0.51 |
| 1:D:1407:THR:HG22 | 1:D:1426:LEU:HD21 | 1.93 | 0.51 |
| 2:E:2145:LEU:HD12 | 2:E:2435:MET:HE1 | 1.93 | 0.51 |
| 3:F:2935[B]:ILE:CD1 | 3:F:2936[B]:GLU:N | 2.73 | 0.51 |
| 3:F:2952[A]:ALA:CB | 3:F:2956[A]:LYS:HB3 | 2.40 | 0.51 |
| 3:F:2952[B]:ALA:CA | 3:F:2956[B]:LYS:HB3 | 2.38 | 0.51 |
| 3:F:2962[A]:GLY:N | 3:F:3111[A]:SER:OG | 2.44 | 0.51 |
| 3:F:2978[B]:CYS:O | 3:a:2977[B]:CYS:SG | 2.68 | 0.51 |
| 3:F:3101[B]:PRO:HG2 | 3:F:3102[B]:TYR:CD1 | 2.46 | 0.51 |
| 3:F:3132[B]:ALA:HB1 | 3:F:3197[B]:ILE:HD13 | 1.89 | 0.51 |
| 3:F:3273[A]:LEU:O | 3:F:3275[A]:LEU:HD12 | 2.11 | 0.51 |
| 1:G:865:LYS:NZ | 1:G:966:SER:OG | 2.43 | 0.51 |
| 1:G:1059:LEU:HD13 | 1:G:1063:ARG:HH21 | 1.74 | 0.51 |
| 3:I:2966[A]:SER:C | 3:I:2967[A]:CYS:SG | 2.94 | 0.51 |
| 3:I:2985[B]:PHE:HE2 | 3:R:2968[B]:GLN:O | 1.93 | 0.51 |
| 3:I:3219[B]:LEU:N | 3:I:3219[B]:LEU:CD2 | 2.73 | 0.51 |
| 3:I:3285[B]:VAL:CG2 | 3:I:3286[B]:THR:N | 2.73 | 0.51 |
| 3:I:3291[B]:ASP:OD2 | 3:I:3293[B]:LYS:NZ | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3300[A]:LEU:N | 3:I:3300[A]:LEU:CD2 | 2.73 | 0.51 |
| 1:J:566:ARG:HH12 | 1:J:803:LYS:NZ | 2.09 | 0.51 |
| 3:L:2962[A]:GLY:N | 3:L:3111[A]:SER:OG | 2.44 | 0.51 |
| 3:L:3139[B]:LEU:CD2 | 3:L:3139[B]:LEU:N | 2.73 | 0.51 |
| 3:L:3273[B]:LEU:O | 3:L:3275[B]:LEU:HD12 | 2.11 | 0.51 |
| 1:M:23:ARG:HA | 1:M:122:VAL:HG11 | 1.93 | 0.51 |
| 1:M:911:LEU:HD21 | 1:M:1095:MET:HE2 | 1.93 | 0.51 |
| 1:M:980:TYR:CE1 | 1:M:1021:LEU:HB3 | 2.45 | 0.51 |
| 3:O:2948[B]:ASP:CB | 3:O:2949[B]:LYS:HA | 2.16 | 0.51 |
| 3:O:2952[A]:ALA:N | 3:O:2953[A]:GLY:HA2 | 2.06 | 0.51 |
| 3:O:3219[B]:LEU:N | 3:O:3219[B]:LEU:CD2 | 2.73 | 0.51 |
| 3:O:3273[B]:LEU:O | 3:O:3275[B]:LEU:HD12 | 2.11 | 0.51 |
| 3:O:3298[A]:ASN:HA | 3:O:3299[A]:LEU:HB3 | 1.88 | 0.51 |
| 3:O:3298[B]:ASN:HA | 3:O:3299[B]:LEU:HB3 | 1.88 | 0.51 |
| 1:P:1210:LYS:HA | 1:P:1211:TYR:HB3 | 1.93 | 0.51 |
| 3:R:2966[B]:SER:C | 3:R:2967[B]:CYS:SG | 2.94 | 0.51 |
| 3:R:3104[B]:MET:HA | 3:R:3110[B]:THR:CG2 | 2.17 | 0.51 |
| 3:R:3151[B]:LEU:HB2 | 3:R:3175[B]:TYR:HE2 | 1.68 | 0.51 |
| 3:R:3273[B]:LEU:O | 3:R:3275[B]:LEU:HD12 | 2.11 | 0.51 |
| 1:S:1348:TRP:CD1 | 1:S:1403:LEU:HD13 | 2.45 | 0.51 |
| 2:T:2625:LEU:HD22 | 2:T:2626:ARG:HB2 | 1.92 | 0.51 |
| 3:U:2945[B]:VAL:HG22 | 3:U:2954[B]:TYR:HB2 | 1.91 | 0.51 |
| 3:U:3096[A]:VAL:HG11 | 3:U:3115[A]:LEU:HD12 | 1.89 | 0.51 |
| 3:U:3110[B]:THR:O | 3:U:3111[B]:SER:C | 2.53 | 0.51 |
| 3:U:3110[B]:THR:C | 3:U:3112[B]:TYR:N | 2.68 | 0.51 |
| 1:V:568:PHE:N | 1:V:568:PHE:CD1 | 2.78 | 0.51 |
| 1:V:846:MET:HE1 | 1:V:854:LEU:HD22 | 1.93 | 0.51 |
| 2:W:2610:ASP:OD1 | 2:W:2610:ASP:N | 2.44 | 0.51 |
| 3:X:3042[B]:ASP:N | 3:X:3042[B]:ASP:OD2 | 2.41 | 0.51 |
| 3:X:3092[B]:ILE:CG2 | 3:X:3096[B]:VAL:CG2 | 2.88 | 0.51 |
| 3:X:3293[A]:LYS:CB | 3:X:3294[A]:SER:CB | 2.54 | 0.51 |
| 1:Y:148:GLN:C | 1:Y:150:GLY:H | 2.18 | 0.51 |
| 3:a:2961[A]:HIS:HB3 | 3:a:3111[A]:SER:HB3 | 1.92 | 0.51 |
| 3:a:2966[A]:SER:C | 3:a:2967[A]:CYS:SG | 2.94 | 0.51 |
| 3:a:3092[A]:ILE:CG2 | 3:a:3096[A]:VAL:CG2 | 2.88 | 0.51 |
| 3:a:3092[B]:ILE:CG2 | 3:a:3096[B]:VAL:CG2 | 2.88 | 0.51 |
| 3:a:3176[A]:LYS:N | 3:a:3176[A]:LYS:CE | 2.73 | 0.51 |
| 3:a:3183[B]:LEU:N | 3:a:3184[B]:ASN:HA | 2.12 | 0.51 |
| 3:a:3228[B]:VAL:HG23 | 3:a:3228[B]:VAL:O | 2.10 | 0.51 |
| 1:b:1074:ILE:O | 1:b:1078:ARG:HG2 | 2.09 | 0.51 |
| 2:c:2517:VAL:HG13 | 2:c:2605:LEU:HD13 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2952[A]:ALA:N | 3:d:2953[A]:GLY:HA2 | 2.06 | 0.51 |
| 3:d:2961[B]:HIS:HB3 | 3:d:3111[B]:SER:HB3 | 1.91 | 0.51 |
| 3:d:3038[B]:ILE:HG23 | 3:d:3040[B]:VAL:HG22 | 1.90 | 0.51 |
| 3:d:3101[B]:PRO:HG2 | 3:d:3102[B]:TYR:CD1 | 2.46 | 0.51 |
| 3:d:3300[A]:LEU:N | 3:d:3300[A]:LEU:CD2 | 2.73 | 0.51 |
| 1:A:569:LYS:C | 1:A:571:PRO:HD3 | 2.36 | 0.51 |
| 1:A:1158:GLU:CD | 1:A:1216:ARG:HE | 2.18 | 0.51 |
| 1:A:1302:SER:HB3 | 1:A:1303:GLU:CA | 2.37 | 0.51 |
| 1:A:1348:TRP:CD1 | 1:A:1403:LEU:HD13 | 2.45 | 0.51 |
| 2:B:2802:ASP:OD2 | 2:B:2903:TYR:OH | 2.20 | 0.51 |
| 3:C:2961[B]:HIS:HB3 | 3:C:3111[B]:SER:HB3 | 1.91 | 0.51 |
| 3:C:3079[B]:CYS:HB3 | 3:L:3161[B]:GLU:CB | 2.41 | 0.51 |
| 3:C:3120[B]:HIS:NE2 | 3:L:2969[B]:TYR:HE2 | 1.94 | 0.51 |
| 1:D:573:LYS:HB3 | 1:D:574:GLY:HA2 | 1.93 | 0.51 |
| 1:D:806:ASN:ND2 | 6:k:1:NAG:C8 | 2.73 | 0.51 |
| 1:D:1082:SER:O | 1:D:1086:LEU:HG | 2.09 | 0.51 |
| 2:E:2546:LEU:H | 2:E:2557:ALA:HA | 1.75 | 0.51 |
| 2:E:2728:ARG:HE | 2:E:2730:LEU:HD12 | 1.75 | 0.51 |
| 3:F:2928[B]:ASN:C | 3:F:2930[B]:LEU:HD22 | 2.36 | 0.51 |
| 3:F:2983[B]:VAL:HG22 | 3:a:3162[B]:ASP:OD1 | 2.11 | 0.51 |
| 3:F:3108[B]:HIS:HE1 | 3:a:3251[B]:ASP:CG | 2.16 | 0.51 |
| 1:G:203:ASP:O | 1:G:206:PHE:HB3 | 2.11 | 0.51 |
| 2:H:2667:GLU:HB3 | 2:H:2730:LEU:HD22 | 1.91 | 0.51 |
| 3:I:2935[A]:ILE:CD1 | 3:I:2936[A]:GLU:N | 2.73 | 0.51 |
| 3:I:3135[B]:LYS:HB2 | 3:I:3141[B]:TYR:HD1 | 1.76 | 0.51 |
| 3:I:3155[B]:MET:HB3 | 3:R:3153[B]:LYS:CD | 2.35 | 0.51 |
| 1:J:527:LEU:HD23 | 1:J:632:LEU:HD12 | 1.92 | 0.51 |
| 1:J:982:LYS:N | 1:J:983:PRO:HD3 | 2.25 | 0.51 |
| 1:J:1033:LEU:HA | 1:J:1036:SER:HB3 | 1.92 | 0.51 |
| 1:J:1145:THR:HB | 1:J:1191:PRO:HB2 | 1.92 | 0.51 |
| 3:L:3101[B]:PRO:HG2 | 3:L:3102[B]:TYR:CD1 | 2.46 | 0.51 |
| 3:L:3176[A]:LYS:N | 3:L:3176[A]:LYS:CE | 2.73 | 0.51 |
| 3:O:2986[B]:PRO:CB | 3:O:3127[B]:TRP:CZ3 | 2.94 | 0.51 |
| 3:O:3114[B]:PRO:CD | 3:O:3115[B]:LEU:N | 2.72 | 0.51 |
| 3:O:3176[B]:LYS:N | 3:O:3176[B]:LYS:CE | 2.73 | 0.51 |
| 3:O:3285[B]:VAL:CG2 | 3:O:3286[B]:THR:N | 2.73 | 0.51 |
| 1:P:132:ASN:HB2 | 1:P:133:LYS:HA | 1.92 | 0.51 |
| 1:P:494:VAL:HG23 | 1:P:671:PHE:CZ | 2.45 | 0.51 |
| 2:Q:2631:TYR:HD1 | 2:Q:2631:TYR:H | 1.58 | 0.51 |
| 3:R:2986[B]:PRO:CB | 3:R:3127[B]:TRP:CZ3 | 2.94 | 0.51 |
| 3:R:3176[A]:LYS:NZ | 3:R:3176[A]:LYS:CB | 2.73 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3273[A]:LEU:O | 3:R:3275[A]:LEU:HD12 | 2.11 | 0.51 |
| 1:S:956:PRO:HB2 | 1:S:957:ASN:C | 2.36 | 0.51 |
| 3:U:2935[A]:ILE:CD1 | 3:U:2936[A]:GLU:N | 2.73 | 0.51 |
| 1:V:43:GLU:HG3 | 1:V:44:PRO:HA | 1.92 | 0.51 |
| 3:X:2935[B]:ILE:CD1 | 3:X:2935[B]:ILE:N | 2.73 | 0.51 |
| 3:X:2961[A]:HIS:HB3 | 3:X:3111[A]:SER:HB3 | 1.92 | 0.51 |
| 3:X:2986[A]:PRO:CB | 3:X:3127[A]:TRP:CZ3 | 2.94 | 0.51 |
| 3:X:3092[A]:ILE:CG2 | 3:X:3096[A]:VAL:CG2 | 2.88 | 0.51 |
| 3:X:3104[B]:MET:HA | 3:X:3110[B]:THR:CG2 | 2.17 | 0.51 |
| 3:X:3196[A]:THR:CA | 3:X:3199[A]:GLN:OE1 | 2.58 | 0.51 |
| 3:X:3285[A]:VAL:CG2 | 3:X:3286[A]:THR:N | 2.73 | 0.51 |
| 3:X:3291[B]:ASP:OD2 | 3:X:3293[B]:LYS:NZ | 2.44 | 0.51 |
| 2:Z:2128:LEU:HB2 | 2:Z:2286:HIS:HB3 | 1.91 | 0.51 |
| 3:a:2952[B]:ALA:CA | 3:a:2956[B]:LYS:HB3 | 2.38 | 0.51 |
| 3:a:2986[B]:PRO:CB | 3:a:3127[B]:TRP:CZ3 | 2.94 | 0.51 |
| 3:a:3139[A]:LEU:CD2 | 3:a:3139[A]:LEU:N | 2.73 | 0.51 |
| 3:a:3176[B]:LYS:NZ | 3:a:3176[B]:LYS:CB | 2.73 | 0.51 |
| 3:a:3300[B]:LEU:CD2 | 3:a:3300[B]:LEU:H | 2.24 | 0.51 |
| 2:c:2234:GLN:HG3 | 2:c:2235:PRO:HD2 | 1.92 | 0.51 |
| 2:c:2562:GLY:H | 2:c:2846:TRP:HB2 | 1.75 | 0.51 |
| 3:d:2952[B]:ALA:CB | 3:d:2956[B]:LYS:HB3 | 2.40 | 0.51 |
| 3:d:3132[B]:ALA:HB1 | 3:d:3197[B]:ILE:HD13 | 1.89 | 0.51 |
| 3:d:3275[B]:LEU:N | 3:d:3275[B]:LEU:CD1 | 2.73 | 0.51 |
| 3:d:3293[A]:LYS:CG | 3:d:3294[A]:SER:HB2 | 2.36 | 0.51 |
| 3:d:3298[A]:ASN:HA | 3:d:3299[A]:LEU:HB3 | 1.88 | 0.51 |
| 4:m:1:NAG:C4 | 4:m:2:NAG:N2 | 2.73 | 0.51 |
| 3:C:2968[B]:GLN:C | 3:L:2985[B]:PHE:CE2 | 2.89 | 0.51 |
| 3:C:2975[B]:PHE:O | 3:L:3254[B]:MET:O | 2.29 | 0.51 |
| 3:C:3114[A]:PRO:CD | 3:C:3115[A]:LEU:N | 2.72 | 0.51 |
| 3:C:3139[B]:LEU:CD2 | 3:C:3139[B]:LEU:N | 2.73 | 0.51 |
| 3:C:3147[B]:GLU:CG | 3:C:3149[B]:ASN:ND2 | 2.73 | 0.51 |
| 3:C:3176[A]:LYS:NZ | 3:C:3176[A]:LYS:CB | 2.73 | 0.51 |
| 1:D:460:GLU:CD | 1:D:1368:ARG:HH21 | 2.18 | 0.51 |
| 1:D:583:LEU:O | 1:D:587:PHE:HD1 | 1.92 | 0.51 |
| 1:D:1276:ASN:OD1 | 1:D:1280:GLN:NE2 | 2.43 | 0.51 |
| 1:D:1321:HIS:CD2 | 1:D:1321:HIS:H | 2.28 | 0.51 |
| 2:E:2180:TRP:HB2 | 2:E:2243:LEU:HD13 | 1.93 | 0.51 |
| 3:F:2937[A]:ASN:ND2 | 3:F:3006[A]:LYS:CD | 2.73 | 0.51 |
| 3:F:2982[B]:MET:CE | 3:a:2977[B]:CYS:HB3 | 2.35 | 0.51 |
| 3:F:3110[B]:THR:O | 3:F:3111[B]:SER:C | 2.53 | 0.51 |
| 3:F:3113[A]:ASP:O | 3:F:3114[A]:PRO:C | 2.53 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3291[B]:ASP:OD2 | 3:F:3293[B]:LYS:NZ | 2.43 | 0.51 |
| 1:G:140:ASP:CG | 1:G:142:ARG:HE | 2.19 | 0.51 |
| 3:I:2935[B]:ILE:CD1 | 3:I:2935[B]:ILE:N | 2.73 | 0.51 |
| 3:I:2937[A]:ASN:ND2 | 3:I:3006[A]:LYS:CD | 2.73 | 0.51 |
| 3:I:2982[B]:MET:HB3 | 3:R:3160[B]:SER:CB | 2.40 | 0.51 |
| 3:I:3092[B]:ILE:CG2 | 3:I:3096[B]:VAL:CG2 | 2.88 | 0.51 |
| 3:I:3093[B]:HIS:CG | 3:R:2971[B]:ASP:O | 2.64 | 0.51 |
| 3:I:3249[B]:GLY:N | 3:R:2974[B]:ALA:N | 2.58 | 0.51 |
| 1:J:320:LYS:NZ | 1:J:337:ASP:HB3 | 2.25 | 0.51 |
| 1:J:598:GLN:HE22 | 1:J:778:LYS:H | 1.58 | 0.51 |
| 1:J:1470:GLU:HB3 | 1:J:1537:ILE:CD1 | 2.41 | 0.51 |
| 3:L:2933[A]:SER:CB | 3:L:2936[A]:GLU:CB | 2.86 | 0.51 |
| 3:L:2937[A]:ASN:ND2 | 3:L:3006[A]:LYS:CD | 2.73 | 0.51 |
| 3:L:2988[A]:TRP:HE3 | 3:L:2989[A]:HIS:CE1 | 2.25 | 0.51 |
| 3:L:3211[A]:ASP:OD1 | 3:L:3211[A]:ASP:N | 2.28 | 0.51 |
| 3:L:3273[A]:LEU:HB2 | 3:L:3275[A]:LEU:CD1 | 2.34 | 0.51 |
| 3:L:3273[A]:LEU:O | 3:L:3275[A]:LEU:HD12 | 2.11 | 0.51 |
| 1:M:2:LEU:H | 1:M:274:TYR:HA | 1.76 | 0.51 |
| 1:M:1230:LEU:H | 1:M:1230:LEU:HD13 | 1.76 | 0.51 |
| 2:N:2821:LEU:HD11 | 2:N:2879:LEU:HD23 | 1.91 | 0.51 |
| 3:O:2937[A]:ASN:ND2 | 3:O:3006[A]:LYS:CD | 2.73 | 0.51 |
| 3:O:2961[B]:HIS:HB3 | 3:O:3111[B]:SER:HB3 | 1.92 | 0.51 |
| 3:O:2962[B]:GLY:N | 3:O:3111[B]:SER:OG | 2.44 | 0.51 |
| 3:O:2986[A]:PRO:CB | 3:O:3127[A]:TRP:CZ3 | 2.94 | 0.51 |
| 3:O:3219[A]:LEU:N | 3:O:3219[A]:LEU:CD2 | 2.73 | 0.51 |
| 1:P:212:ASN:OD1 | 1:P:215:ARG:NH1 | 2.43 | 0.51 |
| 1:P:728:ARG:HE | 1:P:730:PHE:HZ | 1.58 | 0.51 |
| 1:P:1587:ALA:HA | 1:P:1614:GLU:HG2 | 1.91 | 0.51 |
| 3:R:2933[B]:SER:CB | 3:R:2936[B]:GLU:CB | 2.85 | 0.51 |
| 3:R:2961[A]:HIS:HB3 | 3:R:3111[A]:SER:HB3 | 1.92 | 0.51 |
| 3:R:3101[B]:PRO:HG2 | 3:R:3102[B]:TYR:CD1 | 2.46 | 0.51 |
| 3:R:3176[B]:LYS:N | 3:R:3176[B]:LYS:CE | 2.73 | 0.51 |
| 2:T:2128:LEU:HD13 | 2:T:2286:HIS:CG | 2.46 | 0.51 |
| 3:U:2969[B]:TYR:HE1 | 3:d:2978[B]:CYS:SG | 2.28 | 0.51 |
| 3:U:2986[B]:PRO:CB | 3:U:3127[B]:TRP:CZ3 | 2.94 | 0.51 |
| 3:U:3147[A]:GLU:CG | 3:U:3149[A]:ASN:ND2 | 2.73 | 0.51 |
| 3:U:3176[A]:LYS:N | 3:U:3176[A]:LYS:CE | 2.73 | 0.51 |
| 3:U:3183[A]:LEU:N | 3:U:3184[A]:ASN:HA | 2.12 | 0.51 |
| 3:U:3284[A]:LYS:HD3 | 3:U:3284[A]:LYS:C | 2.32 | 0.51 |
| 3:U:3300[B]:LEU:N | 3:U:3300[B]:LEU:CD2 | 2.73 | 0.51 |
| 1:V:1470:GLU:HG3 | 1:V:1530:LEU:HD12 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W:2650:GLY:H | 2:W:2654:SER:HB3 | 1.76 | 0.51 |
| 3:X:3113[A]:ASP:O | 3:X:3114[A]:PRO:C | 2.53 | 0.51 |
| 3:X:3151[B]:LEU:HB2 | 3:X:3175[B]:TYR:HE2 | 1.67 | 0.51 |
| 3:X:3228[B]:VAL:O | 3:X:3228[B]:VAL:HG23 | 2.10 | 0.51 |
| 1:Y:527:LEU:HD23 | 1:Y:632:LEU:HD12 | 1.92 | 0.51 |
| 3:a:2952[A]:ALA:CA | 3:a:2956[A]:LYS:HB3 | 2.38 | 0.51 |
| 3:a:3028[A]:PRO:HG2 | 3:a:3029[A]:LYS:CG | 2.40 | 0.51 |
| 1:b:753:ASN:OD1 | 1:b:753:ASN:N | 2.37 | 0.51 |
| 1:b:1290:ILE:HD13 | 1:b:1329:LEU:HG | 1.93 | 0.51 |
| 1:b:1323:HIS:CD2 | 9:b:2105:CUO:O1 | 2.63 | 0.51 |
| 1:b:1467:ILE:HD13 | 1:b:1532:PHE:HB2 | 1.93 | 0.51 |
| 3:d:2935[B]:ILE:CD1 | 3:d:2935[B]:ILE:N | 2.73 | 0.51 |
| 3:d:3096[A]:VAL:HG11 | 3:d:3115[A]:LEU:HD12 | 1.89 | 0.51 |
| 3:d:3135[A]:LYS:HB2 | 3:d:3141[A]:TYR:HD1 | 1.76 | 0.51 |
| 3:d:3273[A]:LEU:O | 3:d:3275[A]:LEU:HD12 | 2.11 | 0.51 |
| 1:A:1013:ILE:HG21 | 1:A:1192:TYR:CD1 | 2.45 | 0.51 |
| 3:C:2937[A]:ASN:ND2 | 3:C:3006[A]:LYS:CD | 2.73 | 0.51 |
| 3:C:2951[A]:ASP:O | 3:C:2956[A]:LYS:HE2 | 2.09 | 0.51 |
| 3:C:2951[B]:ASP:O | 3:C:2956[B]:LYS:HE2 | 2.09 | 0.51 |
| 3:C:2966[B]:SER:C | 3:C:2967[B]:CYS:SG | 2.94 | 0.51 |
| 3:C:2986[A]:PRO:CB | 3:C:3127[A]:TRP:CZ3 | 2.94 | 0.51 |
| 3:C:3153[B]:LYS:HE3 | 3:L:3155[B]:MET:C | 2.36 | 0.51 |
| 2:E:2172:ILE:HG13 | 2:E:2173:VAL:HG13 | 1.93 | 0.51 |
| 2:E:2580:SER:O | 2:E:2583:ARG:HB3 | 2.11 | 0.51 |
| 3:F:2961[B]:HIS:CD2 | 3:F:2988[B]:TRP:CZ3 | 2.96 | 0.51 |
| 3:F:2971[B]:ASP:OD1 | 3:a:3248[B]:LEU:HD21 | 2.11 | 0.51 |
| 3:F:3101[A]:PRO:HG2 | 3:F:3102[A]:TYR:CD1 | 2.45 | 0.51 |
| 3:F:3196[B]:THR:O | 3:F:3199[B]:GLN:HB2 | 2.11 | 0.51 |
| 1:G:108:PRO:O | 1:G:121:ASN:N | 2.42 | 0.51 |
| 1:G:128:ILE:HG13 | 1:G:130:PHE:O | 2.10 | 0.51 |
| 1:G:1060:GLN:HB2 | 1:G:1067:TYR:HB3 | 1.92 | 0.51 |
| 1:G:1471:LEU:HD11 | 1:G:1540:LEU:HD23 | 1.92 | 0.51 |
| 2:H:2551:PRO:HA | 2:H:2554:PRO:HD2 | 1.91 | 0.51 |
| 3:I:2962[A]:GLY:N | 3:I:3111[A]:SER:OG | 2.44 | 0.51 |
| 3:I:3104[B]:MET:HA | 3:I:3110[B]:THR:CG2 | 2.17 | 0.51 |
| 1:J:7:VAL:HG13 | 1:J:104:LEU:HD22 | 1.93 | 0.51 |
| 1:J:555:ALA:HB3 | 1:J:558:HIS:CE1 | 2.46 | 0.51 |
| 3:L:2928[B]:ASN:C | 3:L:2930[B]:LEU:HD22 | 2.36 | 0.51 |
| 3:L:2962[B]:GLY:N | 3:L:3111[B]:SER:OG | 2.44 | 0.51 |
| 3:L:3113[B]:ASP:O | 3:L:3114[B]:PRO:C | 2.53 | 0.51 |
| 3:L:3287[A]:ILE:O | 3:L:3287[A]:ILE:HG23 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3293[A]:LYS:CG | 3:L:3294[A]:SER:HB2 | 2.36 | 0.51 |
| 1:M:402:THR:HG23 | 1:M:659:CYS:HA | 1.92 | 0.51 |
| 1:M:643:ILE:HD13 | 1:M:708:PHE:HB2 | 1.91 | 0.51 |
| 2:N:2562:GLY:H | 2:N:2846:TRP:HB2 | 1.76 | 0.51 |
| 3:O:2928[A]:ASN:C | 3:O:2930[A]:LEU:HD22 | 2.36 | 0.51 |
| 3:O:2951[B]:ASP:O | 3:O:2956[B]:LYS:HE2 | 2.09 | 0.51 |
| 3:O:2966[B]:SER:C | 3:O:2967[B]:CYS:SG | 2.94 | 0.51 |
| 3:O:3096[B]:VAL:HG11 | 3:O:3115[B]:LEU:HD12 | 1.89 | 0.51 |
| 3:O:3300[B]:LEU:CD2 | 3:O:3300[B]:LEU:H | 2.24 | 0.51 |
| 3:R:2952[A]:ALA:CB | 3:R:2956[A]:LYS:HB3 | 2.40 | 0.51 |
| 3:R:3023[B]:ILE:O | 3:R:3025[B]:VAL:N | 2.44 | 0.51 |
| 3:R:3110[A]:THR:O | 3:R:3111[A]:SER:C | 2.53 | 0.51 |
| 3:R:3114[B]:PRO:CD | 3:R:3115[B]:LEU:N | 2.73 | 0.51 |
| 1:S:77:GLU:O | 1:S:81:VAL:HG23 | 2.11 | 0.51 |
| 1:S:979:LEU:CB | 1:S:980:TYR:HA | 2.38 | 0.51 |
| 3:U:2928[B]:ASN:C | 3:U:2930[B]:LEU:HD22 | 2.36 | 0.51 |
| 3:U:2962[A]:GLY:N | 3:U:3111[A]:SER:OG | 2.44 | 0.51 |
| 3:U:3113[B]:ASP:O | 3:U:3114[B]:PRO:C | 2.53 | 0.51 |
| 3:U:3291[A]:ASP:OD2 | 3:U:3293[A]:LYS:NZ | 2.43 | 0.51 |
| 1:V:150:GLY:HA2 | 1:V:151:GLN:C | 2.35 | 0.51 |
| 1:V:1315:GLY:HA3 | 1:V:1601:TRP:HB2 | 1.91 | 0.51 |
| 2:W:2184:MET:HE3 | 2:W:2231:LEU:HD11 | 1.92 | 0.51 |
| 3:X:2952[A]:ALA:CB | 3:X:2956[A]:LYS:HB3 | 2.40 | 0.51 |
| 3:X:2966[A]:SER:C | 3:X:2967[A]:CYS:SG | 2.94 | 0.51 |
| 3:X:3275[B]:LEU:N | 3:X:3275[B]:LEU:CD1 | 2.73 | 0.51 |
| 1:Y:361:GLU:HG2 | 1:Y:363:THR:HG22 | 1.92 | 0.51 |
| 1:Y:1315:GLY:HA3 | 1:Y:1601:TRP:CG | 2.46 | 0.51 |
| 3:a:2962[A]:GLY:N | 3:a:3111[A]:SER:OG | 2.44 | 0.51 |
| 3:a:2966[B]:SER:C | 3:a:2967[B]:CYS:SG | 2.94 | 0.51 |
| 3:a:3300[B]:LEU:N | 3:a:3300[B]:LEU:CD2 | 2.73 | 0.51 |
| 3:d:2952[A]:ALA:CA | 3:d:2956[A]:LYS:HB3 | 2.38 | 0.51 |
| 3:d:3028[B]:PRO:HG2 | 3:d:3029[B]:LYS:CG | 2.40 | 0.51 |
| 3:d:3101[A]:PRO:HG2 | 3:d:3102[A]:TYR:CD1 | 2.46 | 0.51 |
| 3:d:3273[B]:LEU:O | 3:d:3275[B]:LEU:HD12 | 2.11 | 0.51 |
| 1:A:965:ASP:O | 1:A:969:ALA:N | 2.44 | 0.51 |
| 1:A:1067:TYR:H | 1:A:1067:TYR:HD1 | 1.58 | 0.51 |
| 2:B:2115:SER:OG | 2:B:2116:SER:N | 2.41 | 0.51 |
| 2:B:2619:VAL:HG22 | 1:b:138:ALA:HB2 | 1.92 | 0.51 |
| 3:C:2935[B]:ILE:CD1 | 3:C:2935[B]:ILE:N | 2.73 | 0.51 |
| 3:C:3023[A]:ILE:O | 3:C:3025[A]:VAL:N | 2.44 | 0.51 |
| 3:C:3110[A]:THR:C | 3:C:3112[A]:TYR:N | 2.68 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3115[A]:LEU:HD22 | 3:C:3115[A]:LEU:O | 2.10 | 0.51 |
| 3:C:3153[B]:LYS:O | 3:L:3153[B]:LYS:O | 2.28 | 0.51 |
| 3:C:3196[A]:THR:O | 3:C:3199[A]:GLN:HB2 | 2.11 | 0.51 |
| 3:F:3173[B]:THR:HG21 | 3:a:3173[B]:THR:OG1 | 2.11 | 0.51 |
| 3:F:3176[A]:LYS:H | 3:F:3176[A]:LYS:CE | 2.17 | 0.51 |
| 3:F:3284[B]:LYS:HD3 | 3:F:3284[B]:LYS:C | 2.32 | 0.51 |
| 1:G:1154:SER:HB3 | 1:G:1220:MET:HE2 | 1.93 | 0.51 |
| 3:I:2966[B]:SER:C | 3:I:2967[B]:CYS:SG | 2.94 | 0.51 |
| 3:I:2986[A]:PRO:CB | 3:I:3127[A]:TRP:CZ3 | 2.94 | 0.51 |
| 3:I:3150[B]:LYS:CB | 3:R:3159[B]:SER:O | 2.51 | 0.51 |
| 3:I:3273[A]:LEU:O | 3:I:3275[A]:LEU:HD12 | 2.11 | 0.51 |
| 1:J:552:PHE:HZ | 1:J:623:TYR:HE1 | 1.58 | 0.51 |
| 1:J:837:HIS:HA | 1:J:1113:HIS:O | 2.10 | 0.51 |
| 1:J:1155:LEU:HB2 | 1:J:1177:VAL:CG1 | 2.41 | 0.51 |
| 2:K:2556:TYR:HD1 | 2:K:2557:ALA:N | 2.08 | 0.51 |
| 3:L:2966[A]:SER:C | 3:L:2967[A]:CYS:SG | 2.94 | 0.51 |
| 3:L:3151[B]:LEU:CB | 3:L:3175[B]:TYR:CD2 | 2.93 | 0.51 |
| 3:L:3196[B]:THR:O | 3:L:3200[B]:LEU:N | 2.44 | 0.51 |
| 3:L:3300[B]:LEU:N | 3:L:3300[B]:LEU:CD2 | 2.73 | 0.51 |
| 1:M:563:ILE:O | 1:M:612:GLY:HA3 | 2.11 | 0.51 |
| 1:M:1164:ASP:OD1 | 1:M:1212:HIS:NE2 | 2.27 | 0.51 |
| 3:O:2952[B]:ALA:CB | 3:O:2956[B]:LYS:HB3 | 2.40 | 0.51 |
| 3:O:2966[A]:SER:C | 3:O:2967[A]:CYS:SG | 2.94 | 0.51 |
| 3:O:3023[B]:ILE:O | 3:O:3025[B]:VAL:N | 2.44 | 0.51 |
| 3:O:3028[B]:PRO:HG2 | 3:O:3029[B]:LYS:CG | 2.40 | 0.51 |
| 3:O:3139[B]:LEU:CD2 | 3:O:3139[B]:LEU:N | 2.73 | 0.51 |
| 3:O:3147[A]:GLU:CB | 3:O:3149[A]:ASN:ND2 | 2.73 | 0.51 |
| 3:O:3287[A]:ILE:O | 3:O:3287[A]:ILE:HG23 | 2.10 | 0.51 |
| 3:R:2928[A]:ASN:C | 3:R:2930[A]:LEU:HD22 | 2.36 | 0.51 |
| 3:R:3101[A]:PRO:HG2 | 3:R:3102[A]:TYR:CD1 | 2.46 | 0.51 |
| 3:R:3228[A]:VAL:O | 3:R:3228[A]:VAL:HG23 | 2.10 | 0.51 |
| 3:R:3275[A]:LEU:N | 3:R:3275[A]:LEU:CD1 | 2.73 | 0.51 |
| 1:S:807:GLY:HA2 | 1:S:808:THR:C | 2.36 | 0.51 |
| 3:U:2928[A]:ASN:C | 3:U:2930[A]:LEU:HD22 | 2.36 | 0.51 |
| 3:U:2986[A]:PRO:CB | 3:U:3127[A]:TRP:CZ3 | 2.94 | 0.51 |
| 3:U:3092[B]:ILE:CG2 | 3:U:3096[B]:VAL:CG2 | 2.88 | 0.51 |
| 3:U:3147[A]:GLU:CB | 3:U:3149[A]:ASN:ND2 | 2.73 | 0.51 |
| 3:U:3158[B]:PHE:HB2 | 3:d:3149[B]:ASN:CB | 2.40 | 0.51 |
| 3:U:3228[B]:VAL:HG23 | 3:U:3228[B]:VAL:O | 2.10 | 0.51 |
| 2:W:2361:LYS:HD2 | 2:W:2362:GLN:N | 2.26 | 0.51 |
| 2:W:2554:PRO:HA | 2:W:2555:GLU:HB2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W:2816:SER:HB2 | 2:W:2886:VAL:HG21 | 1.92 | 0.51 |
| 3:X:2937[A]:ASN:ND2 | 3:X:3006[A]:LYS:CD | 2.73 | 0.51 |
| 3:X:2961[B]:HIS:HB3 | 3:X:3111[B]:SER:HB3 | 1.92 | 0.51 |
| 3:X:2969[B]:TYR:CG | 3:X:2970[B]:PRO:HD2 | 2.42 | 0.51 |
| 3:X:3028[B]:PRO:HG2 | 3:X:3029[B]:LYS:CG | 2.40 | 0.51 |
| 3:X:3104[A]:MET:HA | 3:X:3110[A]:THR:CG2 | 2.17 | 0.51 |
| 3:a:3113[B]:ASP:O | 3:a:3114[B]:PRO:C | 2.53 | 0.51 |
| 3:a:3196[A]:THR:OG1 | 3:a:3199[A]:GLN:HB2 | 2.11 | 0.51 |
| 3:a:3219[A]:LEU:N | 3:a:3219[A]:LEU:CD2 | 2.73 | 0.51 |
| 3:a:3273[A]:LEU:O | 3:a:3275[A]:LEU:HD12 | 2.11 | 0.51 |
| 1:b:92:TRP:O | 1:b:212:ASN:ND2 | 2.44 | 0.51 |
| 1:b:521:THR:HA | 1:b:568:PHE:HE2 | 1.76 | 0.51 |
| 3:d:2933[B]:SER:CB | 3:d:2936[B]:GLU:CB | 2.86 | 0.51 |
| 3:d:2935[A]:ILE:CD1 | 3:d:2935[A]:ILE:N | 2.73 | 0.51 |
| 3:d:2962[A]:GLY:N | 3:d:3111[A]:SER:OG | 2.44 | 0.51 |
| 3:d:2966[A]:SER:C | 3:d:2967[A]:CYS:SG | 2.94 | 0.51 |
| 3:d:3023[B]:ILE:O | 3:d:3025[B]:VAL:N | 2.44 | 0.51 |
| 3:d:3113[B]:ASP:O | 3:d:3114[B]:PRO:C | 2.53 | 0.51 |
| 3:d:3114[B]:PRO:CD | 3:d:3115[B]:LEU:N | 2.72 | 0.51 |
| 1:A:931:TRP:CD1 | 1:A:1048:ASN:HD22 | 2.29 | 0.51 |
| 1:A:1573:CYS:HA | 1:A:1583:CYS:O | 2.11 | 0.51 |
| 2:B:2497:GLU:HB2 | 2:B:2498:VAL:HA | 1.91 | 0.51 |
| 3:C:3219[B]:LEU:N | 3:C:3219[B]:LEU:CD2 | 2.73 | 0.51 |
| 3:C:3300[B]:LEU:CD2 | 3:C:3300[B]:LEU:H | 2.24 | 0.51 |
| 1:D:1082:SER:HB3 | 1:D:1083:PRO:HD3 | 1.93 | 0.51 |
| 1:D:1358:LEU:O | 1:D:1375:ASN:ND2 | 2.38 | 0.51 |
| 2:E:2554:PRO:HA | 2:E:2555:GLU:CB | 2.41 | 0.51 |
| 3:F:3023[B]:ILE:O | 3:F:3025[B]:VAL:N | 2.44 | 0.51 |
| 3:F:3113[B]:ASP:O | 3:F:3114[B]:PRO:C | 2.53 | 0.51 |
| 3:F:3300[A]:LEU:CD2 | 3:F:3300[A]:LEU:H | 2.24 | 0.51 |
| 3:I:2952[B]:ALA:HB3 | 3:I:2954[B]:TYR:N | 2.17 | 0.51 |
| 3:I:3023[A]:ILE:O | 3:I:3025[A]:VAL:N | 2.44 | 0.51 |
| 3:I:3150[B]:LYS:O | 3:R:3172[B]:SER:CB | 2.59 | 0.51 |
| 3:I:3255[B]:PRO:HG3 | 3:R:2963[B]:MET:N | 2.25 | 0.51 |
| 1:J:898:GLY:HA2 | 1:J:1186:TRP:CB | 2.41 | 0.51 |
| 2:K:2795:ILE:O | 2:K:2799:LYS:HG3 | 2.10 | 0.51 |
| 2:K:2816:SER:HB2 | 2:K:2886:VAL:HG22 | 1.93 | 0.51 |
| 3:L:2969[A]:TYR:CE2 | 3:L:2970[A]:PRO:CG | 2.86 | 0.51 |
| 1:M:1013:ILE:HG21 | 1:M:1192:TYR:CD1 | 2.46 | 0.51 |
| 3:O:2952[A]:ALA:CA | 3:O:2956[A]:LYS:HB3 | 2.38 | 0.51 |
| 3:O:3141[A]:TYR:CD2 | 3:O:3141[A]:TYR:C | 2.86 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3153[B]:LYS:HG2 | 3:X:3176[B]:LYS:HZ1 | 1.73 | 0.51 |
| 3:O:3196[B]:THR:O | 3:O:3200[B]:LEU:N | 2.44 | 0.51 |
| 3:O:3253[B]:GLU:OE2 | 3:X:3161[B]:GLU:OE1 | 2.26 | 0.51 |
| 3:O:3300[A]:LEU:CD2 | 3:O:3300[A]:LEU:H | 2.24 | 0.51 |
| 1:P:480:CYS:HA | 1:P:490:TRP:CE2 | 2.45 | 0.51 |
| 1:P:533:VAL:HG12 | 1:P:540:THR:HG22 | 1.93 | 0.51 |
| 1:P:883:CYS:HB3 | 1:P:884:PRO:HD2 | 1.93 | 0.51 |
| 1:P:1152:LYS:HZ2 | 1:P:1183:GLU:HG2 | 1.76 | 0.51 |
| 2:Q:2446:GLU:HG2 | 2:Q:2448:THR:HG23 | 1.93 | 0.51 |
| 2:Q:2665:GLU:OE1 | 2:Q:2798:GLN:NE2 | 2.39 | 0.51 |
| 3:R:2952[B]:ALA:CB | 3:R:2956[B]:LYS:HB3 | 2.40 | 0.51 |
| 3:R:3201[A]:GLU:O | 3:R:3205[A]:LYS:HB2 | 2.11 | 0.51 |
| 3:R:3275[B]:LEU:N | 3:R:3275[B]:LEU:CD1 | 2.73 | 0.51 |
| 3:U:2952[B]:ALA:CA | 3:U:2956[B]:LYS:HB3 | 2.38 | 0.51 |
| 3:U:3101[B]:PRO:HG2 | 3:U:3102[B]:TYR:CD1 | 2.45 | 0.51 |
| 3:U:3228[A]:VAL:O | 3:U:3228[A]:VAL:HG23 | 2.10 | 0.51 |
| 1:V:1195:ASP:OD1 | 1:V:1196:ILE:N | 2.44 | 0.51 |
| 2:W:2394:VAL:HG11 | 2:W:2451:LEU:HD12 | 1.93 | 0.51 |
| 3:X:2928[A]:ASN:C | 3:X:2930[A]:LEU:HD22 | 2.36 | 0.51 |
| 3:X:3101[A]:PRO:HG2 | 3:X:3102[A]:TYR:CD1 | 2.46 | 0.51 |
| 3:X:3110[B]:THR:C | 3:X:3112[B]:TYR:N | 2.68 | 0.51 |
| 1:Y:411:ASP:OD1 | 1:Y:411:ASP:N | 2.35 | 0.51 |
| 1:Y:706:LEU:HB2 | 1:Y:713:ILE:HD11 | 1.93 | 0.51 |
| 2:Z:2224:THR:HG23 | 2:Z:2278:GLU:HB3 | 1.93 | 0.51 |
| 3:a:2937[A]:ASN:ND2 | 3:a:3006[A]:LYS:CD | 2.73 | 0.51 |
| 3:a:2952[B]:ALA:CB | 3:a:2956[B]:LYS:HB3 | 2.40 | 0.51 |
| 3:a:2986[A]:PRO:CB | 3:a:3127[A]:TRP:CZ3 | 2.94 | 0.51 |
| 3:a:3110[B]:THR:O | 3:a:3111[B]:SER:C | 2.53 | 0.51 |
| 3:a:3147[A]:GLU:CB | 3:a:3149[A]:ASN:ND2 | 2.73 | 0.51 |
| 3:a:3285[A]:VAL:CG2 | 3:a:3286[A]:THR:N | 2.73 | 0.51 |
| 3:d:2928[B]:ASN:C | 3:d:2930[B]:LEU:HD22 | 2.36 | 0.51 |
| 3:d:3004[B]:GLY:O | 3:d:3006[B]:LYS:N | 2.44 | 0.51 |
| 3:d:3113[A]:ASP:O | 3:d:3114[A]:PRO:C | 2.53 | 0.51 |
| 3:d:3147[A]:GLU:CD | 3:d:3149[A]:ASN:HD21 | 2.17 | 0.51 |
| 3:d:3196[A]:THR:OG1 | 3:d:3199[A]:GLN:HB2 | 2.11 | 0.51 |
| 3:d:3196[B]:THR:O | 3:d:3199[B]:GLN:HB2 | 2.11 | 0.51 |
| 1:A:1046:HIS:HA | 1:A:1049:VAL:HB | 1.93 | 0.51 |
| 3:C:3093[B]:HIS:CE1 | 3:C:3119[B]:HIS:CD2 | 2.92 | 0.51 |
| 3:C:3147[A]:GLU:CB | 3:C:3149[A]:ASN:ND2 | 2.73 | 0.51 |
| 3:C:3176[B]:LYS:N | 3:C:3176[B]:LYS:CE | 2.73 | 0.51 |
| 3:C:3268[A]:LYS:HG2 | 1:D:1539:GLN:HE22 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3273[B]:LEU:O | 3:C:3275[B]:LEU:HD12 | 2.11 | 0.51 |
| 3:C:3284[B]:LYS:HD3 | 3:C:3284[B]:LYS:C | 2.32 | 0.51 |
| 1:D:135:THR:O | 1:D:135:THR:OG1 | 2.28 | 0.51 |
| 1:D:316:ASN:HD21 | 1:D:340:GLN:HE21 | 1.59 | 0.51 |
| 2:E:2802:ASP:OD2 | 2:E:2903:TYR:OH | 2.18 | 0.51 |
| 3:F:2928[A]:ASN:C | 3:F:2930[A]:LEU:HD22 | 2.36 | 0.51 |
| 3:F:3110[A]:THR:C | 3:F:3112[A]:TYR:N | 2.68 | 0.51 |
| 3:F:3110[B]:THR:C | 3:F:3112[B]:TYR:N | 2.68 | 0.51 |
| 3:F:3155[B]:MET:H | 3:a:3153[B]:LYS:HB3 | 1.75 | 0.51 |
| 3:F:3155[B]:MET:O | 3:a:3153[B]:LYS:CB | 2.59 | 0.51 |
| 3:F:3254[B]:MET:CB | 3:a:2966[B]:SER:CB | 2.89 | 0.51 |
| 3:F:3273[B]:LEU:O | 3:F:3275[B]:LEU:HD12 | 2.11 | 0.51 |
| 2:H:2500:ILE:HG13 | 2:H:2501:PRO:HD2 | 1.92 | 0.51 |
| 2:H:2830:GLN:H | 2:H:2863:ARG:NH2 | 2.09 | 0.51 |
| 3:I:2928[B]:ASN:C | 3:I:2930[B]:LEU:HD22 | 2.36 | 0.51 |
| 3:I:3023[B]:ILE:O | 3:I:3025[B]:VAL:N | 2.44 | 0.51 |
| 3:I:3101[A]:PRO:HG2 | 3:I:3102[A]:TYR:CD1 | 2.46 | 0.51 |
| 3:I:3120[B]:HIS:HD2 | 3:R:2969[B]:TYR:HE2 | 1.52 | 0.51 |
| 3:I:3196[A]:THR:OG1 | 3:I:3199[A]:GLN:HB2 | 2.11 | 0.51 |
| 3:I:3228[B]:VAL:O | 3:I:3228[B]:VAL:HG23 | 2.10 | 0.51 |
| 3:I:3300[A]:LEU:CD2 | 3:I:3300[A]:LEU:H | 2.24 | 0.51 |
| 1:J:483:GLY:HA2 | 1:J:773:PHE:CZ | 2.46 | 0.51 |
| 1:J:1300:CYS:HB3 | 1:J:1494:ARG:NH1 | 2.26 | 0.51 |
| 2:K:2547:MET:O | 2:K:2751:TRP:HH2 | 1.94 | 0.51 |
| 2:K:2863:ARG:HB2 | 2:K:2865:ILE:HG12 | 1.93 | 0.51 |
| 3:L:2966[B]:SER:C | 3:L:2967[B]:CYS:SG | 2.94 | 0.51 |
| 3:L:3023[A]:ILE:O | 3:L:3025[A]:VAL:N | 2.44 | 0.51 |
| 3:O:2952[B]:ALA:CA | 3:O:2956[B]:LYS:HB3 | 2.38 | 0.51 |
| 3:O:2969[B]:TYR:CB | 3:X:2988[B]:TRP:O | 2.59 | 0.51 |
| 3:O:2976[B]:ALA:CB | 3:X:3156[B]:MET:HG2 | 2.41 | 0.51 |
| 3:O:3023[A]:ILE:O | 3:O:3025[A]:VAL:N | 2.44 | 0.51 |
| 3:O:3115[A]:LEU:HD22 | 3:O:3115[A]:LEU:O | 2.10 | 0.51 |
| 3:O:3176[A]:LYS:N | 3:O:3176[A]:LYS:CE | 2.73 | 0.51 |
| 3:O:3196[B]:THR:OG1 | 3:O:3199[B]:GLN:HB2 | 2.11 | 0.51 |
| 1:P:59:LEU:HD13 | 1:P:68:TRP:CD1 | 2.45 | 0.51 |
| 1:P:1286:ARG:HD2 | 1:P:1333:GLU:OE1 | 2.11 | 0.51 |
| 2:Q:2191:LEU:HD13 | 2:Q:2296:LEU:HD22 | 1.93 | 0.51 |
| 3:R:3023[A]:ILE:O | 3:R:3025[A]:VAL:N | 2.44 | 0.51 |
| 3:R:3300[A]:LEU:CD2 | 3:R:3300[A]:LEU:H | 2.24 | 0.51 |
| 1:S:895:CYS:O | 1:S:897:HIS:ND1 | 2.42 | 0.51 |
| 2:T:2856:ILE:HG22 | 2:T:2859:VAL:HB | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2952[A]:ALA:CB | 3:U:2956[A]:LYS:HB3 | 2.40 | 0.51 |
| 3:U:2961[B]:HIS:HB3 | 3:U:3111[B]:SER:HB3 | 1.92 | 0.51 |
| 3:U:2962[B]:GLY:N | 3:U:3111[B]:SER:OG | 2.44 | 0.51 |
| 3:U:3042[A]:ASP:N | 3:U:3042[A]:ASP:OD2 | 2.41 | 0.51 |
| 3:U:3114[B]:PRO:CD | 3:U:3115[B]:LEU:N | 2.72 | 0.51 |
| 3:U:3147[B]:GLU:CB | 3:U:3149[B]:ASN:ND2 | 2.73 | 0.51 |
| 3:U:3196[A]:THR:O | 3:U:3199[A]:GLN:HB2 | 2.11 | 0.51 |
| 3:U:3201[B]:GLU:O | 3:U:3205[B]:LYS:HB2 | 2.11 | 0.51 |
| 3:U:3300[B]:LEU:CD2 | 3:U:3300[B]:LEU:H | 2.24 | 0.51 |
| 1:V:841:LYS:HA | 1:V:1117:ASP:HB2 | 1.92 | 0.51 |
| 1:V:926:LEU:HD11 | 1:V:1043:MET:HB3 | 1.92 | 0.51 |
| 1:V:980:TYR:CE2 | 1:V:1021:LEU:HB3 | 2.46 | 0.51 |
| 1:V:1472:GLN:OE1 | 1:V:1475:ARG:NH1 | 2.44 | 0.51 |
| 2:W:2415:PRO:HG2 | 2:W:2417:VAL:O | 2.12 | 0.51 |
| 2:W:2497:GLU:HB2 | 2:W:2498:VAL:HA | 1.92 | 0.51 |
| 2:W:2569:TRP:HA | 2:W:2746:MET:HE3 | 1.92 | 0.51 |
| 3:X:3023[A]:ILE:O | 3:X:3025[A]:VAL:N | 2.44 | 0.51 |
| 3:X:3096[B]:VAL:HG11 | 3:X:3115[B]:LEU:HD12 | 1.89 | 0.51 |
| 3:X:3196[B]:THR:O | 3:X:3199[B]:GLN:HB2 | 2.11 | 0.51 |
| 1:Y:905:TRP:CZ2 | 1:Y:1083:PRO:HG2 | 2.46 | 0.51 |
| 2:Z:2172:ILE:HG13 | 2:Z:2173:VAL:HG13 | 1.93 | 0.51 |
| 3:a:3219[B]:LEU:N | 3:a:3219[B]:LEU:CD2 | 2.73 | 0.51 |
| 1:b:10:LEU:HD12 | 1:b:104:LEU:HD11 | 1.93 | 0.51 |
| 1:b:187:GLY:HA3 | 1:b:195:SER:HB3 | 1.91 | 0.51 |
| 1:b:548:ALA:O | 1:b:559:THR:HG22 | 2.11 | 0.51 |
| 1:b:1542:ARG:O | 1:b:1546:LYS:HG2 | 2.11 | 0.51 |
| 3:d:3188[B]:ASP:N | 3:d:3188[B]:ASP:OD2 | 2.36 | 0.51 |
| 3:d:3228[B]:VAL:O | 3:d:3228[B]:VAL:HG23 | 2.10 | 0.51 |
| 1:A:1596:GLU:O | 1:A:1597:THR:HG22 | 2.12 | 0.50 |
| 3:C:2975[B]:PHE:HZ | 3:L:2961[B]:HIS:CD2 | 2.28 | 0.50 |
| 3:C:3101[A]:PRO:HG2 | 3:C:3102[A]:TYR:CD1 | 2.46 | 0.50 |
| 3:C:3196[B]:THR:OG1 | 3:C:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:C:3196[B]:THR:CA | 3:C:3199[B]:GLN:OE1 | 2.58 | 0.50 |
| 3:C:3223[B]:GLY:C | 3:L:3252[B]:TYR:CZ | 2.88 | 0.50 |
| 3:C:3291[A]:ASP:OD2 | 3:C:3293[A]:LYS:NZ | 2.43 | 0.50 |
| 1:D:468:CYS:HA | 1:D:469:PRO:C | 2.37 | 0.50 |
| 1:D:490:TRP:HE1 | 1:D:670:PRO:HD3 | 1.76 | 0.50 |
| 1:D:1299:GLN:HB2 | 1:D:1311:CYS:SG | 2.52 | 0.50 |
| 2:E:2224:THR:HG23 | 2:E:2278:GLU:HB3 | 1.93 | 0.50 |
| 2:E:2795:ILE:O | 2:E:2798:GLN:HG2 | 2.11 | 0.50 |
| 3:F:2935[A]:ILE:CD1 | 3:F:2936[A]:GLU:N | 2.73 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3157[B]:PRO:CD | 3:a:3153[B]:LYS:NZ | 2.74 | 0.50 |
| 3:F:3163[B]:ASN:CG | 3:a:3149[B]:ASN:HD22 | 2.19 | 0.50 |
| 3:F:3196[B]:THR:O | 3:F:3200[B]:LEU:N | 2.43 | 0.50 |
| 3:F:3201[A]:GLU:O | 3:F:3205[A]:LYS:HB2 | 2.11 | 0.50 |
| 3:F:3255[B]:PRO:HB3 | 3:a:2964[B]:PRO:N | 2.17 | 0.50 |
| 3:F:3293[B]:LYS:CG | 3:F:3294[B]:SER:HB2 | 2.36 | 0.50 |
| 3:I:2949[B]:LYS:C | 3:I:2953[B]:GLY:H | 2.17 | 0.50 |
| 3:I:3114[A]:PRO:CD | 3:I:3115[A]:LEU:N | 2.72 | 0.50 |
| 3:I:3254[B]:MET:CE | 3:R:3157[B]:PRO:HD3 | 2.41 | 0.50 |
| 3:I:3300[B]:LEU:CD2 | 3:I:3300[B]:LEU:H | 2.24 | 0.50 |
| 1:J:622:HIS:HE1 | 1:J:767:LYS:H | 1.54 | 0.50 |
| 3:L:2952[A]:ALA:CA | 3:L:2956[A]:LYS:HB3 | 2.38 | 0.50 |
| 3:L:3147[A]:GLU:CG | 3:L:3149[A]:ASN:ND2 | 2.73 | 0.50 |
| 3:L:3217[A]:PHE:CB | 3:L:3219[A]:LEU:HD21 | 2.42 | 0.50 |
| 1:M:447:MET:HA | 1:M:455:TYR:HB2 | 1.93 | 0.50 |
| 1:M:449:ASP:OD2 | 1:M:1280:GLN:NE2 | 2.44 | 0.50 |
| 1:M:965:ASP:H | 1:M:966:SER:HA | 1.76 | 0.50 |
| 1:M:1542:ARG:O | 1:M:1546:LYS:HG2 | 2.11 | 0.50 |
| 2:N:2132:CYS:HB2 | 2:N:2142:ALA:CB | 2.41 | 0.50 |
| 2:N:2556:TYR:CE1 | 2:N:2844:MET:HG3 | 2.46 | 0.50 |
| 3:O:2935[A]:ILE:CD1 | 3:O:2936[A]:GLU:N | 2.73 | 0.50 |
| 3:O:2937[B]:ASN:ND2 | 3:O:3006[B]:LYS:CD | 2.73 | 0.50 |
| 3:O:3176[B]:LYS:H | 3:O:3176[B]:LYS:CE | 2.17 | 0.50 |
| 3:O:3188[B]:ASP:N | 3:O:3188[B]:ASP:OD2 | 2.36 | 0.50 |
| 1:P:928:TYR:HB2 | 1:P:1048:ASN:HB2 | 1.92 | 0.50 |
| 2:Q:2361:LYS:HD2 | 2:Q:2362:GLN:N | 2.26 | 0.50 |
| 3:R:2961[B]:HIS:HB3 | 3:R:3111[B]:SER:HB3 | 1.92 | 0.50 |
| 3:R:3115[B]:LEU:HD22 | 3:R:3115[B]:LEU:O | 2.10 | 0.50 |
| 3:R:3196[B]:THR:O | 3:R:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:R:3228[B]:VAL:O | 3:R:3228[B]:VAL:HG23 | 2.10 | 0.50 |
| 1:S:516:TRP:CD1 | 1:S:579:LEU:HB3 | 2.45 | 0.50 |
| 3:U:3201[A]:GLU:O | 3:U:3205[A]:LYS:HB2 | 2.11 | 0.50 |
| 3:U:3285[B]:VAL:CG2 | 3:U:3286[B]:THR:N | 2.73 | 0.50 |
| 1:V:905:TRP:HE1 | 1:V:1083:PRO:CD | 2.24 | 0.50 |
| 2:W:2180:TRP:HB3 | 2:W:2184:MET:HE2 | 1.92 | 0.50 |
| 3:X:2961[A]:HIS:CD2 | 3:X:2988[A]:TRP:CZ3 | 2.96 | 0.50 |
| 3:X:2962[B]:GLY:N | 3:X:3111[B]:SER:OG | 2.44 | 0.50 |
| 3:X:3066[B]:TYR:CE1 | 3:X:3193[B]:HIS:CE1 | 2.98 | 0.50 |
| 1:Y:462:HIS:HA | 1:Y:490:TRP:CH2 | 2.45 | 0.50 |
| 2:Z:2610:ASP:HA | 2:Z:2621:GLU:HA | 1.93 | 0.50 |
| 2:Z:2866:PRO:HG2 | 3:a:2933[A]:SER:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2928[A]:ASN:C | 3:a:2930[A]:LEU:HD22 | 2.36 | 0.50 |
| 3:a:3113[A]:ASP:O | 3:a:3114[A]:PRO:C | 2.53 | 0.50 |
| 3:a:3228[A]:VAL:O | 3:a:3228[A]:VAL:HG23 | 2.10 | 0.50 |
| 3:a:3275[B]:LEU:N | 3:a:3275[B]:LEU:CD1 | 2.73 | 0.50 |
| 1:b:1302:SER:HB3 | 1:b:1303:GLU:HA | 1.91 | 0.50 |
| 2:c:2254:THR:HG23 | 2:c:2317:LEU:HD13 | 1.93 | 0.50 |
| 2:c:2560:LEU:HD13 | 2:c:2569:TRP:CD1 | 2.47 | 0.50 |
| 3:d:2962[B]:GLY:N | 3:d:3111[B]:SER:OG | 2.44 | 0.50 |
| 3:d:3110[A]:THR:C | 3:d:3112[A]:TYR:N | 2.68 | 0.50 |
| 3:d:3147[A]:GLU:CB | 3:d:3149[A]:ASN:ND2 | 2.73 | 0.50 |
| 3:d:3151[B]:LEU:CB | 3:d:3175[B]:TYR:CD2 | 2.93 | 0.50 |
| 3:d:3173[B]:THR:HG22 | 3:d:3174[B]:GLY:H | 1.67 | 0.50 |
| 3:C:2964[B]:PRO:O | 3:L:3255[B]:PRO:HA | 2.07 | 0.50 |
| 3:C:3101[B]:PRO:HG2 | 3:C:3102[B]:TYR:CD1 | 2.46 | 0.50 |
| 3:C:3150[B]:LYS:HZ2 | 3:L:3160[B]:SER:CA | 2.19 | 0.50 |
| 3:C:3154[B]:PRO:HD3 | 3:L:3173[B]:THR:O | 2.10 | 0.50 |
| 3:C:3228[A]:VAL:HG23 | 3:C:3228[A]:VAL:O | 2.10 | 0.50 |
| 3:C:3291[B]:ASP:OD2 | 3:C:3293[B]:LYS:NZ | 2.43 | 0.50 |
| 1:D:957:ASN:N | 1:D:958:PRO:HA | 2.26 | 0.50 |
| 1:D:1030:MET:HA | 1:D:1036:SER:HA | 1.93 | 0.50 |
| 3:F:3110[A]:THR:O | 3:F:3111[A]:SER:C | 2.53 | 0.50 |
| 3:F:3135[A]:LYS:HB2 | 3:F:3141[A]:TYR:HD1 | 1.76 | 0.50 |
| 3:F:3155[B]:MET:N | 3:a:3153[B]:LYS:HB3 | 2.27 | 0.50 |
| 3:F:3176[A]:LYS:NZ | 3:F:3176[A]:LYS:CB | 2.73 | 0.50 |
| 2:H:2134:ASN:OD1 | 2:H:2137:ALA:N | 2.45 | 0.50 |
| 2:H:2833:GLY:HA3 | 2:H:2854:MET:HE1 | 1.93 | 0.50 |
| 3:I:2960[A]:PHE:CD2 | 3:I:3157[A]:PRO:CG | 2.74 | 0.50 |
| 3:I:2965[B]:LEU:CA | 3:R:3253[B]:GLU:CD | 2.68 | 0.50 |
| 3:I:2971[A]:ASP:CG | 3:I:2973[A]:THR:HG1 | 2.12 | 0.50 |
| 3:I:2980[B]:HIS:CA | 3:R:2968[B]:GLN:HG2 | 2.36 | 0.50 |
| 3:I:2986[B]:PRO:CB | 3:I:3127[B]:TRP:CZ3 | 2.94 | 0.50 |
| 3:I:3149[B]:ASN:ND2 | 3:R:3163[B]:ASN:C | 2.67 | 0.50 |
| 3:I:3159[B]:SER:HA | 3:R:3150[B]:LYS:CA | 2.32 | 0.50 |
| 3:I:3228[B]:VAL:CG2 | 3:I:3245[B]:PHE:CE2 | 2.89 | 0.50 |
| 1:J:346:GLY:O | 1:J:349:GLU:HB2 | 2.12 | 0.50 |
| 1:J:982:LYS:H | 1:J:983:PRO:HD3 | 1.76 | 0.50 |
| 1:J:1280:GLN:NE2 | 1:J:1337:ARG:HB3 | 2.26 | 0.50 |
| 2:K:2680:HIS:NE2 | 2:K:2684:HIS:CD2 | 2.79 | 0.50 |
| 3:L:2948[B]:ASP:CB | 3:L:2949[B]:LYS:CA | 2.78 | 0.50 |
| 3:L:3113[A]:ASP:O | 3:L:3114[A]:PRO:C | 2.53 | 0.50 |
| 1:M:387:ASN:OD1 | 1:M:387:ASN:N | 2.43 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:765:GLY:O | 1:M:768:GLU:HG2 | 2.10 | 0.50 |
| 2:N:2571:ARG:NH1 | 2:N:2715:ASP:OD1 | 2.44 | 0.50 |
| 3:O:3163[B]:ASN:HD22 | 3:X:3148[B]:ILE:CG2 | 2.22 | 0.50 |
| 3:O:3196[A]:THR:O | 3:O:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 3:O:3254[B]:MET:HG2 | 3:X:3159[B]:SER:CB | 2.40 | 0.50 |
| 1:P:550:ILE:HG13 | 1:P:558:HIS:H | 1.75 | 0.50 |
| 1:P:1438:ASP:OD1 | 1:P:1439:VAL:N | 2.44 | 0.50 |
| 2:Q:2390:GLN:NE2 | 2:Q:2494:GLN:O | 2.44 | 0.50 |
| 3:R:2928[B]:ASN:C | 3:R:2930[B]:LEU:HD22 | 2.36 | 0.50 |
| 3:R:3135[B]:LYS:HB2 | 3:R:3141[B]:TYR:HD1 | 1.76 | 0.50 |
| 3:R:3201[B]:GLU:O | 3:R:3205[B]:LYS:HB2 | 2.12 | 0.50 |
| 1:S:166:GLU:OE2 | 1:S:297:ARG:NH1 | 2.44 | 0.50 |
| 1:S:517:THR:HG21 | 1:S:708:PHE:HE1 | 1.76 | 0.50 |
| 1:S:1565:SER:HB3 | 1:S:1594:GLY:H | 1.75 | 0.50 |
| 1:S:1618:LEU:HD23 | 3:X:3136[B]:TYR:CE2 | 2.47 | 0.50 |
| 2:T:2816:SER:HB2 | 2:T:2886:VAL:HG21 | 1.93 | 0.50 |
| 3:U:3196[B]:THR:CA | 3:U:3199[B]:GLN:OE1 | 2.58 | 0.50 |
| 1:V:1170:MET:SD | 1:V:1199:VAL:HG23 | 2.51 | 0.50 |
| 1:V:1315:GLY:HA3 | 1:V:1601:TRP:CB | 2.41 | 0.50 |
| 2:W:2799:LYS:HA | 2:W:2803:ARG:HH12 | 1.77 | 0.50 |
| 3:X:2937[B]:ASN:ND2 | 3:X:3006[B]:LYS:CD | 2.73 | 0.50 |
| 3:X:2986[B]:PRO:CB | 3:X:3127[B]:TRP:CZ3 | 2.94 | 0.50 |
| 3:X:3228[A]:VAL:O | 3:X:3228[A]:VAL:HG23 | 2.10 | 0.50 |
| 3:X:3273[A]:LEU:O | 3:X:3275[A]:LEU:HD12 | 2.11 | 0.50 |
| 1:Y:94:TRP:CD1 | 1:Y:212:ASN:HD22 | 2.28 | 0.50 |
| 1:Y:643:ILE:HD13 | 1:Y:708:PHE:HB2 | 1.93 | 0.50 |
| 1:Y:705:THR:HG22 | 1:Y:1118:THR:HG23 | 1.92 | 0.50 |
| 1:Y:906:HIS:HA | 1:Y:909:ILE:HB | 1.92 | 0.50 |
| 1:Y:1621:ASN:CA | 3:d:3188[B]:ASP:HB2 | 2.42 | 0.50 |
| 3:a:3135[B]:LYS:HB2 | 3:a:3141[B]:TYR:HD1 | 1.76 | 0.50 |
| 3:a:3285[B]:VAL:CG2 | 3:a:3286[B]:THR:N | 2.73 | 0.50 |
| 1:b:1348:TRP:CD1 | 1:b:1403:LEU:HD13 | 2.45 | 0.50 |
| 3:d:2986[A]:PRO:CB | 3:d:3127[A]:TRP:CZ3 | 2.94 | 0.50 |
| 3:d:2986[B]:PRO:CB | 3:d:3127[B]:TRP:CZ3 | 2.94 | 0.50 |
| 3:d:3042[A]:ASP:N | 3:d:3042[A]:ASP:OD2 | 2.41 | 0.50 |
| 3:d:3201[A]:GLU:O | 3:d:3205[A]:LYS:HB2 | 2.11 | 0.50 |
| 1:A:25:MET:HE2 | 1:A:34:TYR:HA | 1.93 | 0.50 |
| 1:A:704:ASP:OD1 | 1:A:704:ASP:N | 2.41 | 0.50 |
| 1:A:943:LEU:HD13 | 1:A:944:GLU:N | 2.26 | 0.50 |
| 1:A:1299:GLN:O | 1:A:1301:PRO:HD3 | 2.11 | 0.50 |
| 3:C:2962[A]:GLY:N | 3:C:3111[A]:SER:OG | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2969[B]:TYR:CD2 | 3:C:2970[B]:PRO:CD | 2.85 | 0.50 |
| 3:C:2973[B]:THR:N | 3:L:3090[B]:ASN:HB3 | 2.26 | 0.50 |
| 3:C:3196[A]:THR:OG1 | 3:C:3199[A]:GLN:HB2 | 2.12 | 0.50 |
| 3:C:3201[A]:GLU:O | 3:C:3205[A]:LYS:HB2 | 2.11 | 0.50 |
| 1:D:4:ARG:HD2 | 1:D:89:ILE:O | 2.11 | 0.50 |
| 1:D:395:THR:HG22 | 1:D:396:ILE:HG13 | 1.92 | 0.50 |
| 1:D:754:GLU:OE2 | 1:D:799:ARG:NH2 | 2.43 | 0.50 |
| 1:D:1206:HIS:CE1 | 1:D:1209:ASP:HB3 | 2.47 | 0.50 |
| 2:E:2472:ASN:N | 2:E:2473:GLY:HA2 | 2.26 | 0.50 |
| 3:F:2982[B]:MET:CA | 3:a:3160[B]:SER:OG | 2.59 | 0.50 |
| 3:F:3004[A]:GLY:O | 3:F:3006[A]:LYS:N | 2.44 | 0.50 |
| 3:F:3023[A]:ILE:O | 3:F:3025[A]:VAL:N | 2.44 | 0.50 |
| 3:F:3066[A]:TYR:CE1 | 3:F:3193[A]:HIS:CE1 | 2.98 | 0.50 |
| 3:F:3217[B]:PHE:CB | 3:F:3219[B]:LEU:HD21 | 2.42 | 0.50 |
| 3:F:3254[B]:MET:CG | 3:a:2966[B]:SER:CB | 2.77 | 0.50 |
| 1:G:120:LYS:H | 1:G:121:ASN:HA | 1.75 | 0.50 |
| 1:G:975:PRO:HG2 | 1:G:1024:GLY:HA3 | 1.91 | 0.50 |
| 2:H:2683:ILE:O | 2:H:2687:ILE:HG12 | 2.11 | 0.50 |
| 2:H:2811:HIS:HB3 | 2:H:2847:HIS:CD2 | 2.46 | 0.50 |
| 3:I:2928[A]:ASN:C | 3:I:2930[A]:LEU:HD22 | 2.36 | 0.50 |
| 3:I:2962[B]:GLY:N | 3:I:3111[B]:SER:OG | 2.44 | 0.50 |
| 3:I:2967[B]:CYS:HB3 | 3:R:2979[B]:GLN:C | 2.15 | 0.50 |
| 3:I:2973[B]:THR:O | 3:R:3107[B]:LEU:HD12 | 2.10 | 0.50 |
| 3:I:3159[B]:SER:HA | 3:R:3150[B]:LYS:CB | 2.30 | 0.50 |
| 3:I:3161[B]:GLU:HA | 3:R:3147[B]:GLU:HG2 | 1.93 | 0.50 |
| 3:I:3196[B]:THR:OG1 | 3:I:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:I:3201[A]:GLU:O | 3:I:3205[A]:LYS:HB2 | 2.11 | 0.50 |
| 3:I:3228[A]:VAL:O | 3:I:3228[A]:VAL:HG23 | 2.10 | 0.50 |
| 3:I:3273[B]:LEU:O | 3:I:3275[B]:LEU:HD12 | 2.11 | 0.50 |
| 1:J:480:CYS:SG | 1:J:621:LEU:HD11 | 2.51 | 0.50 |
| 1:J:724:LYS:HA | 1:J:728:ARG:HH12 | 1.77 | 0.50 |
| 2:K:2868:GLU:N | 2:K:2868:GLU:OE1 | 2.45 | 0.50 |
| 3:L:2937[B]:ASN:ND2 | 3:L:3006[B]:LYS:CD | 2.73 | 0.50 |
| 3:L:2957[B]:ILE:HA | 3:L:2960[B]:PHE:HE1 | 1.64 | 0.50 |
| 3:L:3196[B]:THR:OG1 | 3:L:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:L:3307[B]:PHE:HE1 | 3:L:3309[B]:PRO:CG | 2.08 | 0.50 |
| 1:M:1348:TRP:HH2 | 1:M:1461:VAL:HG23 | 1.77 | 0.50 |
| 2:N:2180:TRP:HD1 | 2:N:2247:ILE:HD11 | 1.76 | 0.50 |
| 3:O:3110[A]:THR:O | 3:O:3111[A]:SER:C | 2.53 | 0.50 |
| 3:O:3220[A]:ARG:HH11 | 3:O:3220[A]:ARG:CG | 2.12 | 0.50 |
| 1:P:597:VAL:O | 1:P:601:VAL:HG12 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:1407:THR:HG22 | 1:P:1426:LEU:HD21 | 1.93 | 0.50 |
| 2:Q:2132:CYS:O | 2:Q:2334:LYS:HD3 | 2.11 | 0.50 |
| 3:R:3004[B]:GLY:O | 3:R:3006[B]:LYS:N | 2.44 | 0.50 |
| 3:R:3135[A]:LYS:HG3 | 3:R:3141[A]:TYR:CD1 | 2.33 | 0.50 |
| 3:R:3196[B]:THR:OG1 | 3:R:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:U:3196[B]:THR:OG1 | 3:U:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:U:3219[B]:LEU:N | 3:U:3219[B]:LEU:CD2 | 2.73 | 0.50 |
| 3:U:3276[A]:ASP:O | 3:U:3277[A]:ALA:HB3 | 2.12 | 0.50 |
| 1:V:1231:VAL:C | 1:V:1233:SER:H | 2.18 | 0.50 |
| 1:V:1427:HIS:HD2 | 1:V:1457:HIS:CE1 | 2.28 | 0.50 |
| 3:X:2952[B]:ALA:CB | 3:X:2953[B]:GLY:CA | 2.82 | 0.50 |
| 3:X:3110[B]:THR:O | 3:X:3111[B]:SER:C | 2.53 | 0.50 |
| 3:X:3196[A]:THR:O | 3:X:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 1:Y:566:ARG:HH11 | 1:Y:803:LYS:NZ | 2.09 | 0.50 |
| 3:a:2933[B]:SER:CB | 3:a:2936[B]:GLU:CB | 2.85 | 0.50 |
| 1:b:1575:PRO:HA | 1:b:1581:GLU:O | 2.11 | 0.50 |
| 3:d:2928[A]:ASN:C | 3:d:2930[A]:LEU:HD22 | 2.36 | 0.50 |
| 3:d:2961[A]:HIS:HB3 | 3:d:3111[A]:SER:HB3 | 1.92 | 0.50 |
| 3:d:2961[B]:HIS:CD2 | 3:d:2988[B]:TRP:CZ3 | 2.96 | 0.50 |
| 3:d:3196[A]:THR:O | 3:d:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 3:d:3284[A]:LYS:HE2 | 3:d:3284[A]:LYS:CA | 2.30 | 0.50 |
| 3:d:3291[A]:ASP:OD2 | 3:d:3293[A]:LYS:NZ | 2.43 | 0.50 |
| 3:d:3300[A]:LEU:CD2 | 3:d:3300[A]:LEU:H | 2.24 | 0.50 |
| 3:d:3300[B]:LEU:CD2 | 3:d:3300[B]:LEU:H | 2.24 | 0.50 |
| 4:q:1:NAG:C4 | 4:q:2:NAG:HN2 | 2.24 | 0.50 |
| 1:A:269:TYR:HA | 1:A:272:LEU:HD13 | 1.91 | 0.50 |
| 1:A:747:PHE:HB2 | 1:A:799:ARG:HB3 | 1.93 | 0.50 |
| 1:A:1210:LYS:HA | 1:A:1211:TYR:HD2 | 1.76 | 0.50 |
| 1:A:1631:GLU:OE1 | 1:b:328:LYS:NZ | 2.45 | 0.50 |
| 3:C:2928[A]:ASN:C | 3:C:2930[A]:LEU:HD22 | 2.36 | 0.50 |
| 3:C:3156[B]:MET:CG | 3:L:2984[B]:THR:OG1 | 2.59 | 0.50 |
| 1:D:73:LEU:HD11 | 1:D:210:HIS:O | 2.12 | 0.50 |
| 1:D:1249:TRP:HZ2 | 1:D:1537:ILE:HD12 | 1.76 | 0.50 |
| 2:E:2500:ILE:HD11 | 2:E:2775:GLY:O | 2.12 | 0.50 |
| 3:F:2983[B]:VAL:CG2 | 3:a:3161[B]:GLU:CB | 2.86 | 0.50 |
| 3:F:3147[A]:GLU:CG | 3:F:3149[A]:ASN:ND2 | 2.73 | 0.50 |
| 3:F:3176[B]:LYS:NZ | 3:F:3176[B]:LYS:CB | 2.73 | 0.50 |
| 3:F:3196[A]:THR:O | 3:F:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 3:F:3276[A]:ASP:O | 3:F:3277[A]:ALA:HB3 | 2.12 | 0.50 |
| 3:F:3284[A]:LYS:HD3 | 3:F:3284[A]:LYS:C | 2.32 | 0.50 |
| 1:G:37:ILE:O | 1:G:72:TYR:OH | 2.19 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1324:ARG:HG2 | 1:G:1516:VAL:HG12 | 1.93 | 0.50 |
| 3:I:3110[A]:THR:O | 3:I:3111[A]:SER:C | 2.53 | 0.50 |
| 3:I:3160[B]:SER:HA | 3:R:2983[B]:VAL:HB | 1.92 | 0.50 |
| 3:I:3162[B]:ASP:C | 3:R:3147[B]:GLU:OE1 | 2.48 | 0.50 |
| 3:I:3264[A]:TYR:C | 3:I:3264[A]:TYR:CD1 | 2.86 | 0.50 |
| 1:J:110:PHE:N | 1:J:119:LYS:O | 2.37 | 0.50 |
| 3:L:2951[A]:ASP:O | 3:L:2956[A]:LYS:HE2 | 2.09 | 0.50 |
| 3:L:3196[A]:THR:OG1 | 3:L:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 3:L:3228[A]:VAL:O | 3:L:3228[A]:VAL:HG23 | 2.10 | 0.50 |
| 3:L:3264[A]:TYR:C | 3:L:3264[A]:TYR:CD1 | 2.86 | 0.50 |
| 1:M:979:LEU:HB3 | 1:M:980:TYR:CA | 2.42 | 0.50 |
| 3:O:2962[A]:GLY:N | 3:O:3111[A]:SER:OG | 2.44 | 0.50 |
| 3:O:3042[B]:ASP:N | 3:O:3042[B]:ASP:OD2 | 2.41 | 0.50 |
| 3:O:3196[A]:THR:OG1 | 3:O:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 3:O:3276[B]:ASP:O | 3:O:3277[B]:ALA:HB3 | 2.12 | 0.50 |
| 3:O:3288[A]:MET:CA | 3:O:3295[A]:LEU:HG | 2.42 | 0.50 |
| 1:P:566:ARG:HH22 | 1:P:803:LYS:HD3 | 1.76 | 0.50 |
| 1:P:1348:TRP:CH2 | 1:P:1461:VAL:HG23 | 2.46 | 0.50 |
| 1:P:1631:GLU:OE1 | 1:S:329:ARG:NH1 | 2.44 | 0.50 |
| 3:R:2986[A]:PRO:CB | 3:R:3127[A]:TRP:CZ3 | 2.94 | 0.50 |
| 3:R:3183[A]:LEU:H | 3:R:3184[A]:ASN:CA | 2.22 | 0.50 |
| 3:R:3196[A]:THR:OG1 | 3:R:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 3:R:3196[A]:THR:O | 3:R:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 3:R:3196[B]:THR:N | 3:R:3199[B]:GLN:CB | 2.65 | 0.50 |
| 3:R:3276[B]:ASP:O | 3:R:3277[B]:ALA:HB3 | 2.12 | 0.50 |
| 2:T:2630:LYS:C | 2:T:2632:GLU:H | 2.18 | 0.50 |
| 3:U:3135[B]:LYS:HB2 | 3:U:3141[B]:TYR:HD1 | 1.76 | 0.50 |
| 3:U:3273[B]:LEU:O | 3:U:3275[B]:LEU:HD12 | 2.11 | 0.50 |
| 1:V:548:ALA:H | 1:V:559:THR:HG22 | 1.76 | 0.50 |
| 1:V:957:ASN:ND2 | 1:V:960:PHE:HB2 | 2.26 | 0.50 |
| 3:X:2962[A]:GLY:N | 3:X:3111[A]:SER:OG | 2.44 | 0.50 |
| 3:X:3023[B]:ILE:O | 3:X:3025[B]:VAL:N | 2.44 | 0.50 |
| 3:X:3196[A]:THR:O | 3:X:3200[A]:LEU:N | 2.44 | 0.50 |
| 1:Y:305:ASN:N | 1:Y:400:ILE:O | 2.27 | 0.50 |
| 1:Y:1018:ILE:HA | 1:Y:1021:LEU:HB2 | 1.93 | 0.50 |
| 1:Y:1162:ALA:HA | 1:Y:1168:GLN:O | 2.12 | 0.50 |
| 1:Y:1321:HIS:CD2 | 1:Y:1465:TRP:HH2 | 2.30 | 0.50 |
| 2:Z:2265:ILE:HD12 | 2:Z:2443:TYR:CG | 2.46 | 0.50 |
| 3:a:2935[A]:ILE:CD1 | 3:a:2936[A]:GLU:N | 2.73 | 0.50 |
| 3:a:3023[A]:ILE:O | 3:a:3025[A]:VAL:N | 2.44 | 0.50 |
| 1:b:29:GLU:OE2 | 1:b:29:GLU:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:557:VAL:HG22 | 1:b:558:HIS:HA | 1.93 | 0.50 |
| 1:b:1328:SER:HB2 | 1:b:1523:LEU:HD13 | 1.93 | 0.50 |
| 1:b:1636:ASN:C | 1:b:1638:SER:H | 2.19 | 0.50 |
| 3:d:3096[B]:VAL:HG11 | 3:d:3115[B]:LEU:HD12 | 1.89 | 0.50 |
| 3:d:3114[A]:PRO:CD | 3:d:3115[A]:LEU:N | 2.72 | 0.50 |
| 1:A:716:LEU:O | 1:A:720:VAL:HG13 | 2.11 | 0.50 |
| 1:A:1486:LEU:HD12 | 2:E:2486:ILE:HG22 | 1.92 | 0.50 |
| 3:C:2974[B]:ALA:CB | 3:L:3253[B]:GLU:OE1 | 2.58 | 0.50 |
| 3:C:3023[B]:ILE:O | 3:C:3025[B]:VAL:N | 2.44 | 0.50 |
| 3:C:3038[A]:ILE:HG23 | 3:C:3040[A]:VAL:HG22 | 1.90 | 0.50 |
| 3:C:3183[A]:LEU:H | 3:C:3184[A]:ASN:CA | 2.21 | 0.50 |
| 3:C:3220[B]:ARG:HD3 | 3:L:2964[B]:PRO:HB3 | 1.93 | 0.50 |
| 3:C:3256[B]:TRP:CA | 3:L:2965[B]:LEU:O | 2.56 | 0.50 |
| 1:D:1189:ASP:OD2 | 1:D:1190:ARG:NH1 | 2.44 | 0.50 |
| 3:F:2933[A]:SER:CB | 3:F:2936[A]:GLU:CB | 2.85 | 0.50 |
| 3:F:2986[B]:PRO:CB | 3:F:3127[B]:TRP:CZ3 | 2.94 | 0.50 |
| 3:F:3038[A]:ILE:HG23 | 3:F:3040[A]:VAL:HG22 | 1.90 | 0.50 |
| 3:F:3163[B]:ASN:ND2 | 3:a:3149[B]:ASN:CG | 2.70 | 0.50 |
| 3:F:3252[B]:TYR:O | 3:a:3252[B]:TYR:O | 2.30 | 0.50 |
| 3:F:3285[B]:VAL:CG2 | 3:F:3286[B]:THR:N | 2.73 | 0.50 |
| 1:G:197:LEU:HB3 | 1:G:344:LEU:HD13 | 1.94 | 0.50 |
| 1:G:1275:ARG:HH22 | 1:G:1357:ARG:NH1 | 2.10 | 0.50 |
| 3:I:2951[A]:ASP:O | 3:I:2956[A]:LYS:HE2 | 2.09 | 0.50 |
| 3:I:2961[A]:HIS:HB3 | 3:I:3111[A]:SER:HB3 | 1.92 | 0.50 |
| 3:I:3114[B]:PRO:CD | 3:I:3115[B]:LEU:N | 2.72 | 0.50 |
| 1:J:488:PRO:HB2 | 1:J:641:TRP:CE3 | 2.46 | 0.50 |
| 1:J:854:LEU:HG | 1:J:959:PHE:HE2 | 1.76 | 0.50 |
| 2:K:2687:ILE:HD11 | 2:K:2695:MET:HG2 | 1.93 | 0.50 |
| 3:L:2928[A]:ASN:C | 3:L:2930[A]:LEU:HD22 | 2.36 | 0.50 |
| 3:L:3196[A]:THR:O | 3:L:3200[A]:LEU:N | 2.44 | 0.50 |
| 3:L:3196[B]:THR:O | 3:L:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:L:3201[B]:GLU:O | 3:L:3205[B]:LYS:HB2 | 2.11 | 0.50 |
| 3:L:3276[B]:ASP:O | 3:L:3277[B]:ALA:HB3 | 2.12 | 0.50 |
| 2:N:2849:ASP:OD2 | 2:N:2850:ARG:NH2 | 2.45 | 0.50 |
| 3:O:3135[B]:LYS:HB2 | 3:O:3141[B]:TYR:HD1 | 1.76 | 0.50 |
| 2:Q:2240:GLN:HG3 | 2:Q:2241:THR:N | 2.26 | 0.50 |
| 3:R:2962[B]:GLY:N | 3:R:3111[B]:SER:OG | 2.44 | 0.50 |
| 3:R:2965[B]:LEU:CG | 3:R:2974[B]:ALA:CB | 2.85 | 0.50 |
| 3:R:3217[B]:PHE:CB | 3:R:3219[B]:LEU:HD21 | 2.42 | 0.50 |
| 3:R:3284[B]:LYS:HD3 | 3:R:3284[B]:LYS:C | 2.32 | 0.50 |
| 1:S:432:THR:HG23 | 1:S:435:GLU:H | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:551:GLU:OE2 | 1:S:1368:ARG:NH1 | 2.44 | 0.50 |
| 3:U:2969[A]:TYR:CD2 | 3:U:2970[A]:PRO:HD2 | 2.47 | 0.50 |
| 3:U:3066[A]:TYR:CE1 | 3:U:3193[A]:HIS:CE1 | 2.98 | 0.50 |
| 3:U:3101[A]:PRO:HG2 | 3:U:3102[A]:TYR:CD1 | 2.46 | 0.50 |
| 3:U:3113[A]:ASP:O | 3:U:3114[A]:PRO:C | 2.53 | 0.50 |
| 3:U:3172[B]:SER:N | 3:d:3152[B]:LYS:HZ1 | 2.10 | 0.50 |
| 3:U:3176[B]:LYS:N | 3:U:3176[B]:LYS:CE | 2.73 | 0.50 |
| 3:U:3217[A]:PHE:CB | 3:U:3219[A]:LEU:HD21 | 2.42 | 0.50 |
| 3:U:3219[B]:LEU:O | 3:d:2972[B]:GLY:C | 2.55 | 0.50 |
| 3:U:3254[B]:MET:O | 3:d:2975[B]:PHE:CZ | 2.63 | 0.50 |
| 3:U:3288[A]:MET:CA | 3:U:3295[A]:LEU:HG | 2.42 | 0.50 |
| 3:U:3300[A]:LEU:CD2 | 3:U:3300[A]:LEU:H | 2.24 | 0.50 |
| 1:V:622:HIS:HE1 | 1:V:767:LYS:H | 1.60 | 0.50 |
| 1:V:963:ALA:HB3 | 1:V:1038:PHE:O | 2.10 | 0.50 |
| 2:W:2742:MET:HE3 | 2:W:2769:PHE:HE2 | 1.76 | 0.50 |
| 3:X:3276[B]:ASP:O | 3:X:3277[B]:ALA:HB3 | 2.12 | 0.50 |
| 1:Y:492:ARG:NH1 | 1:Y:638:ASP:OD1 | 2.45 | 0.50 |
| 1:Y:566:ARG:N | 1:Y:567:LEU:HA | 2.25 | 0.50 |
| 2:Z:2486:ILE:HB | 1:b:1487:PRO:HD3 | 1.92 | 0.50 |
| 3:a:3023[B]:ILE:O | 3:a:3025[B]:VAL:N | 2.44 | 0.50 |
| 3:a:3151[B]:LEU:CB | 3:a:3175[B]:TYR:CD2 | 2.93 | 0.50 |
| 3:a:3196[B]:THR:O | 3:a:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 1:b:573:LYS:HB3 | 1:b:574:GLY:HA2 | 1.93 | 0.50 |
| 1:b:704:ASP:N | 1:b:704:ASP:OD1 | 2.44 | 0.50 |
| 1:b:1421:VAL:HG23 | 1:b:1422:HIS:HD1 | 1.76 | 0.50 |
| 2:c:2107:LEU:HA | 2:c:2110:MET:HG2 | 1.94 | 0.50 |
| 2:c:2571:ARG:NH1 | 2:c:2715:ASP:OD1 | 2.44 | 0.50 |
| 3:d:2966[B]:SER:C | 3:d:2967[B]:CYS:SG | 2.94 | 0.50 |
| 3:d:3176[A]:LYS:N | 3:d:3176[A]:LYS:CE | 2.73 | 0.50 |
| 3:d:3217[A]:PHE:CB | 3:d:3219[A]:LEU:HD21 | 2.42 | 0.50 |
| 3:C:2966[A]:SER:C | 3:C:2967[A]:CYS:SG | 2.94 | 0.50 |
| 3:C:3285[A]:VAL:CG2 | 3:C:3286[A]:THR:N | 2.73 | 0.50 |
| 3:F:2985[B]:PHE:CE2 | 3:a:2970[B]:PRO:HA | 2.40 | 0.50 |
| 3:F:3028[B]:PRO:HG2 | 3:F:3029[B]:LYS:CG | 2.40 | 0.50 |
| 3:F:3219[B]:LEU:N | 3:F:3219[B]:LEU:CD2 | 2.73 | 0.50 |
| 3:F:3288[A]:MET:CA | 3:F:3295[A]:LEU:HG | 2.42 | 0.50 |
| 1:G:307:ARG:HH12 | 1:G:484:MET:HE1 | 1.77 | 0.50 |
| 1:G:474:LEU:HD22 | 1:G:475:ASN:H | 1.77 | 0.50 |
| 1:G:594:ASP:OD1 | 1:G:775:ARG:NH1 | 2.45 | 0.50 |
| 1:G:896:HIS:HB2 | 1:G:905:TRP:CG | 2.47 | 0.50 |
| 1:G:931:TRP:CZ3 | 1:G:995:ILE:HD11 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:2568:HIS:NE2 | 2:H:2669:TYR:OH | 2.44 | 0.50 |
| 2:H:2800:LYS:O | 3:I:3023[A]:ILE:HD13 | 2.03 | 0.50 |
| 3:I:3147[A]:GLU:CG | 3:I:3149[A]:ASN:ND2 | 2.73 | 0.50 |
| 3:I:3252[B]:TYR:CD1 | 3:R:3108[B]:HIS:CE1 | 2.99 | 0.50 |
| 3:I:3284[A]:LYS:HD3 | 3:I:3284[A]:LYS:C | 2.32 | 0.50 |
| 1:J:1427:HIS:CE1 | 1:J:1457:HIS:CE1 | 2.99 | 0.50 |
| 3:L:2952[B]:ALA:CB | 3:L:2956[B]:LYS:HB3 | 2.40 | 0.50 |
| 3:L:2969[A]:TYR:CD2 | 3:L:2970[A]:PRO:HD2 | 2.47 | 0.50 |
| 3:L:3217[B]:PHE:CB | 3:L:3219[B]:LEU:HD21 | 2.42 | 0.50 |
| 3:L:3300[A]:LEU:CD2 | 3:L:3300[A]:LEU:H | 2.24 | 0.50 |
| 3:L:3300[B]:LEU:CD2 | 3:L:3300[B]:LEU:H | 2.24 | 0.50 |
| 1:M:157:GLU:OE2 | 1:M:296:ARG:NH2 | 2.41 | 0.50 |
| 1:M:1323:HIS:CD2 | 1:M:1458:HIS:CE1 | 3.00 | 0.50 |
| 1:M:1339:SER:CB | 1:M:1340:GLY:HA2 | 2.42 | 0.50 |
| 2:N:2548:CYS:HB2 | 2:N:2558:CYS:HA | 1.93 | 0.50 |
| 2:N:2647:LEU:HD12 | 2:N:2656:LEU:HB2 | 1.94 | 0.50 |
| 3:O:2965[B]:LEU:CG | 3:O:2974[B]:ALA:CB | 2.85 | 0.50 |
| 3:O:3141[B]:TYR:CD2 | 3:O:3141[B]:TYR:C | 2.86 | 0.50 |
| 3:O:3276[A]:ASP:O | 3:O:3277[A]:ALA:HB3 | 2.12 | 0.50 |
| 2:Q:2394:VAL:HG11 | 2:Q:2451:LEU:HD12 | 1.93 | 0.50 |
| 3:R:3217[A]:PHE:CB | 3:R:3219[A]:LEU:HD21 | 2.42 | 0.50 |
| 3:R:3300[B]:LEU:CD2 | 3:R:3300[B]:LEU:H | 2.24 | 0.50 |
| 2:T:2303:ARG:NH2 | 2:T:2372:GLU:O | 2.44 | 0.50 |
| 3:U:3023[B]:ILE:O | 3:U:3025[B]:VAL:N | 2.44 | 0.50 |
| 3:U:3176[B]:LYS:NZ | 3:U:3176[B]:LYS:CB | 2.73 | 0.50 |
| 3:U:3196[B]:THR:O | 3:U:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:U:3273[A]:LEU:O | 3:U:3275[A]:LEU:HD12 | 2.11 | 0.50 |
| 3:U:3291[B]:ASP:OD2 | 3:U:3293[B]:LYS:NZ | 2.43 | 0.50 |
| 1:V:904:HIS:O | 1:V:907:ARG:HB3 | 2.12 | 0.50 |
| 2:W:2390:GLN:NE2 | 2:W:2494:GLN:O | 2.44 | 0.50 |
| 3:X:3196[A]:THR:OG1 | 3:X:3199[A]:GLN:HB2 | 2.12 | 0.50 |
| 3:X:3196[B]:THR:OG1 | 3:X:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:X:3264[B]:TYR:C | 3:X:3264[B]:TYR:CD1 | 2.86 | 0.50 |
| 3:X:3285[B]:VAL:CG2 | 3:X:3286[B]:THR:N | 2.73 | 0.50 |
| 3:X:3300[B]:LEU:CD2 | 3:X:3300[B]:LEU:H | 2.24 | 0.50 |
| 1:Y:1315:GLY:HA3 | 1:Y:1601:TRP:CB | 2.42 | 0.50 |
| 2:Z:2244:PHE:HZ | 2:Z:2376:MET:HE1 | 1.76 | 0.50 |
| 3:a:2935[B]:ILE:CD1 | 3:a:2936[B]:GLU:N | 2.73 | 0.50 |
| 3:a:2969[A]:TYR:CD2 | 3:a:2970[A]:PRO:HD2 | 2.47 | 0.50 |
| 3:a:3101[B]:PRO:HG2 | 3:a:3102[B]:TYR:CD1 | 2.46 | 0.50 |
| 3:a:3217[A]:PHE:CB | 3:a:3219[A]:LEU:HD21 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3023[A]:ILE:O | 3:d:3025[A]:VAL:N | 2.44 | 0.50 |
| 3:d:3135[B]:LYS:HB2 | 3:d:3141[B]:TYR:HD1 | 1.76 | 0.50 |
| 1:A:500:ASN:O | 1:A:504:THR:OG1 | 2.23 | 0.50 |
| 2:B:2242:TRP:O | 2:B:2246:ASN:ND2 | 2.36 | 0.50 |
| 3:C:3196[A]:THR:CA | 3:C:3199[A]:GLN:OE1 | 2.58 | 0.50 |
| 3:C:3196[B]:THR:O | 3:C:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 3:C:3249[B]:GLY:O | 3:L:3252[B]:TYR:CD2 | 2.65 | 0.50 |
| 1:D:1279:LYS:O | 1:D:1282:ALA:N | 2.42 | 0.50 |
| 3:F:2966[A]:SER:C | 3:F:2967[A]:CYS:SG | 2.94 | 0.50 |
| 3:F:2969[A]:TYR:CD2 | 3:F:2970[A]:PRO:HD2 | 2.47 | 0.50 |
| 3:F:3160[B]:SER:OG | 3:a:2982[B]:MET:C | 2.54 | 0.50 |
| 3:F:3160[B]:SER:OG | 3:a:2983[B]:VAL:HG23 | 2.12 | 0.50 |
| 2:H:2546:LEU:HA | 2:H:2557:ALA:HA | 1.93 | 0.50 |
| 3:I:3135[A]:LYS:HB2 | 3:I:3141[A]:TYR:HD1 | 1.76 | 0.50 |
| 3:I:3156[B]:MET:N | 3:R:2979[B]:GLN:NE2 | 2.56 | 0.50 |
| 1:J:516:TRP:HZ3 | 1:J:633:HIS:HD1 | 1.60 | 0.50 |
| 1:J:718:ARG:HG3 | 1:J:832:LYS:HB2 | 1.92 | 0.50 |
| 3:L:3201[A]:GLU:O | 3:L:3205[A]:LYS:HB2 | 2.11 | 0.50 |
| 3:L:3288[B]:MET:CA | 3:L:3295[B]:LEU:HG | 2.42 | 0.50 |
| 1:M:1141:ARG:HB2 | 1:M:1197:THR:OG1 | 2.12 | 0.50 |
| 3:O:2965[B]:LEU:C | 3:X:3254[B]:MET:HE1 | 2.34 | 0.50 |
| 3:O:3147[A]:GLU:CG | 3:O:3149[A]:ASN:ND2 | 2.73 | 0.50 |
| 3:O:3291[B]:ASP:OD2 | 3:O:3293[B]:LYS:NZ | 2.43 | 0.50 |
| 1:P:898:GLY:HA2 | 1:P:1186:TRP:HB2 | 1.93 | 0.50 |
| 3:R:2949[B]:LYS:C | 3:R:2949[B]:LYS:CD | 2.85 | 0.50 |
| 3:R:3298[B]:ASN:HA | 3:R:3299[B]:LEU:HB3 | 1.88 | 0.50 |
| 2:T:2261:VAL:HG21 | 2:T:2441:ARG:HG3 | 1.93 | 0.50 |
| 2:T:2415:PRO:HD3 | 2:T:2454:MET:HE1 | 1.93 | 0.50 |
| 2:T:2830:GLN:OE1 | 2:T:2863:ARG:NH1 | 2.44 | 0.50 |
| 1:V:166:GLU:OE2 | 1:V:297:ARG:NH1 | 2.45 | 0.50 |
| 1:V:718:ARG:HH11 | 1:V:830:ASN:ND2 | 2.10 | 0.50 |
| 3:X:2949[B]:LYS:C | 3:X:2949[B]:LYS:CD | 2.85 | 0.50 |
| 3:X:2949[B]:LYS:C | 3:X:2949[B]:LYS:HZ3 | 2.12 | 0.50 |
| 3:X:3196[B]:THR:CA | 3:X:3199[B]:GLN:OE1 | 2.58 | 0.50 |
| 3:a:2961[A]:HIS:CD2 | 3:a:2988[A]:TRP:CZ3 | 2.96 | 0.50 |
| 3:a:3110[B]:THR:C | 3:a:3112[B]:TYR:N | 2.68 | 0.50 |
| 3:a:3196[A]:THR:O | 3:a:3199[A]:GLN:HB2 | 2.11 | 0.50 |
| 3:a:3217[B]:PHE:CB | 3:a:3219[B]:LEU:HD21 | 2.42 | 0.50 |
| 3:a:3288[A]:MET:CA | 3:a:3295[A]:LEU:HG | 2.42 | 0.50 |
| 3:d:3147[A]:GLU:CG | 3:d:3149[A]:ASN:ND2 | 2.73 | 0.50 |
| 3:d:3211[B]:ASP:OD1 | 3:d:3211[B]:ASP:N | 2.28 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:119:LYS:HB3 | 1:A:120:LYS:HD2 | 1.93 | 0.50 |
| 1:A:637:VAL:HA | 1:A:640:LEU:HD12 | 1.94 | 0.50 |
| 1:A:1078:ARG:NH2 | 2:E:2877:ILE:O | 2.45 | 0.50 |
| 2:B:2749:PHE:O | 2:B:2754:ASN:ND2 | 2.31 | 0.50 |
| 3:C:2935[A]:ILE:CD1 | 3:C:2935[A]:ILE:H | 2.25 | 0.50 |
| 3:C:3110[B]:THR:O | 3:C:3111[B]:SER:C | 2.53 | 0.50 |
| 3:C:3135[B]:LYS:HB2 | 3:C:3141[B]:TYR:HD1 | 1.76 | 0.50 |
| 1:D:443:MET:HE3 | 1:D:447:MET:HE2 | 1.93 | 0.50 |
| 2:E:2157:LEU:O | 2:E:2160:VAL:HG22 | 2.12 | 0.50 |
| 2:E:2248:ILE:HG13 | 2:E:2373:MET:HE2 | 1.94 | 0.50 |
| 3:F:2939[B]:ARG:NE | 3:F:3031[B]:ASN:ND2 | 2.60 | 0.50 |
| 3:F:2962[B]:GLY:N | 3:F:3111[B]:SER:OG | 2.44 | 0.50 |
| 3:F:2986[A]:PRO:CB | 3:F:3127[A]:TRP:CZ3 | 2.94 | 0.50 |
| 3:F:3255[B]:PRO:CA | 3:a:2966[B]:SER:N | 2.75 | 0.50 |
| 3:F:3273[A]:LEU:HB2 | 3:F:3275[A]:LEU:CD1 | 2.34 | 0.50 |
| 3:F:3300[B]:LEU:CD2 | 3:F:3300[B]:LEU:H | 2.24 | 0.50 |
| 1:G:120:LYS:HB3 | 1:G:122:VAL:N | 2.27 | 0.50 |
| 1:G:1087:ALA:HB3 | 1:G:1090:ILE:HG13 | 1.92 | 0.50 |
| 3:I:2949[B]:LYS:C | 3:I:2949[B]:LYS:CD | 2.85 | 0.50 |
| 3:I:2960[A]:PHE:CD1 | 3:I:2960[A]:PHE:N | 2.72 | 0.50 |
| 3:I:3155[B]:MET:HE3 | 3:R:3156[B]:MET:H | 1.77 | 0.50 |
| 1:J:1582:ASN:HB3 | 1:J:1583:CYS:HB3 | 1.94 | 0.50 |
| 3:L:3220[A]:ARG:HH11 | 3:L:3220[A]:ARG:CG | 2.12 | 0.50 |
| 3:L:3293[B]:LYS:HB2 | 3:L:3294[B]:SER:CA | 2.41 | 0.50 |
| 3:O:2969[A]:TYR:CD2 | 3:O:2970[A]:PRO:HD2 | 2.47 | 0.50 |
| 3:O:3159[B]:SER:C | 3:X:3151[B]:LEU:HD12 | 2.37 | 0.50 |
| 3:O:3228[B]:VAL:O | 3:O:3228[B]:VAL:HG23 | 2.10 | 0.50 |
| 1:P:450:LYS:HE3 | 1:P:451:SER:H | 1.77 | 0.50 |
| 1:P:843:VAL:HG22 | 1:P:928:TYR:O | 2.12 | 0.50 |
| 1:P:1132:GLU:OE2 | 1:P:1136:ARG:NE | 2.31 | 0.50 |
| 3:R:2937[B]:ASN:ND2 | 3:R:3006[B]:LYS:CD | 2.73 | 0.50 |
| 3:R:2962[A]:GLY:N | 3:R:3111[A]:SER:OG | 2.44 | 0.50 |
| 3:R:3042[B]:ASP:N | 3:R:3042[B]:ASP:OD2 | 2.41 | 0.50 |
| 3:R:3113[A]:ASP:O | 3:R:3114[A]:PRO:C | 2.53 | 0.50 |
| 3:R:3151[B]:LEU:CB | 3:R:3175[B]:TYR:CD2 | 2.93 | 0.50 |
| 1:S:855:ARG:HD2 | 1:S:947:TYR:CD2 | 2.46 | 0.50 |
| 1:S:930:ASP:OD1 | 1:S:1051:ARG:NH2 | 2.44 | 0.50 |
| 2:T:2097:LEU:HD12 | 2:W:2235:PRO:HG2 | 1.94 | 0.50 |
| 3:U:2948[A]:ASP:CB | 3:U:2949[A]:LYS:CA | 2.78 | 0.50 |
| 3:U:2949[A]:LYS:C | 3:U:2949[A]:LYS:CD | 2.85 | 0.50 |
| 3:U:2949[B]:LYS:C | 3:U:2949[B]:LYS:CD | 2.85 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2960[B]:PHE:CD1 | 3:U:2960[B]:PHE:N | 2.72 | 0.50 |
| 3:U:3258[B]:PHE:N | 3:d:2969[B]:TYR:O | 2.45 | 0.50 |
| 3:U:3293[B]:LYS:HB2 | 3:U:3294[B]:SER:CA | 2.41 | 0.50 |
| 1:V:1423:TYR:OH | 1:V:1461:VAL:O | 2.25 | 0.50 |
| 1:V:1427:HIS:HD2 | 1:V:1457:HIS:HE1 | 1.59 | 0.50 |
| 2:W:2128:LEU:HD23 | 2:W:2216:PHE:HZ | 1.76 | 0.50 |
| 3:X:3004[B]:GLY:O | 3:X:3006[B]:LYS:N | 2.44 | 0.50 |
| 3:X:3110[A]:THR:C | 3:X:3112[A]:TYR:H | 2.20 | 0.50 |
| 3:X:3135[A]:LYS:HB2 | 3:X:3141[A]:TYR:HD1 | 1.76 | 0.50 |
| 3:X:3217[A]:PHE:CB | 3:X:3219[A]:LEU:HD21 | 2.42 | 0.50 |
| 3:X:3288[A]:MET:CA | 3:X:3295[A]:LEU:HG | 2.42 | 0.50 |
| 1:Y:305:ASN:HB3 | 1:Y:400:ILE:HB | 1.94 | 0.50 |
| 1:Y:1008:GLU:HA | 1:Y:1011:TYR:HB3 | 1.93 | 0.50 |
| 3:a:3004[A]:GLY:O | 3:a:3006[A]:LYS:N | 2.44 | 0.50 |
| 3:a:3291[A]:ASP:OD2 | 3:a:3293[A]:LYS:NZ | 2.43 | 0.50 |
| 1:b:1170:MET:HB3 | 1:b:1203:MET:HE2 | 1.94 | 0.50 |
| 2:c:2740:ASP:OD2 | 2:c:2741:GLN:HG2 | 2.12 | 0.50 |
| 3:d:2949[A]:LYS:C | 3:d:2949[A]:LYS:CD | 2.85 | 0.50 |
| 3:d:3110[A]:THR:O | 3:d:3111[A]:SER:C | 2.53 | 0.50 |
| 3:d:3288[B]:MET:CA | 3:d:3295[B]:LEU:HG | 2.42 | 0.50 |
| 1:A:1639:LYS:CB | 1:b:472:ASP:HB3 | 2.40 | 0.50 |
| 2:B:2161:GLN:NE2 | 2:B:2348:THR:HG21 | 2.27 | 0.50 |
| 3:C:2928[B]:ASN:C | 3:C:2930[B]:LEU:HD22 | 2.36 | 0.50 |
| 3:C:3151[B]:LEU:CA | 3:L:3154[B]:PRO:HB2 | 2.40 | 0.50 |
| 3:C:3152[B]:LYS:HG3 | 3:L:3172[B]:SER:HG | 1.75 | 0.50 |
| 3:C:3276[A]:ASP:O | 3:C:3277[A]:ALA:HB3 | 2.12 | 0.50 |
| 1:D:1321:HIS:O | 1:D:1324:ARG:HB3 | 2.11 | 0.50 |
| 2:E:2603:PRO:HG2 | 2:E:2606:LEU:HD12 | 1.93 | 0.50 |
| 3:F:3196[B]:THR:OG1 | 3:F:3199[B]:GLN:HG3 | 2.12 | 0.50 |
| 3:F:3262[A]:PHE:C | 3:F:3263[A]:LEU:HD12 | 2.37 | 0.50 |
| 1:G:127:GLU:CG | 1:G:135:THR:H | 2.24 | 0.50 |
| 3:I:2952[B]:ALA:CA | 3:I:2956[B]:LYS:HB3 | 2.38 | 0.50 |
| 3:I:2969[A]:TYR:CE2 | 3:I:2970[A]:PRO:CG | 2.86 | 0.50 |
| 3:I:2971[B]:ASP:CG | 3:I:2973[B]:THR:HG1 | 2.15 | 0.50 |
| 3:I:3276[A]:ASP:O | 3:I:3277[A]:ALA:HB3 | 2.12 | 0.50 |
| 1:J:41:HIS:NE2 | 1:J:58:CYS:SG | 2.85 | 0.50 |
| 1:J:69:HIS:CD2 | 9:J:5001:CUO:O1 | 2.64 | 0.50 |
| 1:J:931:TRP:CZ3 | 1:J:995:ILE:HD11 | 2.46 | 0.50 |
| 2:K:2282:LEU:HD21 | 2:K:2294:PHE:HA | 1.94 | 0.50 |
| 3:L:2981[A]:GLY:N | 3:L:3086[A]:GLU:OE1 | 2.45 | 0.50 |
| 3:L:3262[A]:PHE:C | 3:L:3263[A]:LEU:HD12 | 2.37 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2960[B]:PHE:CD2 | 3:O:3157[B]:PRO:CG | 2.74 | 0.50 |
| 3:O:3102[B]:TYR:HA | 3:X:2971[B]:ASP:CA | 2.42 | 0.50 |
| 3:O:3196[B]:THR:O | 3:O:3199[B]:GLN:HB2 | 2.11 | 0.50 |
| 1:P:1604:ASP:OD1 | 1:P:1605:ARG:NH1 | 2.44 | 0.50 |
| 3:R:2966[A]:SER:C | 3:R:2967[A]:CYS:SG | 2.94 | 0.50 |
| 3:R:3110[B]:THR:C | 3:R:3112[B]:TYR:N | 2.68 | 0.50 |
| 1:S:514:TRP:CZ2 | 1:S:606:ILE:HD11 | 2.47 | 0.50 |
| 1:S:1231:VAL:O | 1:S:1233:SER:N | 2.44 | 0.50 |
| 1:S:1467:ILE:HD13 | 1:S:1532:PHE:HB2 | 1.93 | 0.50 |
| 2:T:2107:LEU:O | 2:T:2111:GLN:HB2 | 2.12 | 0.50 |
| 3:U:2935[B]:ILE:CD1 | 3:U:2935[B]:ILE:H | 2.25 | 0.50 |
| 3:U:2966[B]:SER:C | 3:U:2967[B]:CYS:SG | 2.94 | 0.50 |
| 3:U:2969[B]:TYR:CD2 | 3:U:2970[B]:PRO:HD2 | 2.47 | 0.50 |
| 3:U:3159[B]:SER:HB2 | 3:d:3150[B]:LYS:HE3 | 1.90 | 0.50 |
| 3:U:3283[A]:ILE:C | 3:U:3283[A]:ILE:CD1 | 2.85 | 0.50 |
| 1:V:372:ALA:O | 1:V:375:SER:OG | 2.26 | 0.50 |
| 1:V:730:PHE:N | 1:V:821:ILE:O | 2.27 | 0.50 |
| 1:V:882:TRP:CD1 | 1:V:1086:LEU:HD11 | 2.47 | 0.50 |
| 1:V:1324:ARG:NH1 | 1:V:1519:TYR:HB3 | 2.26 | 0.50 |
| 3:X:2928[B]:ASN:C | 3:X:2930[B]:LEU:HD22 | 2.36 | 0.50 |
| 3:X:3093[B]:HIS:HB2 | 3:X:3248[B]:LEU:HD13 | 1.94 | 0.50 |
| 3:X:3262[B]:PHE:C | 3:X:3263[B]:LEU:HD12 | 2.37 | 0.50 |
| 2:Z:2736:TYR:HB3 | 1:b:1236:TYR:HB3 | 1.93 | 0.50 |
| 3:a:3004[B]:GLY:O | 3:a:3006[B]:LYS:N | 2.44 | 0.50 |
| 3:a:3300[A]:LEU:CD2 | 3:a:3300[A]:LEU:H | 2.24 | 0.50 |
| 1:b:132:ASN:OD1 | 1:b:132:ASN:N | 2.45 | 0.50 |
| 1:b:757:VAL:O | 1:b:779:HIS:HE1 | 1.95 | 0.50 |
| 1:b:931:TRP:NE1 | 1:b:1048:ASN:HD22 | 2.10 | 0.50 |
| 2:c:2807:GLY:O | 2:c:2899:PRO:HA | 2.12 | 0.50 |
| 3:d:2954[A]:TYR:C | 3:d:2957[A]:ILE:HG22 | 2.37 | 0.50 |
| 3:d:3288[A]:MET:CA | 3:d:3295[A]:LEU:HG | 2.42 | 0.50 |
| 3:d:3293[A]:LYS:HB2 | 3:d:3294[A]:SER:CA | 2.41 | 0.50 |
| 1:A:874:ALA:HA | 1:A:913:PHE:HZ | 1.76 | 0.49 |
| 3:C:2952[A]:ALA:CA | 3:C:2956[A]:LYS:HB3 | 2.38 | 0.49 |
| 3:C:2962[B]:GLY:N | 3:C:3111[B]:SER:OG | 2.44 | 0.49 |
| 3:C:3135[A]:LYS:HB2 | 3:C:3141[A]:TYR:HD1 | 1.76 | 0.49 |
| 3:C:3173[B]:THR:HA | 3:L:3153[B]:LYS:C | 2.37 | 0.49 |
| 3:C:3183[B]:LEU:N | 3:C:3184[B]:ASN:HA | 2.12 | 0.49 |
| 3:C:3201[B]:GLU:O | 3:C:3205[B]:LYS:HB2 | 2.11 | 0.49 |
| 3:C:3262[A]:PHE:C | 3:C:3263[A]:LEU:HD12 | 2.37 | 0.49 |
| 1:D:567:LEU:HD11 | 1:D:579:LEU:HD11 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:891:LYS:HB2 | 1:D:892:TYR:CD2 | 2.47 | 0.49 |
| 1:D:1361:GLU:HG3 | 1:D:1363:THR:H | 1.77 | 0.49 |
| 3:F:3150[B]:LYS:C | 3:a:3172[B]:SER:CB | 2.85 | 0.49 |
| 3:F:3151[A]:LEU:CB | 3:F:3175[A]:TYR:CD2 | 2.93 | 0.49 |
| 3:F:3151[B]:LEU:CB | 3:F:3175[B]:TYR:CD2 | 2.93 | 0.49 |
| 3:F:3154[B]:PRO:CG | 3:a:3174[B]:GLY:CA | 2.86 | 0.49 |
| 3:F:3160[B]:SER:CB | 3:a:2983[B]:VAL:HG23 | 2.37 | 0.49 |
| 3:F:3173[B]:THR:HG22 | 3:F:3174[B]:GLY:H | 1.67 | 0.49 |
| 3:F:3252[B]:TYR:O | 3:a:3253[B]:GLU:HA | 2.12 | 0.49 |
| 3:F:3255[B]:PRO:HG3 | 3:a:2963[B]:MET:CA | 2.41 | 0.49 |
| 1:G:1033:LEU:HD11 | 1:G:1183:GLU:HB2 | 1.93 | 0.49 |
| 3:I:2949[A]:LYS:C | 3:I:2949[A]:LYS:CD | 2.85 | 0.49 |
| 3:I:2952[A]:ALA:N | 3:I:2953[A]:GLY:HA2 | 2.06 | 0.49 |
| 3:I:3110[B]:THR:C | 3:I:3112[B]:TYR:H | 2.20 | 0.49 |
| 3:I:3196[B]:THR:O | 3:I:3199[B]:GLN:HB2 | 2.11 | 0.49 |
| 3:I:3288[B]:MET:CA | 3:I:3295[B]:LEU:HG | 2.42 | 0.49 |
| 1:J:329:ARG:HB3 | 1:M:1584:GLY:N | 2.26 | 0.49 |
| 1:J:972:SER:HA | 1:J:1028:VAL:HG22 | 1.94 | 0.49 |
| 1:J:1316:MET:HB3 | 1:J:1318:VAL:HG22 | 1.94 | 0.49 |
| 3:L:2954[A]:TYR:C | 3:L:2957[A]:ILE:HG22 | 2.37 | 0.49 |
| 3:L:2986[A]:PRO:CB | 3:L:3127[A]:TRP:CZ3 | 2.94 | 0.49 |
| 3:L:2986[B]:PRO:CB | 3:L:3127[B]:TRP:CZ3 | 2.94 | 0.49 |
| 3:L:3176[B]:LYS:NZ | 3:L:3176[B]:LYS:CB | 2.73 | 0.49 |
| 3:O:2939[B]:ARG:NE | 3:O:3031[B]:ASN:ND2 | 2.60 | 0.49 |
| 3:O:2969[B]:TYR:CG | 3:O:2970[B]:PRO:HD2 | 2.42 | 0.49 |
| 3:O:3038[A]:ILE:HG23 | 3:O:3040[A]:VAL:HG22 | 1.90 | 0.49 |
| 3:O:3093[A]:HIS:HB2 | 3:O:3248[A]:LEU:HD13 | 1.94 | 0.49 |
| 1:P:1034:GLU:HB2 | 1:P:1180:SER:OG | 2.12 | 0.49 |
| 1:P:1475:ARG:NE | 1:P:1541:GLU:OE2 | 2.30 | 0.49 |
| 3:R:3066[A]:TYR:CE1 | 3:R:3193[A]:HIS:CE1 | 2.98 | 0.49 |
| 3:R:3176[A]:LYS:N | 3:R:3176[A]:LYS:CE | 2.73 | 0.49 |
| 3:R:3196[B]:THR:OG1 | 3:R:3199[B]:GLN:HG3 | 2.12 | 0.49 |
| 3:R:3262[B]:PHE:C | 3:R:3263[B]:LEU:HD12 | 2.37 | 0.49 |
| 3:R:3293[A]:LYS:HB2 | 3:R:3294[A]:SER:CA | 2.41 | 0.49 |
| 3:U:2939[A]:ARG:NE | 3:U:3031[A]:ASN:ND2 | 2.60 | 0.49 |
| 3:U:2954[B]:TYR:C | 3:U:2957[B]:ILE:HG22 | 2.37 | 0.49 |
| 3:U:3093[B]:HIS:HB2 | 3:U:3248[B]:LEU:HD13 | 1.94 | 0.49 |
| 3:U:3104[A]:MET:HA | 3:U:3110[A]:THR:CG2 | 2.17 | 0.49 |
| 3:U:3135[A]:LYS:HB2 | 3:U:3141[A]:TYR:HD1 | 1.76 | 0.49 |
| 3:U:3196[A]:THR:OG1 | 3:U:3199[A]:GLN:HB2 | 2.12 | 0.49 |
| 3:U:3256[B]:TRP:CA | 3:d:2969[B]:TYR:H | 2.25 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:843:VAL:HG11 | 1:V:1044:LEU:HD13 | 1.93 | 0.49 |
| 1:V:1396:GLU:OE2 | 1:V:1569:ARG:NH2 | 2.45 | 0.49 |
| 2:W:2257:CYS:O | 2:W:2261:VAL:HG23 | 2.12 | 0.49 |
| 3:X:2935[A]:ILE:CD1 | 3:X:2935[A]:ILE:H | 2.25 | 0.49 |
| 3:X:2939[A]:ARG:NE | 3:X:3031[A]:ASN:ND2 | 2.60 | 0.49 |
| 3:X:3113[B]:ASP:O | 3:X:3114[B]:PRO:C | 2.53 | 0.49 |
| 3:X:3135[B]:LYS:HB2 | 3:X:3141[B]:TYR:HD1 | 1.76 | 0.49 |
| 1:Y:126:GLY:HA3 | 1:Y:202:TYR:O | 2.11 | 0.49 |
| 1:Y:238:ASN:OD1 | 1:Y:238:ASN:N | 2.40 | 0.49 |
| 1:Y:1492:PRO:HA | 1:Y:1512:ARG:HA | 1.94 | 0.49 |
| 2:Z:2154:TRP:HD1 | 2:Z:2333:LEU:HD12 | 1.77 | 0.49 |
| 3:a:3151[A]:LEU:CB | 3:a:3175[A]:TYR:CD2 | 2.93 | 0.49 |
| 3:a:3201[B]:GLU:O | 3:a:3205[B]:LYS:HB2 | 2.11 | 0.49 |
| 3:a:3273[B]:LEU:O | 3:a:3275[B]:LEU:HD12 | 2.11 | 0.49 |
| 2:c:2570:HIS:HD2 | 2:c:2711:HIS:HE1 | 1.58 | 0.49 |
| 2:c:2606:LEU:HD21 | 2:c:2709:VAL:HG21 | 1.92 | 0.49 |
| 3:d:2935[B]:ILE:CD1 | 3:d:2935[B]:ILE:H | 2.25 | 0.49 |
| 3:d:3141[A]:TYR:CD2 | 3:d:3141[A]:TYR:C | 2.86 | 0.49 |
| 3:C:2935[B]:ILE:CD1 | 3:C:2935[B]:ILE:H | 2.25 | 0.49 |
| 3:C:3024[B]:LEU:CD1 | 3:C:3024[B]:LEU:C | 2.85 | 0.49 |
| 3:C:3217[B]:PHE:CB | 3:C:3219[B]:LEU:HD21 | 2.42 | 0.49 |
| 3:C:3262[B]:PHE:C | 3:C:3263[B]:LEU:HD12 | 2.37 | 0.49 |
| 1:D:711:LEU:HD21 | 1:D:719:TYR:HD2 | 1.76 | 0.49 |
| 2:E:2647:LEU:HG | 2:E:2656:LEU:HG | 1.93 | 0.49 |
| 3:F:2935[B]:ILE:CD1 | 3:F:2935[B]:ILE:H | 2.25 | 0.49 |
| 3:F:3196[B]:THR:OG1 | 3:F:3199[B]:GLN:HB2 | 2.11 | 0.49 |
| 1:G:37:ILE:HD13 | 1:G:75:GLN:HG3 | 1.94 | 0.49 |
| 3:I:2935[A]:ILE:CD1 | 3:I:2935[A]:ILE:H | 2.25 | 0.49 |
| 3:I:2939[A]:ARG:NE | 3:I:3031[A]:ASN:ND2 | 2.60 | 0.49 |
| 3:I:3066[A]:TYR:CE1 | 3:I:3193[A]:HIS:CE1 | 2.98 | 0.49 |
| 3:I:3113[B]:ASP:O | 3:I:3114[B]:PRO:C | 2.53 | 0.49 |
| 3:I:3155[B]:MET:HA | 3:R:2979[B]:GLN:HE21 | 1.77 | 0.49 |
| 3:I:3196[A]:THR:O | 3:I:3199[A]:GLN:HB2 | 2.11 | 0.49 |
| 3:I:3219[A]:LEU:N | 3:I:3219[A]:LEU:CD2 | 2.73 | 0.49 |
| 1:J:1583:CYS:O | 1:M:329:ARG:HA | 2.12 | 0.49 |
| 2:K:2746:MET:HE2 | 2:K:2765:PRO:HG3 | 1.93 | 0.49 |
| 3:L:2935[A]:ILE:CD1 | 3:L:2936[A]:GLU:N | 2.73 | 0.49 |
| 3:L:2935[B]:ILE:CD1 | 3:L:2936[B]:GLU:N | 2.73 | 0.49 |
| 3:L:3066[B]:TYR:CE1 | 3:L:3193[B]:HIS:CE1 | 2.98 | 0.49 |
| 3:L:3096[A]:VAL:HG11 | 3:L:3115[A]:LEU:HD12 | 1.89 | 0.49 |
| 3:L:3110[A]:THR:C | 3:L:3112[A]:TYR:N | 2.68 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3284[B]:LYS:CE | 3:L:3284[B]:LYS:CA | 2.85 | 0.49 |
| 3:L:3298[A]:ASN:CA | 3:L:3299[A]:LEU:C | 2.85 | 0.49 |
| 1:M:81:VAL:HA | 1:M:85:SER:HB3 | 1.94 | 0.49 |
| 1:M:137:ARG:NH2 | 1:M:203:ASP:OD1 | 2.37 | 0.49 |
| 1:M:329:ARG:HH11 | 1:M:329:ARG:HB3 | 1.76 | 0.49 |
| 1:M:804:ASP:H | 1:M:810:LEU:HD13 | 1.77 | 0.49 |
| 1:M:861:PHE:CD2 | 1:M:870:TYR:HB2 | 2.47 | 0.49 |
| 1:M:1622:GLN:HG2 | 1:M:1652:PHE:CD1 | 2.47 | 0.49 |
| 3:O:2948[B]:ASP:CB | 3:O:2949[B]:LYS:CA | 2.78 | 0.49 |
| 3:O:3066[B]:TYR:CE1 | 3:O:3193[B]:HIS:CE1 | 2.98 | 0.49 |
| 3:O:3113[B]:ASP:O | 3:O:3114[B]:PRO:C | 2.53 | 0.49 |
| 3:O:3135[A]:LYS:HB2 | 3:O:3141[A]:TYR:HD1 | 1.76 | 0.49 |
| 3:O:3201[B]:GLU:O | 3:O:3205[B]:LYS:HB2 | 2.11 | 0.49 |
| 3:O:3262[A]:PHE:C | 3:O:3263[A]:LEU:HD12 | 2.37 | 0.49 |
| 3:O:3275[A]:LEU:N | 3:O:3275[A]:LEU:CD1 | 2.73 | 0.49 |
| 3:O:3275[B]:LEU:N | 3:O:3275[B]:LEU:CD1 | 2.73 | 0.49 |
| 3:R:3232[B]:VAL:HG23 | 3:R:3273[B]:LEU:HD11 | 1.94 | 0.49 |
| 3:R:3291[A]:ASP:OD2 | 3:R:3293[A]:LYS:NZ | 2.43 | 0.49 |
| 1:S:1219:ASP:N | 1:S:1223:ALA:O | 2.36 | 0.49 |
| 1:S:1362:ALA:HA | 1:S:1378:PHE:CG | 2.47 | 0.49 |
| 2:T:2867:PRO:HG2 | 3:U:2932[A]:PRO:HG2 | 1.93 | 0.49 |
| 3:U:2939[B]:ARG:NE | 3:U:3031[B]:ASN:ND2 | 2.60 | 0.49 |
| 3:U:3023[A]:ILE:O | 3:U:3025[A]:VAL:N | 2.44 | 0.49 |
| 3:U:3232[A]:VAL:HG23 | 3:U:3273[A]:LEU:HD11 | 1.94 | 0.49 |
| 3:U:3276[B]:ASP:O | 3:U:3277[B]:ALA:HB3 | 2.12 | 0.49 |
| 1:V:559:THR:HG21 | 1:V:627:ASP:HA | 1.94 | 0.49 |
| 1:V:1322:TRP:CD1 | 1:V:1493:MET:HB3 | 2.47 | 0.49 |
| 3:X:2954[A]:TYR:C | 3:X:2957[A]:ILE:HG22 | 2.37 | 0.49 |
| 3:X:3176[B]:LYS:CE | 3:X:3176[B]:LYS:N | 2.73 | 0.49 |
| 1:Y:483:GLY:HA2 | 1:Y:773:PHE:CZ | 2.46 | 0.49 |
| 1:Y:499:GLU:HG3 | 1:Y:511:VAL:HG12 | 1.95 | 0.49 |
| 3:a:2949[A]:LYS:C | 3:a:2949[A]:LYS:CD | 2.85 | 0.49 |
| 3:a:2962[B]:GLY:N | 3:a:3111[B]:SER:OG | 2.44 | 0.49 |
| 3:a:3093[A]:HIS:HB2 | 3:a:3248[A]:LEU:HD13 | 1.94 | 0.49 |
| 3:a:3135[A]:LYS:HB2 | 3:a:3141[A]:TYR:HD1 | 1.76 | 0.49 |
| 3:d:2935[A]:ILE:CD1 | 3:d:2935[A]:ILE:H | 2.26 | 0.49 |
| 3:d:3151[A]:LEU:CB | 3:d:3175[A]:TYR:CD2 | 2.93 | 0.49 |
| 3:d:3219[B]:LEU:N | 3:d:3219[B]:LEU:CD2 | 2.73 | 0.49 |
| 1:A:449:ASP:HB3 | 1:A:1276:ASN:OD1 | 2.12 | 0.49 |
| 1:A:572:SER:O | 1:A:578:PHE:HB2 | 2.12 | 0.49 |
| 3:C:3151[B]:LEU:CB | 3:C:3175[B]:TYR:CD2 | 2.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:256:ILE:O | 1:D:260:ASN:ND2 | 2.45 | 0.49 |
| 1:D:668:MET:HE2 | 1:D:668:MET:HA | 1.95 | 0.49 |
| 2:E:2451:LEU:HD22 | 2:E:2456:LEU:HD11 | 1.94 | 0.49 |
| 3:F:2949[B]:LYS:C | 3:F:2949[B]:LYS:CD | 2.85 | 0.49 |
| 3:F:2985[B]:PHE:CD2 | 3:a:2968[B]:GLN:O | 2.64 | 0.49 |
| 3:F:3114[B]:PRO:CD | 3:F:3115[B]:LEU:N | 2.72 | 0.49 |
| 3:F:3196[A]:THR:OG1 | 3:F:3199[A]:GLN:HB2 | 2.11 | 0.49 |
| 3:F:3276[B]:ASP:O | 3:F:3277[B]:ALA:HB3 | 2.12 | 0.49 |
| 1:G:489:HIS:HB3 | 1:G:689:PRO:HB3 | 1.95 | 0.49 |
| 2:H:2542:TYR:HB2 | 2:H:2573:TYR:HE1 | 1.77 | 0.49 |
| 2:H:2650:GLY:N | 2:H:2651:GLN:HA | 2.27 | 0.49 |
| 3:I:2954[A]:TYR:C | 3:I:2957[A]:ILE:HG22 | 2.37 | 0.49 |
| 3:I:2954[B]:TYR:C | 3:I:2957[B]:ILE:HG22 | 2.37 | 0.49 |
| 3:I:3110[A]:THR:C | 3:I:3112[A]:TYR:H | 2.20 | 0.49 |
| 3:I:3160[B]:SER:CA | 3:R:2983[B]:VAL:HB | 2.42 | 0.49 |
| 3:I:3176[A]:LYS:H | 3:I:3176[A]:LYS:CE | 2.17 | 0.49 |
| 3:I:3196[A]:THR:OG1 | 3:I:3199[A]:GLN:HG3 | 2.12 | 0.49 |
| 3:I:3201[B]:GLU:O | 3:I:3205[B]:LYS:HB2 | 2.11 | 0.49 |
| 2:K:2735:ALA:HB2 | 2:K:2769:PHE:CZ | 2.47 | 0.49 |
| 3:L:3023[B]:ILE:O | 3:L:3025[B]:VAL:N | 2.44 | 0.49 |
| 3:L:3110[A]:THR:O | 3:L:3111[A]:SER:C | 2.53 | 0.49 |
| 3:L:3191[A]:ASN:C | 3:L:3192[A]:PHE:O | 2.52 | 0.49 |
| 3:L:3283[B]:ILE:C | 3:L:3283[B]:ILE:CD1 | 2.85 | 0.49 |
| 1:M:639:ARG:HB2 | 1:M:703:TYR:CE2 | 2.47 | 0.49 |
| 2:N:2595:TRP:CE2 | 2:N:2683:ILE:HG13 | 2.47 | 0.49 |
| 3:O:3114[A]:PRO:CD | 3:O:3115[A]:LEU:N | 2.72 | 0.49 |
| 3:O:3217[A]:PHE:CB | 3:O:3219[A]:LEU:HD21 | 2.42 | 0.49 |
| 1:P:324:PRO:HG2 | 1:P:376:ASN:OD1 | 2.12 | 0.49 |
| 1:P:744:VAL:HG12 | 1:P:802:ILE:HG23 | 1.94 | 0.49 |
| 3:R:2939[A]:ARG:NE | 3:R:3031[A]:ASN:ND2 | 2.60 | 0.49 |
| 3:R:2969[A]:TYR:CD2 | 3:R:2970[A]:PRO:HD2 | 2.47 | 0.49 |
| 3:R:2981[B]:GLY:N | 3:R:3086[B]:GLU:OE1 | 2.45 | 0.49 |
| 3:U:2935[A]:ILE:CD1 | 3:U:2935[A]:ILE:H | 2.25 | 0.49 |
| 3:U:2952[A]:ALA:CA | 3:U:2956[A]:LYS:HB3 | 2.38 | 0.49 |
| 3:U:3004[A]:GLY:O | 3:U:3006[A]:LYS:N | 2.44 | 0.49 |
| 1:V:567:LEU:HD13 | 1:V:609:TRP:CD1 | 2.46 | 0.49 |
| 3:X:2935[B]:ILE:CD1 | 3:X:2935[B]:ILE:H | 2.25 | 0.49 |
| 3:X:3027[B]:GLU:CD | 3:X:3028[B]:PRO:CD | 2.86 | 0.49 |
| 3:X:3191[B]:ASN:C | 3:X:3192[B]:PHE:O | 2.52 | 0.49 |
| 3:X:3201[B]:GLU:O | 3:X:3205[B]:LYS:HB2 | 2.11 | 0.49 |
| 3:X:3298[B]:ASN:CA | 3:X:3299[B]:LEU:C | 2.86 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:1302:SER:HB3 | 1:Y:1303:GLU:CD | 2.37 | 0.49 |
| 1:Y:1312:CYS:HA | 1:Y:1322:TRP:CE2 | 2.47 | 0.49 |
| 1:Y:1492:PRO:HB2 | 1:Y:1497:SER:HB3 | 1.94 | 0.49 |
| 3:a:2939[B]:ARG:NE | 3:a:3031[B]:ASN:ND2 | 2.60 | 0.49 |
| 3:a:3291[B]:ASP:OD2 | 3:a:3293[B]:LYS:NZ | 2.43 | 0.49 |
| 1:b:552:PHE:HZ | 1:b:623:TYR:HE1 | 1.58 | 0.49 |
| 3:d:2949[B]:LYS:C | 3:d:2949[B]:LYS:CD | 2.85 | 0.49 |
| 3:d:2961[A]:HIS:CD2 | 3:d:2988[A]:TRP:CZ3 | 2.96 | 0.49 |
| 3:d:3110[B]:THR:C | 3:d:3112[B]:TYR:H | 2.20 | 0.49 |
| 3:d:3293[A]:LYS:CB | 3:d:3294[A]:SER:CB | 2.54 | 0.49 |
| 3:d:3298[B]:ASN:CB | 3:d:3299[B]:LEU:C | 2.85 | 0.49 |
| 7:z:3:BMA:H2 | 7:z:4:MAN:C3 | 2.31 | 0.49 |
| 1:A:456:GLN:HG2 | 1:A:551:GLU:HB3 | 1.95 | 0.49 |
| 1:A:1441:SER:OG | 1:A:1442:MET:N | 2.43 | 0.49 |
| 2:B:2680:HIS:CD2 | 2:B:2684:HIS:HD2 | 2.31 | 0.49 |
| 3:C:2949[B]:LYS:C | 3:C:2949[B]:LYS:CD | 2.85 | 0.49 |
| 3:C:2960[A]:PHE:CD2 | 3:C:3157[A]:PRO:CG | 2.74 | 0.49 |
| 3:C:3066[B]:TYR:CE1 | 3:C:3193[B]:HIS:CE1 | 2.98 | 0.49 |
| 1:D:730:PHE:CE1 | 1:D:780:GLU:HG2 | 2.47 | 0.49 |
| 1:D:1324:ARG:NH1 | 1:D:1516:VAL:O | 2.46 | 0.49 |
| 3:F:2978[B]:CYS:O | 3:a:2975[B]:PHE:HB3 | 2.11 | 0.49 |
| 3:F:2982[B]:MET:C | 3:a:3160[B]:SER:OG | 2.53 | 0.49 |
| 3:F:3135[B]:LYS:HB2 | 3:F:3141[B]:TYR:HD1 | 1.76 | 0.49 |
| 3:F:3283[B]:ILE:C | 3:F:3283[B]:ILE:CD1 | 2.85 | 0.49 |
| 2:H:2361:LYS:HD2 | 2:H:2362:GLN:H | 1.77 | 0.49 |
| 3:I:2935[B]:ILE:CD1 | 3:I:2935[B]:ILE:H | 2.25 | 0.49 |
| 3:I:2965[B]:LEU:CD2 | 3:R:3250[B]:GLY:H | 2.25 | 0.49 |
| 3:I:3066[B]:TYR:CE1 | 3:I:3193[B]:HIS:CE1 | 2.98 | 0.49 |
| 3:I:3268[A]:LYS:CG | 1:J:1539:GLN:HE22 | 2.25 | 0.49 |
| 1:J:194:MET:HA | 1:J:200:THR:HA | 1.95 | 0.49 |
| 3:L:3014[B]:TRP:HH2 | 3:L:3123[B]:THR:HG23 | 1.78 | 0.49 |
| 3:L:3276[A]:ASP:O | 3:L:3277[A]:ALA:HB3 | 2.12 | 0.49 |
| 3:L:3291[A]:ASP:OD2 | 3:L:3293[A]:LYS:NZ | 2.43 | 0.49 |
| 1:M:127:GLU:OE2 | 1:M:135:THR:N | 2.42 | 0.49 |
| 3:O:2963[B]:MET:SD | 3:X:2975[B]:PHE:CZ | 3.02 | 0.49 |
| 3:O:3110[A]:THR:C | 3:O:3112[A]:TYR:H | 2.20 | 0.49 |
| 3:O:3196[A]:THR:O | 3:O:3200[A]:LEU:N | 2.43 | 0.49 |
| 3:O:3201[A]:GLU:O | 3:O:3205[A]:LYS:HB2 | 2.11 | 0.49 |
| 3:O:3252[B]:TYR:CB | 3:X:3156[B]:MET:CB | 2.66 | 0.49 |
| 3:O:3291[A]:ASP:OD2 | 3:O:3293[A]:LYS:NZ | 2.43 | 0.49 |
| 1:P:432:THR:HG23 | 1:P:435:GLU:H | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:1562:ILE:HD11 | 1:P:1645:PHE:CZ | 2.48 | 0.49 |
| 2:Q:2568:HIS:ND1 | 2:Q:2765:PRO:HB3 | 2.28 | 0.49 |
| 3:R:3014[B]:TRP:HH2 | 3:R:3123[B]:THR:HG23 | 1.78 | 0.49 |
| 3:R:3298[B]:ASN:CB | 3:R:3299[B]:LEU:C | 2.85 | 0.49 |
| 1:S:598:GLN:O | 1:S:602:THR:OG1 | 2.23 | 0.49 |
| 1:S:949:ASP:OD1 | 1:S:950:ALA:N | 2.40 | 0.49 |
| 3:U:3110[A]:THR:C | 3:U:3112[A]:TYR:H | 2.20 | 0.49 |
| 3:U:3147[B]:GLU:CG | 3:U:3149[B]:ASN:ND2 | 2.73 | 0.49 |
| 1:V:460:GLU:O | 1:V:467:LYS:NZ | 2.36 | 0.49 |
| 1:V:1019:HIS:CE1 | 1:V:1046:HIS:HE1 | 2.31 | 0.49 |
| 3:X:2939[B]:ARG:HG3 | 3:X:2939[B]:ARG:NH1 | 2.28 | 0.49 |
| 3:X:2939[B]:ARG:NE | 3:X:3031[B]:ASN:ND2 | 2.60 | 0.49 |
| 3:X:2969[A]:TYR:CD2 | 3:X:2970[A]:PRO:HD2 | 2.47 | 0.49 |
| 3:X:3298[A]:ASN:CA | 3:X:3299[A]:LEU:C | 2.85 | 0.49 |
| 1:Y:1470:GLU:HB3 | 1:Y:1537:ILE:CD1 | 2.42 | 0.49 |
| 3:a:2954[B]:TYR:C | 3:a:2957[B]:ILE:HG22 | 2.37 | 0.49 |
| 3:a:3262[A]:PHE:C | 3:a:3263[A]:LEU:HD12 | 2.37 | 0.49 |
| 3:a:3284[B]:LYS:HE2 | 3:a:3284[B]:LYS:CA | 2.30 | 0.49 |
| 1:b:567:LEU:HB3 | 1:b:570:GLN:O | 2.12 | 0.49 |
| 2:c:2312:GLN:OE1 | 2:c:2315:ARG:NH1 | 2.46 | 0.49 |
| 2:c:2404:GLY:HA2 | 2:c:2405:SER:C | 2.37 | 0.49 |
| 2:c:2722:GLN:NE2 | 2:c:2769:PHE:O | 2.39 | 0.49 |
| 3:d:2988[B]:TRP:HE3 | 3:d:2989[B]:HIS:CE1 | 2.25 | 0.49 |
| 3:d:3027[A]:GLU:CD | 3:d:3028[A]:PRO:CD | 2.86 | 0.49 |
| 3:d:3201[B]:GLU:O | 3:d:3205[B]:LYS:HB2 | 2.11 | 0.49 |
| 3:d:3217[B]:PHE:CB | 3:d:3219[B]:LEU:HD21 | 2.42 | 0.49 |
| 3:d:3298[A]:ASN:CA | 3:d:3299[A]:LEU:C | 2.86 | 0.49 |
| 1:A:1301:PRO:HA | 1:A:1308:VAL:HA | 1.95 | 0.49 |
| 2:B:2680:HIS:HB2 | 2:B:2714:VAL:HG11 | 1.93 | 0.49 |
| 3:C:2969[A]:TYR:CD2 | 3:C:2970[A]:PRO:HD2 | 2.47 | 0.49 |
| 3:C:2986[B]:PRO:CB | 3:C:3127[B]:TRP:CZ3 | 2.94 | 0.49 |
| 3:C:3014[A]:TRP:HH2 | 3:C:3123[A]:THR:HG23 | 1.78 | 0.49 |
| 3:C:3086[B]:GLU:CG | 3:L:2968[B]:GLN:NE2 | 2.70 | 0.49 |
| 3:C:3217[A]:PHE:CB | 3:C:3219[A]:LEU:HD21 | 2.42 | 0.49 |
| 3:C:3256[B]:TRP:CD1 | 3:L:2975[B]:PHE:O | 2.65 | 0.49 |
| 3:C:3298[B]:ASN:CB | 3:C:3299[B]:LEU:C | 2.85 | 0.49 |
| 2:E:2533:ASP:OD1 | 2:E:2533:ASP:N | 2.44 | 0.49 |
| 3:F:3027[B]:GLU:CD | 3:F:3028[B]:PRO:CD | 2.86 | 0.49 |
| 3:F:3155[B]:MET:O | 3:a:3153[B]:LYS:HD2 | 2.07 | 0.49 |
| 3:F:3298[B]:ASN:CB | 3:F:3299[B]:LEU:C | 2.86 | 0.49 |
| 1:G:1339:SER:CB | 1:G:1340:GLY:HA2 | 2.38 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:2553:ALA:N | 2:H:2554:PRO:HD2 | 2.28 | 0.49 |
| 3:I:2933[B]:SER:CB | 3:I:2936[B]:GLU:CB | 2.85 | 0.49 |
| 3:I:2980[B]:HIS:HD2 | 3:R:2969[B]:TYR:O | 1.94 | 0.49 |
| 3:I:3248[B]:LEU:C | 3:R:2974[B]:ALA:H | 2.20 | 0.49 |
| 3:I:3252[B]:TYR:CD2 | 3:R:3108[B]:HIS:CE1 | 3.00 | 0.49 |
| 3:I:3283[B]:ILE:C | 3:I:3283[B]:ILE:CD1 | 2.85 | 0.49 |
| 3:I:3288[A]:MET:CA | 3:I:3295[A]:LEU:HG | 2.42 | 0.49 |
| 3:I:3298[A]:ASN:CA | 3:I:3299[A]:LEU:C | 2.86 | 0.49 |
| 1:J:428:ILE:HD12 | 1:J:514:TRP:HB3 | 1.94 | 0.49 |
| 1:J:1215:LEU:HD22 | 1:J:1229:LYS:NZ | 2.27 | 0.49 |
| 3:L:3285[B]:VAL:CG2 | 3:L:3286[B]:THR:N | 2.73 | 0.49 |
| 3:L:3298[B]:ASN:HA | 3:L:3299[B]:LEU:HB3 | 1.88 | 0.49 |
| 2:N:2866:PRO:HB2 | 2:N:2868:GLU:OE1 | 2.11 | 0.49 |
| 3:O:3109[B]:TYR:CD2 | 3:X:2969[B]:TYR:C | 2.81 | 0.49 |
| 3:O:3110[B]:THR:C | 3:O:3112[B]:TYR:H | 2.20 | 0.49 |
| 3:O:3183[B]:LEU:H | 3:O:3184[B]:ASN:CA | 2.22 | 0.49 |
| 3:O:3228[A]:VAL:HG23 | 3:O:3228[A]:VAL:O | 2.10 | 0.49 |
| 1:P:483:GLY:HA2 | 1:P:773:PHE:CZ | 2.48 | 0.49 |
| 1:P:1015:HIS:CD2 | 1:P:1045:HIS:HE1 | 2.31 | 0.49 |
| 2:Q:2525:LYS:NZ | 2:Q:2526:ARG:HH12 | 2.11 | 0.49 |
| 2:Q:2553:ALA:N | 2:Q:2554:PRO:HD2 | 2.28 | 0.49 |
| 2:Q:2805:PHE:CE1 | 2:Q:2855:ASP:HB3 | 2.47 | 0.49 |
| 3:R:2939[A]:ARG:HG3 | 3:R:2939[A]:ARG:NH1 | 2.28 | 0.49 |
| 3:R:3110[A]:THR:C | 3:R:3112[A]:TYR:H | 2.21 | 0.49 |
| 3:R:3262[A]:PHE:C | 3:R:3263[A]:LEU:HD12 | 2.37 | 0.49 |
| 3:R:3283[B]:ILE:C | 3:R:3283[B]:ILE:CD1 | 2.85 | 0.49 |
| 1:S:462:HIS:HA | 1:S:490:TRP:CH2 | 2.47 | 0.49 |
| 2:T:2825:ILE:HG22 | 2:T:2863:ARG:HH21 | 1.76 | 0.49 |
| 1:V:898:GLY:N | 1:V:899:MET:SD | 2.73 | 0.49 |
| 1:V:1351:PRO:HA | 1:V:1400:ASN:HB2 | 1.92 | 0.49 |
| 2:W:2180:TRP:CH2 | 2:W:2300:ASN:HB3 | 2.48 | 0.49 |
| 2:W:2571:ARG:NH1 | 2:W:2771:TYR:HB3 | 2.27 | 0.49 |
| 3:X:3110[B]:THR:C | 3:X:3112[B]:TYR:H | 2.20 | 0.49 |
| 3:X:3232[B]:VAL:HG23 | 3:X:3273[B]:LEU:HD11 | 1.95 | 0.49 |
| 3:X:3276[A]:ASP:O | 3:X:3277[A]:ALA:HB3 | 2.12 | 0.49 |
| 1:Y:215:ARG:NE | 1:Y:279:LEU:HA | 2.28 | 0.49 |
| 2:Z:2090:LYS:NZ | 2:Z:2099:GLU:OE2 | 2.45 | 0.49 |
| 2:Z:2121:THR:O | 2:Z:2124:SER:HB3 | 2.13 | 0.49 |
| 3:a:2935[B]:ILE:CD1 | 3:a:2935[B]:ILE:H | 2.25 | 0.49 |
| 3:a:3196[B]:THR:OG1 | 3:a:3199[B]:GLN:HG3 | 2.12 | 0.49 |
| 3:a:3201[A]:GLU:O | 3:a:3205[A]:LYS:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3232[A]:VAL:HG23 | 3:a:3273[A]:LEU:HD11 | 1.94 | 0.49 |
| 1:b:1582:ASN:HB3 | 1:b:1583:CYS:CB | 2.34 | 0.49 |
| 2:c:2603:PRO:HG2 | 2:c:2606:LEU:HD12 | 1.93 | 0.49 |
| 3:d:3014[A]:TRP:HH2 | 3:d:3123[A]:THR:HG23 | 1.78 | 0.49 |
| 3:d:3089[B]:HIS:CE1 | 3:d:3093[B]:HIS:CE1 | 3.01 | 0.49 |
| 3:d:3176[B]:LYS:N | 3:d:3176[B]:LYS:CE | 2.73 | 0.49 |
| 3:d:3196[B]:THR:OG1 | 3:d:3199[B]:GLN:HB2 | 2.12 | 0.49 |
| 1:A:105:VAL:HB | 1:A:137:ARG:HH12 | 1.77 | 0.49 |
| 1:A:372:ALA:O | 1:A:375:SER:OG | 2.31 | 0.49 |
| 1:A:646:ALA:O | 1:A:649:ILE:HG12 | 2.12 | 0.49 |
| 3:C:2954[B]:TYR:C | 3:C:2957[B]:ILE:HG22 | 2.37 | 0.49 |
| 3:C:2971[B]:ASP:OD2 | 3:L:3248[B]:LEU:CD2 | 2.60 | 0.49 |
| 3:C:3113[A]:ASP:O | 3:C:3114[A]:PRO:C | 2.53 | 0.49 |
| 3:C:3228[B]:VAL:O | 3:C:3228[B]:VAL:HG23 | 2.10 | 0.49 |
| 3:C:3232[A]:VAL:HG23 | 3:C:3273[A]:LEU:HD11 | 1.95 | 0.49 |
| 3:C:3275[A]:LEU:N | 3:C:3275[A]:LEU:CD1 | 2.73 | 0.49 |
| 3:C:3300[A]:LEU:CD2 | 3:C:3300[A]:LEU:H | 2.24 | 0.49 |
| 9:C:3401[A]:CUO:O1 | 3:L:3120[A]:HIS:CE1 | 2.66 | 0.49 |
| 1:D:467:LYS:HB2 | 1:D:471:PRO:HG3 | 1.94 | 0.49 |
| 2:E:2472:ASN:HB2 | 2:E:2474:THR:N | 2.28 | 0.49 |
| 3:F:3120[A]:HIS:CE1 | 9:a:3401[A]:CUO:O1 | 2.66 | 0.49 |
| 3:F:3191[B]:ASN:C | 3:F:3192[B]:PHE:O | 2.52 | 0.49 |
| 3:F:3201[B]:GLU:O | 3:F:3205[B]:LYS:HB2 | 2.11 | 0.49 |
| 3:F:3255[B]:PRO:CB | 3:a:2964[B]:PRO:HD2 | 2.43 | 0.49 |
| 3:F:3262[B]:PHE:C | 3:F:3263[B]:LEU:HD12 | 2.37 | 0.49 |
| 3:F:3283[A]:ILE:C | 3:F:3283[A]:ILE:CD1 | 2.85 | 0.49 |
| 1:G:145:GLN:HG2 | 1:G:151:GLN:HB2 | 1.95 | 0.49 |
| 1:G:293:LEU:O | 1:G:296:ARG:HG2 | 2.12 | 0.49 |
| 2:H:2866:PRO:CB | 2:H:2868:GLU:HG3 | 2.43 | 0.49 |
| 3:I:3107[B]:LEU:HD12 | 3:R:2973[B]:THR:C | 2.37 | 0.49 |
| 3:L:3151[A]:LEU:CB | 3:L:3175[A]:TYR:CD2 | 2.93 | 0.49 |
| 1:M:899:MET:HB3 | 1:M:1012:GLU:OE1 | 2.13 | 0.49 |
| 1:M:901:THR:HG22 | 1:M:904:HIS:HB2 | 1.94 | 0.49 |
| 1:M:1166:THR:H | 1:M:1167:ASP:HA | 1.77 | 0.49 |
| 1:M:1290:ILE:HD13 | 1:M:1329:LEU:HG | 1.93 | 0.49 |
| 1:M:1315:GLY:HA3 | 1:M:1601:TRP:CG | 2.47 | 0.49 |
| 3:O:2939[B]:ARG:HG3 | 3:O:2939[B]:ARG:NH1 | 2.28 | 0.49 |
| 3:O:3014[A]:TRP:HH2 | 3:O:3123[A]:THR:HG23 | 1.78 | 0.49 |
| 3:O:3120[B]:HIS:CE1 | 9:O:3401[B]:CUO:O1 | 2.66 | 0.49 |
| 3:O:3196[B]:THR:OG1 | 3:O:3199[B]:GLN:HG3 | 2.12 | 0.49 |
| 3:O:3232[A]:VAL:HG23 | 3:O:3273[A]:LEU:HD11 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2935[B]:ILE:CD1 | 3:R:2936[B]:GLU:N | 2.73 | 0.49 |
| 3:R:2939[B]:ARG:NE | 3:R:3031[B]:ASN:ND2 | 2.60 | 0.49 |
| 3:R:3196[A]:THR:CA | 3:R:3199[A]:GLN:OE1 | 2.58 | 0.49 |
| 3:R:3276[A]:ASP:O | 3:R:3277[A]:ALA:HB3 | 2.12 | 0.49 |
| 3:R:3283[A]:ILE:C | 3:R:3283[A]:ILE:CD1 | 2.85 | 0.49 |
| 1:S:49:ALA:H | 1:S:55:ILE:HD12 | 1.78 | 0.49 |
| 1:S:462:HIS:HA | 1:S:490:TRP:HH2 | 1.77 | 0.49 |
| 2:T:2808:PHE:HZ | 2:T:2821:LEU:HD13 | 1.78 | 0.49 |
| 3:U:2975[B]:PHE:CZ | 3:d:3256[B]:TRP:HD1 | 2.30 | 0.49 |
| 3:U:3089[B]:HIS:CE1 | 3:U:3093[B]:HIS:CE1 | 3.01 | 0.49 |
| 3:U:3191[A]:ASN:ND2 | 3:U:3191[A]:ASN:N | 2.60 | 0.49 |
| 3:U:3211[B]:ASP:OD1 | 3:U:3211[B]:ASP:N | 2.28 | 0.49 |
| 2:W:2762:VAL:O | 2:W:2768:LEU:HD23 | 2.13 | 0.49 |
| 3:X:3089[B]:HIS:CE1 | 3:X:3093[B]:HIS:CE1 | 3.01 | 0.49 |
| 3:X:3293[A]:LYS:HB2 | 3:X:3294[A]:SER:CA | 2.41 | 0.49 |
| 3:X:3300[A]:LEU:CD2 | 3:X:3300[A]:LEU:H | 2.24 | 0.49 |
| 2:Z:2849:ASP:HB3 | 2:Z:2850:ARG:NE | 2.27 | 0.49 |
| 3:a:3027[B]:GLU:CD | 3:a:3028[B]:PRO:CD | 2.86 | 0.49 |
| 3:a:3110[A]:THR:O | 3:a:3111[A]:SER:C | 2.53 | 0.49 |
| 3:a:3283[B]:ILE:C | 3:a:3283[B]:ILE:CD1 | 2.85 | 0.49 |
| 3:a:3298[A]:ASN:CB | 3:a:3299[A]:LEU:C | 2.85 | 0.49 |
| 1:b:411:ASP:OD1 | 1:b:411:ASP:N | 2.46 | 0.49 |
| 3:d:3027[B]:GLU:CD | 3:d:3028[B]:PRO:CD | 2.86 | 0.49 |
| 3:d:3196[B]:THR:OG1 | 3:d:3199[B]:GLN:HG3 | 2.12 | 0.49 |
| 1:A:480:CYS:HA | 1:A:490:TRP:CE2 | 2.48 | 0.49 |
| 1:A:717:GLN:O | 1:A:720:VAL:HG22 | 2.13 | 0.49 |
| 1:A:1074:ILE:HB | 2:E:2901:LEU:HB2 | 1.94 | 0.49 |
| 2:B:2573:TYR:CE2 | 2:B:2707:PHE:HE2 | 2.28 | 0.49 |
| 3:C:2939[B]:ARG:NE | 3:C:3031[B]:ASN:ND2 | 2.60 | 0.49 |
| 3:C:2949[A]:LYS:C | 3:C:2949[A]:LYS:CD | 2.85 | 0.49 |
| 3:C:2954[A]:TYR:C | 3:C:2957[A]:ILE:HG22 | 2.37 | 0.49 |
| 3:C:3089[A]:HIS:CE1 | 3:C:3093[A]:HIS:CE1 | 3.01 | 0.49 |
| 3:C:3120[B]:HIS:NE2 | 9:L:3401[B]:CUO:O1 | 2.30 | 0.49 |
| 3:C:3196[B]:THR:O | 3:C:3200[B]:LEU:N | 2.43 | 0.49 |
| 1:D:644:TRP:O | 1:D:647:LEU:HB2 | 2.12 | 0.49 |
| 1:D:830:ASN:HB3 | 1:D:832:LYS:HB2 | 1.95 | 0.49 |
| 3:F:2967[B]:CYS:HB3 | 3:a:2980[B]:HIS:N | 2.16 | 0.49 |
| 3:F:3014[B]:TRP:HH2 | 3:F:3123[B]:THR:HG23 | 1.78 | 0.49 |
| 3:F:3093[A]:HIS:HB2 | 3:F:3248[A]:LEU:HD13 | 1.94 | 0.49 |
| 3:F:3110[A]:THR:C | 3:F:3112[A]:TYR:H | 2.20 | 0.49 |
| 3:F:3110[B]:THR:C | 3:F:3112[B]:TYR:H | 2.20 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:306:PHE:HB3 | 1:G:308:LEU:HD13 | 1.94 | 0.49 |
| 1:G:655:TYR:HE2 | 1:G:693:TYR:HB3 | 1.78 | 0.49 |
| 1:G:1284:GLU:OE1 | 1:G:1337:ARG:NH1 | 2.46 | 0.49 |
| 1:G:1636:ASN:OD1 | 6:r:1:NAG:C7 | 2.60 | 0.49 |
| 1:G:1636:ASN:OD1 | 6:r:1:NAG:N2 | 2.46 | 0.49 |
| 2:H:2457:LYS:HZ1 | 1:J:1206:HIS:HB3 | 1.78 | 0.49 |
| 2:H:2680:HIS:NE2 | 2:H:2684:HIS:CD2 | 2.81 | 0.49 |
| 3:I:3262[A]:PHE:C | 3:I:3263[A]:LEU:HD12 | 2.38 | 0.49 |
| 1:J:63:PRO:HA | 1:J:172:GLU:HG3 | 1.94 | 0.49 |
| 1:J:618:MET:HE2 | 1:J:629:MET:HE2 | 1.95 | 0.49 |
| 1:J:1361:GLU:HG3 | 1:J:1363:THR:H | 1.77 | 0.49 |
| 2:K:2279:LEU:HD12 | 2:K:2284:HIS:HD2 | 1.78 | 0.49 |
| 3:L:2935[B]:ILE:CD1 | 3:L:2935[B]:ILE:H | 2.25 | 0.49 |
| 3:L:2939[B]:ARG:NE | 3:L:3031[B]:ASN:ND2 | 2.60 | 0.49 |
| 3:L:2949[A]:LYS:C | 3:L:2949[A]:LYS:CD | 2.85 | 0.49 |
| 3:L:3110[B]:THR:O | 3:L:3111[B]:SER:C | 2.53 | 0.49 |
| 3:L:3196[B]:THR:OG1 | 3:L:3199[B]:GLN:HG3 | 2.12 | 0.49 |
| 1:M:1103:PHE:HE2 | 2:Q:2871:PHE:HA | 1.78 | 0.49 |
| 2:N:2536:PHE:HE1 | 2:N:2708:TYR:HE2 | 1.60 | 0.49 |
| 3:O:2949[B]:LYS:C | 3:O:2949[B]:LYS:HZ3 | 2.11 | 0.49 |
| 3:O:2968[B]:GLN:CD | 3:X:2984[B]:THR:HG1 | 2.11 | 0.49 |
| 3:O:2981[A]:GLY:N | 3:O:3086[A]:GLU:OE1 | 2.45 | 0.49 |
| 3:O:3120[A]:HIS:CE1 | 9:O:3401[A]:CUO:O1 | 2.66 | 0.49 |
| 2:Q:2336:PHE:HB3 | 2:Q:2348:THR:HG22 | 1.94 | 0.49 |
| 3:R:2935[A]:ILE:CD1 | 3:R:2935[A]:ILE:H | 2.25 | 0.49 |
| 3:R:2935[B]:ILE:CD1 | 3:R:2935[B]:ILE:H | 2.25 | 0.49 |
| 3:R:2954[A]:TYR:C | 3:R:2957[A]:ILE:HG22 | 2.37 | 0.49 |
| 3:R:3027[B]:GLU:CD | 3:R:3028[B]:PRO:CD | 2.86 | 0.49 |
| 3:R:3093[A]:HIS:HB2 | 3:R:3248[A]:LEU:HD13 | 1.94 | 0.49 |
| 3:R:3288[B]:MET:CA | 3:R:3295[B]:LEU:HG | 2.42 | 0.49 |
| 1:S:1063:ARG:HB3 | 1:S:1065:LYS:HE3 | 1.95 | 0.49 |
| 1:S:1558:LEU:HD13 | 2:W:2440:ASP:HA | 1.94 | 0.49 |
| 2:T:2665:GLU:OE1 | 2:T:2798:GLN:NE2 | 2.46 | 0.49 |
| 3:U:2939[B]:ARG:HG3 | 3:U:2939[B]:ARG:NH1 | 2.28 | 0.49 |
| 3:U:3176[A]:LYS:NZ | 3:U:3176[A]:LYS:CB | 2.73 | 0.49 |
| 3:U:3176[B]:LYS:C | 3:U:3177[B]:SER:HG | 2.08 | 0.49 |
| 3:U:3196[A]:THR:CA | 3:U:3199[A]:GLN:OE1 | 2.58 | 0.49 |
| 3:U:3262[A]:PHE:C | 3:U:3263[A]:LEU:HD12 | 2.37 | 0.49 |
| 3:U:3298[A]:ASN:CA | 3:U:3299[A]:LEU:C | 2.85 | 0.49 |
| 3:X:2960[A]:PHE:CD2 | 3:X:3157[A]:PRO:CG | 2.74 | 0.49 |
| 3:X:3014[B]:TRP:HH2 | 3:X:3123[B]:THR:HG23 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3201[A]:GLU:O | 3:X:3205[A]:LYS:HB2 | 2.11 | 0.49 |
| 3:X:3217[B]:PHE:CB | 3:X:3219[B]:LEU:HD21 | 2.42 | 0.49 |
| 3:a:2939[A]:ARG:NE | 3:a:3031[A]:ASN:ND2 | 2.60 | 0.49 |
| 3:a:2960[A]:PHE:CD2 | 3:a:3157[A]:PRO:CG | 2.74 | 0.49 |
| 3:a:3176[A]:LYS:C | 3:a:3177[A]:SER:HG | 2.10 | 0.49 |
| 3:a:3191[B]:ASN:C | 3:a:3192[B]:PHE:O | 2.52 | 0.49 |
| 3:a:3276[B]:ASP:O | 3:a:3277[B]:ALA:HB3 | 2.12 | 0.49 |
| 1:b:389:THR:OG1 | 6:NA:1:NAG:H82 | 2.12 | 0.49 |
| 1:b:464:LEU:HD13 | 1:b:622:HIS:CE1 | 2.47 | 0.49 |
| 1:b:1148:LEU:HB2 | 1:b:1188:PHE:HD2 | 1.78 | 0.49 |
| 1:b:1316:MET:HB3 | 1:b:1318:VAL:HG22 | 1.95 | 0.49 |
| 3:d:3196[A]:THR:CA | 3:d:3199[A]:GLN:OE1 | 2.58 | 0.49 |
| 3:d:3275[A]:LEU:N | 3:d:3275[A]:LEU:CD1 | 2.73 | 0.49 |
| 1:A:611:GLY:HA2 | 1:A:617:SER:HB2 | 1.94 | 0.49 |
| 1:A:1018:ILE:HA | 1:A:1021:LEU:HB2 | 1.95 | 0.49 |
| 2:B:2252:GLU:CD | 2:B:2393:ARG:HH12 | 2.20 | 0.49 |
| 3:C:3027[A]:GLU:CD | 3:C:3028[A]:PRO:CD | 2.86 | 0.49 |
| 2:E:2099:GLU:HA | 2:E:2172:ILE:HD11 | 1.95 | 0.49 |
| 3:F:2939[B]:ARG:HG3 | 3:F:2939[B]:ARG:NH1 | 2.28 | 0.49 |
| 3:F:3293[A]:LYS:CG | 3:F:3294[A]:SER:HB2 | 2.36 | 0.49 |
| 3:F:3298[A]:ASN:CB | 3:F:3299[A]:LEU:C | 2.85 | 0.49 |
| 9:F:3401[A]:CUO:O1 | 3:a:3120[A]:HIS:CE1 | 2.66 | 0.49 |
| 3:I:2989[B]:HIS:HD2 | 3:R:2970[B]:PRO:HA | 1.72 | 0.49 |
| 3:I:3014[A]:TRP:HH2 | 3:I:3123[A]:THR:HG23 | 1.78 | 0.49 |
| 3:I:3160[B]:SER:CB | 3:R:3150[B]:LYS:NZ | 2.62 | 0.49 |
| 1:J:135:THR:HG22 | 1:J:192:HIS:HB3 | 1.94 | 0.49 |
| 1:J:139:VAL:HG11 | 1:J:144:TYR:OH | 2.13 | 0.49 |
| 1:J:1279:LYS:HE3 | 1:J:1376:PRO:HG3 | 1.93 | 0.49 |
| 3:L:3147[B]:GLU:CG | 3:L:3149[B]:ASN:ND2 | 2.73 | 0.49 |
| 3:L:3219[A]:LEU:N | 3:L:3219[A]:LEU:CD2 | 2.73 | 0.49 |
| 1:M:142:ARG:NH1 | 1:M:340:GLN:OE1 | 2.45 | 0.49 |
| 1:M:552:PHE:HZ | 1:M:623:TYR:HE1 | 1.61 | 0.49 |
| 1:M:801:ASP:N | 1:M:801:ASP:OD1 | 2.45 | 0.49 |
| 1:M:1081:MET:HG2 | 1:M:1100:SER:O | 2.12 | 0.49 |
| 3:O:3027[A]:GLU:CD | 3:O:3028[A]:PRO:CD | 2.86 | 0.49 |
| 3:O:3157[B]:PRO:HB3 | 3:X:3150[B]:LYS:HA | 1.93 | 0.49 |
| 3:O:3169[B]:LYS:HA | 3:X:3148[B]:ILE:HG21 | 1.91 | 0.49 |
| 3:O:3255[B]:PRO:N | 3:X:3169[B]:LYS:HG3 | 2.27 | 0.49 |
| 3:R:2954[B]:TYR:C | 3:R:2957[B]:ILE:HG22 | 2.37 | 0.49 |
| 3:R:2961[B]:HIS:CD2 | 3:R:2988[B]:TRP:CZ3 | 2.96 | 0.49 |
| 3:R:3110[B]:THR:C | 3:R:3112[B]:TYR:H | 2.20 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1315:GLY:HA3 | 1:S:1601:TRP:HB2 | 1.94 | 0.49 |
| 1:S:1333:GLU:O | 1:S:1337:ARG:HG3 | 2.12 | 0.49 |
| 2:T:2625:LEU:HA | 2:T:2638:ARG:NH2 | 2.27 | 0.49 |
| 3:U:2954[B]:TYR:CA | 3:U:2957[B]:ILE:HG22 | 2.43 | 0.49 |
| 3:U:2960[B]:PHE:CD2 | 3:U:3157[B]:PRO:CG | 2.74 | 0.49 |
| 3:U:3014[B]:TRP:HH2 | 3:U:3123[B]:THR:HG23 | 1.78 | 0.49 |
| 3:U:3089[A]:HIS:CE1 | 3:U:3093[A]:HIS:CE1 | 3.01 | 0.49 |
| 3:U:3288[B]:MET:CA | 3:U:3295[B]:LEU:HG | 2.42 | 0.49 |
| 2:W:2903:TYR:OH | 3:X:2932[A]:PRO:HD2 | 2.12 | 0.49 |
| 3:X:3014[A]:TRP:HH2 | 3:X:3123[A]:THR:HG23 | 1.77 | 0.49 |
| 3:a:2949[B]:LYS:C | 3:a:2949[B]:LYS:CD | 2.85 | 0.49 |
| 3:a:3014[B]:TRP:HH2 | 3:a:3123[B]:THR:HG23 | 1.78 | 0.49 |
| 3:a:3110[B]:THR:C | 3:a:3112[B]:TYR:H | 2.20 | 0.49 |
| 3:a:3298[B]:ASN:CA | 3:a:3299[B]:LEU:C | 2.85 | 0.49 |
| 1:b:318:ARG:HB2 | 1:b:382:GLU:HB2 | 1.94 | 0.49 |
| 1:b:1505:ARG:O | 1:b:1509:THR:OG1 | 2.31 | 0.49 |
| 1:b:1636:ASN:ND2 | 4:QA:1:NAG:O7 | 2.46 | 0.49 |
| 2:c:2599:SER:O | 2:c:2645:PHE:HB3 | 2.13 | 0.49 |
| 2:c:2687:ILE:HD11 | 2:c:2695:MET:HE3 | 1.95 | 0.49 |
| 3:d:2954[B]:TYR:C | 3:d:2957[B]:ILE:HG22 | 2.37 | 0.49 |
| 3:d:3066[A]:TYR:CE1 | 3:d:3193[A]:HIS:CE1 | 2.98 | 0.49 |
| 3:d:3110[B]:THR:C | 3:d:3112[B]:TYR:N | 2.68 | 0.49 |
| 5:l:1:NAG:H61 | 5:l:2:NAG:C1 | 2.43 | 0.49 |
| 1:A:980:TYR:HE1 | 1:A:1021:LEU:HD13 | 1.77 | 0.49 |
| 1:A:1205:LEU:HD23 | 1:A:1211:TYR:HB2 | 1.94 | 0.49 |
| 1:A:1348:TRP:HD1 | 1:A:1403:LEU:HD13 | 1.76 | 0.49 |
| 3:C:2969[B]:TYR:CD2 | 3:L:3093[B]:HIS:NE2 | 2.79 | 0.49 |
| 3:C:3004[A]:GLY:O | 3:C:3006[A]:LYS:N | 2.44 | 0.49 |
| 3:C:3014[B]:TRP:HH2 | 3:C:3123[B]:THR:HG23 | 1.78 | 0.49 |
| 3:C:3156[B]:MET:CE | 3:L:2979[B]:GLN:HB3 | 2.32 | 0.49 |
| 3:C:3196[A]:THR:O | 3:C:3200[A]:LEU:N | 2.44 | 0.49 |
| 3:C:3232[B]:VAL:HG23 | 3:C:3273[B]:LEU:HD11 | 1.94 | 0.49 |
| 3:C:3255[B]:PRO:CD | 3:L:2959[B]:SER:O | 2.61 | 0.49 |
| 3:C:3276[B]:ASP:O | 3:C:3277[B]:ALA:HB3 | 2.12 | 0.49 |
| 3:C:3293[B]:LYS:HB2 | 3:C:3294[B]:SER:CA | 2.41 | 0.49 |
| 3:C:3298[A]:ASN:CB | 3:C:3299[A]:LEU:C | 2.86 | 0.49 |
| 1:D:398:ARG:NH2 | 1:D:484:MET:HE2 | 2.28 | 0.49 |
| 3:F:2949[A]:LYS:C | 3:F:2949[A]:LYS:CD | 2.85 | 0.49 |
| 3:F:2954[B]:TYR:C | 3:F:2957[B]:ILE:HG22 | 2.37 | 0.49 |
| 3:F:2968[B]:GLN:HG2 | 3:a:2980[B]:HIS:CA | 2.34 | 0.49 |
| 3:F:3172[B]:SER:HB2 | 3:a:3150[B]:LYS:O | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3196[B]:THR:CA | 3:F:3199[B]:GLN:OE1 | 2.58 | 0.49 |
| 2:H:2411:PHE:HE2 | 2:H:2445:MET:HE3 | 1.77 | 0.49 |
| 2:H:2615:TRP:NE1 | 2:K:2121:THR:HG23 | 2.28 | 0.49 |
| 2:H:2813:ILE:CG2 | 2:H:2896:LEU:HD21 | 2.42 | 0.49 |
| 3:I:2935[B]:ILE:CD1 | 3:I:2936[B]:GLU:N | 2.73 | 0.49 |
| 3:I:2969[A]:TYR:CD2 | 3:I:2970[A]:PRO:HD2 | 2.47 | 0.49 |
| 3:I:2970[B]:PRO:HD3 | 3:R:2989[B]:HIS:ND1 | 2.21 | 0.49 |
| 3:I:3183[B]:LEU:N | 3:I:3184[B]:ASN:HA | 2.11 | 0.49 |
| 3:I:3262[B]:PHE:C | 3:I:3263[B]:LEU:HD12 | 2.37 | 0.49 |
| 3:I:3283[A]:ILE:C | 3:I:3283[A]:ILE:CD1 | 2.85 | 0.49 |
| 1:J:195:SER:CB | 1:J:386:ILE:HD11 | 2.43 | 0.49 |
| 1:J:570:GLN:HA | 1:J:571:PRO:C | 2.38 | 0.49 |
| 2:K:2679:ILE:O | 2:K:2682:SER:HB3 | 2.13 | 0.49 |
| 3:L:2933[B]:SER:CB | 3:L:2936[B]:GLU:CB | 2.85 | 0.49 |
| 3:L:2949[B]:LYS:C | 3:L:2949[B]:LYS:CD | 2.85 | 0.49 |
| 3:L:3027[A]:GLU:CD | 3:L:3028[A]:PRO:CD | 2.86 | 0.49 |
| 3:L:3066[A]:TYR:CE1 | 3:L:3193[A]:HIS:CE1 | 2.98 | 0.49 |
| 3:L:3196[B]:THR:CA | 3:L:3199[B]:GLN:HB2 | 2.43 | 0.49 |
| 3:L:3275[B]:LEU:N | 3:L:3275[B]:LEU:CD1 | 2.73 | 0.49 |
| 1:M:289:LEU:HD22 | 1:M:293:LEU:HD13 | 1.93 | 0.49 |
| 1:M:425:ARG:NE | 1:M:499:GLU:OE2 | 2.38 | 0.49 |
| 1:M:898:GLY:HA2 | 1:M:1186:TRP:HB2 | 1.95 | 0.49 |
| 2:N:2329:MET:HA | 2:N:2354:PRO:HG2 | 1.95 | 0.49 |
| 2:N:2866:PRO:HB2 | 2:N:2868:GLU:CD | 2.37 | 0.49 |
| 3:O:2954[A]:TYR:C | 3:O:2957[A]:ILE:HG22 | 2.37 | 0.49 |
| 3:O:3089[A]:HIS:CE1 | 3:O:3093[A]:HIS:CE1 | 3.01 | 0.49 |
| 3:O:3196[A]:THR:CG2 | 1:P:416:ASN:ND2 | 2.59 | 0.49 |
| 3:O:3196[B]:THR:CA | 3:O:3199[B]:GLN:OE1 | 2.58 | 0.49 |
| 1:P:449:ASP:HB3 | 1:P:1280:GLN:NE2 | 2.28 | 0.49 |
| 1:P:1086:LEU:CD1 | 1:P:1090:ILE:HD11 | 2.43 | 0.49 |
| 2:Q:2340:ALA:HB1 | 2:Q:2341:PRO:CD | 2.42 | 0.49 |
| 3:R:3089[A]:HIS:CE1 | 3:R:3093[A]:HIS:CE1 | 3.01 | 0.49 |
| 3:R:3211[B]:ASP:OD1 | 3:R:3211[B]:ASP:N | 2.28 | 0.49 |
| 1:S:557:VAL:HB | 1:S:558:HIS:HA | 1.95 | 0.49 |
| 3:U:2965[B]:LEU:HG | 3:d:3220[B]:ARG:C | 2.37 | 0.49 |
| 3:U:3120[A]:HIS:CE1 | 9:U:3401[A]:CUO:O1 | 2.66 | 0.49 |
| 3:U:3196[B]:THR:OG1 | 3:U:3199[B]:GLN:HG3 | 2.12 | 0.49 |
| 3:U:3217[B]:PHE:CB | 3:U:3219[B]:LEU:HD21 | 2.42 | 0.49 |
| 2:W:2240:GLN:HE21 | 2:W:2241:THR:HG22 | 1.78 | 0.49 |
| 2:W:2451:LEU:HD22 | 2:W:2456:LEU:HD11 | 1.95 | 0.49 |
| 3:X:2954[B]:TYR:C | 3:X:2957[B]:ILE:HG22 | 2.37 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2961[B]:HIS:CD2 | 3:X:2988[B]:TRP:CZ3 | 2.96 | 0.49 |
| 3:X:3151[A]:LEU:CB | 3:X:3175[A]:TYR:CD2 | 2.93 | 0.49 |
| 3:X:3200[A]:LEU:HD22 | 3:X:3204[A]:LEU:HD11 | 1.95 | 0.49 |
| 3:X:3262[A]:PHE:C | 3:X:3263[A]:LEU:HD12 | 2.37 | 0.49 |
| 1:Y:1422:HIS:NE2 | 1:Y:1608:ARG:HB2 | 2.28 | 0.49 |
| 2:Z:2240:GLN:HG2 | 2:Z:2244:PHE:CD1 | 2.48 | 0.49 |
| 3:a:3014[A]:TRP:HH2 | 3:a:3123[A]:THR:HG23 | 1.78 | 0.49 |
| 3:a:3110[A]:THR:C | 3:a:3112[A]:TYR:H | 2.21 | 0.49 |
| 3:a:3284[B]:LYS:CD | 3:a:3284[B]:LYS:C | 2.86 | 0.49 |
| 1:b:1494:ARG:HG3 | 1:b:1494:ARG:HH11 | 1.77 | 0.49 |
| 2:c:2110:MET:HE1 | 2:c:2122:ILE:HD12 | 1.94 | 0.49 |
| 3:d:2939[A]:ARG:HG3 | 3:d:2939[A]:ARG:NH1 | 2.28 | 0.49 |
| 3:d:2939[B]:ARG:NE | 3:d:3031[B]:ASN:ND2 | 2.60 | 0.49 |
| 3:d:3014[B]:TRP:HH2 | 3:d:3123[B]:THR:HG23 | 1.78 | 0.49 |
| 3:d:3141[B]:TYR:CD2 | 3:d:3141[B]:TYR:C | 2.86 | 0.49 |
| 3:d:3196[A]:THR:OG1 | 3:d:3199[A]:GLN:HG3 | 2.12 | 0.49 |
| 3:d:3262[A]:PHE:C | 3:d:3263[A]:LEU:HD12 | 2.38 | 0.49 |
| 3:d:3276[B]:ASP:O | 3:d:3277[B]:ALA:HB3 | 2.12 | 0.49 |
| 2:B:2887:ASP:OD1 | 2:B:2887:ASP:N | 2.34 | 0.49 |
| 3:C:3086[B]:GLU:HG2 | 3:L:2968[B]:GLN:HE21 | 1.78 | 0.49 |
| 3:C:3151[A]:LEU:CB | 3:C:3175[A]:TYR:CD2 | 2.93 | 0.49 |
| 3:C:3253[B]:GLU:HB3 | 3:L:3252[B]:TYR:CB | 2.42 | 0.49 |
| 1:D:215:ARG:NE | 1:D:279:LEU:HA | 2.27 | 0.49 |
| 1:D:947:TYR:HE1 | 1:D:956:PRO:HG2 | 1.78 | 0.49 |
| 2:E:2819:VAL:HG22 | 2:E:2883:ILE:HG13 | 1.94 | 0.49 |
| 3:F:2971[B]:ASP:N | 3:a:3093[B]:HIS:NE2 | 2.13 | 0.49 |
| 3:F:3089[A]:HIS:CE1 | 3:F:3093[A]:HIS:CE1 | 3.01 | 0.49 |
| 3:F:3143[B]:SER:OG | 3:F:3144[B]:ALA:N | 2.46 | 0.49 |
| 3:F:3232[A]:VAL:HG23 | 3:F:3273[A]:LEU:HD11 | 1.94 | 0.49 |
| 1:G:277:ASP:OD1 | 1:G:278:ASP:N | 2.46 | 0.49 |
| 1:G:1245:GLU:CD | 1:G:1245:GLU:H | 2.17 | 0.49 |
| 1:G:1260:ARG:HD3 | 1:G:1331:GLU:OE1 | 2.13 | 0.49 |
| 2:H:2572:VAL:HG22 | 2:H:2768:LEU:HD22 | 1.95 | 0.49 |
| 2:H:2744:PHE:HZ | 1:J:1212:HIS:HB3 | 1.78 | 0.49 |
| 3:I:2939[A]:ARG:HG3 | 3:I:2939[A]:ARG:NH1 | 2.28 | 0.49 |
| 3:I:2965[B]:LEU:CG | 3:I:2974[B]:ALA:CB | 2.85 | 0.49 |
| 3:I:3096[A]:VAL:HG11 | 3:I:3115[A]:LEU:HD12 | 1.89 | 0.49 |
| 3:I:3151[B]:LEU:HB2 | 3:I:3175[B]:TYR:HE2 | 1.68 | 0.49 |
| 3:I:3155[B]:MET:SD | 3:R:3154[B]:PRO:HD2 | 2.53 | 0.49 |
| 3:I:3183[A]:LEU:H | 3:I:3184[A]:ASN:CA | 2.22 | 0.49 |
| 3:I:3217[A]:PHE:CB | 3:I:3219[A]:LEU:HD21 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:120:LYS:N | 1:J:121:ASN:HA | 2.27 | 0.49 |
| 1:J:1335:LEU:HA | 1:J:1339:SER:HB3 | 1.93 | 0.49 |
| 3:L:2954[B]:TYR:C | 3:L:2957[B]:ILE:HG22 | 2.37 | 0.49 |
| 3:L:3176[B]:LYS:N | 3:L:3176[B]:LYS:CE | 2.73 | 0.49 |
| 1:M:1400:ASN:ND2 | 1:M:1433:TRP:HZ3 | 2.11 | 0.49 |
| 2:N:2374:ASN:ND2 | 2:Q:2098:GLN:HE22 | 2.11 | 0.49 |
| 2:N:2805:PHE:CE1 | 2:N:2855:ASP:HB3 | 2.48 | 0.49 |
| 3:O:2949[A]:LYS:C | 3:O:2949[A]:LYS:CD | 2.85 | 0.49 |
| 3:O:3196[A]:THR:OG1 | 3:O:3199[A]:GLN:HG3 | 2.12 | 0.49 |
| 3:O:3196[A]:THR:CA | 3:O:3199[A]:GLN:HB2 | 2.43 | 0.49 |
| 3:O:3217[B]:PHE:HD2 | 3:O:3300[B]:LEU:HD12 | 1.78 | 0.49 |
| 3:R:3113[B]:ASP:O | 3:R:3114[B]:PRO:C | 2.53 | 0.49 |
| 3:R:3191[B]:ASN:C | 3:R:3192[B]:PHE:O | 2.52 | 0.49 |
| 3:R:3196[A]:THR:O | 3:R:3200[A]:LEU:N | 2.43 | 0.49 |
| 3:R:3219[A]:LEU:N | 3:R:3219[A]:LEU:CD2 | 2.73 | 0.49 |
| 1:S:834:ASP:OD1 | 1:S:834:ASP:N | 2.38 | 0.49 |
| 3:U:2952[A]:ALA:CB | 3:U:2953[A]:GLY:CA | 2.82 | 0.49 |
| 3:U:2969[B]:TYR:C | 3:d:2981[B]:GLY:N | 2.70 | 0.49 |
| 3:U:2975[B]:PHE:HB2 | 3:d:3256[B]:TRP:CB | 1.78 | 0.49 |
| 3:U:3154[B]:PRO:HG3 | 3:d:2984[B]:THR:HG22 | 1.77 | 0.49 |
| 3:U:3191[B]:ASN:ND2 | 3:U:3191[B]:ASN:N | 2.60 | 0.49 |
| 3:U:3196[A]:THR:OG1 | 3:U:3199[A]:GLN:HG3 | 2.12 | 0.49 |
| 3:U:3196[A]:THR:O | 3:U:3200[A]:LEU:N | 2.43 | 0.49 |
| 3:U:3262[B]:PHE:C | 3:U:3263[B]:LEU:HD12 | 2.37 | 0.49 |
| 1:V:49:ALA:HB3 | 1:V:55:ILE:HD12 | 1.94 | 0.49 |
| 1:V:137:ARG:NH1 | 1:V:203:ASP:OD1 | 2.46 | 0.49 |
| 1:V:745:ASP:HB2 | 1:V:801:ASP:OD1 | 2.12 | 0.49 |
| 1:V:949:ASP:C | 1:V:952:GLY:H | 2.21 | 0.49 |
| 3:X:2933[B]:SER:HA | 3:X:2935[B]:ILE:HD11 | 1.95 | 0.49 |
| 1:Y:22:LEU:HG | 1:Y:122:VAL:HG11 | 1.94 | 0.49 |
| 1:Y:392:PRO:HB2 | 1:Y:394:GLN:HG2 | 1.95 | 0.49 |
| 1:Y:1299:GLN:HB2 | 1:Y:1311:CYS:SG | 2.53 | 0.49 |
| 1:Y:1365:TYR:CD1 | 1:Y:1372:ILE:HG22 | 2.35 | 0.49 |
| 1:Y:1622:GLN:O | 2:c:2326:ILE:HD11 | 2.13 | 0.49 |
| 1:Y:1639:LYS:NZ | 1:Y:1642:GLN:HG3 | 2.28 | 0.49 |
| 3:a:3196[A]:THR:CA | 3:a:3199[A]:GLN:HB2 | 2.43 | 0.49 |
| 3:a:3196[B]:THR:OG1 | 3:a:3199[B]:GLN:HB2 | 2.12 | 0.49 |
| 3:a:3217[A]:PHE:HD2 | 3:a:3300[A]:LEU:HD12 | 1.78 | 0.49 |
| 3:a:3232[B]:VAL:HG23 | 3:a:3273[B]:LEU:HD11 | 1.94 | 0.49 |
| 1:b:1390:ASP:HB2 | 1:b:1438:ASP:OD2 | 2.12 | 0.49 |
| 3:d:2954[B]:TYR:CA | 3:d:2957[B]:ILE:HG22 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3196[A]:THR:O | 3:d:3200[A]:LEU:N | 2.44 | 0.49 |
| 3:d:3232[B]:VAL:HG23 | 3:d:3273[B]:LEU:HD11 | 1.95 | 0.49 |
| 1:A:187:GLY:HA3 | 1:A:195:SER:N | 2.27 | 0.48 |
| 1:A:1627:ARG:NH2 | 1:A:1629:GLU:OE1 | 2.43 | 0.48 |
| 2:B:2597:MET:HE2 | 2:B:2598:PRO:HD2 | 1.93 | 0.48 |
| 2:B:2670:CYS:N | 2:B:2737:CYS:SG | 2.86 | 0.48 |
| 2:B:2740:ASP:OD2 | 1:D:1232:THR:OG1 | 2.23 | 0.48 |
| 3:C:2939[B]:ARG:HG3 | 3:C:2939[B]:ARG:NH1 | 2.28 | 0.48 |
| 3:C:2961[B]:HIS:CD2 | 3:C:2988[B]:TRP:CZ3 | 2.96 | 0.48 |
| 3:C:3089[B]:HIS:CE1 | 3:L:2971[B]:ASP:HB3 | 2.47 | 0.48 |
| 3:C:3283[A]:ILE:C | 3:C:3283[A]:ILE:CD1 | 2.85 | 0.48 |
| 3:C:3288[A]:MET:CA | 3:C:3295[A]:LEU:HG | 2.42 | 0.48 |
| 1:D:104:LEU:HB3 | 1:D:123:PHE:HD2 | 1.77 | 0.48 |
| 1:D:514:TRP:CZ2 | 1:D:606:ILE:HD11 | 2.48 | 0.48 |
| 1:D:664:VAL:O | 1:D:689:PRO:HD2 | 2.13 | 0.48 |
| 1:D:902:PHE:HB3 | 1:D:903:PRO:HD3 | 1.93 | 0.48 |
| 1:D:1296:VAL:HG13 | 1:D:1384:PHE:HZ | 1.78 | 0.48 |
| 3:F:2969[B]:TYR:HE2 | 3:a:3120[B]:HIS:NE2 | 2.09 | 0.48 |
| 3:F:3089[B]:HIS:CE1 | 3:F:3093[B]:HIS:CE1 | 3.01 | 0.48 |
| 3:F:3147[B]:GLU:CG | 3:F:3149[B]:ASN:ND2 | 2.73 | 0.48 |
| 3:F:3149[B]:ASN:HB3 | 3:a:3165[B]:ASN:O | 2.12 | 0.48 |
| 3:F:3217[A]:PHE:CB | 3:F:3219[A]:LEU:HD21 | 2.42 | 0.48 |
| 1:G:954:ALA:O | 1:G:956:PRO:HD3 | 2.13 | 0.48 |
| 2:H:2402:GLY:HA3 | 2:H:2403:PHE:HD1 | 1.78 | 0.48 |
| 3:I:2971[B]:ASP:O | 3:R:3093[B]:HIS:HB2 | 2.13 | 0.48 |
| 3:I:2981[A]:GLY:N | 3:I:3086[A]:GLU:OE1 | 2.45 | 0.48 |
| 3:I:2991[A]:LEU:HD23 | 3:I:3158[A]:PHE:CE1 | 2.48 | 0.48 |
| 3:I:3089[A]:HIS:CE1 | 3:I:3093[A]:HIS:CE1 | 3.01 | 0.48 |
| 3:I:3256[B]:TRP:NE1 | 3:R:2965[B]:LEU:HD12 | 2.26 | 0.48 |
| 1:J:1302:SER:HB3 | 1:J:1494:ARG:NH2 | 2.28 | 0.48 |
| 3:L:2939[B]:ARG:HG3 | 3:L:2939[B]:ARG:NH1 | 2.28 | 0.48 |
| 3:L:2948[A]:ASP:CB | 3:L:2949[A]:LYS:CA | 2.78 | 0.48 |
| 3:L:3110[A]:THR:C | 3:L:3112[A]:TYR:H | 2.20 | 0.48 |
| 3:L:3135[B]:LYS:HB2 | 3:L:3141[B]:TYR:HD1 | 1.76 | 0.48 |
| 3:L:3284[A]:LYS:CE | 3:L:3284[A]:LYS:CA | 2.85 | 0.48 |
| 1:M:622:HIS:HE1 | 1:M:767:LYS:H | 1.59 | 0.48 |
| 1:M:1324:ARG:NH1 | 1:M:1519:TYR:HB3 | 2.28 | 0.48 |
| 1:M:1427:HIS:CE1 | 1:M:1458:HIS:CE1 | 3.00 | 0.48 |
| 3:O:2935[B]:ILE:CD1 | 3:O:2935[B]:ILE:H | 2.25 | 0.48 |
| 3:O:2949[B]:LYS:C | 3:O:2949[B]:LYS:CD | 2.85 | 0.48 |
| 3:O:2954[B]:TYR:C | 3:O:2957[B]:ILE:HG22 | 2.37 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2954[B]:TYR:CA | 3:O:2957[B]:ILE:HG22 | 2.43 | 0.48 |
| 3:O:3157[B]:PRO:CA | 3:X:3153[B]:LYS:N | 2.60 | 0.48 |
| 3:O:3252[B]:TYR:CD2 | 3:X:2966[B]:SER:O | 2.53 | 0.48 |
| 1:P:563:ILE:O | 1:P:612:GLY:HA3 | 2.13 | 0.48 |
| 3:R:2937[B]:ASN:CB | 3:R:3006[B]:LYS:CE | 2.86 | 0.48 |
| 3:R:2952[A]:ALA:CB | 3:R:2953[A]:GLY:CA | 2.82 | 0.48 |
| 3:R:3135[A]:LYS:HB2 | 3:R:3141[A]:TYR:HD1 | 1.76 | 0.48 |
| 3:R:3147[B]:GLU:CG | 3:R:3149[B]:ASN:ND2 | 2.73 | 0.48 |
| 3:R:3191[A]:ASN:ND2 | 3:R:3191[A]:ASN:N | 2.60 | 0.48 |
| 3:R:3196[A]:THR:OG1 | 3:R:3199[A]:GLN:HG3 | 2.12 | 0.48 |
| 3:R:3298[B]:ASN:CA | 3:R:3299[B]:LEU:C | 2.85 | 0.48 |
| 1:S:14:GLU:O | 1:S:17:ASN:ND2 | 2.46 | 0.48 |
| 2:T:2341:PRO:HG2 | 2:T:2342:TYR:CD1 | 2.47 | 0.48 |
| 3:U:2954[A]:TYR:C | 3:U:2957[A]:ILE:HG22 | 2.37 | 0.48 |
| 3:U:3183[B]:LEU:H | 3:U:3184[B]:ASN:CA | 2.22 | 0.48 |
| 3:U:3217[A]:PHE:HD2 | 3:U:3300[A]:LEU:HD12 | 1.79 | 0.48 |
| 1:V:140:ASP:OD1 | 1:V:142:ARG:NE | 2.38 | 0.48 |
| 1:V:1156:LEU:HD13 | 1:V:1176:TYR:CE1 | 2.48 | 0.48 |
| 1:V:1583:CYS:C | 1:Y:329:ARG:HB3 | 2.38 | 0.48 |
| 2:W:2370:MET:HE3 | 2:W:2370:MET:HB2 | 1.75 | 0.48 |
| 2:W:2612:TYR:OH | 2:W:2617:ASP:OD1 | 2.28 | 0.48 |
| 2:W:2786:MET:HE1 | 2:W:2794:LEU:HD13 | 1.94 | 0.48 |
| 3:X:3120[B]:HIS:CE1 | 9:X:3401[B]:CUO:O1 | 2.66 | 0.48 |
| 3:X:3232[A]:VAL:HG23 | 3:X:3273[A]:LEU:HD11 | 1.94 | 0.48 |
| 1:Y:826:ILE:HG12 | 1:Y:827:ALA:N | 2.28 | 0.48 |
| 1:Y:975:PRO:HG3 | 1:Y:1026:GLU:HG3 | 1.95 | 0.48 |
| 3:a:3114[A]:PRO:CD | 3:a:3115[A]:LEU:N | 2.72 | 0.48 |
| 3:d:2954[A]:TYR:CA | 3:d:2957[A]:ILE:HG22 | 2.43 | 0.48 |
| 3:d:3191[A]:ASN:ND2 | 3:d:3191[A]:ASN:N | 2.60 | 0.48 |
| 3:d:3276[A]:ASP:O | 3:d:3277[A]:ALA:HB3 | 2.12 | 0.48 |
| 6:GA:1:NAG:O3 | 6:GA:2:NAG:C1 | 2.60 | 0.48 |
| 3:C:2933[B]:SER:HA | 3:C:2935[B]:ILE:HD11 | 1.95 | 0.48 |
| 3:C:2971[A]:ASP:CG | 3:C:2973[A]:THR:HG1 | 2.17 | 0.48 |
| 3:C:3027[B]:GLU:CD | 3:C:3028[B]:PRO:CD | 2.86 | 0.48 |
| 3:C:3110[A]:THR:C | 3:C:3112[A]:TYR:H | 2.20 | 0.48 |
| 3:C:3149[B]:ASN:O | 3:L:3172[B]:SER:CA | 2.60 | 0.48 |
| 3:C:3191[B]:ASN:ND2 | 3:C:3191[B]:ASN:N | 2.60 | 0.48 |
| 1:D:462:HIS:HA | 1:D:490:TRP:CH2 | 2.47 | 0.48 |
| 3:F:2939[A]:ARG:NE | 3:F:3031[A]:ASN:ND2 | 2.60 | 0.48 |
| 3:F:2954[B]:TYR:CA | 3:F:2957[B]:ILE:HG22 | 2.43 | 0.48 |
| 3:F:3027[A]:GLU:CD | 3:F:3028[A]:PRO:CD | 2.86 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3298[B]:ASN:CA | 3:F:3299[B]:LEU:C | 2.86 | 0.48 |
| 1:G:902:PHE:HB3 | 1:G:903:PRO:HD3 | 1.93 | 0.48 |
| 3:I:2939[B]:ARG:NE | 3:I:3031[B]:ASN:ND2 | 2.60 | 0.48 |
| 3:I:2985[B]:PHE:CD2 | 3:R:2968[B]:GLN:O | 2.67 | 0.48 |
| 3:I:3027[A]:GLU:CD | 3:I:3028[A]:PRO:CD | 2.86 | 0.48 |
| 3:I:3150[B]:LYS:CD | 3:R:3160[B]:SER:CB | 2.91 | 0.48 |
| 3:I:3155[B]:MET:H | 3:R:3153[B]:LYS:C | 2.10 | 0.48 |
| 3:I:3157[B]:PRO:HD3 | 3:R:2982[B]:MET:CE | 2.43 | 0.48 |
| 3:I:3171[B]:HIS:HA | 3:R:3152[B]:LYS:HB3 | 1.95 | 0.48 |
| 3:I:3176[B]:LYS:N | 3:I:3176[B]:LYS:CE | 2.73 | 0.48 |
| 3:I:3217[B]:PHE:CB | 3:I:3219[B]:LEU:HD21 | 2.42 | 0.48 |
| 3:I:3298[B]:ASN:CB | 3:I:3299[B]:LEU:C | 2.85 | 0.48 |
| 2:K:2179:ASP:HB3 | 2:K:2303:ARG:HH12 | 1.78 | 0.48 |
| 3:L:3014[A]:TRP:HH2 | 3:L:3123[A]:THR:HG23 | 1.78 | 0.48 |
| 3:L:3191[A]:ASN:ND2 | 3:L:3191[A]:ASN:N | 2.60 | 0.48 |
| 3:L:3196[A]:THR:O | 3:L:3199[A]:GLN:HB2 | 2.11 | 0.48 |
| 1:M:294:LYS:HA | 1:M:297:ARG:HD2 | 1.95 | 0.48 |
| 2:N:2373:MET:HB3 | 2:N:2381:LEU:HD11 | 1.96 | 0.48 |
| 3:O:2939[A]:ARG:NE | 3:O:3031[A]:ASN:ND2 | 2.60 | 0.48 |
| 3:O:2949[A]:LYS:C | 3:O:2949[A]:LYS:HZ3 | 2.15 | 0.48 |
| 3:O:3110[B]:THR:C | 3:O:3112[B]:TYR:N | 2.68 | 0.48 |
| 3:O:3143[A]:SER:OG | 3:O:3144[A]:ALA:N | 2.46 | 0.48 |
| 3:O:3217[A]:PHE:HD2 | 3:O:3300[A]:LEU:HD12 | 1.79 | 0.48 |
| 1:P:1145:THR:OG1 | 1:P:1233:SER:HB3 | 2.13 | 0.48 |
| 3:R:2933[A]:SER:HA | 3:R:2935[A]:ILE:HD11 | 1.95 | 0.48 |
| 3:R:2939[B]:ARG:HG3 | 3:R:2939[B]:ARG:NH1 | 2.28 | 0.48 |
| 3:R:3183[B]:LEU:H | 3:R:3184[B]:ASN:CA | 2.22 | 0.48 |
| 1:S:597:VAL:O | 1:S:601:VAL:HG12 | 2.13 | 0.48 |
| 2:T:2172:ILE:HG13 | 2:T:2173:VAL:HG13 | 1.95 | 0.48 |
| 2:T:2265:ILE:HD12 | 2:T:2443:TYR:CD1 | 2.47 | 0.48 |
| 2:T:2279:LEU:HD12 | 2:T:2284:HIS:HD2 | 1.78 | 0.48 |
| 2:T:2504:ARG:HD3 | 2:T:2775:GLY:O | 2.13 | 0.48 |
| 3:U:3004[B]:GLY:O | 3:U:3006[B]:LYS:N | 2.44 | 0.48 |
| 3:U:3298[B]:ASN:CA | 3:U:3299[B]:LEU:C | 2.85 | 0.48 |
| 1:V:904:HIS:HB3 | 1:V:1105:VAL:HG21 | 1.95 | 0.48 |
| 3:X:3024[A]:LEU:CD1 | 3:X:3024[A]:LEU:C | 2.85 | 0.48 |
| 2:Z:2562:GLY:H | 2:Z:2846:TRP:HB2 | 1.78 | 0.48 |
| 3:a:2935[A]:ILE:CD1 | 3:a:2935[A]:ILE:H | 2.25 | 0.48 |
| 3:a:3027[A]:GLU:CD | 3:a:3028[A]:PRO:CD | 2.86 | 0.48 |
| 3:a:3262[B]:PHE:C | 3:a:3263[B]:LEU:HD12 | 2.37 | 0.48 |
| 1:b:22:LEU:HD23 | 1:b:122:VAL:HB | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3298[A]:ASN:CB | 3:d:3299[A]:LEU:C | 2.86 | 0.48 |
| 3:d:3298[B]:ASN:CB | 3:d:3300[B]:LEU:CD2 | 2.61 | 0.48 |
| 1:A:213:VAL:HA | 1:A:216:HIS:ND1 | 2.29 | 0.48 |
| 1:A:494:VAL:HG23 | 1:A:671:PHE:CZ | 2.48 | 0.48 |
| 1:A:1148:LEU:HB2 | 1:A:1188:PHE:CD2 | 2.48 | 0.48 |
| 2:B:2268:ASN:HD22 | 2:B:2428:VAL:HA | 1.78 | 0.48 |
| 3:C:2939[A]:ARG:NE | 3:C:3031[A]:ASN:ND2 | 2.60 | 0.48 |
| 3:C:2961[A]:HIS:CD2 | 3:C:2988[A]:TRP:CZ3 | 2.97 | 0.48 |
| 3:C:3093[B]:HIS:HB2 | 3:C:3248[B]:LEU:HD13 | 1.94 | 0.48 |
| 3:C:3196[B]:THR:OG1 | 3:C:3199[B]:GLN:HG3 | 2.12 | 0.48 |
| 3:C:3219[A]:LEU:N | 3:C:3219[A]:LEU:CD2 | 2.73 | 0.48 |
| 1:D:145:GLN:HB3 | 1:D:146:ALA:H | 1.48 | 0.48 |
| 1:D:449:ASP:OD1 | 1:D:449:ASP:N | 2.46 | 0.48 |
| 3:F:2933[B]:SER:HA | 3:F:2935[B]:ILE:HD11 | 1.95 | 0.48 |
| 3:F:3155[B]:MET:CB | 3:a:3153[B]:LYS:HB3 | 2.43 | 0.48 |
| 3:F:3228[B]:VAL:CG2 | 3:F:3245[B]:PHE:CE1 | 2.97 | 0.48 |
| 1:G:398:ARG:HH21 | 1:G:663:GLU:CD | 2.21 | 0.48 |
| 2:H:2300:ASN:OD1 | 2:H:2303:ARG:NH1 | 2.47 | 0.48 |
| 2:H:2887:ASP:HB2 | 2:H:2890:VAL:HG23 | 1.95 | 0.48 |
| 3:I:2933[A]:SER:CB | 3:I:2936[A]:GLU:CB | 2.85 | 0.48 |
| 3:I:2975[B]:PHE:CB | 3:R:3107[B]:LEU:HD11 | 2.19 | 0.48 |
| 3:I:3014[B]:TRP:HH2 | 3:I:3123[B]:THR:HG23 | 1.78 | 0.48 |
| 3:I:3090[B]:ASN:CB | 3:R:2971[B]:ASP:O | 2.61 | 0.48 |
| 3:I:3153[B]:LYS:HB3 | 3:R:3155[B]:MET:CA | 2.42 | 0.48 |
| 3:I:3196[B]:THR:O | 3:I:3200[B]:LEU:N | 2.44 | 0.48 |
| 3:I:3276[B]:ASP:O | 3:I:3277[B]:ALA:HB3 | 2.12 | 0.48 |
| 3:I:3291[A]:ASP:OD2 | 3:I:3293[A]:LYS:NZ | 2.43 | 0.48 |
| 1:J:308:LEU:O | 1:J:772:ARG:NH2 | 2.46 | 0.48 |
| 1:J:555:ALA:HB3 | 1:J:558:HIS:HE1 | 1.77 | 0.48 |
| 1:J:1157:VAL:HG21 | 1:J:1229:LYS:HE2 | 1.93 | 0.48 |
| 1:J:1403:LEU:HD21 | 1:J:1429:THR:HG21 | 1.96 | 0.48 |
| 1:J:1563:LYS:H | 1:J:1563:LYS:HG2 | 1.38 | 0.48 |
| 2:K:2336:PHE:HB3 | 2:K:2348:THR:HG22 | 1.95 | 0.48 |
| 2:K:2903:TYR:OH | 3:L:2932[A]:PRO:HD2 | 2.13 | 0.48 |
| 3:L:3093[B]:HIS:HB2 | 3:L:3248[B]:LEU:HD13 | 1.94 | 0.48 |
| 3:L:3191[B]:ASN:C | 3:L:3192[B]:PHE:O | 2.52 | 0.48 |
| 3:L:3196[A]:THR:CA | 3:L:3199[A]:GLN:HB2 | 2.43 | 0.48 |
| 3:L:3220[B]:ARG:HH11 | 3:L:3220[B]:ARG:CG | 2.12 | 0.48 |
| 3:L:3262[B]:PHE:C | 3:L:3263[B]:LEU:HD12 | 2.37 | 0.48 |
| 3:L:3283[A]:ILE:C | 3:L:3283[A]:ILE:CD1 | 2.85 | 0.48 |
| 1:M:1028:VAL:HA | 1:M:1035:TYR:CD2 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1078:ARG:NH1 | 2:Q:2870:LEU:O | 2.45 | 0.48 |
| 2:N:2240:GLN:HG2 | 2:N:2244:PHE:CD1 | 2.48 | 0.48 |
| 3:O:2933[A]:SER:CB | 3:O:2936[A]:GLU:CB | 2.85 | 0.48 |
| 3:O:2935[A]:ILE:CD1 | 3:O:2935[A]:ILE:H | 2.25 | 0.48 |
| 3:O:2991[B]:LEU:HD23 | 3:O:3158[B]:PHE:CE1 | 2.47 | 0.48 |
| 3:O:3262[B]:PHE:C | 3:O:3263[B]:LEU:HD12 | 2.37 | 0.48 |
| 1:P:4:ARG:HD3 | 1:P:77:GLU:OE2 | 2.13 | 0.48 |
| 1:P:879:SER:O | 1:P:879:SER:OG | 2.31 | 0.48 |
| 1:P:999:LEU:HB3 | 1:P:1133:ILE:HD11 | 1.95 | 0.48 |
| 1:P:1348:TRP:CG | 1:P:1430:ILE:HD11 | 2.48 | 0.48 |
| 2:Q:2627:GLY:HA3 | 2:Q:2703:PHE:O | 2.13 | 0.48 |
| 3:R:2952[A]:ALA:HB3 | 3:R:2954[A]:TYR:N | 2.17 | 0.48 |
| 3:R:3027[A]:GLU:CD | 3:R:3028[A]:PRO:CD | 2.86 | 0.48 |
| 3:R:3114[A]:PRO:CD | 3:R:3115[A]:LEU:N | 2.72 | 0.48 |
| 3:R:3196[B]:THR:HG23 | 3:R:3199[B]:GLN:OE1 | 2.14 | 0.48 |
| 3:R:3228[A]:VAL:CG2 | 3:R:3245[A]:PHE:CE1 | 2.97 | 0.48 |
| 3:R:3291[B]:ASP:OD2 | 3:R:3293[B]:LYS:NZ | 2.43 | 0.48 |
| 3:R:3298[A]:ASN:CA | 3:R:3299[A]:LEU:C | 2.86 | 0.48 |
| 1:S:1465:TRP:O | 1:S:1469:GLN:HG3 | 2.12 | 0.48 |
| 2:T:2730:LEU:HA | 1:V:1245:GLU:HB3 | 1.95 | 0.48 |
| 3:U:3027[B]:GLU:CD | 3:U:3028[B]:PRO:CD | 2.86 | 0.48 |
| 3:U:3110[B]:THR:C | 3:U:3112[B]:TYR:H | 2.21 | 0.48 |
| 3:U:3120[B]:HIS:CE1 | 9:U:3401[B]:CUO:O1 | 2.66 | 0.48 |
| 3:U:3170[B]:ALA:HA | 3:d:3148[B]:ILE:CB | 2.38 | 0.48 |
| 3:U:3196[A]:THR:CA | 3:U:3199[A]:GLN:HB2 | 2.43 | 0.48 |
| 3:U:3298[A]:ASN:CB | 3:U:3299[A]:LEU:C | 2.85 | 0.48 |
| 1:V:307:ARG:HH21 | 1:V:397:PRO:HB3 | 1.78 | 0.48 |
| 1:V:914:GLU:OE1 | 1:V:926:LEU:N | 2.35 | 0.48 |
| 1:V:1013:ILE:HD11 | 1:V:1148:LEU:CD1 | 2.43 | 0.48 |
| 1:V:1037:ALA:C | 1:V:1039:ASP:H | 2.21 | 0.48 |
| 1:V:1150:GLY:N | 1:V:1186:TRP:O | 2.41 | 0.48 |
| 1:V:1427:HIS:CD2 | 1:V:1457:HIS:HE1 | 2.31 | 0.48 |
| 3:X:3143[A]:SER:OG | 3:X:3144[A]:ALA:N | 2.46 | 0.48 |
| 3:X:3217[A]:PHE:HD2 | 3:X:3300[A]:LEU:HD12 | 1.78 | 0.48 |
| 1:Y:1613:ASP:OD1 | 3:d:3185[B]:TYR:CA | 2.61 | 0.48 |
| 1:Y:1656:ASP:C | 3:d:2937[B]:ASN:HD21 | 2.03 | 0.48 |
| 3:a:2933[B]:SER:HA | 3:a:2935[B]:ILE:HD11 | 1.95 | 0.48 |
| 3:a:2954[A]:TYR:C | 3:a:2957[A]:ILE:HG22 | 2.37 | 0.48 |
| 3:a:3096[A]:VAL:HG11 | 3:a:3115[A]:LEU:HD12 | 1.89 | 0.48 |
| 3:a:3141[B]:TYR:CD2 | 3:a:3141[B]:TYR:C | 2.86 | 0.48 |
| 3:a:3196[A]:THR:O | 3:a:3200[A]:LEU:N | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3217[B]:PHE:HD2 | 3:a:3300[B]:LEU:HD12 | 1.79 | 0.48 |
| 1:b:914:GLU:OE1 | 1:b:926:LEU:N | 2.34 | 0.48 |
| 2:c:2569:TRP:HZ2 | 2:c:2748:PRO:HG3 | 1.78 | 0.48 |
| 2:c:2627:GLY:HA3 | 2:c:2703:PHE:O | 2.13 | 0.48 |
| 2:c:2830:GLN:HB2 | 2:c:2863:ARG:NH2 | 2.28 | 0.48 |
| 3:d:2931[A]:THR:HG1 | 3:d:2934[A]:GLU:CD | 2.04 | 0.48 |
| 3:d:3004[A]:GLY:O | 3:d:3006[A]:LYS:N | 2.44 | 0.48 |
| 3:d:3232[A]:VAL:HG23 | 3:d:3273[A]:LEU:HD11 | 1.95 | 0.48 |
| 3:d:3262[B]:PHE:C | 3:d:3263[B]:LEU:HD12 | 2.37 | 0.48 |
| 1:A:989:THR:OG1 | 1:A:990:HIS:N | 2.44 | 0.48 |
| 3:C:3089[B]:HIS:CE1 | 3:C:3093[B]:HIS:CE1 | 3.01 | 0.48 |
| 3:C:3153[B]:LYS:NZ | 3:L:3158[B]:PHE:HE2 | 2.03 | 0.48 |
| 3:C:3196[B]:THR:CA | 3:C:3199[B]:GLN:HB2 | 2.43 | 0.48 |
| 1:D:897:HIS:HB3 | 1:D:899:MET:HE1 | 1.94 | 0.48 |
| 3:F:2935[A]:ILE:CD1 | 3:F:2935[A]:ILE:H | 2.25 | 0.48 |
| 3:F:2969[B]:TYR:C | 3:a:2985[B]:PHE:HE2 | 2.21 | 0.48 |
| 3:F:2969[B]:TYR:HE1 | 3:a:2992[B]:TYR:HE2 | 1.61 | 0.48 |
| 3:F:3143[A]:SER:OG | 3:F:3144[A]:ALA:N | 2.46 | 0.48 |
| 3:F:3200[B]:LEU:HD22 | 3:F:3204[B]:LEU:HD11 | 1.95 | 0.48 |
| 3:F:3219[A]:LEU:N | 3:F:3219[A]:LEU:CD2 | 2.73 | 0.48 |
| 1:G:572:SER:O | 1:G:578:PHE:HB2 | 2.13 | 0.48 |
| 1:G:931:TRP:CD1 | 1:G:1048:ASN:HD22 | 2.32 | 0.48 |
| 1:G:1494:ARG:HG3 | 1:G:1494:ARG:NH1 | 2.28 | 0.48 |
| 2:H:2180:TRP:HB3 | 2:H:2184:MET:HE2 | 1.95 | 0.48 |
| 2:H:2797:LYS:HZ3 | 3:I:3028[A]:PRO:CD | 2.13 | 0.48 |
| 3:I:2951[A]:ASP:C | 3:I:2956[A]:LYS:HZ1 | 2.15 | 0.48 |
| 3:I:2961[A]:HIS:CD2 | 3:I:2988[A]:TRP:CZ3 | 2.96 | 0.48 |
| 3:I:2973[B]:THR:C | 3:R:3107[B]:LEU:HD12 | 2.38 | 0.48 |
| 3:I:2982[B]:MET:CG | 3:R:3156[B]:MET:CB | 2.84 | 0.48 |
| 3:I:3027[B]:GLU:CD | 3:I:3028[B]:PRO:CD | 2.86 | 0.48 |
| 3:I:3113[A]:ASP:O | 3:I:3114[A]:PRO:C | 2.53 | 0.48 |
| 3:I:3120[A]:HIS:CE1 | 9:R:3401[A]:CUO:O1 | 2.66 | 0.48 |
| 3:I:3147[B]:GLU:N | 3:R:3161[B]:GLU:HA | 2.27 | 0.48 |
| 3:I:3149[B]:ASN:ND2 | 3:R:3163[B]:ASN:CA | 2.76 | 0.48 |
| 3:I:3196[B]:THR:HG23 | 3:I:3199[B]:GLN:OE1 | 2.14 | 0.48 |
| 1:J:1414:THR:HG23 | 1:J:1477:LEU:HD13 | 1.95 | 0.48 |
| 1:J:1427:HIS:HE1 | 1:J:1458:HIS:CD2 | 2.32 | 0.48 |
| 3:L:3089[A]:HIS:CE1 | 3:L:3093[A]:HIS:CE1 | 3.01 | 0.48 |
| 3:L:3196[A]:THR:OG1 | 3:L:3199[A]:GLN:HG3 | 2.12 | 0.48 |
| 3:L:3228[B]:VAL:CG2 | 3:L:3245[B]:PHE:CE1 | 2.97 | 0.48 |
| 3:L:3232[B]:VAL:HG23 | 3:L:3273[B]:LEU:HD11 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3298[B]:ASN:CA | 3:L:3299[B]:LEU:C | 2.85 | 0.48 |
| 1:M:841:LYS:HA | 1:M:1117:ASP:HB2 | 1.95 | 0.48 |
| 3:O:2939[A]:ARG:HG3 | 3:O:2939[A]:ARG:NH1 | 2.28 | 0.48 |
| 3:O:2969[B]:TYR:HD1 | 3:X:3158[B]:PHE:HD1 | 1.44 | 0.48 |
| 3:O:3101[B]:PRO:O | 3:X:2971[B]:ASP:CA | 2.59 | 0.48 |
| 3:O:3163[B]:ASN:HB2 | 3:X:3149[B]:ASN:HB3 | 1.91 | 0.48 |
| 3:O:3298[B]:ASN:CB | 3:O:3299[B]:LEU:C | 2.86 | 0.48 |
| 1:P:61:GLY:HA3 | 1:P:352:TRP:CG | 2.47 | 0.48 |
| 1:P:112:ASP:N | 1:P:112:ASP:OD1 | 2.42 | 0.48 |
| 1:P:945:ALA:C | 1:P:957:ASN:HD22 | 2.21 | 0.48 |
| 2:Q:2509:ILE:HD11 | 2:Q:2605:LEU:HD23 | 1.94 | 0.48 |
| 3:R:2949[A]:LYS:C | 3:R:2949[A]:LYS:CD | 2.85 | 0.48 |
| 3:R:3143[B]:SER:OG | 3:R:3144[B]:ALA:N | 2.47 | 0.48 |
| 3:R:3196[B]:THR:CA | 3:R:3199[B]:GLN:HB2 | 2.43 | 0.48 |
| 1:S:633:HIS:C | 1:S:633:HIS:HD1 | 2.20 | 0.48 |
| 1:S:717:GLN:O | 1:S:721:GLU:HG2 | 2.14 | 0.48 |
| 2:T:2502:LEU:HD12 | 2:T:2505:ILE:HD11 | 1.96 | 0.48 |
| 2:T:2825:ILE:HG13 | 2:T:2877:ILE:HG12 | 1.94 | 0.48 |
| 3:U:2954[A]:TYR:CA | 3:U:2957[A]:ILE:HG22 | 2.43 | 0.48 |
| 3:U:3014[A]:TRP:HH2 | 3:U:3123[A]:THR:HG23 | 1.78 | 0.48 |
| 3:U:3027[A]:GLU:CD | 3:U:3028[A]:PRO:CD | 2.86 | 0.48 |
| 3:U:3169[B]:LYS:C | 3:d:3148[B]:ILE:CG2 | 2.78 | 0.48 |
| 3:U:3183[A]:LEU:H | 3:U:3184[A]:ASN:CA | 2.22 | 0.48 |
| 3:U:3196[B]:THR:HG23 | 3:U:3199[B]:GLN:OE1 | 2.14 | 0.48 |
| 3:U:3254[B]:MET:CE | 3:d:3254[B]:MET:HE2 | 2.26 | 0.48 |
| 1:V:468:CYS:SG | 1:V:669:LYS:HB3 | 2.53 | 0.48 |
| 1:V:597:VAL:HG11 | 1:V:775:ARG:HB2 | 1.95 | 0.48 |
| 1:V:1143:ALA:HA | 1:V:1195:ASP:HA | 1.96 | 0.48 |
| 2:W:2671:ASP:O | 2:W:2675:GLN:HG2 | 2.14 | 0.48 |
| 3:X:3004[A]:GLY:O | 3:X:3006[A]:LYS:N | 2.44 | 0.48 |
| 3:X:3066[A]:TYR:CE1 | 3:X:3193[A]:HIS:CE1 | 2.98 | 0.48 |
| 3:X:3275[A]:LEU:N | 3:X:3275[A]:LEU:CD1 | 2.73 | 0.48 |
| 1:Y:566:ARG:HH12 | 1:Y:745:ASP:CG | 2.21 | 0.48 |
| 1:Y:668:MET:N | 1:Y:687:SER:O | 2.27 | 0.48 |
| 1:Y:1074:ILE:HA | 1:Y:1077:LEU:HB2 | 1.96 | 0.48 |
| 3:a:2933[A]:SER:HA | 3:a:2935[A]:ILE:HD11 | 1.95 | 0.48 |
| 3:a:3104[A]:MET:HA | 3:a:3110[A]:THR:CG2 | 2.17 | 0.48 |
| 1:b:1053:TRP:O | 1:b:1057:GLN:HG3 | 2.13 | 0.48 |
| 1:b:1494:ARG:HG3 | 1:b:1494:ARG:NH1 | 2.28 | 0.48 |
| 2:c:2212:GLY:HA3 | 2:c:2290:TYR:O | 2.13 | 0.48 |
| 3:d:2960[A]:PHE:CD1 | 3:d:2960[A]:PHE:N | 2.72 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3200[B]:LEU:HD22 | 3:d:3204[B]:LEU:HD11 | 1.95 | 0.48 |
| 3:C:2939[A]:ARG:HG3 | 3:C:2939[A]:ARG:NH1 | 2.28 | 0.48 |
| 3:C:2952[B]:ALA:CA | 3:C:2956[B]:LYS:HB3 | 2.38 | 0.48 |
| 3:C:2965[B]:LEU:HB3 | 3:L:3256[B]:TRP:CH2 | 2.39 | 0.48 |
| 3:C:2982[B]:MET:HG3 | 3:L:3156[B]:MET:HG3 | 1.84 | 0.48 |
| 3:C:3149[B]:ASN:CB | 3:L:3169[B]:LYS:H | 2.22 | 0.48 |
| 3:C:3155[B]:MET:H | 3:L:3153[B]:LYS:CA | 2.25 | 0.48 |
| 3:C:3170[B]:ALA:CA | 3:L:3148[B]:ILE:HG22 | 2.44 | 0.48 |
| 3:C:3180[B]:TYR:CB | 3:C:3183[B]:LEU:CD2 | 2.90 | 0.48 |
| 3:C:3298[A]:ASN:CB | 3:C:3300[A]:LEU:CD2 | 2.61 | 0.48 |
| 1:D:447:MET:HA | 1:D:455:TYR:HB3 | 1.96 | 0.48 |
| 1:D:806:ASN:OD1 | 1:D:808:THR:OG1 | 2.28 | 0.48 |
| 3:F:2954[A]:TYR:C | 3:F:2957[A]:ILE:HG22 | 2.37 | 0.48 |
| 3:F:2969[B]:TYR:HA | 3:a:2989[B]:HIS:NE2 | 2.29 | 0.48 |
| 3:F:2982[B]:MET:HG3 | 3:a:3156[B]:MET:CB | 2.41 | 0.48 |
| 3:F:3293[B]:LYS:CD | 3:F:3294[B]:SER:N | 2.64 | 0.48 |
| 3:I:2939[B]:ARG:HG3 | 3:I:2939[B]:ARG:NH1 | 2.28 | 0.48 |
| 3:I:3093[B]:HIS:HB2 | 3:I:3248[B]:LEU:HD13 | 1.94 | 0.48 |
| 3:I:3155[B]:MET:HA | 3:R:3155[B]:MET:HE3 | 1.94 | 0.48 |
| 3:I:3173[A]:THR:HG22 | 3:I:3174[A]:GLY:H | 1.67 | 0.48 |
| 3:I:3196[A]:THR:CA | 3:I:3199[A]:GLN:HB2 | 2.43 | 0.48 |
| 1:J:92:TRP:CE3 | 1:J:102:PRO:HD3 | 2.49 | 0.48 |
| 1:J:497:GLN:NE2 | 1:J:683:THR:OG1 | 2.46 | 0.48 |
| 1:J:885:SER:HB2 | 1:J:886:PRO:HA | 1.96 | 0.48 |
| 3:L:3024[A]:LEU:CD1 | 3:L:3024[A]:LEU:C | 2.85 | 0.48 |
| 3:L:3196[A]:THR:HG23 | 3:L:3199[A]:GLN:OE1 | 2.14 | 0.48 |
| 1:M:473:ALA:O | 1:M:476:ARG:NH1 | 2.45 | 0.48 |
| 1:M:904:HIS:HB3 | 1:M:1105:VAL:HG21 | 1.96 | 0.48 |
| 1:M:1520:GLN:HE21 | 1:M:1526:LYS:HG3 | 1.78 | 0.48 |
| 3:O:3089[B]:HIS:CE1 | 3:O:3093[B]:HIS:CE1 | 3.01 | 0.48 |
| 3:O:3217[B]:PHE:CB | 3:O:3219[B]:LEU:HD21 | 2.42 | 0.48 |
| 1:P:120:LYS:H | 1:P:121:ASN:HA | 1.78 | 0.48 |
| 2:Q:2310:GLU:HG3 | 2:Q:2371:LEU:HD13 | 1.94 | 0.48 |
| 2:Q:2628:HIS:HB2 | 2:Q:2635:TYR:CE2 | 2.49 | 0.48 |
| 3:R:2933[B]:SER:HA | 3:R:2935[B]:ILE:HD11 | 1.95 | 0.48 |
| 3:R:2991[A]:LEU:HD23 | 3:R:3158[A]:PHE:CE1 | 2.48 | 0.48 |
| 3:R:3004[A]:GLY:O | 3:R:3006[A]:LYS:N | 2.44 | 0.48 |
| 3:R:3093[B]:HIS:HB2 | 3:R:3248[B]:LEU:HD13 | 1.94 | 0.48 |
| 3:R:3232[A]:VAL:HG23 | 3:R:3273[A]:LEU:HD11 | 1.95 | 0.48 |
| 3:R:3298[A]:ASN:CB | 3:R:3299[A]:LEU:C | 2.86 | 0.48 |
| 1:S:691:ASP:O | 1:S:698:GLU:HG3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1002:GLU:HG3 | 1:S:1065:LYS:HD2 | 1.93 | 0.48 |
| 1:S:1163:ALA:O | 1:S:1167:ASP:HB3 | 2.13 | 0.48 |
| 2:T:2156:ARG:HD2 | 2:T:2357:VAL:HG12 | 1.95 | 0.48 |
| 3:U:2965[B]:LEU:HD23 | 3:d:3220[B]:ARG:NH1 | 2.29 | 0.48 |
| 3:U:3171[B]:HIS:CA | 3:d:3152[B]:LYS:HZ1 | 2.27 | 0.48 |
| 3:U:3191[A]:ASN:C | 3:U:3192[A]:PHE:O | 2.52 | 0.48 |
| 3:U:3232[B]:VAL:HG23 | 3:U:3273[B]:LEU:HD11 | 1.94 | 0.48 |
| 1:V:1356:PRO:HD2 | 1:V:1359:ILE:HD11 | 1.94 | 0.48 |
| 3:X:2949[A]:LYS:C | 3:X:2949[A]:LYS:CD | 2.85 | 0.48 |
| 3:X:3120[A]:HIS:CE1 | 9:X:3401[A]:CUO:O1 | 2.66 | 0.48 |
| 3:X:3196[A]:THR:OG1 | 3:X:3199[A]:GLN:CD | 2.57 | 0.48 |
| 3:X:3283[B]:ILE:C | 3:X:3283[B]:ILE:CD1 | 2.85 | 0.48 |
| 1:Y:306:PHE:HB3 | 1:Y:308:LEU:HD13 | 1.96 | 0.48 |
| 2:Z:2116:SER:HA | 2:Z:2121:THR:HG21 | 1.94 | 0.48 |
| 3:a:3191[A]:ASN:ND2 | 3:a:3191[A]:ASN:N | 2.60 | 0.48 |
| 2:c:2471:HIS:ND1 | 2:c:2471:HIS:O | 2.46 | 0.48 |
| 3:d:2933[B]:SER:HA | 3:d:2935[B]:ILE:HD11 | 1.96 | 0.48 |
| 3:d:2952[B]:ALA:HB3 | 3:d:2954[B]:TYR:N | 2.17 | 0.48 |
| 3:d:3196[A]:THR:OG1 | 3:d:3199[A]:GLN:CD | 2.57 | 0.48 |
| 3:d:3196[A]:THR:CA | 3:d:3199[A]:GLN:HB2 | 2.43 | 0.48 |
| 3:d:3283[B]:ILE:C | 3:d:3283[B]:ILE:CD1 | 2.85 | 0.48 |
| 3:d:3291[B]:ASP:OD2 | 3:d:3293[B]:LYS:NZ | 2.43 | 0.48 |
| 1:A:201:SER:HA | 1:A:206:PHE:CD2 | 2.49 | 0.48 |
| 1:A:240:PHE:HA | 1:A:263:ALA:HB3 | 1.94 | 0.48 |
| 2:B:2263:PHE:HE1 | 2:B:2304:LEU:HB3 | 1.79 | 0.48 |
| 2:B:2412:GLN:HG2 | 2:B:2422:GLU:HA | 1.94 | 0.48 |
| 3:C:2968[B]:GLN:HA | 3:C:2973[B]:THR:O | 2.14 | 0.48 |
| 3:C:3217[A]:PHE:HD2 | 3:C:3300[A]:LEU:HD12 | 1.79 | 0.48 |
| 3:C:3220[A]:ARG:HH11 | 3:C:3220[A]:ARG:CG | 2.12 | 0.48 |
| 1:D:1149:GLU:HG3 | 1:D:1187:LYS:HB3 | 1.95 | 0.48 |
| 2:E:2868:GLU:CG | 3:F:2932[A]:PRO:C | 2.71 | 0.48 |
| 3:F:2939[A]:ARG:HG3 | 3:F:2939[A]:ARG:NH1 | 2.28 | 0.48 |
| 3:F:2982[B]:MET:HA | 3:a:3160[B]:SER:OG | 2.12 | 0.48 |
| 3:F:2994[B]:LYS:HE2 | 3:F:3183[B]:LEU:O | 2.14 | 0.48 |
| 3:F:3196[A]:THR:OG1 | 3:F:3199[A]:GLN:HG3 | 2.12 | 0.48 |
| 3:F:3284[B]:LYS:CD | 3:F:3284[B]:LYS:C | 2.86 | 0.48 |
| 1:G:430:SER:O | 1:G:933:ARG:NH2 | 2.46 | 0.48 |
| 3:I:2954[B]:TYR:CA | 3:I:2957[B]:ILE:HG22 | 2.43 | 0.48 |
| 3:I:2982[B]:MET:HB2 | 3:R:3156[B]:MET:HB3 | 1.94 | 0.48 |
| 3:I:3153[B]:LYS:HE3 | 3:R:3158[B]:PHE:N | 1.92 | 0.48 |
| 3:I:3160[B]:SER:OG | 3:R:2983[B]:VAL:HG23 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3251[B]:ASP:HB2 | 3:R:3251[B]:ASP:CG | 2.38 | 0.48 |
| 9:I:3401[A]:CUO:O1 | 3:R:3120[A]:HIS:CE1 | 2.66 | 0.48 |
| 1:J:903:PRO:HG2 | 1:J:904:HIS:CD2 | 2.49 | 0.48 |
| 1:J:991:LEU:O | 1:J:995:ILE:HG13 | 2.14 | 0.48 |
| 2:K:2457:LYS:O | 2:K:2460:SER:OG | 2.30 | 0.48 |
| 3:L:2939[A]:ARG:NE | 3:L:3031[A]:ASN:ND2 | 2.60 | 0.48 |
| 3:L:2952[B]:ALA:HB3 | 3:L:2954[B]:TYR:N | 2.17 | 0.48 |
| 3:L:2994[B]:LYS:HE2 | 3:L:3183[B]:LEU:O | 2.14 | 0.48 |
| 3:L:3217[A]:PHE:HD2 | 3:L:3300[A]:LEU:HD12 | 1.78 | 0.48 |
| 1:M:897:HIS:HB3 | 1:M:899:MET:HE1 | 1.95 | 0.48 |
| 1:M:1361:GLU:HG3 | 1:M:1363:THR:H | 1.78 | 0.48 |
| 2:N:2128:LEU:HD13 | 2:N:2286:HIS:HB3 | 1.96 | 0.48 |
| 3:O:3004[A]:GLY:O | 3:O:3006[A]:LYS:N | 2.44 | 0.48 |
| 3:O:3038[B]:ILE:HG23 | 3:X:2969[B]:TYR:HE1 | 1.71 | 0.48 |
| 3:O:3093[B]:HIS:HB2 | 3:O:3248[B]:LEU:HD13 | 1.94 | 0.48 |
| 3:O:3196[A]:THR:OG1 | 3:O:3199[A]:GLN:CD | 2.57 | 0.48 |
| 3:O:3298[B]:ASN:CA | 3:O:3299[B]:LEU:C | 2.86 | 0.48 |
| 1:P:164:GLU:OE1 | 1:P:296:ARG:NH1 | 2.46 | 0.48 |
| 1:P:361:GLU:HG2 | 1:P:363:THR:HG22 | 1.94 | 0.48 |
| 1:P:954:ALA:O | 1:P:956:PRO:HD3 | 2.13 | 0.48 |
| 3:R:3200[A]:LEU:HD22 | 3:R:3204[A]:LEU:HD11 | 1.95 | 0.48 |
| 3:R:3217[A]:PHE:HD2 | 3:R:3300[A]:LEU:HD12 | 1.79 | 0.48 |
| 3:U:3143[B]:SER:OG | 3:U:3144[B]:ALA:N | 2.47 | 0.48 |
| 1:V:450:LYS:HD2 | 1:V:450:LYS:HA | 1.40 | 0.48 |
| 1:V:757:VAL:HG21 | 1:V:781:ILE:HG22 | 1.94 | 0.48 |
| 1:V:858:MET:HG3 | 1:V:959:PHE:CZ | 2.48 | 0.48 |
| 3:X:3110[A]:THR:C | 3:X:3112[A]:TYR:N | 2.68 | 0.48 |
| 1:Y:133:LYS:HE3 | 1:Y:134:VAL:HG23 | 1.95 | 0.48 |
| 1:Y:547:LYS:HD2 | 1:Y:558:HIS:HD2 | 1.78 | 0.48 |
| 1:Y:854:LEU:HD23 | 1:Y:941:LEU:HD21 | 1.96 | 0.48 |
| 1:Y:862:ALA:HA | 1:Y:870:TYR:HB3 | 1.95 | 0.48 |
| 2:Z:2189:GLY:HA2 | 2:Z:2192:THR:HG22 | 1.94 | 0.48 |
| 3:a:3093[B]:HIS:HB2 | 3:a:3248[B]:LEU:HD13 | 1.94 | 0.48 |
| 3:a:3151[B]:LEU:HB2 | 3:a:3175[B]:TYR:HE2 | 1.67 | 0.48 |
| 1:b:483:GLY:HA2 | 1:b:773:PHE:CE1 | 2.48 | 0.48 |
| 2:c:2265:ILE:HD12 | 2:c:2443:TYR:CD1 | 2.49 | 0.48 |
| 3:d:3093[B]:HIS:HB2 | 3:d:3248[B]:LEU:HD13 | 1.94 | 0.48 |
| 3:d:3183[A]:LEU:H | 3:d:3184[A]:ASN:CA | 2.22 | 0.48 |
| 3:d:3191[A]:ASN:C | 3:d:3192[A]:PHE:O | 2.52 | 0.48 |
| 4:7:1:NAG:H61 | 4:7:2:NAG:C1 | 2.43 | 0.48 |
| 4:OA:1:NAG:O4 | 4:OA:2:NAG:O7 | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:554:LYS:HD3 | 1:A:554:LYS:HA | 1.72 | 0.48 |
| 2:B:2500:ILE:HD11 | 2:B:2775:GLY:O | 2.13 | 0.48 |
| 3:C:3110[B]:THR:C | 3:C:3112[B]:TYR:H | 2.20 | 0.48 |
| 3:C:3120[A]:HIS:CE1 | 9:L:3401[A]:CUO:O1 | 2.66 | 0.48 |
| 3:C:3176[A]:LYS:N | 3:C:3176[A]:LYS:CE | 2.73 | 0.48 |
| 3:C:3191[B]:ASN:C | 3:C:3192[B]:PHE:O | 2.52 | 0.48 |
| 3:C:3200[A]:LEU:HD22 | 3:C:3204[A]:LEU:HD11 | 1.95 | 0.48 |
| 3:C:3298[A]:ASN:CA | 3:C:3299[A]:LEU:C | 2.85 | 0.48 |
| 1:D:69:HIS:NE2 | 9:D:5001:CUO:O1 | 2.47 | 0.48 |
| 2:E:2086:ASN:OD1 | 2:E:2086:ASN:N | 2.44 | 0.48 |
| 3:F:2975[B]:PHE:CA | 3:a:3107[B]:LEU:CD1 | 2.92 | 0.48 |
| 3:F:3013[B]:ASP:CG | 3:F:3015[B]:THR:HG1 | 2.21 | 0.48 |
| 3:F:3148[B]:ILE:HG22 | 3:F:3152[B]:LYS:CE | 2.44 | 0.48 |
| 3:F:3183[B]:LEU:H | 3:F:3184[B]:ASN:CA | 2.21 | 0.48 |
| 3:F:3229[A]:ASN:OD1 | 3:F:3244[A]:THR:HB | 2.14 | 0.48 |
| 1:G:1392:ASP:OD2 | 1:G:1437:ARG:NE | 2.46 | 0.48 |
| 2:H:2097:LEU:HD12 | 2:K:2235:PRO:HG2 | 1.96 | 0.48 |
| 2:H:2130:PRO:HG2 | 2:H:2140:ARG:HB2 | 1.94 | 0.48 |
| 2:H:2515:ARG:HD2 | 2:K:2168:ARG:NH2 | 2.29 | 0.48 |
| 3:I:3093[A]:HIS:HB2 | 3:I:3248[A]:LEU:HD13 | 1.94 | 0.48 |
| 3:I:3153[B]:LYS:NZ | 3:R:3157[B]:PRO:N | 2.62 | 0.48 |
| 3:I:3159[B]:SER:O | 3:R:3150[B]:LYS:CB | 2.55 | 0.48 |
| 3:I:3196[B]:THR:OG1 | 3:I:3199[B]:GLN:CD | 2.57 | 0.48 |
| 3:I:3217[A]:PHE:HD2 | 3:I:3300[A]:LEU:HD12 | 1.78 | 0.48 |
| 3:I:3221[B]:ALA:HB3 | 3:R:2964[B]:PRO:HB2 | 1.81 | 0.48 |
| 3:I:3285[B]:VAL:CG2 | 3:I:3286[B]:THR:H | 2.27 | 0.48 |
| 1:J:447:MET:HA | 1:J:455:TYR:CB | 2.43 | 0.48 |
| 3:L:2933[A]:SER:HA | 3:L:2935[A]:ILE:HD11 | 1.95 | 0.48 |
| 3:L:3027[B]:GLU:CD | 3:L:3028[B]:PRO:CD | 2.86 | 0.48 |
| 3:L:3093[A]:HIS:HB2 | 3:L:3248[A]:LEU:HD13 | 1.94 | 0.48 |
| 3:L:3217[B]:PHE:HD2 | 3:L:3300[B]:LEU:HD12 | 1.79 | 0.48 |
| 1:M:494:VAL:HG13 | 1:M:631:TRP:HZ3 | 1.79 | 0.48 |
| 2:N:2440:ASP:OD2 | 2:N:2441:ARG:NH1 | 2.47 | 0.48 |
| 2:N:2819:VAL:HB | 2:N:2835:ILE:HB | 1.96 | 0.48 |
| 3:O:2937[A]:ASN:CB | 3:O:3006[A]:LYS:CE | 2.86 | 0.48 |
| 3:O:2981[B]:GLY:N | 3:O:3086[B]:GLU:OE1 | 2.45 | 0.48 |
| 3:O:2994[A]:LYS:HE2 | 3:O:3183[A]:LEU:O | 2.14 | 0.48 |
| 3:O:3027[B]:GLU:CD | 3:O:3028[B]:PRO:CD | 2.86 | 0.48 |
| 3:O:3161[B]:GLU:HG2 | 3:X:3146[B]:CYS:SG | 2.54 | 0.48 |
| 3:O:3196[A]:THR:HG23 | 3:O:3199[A]:GLN:OE1 | 2.14 | 0.48 |
| 3:O:3196[B]:THR:CA | 3:O:3199[B]:GLN:HB2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:43:GLU:HG3 | 1:P:44:PRO:HA | 1.94 | 0.48 |
| 3:R:3066[B]:TYR:CE1 | 3:R:3193[B]:HIS:CE1 | 2.98 | 0.48 |
| 3:R:3228[B]:VAL:CG2 | 3:R:3245[B]:PHE:CE1 | 2.97 | 0.48 |
| 3:R:3229[A]:ASN:OD1 | 3:R:3244[A]:THR:HB | 2.14 | 0.48 |
| 1:S:236:GLY:HA2 | 1:S:819:ILE:HB | 1.96 | 0.48 |
| 1:S:980:TYR:OH | 1:S:1021:LEU:HD22 | 2.14 | 0.48 |
| 1:S:1346:TRP:O | 1:S:1460:ASN:ND2 | 2.47 | 0.48 |
| 3:U:2937[A]:ASN:CB | 3:U:3006[A]:LYS:CE | 2.86 | 0.48 |
| 3:U:2971[B]:ASP:HA | 3:d:3090[B]:ASN:CG | 2.31 | 0.48 |
| 3:U:2994[B]:LYS:HE2 | 3:U:3183[B]:LEU:O | 2.14 | 0.48 |
| 1:V:597:VAL:HG12 | 1:V:773:PHE:CD1 | 2.49 | 0.48 |
| 1:V:1005:CYS:O | 1:V:1009:VAL:HG23 | 2.14 | 0.48 |
| 3:X:2933[A]:SER:HA | 3:X:2935[A]:ILE:HD11 | 1.95 | 0.48 |
| 1:Y:527:LEU:HD22 | 1:Y:629:MET:HG3 | 1.96 | 0.48 |
| 2:Z:2546:LEU:H | 2:Z:2557:ALA:HA | 1.79 | 0.48 |
| 3:a:3089[A]:HIS:CE1 | 3:a:3093[A]:HIS:CE1 | 3.01 | 0.48 |
| 3:a:3183[B]:LEU:H | 3:a:3184[B]:ASN:CA | 2.22 | 0.48 |
| 3:a:3196[A]:THR:OG1 | 3:a:3199[A]:GLN:CD | 2.57 | 0.48 |
| 3:a:3276[A]:ASP:O | 3:a:3277[A]:ALA:HB3 | 2.12 | 0.48 |
| 1:b:137:ARG:NH1 | 1:b:203:ASP:OD1 | 2.47 | 0.48 |
| 1:b:957:ASN:HB3 | 1:b:960:PHE:H | 1.77 | 0.48 |
| 2:c:2107:LEU:O | 2:c:2111:GLN:HB2 | 2.13 | 0.48 |
| 3:d:2939[A]:ARG:NE | 3:d:3031[A]:ASN:ND2 | 2.60 | 0.48 |
| 3:d:3120[A]:HIS:CE1 | 9:d:3401[A]:CUO:O1 | 2.66 | 0.48 |
| 1:A:572:SER:HA | 1:A:573:LYS:HA | 1.47 | 0.48 |
| 1:A:835:GLU:C | 1:A:836:GLN:HE21 | 2.21 | 0.48 |
| 2:B:2157:LEU:O | 2:B:2160:VAL:HG22 | 2.14 | 0.48 |
| 3:C:3196[A]:THR:CA | 3:C:3199[A]:GLN:HB2 | 2.43 | 0.48 |
| 3:C:3196[B]:THR:HG23 | 3:C:3199[B]:GLN:OE1 | 2.14 | 0.48 |
| 1:D:47:CYS:N | 1:D:57:CYS:SG | 2.87 | 0.48 |
| 1:D:203:ASP:O | 1:D:206:PHE:HB3 | 2.14 | 0.48 |
| 1:D:480:CYS:HA | 1:D:490:TRP:CE2 | 2.49 | 0.48 |
| 1:D:1013:ILE:HG21 | 1:D:1192:TYR:CD1 | 2.48 | 0.48 |
| 1:D:1584:GLY:HA3 | 1:G:329:ARG:HB2 | 1.96 | 0.48 |
| 3:F:2952[B]:ALA:HB1 | 3:F:2957[B]:ILE:H | 1.79 | 0.48 |
| 3:F:3196[A]:THR:OG1 | 3:F:3199[A]:GLN:CD | 2.57 | 0.48 |
| 3:F:3220[B]:ARG:HH11 | 3:F:3220[B]:ARG:CG | 2.12 | 0.48 |
| 1:G:387:ASN:ND2 | 4:o:1:NAG:C6 | 2.77 | 0.48 |
| 2:H:2807:GLY:O | 2:H:2899:PRO:HA | 2.14 | 0.48 |
| 3:I:2988[B]:TRP:CZ2 | 3:R:2975[B]:PHE:HE2 | 2.31 | 0.48 |
| 3:I:3148[A]:ILE:HG22 | 3:I:3152[A]:LYS:CE | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3183[B]:LEU:H | 3:I:3184[B]:ASN:CA | 2.22 | 0.48 |
| 3:I:3196[A]:THR:OG1 | 3:I:3199[A]:GLN:CD | 2.57 | 0.48 |
| 3:I:3196[B]:THR:OG1 | 3:I:3199[B]:GLN:HG3 | 2.12 | 0.48 |
| 3:I:3217[B]:PHE:HD2 | 3:I:3300[B]:LEU:HD12 | 1.78 | 0.48 |
| 2:K:2265:ILE:HD12 | 2:K:2443:TYR:CD1 | 2.49 | 0.48 |
| 3:L:2935[A]:ILE:CD1 | 3:L:2935[A]:ILE:H | 2.25 | 0.48 |
| 3:L:3089[B]:HIS:CE1 | 3:L:3093[B]:HIS:CE1 | 3.01 | 0.48 |
| 3:L:3228[A]:VAL:CG2 | 3:L:3245[A]:PHE:CE1 | 2.97 | 0.48 |
| 3:O:2954[A]:TYR:CA | 3:O:2957[A]:ILE:HG22 | 2.43 | 0.48 |
| 3:O:2976[B]:ALA:CB | 3:X:3156[B]:MET:CG | 2.91 | 0.48 |
| 3:O:3200[A]:LEU:HD22 | 3:O:3204[A]:LEU:HD11 | 1.95 | 0.48 |
| 3:O:3228[A]:VAL:CG2 | 3:O:3245[A]:PHE:CE1 | 2.97 | 0.48 |
| 1:P:695:TYR:OH | 1:P:703:TYR:HD2 | 1.97 | 0.48 |
| 1:P:855:ARG:HH21 | 1:P:941:LEU:HA | 1.79 | 0.48 |
| 2:Q:2184:MET:HE3 | 2:Q:2231:LEU:HD11 | 1.96 | 0.48 |
| 2:Q:2668:ASP:OD1 | 2:Q:2669:TYR:N | 2.47 | 0.48 |
| 2:Q:2825:ILE:HG23 | 2:Q:2826:GLU:N | 2.28 | 0.48 |
| 2:Q:2856:ILE:HG22 | 2:Q:2859:VAL:HB | 1.95 | 0.48 |
| 1:S:873:VAL:HA | 1:S:876:PHE:CE2 | 2.48 | 0.48 |
| 1:S:1239:GLY:O | 1:S:1242:ASN:ND2 | 2.46 | 0.48 |
| 1:S:1491:GLN:OE1 | 1:S:1491:GLN:N | 2.46 | 0.48 |
| 2:T:2682:SER:HA | 2:T:2836:PHE:CD1 | 2.48 | 0.48 |
| 2:T:2824:CYS:O | 2:T:2877:ILE:HA | 2.13 | 0.48 |
| 3:U:2952[B]:ALA:HB1 | 3:U:2957[B]:ILE:H | 1.79 | 0.48 |
| 3:U:2961[A]:HIS:CD2 | 3:U:2988[A]:TRP:CZ3 | 2.97 | 0.48 |
| 3:U:2973[B]:THR:HG21 | 3:d:3222[B]:ILE:O | 2.14 | 0.48 |
| 3:U:3143[A]:SER:OG | 3:U:3144[A]:ALA:N | 2.47 | 0.48 |
| 3:U:3151[B]:LEU:CB | 3:U:3175[B]:TYR:CD2 | 2.93 | 0.48 |
| 3:U:3229[A]:ASN:OD1 | 3:U:3244[A]:THR:HB | 2.14 | 0.48 |
| 1:V:951:ASN:N | 1:V:951:ASN:OD1 | 2.46 | 0.48 |
| 3:X:2952[B]:ALA:N | 3:X:2953[B]:GLY:CA | 2.71 | 0.48 |
| 3:X:2994[A]:LYS:HE2 | 3:X:3183[A]:LEU:O | 2.14 | 0.48 |
| 3:X:3027[A]:GLU:CD | 3:X:3028[A]:PRO:CD | 2.86 | 0.48 |
| 3:X:3089[A]:HIS:CE1 | 3:X:3093[A]:HIS:CE1 | 3.01 | 0.48 |
| 3:X:3114[B]:PRO:CD | 3:X:3115[B]:LEU:N | 2.72 | 0.48 |
| 3:X:3196[A]:THR:OG1 | 3:X:3199[A]:GLN:HG3 | 2.12 | 0.48 |
| 1:Y:972:SER:HA | 1:Y:1028:VAL:HG22 | 1.96 | 0.48 |
| 2:Z:2134:ASN:HD22 | 2:Z:2134:ASN:C | 2.22 | 0.48 |
| 3:a:2939[A]:ARG:HG3 | 3:a:2939[A]:ARG:NH1 | 2.28 | 0.48 |
| 3:a:3196[B]:THR:OG1 | 3:a:3199[B]:GLN:CD | 2.57 | 0.48 |
| 1:b:843:VAL:HG13 | 1:b:927:PRO:HB2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:1636:ASN:HB3 | 1:b:1638:SER:H | 1.79 | 0.48 |
| 2:c:2658:LYS:NZ | 2:c:2858:ASP:OD2 | 2.30 | 0.48 |
| 3:d:3093[A]:HIS:HB2 | 3:d:3248[A]:LEU:HD13 | 1.94 | 0.48 |
| 3:d:3110[A]:THR:C | 3:d:3112[A]:TYR:H | 2.20 | 0.48 |
| 3:d:3120[B]:HIS:CE1 | 9:d:3401[B]:CUO:O1 | 2.66 | 0.48 |
| 3:d:3143[A]:SER:OG | 3:d:3144[A]:ALA:N | 2.47 | 0.48 |
| 1:A:646:ALA:HB1 | 1:A:713:ILE:HD12 | 1.95 | 0.48 |
| 1:A:893:ALA:HB2 | 1:A:1182:ASN:HB2 | 1.96 | 0.48 |
| 1:A:899:MET:HE2 | 1:A:1186:TRP:CD2 | 2.49 | 0.48 |
| 1:A:1145:THR:HB | 1:A:1191:PRO:HB2 | 1.96 | 0.48 |
| 2:B:2826:GLU:OE1 | 2:B:2876:LYS:NZ | 2.44 | 0.48 |
| 3:C:2976[B]:ALA:HB2 | 3:L:3253[B]:GLU:HG3 | 1.96 | 0.48 |
| 3:C:2985[B]:PHE:CZ | 3:L:2969[B]:TYR:O | 2.66 | 0.48 |
| 1:D:258:LYS:O | 1:D:261:SER:OG | 2.32 | 0.48 |
| 1:D:630:PHE:O | 1:D:633:HIS:HB3 | 2.14 | 0.48 |
| 1:D:1058:ALA:HB1 | 1:D:1126:ILE:HD12 | 1.95 | 0.48 |
| 1:D:1171:LYS:HG2 | 1:D:1173:GLY:H | 1.79 | 0.48 |
| 1:D:1630:MET:HE2 | 1:D:1648:PRO:HD3 | 1.96 | 0.48 |
| 2:E:2225:ARG:NH1 | 2:E:2291:ASP:OD1 | 2.47 | 0.48 |
| 2:E:2575:LEU:HD23 | 2:E:2575:LEU:HA | 1.73 | 0.48 |
| 3:F:2952[A]:ALA:N | 3:F:2953[A]:GLY:HA2 | 2.06 | 0.48 |
| 3:F:3217[A]:PHE:HD2 | 3:F:3300[A]:LEU:HD12 | 1.78 | 0.48 |
| 3:F:3252[B]:TYR:O | 3:a:3253[B]:GLU:N | 2.46 | 0.48 |
| 3:F:3298[A]:ASN:CA | 3:F:3299[A]:LEU:C | 2.85 | 0.48 |
| 1:G:278:ASP:O | 1:G:279:LEU:HG | 2.13 | 0.48 |
| 1:G:1574:VAL:HG22 | 1:G:1620:LEU:HD21 | 1.95 | 0.48 |
| 3:I:2954[A]:TYR:CA | 3:I:2957[A]:ILE:HG22 | 2.43 | 0.48 |
| 3:I:3004[A]:GLY:O | 3:I:3006[A]:LYS:N | 2.44 | 0.48 |
| 3:I:3108[B]:HIS:CE1 | 3:R:3251[B]:ASP:CB | 2.97 | 0.48 |
| 3:I:3151[A]:LEU:CB | 3:I:3175[A]:TYR:CD2 | 2.93 | 0.48 |
| 3:I:3196[A]:THR:HG23 | 3:I:3199[A]:GLN:OE1 | 2.14 | 0.48 |
| 3:I:3211[B]:ASP:OD1 | 3:I:3211[B]:ASP:N | 2.27 | 0.48 |
| 1:J:331:SER:HA | 1:M:1581:GLU:HG3 | 1.94 | 0.48 |
| 1:J:753:ASN:OD1 | 1:J:753:ASN:N | 2.46 | 0.48 |
| 1:J:1400:ASN:HD22 | 1:J:1403:LEU:HG | 1.79 | 0.48 |
| 3:L:2937[A]:ASN:CB | 3:L:3006[A]:LYS:CE | 2.85 | 0.48 |
| 3:L:2952[B]:ALA:HB1 | 3:L:2957[B]:ILE:H | 1.79 | 0.48 |
| 3:L:3104[A]:MET:HA | 3:L:3110[A]:THR:CG2 | 2.17 | 0.48 |
| 3:L:3141[B]:TYR:CD2 | 3:L:3141[B]:TYR:C | 2.86 | 0.48 |
| 3:L:3148[A]:ILE:HG22 | 3:L:3152[A]:LYS:CE | 2.44 | 0.48 |
| 3:L:3196[A]:THR:OG1 | 3:L:3199[A]:GLN:CD | 2.57 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3225[A]:SER:C | 3:L:3290[A]:ILE:HG23 | 2.39 | 0.48 |
| 1:M:151:GLN:N | 1:M:151:GLN:OE1 | 2.47 | 0.48 |
| 1:M:588:GLU:OE2 | 1:M:728:ARG:NH2 | 2.36 | 0.48 |
| 1:M:1348:TRP:CH2 | 1:M:1461:VAL:HG23 | 2.49 | 0.48 |
| 3:O:2968[B]:GLN:C | 3:X:2988[B]:TRP:CB | 2.87 | 0.48 |
| 3:O:3014[B]:TRP:HH2 | 3:O:3123[B]:THR:HG23 | 1.78 | 0.48 |
| 3:O:3196[B]:THR:OG1 | 3:O:3199[B]:GLN:CD | 2.57 | 0.48 |
| 3:O:3225[B]:SER:C | 3:O:3290[B]:ILE:HG23 | 2.39 | 0.48 |
| 3:R:2970[A]:PRO:C | 3:R:2972[A]:GLY:N | 2.72 | 0.48 |
| 3:R:3196[A]:THR:OG1 | 3:R:3199[A]:GLN:CD | 2.57 | 0.48 |
| 3:R:3284[A]:LYS:CE | 3:R:3284[A]:LYS:CA | 2.85 | 0.48 |
| 1:S:906:HIS:CD2 | 9:S:2104:CUO:O1 | 2.67 | 0.48 |
| 1:S:1421:VAL:HG23 | 1:S:1422:HIS:HD1 | 1.78 | 0.48 |
| 1:S:1596:GLU:O | 1:S:1597:THR:HG22 | 2.14 | 0.48 |
| 1:S:1604:ASP:OD1 | 1:S:1605:ARG:NH1 | 2.47 | 0.48 |
| 2:T:2168:ARG:NH2 | 2:W:2515:ARG:HD2 | 2.28 | 0.48 |
| 3:U:2933[A]:SER:HA | 3:U:2935[A]:ILE:HD11 | 1.96 | 0.48 |
| 3:U:2968[A]:GLN:HA | 3:U:2973[A]:THR:O | 2.14 | 0.48 |
| 3:U:2994[A]:LYS:HE2 | 3:U:3183[A]:LEU:O | 2.14 | 0.48 |
| 3:U:3151[A]:LEU:CB | 3:U:3175[A]:TYR:CD2 | 2.93 | 0.48 |
| 3:U:3196[A]:THR:HG23 | 3:U:3199[A]:GLN:OE1 | 2.14 | 0.48 |
| 2:W:2336:PHE:HB3 | 2:W:2348:THR:HG22 | 1.95 | 0.48 |
| 2:W:2343:ASN:HD22 | 2:W:2349:THR:HG23 | 1.77 | 0.48 |
| 2:W:2802:ASP:OD2 | 3:X:2932[A]:PRO:CD | 2.62 | 0.48 |
| 3:X:3217[B]:PHE:HD2 | 3:X:3300[B]:LEU:HD12 | 1.78 | 0.48 |
| 1:Y:1471:LEU:HD12 | 1:Y:1537:ILE:HD13 | 1.95 | 0.48 |
| 1:Y:1565:SER:HB3 | 1:Y:1594:GLY:H | 1.79 | 0.48 |
| 2:Z:2746:MET:O | 2:Z:2750:ILE:HG13 | 2.14 | 0.48 |
| 3:a:2968[A]:GLN:HA | 3:a:2973[A]:THR:O | 2.14 | 0.48 |
| 3:a:3143[B]:SER:OG | 3:a:3144[B]:ALA:N | 2.46 | 0.48 |
| 3:a:3147[A]:GLU:CG | 3:a:3149[A]:ASN:ND2 | 2.73 | 0.48 |
| 3:a:3298[A]:ASN:CA | 3:a:3299[A]:LEU:C | 2.86 | 0.48 |
| 2:c:2547:MET:O | 2:c:2751:TRP:HH2 | 1.96 | 0.48 |
| 3:d:3089[A]:HIS:CE1 | 3:d:3093[A]:HIS:CE1 | 3.01 | 0.48 |
| 4:q:2:NAG:H83 | 4:q:2:NAG:O3 | 2.14 | 0.48 |
| 1:A:177:VAL:HA | 1:A:180:ASN:OD1 | 2.14 | 0.48 |
| 1:A:641:TRP:C | 1:A:641:TRP:CD1 | 2.91 | 0.48 |
| 1:A:944:GLU:O | 1:A:957:ASN:ND2 | 2.47 | 0.48 |
| 1:A:954:ALA:O | 1:A:956:PRO:HD3 | 2.13 | 0.48 |
| 2:B:2370:MET:HE3 | 2:B:2370:MET:HB2 | 1.73 | 0.48 |
| 2:B:2650:GLY:N | 2:B:2651:GLN:HA | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2952[B]:ALA:N | 3:C:2953[B]:GLY:HA2 | 2.06 | 0.48 |
| 3:C:2970[B]:PRO:C | 3:C:2972[B]:GLY:N | 2.72 | 0.48 |
| 3:C:3093[A]:HIS:HB2 | 3:C:3248[A]:LEU:HD13 | 1.94 | 0.48 |
| 3:C:3104[B]:MET:HA | 3:C:3110[B]:THR:CG2 | 2.17 | 0.48 |
| 3:C:3172[B]:SER:CB | 3:L:3152[B]:LYS:HB2 | 2.42 | 0.48 |
| 3:C:3196[A]:THR:HG23 | 3:C:3199[A]:GLN:OE1 | 2.14 | 0.48 |
| 3:C:3285[B]:VAL:CG2 | 3:C:3286[B]:THR:H | 2.27 | 0.48 |
| 1:D:456:GLN:HG2 | 1:D:551:GLU:HB3 | 1.96 | 0.48 |
| 1:D:928:TYR:HB2 | 1:D:1048:ASN:HB2 | 1.95 | 0.48 |
| 1:D:1257:SER:O | 1:D:1525:TYR:HA | 2.13 | 0.48 |
| 1:D:1396:GLU:O | 1:D:1400:ASN:ND2 | 2.47 | 0.48 |
| 2:E:2158:TYR:O | 2:E:2161:GLN:HB3 | 2.14 | 0.48 |
| 2:E:2652:LYS:HE2 | 2:E:2657:PHE:CZ | 2.49 | 0.48 |
| 2:E:2800:LYS:HB3 | 3:F:3023[A]:ILE:HD13 | 1.95 | 0.48 |
| 3:F:2983[B]:VAL:CG2 | 3:a:3162[B]:ASP:OD1 | 2.62 | 0.48 |
| 3:F:3125[B]:ARG:O | 3:F:3129[B]:ILE:HG13 | 2.14 | 0.48 |
| 3:F:3196[A]:THR:HG23 | 3:F:3199[A]:GLN:OE1 | 2.14 | 0.48 |
| 3:F:3196[B]:THR:CA | 3:F:3199[B]:GLN:HB2 | 2.43 | 0.48 |
| 3:F:3217[B]:PHE:HD2 | 3:F:3300[B]:LEU:HD12 | 1.78 | 0.48 |
| 3:F:3275[B]:LEU:N | 3:F:3275[B]:LEU:CD1 | 2.73 | 0.48 |
| 1:G:346:GLY:O | 1:G:349:GLU:HB3 | 2.14 | 0.48 |
| 2:H:2414:CYS:SG | 2:H:2465:LYS:HD2 | 2.54 | 0.48 |
| 2:H:2622:ASN:O | 2:H:2625:LEU:HD12 | 2.14 | 0.48 |
| 2:H:2695:MET:CE | 2:H:2707:PHE:HB2 | 2.43 | 0.48 |
| 2:H:2866:PRO:HB2 | 2:H:2868:GLU:HG3 | 1.96 | 0.48 |
| 1:J:415:VAL:HG21 | 1:J:697:ALA:HB2 | 1.94 | 0.48 |
| 2:K:2322:SER:HB3 | 2:K:2329:MET:HE2 | 1.96 | 0.48 |
| 2:K:2653:GLU:H | 2:K:2653:GLU:HG3 | 1.53 | 0.48 |
| 3:L:2933[B]:SER:HA | 3:L:2935[B]:ILE:HD11 | 1.96 | 0.48 |
| 3:L:2952[A]:ALA:HB1 | 3:L:2957[A]:ILE:H | 1.79 | 0.48 |
| 3:L:2970[A]:PRO:C | 3:L:2972[A]:GLY:N | 2.72 | 0.48 |
| 3:L:2994[A]:LYS:HE2 | 3:L:3183[A]:LEU:O | 2.14 | 0.48 |
| 3:L:3135[A]:LYS:HB2 | 3:L:3141[A]:TYR:HD1 | 1.76 | 0.48 |
| 1:M:127:GLU:CD | 1:M:134:VAL:HB | 2.39 | 0.48 |
| 1:M:494:VAL:HG23 | 1:M:671:PHE:CZ | 2.49 | 0.48 |
| 2:N:2153:GLN:HG3 | 2:N:2305:TRP:HH2 | 1.79 | 0.48 |
| 3:O:3066[A]:TYR:CE1 | 3:O:3193[A]:HIS:CE1 | 2.98 | 0.48 |
| 3:O:3232[B]:VAL:HG23 | 3:O:3273[B]:LEU:HD11 | 1.94 | 0.48 |
| 1:P:447:MET:HA | 1:P:455:TYR:CB | 2.42 | 0.48 |
| 1:P:904:HIS:O | 1:P:907:ARG:HB3 | 2.14 | 0.48 |
| 2:Q:2504:ARG:HG2 | 2:Q:2582:ARG:HH21 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2968[A]:GLN:HA | 3:R:2973[A]:THR:O | 2.14 | 0.48 |
| 3:R:2968[B]:GLN:HA | 3:R:2973[B]:THR:O | 2.14 | 0.48 |
| 3:R:3014[A]:TRP:HH2 | 3:R:3123[A]:THR:HG23 | 1.78 | 0.48 |
| 3:R:3151[A]:LEU:CB | 3:R:3175[A]:TYR:CD2 | 2.93 | 0.48 |
| 3:R:3196[B]:THR:O | 3:R:3200[B]:LEU:N | 2.44 | 0.48 |
| 1:S:904:HIS:O | 1:S:907:ARG:HB3 | 2.13 | 0.48 |
| 1:V:560:SER:O | 1:V:617:SER:HB3 | 2.14 | 0.48 |
| 1:V:597:VAL:O | 1:V:601:VAL:HG12 | 2.14 | 0.48 |
| 3:X:2994[B]:LYS:HE2 | 3:X:3183[B]:LEU:O | 2.14 | 0.48 |
| 3:X:3161[A]:GLU:H | 3:X:3161[A]:GLU:CD | 2.18 | 0.48 |
| 3:X:3196[B]:THR:OG1 | 3:X:3199[B]:GLN:CD | 2.57 | 0.48 |
| 3:X:3196[B]:THR:OG1 | 3:X:3199[B]:GLN:HG3 | 2.12 | 0.48 |
| 3:X:3288[B]:MET:CA | 3:X:3295[B]:LEU:HG | 2.42 | 0.48 |
| 1:Y:593:CYS:HB3 | 1:Y:775:ARG:NE | 2.29 | 0.48 |
| 1:Y:896:HIS:HB2 | 1:Y:905:TRP:CG | 2.48 | 0.48 |
| 1:Y:1055:THR:HA | 1:Y:1119:LEU:HD13 | 1.95 | 0.48 |
| 1:Y:1315:GLY:HA3 | 1:Y:1601:TRP:HB2 | 1.95 | 0.48 |
| 2:Z:2131:LEU:HD12 | 2:Z:2335:PRO:HB3 | 1.95 | 0.48 |
| 2:Z:2805:PHE:CE1 | 2:Z:2855:ASP:HB3 | 2.49 | 0.48 |
| 3:a:2994[B]:LYS:HE2 | 3:a:3183[B]:LEU:O | 2.14 | 0.48 |
| 3:a:3089[B]:HIS:CE1 | 3:a:3093[B]:HIS:CE1 | 3.01 | 0.48 |
| 3:a:3125[B]:ARG:O | 3:a:3129[B]:ILE:HG13 | 2.14 | 0.48 |
| 1:b:126:GLY:HA2 | 1:b:127:GLU:HA | 1.35 | 0.48 |
| 1:b:240:PHE:HA | 1:b:263:ALA:HB3 | 1.96 | 0.48 |
| 2:c:2142:ALA:HB1 | 2:c:2143:CYS:HB2 | 1.95 | 0.48 |
| 2:c:2225:ARG:HD2 | 2:c:2274:LEU:HD22 | 1.95 | 0.48 |
| 2:c:2552:GLU:HB3 | 2:c:2553:ALA:HB2 | 1.95 | 0.48 |
| 2:c:2573:TYR:HE2 | 2:c:2707:PHE:HE2 | 1.61 | 0.48 |
| 3:d:2937[B]:ASN:CB | 3:d:3006[B]:LYS:CE | 2.85 | 0.48 |
| 3:d:2969[A]:TYR:CD2 | 3:d:2970[A]:PRO:HD2 | 2.47 | 0.48 |
| 3:d:2994[B]:LYS:HE2 | 3:d:3183[B]:LEU:O | 2.14 | 0.48 |
| 3:d:3196[B]:THR:CA | 3:d:3199[B]:GLN:HB2 | 2.43 | 0.48 |
| 3:d:3228[A]:VAL:CG2 | 3:d:3245[A]:PHE:CE1 | 2.97 | 0.48 |
| 1:A:611:GLY:HA3 | 1:A:619:SER:HB3 | 1.96 | 0.47 |
| 1:A:905:TRP:HE1 | 1:A:1083:PRO:HD2 | 1.79 | 0.47 |
| 1:A:1571:TYR:HE1 | 1:A:1631:GLU:HB3 | 1.78 | 0.47 |
| 3:C:2949[B]:LYS:C | 3:C:2953[B]:GLY:N | 2.72 | 0.47 |
| 3:C:2981[A]:GLY:N | 3:C:3086[A]:GLU:OE1 | 2.45 | 0.47 |
| 3:C:3125[A]:ARG:O | 3:C:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:C:3125[B]:ARG:O | 3:C:3129[B]:ILE:HG13 | 2.14 | 0.47 |
| 3:C:3191[A]:ASN:ND2 | 3:C:3191[A]:ASN:N | 2.60 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3217[B]:PHE:HD2 | 3:C:3300[B]:LEU:HD12 | 1.78 | 0.47 |
| 1:D:464:LEU:HD11 | 1:D:767:LYS:HD3 | 1.96 | 0.47 |
| 2:E:2783:PHE:HB3 | 2:E:2791:LEU:HD21 | 1.95 | 0.47 |
| 3:F:2965[B]:LEU:HB3 | 3:a:3256[B]:TRP:CZ2 | 2.48 | 0.47 |
| 3:F:3196[A]:THR:CA | 3:F:3199[A]:GLN:HB2 | 2.43 | 0.47 |
| 3:F:3284[A]:LYS:CE | 3:F:3284[A]:LYS:CA | 2.85 | 0.47 |
| 1:G:148:GLN:HA | 1:G:149:GLU:C | 2.38 | 0.47 |
| 1:G:301:ARG:HD2 | 1:G:361:GLU:OE2 | 2.14 | 0.47 |
| 3:I:2968[B]:GLN:HG2 | 3:R:2981[B]:GLY:N | 2.28 | 0.47 |
| 3:I:3298[B]:ASN:CA | 3:I:3299[B]:LEU:C | 2.86 | 0.47 |
| 1:J:1085:SER:HB2 | 1:J:1100:SER:HB2 | 1.96 | 0.47 |
| 3:L:3200[A]:LEU:HD22 | 3:L:3204[A]:LEU:HD11 | 1.95 | 0.47 |
| 1:M:1018:ILE:HD12 | 1:M:1045:HIS:CD2 | 2.49 | 0.47 |
| 1:M:1348:TRP:CZ3 | 1:M:1460:ASN:HB3 | 2.49 | 0.47 |
| 2:N:2603:PRO:HG2 | 2:N:2606:LEU:HD12 | 1.96 | 0.47 |
| 2:N:2665:GLU:HB2 | 2:N:2798:GLN:NE2 | 2.29 | 0.47 |
| 3:O:2975[B]:PHE:CA | 3:X:3156[B]:MET:CG | 2.90 | 0.47 |
| 3:O:2991[A]:LEU:HD23 | 3:O:3158[A]:PHE:CE1 | 2.48 | 0.47 |
| 3:O:3104[B]:MET:HA | 3:O:3110[B]:THR:CG2 | 2.17 | 0.47 |
| 3:O:3160[B]:SER:HB3 | 3:X:3149[B]:ASN:N | 2.28 | 0.47 |
| 3:O:3196[A]:THR:CA | 3:O:3199[A]:GLN:OE1 | 2.58 | 0.47 |
| 3:O:3283[A]:ILE:C | 3:O:3283[A]:ILE:CD1 | 2.85 | 0.47 |
| 1:P:979:LEU:HB2 | 1:P:980:TYR:CA | 2.38 | 0.47 |
| 1:P:1033:LEU:HG | 1:P:1180:SER:HB3 | 1.96 | 0.47 |
| 3:R:3125[B]:ARG:O | 3:R:3129[B]:ILE:HG13 | 2.14 | 0.47 |
| 1:S:194:MET:HA | 1:S:200:THR:HA | 1.96 | 0.47 |
| 1:S:906:HIS:NE2 | 9:S:2104:CUO:O1 | 2.47 | 0.47 |
| 1:S:1228:LEU:H | 1:S:1228:LEU:HD13 | 1.78 | 0.47 |
| 2:T:2361:LYS:HD2 | 2:T:2362:GLN:N | 2.29 | 0.47 |
| 3:U:3093[A]:HIS:HB2 | 3:U:3248[A]:LEU:HD13 | 1.95 | 0.47 |
| 3:U:3191[B]:ASN:C | 3:U:3192[B]:PHE:O | 2.52 | 0.47 |
| 3:U:3196[B]:THR:OG1 | 3:U:3199[B]:GLN:CD | 2.57 | 0.47 |
| 3:U:3229[B]:ASN:OD1 | 3:U:3244[B]:THR:HB | 2.14 | 0.47 |
| 3:U:3230[A]:PHE:H | 3:U:3243[A]:GLY:HA3 | 1.79 | 0.47 |
| 1:V:668:MET:HE2 | 1:V:668:MET:HA | 1.95 | 0.47 |
| 3:X:2968[A]:GLN:HA | 3:X:2973[A]:THR:O | 2.14 | 0.47 |
| 3:X:3093[A]:HIS:HB2 | 3:X:3248[A]:LEU:HD13 | 1.95 | 0.47 |
| 3:X:3125[A]:ARG:O | 3:X:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:X:3228[B]:VAL:CG2 | 3:X:3245[B]:PHE:CE1 | 2.97 | 0.47 |
| 3:X:3291[A]:ASP:OD2 | 3:X:3293[A]:LYS:NZ | 2.43 | 0.47 |
| 3:X:3298[A]:ASN:CB | 3:X:3299[A]:LEU:C | 2.85 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:321:LEU:HD11 | 1:Y:377:TYR:CD1 | 2.49 | 0.47 |
| 1:Y:664:VAL:O | 1:Y:689:PRO:HD2 | 2.14 | 0.47 |
| 1:Y:684:ARG:HH11 | 1:Y:684:ARG:HB3 | 1.78 | 0.47 |
| 1:Y:906:HIS:CD2 | 9:Y:2104:CUO:O1 | 2.66 | 0.47 |
| 1:Y:1013:ILE:HG21 | 1:Y:1192:TYR:CD1 | 2.49 | 0.47 |
| 1:Y:1563:LYS:HE3 | 6:LA:2:NAG:H3 | 1.96 | 0.47 |
| 1:Y:1617:LYS:HE2 | 3:d:3180[B]:TYR:CD2 | 2.48 | 0.47 |
| 2:Z:2168:ARG:NH2 | 2:c:2515:ARG:HD2 | 2.29 | 0.47 |
| 2:Z:2823:ILE:HG13 | 2:Z:2832:ALA:HB2 | 1.96 | 0.47 |
| 3:a:2952[B]:ALA:HB1 | 3:a:2957[B]:ILE:H | 1.79 | 0.47 |
| 3:a:2968[B]:GLN:HA | 3:a:2973[B]:THR:O | 2.14 | 0.47 |
| 3:a:3066[B]:TYR:CE1 | 3:a:3193[B]:HIS:CE1 | 2.98 | 0.47 |
| 3:a:3196[A]:THR:OG1 | 3:a:3199[A]:GLN:HG3 | 2.12 | 0.47 |
| 3:a:3196[A]:THR:HG23 | 3:a:3199[A]:GLN:OE1 | 2.14 | 0.47 |
| 3:a:3196[B]:THR:HG23 | 3:a:3199[B]:GLN:OE1 | 2.14 | 0.47 |
| 3:a:3230[B]:PHE:H | 3:a:3243[B]:GLY:HA3 | 1.79 | 0.47 |
| 1:b:1162:ALA:HB3 | 1:b:1212:HIS:CE1 | 2.49 | 0.47 |
| 1:b:1315:GLY:HA3 | 1:b:1601:TRP:CB | 2.43 | 0.47 |
| 2:c:2411:PHE:HE1 | 2:c:2445:MET:HE3 | 1.79 | 0.47 |
| 3:d:3089[A]:HIS:CE1 | 3:d:3119[A]:HIS:CE1 | 2.81 | 0.47 |
| 3:d:3125[A]:ARG:O | 3:d:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:d:3285[B]:VAL:CG2 | 3:d:3286[B]:THR:H | 2.27 | 0.47 |
| 1:A:72:TYR:HE2 | 1:A:206:PHE:HE2 | 1.61 | 0.47 |
| 2:B:2472:ASN:ND2 | 4:i:1:NAG:C7 | 2.75 | 0.47 |
| 2:B:2551:PRO:HA | 2:B:2552:GLU:HA | 1.49 | 0.47 |
| 2:B:2887:ASP:C | 2:B:2889:ALA:HA | 2.40 | 0.47 |
| 3:C:2937[A]:ASN:CB | 3:C:3006[A]:LYS:CE | 2.86 | 0.47 |
| 3:C:2954[A]:TYR:CA | 3:C:2957[A]:ILE:HG22 | 2.43 | 0.47 |
| 3:C:2971[B]:ASP:HA | 3:L:3089[B]:HIS:C | 2.38 | 0.47 |
| 3:C:2972[B]:GLY:CA | 3:L:3086[B]:GLU:HG2 | 2.42 | 0.47 |
| 3:C:2985[B]:PHE:CZ | 3:L:2970[B]:PRO:CB | 2.84 | 0.47 |
| 3:C:3120[B]:HIS:HD2 | 3:L:2969[B]:TYR:OH | 1.91 | 0.47 |
| 3:C:3149[B]:ASN:CG | 3:L:3169[B]:LYS:HE3 | 2.17 | 0.47 |
| 3:C:3153[B]:LYS:HZ2 | 3:L:3156[B]:MET:C | 2.17 | 0.47 |
| 1:D:670:PRO:HD2 | 1:D:671:PHE:HD1 | 1.79 | 0.47 |
| 1:D:1002:GLU:HB3 | 1:D:1065:LYS:NZ | 2.29 | 0.47 |
| 2:E:2651:GLN:HE21 | 2:E:2652:LYS:HG3 | 1.78 | 0.47 |
| 2:E:2672:PHE:HZ | 2:E:2718:TRP:HA | 1.79 | 0.47 |
| 3:F:2968[B]:GLN:HA | 3:F:2973[B]:THR:O | 2.14 | 0.47 |
| 3:F:3150[B]:LYS:HZ1 | 3:a:3162[B]:ASP:C | 2.20 | 0.47 |
| 3:F:3165[B]:ASN:O | 3:a:3149[B]:ASN:HB3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3169[B]:LYS:CE | 3:a:3147[B]:GLU:N | 2.58 | 0.47 |
| 3:F:3225[A]:SER:C | 3:F:3290[A]:ILE:HG23 | 2.39 | 0.47 |
| 3:F:3229[B]:ASN:OD1 | 3:F:3244[B]:THR:HB | 2.14 | 0.47 |
| 3:F:3230[A]:PHE:H | 3:F:3243[A]:GLY:HA3 | 1.79 | 0.47 |
| 3:F:3255[B]:PRO:O | 3:a:2966[B]:SER:HA | 2.13 | 0.47 |
| 1:G:177:VAL:HG11 | 1:G:358:TYR:CE1 | 2.50 | 0.47 |
| 1:G:1034:GLU:HB2 | 1:G:1182:ASN:ND2 | 2.29 | 0.47 |
| 2:H:2122:ILE:O | 2:H:2125:PHE:HB2 | 2.13 | 0.47 |
| 2:H:2644:LEU:HB2 | 2:H:2686:LEU:HB3 | 1.96 | 0.47 |
| 3:I:2952[B]:ALA:HB1 | 3:I:2957[B]:ILE:H | 1.79 | 0.47 |
| 3:I:3004[B]:GLY:O | 3:I:3006[B]:LYS:N | 2.44 | 0.47 |
| 3:I:3196[A]:THR:O | 3:I:3200[A]:LEU:N | 2.43 | 0.47 |
| 3:I:3200[B]:LEU:HD22 | 3:I:3204[B]:LEU:HD11 | 1.95 | 0.47 |
| 3:I:3228[B]:VAL:CG2 | 3:I:3245[B]:PHE:CE1 | 2.97 | 0.47 |
| 3:I:3232[A]:VAL:HG23 | 3:I:3273[A]:LEU:HD11 | 1.95 | 0.47 |
| 1:J:1438:ASP:HB2 | 1:M:1372:ILE:HD12 | 1.96 | 0.47 |
| 2:K:2496:LEU:HB3 | 2:K:2498:VAL:HG22 | 1.95 | 0.47 |
| 3:L:2968[B]:GLN:HA | 3:L:2973[B]:THR:O | 2.14 | 0.47 |
| 3:L:3110[B]:THR:C | 3:L:3112[B]:TYR:H | 2.21 | 0.47 |
| 3:L:3196[B]:THR:HG23 | 3:L:3199[B]:GLN:OE1 | 2.14 | 0.47 |
| 1:M:1442:MET:HE1 | 1:M:1454:PHE:HA | 1.95 | 0.47 |
| 1:M:1575:PRO:HA | 1:M:1581:GLU:O | 2.14 | 0.47 |
| 2:N:2129:PRO:O | 2:N:2131:LEU:HD23 | 2.14 | 0.47 |
| 3:O:2933[B]:SER:HA | 3:O:2935[B]:ILE:HD11 | 1.95 | 0.47 |
| 3:O:2976[B]:ALA:H | 3:X:3156[B]:MET:CG | 1.99 | 0.47 |
| 3:O:3125[A]:ARG:O | 3:O:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:O:3143[B]:SER:OG | 3:O:3144[B]:ALA:N | 2.46 | 0.47 |
| 3:O:3151[B]:LEU:CB | 3:O:3175[B]:TYR:CD2 | 2.93 | 0.47 |
| 3:O:3191[A]:ASN:C | 3:O:3192[A]:PHE:O | 2.52 | 0.47 |
| 3:O:3293[A]:LYS:HB2 | 3:O:3294[A]:SER:CA | 2.41 | 0.47 |
| 1:P:829:ALA:HA | 1:P:830:ASN:CG | 2.39 | 0.47 |
| 1:P:961:SER:HB2 | 1:P:973:ARG:HA | 1.95 | 0.47 |
| 1:P:981:GLU:HG2 | 1:P:983:PRO:HD2 | 1.96 | 0.47 |
| 1:P:1551:ASP:OD1 | 1:P:1551:ASP:N | 2.47 | 0.47 |
| 2:Q:2240:GLN:HG2 | 2:Q:2244:PHE:CD1 | 2.49 | 0.47 |
| 2:Q:2840:GLY:O | 2:Q:2843:GLU:HB2 | 2.15 | 0.47 |
| 3:R:2994[A]:LYS:HE2 | 3:R:3183[A]:LEU:O | 2.14 | 0.47 |
| 3:R:3110[A]:THR:C | 3:R:3112[A]:TYR:N | 2.68 | 0.47 |
| 3:R:3125[A]:ARG:O | 3:R:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:R:3298[A]:ASN:CA | 3:R:3299[A]:LEU:CB | 2.85 | 0.47 |
| 1:S:411:ASP:HB2 | 1:S:654:PRO:HA | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:750:ALA:HA | 1:S:796:TYR:HB3 | 1.96 | 0.47 |
| 1:S:929:TRP:O | 1:S:1048:ASN:ND2 | 2.47 | 0.47 |
| 2:T:2327:GLU:H | 2:T:2327:GLU:HG3 | 1.44 | 0.47 |
| 2:T:2597:MET:SD | 2:T:2651:GLN:NE2 | 2.76 | 0.47 |
| 3:U:2933[B]:SER:HA | 3:U:2935[B]:ILE:HD11 | 1.95 | 0.47 |
| 3:U:3200[A]:LEU:HD22 | 3:U:3204[A]:LEU:HD11 | 1.95 | 0.47 |
| 1:V:215:ARG:HE | 1:V:279:LEU:HA | 1.78 | 0.47 |
| 1:V:564:ASP:OD1 | 1:V:564:ASP:N | 2.38 | 0.47 |
| 1:V:1642:GLN:CD | 1:V:1642:GLN:H | 2.21 | 0.47 |
| 3:X:2991[A]:LEU:HD23 | 3:X:3158[A]:PHE:CE1 | 2.47 | 0.47 |
| 3:X:3143[B]:SER:OG | 3:X:3144[B]:ALA:N | 2.47 | 0.47 |
| 3:X:3147[A]:GLU:CG | 3:X:3149[A]:ASN:ND2 | 2.73 | 0.47 |
| 3:X:3196[A]:THR:HG23 | 3:X:3199[A]:GLN:OE1 | 2.14 | 0.47 |
| 3:X:3196[B]:THR:HG23 | 3:X:3199[B]:GLN:OE1 | 2.14 | 0.47 |
| 1:Y:127:GLU:HA | 1:Y:134:VAL:HG13 | 1.95 | 0.47 |
| 1:Y:760:ILE:HG21 | 1:Y:777:TYR:HE2 | 1.79 | 0.47 |
| 1:Y:871:GLN:NE2 | 1:Y:964:ILE:O | 2.47 | 0.47 |
| 1:Y:1161:ILE:O | 1:Y:1203:MET:HE1 | 2.14 | 0.47 |
| 2:Z:2730:LEU:HA | 1:b:1245:GLU:HB3 | 1.95 | 0.47 |
| 2:Z:2879:LEU:HD12 | 2:Z:2899:PRO:HB2 | 1.96 | 0.47 |
| 2:Z:2901:LEU:HB2 | 1:b:1074:ILE:HB | 1.96 | 0.47 |
| 3:a:2949[A]:LYS:C | 3:a:2953[A]:GLY:N | 2.72 | 0.47 |
| 3:a:3298[B]:ASN:CB | 3:a:3299[B]:LEU:C | 2.85 | 0.47 |
| 1:b:1018:ILE:HD12 | 1:b:1045:HIS:CD2 | 2.49 | 0.47 |
| 3:d:2968[A]:GLN:HA | 3:d:2973[A]:THR:O | 2.14 | 0.47 |
| 3:d:3196[B]:THR:OG1 | 3:d:3199[B]:GLN:CD | 2.57 | 0.47 |
| 3:d:3196[B]:THR:HG23 | 3:d:3199[B]:GLN:OE1 | 2.14 | 0.47 |
| 3:d:3230[A]:PHE:H | 3:d:3243[A]:GLY:HA3 | 1.80 | 0.47 |
| 3:d:3230[B]:PHE:H | 3:d:3243[B]:GLY:HA3 | 1.80 | 0.47 |
| 4:7:1:NAG:H61 | 4:7:2:NAG:N2 | 2.30 | 0.47 |
| 1:A:466:ALA:HB1 | 1:A:476:ARG:HG3 | 1.95 | 0.47 |
| 1:A:1145:THR:OG1 | 1:A:1233:SER:HB3 | 2.14 | 0.47 |
| 1:A:1154:SER:HB2 | 1:A:1220:MET:HE2 | 1.95 | 0.47 |
| 1:A:1578:ILE:HA | 1:A:1579:GLY:HA2 | 1.58 | 0.47 |
| 2:B:2568:HIS:HD2 | 2:B:2765:PRO:HB3 | 1.79 | 0.47 |
| 3:C:2952[B]:ALA:HB1 | 3:C:2957[B]:ILE:H | 1.79 | 0.47 |
| 3:C:3143[B]:SER:OG | 3:C:3144[B]:ALA:N | 2.47 | 0.47 |
| 3:C:3169[B]:LYS:O | 3:L:3152[B]:LYS:CD | 2.62 | 0.47 |
| 3:C:3172[B]:SER:CB | 3:L:3150[B]:LYS:HA | 2.27 | 0.47 |
| 3:C:3228[B]:VAL:CG2 | 3:C:3245[B]:PHE:CE1 | 2.97 | 0.47 |
| 3:F:2991[B]:LEU:HD23 | 3:F:3158[B]:PHE:CE1 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3157[B]:PRO:O | 3:a:3150[B]:LYS:CG | 2.54 | 0.47 |
| 3:F:3163[B]:ASN:HD22 | 3:a:3150[B]:LYS:CG | 2.07 | 0.47 |
| 3:F:3228[A]:VAL:CG2 | 3:F:3245[A]:PHE:CE1 | 2.97 | 0.47 |
| 3:F:3257[B]:ALA:HB3 | 3:a:2956[B]:LYS:HD2 | 1.97 | 0.47 |
| 3:F:3285[A]:VAL:CG2 | 3:F:3286[A]:THR:H | 2.27 | 0.47 |
| 1:G:872:GLN:O | 1:G:875:ALA:N | 2.45 | 0.47 |
| 1:G:1358:LEU:O | 1:G:1375:ASN:ND2 | 2.42 | 0.47 |
| 1:G:1559:LEU:HD21 | 1:G:1590:PHE:CE1 | 2.49 | 0.47 |
| 2:H:2166:LEU:HA | 2:H:2169:HIS:HB2 | 1.95 | 0.47 |
| 2:H:2728:ARG:HB3 | 2:H:2730:LEU:HD12 | 1.96 | 0.47 |
| 3:I:2933[A]:SER:HA | 3:I:2935[A]:ILE:HD11 | 1.95 | 0.47 |
| 3:I:2949[B]:LYS:C | 3:I:2953[B]:GLY:N | 2.72 | 0.47 |
| 3:I:2959[B]:SER:HA | 3:R:3255[B]:PRO:HG2 | 1.50 | 0.47 |
| 3:I:3148[B]:ILE:HG22 | 3:I:3152[B]:LYS:CE | 2.44 | 0.47 |
| 3:I:3221[B]:ALA:HB2 | 3:R:2964[B]:PRO:C | 2.23 | 0.47 |
| 3:I:3225[B]:SER:C | 3:I:3290[B]:ILE:HG23 | 2.39 | 0.47 |
| 3:I:3293[A]:LYS:HB2 | 3:I:3294[A]:SER:CA | 2.41 | 0.47 |
| 3:I:3298[A]:ASN:CB | 3:I:3299[A]:LEU:C | 2.86 | 0.47 |
| 1:J:40:TYR:HE2 | 1:J:75:GLN:HE21 | 1.61 | 0.47 |
| 1:J:324:PRO:HA | 1:J:332:ASP:OD1 | 2.14 | 0.47 |
| 1:J:855:ARG:HH21 | 1:J:941:LEU:HA | 1.79 | 0.47 |
| 1:J:946:GLU:HA | 1:J:955:LYS:HB3 | 1.96 | 0.47 |
| 2:K:2240:GLN:HE21 | 2:K:2241:THR:HG22 | 1.79 | 0.47 |
| 3:L:2954[A]:TYR:CA | 3:L:2957[A]:ILE:HG22 | 2.43 | 0.47 |
| 3:L:3125[A]:ARG:O | 3:L:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:L:3143[B]:SER:OG | 3:L:3144[B]:ALA:N | 2.46 | 0.47 |
| 3:L:3196[B]:THR:OG1 | 3:L:3199[B]:GLN:CD | 2.57 | 0.47 |
| 3:L:3200[B]:LEU:HD22 | 3:L:3204[B]:LEU:HD11 | 1.95 | 0.47 |
| 3:L:3229[B]:ASN:OD1 | 3:L:3244[B]:THR:HB | 2.14 | 0.47 |
| 3:L:3230[A]:PHE:H | 3:L:3243[A]:GLY:HA3 | 1.80 | 0.47 |
| 3:O:2968[A]:GLN:HA | 3:O:2973[A]:THR:O | 2.14 | 0.47 |
| 3:O:3191[B]:ASN:C | 3:O:3192[B]:PHE:O | 2.52 | 0.47 |
| 3:O:3196[B]:THR:HG23 | 3:O:3199[B]:GLN:OE1 | 2.14 | 0.47 |
| 3:O:3298[A]:ASN:CB | 3:O:3299[A]:LEU:C | 2.85 | 0.47 |
| 1:P:837:HIS:HA | 1:P:1113:HIS:O | 2.13 | 0.47 |
| 1:P:1279:LYS:HB2 | 1:P:1376:PRO:HG3 | 1.96 | 0.47 |
| 1:P:1324:ARG:NE | 1:P:1462:ASP:OD1 | 2.44 | 0.47 |
| 3:R:2994[B]:LYS:HE2 | 3:R:3183[B]:LEU:O | 2.14 | 0.47 |
| 3:R:3141[A]:TYR:CD2 | 3:R:3141[A]:TYR:C | 2.86 | 0.47 |
| 3:R:3148[A]:ILE:HG22 | 3:R:3152[A]:LYS:CE | 2.44 | 0.47 |
| 3:R:3217[B]:PHE:HD2 | 3:R:3300[B]:LEU:HD12 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:898:GLY:N | 1:S:899:MET:SD | 2.74 | 0.47 |
| 1:S:1179:GLY:HA2 | 1:S:1183:GLU:OE1 | 2.14 | 0.47 |
| 1:S:1286:ARG:HG3 | 1:S:1337:ARG:NH2 | 2.29 | 0.47 |
| 2:T:2435:MET:SD | 2:T:2436:PRO:HD2 | 2.54 | 0.47 |
| 1:V:1578:ILE:HA | 1:V:1579:GLY:HA2 | 1.55 | 0.47 |
| 2:W:2728:ARG:HB3 | 2:W:2730:LEU:HD12 | 1.96 | 0.47 |
| 3:X:2968[B]:GLN:HA | 3:X:2973[B]:THR:O | 2.14 | 0.47 |
| 3:X:2981[B]:GLY:N | 3:X:3086[B]:GLU:OE1 | 2.45 | 0.47 |
| 3:X:3200[B]:LEU:HD22 | 3:X:3204[B]:LEU:HD11 | 1.95 | 0.47 |
| 3:X:3225[A]:SER:C | 3:X:3290[A]:ILE:HG23 | 2.39 | 0.47 |
| 3:X:3230[A]:PHE:H | 3:X:3243[A]:GLY:HA3 | 1.79 | 0.47 |
| 3:X:3230[B]:PHE:H | 3:X:3243[B]:GLY:HA3 | 1.79 | 0.47 |
| 1:Y:325:THR:N | 1:Y:332:ASP:OD1 | 2.47 | 0.47 |
| 1:Y:1475:ARG:NE | 1:Y:1541:GLU:OE2 | 2.32 | 0.47 |
| 2:Z:2286:HIS:NE2 | 2:Z:2433:THR:HG22 | 2.29 | 0.47 |
| 2:Z:2625:LEU:O | 2:Z:2638:ARG:NH2 | 2.47 | 0.47 |
| 3:a:2994[A]:LYS:HE2 | 3:a:3183[A]:LEU:O | 2.14 | 0.47 |
| 3:a:3229[A]:ASN:OD1 | 3:a:3244[A]:THR:HB | 2.14 | 0.47 |
| 1:b:1077:LEU:HD23 | 1:b:1103:PHE:HE1 | 1.79 | 0.47 |
| 1:b:1161:ILE:O | 1:b:1203:MET:HE1 | 2.14 | 0.47 |
| 3:d:3143[B]:SER:OG | 3:d:3144[B]:ALA:N | 2.46 | 0.47 |
| 3:d:3146[A]:CYS:HA | 3:d:3147[A]:GLU:HA | 1.70 | 0.47 |
| 3:d:3217[A]:PHE:HD2 | 3:d:3300[A]:LEU:HD12 | 1.79 | 0.47 |
| 3:d:3229[B]:ASN:OD1 | 3:d:3244[B]:THR:HB | 2.14 | 0.47 |
| 1:A:398:ARG:NH2 | 1:A:484:MET:HE2 | 2.29 | 0.47 |
| 3:C:3074[A]:GLU:CD | 3:C:3212[A]:ARG:NH2 | 2.73 | 0.47 |
| 3:C:3154[B]:PRO:CA | 3:L:3174[B]:GLY:N | 2.77 | 0.47 |
| 1:D:841:LYS:HA | 1:D:1117:ASP:HB2 | 1.95 | 0.47 |
| 2:E:2823:ILE:HD11 | 2:E:2859:VAL:HG12 | 1.96 | 0.47 |
| 3:F:2949[B]:LYS:NZ | 3:F:2949[B]:LYS:C | 2.73 | 0.47 |
| 3:F:2994[A]:LYS:HE2 | 3:F:3183[A]:LEU:O | 2.14 | 0.47 |
| 3:F:3150[B]:LYS:HD2 | 3:a:3160[B]:SER:O | 2.06 | 0.47 |
| 1:G:293:LEU:O | 1:G:297:ARG:HG3 | 2.14 | 0.47 |
| 1:G:1348:TRP:HD1 | 1:G:1403:LEU:HD13 | 1.78 | 0.47 |
| 1:G:1578:ILE:HA | 1:G:1579:GLY:HA2 | 1.55 | 0.47 |
| 2:H:2340:ALA:HB1 | 2:H:2341:PRO:CD | 2.41 | 0.47 |
| 3:I:2933[B]:SER:HA | 3:I:2935[B]:ILE:HD11 | 1.96 | 0.47 |
| 3:I:2994[A]:LYS:HE2 | 3:I:3183[A]:LEU:O | 2.14 | 0.47 |
| 3:I:2994[B]:LYS:HE2 | 3:I:3183[B]:LEU:O | 2.14 | 0.47 |
| 3:I:3146[A]:CYS:HA | 3:I:3147[A]:GLU:HA | 1.70 | 0.47 |
| 3:I:3169[B]:LYS:HE2 | 3:R:3147[B]:GLU:H | 1.07 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3196[B]:THR:CA | 3:I:3199[B]:GLN:HB2 | 2.43 | 0.47 |
| 1:J:73:LEU:HD21 | 1:J:210:HIS:HB2 | 1.96 | 0.47 |
| 2:K:2400:LEU:HB2 | 2:K:2439:PHE:HD2 | 1.80 | 0.47 |
| 3:L:2932[B]:PRO:CA | 3:L:2935[B]:ILE:CD1 | 2.85 | 0.47 |
| 3:L:2949[A]:LYS:C | 3:L:2953[A]:GLY:N | 2.72 | 0.47 |
| 1:M:394:GLN:H | 1:M:394:GLN:HG3 | 1.36 | 0.47 |
| 1:M:516:TRP:CD1 | 1:M:579:LEU:HD22 | 2.50 | 0.47 |
| 1:M:979:LEU:HB3 | 1:M:980:TYR:HA | 1.96 | 0.47 |
| 1:M:1470:GLU:OE2 | 1:M:1473:ARG:NH1 | 2.47 | 0.47 |
| 3:O:2952[A]:ALA:HB1 | 3:O:2957[A]:ILE:H | 1.79 | 0.47 |
| 3:O:3183[A]:LEU:H | 3:O:3184[A]:ASN:CA | 2.22 | 0.47 |
| 3:O:3229[A]:ASN:OD1 | 3:O:3244[A]:THR:HB | 2.14 | 0.47 |
| 3:O:3288[B]:MET:CA | 3:O:3295[B]:LEU:HG | 2.42 | 0.47 |
| 1:P:1258:ARG:HD2 | 1:P:1524:HIS:O | 2.14 | 0.47 |
| 3:R:2981[A]:GLY:N | 3:R:3086[A]:GLU:OE1 | 2.45 | 0.47 |
| 3:R:3196[A]:THR:HG23 | 3:R:3199[A]:GLN:OE1 | 2.14 | 0.47 |
| 3:R:3229[B]:ASN:OD1 | 3:R:3244[B]:THR:HB | 2.14 | 0.47 |
| 1:S:151:GLN:OE1 | 1:S:151:GLN:N | 2.42 | 0.47 |
| 1:V:618:MET:HE3 | 1:V:618:MET:HB3 | 1.77 | 0.47 |
| 1:V:838:ARG:NH2 | 1:V:915:ASN:OD1 | 2.47 | 0.47 |
| 3:X:3229[B]:ASN:OD1 | 3:X:3244[B]:THR:HB | 2.14 | 0.47 |
| 1:Y:25:MET:HE2 | 1:Y:34:TYR:HA | 1.95 | 0.47 |
| 1:Y:387:ASN:OD1 | 1:Y:387:ASN:N | 2.39 | 0.47 |
| 1:Y:836:GLN:HB2 | 1:Y:1113:HIS:CG | 2.49 | 0.47 |
| 1:Y:1619:GLY:N | 3:d:3190[B]:LEU:HG | 2.30 | 0.47 |
| 2:Z:2565:THR:OG1 | 2:Z:2741:GLN:NE2 | 2.47 | 0.47 |
| 3:a:2939[B]:ARG:HG3 | 3:a:2939[B]:ARG:NH1 | 2.28 | 0.47 |
| 3:a:2952[A]:ALA:HB1 | 3:a:2957[A]:ILE:H | 1.79 | 0.47 |
| 3:a:2954[B]:TYR:CA | 3:a:2957[B]:ILE:HG22 | 2.43 | 0.47 |
| 3:a:3066[A]:TYR:CE1 | 3:a:3193[A]:HIS:CE1 | 2.98 | 0.47 |
| 3:a:3143[A]:SER:OG | 3:a:3144[A]:ALA:N | 2.46 | 0.47 |
| 3:a:3229[B]:ASN:OD1 | 3:a:3244[B]:THR:HB | 2.14 | 0.47 |
| 3:a:3288[B]:MET:CA | 3:a:3295[B]:LEU:HG | 2.42 | 0.47 |
| 1:b:806:ASN:ND2 | 4:OA:1:NAG:O7 | 2.47 | 0.47 |
| 1:b:1280:GLN:HG2 | 1:b:1337:ARG:HD2 | 1.96 | 0.47 |
| 1:b:1578:ILE:HA | 1:b:1579:GLY:HA2 | 1.71 | 0.47 |
| 3:d:2939[B]:ARG:HG3 | 3:d:2939[B]:ARG:NH1 | 2.28 | 0.47 |
| 3:d:2985[A]:PHE:CE2 | 3:d:2989[A]:HIS:NE2 | 2.83 | 0.47 |
| 3:d:2994[A]:LYS:HE2 | 3:d:3183[A]:LEU:O | 2.14 | 0.47 |
| 4:MA:1:NAG:C6 | 4:MA:2:NAG:HN2 | 2.27 | 0.47 |
| 1:A:907:ARG:HG3 | 1:A:1112:PHE:HE2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2940[A]:ASN:O | 3:C:2944[A]:ALA:N | 2.48 | 0.47 |
| 3:C:2991[B]:LEU:HD23 | 3:C:3158[B]:PHE:CE1 | 2.48 | 0.47 |
| 3:C:2994[B]:LYS:HE2 | 3:C:3183[B]:LEU:O | 2.14 | 0.47 |
| 3:C:3089[B]:HIS:CE1 | 3:C:3119[B]:HIS:CE1 | 2.81 | 0.47 |
| 3:C:3096[B]:VAL:HG11 | 3:C:3115[B]:LEU:HD12 | 1.89 | 0.47 |
| 3:C:3196[B]:THR:OG1 | 3:C:3199[B]:GLN:CD | 2.57 | 0.47 |
| 3:C:3223[B]:GLY:C | 3:L:3252[B]:TYR:CD1 | 2.88 | 0.47 |
| 3:C:3228[A]:VAL:CG2 | 3:C:3245[A]:PHE:CE1 | 2.97 | 0.47 |
| 1:D:1156:LEU:HB2 | 1:D:1176:TYR:CE1 | 2.50 | 0.47 |
| 2:E:2090:LYS:NZ | 2:E:2099:GLU:OE2 | 2.46 | 0.47 |
| 2:E:2570:HIS:CD2 | 2:E:2711:HIS:CE1 | 2.98 | 0.47 |
| 3:F:2965[B]:LEU:C | 3:a:3255[B]:PRO:CA | 2.83 | 0.47 |
| 3:F:2968[A]:GLN:HA | 3:F:2973[A]:THR:O | 2.14 | 0.47 |
| 3:F:3096[A]:VAL:HG11 | 3:F:3115[A]:LEU:HD12 | 1.89 | 0.47 |
| 3:F:3141[A]:TYR:CD2 | 3:F:3141[A]:TYR:C | 2.86 | 0.47 |
| 3:F:3148[A]:ILE:HG22 | 3:F:3152[A]:LYS:CE | 2.44 | 0.47 |
| 3:F:3169[B]:LYS:HA | 3:a:3150[B]:LYS:CA | 2.16 | 0.47 |
| 3:F:3200[A]:LEU:HD22 | 3:F:3204[A]:LEU:HD11 | 1.95 | 0.47 |
| 3:F:3293[B]:LYS:HB2 | 3:F:3294[B]:SER:CA | 2.41 | 0.47 |
| 1:G:497:GLN:HG2 | 1:G:683:THR:HG21 | 1.96 | 0.47 |
| 2:H:2704:ASP:O | 2:H:2707:PHE:HB3 | 2.15 | 0.47 |
| 3:I:3150[B]:LYS:HG3 | 3:R:3163[B]:ASN:CG | 2.34 | 0.47 |
| 3:I:3285[A]:VAL:CG2 | 3:I:3286[A]:THR:H | 2.27 | 0.47 |
| 1:J:1019:HIS:HD1 | 1:J:1030:MET:HE2 | 1.80 | 0.47 |
| 1:J:1280:GLN:NE2 | 1:J:1337:ARG:HD3 | 2.30 | 0.47 |
| 2:K:2128:LEU:O | 2:K:2130:PRO:HD3 | 2.13 | 0.47 |
| 2:K:2158:TYR:O | 2:K:2161:GLN:HB3 | 2.14 | 0.47 |
| 2:K:2309:GLN:NE2 | 2:K:2319:ALA:O | 2.40 | 0.47 |
| 2:K:2572:VAL:HG22 | 2:K:2768:LEU:HD13 | 1.96 | 0.47 |
| 3:L:2961[A]:HIS:CD2 | 3:L:2988[A]:TRP:CZ3 | 2.96 | 0.47 |
| 3:L:3180[B]:TYR:CB | 3:L:3183[B]:LEU:CD2 | 2.90 | 0.47 |
| 3:L:3191[B]:ASN:ND2 | 3:L:3191[B]:ASN:N | 2.60 | 0.47 |
| 3:O:2949[B]:LYS:C | 3:O:2953[B]:GLY:N | 2.72 | 0.47 |
| 3:O:2960[A]:PHE:CD1 | 3:O:2960[A]:PHE:N | 2.72 | 0.47 |
| 3:O:3229[B]:ASN:OD1 | 3:O:3244[B]:THR:HB | 2.14 | 0.47 |
| 3:O:3283[A]:ILE:HB | 3:O:3305[A]:ILE:HD11 | 1.97 | 0.47 |
| 3:O:3298[A]:ASN:CA | 3:O:3299[A]:LEU:C | 2.85 | 0.47 |
| 1:P:1638:SER:OG | 1:S:472:ASP:OD2 | 2.29 | 0.47 |
| 3:R:2949[A]:LYS:NZ | 3:R:2949[A]:LYS:C | 2.73 | 0.47 |
| 3:R:3225[B]:SER:C | 3:R:3290[B]:ILE:HG23 | 2.39 | 0.47 |
| 3:R:3230[A]:PHE:H | 3:R:3243[A]:GLY:HA3 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:43:GLU:HG3 | 1:S:44:PRO:HA | 1.97 | 0.47 |
| 1:S:187:GLY:HA2 | 1:S:193:SER:HB2 | 1.97 | 0.47 |
| 1:S:277:ASP:OD1 | 1:S:278:ASP:N | 2.46 | 0.47 |
| 1:S:876:PHE:CD1 | 1:S:1083:PRO:HB2 | 2.48 | 0.47 |
| 2:T:2844:MET:O | 2:T:2846:TRP:HD1 | 1.98 | 0.47 |
| 3:U:2940[B]:ASN:O | 3:U:2944[B]:ALA:N | 2.48 | 0.47 |
| 1:V:92:TRP:CE3 | 1:V:102:PRO:HD3 | 2.49 | 0.47 |
| 1:V:547:LYS:HE2 | 1:V:558:HIS:CD2 | 2.50 | 0.47 |
| 1:V:843:VAL:HG13 | 1:V:927:PRO:HB2 | 1.97 | 0.47 |
| 1:V:1407:THR:HG22 | 1:V:1426:LEU:HD21 | 1.96 | 0.47 |
| 1:V:1574:VAL:HG22 | 1:V:1620:LEU:HD21 | 1.96 | 0.47 |
| 3:X:2935[A]:ILE:CG1 | 3:X:2936[A]:GLU:N | 2.78 | 0.47 |
| 1:Y:1487:PRO:HD3 | 2:c:2486:ILE:HB | 1.95 | 0.47 |
| 1:Y:1546:LYS:HG3 | 3:d:3001[B]:LYS:CD | 2.44 | 0.47 |
| 1:Y:1550:ARG:NE | 3:d:3008[B]:GLY:C | 2.72 | 0.47 |
| 2:Z:2279:LEU:HD12 | 2:Z:2284:HIS:HD2 | 1.77 | 0.47 |
| 3:a:2940[A]:ASN:O | 3:a:2944[A]:ALA:N | 2.48 | 0.47 |
| 3:a:2940[B]:ASN:O | 3:a:2944[B]:ALA:N | 2.48 | 0.47 |
| 3:a:2970[B]:PRO:C | 3:a:2972[B]:GLY:N | 2.72 | 0.47 |
| 3:a:2971[B]:ASP:OD1 | 9:a:3401[B]:CUO:O2 | 2.33 | 0.47 |
| 1:b:479:CYS:HB3 | 1:b:670:PRO:HD3 | 1.96 | 0.47 |
| 1:b:572:SER:HA | 1:b:573:LYS:HA | 1.39 | 0.47 |
| 2:c:2370:MET:HE3 | 2:c:2370:MET:HB2 | 1.71 | 0.47 |
| 2:c:2462:PHE:CE1 | 2:c:2486:ILE:HD13 | 2.49 | 0.47 |
| 2:c:2699:MET:HG3 | 2:c:2840:GLY:HA3 | 1.96 | 0.47 |
| 3:d:2935[B]:ILE:CG1 | 3:d:2936[B]:GLU:N | 2.78 | 0.47 |
| 3:d:3196[A]:THR:HG23 | 3:d:3199[A]:GLN:OE1 | 2.14 | 0.47 |
| 3:d:3285[B]:VAL:CG2 | 3:d:3286[B]:THR:N | 2.73 | 0.47 |
| 1:A:490:TRP:HE1 | 1:A:670:PRO:HD3 | 1.79 | 0.47 |
| 2:B:2294:PHE:O | 2:B:2297:HIS:HB3 | 2.14 | 0.47 |
| 3:C:2933[A]:SER:HA | 3:C:2935[A]:ILE:HD11 | 1.95 | 0.47 |
| 3:C:2937[B]:ASN:CB | 3:C:3006[B]:LYS:CE | 2.86 | 0.47 |
| 3:C:2952[A]:ALA:HB1 | 3:C:2957[A]:ILE:H | 1.79 | 0.47 |
| 3:C:2968[A]:GLN:HA | 3:C:2973[A]:THR:O | 2.14 | 0.47 |
| 3:C:3151[B]:LEU:C | 3:L:3154[B]:PRO:HB3 | 2.36 | 0.47 |
| 3:C:3255[B]:PRO:HA | 3:L:2964[B]:PRO:O | 2.12 | 0.47 |
| 1:D:745:ASP:HB2 | 1:D:801:ASP:OD1 | 2.14 | 0.47 |
| 1:D:855:ARG:HD3 | 1:D:959:PHE:CD2 | 2.49 | 0.47 |
| 1:D:1018:ILE:HA | 1:D:1021:LEU:HB2 | 1.96 | 0.47 |
| 1:D:1258:ARG:HB3 | 1:D:1342:ALA:HB2 | 1.97 | 0.47 |
| 1:D:1283:ASP:OD1 | 1:D:1283:ASP:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3014[A]:TRP:HH2 | 3:F:3123[A]:THR:HG23 | 1.78 | 0.47 |
| 3:F:3151[A]:LEU:HB2 | 3:F:3175[A]:TYR:HE2 | 1.68 | 0.47 |
| 1:G:321:LEU:HD11 | 1:G:377:TYR:CD2 | 2.50 | 0.47 |
| 1:G:597:VAL:O | 1:G:601:VAL:HG12 | 2.14 | 0.47 |
| 2:H:2800:LYS:HB3 | 3:I:3023[A]:ILE:CD1 | 2.45 | 0.47 |
| 3:I:2959[B]:SER:HB3 | 3:R:3255[B]:PRO:CB | 2.36 | 0.47 |
| 3:I:2985[B]:PHE:CE2 | 3:I:2989[B]:HIS:NE2 | 2.83 | 0.47 |
| 3:I:3078[B]:PHE:HE2 | 3:R:3161[B]:GLU:OE1 | 1.98 | 0.47 |
| 3:I:3155[B]:MET:HA | 3:R:2979[B]:GLN:NE2 | 2.29 | 0.47 |
| 3:I:3173[B]:THR:HA | 3:R:3154[B]:PRO:HA | 1.96 | 0.47 |
| 3:I:3255[B]:PRO:N | 3:R:2966[B]:SER:OG | 2.47 | 0.47 |
| 1:J:177:VAL:O | 1:J:181:PRO:HD3 | 2.14 | 0.47 |
| 1:J:980:TYR:CE1 | 1:J:1021:LEU:HD13 | 2.49 | 0.47 |
| 2:K:2521:MET:HE3 | 2:K:2605:LEU:HD12 | 1.97 | 0.47 |
| 2:K:2616:THR:HB | 2:K:2618:SER:H | 1.78 | 0.47 |
| 3:L:2935[B]:ILE:CG1 | 3:L:2936[B]:GLU:N | 2.78 | 0.47 |
| 3:L:3183[B]:LEU:H | 3:L:3184[B]:ASN:CA | 2.22 | 0.47 |
| 3:L:3229[A]:ASN:OD1 | 3:L:3244[A]:THR:HB | 2.14 | 0.47 |
| 3:L:3230[B]:PHE:H | 3:L:3243[B]:GLY:HA3 | 1.79 | 0.47 |
| 1:M:127:GLU:CD | 1:M:135:THR:H | 2.22 | 0.47 |
| 1:M:909:ILE:HG12 | 1:M:1084:PHE:HZ | 1.79 | 0.47 |
| 3:O:2949[A]:LYS:NZ | 3:O:2949[A]:LYS:C | 2.73 | 0.47 |
| 1:P:1462:ASP:OD2 | 1:P:1525:TYR:OH | 2.23 | 0.47 |
| 3:R:2949[B]:LYS:C | 3:R:2953[B]:GLY:N | 2.72 | 0.47 |
| 3:R:2952[A]:ALA:N | 3:R:2953[A]:GLY:HA2 | 2.06 | 0.47 |
| 1:S:500:ASN:O | 1:S:504:THR:OG1 | 2.32 | 0.47 |
| 3:U:2935[A]:ILE:CG1 | 3:U:2936[A]:GLU:N | 2.78 | 0.47 |
| 3:U:2939[A]:ARG:HG3 | 3:U:2939[A]:ARG:NH1 | 2.28 | 0.47 |
| 3:U:2965[B]:LEU:CG | 3:d:3221[B]:ALA:H | 2.18 | 0.47 |
| 3:U:3257[B]:ALA:C | 3:d:2969[B]:TYR:O | 2.58 | 0.47 |
| 3:U:3284[B]:LYS:CD | 3:U:3284[B]:LYS:C | 2.86 | 0.47 |
| 1:V:840:ARG:HD2 | 1:V:1116:TYR:CZ | 2.50 | 0.47 |
| 2:W:2225:ARG:HD2 | 2:W:2274:LEU:HD22 | 1.96 | 0.47 |
| 2:W:2560:LEU:HD13 | 2:W:2569:TRP:CD1 | 2.50 | 0.47 |
| 2:W:2867:PRO:HG2 | 3:X:2932[A]:PRO:CG | 2.45 | 0.47 |
| 3:X:3148[A]:ILE:HG22 | 3:X:3152[A]:LYS:CE | 2.44 | 0.47 |
| 3:X:3228[A]:VAL:CG2 | 3:X:3245[A]:PHE:CE1 | 2.97 | 0.47 |
| 3:X:3298[B]:ASN:CB | 3:X:3299[B]:LEU:C | 2.86 | 0.47 |
| 1:Y:4:ARG:NH1 | 1:Y:77:GLU:OE1 | 2.48 | 0.47 |
| 1:Y:81:VAL:HA | 1:Y:85:SER:H | 1.79 | 0.47 |
| 1:Y:1075:GLU:HG2 | 2:c:2901:LEU:H | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:2985[A]:PHE:CE2 | 3:a:2989[A]:HIS:NE2 | 2.83 | 0.47 |
| 3:a:3074[B]:GLU:CD | 3:a:3212[B]:ARG:NH2 | 2.73 | 0.47 |
| 3:a:3141[A]:TYR:CD2 | 3:a:3141[A]:TYR:C | 2.86 | 0.47 |
| 3:a:3151[A]:LEU:HB2 | 3:a:3175[A]:TYR:HE2 | 1.68 | 0.47 |
| 3:a:3283[B]:ILE:HB | 3:a:3305[B]:ILE:HD11 | 1.97 | 0.47 |
| 1:b:858:MET:HE1 | 1:b:870:TYR:CE2 | 2.50 | 0.47 |
| 3:d:3148[B]:ILE:HG22 | 3:d:3152[B]:LYS:CE | 2.44 | 0.47 |
| 3:d:3219[A]:LEU:N | 3:d:3219[A]:LEU:CD2 | 2.73 | 0.47 |
| 1:A:81:VAL:HA | 1:A:85:SER:HB3 | 1.96 | 0.47 |
| 1:A:482:HIS:CE1 | 1:A:621:LEU:HD11 | 2.50 | 0.47 |
| 1:A:760:ILE:HG21 | 1:A:777:TYR:HE2 | 1.80 | 0.47 |
| 1:A:965:ASP:HB3 | 1:A:1038:PHE:CE2 | 2.50 | 0.47 |
| 1:A:1156:LEU:HB2 | 1:A:1176:TYR:CE2 | 2.50 | 0.47 |
| 1:A:1403:LEU:HD21 | 1:A:1429:THR:HG21 | 1.96 | 0.47 |
| 2:B:2554:PRO:HA | 2:B:2555:GLU:CB | 2.45 | 0.47 |
| 2:B:2903:TYR:OH | 3:C:2932[A]:PRO:HD2 | 2.14 | 0.47 |
| 3:C:2951[A]:ASP:C | 3:C:2956[A]:LYS:HZ1 | 2.09 | 0.47 |
| 3:C:2968[B]:GLN:CG | 3:L:2981[B]:GLY:N | 2.75 | 0.47 |
| 3:C:2994[A]:LYS:HE2 | 3:C:3183[A]:LEU:O | 2.14 | 0.47 |
| 3:C:3148[A]:ILE:HG22 | 3:C:3152[A]:LYS:CE | 2.44 | 0.47 |
| 3:C:3196[A]:THR:OG1 | 3:C:3199[A]:GLN:CD | 2.57 | 0.47 |
| 3:C:3200[B]:LEU:CD2 | 3:C:3204[B]:LEU:CD1 | 2.93 | 0.47 |
| 3:C:3229[A]:ASN:OD1 | 3:C:3244[A]:THR:HB | 2.14 | 0.47 |
| 3:C:3283[B]:ILE:C | 3:C:3283[B]:ILE:CD1 | 2.85 | 0.47 |
| 1:D:118:ALA:HB1 | 1:D:119:LYS:HA | 1.96 | 0.47 |
| 1:D:353:ASN:HD22 | 1:D:772:ARG:NH2 | 2.13 | 0.47 |
| 1:D:961:SER:HB3 | 1:D:972:SER:O | 2.14 | 0.47 |
| 1:D:964:ILE:HG22 | 1:D:970:SER:C | 2.40 | 0.47 |
| 3:F:2935[B]:ILE:CG1 | 3:F:2936[B]:GLU:N | 2.78 | 0.47 |
| 3:F:2952[A]:ALA:CB | 3:F:2953[A]:GLY:CA | 2.82 | 0.47 |
| 3:F:2969[B]:TYR:CE2 | 3:F:2970[B]:PRO:CG | 2.86 | 0.47 |
| 3:F:2983[B]:VAL:H | 3:a:3160[B]:SER:CA | 2.27 | 0.47 |
| 3:F:2985[B]:PHE:CE2 | 3:F:2989[B]:HIS:NE2 | 2.83 | 0.47 |
| 3:F:3152[B]:LYS:CB | 3:a:3170[B]:ALA:C | 2.86 | 0.47 |
| 3:F:3183[A]:LEU:H | 3:F:3184[A]:ASN:CA | 2.22 | 0.47 |
| 3:F:3196[B]:THR:HG23 | 3:F:3199[B]:GLN:OE1 | 2.14 | 0.47 |
| 3:F:3232[B]:VAL:HG23 | 3:F:3273[B]:LEU:HD11 | 1.95 | 0.47 |
| 3:F:3253[B]:GLU:HB3 | 3:a:3252[B]:TYR:HB3 | 1.97 | 0.47 |
| 3:F:3255[B]:PRO:CD | 3:a:2962[B]:GLY:C | 2.69 | 0.47 |
| 1:G:440:ARG:O | 1:G:444:GLU:HB2 | 2.14 | 0.47 |
| 1:G:460:GLU:CD | 1:G:1368:ARG:HH21 | 2.23 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:664:VAL:O | 1:G:689:PRO:HD2 | 2.15 | 0.47 |
| 1:G:1636:ASN:HB3 | 1:G:1639:LYS:HD3 | 1.95 | 0.47 |
| 2:H:2564:PRO:HA | 2:H:2673:GLU:HG3 | 1.97 | 0.47 |
| 2:H:2900:SER:HA | 1:J:1075:GLU:HG2 | 1.97 | 0.47 |
| 3:I:2935[A]:ILE:CG1 | 3:I:2936[A]:GLU:N | 2.78 | 0.47 |
| 3:I:2935[B]:ILE:CG1 | 3:I:2936[B]:GLU:N | 2.78 | 0.47 |
| 3:I:2952[A]:ALA:HB1 | 3:I:2957[A]:ILE:H | 1.79 | 0.47 |
| 3:I:2964[B]:PRO:N | 3:R:3255[B]:PRO:HG3 | 2.30 | 0.47 |
| 3:I:2968[B]:GLN:HA | 3:I:2973[B]:THR:O | 2.14 | 0.47 |
| 3:I:2969[A]:TYR:CD2 | 3:I:2970[A]:PRO:N | 2.83 | 0.47 |
| 3:I:2985[A]:PHE:CE2 | 3:I:2989[A]:HIS:NE2 | 2.83 | 0.47 |
| 3:I:2992[B]:TYR:CE2 | 3:R:2969[B]:TYR:HE1 | 2.31 | 0.47 |
| 3:I:3107[B]:LEU:HD22 | 3:R:3252[B]:TYR:HB3 | 1.97 | 0.47 |
| 3:I:3125[A]:ARG:O | 3:I:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:I:3125[B]:ARG:O | 3:I:3129[B]:ILE:HG13 | 2.14 | 0.47 |
| 3:I:3143[B]:SER:OG | 3:I:3144[B]:ALA:N | 2.46 | 0.47 |
| 3:I:3155[B]:MET:HB2 | 3:R:3153[B]:LYS:HG2 | 1.83 | 0.47 |
| 3:I:3191[A]:ASN:ND2 | 3:I:3191[A]:ASN:N | 2.60 | 0.47 |
| 3:I:3229[B]:ASN:OD1 | 3:I:3244[B]:THR:HB | 2.14 | 0.47 |
| 3:I:3232[B]:VAL:HG23 | 3:I:3273[B]:LEU:HD11 | 1.94 | 0.47 |
| 1:J:163:LEU:HB3 | 1:J:293:LEU:HD21 | 1.96 | 0.47 |
| 1:J:882:TRP:HB3 | 1:J:1086:LEU:HD11 | 1.97 | 0.47 |
| 1:J:1596:GLU:O | 1:J:1597:THR:HG22 | 2.14 | 0.47 |
| 2:K:2149:ALA:HA | 2:K:2260:GLU:HG2 | 1.97 | 0.47 |
| 2:K:2235:PRO:HG3 | 2:K:2240:GLN:NE2 | 2.27 | 0.47 |
| 2:K:2568:HIS:HD2 | 2:K:2718:TRP:CH2 | 2.33 | 0.47 |
| 3:L:2954[B]:TYR:CA | 3:L:2957[B]:ILE:HG22 | 2.43 | 0.47 |
| 3:L:2985[B]:PHE:CE2 | 3:L:2989[B]:HIS:NE2 | 2.83 | 0.47 |
| 3:L:3125[B]:ARG:O | 3:L:3129[B]:ILE:HG13 | 2.14 | 0.47 |
| 3:L:3141[A]:TYR:CD2 | 3:L:3141[A]:TYR:C | 2.86 | 0.47 |
| 3:L:3182[B]:GLN:H | 3:L:3182[B]:GLN:HG2 | 1.56 | 0.47 |
| 3:L:3200[B]:LEU:CD2 | 3:L:3204[B]:LEU:CD1 | 2.93 | 0.47 |
| 3:L:3225[B]:SER:C | 3:L:3290[B]:ILE:HG23 | 2.39 | 0.47 |
| 3:L:3285[A]:VAL:CG2 | 3:L:3286[A]:THR:H | 2.27 | 0.47 |
| 1:M:1019:HIS:NE2 | 1:M:1046:HIS:CE1 | 2.83 | 0.47 |
| 1:M:1274:LEU:HD21 | 1:M:1344:PRO:HD3 | 1.96 | 0.47 |
| 2:N:2509:ILE:HD11 | 2:N:2605:LEU:HD23 | 1.97 | 0.47 |
| 2:N:2567:MET:HE3 | 2:N:2718:TRP:HB2 | 1.97 | 0.47 |
| 3:O:2933[A]:SER:HA | 3:O:2935[A]:ILE:HD11 | 1.95 | 0.47 |
| 3:O:3148[B]:ILE:HG22 | 3:O:3152[B]:LYS:CE | 2.44 | 0.47 |
| 3:O:3154[B]:PRO:CG | 3:X:3175[B]:TYR:CG | 2.94 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3162[B]:ASP:OD2 | 3:X:3150[B]:LYS:CE | 2.62 | 0.47 |
| 1:P:419:THR:HA | 1:P:420:SER:HA | 1.68 | 0.47 |
| 1:P:480:CYS:SG | 1:P:621:LEU:HD11 | 2.54 | 0.47 |
| 1:P:832:LYS:HA | 1:P:832:LYS:NZ | 2.29 | 0.47 |
| 1:P:879:SER:HA | 1:P:893:ALA:HA | 1.96 | 0.47 |
| 1:P:979:LEU:HD23 | 1:P:980:TYR:HD1 | 1.80 | 0.47 |
| 1:P:1199:VAL:O | 1:P:1203:MET:HG3 | 2.15 | 0.47 |
| 2:Q:2149:ALA:HA | 2:Q:2260:GLU:HG2 | 1.97 | 0.47 |
| 2:Q:2551:PRO:HA | 2:Q:2552:GLU:HA | 1.56 | 0.47 |
| 2:Q:2726:LYS:HB2 | 2:Q:2726:LYS:HE3 | 1.77 | 0.47 |
| 2:Q:2833:GLY:HA3 | 2:Q:2854:MET:HE1 | 1.95 | 0.47 |
| 3:R:2935[A]:ILE:CG1 | 3:R:2936[A]:GLU:N | 2.78 | 0.47 |
| 3:R:2937[A]:ASN:CB | 3:R:3006[A]:LYS:CE | 2.85 | 0.47 |
| 3:R:2940[A]:ASN:O | 3:R:2944[A]:ALA:N | 2.48 | 0.47 |
| 3:R:2952[A]:ALA:HB1 | 3:R:2957[A]:ILE:H | 1.79 | 0.47 |
| 3:R:2952[B]:ALA:HB1 | 3:R:2957[B]:ILE:H | 1.79 | 0.47 |
| 3:R:3143[A]:SER:OG | 3:R:3144[A]:ALA:N | 2.46 | 0.47 |
| 3:R:3196[B]:THR:OG1 | 3:R:3199[B]:GLN:CD | 2.57 | 0.47 |
| 3:R:3200[B]:LEU:HD22 | 3:R:3204[B]:LEU:HD11 | 1.95 | 0.47 |
| 3:R:3225[A]:SER:C | 3:R:3290[A]:ILE:HG23 | 2.39 | 0.47 |
| 3:R:3285[B]:VAL:CG2 | 3:R:3286[B]:THR:H | 2.27 | 0.47 |
| 1:S:931:TRP:CZ3 | 1:S:995:ILE:HD11 | 2.50 | 0.47 |
| 1:S:962:GLY:HA2 | 1:S:971:THR:HB | 1.97 | 0.47 |
| 2:T:2240:GLN:HG2 | 2:T:2244:PHE:CD1 | 2.50 | 0.47 |
| 2:T:2749:PHE:HA | 2:T:2754:ASN:HD22 | 1.79 | 0.47 |
| 3:U:2970[B]:PRO:C | 3:d:3086[B]:GLU:HG2 | 2.40 | 0.47 |
| 3:U:2970[B]:PRO:C | 3:U:2972[B]:GLY:H | 2.23 | 0.47 |
| 3:U:2985[A]:PHE:CE2 | 3:U:2989[A]:HIS:NE2 | 2.83 | 0.47 |
| 3:U:3125[A]:ARG:O | 3:U:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:U:3228[A]:VAL:CG2 | 3:U:3245[A]:PHE:CE1 | 2.97 | 0.47 |
| 3:U:3255[B]:PRO:HB3 | 3:d:2974[B]:ALA:O | 2.12 | 0.47 |
| 1:V:547:LYS:HG3 | 1:V:559:THR:O | 2.15 | 0.47 |
| 1:V:583:LEU:HG | 1:V:602:THR:HG21 | 1.97 | 0.47 |
| 1:V:843:VAL:HG22 | 1:V:928:TYR:O | 2.14 | 0.47 |
| 1:V:1302:SER:HA | 1:V:1303:GLU:HA | 1.66 | 0.47 |
| 1:V:1493:MET:HG2 | 1:V:1511:SER:O | 2.14 | 0.47 |
| 2:W:2177:TYR:HB2 | 2:W:2300:ASN:HB2 | 1.97 | 0.47 |
| 3:X:2935[B]:ILE:CG1 | 3:X:2936[B]:GLU:N | 2.78 | 0.47 |
| 3:X:2949[A]:LYS:NZ | 3:X:2949[A]:LYS:C | 2.73 | 0.47 |
| 3:X:2949[B]:LYS:NZ | 3:X:2949[B]:LYS:C | 2.73 | 0.47 |
| 3:X:2954[B]:TYR:CA | 3:X:2957[B]:ILE:HG22 | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2988[B]:TRP:HE3 | 3:X:2989[B]:HIS:CE1 | 2.25 | 0.47 |
| 3:X:3014[B]:TRP:CD2 | 3:X:3092[B]:ILE:CD1 | 2.98 | 0.47 |
| 3:X:3074[A]:GLU:CD | 3:X:3212[A]:ARG:NH2 | 2.73 | 0.47 |
| 3:X:3125[B]:ARG:O | 3:X:3129[B]:ILE:HG13 | 2.14 | 0.47 |
| 3:X:3137[A]:ARG:HB3 | 3:X:3139[A]:LEU:HD21 | 1.97 | 0.47 |
| 3:X:3182[A]:GLN:H | 3:X:3182[A]:GLN:HG2 | 1.56 | 0.47 |
| 3:X:3196[A]:THR:CA | 3:X:3199[A]:GLN:HB2 | 2.43 | 0.47 |
| 3:X:3283[A]:ILE:C | 3:X:3283[A]:ILE:CD1 | 2.85 | 0.47 |
| 1:Y:327:ASP:HB3 | 1:Y:329:ARG:HG3 | 1.97 | 0.47 |
| 1:Y:860:ALA:HB3 | 1:Y:920:ASN:ND2 | 2.29 | 0.47 |
| 1:Y:867:VAL:HG12 | 1:Y:872:GLN:NE2 | 2.30 | 0.47 |
| 1:Y:977:GLU:HG2 | 1:Y:1021:LEU:HD22 | 1.97 | 0.47 |
| 1:Y:1536:SER:O | 1:Y:1539:GLN:HG2 | 2.15 | 0.47 |
| 2:Z:2556:TYR:HE1 | 2:Z:2845:PRO:HD2 | 1.78 | 0.47 |
| 3:a:2969[A]:TYR:CD2 | 3:a:2970[A]:PRO:N | 2.83 | 0.47 |
| 3:a:3148[A]:ILE:HG22 | 3:a:3152[A]:LYS:CE | 2.44 | 0.47 |
| 3:a:3228[B]:VAL:CG2 | 3:a:3245[B]:PHE:CE1 | 2.97 | 0.47 |
| 3:a:3284[A]:LYS:CE | 3:a:3284[A]:LYS:CA | 2.85 | 0.47 |
| 1:b:490:TRP:HE1 | 1:b:670:PRO:CD | 2.28 | 0.47 |
| 1:b:566:ARG:H | 1:b:567:LEU:HD12 | 1.80 | 0.47 |
| 1:b:618:MET:HE3 | 1:b:618:MET:HB3 | 1.72 | 0.47 |
| 1:b:741:SER:O | 1:b:805:VAL:HG23 | 2.14 | 0.47 |
| 1:b:879:SER:HA | 1:b:893:ALA:HA | 1.95 | 0.47 |
| 1:b:1160:PHE:HD1 | 1:b:1171:LYS:HA | 1.80 | 0.47 |
| 2:c:2190:LEU:HD23 | 2:c:2296:LEU:HD21 | 1.96 | 0.47 |
| 3:d:2933[A]:SER:HA | 3:d:2935[A]:ILE:HD11 | 1.95 | 0.47 |
| 3:d:3066[B]:TYR:CE1 | 3:d:3193[B]:HIS:CE1 | 2.98 | 0.47 |
| 3:d:3125[B]:ARG:O | 3:d:3129[B]:ILE:HG13 | 2.14 | 0.47 |
| 3:d:3148[A]:ILE:HG22 | 3:d:3152[A]:LYS:CE | 2.44 | 0.47 |
| 3:d:3200[A]:LEU:HD22 | 3:d:3204[A]:LEU:HD11 | 1.95 | 0.47 |
| 3:d:3217[B]:PHE:HD2 | 3:d:3300[B]:LEU:HD12 | 1.79 | 0.47 |
| 3:d:3218[A]:LEU:HD12 | 3:d:3218[A]:LEU:HA | 1.78 | 0.47 |
| 3:d:3228[B]:VAL:CG2 | 3:d:3245[B]:PHE:CE1 | 2.97 | 0.47 |
| 3:d:3298[B]:ASN:CA | 3:d:3299[B]:LEU:C | 2.85 | 0.47 |
| 4:q:2:NAG:C3 | 4:q:2:NAG:C8 | 2.85 | 0.47 |
| 4:BA:1:NAG:O7 | 4:BA:1:NAG:H3 | 2.15 | 0.47 |
| 5:PA:1:NAG:H62 | 5:PA:2:NAG:C7 | 2.45 | 0.47 |
| 1:A:1211:TYR:O | 1:A:1211:TYR:CG | 2.67 | 0.47 |
| 1:A:1316:MET:SD | 1:A:1316:MET:N | 2.88 | 0.47 |
| 3:C:2940[B]:ASN:O | 3:C:2944[B]:ALA:N | 2.48 | 0.47 |
| 3:C:2984[B]:THR:OG1 | 3:L:3156[B]:MET:HG2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2985[A]:PHE:CE2 | 3:C:2989[A]:HIS:NE2 | 2.83 | 0.47 |
| 3:C:3169[B]:LYS:HG3 | 3:L:3150[B]:LYS:N | 2.30 | 0.47 |
| 3:C:3230[A]:PHE:H | 3:C:3243[A]:GLY:HA3 | 1.79 | 0.47 |
| 3:C:3230[B]:PHE:H | 3:C:3243[B]:GLY:HA3 | 1.80 | 0.47 |
| 3:C:3252[B]:TYR:CZ | 3:L:3224[B]:GLN:HA | 2.49 | 0.47 |
| 3:C:3285[A]:VAL:CG2 | 3:C:3286[A]:THR:H | 2.27 | 0.47 |
| 3:C:3288[B]:MET:CA | 3:C:3295[B]:LEU:HG | 2.42 | 0.47 |
| 1:D:188:GLY:O | 1:D:386:ILE:HD11 | 2.15 | 0.47 |
| 1:D:589:GLN:HG2 | 1:D:594:ASP:HB3 | 1.97 | 0.47 |
| 2:E:2272:SER:HA | 2:E:2283:ASN:ND2 | 2.29 | 0.47 |
| 2:E:2844:MET:O | 2:E:2846:TRP:HD1 | 1.97 | 0.47 |
| 3:F:2952[A]:ALA:HB1 | 3:F:2957[A]:ILE:H | 1.79 | 0.47 |
| 3:F:2975[B]:PHE:CE1 | 3:a:3107[B]:LEU:CD1 | 2.86 | 0.47 |
| 3:F:2985[A]:PHE:CE2 | 3:F:2989[A]:HIS:NE2 | 2.83 | 0.47 |
| 3:F:3004[B]:GLY:O | 3:F:3006[B]:LYS:N | 2.44 | 0.47 |
| 3:F:3152[B]:LYS:HG3 | 3:a:3172[B]:SER:OG | 2.06 | 0.47 |
| 3:F:3196[A]:THR:O | 3:F:3200[A]:LEU:N | 2.44 | 0.47 |
| 1:G:1321:HIS:ND1 | 1:G:1513:PRO:HB3 | 2.29 | 0.47 |
| 1:G:1348:TRP:CD1 | 1:G:1403:LEU:HD13 | 2.50 | 0.47 |
| 2:H:2270:ILE:HB | 2:H:2297:HIS:CD2 | 2.50 | 0.47 |
| 3:I:2981[B]:GLY:N | 3:I:3086[B]:GLU:OE1 | 2.45 | 0.47 |
| 3:I:3089[B]:HIS:CD2 | 3:R:2972[B]:GLY:H | 2.32 | 0.47 |
| 3:I:3147[B]:GLU:OE2 | 3:R:3163[B]:ASN:O | 2.33 | 0.47 |
| 3:I:3171[B]:HIS:C | 3:R:3152[B]:LYS:O | 2.53 | 0.47 |
| 3:I:3176[A]:LYS:C | 3:I:3177[A]:SER:HG | 2.09 | 0.47 |
| 1:J:634:HIS:HA | 1:J:637:VAL:HG23 | 1.95 | 0.47 |
| 1:J:745:ASP:HB2 | 1:J:801:ASP:OD1 | 2.15 | 0.47 |
| 1:J:1242:ASN:HB3 | 1:J:1479:TYR:OH | 2.15 | 0.47 |
| 2:K:2302:ASP:HB3 | 2:K:2368:TYR:OH | 2.15 | 0.47 |
| 2:K:2506:ARG:HG3 | 2:K:2589:ALA:HB1 | 1.97 | 0.47 |
| 2:K:2879:LEU:HD22 | 2:K:2901:LEU:HD11 | 1.96 | 0.47 |
| 3:L:2968[A]:GLN:HA | 3:L:2973[A]:THR:O | 2.14 | 0.47 |
| 3:L:3074[B]:GLU:OE2 | 3:L:3208[B]:GLN:HG2 | 2.15 | 0.47 |
| 3:L:3298[B]:ASN:CB | 3:L:3299[B]:LEU:C | 2.86 | 0.47 |
| 1:M:995:ILE:HG22 | 1:M:999:LEU:HD22 | 1.97 | 0.47 |
| 3:O:2968[B]:GLN:C | 3:X:2988[B]:TRP:CA | 2.70 | 0.47 |
| 3:O:3109[B]:TYR:OH | 3:X:2973[B]:THR:OG1 | 2.14 | 0.47 |
| 3:O:3137[A]:ARG:HB3 | 3:O:3139[A]:LEU:HD21 | 1.97 | 0.47 |
| 1:P:4:ARG:HD2 | 1:P:89:ILE:O | 2.14 | 0.47 |
| 1:P:329:ARG:NH2 | 1:S:1574:VAL:H | 2.13 | 0.47 |
| 1:P:411:ASP:HB3 | 1:P:658:TYR:OH | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:473:ALA:HB3 | 1:P:476:ARG:HG2 | 1.96 | 0.47 |
| 2:Q:2685:TYR:OH | 2:Q:2886:VAL:HA | 2.15 | 0.47 |
| 3:R:2935[B]:ILE:CG1 | 3:R:2936[B]:GLU:N | 2.78 | 0.47 |
| 3:R:2970[B]:PRO:C | 3:R:2972[B]:GLY:H | 2.23 | 0.47 |
| 3:R:3230[B]:PHE:H | 3:R:3243[B]:GLY:HA3 | 1.80 | 0.47 |
| 1:S:210:HIS:HA | 1:S:213:VAL:HG22 | 1.97 | 0.47 |
| 1:S:245:GLU:OE1 | 1:S:249:ARG:NH1 | 2.48 | 0.47 |
| 1:S:428:ILE:HD12 | 1:S:514:TRP:HB3 | 1.96 | 0.47 |
| 1:S:904:HIS:HB3 | 1:S:1105:VAL:HG21 | 1.96 | 0.47 |
| 1:S:920:ASN:OD1 | 1:S:920:ASN:N | 2.47 | 0.47 |
| 3:U:2935[B]:ILE:CG1 | 3:U:2936[B]:GLU:N | 2.78 | 0.47 |
| 3:U:2960[A]:PHE:CD2 | 3:U:3157[A]:PRO:CG | 2.74 | 0.47 |
| 3:U:3180[A]:TYR:CB | 3:U:3183[A]:LEU:CD2 | 2.90 | 0.47 |
| 3:U:3196[B]:THR:CA | 3:U:3199[B]:GLN:HB2 | 2.43 | 0.47 |
| 3:U:3200[B]:LEU:CD2 | 3:U:3204[B]:LEU:CD1 | 2.93 | 0.47 |
| 3:U:3217[B]:PHE:HD2 | 3:U:3300[B]:LEU:HD12 | 1.78 | 0.47 |
| 3:U:3228[B]:VAL:CG2 | 3:U:3245[B]:PHE:CE1 | 2.97 | 0.47 |
| 3:U:3256[B]:TRP:CE3 | 3:d:2973[B]:THR:N | 2.77 | 0.47 |
| 3:U:3298[B]:ASN:CB | 3:U:3299[B]:LEU:C | 2.86 | 0.47 |
| 1:V:103:GLU:OE2 | 1:V:106:GLN:NE2 | 2.48 | 0.47 |
| 1:V:847:THR:O | 1:V:851:MET:HG3 | 2.14 | 0.47 |
| 2:W:2286:HIS:CD2 | 2:W:2433:THR:HG22 | 2.50 | 0.47 |
| 3:X:2952[B]:ALA:N | 3:X:2953[B]:GLY:HA2 | 2.06 | 0.47 |
| 3:X:3173[A]:THR:HG22 | 3:X:3174[A]:GLY:H | 1.67 | 0.47 |
| 3:X:3196[B]:THR:O | 3:X:3200[B]:LEU:N | 2.44 | 0.47 |
| 3:X:3229[A]:ASN:OD1 | 3:X:3244[A]:THR:HB | 2.14 | 0.47 |
| 3:X:3298[A]:ASN:CA | 3:X:3299[A]:LEU:HB2 | 2.44 | 0.47 |
| 1:Y:59:LEU:HD13 | 1:Y:68:TRP:CD1 | 2.49 | 0.47 |
| 2:Z:2426:PHE:HB3 | 2:Z:2445:MET:HE1 | 1.97 | 0.47 |
| 2:Z:2661:MET:HE2 | 2:Z:2794:LEU:HD23 | 1.97 | 0.47 |
| 3:a:2937[A]:ASN:CB | 3:a:3006[A]:LYS:CE | 2.86 | 0.47 |
| 3:a:2960[B]:PHE:CD2 | 3:a:3157[B]:PRO:CG | 2.74 | 0.47 |
| 3:a:2970[A]:PRO:C | 3:a:2972[A]:GLY:H | 2.23 | 0.47 |
| 3:a:2985[B]:PHE:CE2 | 3:a:2989[B]:HIS:NE2 | 2.83 | 0.47 |
| 3:a:3038[A]:ILE:HG23 | 3:a:3040[A]:VAL:HG22 | 1.90 | 0.47 |
| 2:c:2544:GLY:HA3 | 2:c:2699:MET:O | 2.14 | 0.47 |
| 2:c:2571:ARG:HG3 | 2:c:2715:ASP:OD1 | 2.15 | 0.47 |
| 3:d:2952[A]:ALA:HB1 | 3:d:2957[A]:ILE:H | 1.79 | 0.47 |
| 3:d:2952[B]:ALA:HB1 | 3:d:2957[B]:ILE:H | 1.79 | 0.47 |
| 3:d:3161[A]:GLU:H | 3:d:3161[A]:GLU:CD | 2.19 | 0.47 |
| 3:d:3229[A]:ASN:OD1 | 3:d:3244[A]:THR:HB | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:566:ARG:HH12 | 1:A:743:ASN:CB | 2.25 | 0.47 |
| 1:A:854:LEU:HG | 1:A:959:PHE:HE2 | 1.80 | 0.47 |
| 1:A:1493:MET:O | 1:A:1497:SER:HB3 | 2.15 | 0.47 |
| 1:A:1500:THR:HA | 1:A:1501:ALA:HA | 1.67 | 0.47 |
| 2:B:2189:GLY:HA2 | 2:B:2192:THR:HG22 | 1.96 | 0.47 |
| 3:C:2985[B]:PHE:CE2 | 3:C:2989[B]:HIS:NE2 | 2.83 | 0.47 |
| 3:C:3196[A]:THR:OG1 | 3:C:3199[A]:GLN:HG3 | 2.12 | 0.47 |
| 3:C:3225[A]:SER:C | 3:C:3290[A]:ILE:HG23 | 2.39 | 0.47 |
| 1:D:830:ASN:HA | 1:D:831:VAL:C | 2.39 | 0.47 |
| 2:E:2504:ARG:HD3 | 2:E:2775:GLY:O | 2.15 | 0.47 |
| 3:F:2970[A]:PRO:C | 3:F:2972[A]:GLY:N | 2.72 | 0.47 |
| 3:F:3074[B]:GLU:OE2 | 3:F:3208[B]:GLN:HG2 | 2.15 | 0.47 |
| 3:F:3074[B]:GLU:CD | 3:F:3212[B]:ARG:NH2 | 2.73 | 0.47 |
| 3:F:3093[B]:HIS:HB2 | 3:F:3248[B]:LEU:HD13 | 1.94 | 0.47 |
| 3:F:3096[B]:VAL:HG11 | 3:F:3115[B]:LEU:HD12 | 1.89 | 0.47 |
| 3:F:3125[A]:ARG:O | 3:F:3129[A]:ILE:HG13 | 2.14 | 0.47 |
| 3:F:3160[B]:SER:CB | 3:a:2982[B]:MET:HB3 | 2.45 | 0.47 |
| 3:F:3196[B]:THR:OG1 | 3:F:3199[B]:GLN:CD | 2.57 | 0.47 |
| 3:F:3255[B]:PRO:HG3 | 3:a:2963[B]:MET:N | 2.30 | 0.47 |
| 3:F:3283[B]:ILE:HB | 3:F:3305[B]:ILE:HD11 | 1.97 | 0.47 |
| 3:F:3284[A]:LYS:CE | 3:F:3285[A]:VAL:H | 2.28 | 0.47 |
| 1:G:180:ASN:OD1 | 1:G:344:LEU:HB2 | 2.15 | 0.47 |
| 1:G:223:LEU:HG | 1:G:290:GLU:OE2 | 2.14 | 0.47 |
| 1:G:391:MET:HE3 | 1:G:391:MET:HB3 | 1.79 | 0.47 |
| 1:G:533:VAL:HG12 | 1:G:540:THR:HG22 | 1.96 | 0.47 |
| 1:G:852:ASN:O | 1:G:856:THR:OG1 | 2.33 | 0.47 |
| 1:G:1302:SER:OG | 1:G:1494:ARG:NH2 | 2.48 | 0.47 |
| 2:H:2151:PHE:HB3 | 2:H:2152:PRO:HD3 | 1.96 | 0.47 |
| 2:H:2161:GLN:OE1 | 2:H:2348:THR:HG21 | 2.14 | 0.47 |
| 2:H:2603:PRO:HG2 | 2:H:2606:LEU:HD12 | 1.96 | 0.47 |
| 3:I:3143[A]:SER:OG | 3:I:3144[A]:ALA:N | 2.46 | 0.47 |
| 3:I:3176[A]:LYS:N | 3:I:3176[A]:LYS:CE | 2.73 | 0.47 |
| 3:I:3196[A]:THR:CA | 3:I:3199[A]:GLN:OE1 | 2.58 | 0.47 |
| 1:J:458:LEU:O | 1:J:461:PHE:HB2 | 2.15 | 0.47 |
| 2:K:2571:ARG:HG3 | 2:K:2715:ASP:OD1 | 2.15 | 0.47 |
| 3:L:3004[B]:GLY:O | 3:L:3006[B]:LYS:N | 2.44 | 0.47 |
| 3:L:3014[B]:TRP:CD2 | 3:L:3092[B]:ILE:CD1 | 2.98 | 0.47 |
| 3:L:3196[A]:THR:CA | 3:L:3199[A]:GLN:OE1 | 2.58 | 0.47 |
| 1:M:51:ASP:HA | 1:M:52:GLY:HA2 | 1.58 | 0.47 |
| 1:M:931:TRP:HE3 | 1:M:991:LEU:HD13 | 1.80 | 0.47 |
| 1:M:958:PRO:O | 1:M:959:PHE:HB2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1596:GLU:O | 1:M:1597:THR:HG22 | 2.14 | 0.47 |
| 3:O:2952[B]:ALA:HB1 | 3:O:2957[B]:ILE:H | 1.79 | 0.47 |
| 3:O:3014[B]:TRP:CG | 3:O:3092[B]:ILE:CD1 | 2.98 | 0.47 |
| 1:P:1018:ILE:HD12 | 1:P:1045:HIS:HD2 | 1.80 | 0.47 |
| 3:R:2985[A]:PHE:CE2 | 3:R:2989[A]:HIS:NE2 | 2.83 | 0.47 |
| 1:S:372:ALA:HB3 | 1:S:375:SER:HB3 | 1.96 | 0.47 |
| 1:S:855:ARG:HH21 | 1:S:941:LEU:HA | 1.79 | 0.47 |
| 1:S:931:TRP:CD1 | 1:S:1048:ASN:HD22 | 2.33 | 0.47 |
| 1:S:1639:LYS:HZ1 | 4:BA:2:NAG:C8 | 2.28 | 0.47 |
| 2:T:2556:TYR:CE1 | 2:T:2844:MET:HG3 | 2.50 | 0.47 |
| 2:T:2745:PRO:HB2 | 2:T:2750:ILE:HD12 | 1.97 | 0.47 |
| 3:U:3125[B]:ARG:O | 3:U:3129[B]:ILE:HG13 | 2.14 | 0.47 |
| 3:U:3148[A]:ILE:HG22 | 3:U:3152[A]:LYS:CE | 2.44 | 0.47 |
| 3:U:3196[A]:THR:OG1 | 3:U:3199[A]:GLN:CD | 2.57 | 0.47 |
| 1:V:1147:MET:HE1 | 1:V:1191:PRO:HG3 | 1.96 | 0.47 |
| 3:X:2933[B]:SER:CB | 3:X:2936[B]:GLU:CB | 2.85 | 0.47 |
| 3:X:2939[A]:ARG:HG3 | 3:X:2939[A]:ARG:NH1 | 2.28 | 0.47 |
| 3:X:2952[A]:ALA:HB1 | 3:X:2957[A]:ILE:H | 1.79 | 0.47 |
| 3:X:3137[B]:ARG:HB3 | 3:X:3139[B]:LEU:HD21 | 1.97 | 0.47 |
| 3:X:3183[B]:LEU:N | 3:X:3184[B]:ASN:HA | 2.12 | 0.47 |
| 1:Y:531:THR:HG22 | 1:Y:542:PRO:HA | 1.95 | 0.47 |
| 1:Y:602:THR:O | 1:Y:605:SER:OG | 2.29 | 0.47 |
| 1:Y:1620:LEU:CD1 | 3:d:3189[B]:ASN:CB | 2.93 | 0.47 |
| 3:a:2954[A]:TYR:CA | 3:a:2957[A]:ILE:HG22 | 2.43 | 0.47 |
| 3:a:3180[B]:TYR:CB | 3:a:3183[B]:LEU:CD2 | 2.90 | 0.47 |
| 3:a:3196[B]:THR:O | 3:a:3200[B]:LEU:N | 2.44 | 0.47 |
| 1:b:48:LYS:HA | 1:b:55:ILE:HG13 | 1.97 | 0.47 |
| 1:b:119:LYS:HB2 | 1:b:120:LYS:C | 2.40 | 0.47 |
| 2:c:2180:TRP:HB2 | 2:c:2243:LEU:HD13 | 1.97 | 0.47 |
| 3:d:3014[A]:TRP:CD2 | 3:d:3092[A]:ILE:CD1 | 2.98 | 0.47 |
| 3:d:3284[B]:LYS:CE | 3:d:3284[B]:LYS:CA | 2.85 | 0.47 |
| 3:d:3284[B]:LYS:CE | 3:d:3285[B]:VAL:H | 2.28 | 0.47 |
| 1:A:467:LYS:HB2 | 1:A:479:CYS:SG | 2.54 | 0.47 |
| 1:A:874:ALA:HA | 1:A:913:PHE:CZ | 2.50 | 0.47 |
| 1:A:949:ASP:OD1 | 1:A:950:ALA:N | 2.47 | 0.47 |
| 3:C:3298[B]:ASN:CA | 3:C:3299[B]:LEU:HB2 | 2.44 | 0.47 |
| 1:D:17:ASN:OD1 | 1:D:85:SER:N | 2.47 | 0.47 |
| 1:D:456:GLN:O | 1:D:460:GLU:HG3 | 2.15 | 0.47 |
| 3:F:2933[A]:SER:HA | 3:F:2935[A]:ILE:HD11 | 1.95 | 0.47 |
| 3:F:2949[A]:LYS:C | 3:F:2953[A]:GLY:N | 2.73 | 0.47 |
| 3:F:2949[B]:LYS:C | 3:F:2953[B]:GLY:N | 2.72 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2965[A]:LEU:HD22 | 3:F:2975[A]:PHE:O | 2.15 | 0.47 |
| 3:F:2967[B]:CYS:HB2 | 3:a:2980[B]:HIS:N | 2.30 | 0.47 |
| 3:F:2970[B]:PRO:C | 3:F:2972[B]:GLY:N | 2.72 | 0.47 |
| 3:F:3150[B]:LYS:CA | 3:a:3172[B]:SER:HB3 | 2.45 | 0.47 |
| 3:F:3191[A]:ASN:C | 3:F:3192[A]:PHE:O | 2.52 | 0.47 |
| 3:F:3200[B]:LEU:CD2 | 3:F:3204[B]:LEU:CD1 | 2.93 | 0.47 |
| 1:G:1319:PHE:CE2 | 1:G:1424:GLU:HG3 | 2.50 | 0.47 |
| 3:I:3283[A]:ILE:HB | 3:I:3305[A]:ILE:HD11 | 1.97 | 0.47 |
| 1:J:1209:ASP:O | 1:J:1211:TYR:HD2 | 1.98 | 0.47 |
| 2:K:2132:CYS:HB2 | 2:K:2142:ALA:CB | 2.45 | 0.47 |
| 3:L:2935[A]:ILE:CG1 | 3:L:2936[A]:GLU:N | 2.78 | 0.47 |
| 3:L:2940[B]:ASN:O | 3:L:2944[B]:ALA:N | 2.48 | 0.47 |
| 3:L:3148[B]:ILE:HG22 | 3:L:3152[B]:LYS:CE | 2.44 | 0.47 |
| 1:M:67:MET:HE1 | 1:M:233:PRO:CG | 2.45 | 0.47 |
| 2:N:2115:SER:OG | 2:N:2116:SER:N | 2.47 | 0.47 |
| 2:N:2382:GLU:O | 2:N:2386:ARG:HG3 | 2.14 | 0.47 |
| 3:O:2940[A]:ASN:O | 3:O:2944[A]:ALA:N | 2.48 | 0.47 |
| 3:O:2985[A]:PHE:CE2 | 3:O:2989[A]:HIS:NE2 | 2.83 | 0.47 |
| 3:O:3200[B]:LEU:CD2 | 3:O:3204[B]:LEU:CD1 | 2.93 | 0.47 |
| 3:O:3220[B]:ARG:HH11 | 3:O:3220[B]:ARG:CG | 2.12 | 0.47 |
| 3:O:3293[B]:LYS:HB2 | 3:O:3294[B]:SER:CA | 2.41 | 0.47 |
| 1:P:103:GLU:OE2 | 1:P:106:GLN:NE2 | 2.48 | 0.47 |
| 1:P:739:GLN:N | 1:P:739:GLN:OE1 | 2.48 | 0.47 |
| 1:P:797:THR:HG22 | 1:P:798:LEU:H | 1.80 | 0.47 |
| 2:Q:2190:LEU:O | 2:Q:2209:PHE:HB2 | 2.15 | 0.47 |
| 3:R:2954[A]:TYR:CA | 3:R:2957[A]:ILE:HG22 | 2.43 | 0.47 |
| 3:R:2965[B]:LEU:HD22 | 3:R:2975[B]:PHE:O | 2.15 | 0.47 |
| 3:R:2980[A]:HIS:ND1 | 3:R:2980[A]:HIS:N | 2.60 | 0.47 |
| 3:R:3074[A]:GLU:OE2 | 3:R:3208[A]:GLN:HG2 | 2.15 | 0.47 |
| 1:S:712:SER:O | 1:S:716:LEU:N | 2.48 | 0.47 |
| 1:S:1019:HIS:CE1 | 1:S:1046:HIS:HE1 | 2.31 | 0.47 |
| 1:S:1462:ASP:O | 1:S:1465:TRP:HB3 | 2.15 | 0.47 |
| 1:S:1578:ILE:HA | 1:S:1579:GLY:HA2 | 1.64 | 0.47 |
| 2:T:2569:TRP:O | 2:T:2572:VAL:HG23 | 2.14 | 0.47 |
| 3:U:2985[B]:PHE:CE2 | 3:U:2989[B]:HIS:NE2 | 2.83 | 0.47 |
| 3:U:3014[B]:TRP:CD2 | 3:U:3092[B]:ILE:CD1 | 2.98 | 0.47 |
| 3:U:3148[B]:ILE:HG22 | 3:U:3152[B]:LYS:CE | 2.44 | 0.47 |
| 3:U:3196[B]:THR:O | 3:U:3200[B]:LEU:N | 2.43 | 0.47 |
| 3:U:3298[A]:ASN:CB | 3:U:3300[A]:LEU:CD2 | 2.61 | 0.47 |
| 1:V:430:SER:O | 1:V:933:ARG:NH2 | 2.41 | 0.47 |
| 1:V:554:LYS:HA | 1:V:554:LYS:HD3 | 1.70 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:871:GLN:O | 1:V:875:ALA:N | 2.48 | 0.47 |
| 1:V:1019:HIS:NE2 | 1:V:1046:HIS:HE1 | 2.13 | 0.47 |
| 2:W:2089:ARG:HB2 | 2:W:2368:TYR:CD1 | 2.50 | 0.47 |
| 2:W:2344:LEU:HD23 | 2:W:2349:THR:OG1 | 2.15 | 0.47 |
| 2:W:2562:GLY:H | 2:W:2846:TRP:HB2 | 1.79 | 0.47 |
| 3:X:2940[B]:ASN:O | 3:X:2944[B]:ALA:N | 2.48 | 0.47 |
| 3:X:2952[A]:ALA:N | 3:X:2953[A]:GLY:HA2 | 2.06 | 0.47 |
| 3:X:2952[B]:ALA:HB1 | 3:X:2957[B]:ILE:H | 1.79 | 0.47 |
| 3:X:3203[B]:HIS:O | 3:X:3206[B]:LYS:HB3 | 2.15 | 0.47 |
| 3:X:3218[B]:LEU:HD12 | 3:X:3218[B]:LEU:HA | 1.78 | 0.47 |
| 1:Y:830:ASN:OD1 | 1:Y:832:LYS:HB2 | 2.15 | 0.47 |
| 1:Y:1427:HIS:HD2 | 1:Y:1457:HIS:CE1 | 2.33 | 0.47 |
| 1:Y:1617:LYS:CE | 3:d:3180[B]:TYR:CZ | 2.97 | 0.47 |
| 3:a:2949[B]:LYS:C | 3:a:2953[B]:GLY:N | 2.73 | 0.47 |
| 3:a:3014[B]:TRP:CG | 3:a:3092[B]:ILE:CD1 | 2.98 | 0.47 |
| 3:a:3148[B]:ILE:HG22 | 3:a:3152[B]:LYS:CE | 2.44 | 0.47 |
| 3:a:3228[A]:VAL:CG2 | 3:a:3245[A]:PHE:CE1 | 2.97 | 0.47 |
| 1:b:1013:ILE:HG21 | 1:b:1192:TYR:CD1 | 2.49 | 0.47 |
| 1:b:1142:VAL:HG22 | 1:b:1236:TYR:HD1 | 1.80 | 0.47 |
| 2:c:2669:TYR:HA | 2:c:2721:TRP:CH2 | 2.50 | 0.47 |
| 3:d:2935[A]:ILE:CG1 | 3:d:2936[A]:GLU:N | 2.78 | 0.47 |
| 3:d:3191[B]:ASN:C | 3:d:3192[B]:PHE:O | 2.52 | 0.47 |
| 3:d:3225[A]:SER:C | 3:d:3290[A]:ILE:HG23 | 2.39 | 0.47 |
| 5:FA:1:NAG:H61 | 5:FA:2:NAG:C1 | 2.45 | 0.47 |
| 1:A:104:LEU:HD23 | 1:A:123:PHE:CE2 | 2.50 | 0.46 |
| 1:A:1160:PHE:HB3 | 1:A:1171:LYS:HA | 1.97 | 0.46 |
| 1:A:1324:ARG:NH1 | 1:A:1516:VAL:O | 2.48 | 0.46 |
| 3:C:2965[B]:LEU:HD22 | 3:C:2975[B]:PHE:O | 2.16 | 0.46 |
| 3:C:3293[A]:LYS:HB2 | 3:C:3294[A]:SER:CA | 2.41 | 0.46 |
| 1:D:637:VAL:HA | 1:D:640:LEU:HD12 | 1.96 | 0.46 |
| 2:E:2128:LEU:HD13 | 2:E:2286:HIS:CG | 2.50 | 0.46 |
| 2:E:2867:PRO:O | 2:E:2870:LEU:HB3 | 2.14 | 0.46 |
| 3:F:3014[B]:TRP:CG | 3:F:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:F:3079[A]:CYS:SG | 3:F:3146[A]:CYS:O | 2.73 | 0.46 |
| 3:F:3160[B]:SER:CB | 3:a:2983[B]:VAL:H | 2.28 | 0.46 |
| 1:G:695:TYR:N | 1:G:695:TYR:CD1 | 2.81 | 0.46 |
| 1:G:883:CYS:O | 1:G:885:SER:N | 2.48 | 0.46 |
| 3:I:2940[A]:ASN:O | 3:I:2944[A]:ALA:N | 2.48 | 0.46 |
| 3:I:2940[B]:ASN:O | 3:I:2944[B]:ALA:N | 2.48 | 0.46 |
| 3:I:2968[B]:GLN:HE21 | 3:R:3086[B]:GLU:HG2 | 0.41 | 0.46 |
| 3:I:2970[A]:PRO:C | 3:I:2972[A]:GLY:H | 2.23 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2982[B]:MET:SD | 3:R:2967[B]:CYS:SG | 3.13 | 0.46 |
| 3:I:3074[B]:GLU:OE2 | 3:I:3208[B]:GLN:HG2 | 2.15 | 0.46 |
| 3:I:3119[B]:HIS:NE2 | 3:R:2971[B]:ASP:HA | 2.24 | 0.46 |
| 3:I:3160[B]:SER:CA | 3:R:2983[B]:VAL:N | 2.35 | 0.46 |
| 3:I:3229[A]:ASN:OD1 | 3:I:3244[A]:THR:HB | 2.14 | 0.46 |
| 3:I:3283[B]:ILE:HB | 3:I:3305[B]:ILE:HD11 | 1.97 | 0.46 |
| 1:J:232:ARG:HA | 1:J:233:PRO:HD3 | 1.79 | 0.46 |
| 1:J:1299:GLN:O | 1:J:1301:PRO:HD3 | 2.14 | 0.46 |
| 1:J:1404:TYR:O | 1:J:1407:THR:OG1 | 2.29 | 0.46 |
| 2:K:2822:LYS:HG2 | 2:K:2831:GLU:HA | 1.96 | 0.46 |
| 3:L:3014[A]:TRP:CD2 | 3:L:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:L:3014[B]:TRP:CG | 3:L:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:L:3183[A]:LEU:H | 3:L:3184[A]:ASN:CA | 2.22 | 0.46 |
| 3:L:3284[A]:LYS:CE | 3:L:3285[A]:VAL:H | 2.28 | 0.46 |
| 3:L:3284[B]:LYS:HD3 | 3:L:3285[B]:VAL:O | 2.16 | 0.46 |
| 1:M:306:PHE:HB3 | 1:M:308:LEU:HD13 | 1.96 | 0.46 |
| 1:M:330:GLN:H | 1:M:330:GLN:HG3 | 1.49 | 0.46 |
| 1:M:1505:ARG:O | 1:M:1509:THR:OG1 | 2.33 | 0.46 |
| 2:N:2377:SER:HB3 | 2:N:2380:GLN:HG3 | 1.96 | 0.46 |
| 2:N:2622:ASN:O | 2:N:2625:LEU:HD12 | 2.15 | 0.46 |
| 3:O:2994[B]:LYS:HE2 | 3:O:3183[B]:LEU:O | 2.14 | 0.46 |
| 3:O:3200[A]:LEU:CD2 | 3:O:3204[A]:LEU:CD1 | 2.93 | 0.46 |
| 3:O:3230[A]:PHE:H | 3:O:3243[A]:GLY:HA3 | 1.79 | 0.46 |
| 3:O:3255[B]:PRO:HG2 | 3:X:3163[B]:ASN:ND2 | 2.29 | 0.46 |
| 1:P:643:ILE:HD13 | 1:P:708:PHE:HB2 | 1.97 | 0.46 |
| 1:P:656:LYS:HB2 | 1:P:658:TYR:CE1 | 2.50 | 0.46 |
| 1:P:867:VAL:O | 1:P:868:THR:OG1 | 2.22 | 0.46 |
| 1:P:949:ASP:CG | 1:P:950:ALA:H | 2.22 | 0.46 |
| 1:P:1046:HIS:HA | 1:P:1049:VAL:HB | 1.97 | 0.46 |
| 1:P:1143:ALA:HA | 1:P:1195:ASP:O | 2.15 | 0.46 |
| 1:P:1180:SER:OG | 1:P:1181:GLU:N | 2.47 | 0.46 |
| 1:P:1313:LEU:HD23 | 1:P:1318:VAL:HG23 | 1.96 | 0.46 |
| 2:Q:2572:VAL:HG13 | 2:Q:2768:LEU:HD21 | 1.95 | 0.46 |
| 2:Q:2599:SER:O | 2:Q:2645:PHE:HB3 | 2.15 | 0.46 |
| 3:R:2965[B]:LEU:CD1 | 3:R:2974[B]:ALA:CA | 2.89 | 0.46 |
| 3:R:2987[A]:HIS:O | 3:R:2991[A]:LEU:HB2 | 2.15 | 0.46 |
| 3:R:3014[A]:TRP:CD2 | 3:R:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:R:3079[B]:CYS:SG | 3:R:3146[B]:CYS:O | 2.74 | 0.46 |
| 3:R:3148[B]:ILE:HG22 | 3:R:3152[B]:LYS:CE | 2.44 | 0.46 |
| 1:S:353:ASN:HD22 | 1:S:772:ARG:NH2 | 2.12 | 0.46 |
| 1:S:588:GLU:HG3 | 1:S:724:LYS:HD2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:2871:PHE:HZ | 1:V:1071:ASN:HD22 | 1.61 | 0.46 |
| 3:U:2961[B]:HIS:CD2 | 3:U:2988[B]:TRP:CZ3 | 2.96 | 0.46 |
| 3:U:3014[A]:TRP:CG | 3:U:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:U:3074[B]:GLU:CD | 3:U:3212[B]:ARG:NH2 | 2.73 | 0.46 |
| 1:V:324:PRO:HG2 | 1:V:376:ASN:ND2 | 2.30 | 0.46 |
| 1:V:331:SER:HB2 | 1:Y:1581:GLU:OE2 | 2.14 | 0.46 |
| 2:W:2218:SER:OG | 2:W:2221:THR:OG1 | 2.24 | 0.46 |
| 3:X:2932[B]:PRO:CA | 3:X:2935[B]:ILE:CD1 | 2.85 | 0.46 |
| 3:X:3074[A]:GLU:OE2 | 3:X:3208[A]:GLN:HG2 | 2.15 | 0.46 |
| 3:X:3074[B]:GLU:OE2 | 3:X:3208[B]:GLN:HG2 | 2.15 | 0.46 |
| 3:X:3225[B]:SER:C | 3:X:3290[B]:ILE:HG23 | 2.39 | 0.46 |
| 1:Y:630:PHE:O | 1:Y:633:HIS:HB3 | 2.15 | 0.46 |
| 1:Y:859:ALA:N | 1:Y:957:ASN:HD21 | 2.13 | 0.46 |
| 2:Z:2866:PRO:CG | 3:a:2933[A]:SER:CB | 2.93 | 0.46 |
| 3:a:3114[B]:PRO:CD | 3:a:3115[B]:LEU:N | 2.72 | 0.46 |
| 3:a:3180[A]:TYR:CB | 3:a:3183[A]:LEU:CD2 | 2.89 | 0.46 |
| 1:b:385:ALA:HB2 | 1:b:391:MET:HG3 | 1.97 | 0.46 |
| 2:c:2638:ARG:NH1 | 2:c:2706:ILE:HG13 | 2.30 | 0.46 |
| 3:d:3273[B]:LEU:HB2 | 3:d:3275[B]:LEU:CD1 | 2.34 | 0.46 |
| 3:d:3284[B]:LYS:HD3 | 3:d:3285[B]:VAL:O | 2.16 | 0.46 |
| 1:A:121:ASN:HD21 | 1:A:123:PHE:HB2 | 1.80 | 0.46 |
| 1:A:1163:ALA:HA | 1:A:1211:TYR:H | 1.80 | 0.46 |
| 2:B:2539:ILE:O | 2:B:2573:TYR:OH | 2.14 | 0.46 |
| 2:B:2830:GLN:HB2 | 2:B:2863:ARG:NH1 | 2.31 | 0.46 |
| 3:C:2969[B]:TYR:CD2 | 3:C:2970[B]:PRO:N | 2.83 | 0.46 |
| 3:C:2975[B]:PHE:O | 3:L:3256[B]:TRP:NE1 | 2.49 | 0.46 |
| 3:C:3229[B]:ASN:OD1 | 3:C:3244[B]:THR:HB | 2.14 | 0.46 |
| 1:D:452:ILE:HD11 | 1:D:676:PRO:O | 2.16 | 0.46 |
| 1:D:729:VAL:HG11 | 1:D:785:LEU:HD12 | 1.97 | 0.46 |
| 1:D:1551:ASP:HB3 | 1:D:1652:PHE:HE1 | 1.79 | 0.46 |
| 2:E:2131:LEU:HD12 | 2:E:2335:PRO:HG3 | 1.97 | 0.46 |
| 3:F:2940[B]:ASN:O | 3:F:2944[B]:ALA:N | 2.48 | 0.46 |
| 3:F:2949[A]:LYS:NZ | 3:F:2949[A]:LYS:C | 2.73 | 0.46 |
| 3:F:2954[A]:TYR:CA | 3:F:2957[A]:ILE:HG22 | 2.43 | 0.46 |
| 3:F:2987[B]:HIS:O | 3:F:2991[B]:LEU:HB2 | 2.16 | 0.46 |
| 3:F:3004[B]:GLY:C | 3:F:3006[B]:LYS:N | 2.74 | 0.46 |
| 3:F:3014[A]:TRP:CG | 3:F:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:F:3151[B]:LEU:HB2 | 3:F:3175[B]:TYR:HE2 | 1.68 | 0.46 |
| 3:F:3153[B]:LYS:HB3 | 3:a:3155[B]:MET:N | 2.30 | 0.46 |
| 3:F:3258[B]:PHE:HA | 3:a:3162[B]:ASP:OD2 | 2.15 | 0.46 |
| 3:F:3284[B]:LYS:HD3 | 3:F:3285[B]:VAL:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:801:ASP:OD1 | 1:G:801:ASP:N | 2.46 | 0.46 |
| 1:G:1013:ILE:HG21 | 1:G:1192:TYR:CD1 | 2.50 | 0.46 |
| 1:G:1482:ALA:HB2 | 1:G:1517:PHE:HZ | 1.80 | 0.46 |
| 3:I:3014[B]:TRP:CD2 | 3:I:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:I:3079[A]:CYS:SG | 3:I:3146[A]:CYS:O | 2.74 | 0.46 |
| 3:I:3223[B]:GLY:N | 3:R:2963[B]:MET:HE1 | 2.30 | 0.46 |
| 1:J:136:ALA:HB3 | 2:N:2619:VAL:HB | 1.97 | 0.46 |
| 3:L:2949[B]:LYS:C | 3:L:2953[B]:GLY:N | 2.73 | 0.46 |
| 3:L:3146[A]:CYS:HA | 3:L:3147[A]:GLU:HA | 1.70 | 0.46 |
| 3:L:3146[B]:CYS:HA | 3:L:3147[B]:GLU:HA | 1.70 | 0.46 |
| 3:L:3288[A]:MET:CA | 3:L:3295[A]:LEU:HG | 2.42 | 0.46 |
| 1:M:302:ALA:H | 1:M:363:THR:HB | 1.81 | 0.46 |
| 1:M:464:LEU:HD22 | 1:M:622:HIS:HB3 | 1.97 | 0.46 |
| 1:M:996:ILE:HG23 | 1:M:1133:ILE:HG22 | 1.97 | 0.46 |
| 1:M:1045:HIS:HB3 | 1:M:1046:HIS:HD1 | 1.81 | 0.46 |
| 1:M:1303:GLU:N | 1:M:1303:GLU:OE1 | 2.48 | 0.46 |
| 1:M:1331:GLU:HB2 | 1:M:1343:VAL:CG2 | 2.45 | 0.46 |
| 2:N:2590:VAL:HA | 2:N:2591:PRO:HD3 | 1.81 | 0.46 |
| 3:O:2949[A]:LYS:C | 3:O:2953[A]:GLY:N | 2.72 | 0.46 |
| 3:O:2970[A]:PRO:C | 3:O:2972[A]:GLY:H | 2.23 | 0.46 |
| 3:O:2971[B]:ASP:C | 3:X:2988[B]:TRP:HE3 | 2.23 | 0.46 |
| 3:O:3014[B]:TRP:CD2 | 3:O:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:O:3147[B]:GLU:CG | 3:O:3149[B]:ASN:ND2 | 2.73 | 0.46 |
| 3:O:3151[A]:LEU:CB | 3:O:3175[A]:TYR:CD2 | 2.93 | 0.46 |
| 3:O:3203[B]:HIS:O | 3:O:3206[B]:LYS:HB3 | 2.16 | 0.46 |
| 3:O:3298[B]:ASN:CA | 3:O:3299[B]:LEU:HB2 | 2.44 | 0.46 |
| 1:P:416:ASN:HD22 | 1:P:416:ASN:H | 1.62 | 0.46 |
| 2:Q:2903:TYR:O | 2:Q:2905:PRO:HD3 | 2.16 | 0.46 |
| 3:R:2965[A]:LEU:HD13 | 3:R:2975[A]:PHE:O | 2.16 | 0.46 |
| 3:R:3151[A]:LEU:HB2 | 3:R:3175[A]:TYR:HE2 | 1.68 | 0.46 |
| 3:R:3284[A]:LYS:HD3 | 3:R:3285[A]:VAL:O | 2.16 | 0.46 |
| 3:R:3298[B]:ASN:CA | 3:R:3299[B]:LEU:CB | 2.85 | 0.46 |
| 1:S:4:ARG:HD2 | 1:S:89:ILE:O | 2.15 | 0.46 |
| 1:S:1438:ASP:OD1 | 1:S:1439:VAL:N | 2.48 | 0.46 |
| 2:T:2131:LEU:CD1 | 2:T:2335:PRO:HB3 | 2.46 | 0.46 |
| 3:U:2949[A]:LYS:NZ | 3:U:2949[A]:LYS:C | 2.73 | 0.46 |
| 3:U:2949[B]:LYS:NZ | 3:U:2949[B]:LYS:C | 2.73 | 0.46 |
| 3:U:2970[A]:PRO:C | 3:U:2972[A]:GLY:H | 2.23 | 0.46 |
| 3:U:3074[B]:GLU:OE2 | 3:U:3208[B]:GLN:HG2 | 2.15 | 0.46 |
| 3:U:3137[A]:ARG:HB3 | 3:U:3139[A]:LEU:HD21 | 1.97 | 0.46 |
| 3:X:3219[A]:LEU:N | 3:X:3219[A]:LEU:CD2 | 2.73 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3284[A]:LYS:HD3 | 3:X:3285[A]:VAL:O | 2.16 | 0.46 |
| 1:Y:220:TRP:CZ3 | 1:Y:223:LEU:HD22 | 2.50 | 0.46 |
| 3:a:2935[B]:ILE:CG1 | 3:a:2936[B]:GLU:N | 2.78 | 0.46 |
| 3:a:3014[B]:TRP:CD2 | 3:a:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:a:3104[B]:MET:HA | 3:a:3110[B]:THR:CG2 | 2.17 | 0.46 |
| 3:a:3125[A]:ARG:O | 3:a:3129[A]:ILE:HG13 | 2.14 | 0.46 |
| 3:a:3230[A]:PHE:H | 3:a:3243[A]:GLY:HA3 | 1.79 | 0.46 |
| 3:d:2938[B]:LEU:O | 3:d:2939[B]:ARG:C | 2.58 | 0.46 |
| 3:d:2940[B]:ASN:O | 3:d:2944[B]:ALA:N | 2.48 | 0.46 |
| 3:d:2965[A]:LEU:HD22 | 3:d:2975[A]:PHE:O | 2.15 | 0.46 |
| 3:d:2969[B]:TYR:CD2 | 3:d:2970[B]:PRO:N | 2.83 | 0.46 |
| 3:d:3146[B]:CYS:HA | 3:d:3147[B]:GLU:HA | 1.70 | 0.46 |
| 1:A:733:PHE:CE2 | 1:A:818:PRO:HG3 | 2.51 | 0.46 |
| 2:B:2743:ALA:HB1 | 1:D:1210:LYS:HG3 | 1.97 | 0.46 |
| 3:C:2965[A]:LEU:HD13 | 3:C:2975[A]:PHE:O | 2.16 | 0.46 |
| 3:C:2969[A]:TYR:CD2 | 3:C:2970[A]:PRO:N | 2.83 | 0.46 |
| 3:C:3014[A]:TRP:CD2 | 3:C:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:C:3137[A]:ARG:HD3 | 3:C:3137[A]:ARG:HA | 1.71 | 0.46 |
| 3:C:3284[B]:LYS:CE | 3:C:3285[B]:VAL:H | 2.29 | 0.46 |
| 1:D:493:LEU:HD12 | 1:D:668:MET:HG3 | 1.97 | 0.46 |
| 1:D:1271:MET:HG2 | 1:D:1358:LEU:HD13 | 1.97 | 0.46 |
| 1:D:1323:HIS:CD2 | 9:D:5004:CUO:O1 | 2.68 | 0.46 |
| 1:D:1622:GLN:HG2 | 1:D:1652:PHE:CD1 | 2.50 | 0.46 |
| 2:E:2582:ARG:HA | 2:E:2586:ALA:HB3 | 1.97 | 0.46 |
| 2:E:2720:ILE:HG12 | 2:E:2781:LEU:HG | 1.97 | 0.46 |
| 3:F:3074[A]:GLU:OE2 | 3:F:3208[A]:GLN:HG2 | 2.16 | 0.46 |
| 3:F:3230[B]:PHE:H | 3:F:3243[B]:GLY:HA3 | 1.80 | 0.46 |
| 1:G:252:ASN:HD22 | 1:G:258:LYS:HB2 | 1.81 | 0.46 |
| 1:G:357:PRO:HB3 | 1:G:774:ASP:HB2 | 1.97 | 0.46 |
| 1:G:403:TYR:O | 1:G:658:TYR:HB3 | 2.15 | 0.46 |
| 1:G:928:TYR:HB2 | 1:G:1048:ASN:HB2 | 1.98 | 0.46 |
| 1:G:1146:PHE:HZ | 1:G:1159:TYR:CG | 2.33 | 0.46 |
| 1:G:1250:ILE:O | 1:G:1473:ARG:NH2 | 2.47 | 0.46 |
| 3:I:2965[A]:LEU:HD22 | 3:I:2975[A]:PHE:O | 2.15 | 0.46 |
| 3:I:2968[A]:GLN:HA | 3:I:2973[A]:THR:O | 2.14 | 0.46 |
| 3:I:2968[B]:GLN:OE1 | 3:R:2981[B]:GLY:HA2 | 2.15 | 0.46 |
| 3:I:2970[B]:PRO:C | 3:I:2972[B]:GLY:H | 2.23 | 0.46 |
| 3:I:2988[B]:TRP:CD1 | 3:R:3153[B]:LYS:HD3 | 2.51 | 0.46 |
| 3:I:2992[B]:TYR:HE2 | 3:R:2969[B]:TYR:CE1 | 2.33 | 0.46 |
| 3:I:3004[B]:GLY:C | 3:I:3006[B]:LYS:N | 2.74 | 0.46 |
| 3:I:3074[A]:GLU:OE2 | 3:I:3208[A]:GLN:HG2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3106[B]:THR:C | 3:R:2973[B]:THR:HG21 | 2.40 | 0.46 |
| 1:J:55:ILE:HG21 | 1:J:350:MET:HA | 1.97 | 0.46 |
| 1:J:640:LEU:HD23 | 1:J:643:ILE:HD12 | 1.98 | 0.46 |
| 2:K:2533:ASP:OD1 | 2:K:2533:ASP:N | 2.49 | 0.46 |
| 3:L:2965[A]:LEU:HD22 | 3:L:2975[A]:PHE:O | 2.15 | 0.46 |
| 3:L:3074[A]:GLU:OE2 | 3:L:3208[A]:GLN:HG2 | 2.15 | 0.46 |
| 3:L:3200[A]:LEU:CD2 | 3:L:3204[A]:LEU:CD1 | 2.93 | 0.46 |
| 3:L:3298[A]:ASN:CB | 3:L:3299[A]:LEU:C | 2.86 | 0.46 |
| 1:M:4:ARG:NH1 | 1:M:77:GLU:OE1 | 2.48 | 0.46 |
| 1:M:148:GLN:O | 1:M:150:GLY:N | 2.49 | 0.46 |
| 1:M:450:LYS:HE3 | 1:M:451:SER:H | 1.80 | 0.46 |
| 3:O:2935[A]:ILE:CG1 | 3:O:2936[A]:GLU:N | 2.78 | 0.46 |
| 3:O:2935[B]:ILE:CG1 | 3:O:2936[B]:GLU:N | 2.78 | 0.46 |
| 3:O:2970[A]:PRO:C | 3:O:2972[A]:GLY:N | 2.72 | 0.46 |
| 3:O:2970[B]:PRO:O | 3:X:2989[B]:HIS:CB | 2.63 | 0.46 |
| 3:O:3074[A]:GLU:CD | 3:O:3212[A]:ARG:NH2 | 2.73 | 0.46 |
| 3:O:3074[B]:GLU:CD | 3:O:3212[B]:ARG:NH2 | 2.73 | 0.46 |
| 3:O:3079[B]:CYS:SG | 3:O:3146[B]:CYS:O | 2.73 | 0.46 |
| 3:O:3156[B]:MET:CE | 3:X:3173[B]:THR:HG23 | 2.45 | 0.46 |
| 3:O:3159[B]:SER:N | 3:X:3148[B]:ILE:O | 2.47 | 0.46 |
| 3:O:3203[A]:HIS:O | 3:O:3206[A]:LYS:HB3 | 2.16 | 0.46 |
| 3:O:3284[A]:LYS:HD3 | 3:O:3285[A]:VAL:O | 2.16 | 0.46 |
| 1:P:53:SER:O | 1:P:55:ILE:HG13 | 2.15 | 0.46 |
| 3:R:2985[B]:PHE:CE2 | 3:R:2989[B]:HIS:NE2 | 2.83 | 0.46 |
| 3:R:3014[A]:TRP:CG | 3:R:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 1:S:227:ARG:HE | 1:S:227:ARG:HB2 | 1.34 | 0.46 |
| 1:S:355:ALA:HA | 1:S:734:LEU:HD12 | 1.97 | 0.46 |
| 1:S:881:GLN:OE1 | 1:S:891:LYS:HE2 | 2.15 | 0.46 |
| 1:S:1403:LEU:HD21 | 1:S:1429:THR:HG21 | 1.95 | 0.46 |
| 2:T:2168:ARG:O | 2:W:2503:ASN:HB3 | 2.15 | 0.46 |
| 2:T:2235:PRO:HG3 | 2:T:2240:GLN:NE2 | 2.30 | 0.46 |
| 2:T:2528:LYS:HA | 2:T:2536:PHE:HB3 | 1.97 | 0.46 |
| 2:T:2651:GLN:H | 2:T:2652:LYS:HE2 | 1.79 | 0.46 |
| 3:U:2987[B]:HIS:O | 3:U:2991[B]:LEU:HB2 | 2.16 | 0.46 |
| 3:U:3014[A]:TRP:CD2 | 3:U:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:U:3220[B]:ARG:HG2 | 3:U:3221[B]:ALA:N | 2.09 | 0.46 |
| 3:U:3220[B]:ARG:HH11 | 3:U:3220[B]:ARG:CG | 2.12 | 0.46 |
| 3:U:3293[A]:LYS:HB2 | 3:U:3294[A]:SER:CA | 2.41 | 0.46 |
| 1:V:133:LYS:HA | 1:V:134:VAL:HA | 1.82 | 0.46 |
| 1:V:1016:ASN:HD22 | 1:V:1177:VAL:HA | 1.81 | 0.46 |
| 3:X:2985[B]:PHE:CE2 | 3:X:2989[B]:HIS:NE2 | 2.83 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3014[B]:TRP:CG | 3:X:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:X:3079[A]:CYS:SG | 3:X:3146[A]:CYS:O | 2.74 | 0.46 |
| 3:X:3151[B]:LEU:CB | 3:X:3175[B]:TYR:CD2 | 2.93 | 0.46 |
| 3:X:3203[A]:HIS:O | 3:X:3206[A]:LYS:HB3 | 2.16 | 0.46 |
| 1:Y:250:ASP:HA | 1:Y:258:LYS:NZ | 2.30 | 0.46 |
| 1:Y:1149:GLU:HG3 | 1:Y:1187:LYS:HB3 | 1.97 | 0.46 |
| 1:Y:1166:THR:N | 1:Y:1167:ASP:HA | 2.30 | 0.46 |
| 2:Z:2094:ARG:CZ | 2:c:2370:MET:HE1 | 2.45 | 0.46 |
| 2:Z:2156:ARG:HD2 | 2:Z:2357:VAL:HG12 | 1.97 | 0.46 |
| 2:Z:2572:VAL:HG22 | 2:Z:2768:LEU:CD2 | 2.44 | 0.46 |
| 2:Z:2800:LYS:C | 3:a:3023[A]:ILE:HD13 | 2.40 | 0.46 |
| 2:Z:2816:SER:HB2 | 2:Z:2886:VAL:HB | 1.97 | 0.46 |
| 3:a:3024[B]:LEU:CD1 | 3:a:3024[B]:LEU:C | 2.85 | 0.46 |
| 3:a:3185[B]:TYR:CE2 | 3:a:3187[B]:TYR:HE2 | 2.31 | 0.46 |
| 1:b:306:PHE:HB3 | 1:b:308:LEU:HD13 | 1.98 | 0.46 |
| 2:c:2495:ASN:HD22 | 2:c:2495:ASN:HA | 1.57 | 0.46 |
| 2:c:2885:SER:OG | 2:c:2886:VAL:N | 2.49 | 0.46 |
| 3:d:2940[A]:ASN:O | 3:d:2944[A]:ALA:N | 2.48 | 0.46 |
| 3:d:2965[A]:LEU:HD13 | 3:d:2975[A]:PHE:O | 2.16 | 0.46 |
| 3:d:2965[B]:LEU:HD22 | 3:d:2975[B]:PHE:O | 2.15 | 0.46 |
| 3:d:2985[B]:PHE:CE2 | 3:d:2989[B]:HIS:NE2 | 2.83 | 0.46 |
| 3:d:3014[A]:TRP:CG | 3:d:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:d:3074[B]:GLU:OE2 | 3:d:3208[B]:GLN:HG2 | 2.15 | 0.46 |
| 3:d:3180[B]:TYR:CB | 3:d:3183[B]:LEU:CD2 | 2.89 | 0.46 |
| 3:d:3225[B]:SER:C | 3:d:3290[B]:ILE:HG23 | 2.39 | 0.46 |
| 4:7:1:NAG:H62 | 4:7:2:NAG:N2 | 2.31 | 0.46 |
| 1:A:150:GLY:HA2 | 1:A:152:LYS:N | 2.30 | 0.46 |
| 1:A:361:GLU:HG2 | 1:A:363:THR:HG22 | 1.97 | 0.46 |
| 1:A:885:SER:HB3 | 1:A:891:LYS:NZ | 2.29 | 0.46 |
| 1:A:1059:LEU:HD11 | 1:A:1129:LEU:HD23 | 1.97 | 0.46 |
| 1:A:1485:ALA:O | 1:A:1489:MET:HG2 | 2.15 | 0.46 |
| 2:B:2394:VAL:HG11 | 2:B:2451:LEU:HD12 | 1.98 | 0.46 |
| 3:C:2970[B]:PRO:C | 3:C:2972[B]:GLY:H | 2.23 | 0.46 |
| 3:C:2987[B]:HIS:O | 3:C:2991[B]:LEU:HB2 | 2.16 | 0.46 |
| 3:C:3004[B]:GLY:C | 3:C:3006[B]:LYS:N | 2.73 | 0.46 |
| 3:C:3079[A]:CYS:SG | 3:C:3146[A]:CYS:O | 2.74 | 0.46 |
| 3:C:3159[B]:SER:OG | 3:L:3151[B]:LEU:HA | 2.15 | 0.46 |
| 3:C:3169[B]:LYS:CG | 3:L:3149[B]:ASN:CG | 2.49 | 0.46 |
| 3:C:3173[B]:THR:HG23 | 3:L:3173[B]:THR:OG1 | 2.16 | 0.46 |
| 3:C:3283[B]:ILE:HB | 3:C:3305[B]:ILE:HD11 | 1.97 | 0.46 |
| 3:C:3284[B]:LYS:HD3 | 3:C:3285[B]:VAL:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:987:LYS:HD2 | 1:D:988:TYR:CE1 | 2.51 | 0.46 |
| 2:E:2472:ASN:HB2 | 2:E:2474:THR:H | 1.80 | 0.46 |
| 3:F:2940[A]:ASN:O | 3:F:2944[A]:ALA:N | 2.48 | 0.46 |
| 3:F:3155[B]:MET:HG3 | 3:a:3154[B]:PRO:HD2 | 1.97 | 0.46 |
| 3:F:3161[A]:GLU:H | 3:F:3161[A]:GLU:CD | 2.19 | 0.46 |
| 3:F:3174[B]:GLY:CA | 3:a:3154[B]:PRO:CD | 2.85 | 0.46 |
| 3:F:3209[B]:GLU:O | 3:F:3310[B]:GLY:C | 2.59 | 0.46 |
| 3:F:3288[B]:MET:CA | 3:F:3295[B]:LEU:HG | 2.42 | 0.46 |
| 1:G:1617:LYS:O | 3:L:3197[B]:ILE:HD12 | 2.14 | 0.46 |
| 3:I:2937[A]:ASN:CB | 3:I:3006[A]:LYS:CE | 2.86 | 0.46 |
| 3:I:3161[B]:GLU:CA | 3:R:3147[B]:GLU:HG2 | 2.46 | 0.46 |
| 3:I:3161[B]:GLU:C | 3:R:3147[B]:GLU:HG3 | 2.40 | 0.46 |
| 3:I:3255[B]:PRO:CB | 3:R:2959[B]:SER:HB3 | 2.40 | 0.46 |
| 3:I:3264[A]:TYR:HD1 | 3:I:3265[A]:ASP:N | 2.14 | 0.46 |
| 3:I:3284[B]:LYS:HD3 | 3:I:3285[B]:VAL:O | 2.15 | 0.46 |
| 1:J:164:GLU:CG | 1:J:297:ARG:HE | 2.28 | 0.46 |
| 1:J:518:LYS:HD2 | 1:J:519:PRO:HD2 | 1.96 | 0.46 |
| 1:J:912:ASN:ND2 | 1:J:1093:ASP:OD2 | 2.48 | 0.46 |
| 1:J:1163:ALA:O | 1:J:1167:ASP:HB3 | 2.16 | 0.46 |
| 2:K:2682:SER:HA | 2:K:2836:PHE:CD2 | 2.51 | 0.46 |
| 2:K:2792:GLU:OE2 | 2:K:2796:GLN:NE2 | 2.41 | 0.46 |
| 3:L:2965[B]:LEU:HD13 | 3:L:2975[B]:PHE:O | 2.16 | 0.46 |
| 3:L:2969[A]:TYR:CD2 | 3:L:2970[A]:PRO:N | 2.83 | 0.46 |
| 3:L:2985[A]:PHE:CE2 | 3:L:2989[A]:HIS:NE2 | 2.83 | 0.46 |
| 3:L:3196[B]:THR:CA | 3:L:3199[B]:GLN:OE1 | 2.58 | 0.46 |
| 3:L:3203[B]:HIS:O | 3:L:3206[B]:LYS:HB3 | 2.16 | 0.46 |
| 3:L:3232[A]:VAL:HG23 | 3:L:3273[A]:LEU:HD11 | 1.95 | 0.46 |
| 3:L:3298[B]:ASN:CA | 3:L:3299[B]:LEU:CB | 2.86 | 0.46 |
| 1:M:729:VAL:HG11 | 1:M:785:LEU:HD12 | 1.98 | 0.46 |
| 2:N:2631:TYR:H | 2:N:2631:TYR:HD1 | 1.63 | 0.46 |
| 3:O:2965[A]:LEU:HD22 | 3:O:2975[A]:PHE:O | 2.15 | 0.46 |
| 3:O:2969[A]:TYR:CD2 | 3:O:2970[A]:PRO:N | 2.83 | 0.46 |
| 3:O:2985[B]:PHE:CE2 | 3:O:2989[B]:HIS:NE2 | 2.83 | 0.46 |
| 3:O:3014[A]:TRP:CD2 | 3:O:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:O:3038[B]:ILE:HG23 | 3:O:3040[B]:VAL:HG22 | 1.90 | 0.46 |
| 3:O:3074[A]:GLU:OE2 | 3:O:3208[A]:GLN:HG2 | 2.15 | 0.46 |
| 3:O:3209[A]:GLU:O | 3:O:3310[A]:GLY:C | 2.59 | 0.46 |
| 3:O:3283[B]:ILE:C | 3:O:3283[B]:ILE:CD1 | 2.85 | 0.46 |
| 3:O:3284[B]:LYS:HD3 | 3:O:3285[B]:VAL:O | 2.16 | 0.46 |
| 1:P:187:GLY:HA3 | 1:P:195:SER:HB3 | 1.97 | 0.46 |
| 1:P:575:ASP:OD1 | 1:P:575:ASP:N | 2.42 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:792:MET:HB2 | 1:P:793:PHE:HD1 | 1.80 | 0.46 |
| 3:R:2970[A]:PRO:C | 3:R:2972[A]:GLY:H | 2.23 | 0.46 |
| 3:R:3014[B]:TRP:CD2 | 3:R:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:R:3203[B]:HIS:O | 3:R:3206[B]:LYS:HB3 | 2.16 | 0.46 |
| 3:R:3288[A]:MET:CA | 3:R:3295[A]:LEU:HG | 2.42 | 0.46 |
| 3:R:3298[A]:ASN:CA | 3:R:3299[A]:LEU:HB2 | 2.44 | 0.46 |
| 1:S:120:LYS:HB3 | 1:S:121:ASN:HA | 1.98 | 0.46 |
| 1:S:226:HIS:HA | 1:S:227:ARG:HB2 | 1.97 | 0.46 |
| 2:T:2370:MET:HE2 | 2:T:2370:MET:HB2 | 1.66 | 0.46 |
| 3:U:2949[B]:LYS:C | 3:U:2953[B]:GLY:N | 2.73 | 0.46 |
| 3:U:3079[A]:CYS:SG | 3:U:3146[A]:CYS:O | 2.74 | 0.46 |
| 3:U:3079[B]:CYS:SG | 3:U:3146[B]:CYS:O | 2.74 | 0.46 |
| 3:U:3284[B]:LYS:CE | 3:U:3285[B]:VAL:H | 2.28 | 0.46 |
| 1:V:949:ASP:CB | 1:V:953:GLU:HB2 | 2.41 | 0.46 |
| 1:V:1250:ILE:O | 1:V:1473:ARG:NH2 | 2.49 | 0.46 |
| 2:W:2398:PHE:HE1 | 2:W:2466:THR:HG21 | 1.79 | 0.46 |
| 3:X:2965[B]:LEU:HD22 | 3:X:2975[B]:PHE:O | 2.15 | 0.46 |
| 3:X:2987[A]:HIS:O | 3:X:2991[A]:LEU:HB2 | 2.16 | 0.46 |
| 3:X:3196[B]:THR:CA | 3:X:3199[B]:GLN:HB2 | 2.43 | 0.46 |
| 3:X:3298[B]:ASN:CA | 3:X:3299[B]:LEU:HB2 | 2.44 | 0.46 |
| 1:Y:212:ASN:OD1 | 1:Y:215:ARG:NH1 | 2.48 | 0.46 |
| 1:Y:1166:THR:HB | 1:Y:1167:ASP:C | 2.40 | 0.46 |
| 1:Y:1423:TYR:OH | 1:Y:1461:VAL:O | 2.31 | 0.46 |
| 2:Z:2168:ARG:HA | 2:c:2502:LEU:HB3 | 1.96 | 0.46 |
| 2:Z:2225:ARG:NH1 | 2:Z:2291:ASP:OD1 | 2.48 | 0.46 |
| 3:a:2970[A]:PRO:C | 3:a:2972[A]:GLY:N | 2.72 | 0.46 |
| 3:a:3079[A]:CYS:SG | 3:a:3146[A]:CYS:O | 2.74 | 0.46 |
| 3:a:3203[B]:HIS:O | 3:a:3206[B]:LYS:HB3 | 2.16 | 0.46 |
| 1:b:462:HIS:CE1 | 1:b:621:LEU:HD12 | 2.51 | 0.46 |
| 1:b:1392:ASP:H | 1:b:1435:GLY:HA2 | 1.80 | 0.46 |
| 2:c:2702:SER:HA | 2:c:2707:PHE:CD2 | 2.49 | 0.46 |
| 3:d:2949[B]:LYS:C | 3:d:2953[B]:GLY:N | 2.72 | 0.46 |
| 3:d:3014[B]:TRP:CD2 | 3:d:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:d:3079[B]:CYS:SG | 3:d:3146[B]:CYS:O | 2.74 | 0.46 |
| 3:d:3182[A]:GLN:H | 3:d:3182[A]:GLN:HG2 | 1.56 | 0.46 |
| 3:d:3200[B]:LEU:CD2 | 3:d:3204[B]:LEU:CD1 | 2.93 | 0.46 |
| 3:d:3284[A]:LYS:HD3 | 3:d:3285[A]:VAL:O | 2.16 | 0.46 |
| 1:A:184:TYR:CE2 | 1:A:386:ILE:HG12 | 2.50 | 0.46 |
| 1:A:877:HIS:CE1 | 1:A:905:TRP:HZ3 | 2.33 | 0.46 |
| 1:A:979:LEU:HB2 | 1:A:980:TYR:CD1 | 2.50 | 0.46 |
| 2:B:2472:ASN:N | 2:B:2473:GLY:HA2 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2935[B]:ILE:CG1 | 3:C:2936[B]:GLU:N | 2.78 | 0.46 |
| 3:C:2938[A]:LEU:O | 3:C:2939[A]:ARG:C | 2.58 | 0.46 |
| 3:C:2961[B]:HIS:C | 3:L:3255[B]:PRO:CD | 2.88 | 0.46 |
| 3:C:3141[A]:TYR:CD2 | 3:C:3141[A]:TYR:C | 2.86 | 0.46 |
| 3:C:3203[A]:HIS:O | 3:C:3206[A]:LYS:HB3 | 2.16 | 0.46 |
| 1:D:432:THR:HG23 | 1:D:435:GLU:H | 1.81 | 0.46 |
| 1:D:440:ARG:O | 1:D:444:GLU:HB2 | 2.15 | 0.46 |
| 3:F:2935[A]:ILE:CG1 | 3:F:2936[A]:GLU:N | 2.78 | 0.46 |
| 3:F:2970[B]:PRO:C | 3:F:2972[B]:GLY:H | 2.23 | 0.46 |
| 3:F:2984[B]:THR:CB | 3:a:3159[B]:SER:CB | 2.80 | 0.46 |
| 3:F:2985[A]:PHE:CE2 | 3:F:2989[A]:HIS:CD2 | 3.04 | 0.46 |
| 3:F:3004[A]:GLY:C | 3:F:3006[A]:LYS:N | 2.73 | 0.46 |
| 3:F:3180[B]:TYR:CB | 3:F:3183[B]:LEU:CD2 | 2.90 | 0.46 |
| 3:F:3264[B]:TYR:HD1 | 3:F:3265[B]:ASP:N | 2.14 | 0.46 |
| 1:G:163:LEU:HB3 | 1:G:293:LEU:HD21 | 1.96 | 0.46 |
| 1:G:630:PHE:O | 1:G:633:HIS:HB3 | 2.16 | 0.46 |
| 1:G:956:PRO:HB2 | 1:G:957:ASN:C | 2.40 | 0.46 |
| 2:H:2344:LEU:HA | 2:H:2345:ASN:C | 2.40 | 0.46 |
| 2:H:2779:ASP:HA | 2:H:2780:HIS:HA | 1.45 | 0.46 |
| 3:I:2949[A]:LYS:NZ | 3:I:2949[A]:LYS:C | 2.73 | 0.46 |
| 3:I:2949[B]:LYS:NZ | 3:I:2949[B]:LYS:C | 2.73 | 0.46 |
| 3:I:3150[B]:LYS:HE2 | 3:R:3157[B]:PRO:HB2 | 1.96 | 0.46 |
| 3:I:3200[A]:LEU:HD22 | 3:I:3204[A]:LEU:HD11 | 1.95 | 0.46 |
| 3:I:3200[B]:LEU:CD2 | 3:I:3204[B]:LEU:CD1 | 2.93 | 0.46 |
| 3:I:3203[B]:HIS:O | 3:I:3206[B]:LYS:HB3 | 2.16 | 0.46 |
| 3:I:3228[A]:VAL:CG2 | 3:I:3245[A]:PHE:CE1 | 2.96 | 0.46 |
| 3:I:3230[B]:PHE:H | 3:I:3243[B]:GLY:HA3 | 1.79 | 0.46 |
| 3:I:3284[B]:LYS:CE | 3:I:3284[B]:LYS:CA | 2.85 | 0.46 |
| 3:I:3293[B]:LYS:HB2 | 3:I:3294[B]:SER:CA | 2.41 | 0.46 |
| 3:I:3298[A]:ASN:CA | 3:I:3299[A]:LEU:HB2 | 2.44 | 0.46 |
| 3:L:3284[B]:LYS:CE | 3:L:3285[B]:VAL:H | 2.28 | 0.46 |
| 3:L:3298[B]:ASN:CA | 3:L:3299[B]:LEU:HB2 | 2.45 | 0.46 |
| 1:M:1059:LEU:HD13 | 1:M:1063:ARG:NH2 | 2.31 | 0.46 |
| 2:N:2234:GLN:HG3 | 2:N:2235:PRO:HD2 | 1.98 | 0.46 |
| 2:N:2235:PRO:HG3 | 2:N:2240:GLN:NE2 | 2.31 | 0.46 |
| 2:N:2426:PHE:HB3 | 2:N:2445:MET:HE1 | 1.96 | 0.46 |
| 3:O:2968[B]:GLN:HA | 3:X:2979[B]:GLN:HG2 | 1.96 | 0.46 |
| 3:O:2976[A]:ALA:O | 3:O:2978[A]:CYS:N | 2.46 | 0.46 |
| 3:O:2987[A]:HIS:O | 3:O:2991[A]:LEU:HB2 | 2.15 | 0.46 |
| 3:O:3176[A]:LYS:C | 3:O:3177[A]:SER:HG | 2.10 | 0.46 |
| 3:O:3284[A]:LYS:CE | 3:O:3285[A]:VAL:H | 2.28 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3284[B]:LYS:CE | 3:O:3285[B]:VAL:H | 2.28 | 0.46 |
| 1:P:1339:SER:HB2 | 1:P:1340:GLY:CA | 2.46 | 0.46 |
| 2:Q:2885:SER:HB3 | 2:Q:2890:VAL:HG12 | 1.96 | 0.46 |
| 3:R:2949[A]:LYS:C | 3:R:2953[A]:GLY:N | 2.73 | 0.46 |
| 3:R:3146[B]:CYS:HA | 3:R:3147[B]:GLU:HA | 1.70 | 0.46 |
| 3:R:3196[B]:THR:CA | 3:R:3199[B]:GLN:OE1 | 2.58 | 0.46 |
| 3:R:3281[A]:PHE:HE1 | 3:R:3305[A]:ILE:HG21 | 1.81 | 0.46 |
| 3:R:3293[B]:LYS:HB2 | 3:R:3294[B]:SER:CA | 2.41 | 0.46 |
| 1:S:191:THR:HG1 | 1:S:192:HIS:HD1 | 1.62 | 0.46 |
| 1:S:618:MET:HA | 1:S:624:THR:HB | 1.97 | 0.46 |
| 1:S:673:PHE:HB3 | 1:S:677:LEU:HB2 | 1.97 | 0.46 |
| 1:S:748:VAL:HG22 | 1:S:781:ILE:HD11 | 1.97 | 0.46 |
| 1:S:760:ILE:HG21 | 1:S:777:TYR:HE2 | 1.80 | 0.46 |
| 1:S:1487:PRO:HD3 | 2:W:2486:ILE:HB | 1.97 | 0.46 |
| 2:T:2786:MET:HE1 | 2:T:2794:LEU:HD22 | 1.97 | 0.46 |
| 3:U:2969[B]:TYR:C | 3:d:2981[B]:GLY:CA | 2.88 | 0.46 |
| 3:U:3264[A]:TYR:HD1 | 3:U:3265[A]:ASP:N | 2.14 | 0.46 |
| 3:U:3284[A]:LYS:HD3 | 3:U:3285[A]:VAL:O | 2.16 | 0.46 |
| 3:U:3284[B]:LYS:HD3 | 3:U:3285[B]:VAL:O | 2.16 | 0.46 |
| 1:V:883:CYS:N | 1:V:894:CYS:SG | 2.88 | 0.46 |
| 1:V:1002:GLU:HB3 | 1:V:1065:LYS:HD3 | 1.97 | 0.46 |
| 1:V:1082:SER:OG | 1:V:1083:PRO:HD3 | 2.16 | 0.46 |
| 3:X:2965[A]:LEU:HD22 | 3:X:2975[A]:PHE:O | 2.15 | 0.46 |
| 3:X:3209[A]:GLU:O | 3:X:3310[A]:GLY:C | 2.59 | 0.46 |
| 3:X:3209[B]:GLU:O | 3:X:3310[B]:GLY:C | 2.59 | 0.46 |
| 3:X:3284[A]:LYS:CE | 3:X:3285[A]:VAL:H | 2.29 | 0.46 |
| 3:X:3284[B]:LYS:HD3 | 3:X:3285[B]:VAL:O | 2.16 | 0.46 |
| 1:Y:958:PRO:CA | 1:Y:959:PHE:HB2 | 2.44 | 0.46 |
| 2:Z:2155:HIS:O | 2:Z:2159:VAL:HG23 | 2.15 | 0.46 |
| 2:Z:2244:PHE:CZ | 2:Z:2376:MET:HE1 | 2.51 | 0.46 |
| 2:Z:2795:ILE:O | 2:Z:2799:LYS:HG3 | 2.16 | 0.46 |
| 3:a:2935[A]:ILE:CG1 | 3:a:2936[A]:GLU:N | 2.78 | 0.46 |
| 3:a:3203[A]:HIS:O | 3:a:3206[A]:LYS:HB3 | 2.16 | 0.46 |
| 3:a:3209[A]:GLU:O | 3:a:3310[A]:GLY:C | 2.59 | 0.46 |
| 3:a:3284[A]:LYS:HD3 | 3:a:3285[A]:VAL:O | 2.15 | 0.46 |
| 3:a:3284[A]:LYS:CE | 3:a:3285[A]:VAL:H | 2.28 | 0.46 |
| 1:b:1302:SER:CB | 1:b:1303:GLU:HA | 2.45 | 0.46 |
| 3:d:2949[A]:LYS:C | 3:d:2953[A]:GLY:N | 2.72 | 0.46 |
| 3:d:2969[A]:TYR:CD2 | 3:d:2970[A]:PRO:N | 2.83 | 0.46 |
| 3:d:3079[A]:CYS:SG | 3:d:3146[A]:CYS:O | 2.74 | 0.46 |
| 6:r:1:NAG:O4 | 6:r:1:NAG:O6 | 2.23 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:135:THR:HB | 1:A:193:SER:HB3 | 1.96 | 0.46 |
| 1:A:904:HIS:HE2 | 1:A:1004:PHE:HE2 | 1.62 | 0.46 |
| 1:A:1210:LYS:HG3 | 2:E:2743:ALA:CB | 2.46 | 0.46 |
| 2:B:2086:ASN:ND2 | 2:B:2086:ASN:H | 2.14 | 0.46 |
| 2:B:2344:LEU:O | 2:E:2515:ARG:HB3 | 2.15 | 0.46 |
| 3:C:2935[A]:ILE:CG1 | 3:C:2936[A]:GLU:N | 2.78 | 0.46 |
| 3:C:2949[A]:LYS:C | 3:C:2953[A]:GLY:N | 2.72 | 0.46 |
| 3:C:2956[B]:LYS:O | 3:C:2959[B]:SER:OG | 2.33 | 0.46 |
| 3:C:2985[B]:PHE:CE2 | 3:C:2989[B]:HIS:CD2 | 3.04 | 0.46 |
| 3:C:2987[A]:HIS:O | 3:C:2991[A]:LEU:HB2 | 2.15 | 0.46 |
| 3:C:2991[A]:LEU:HD23 | 3:C:3158[A]:PHE:CE1 | 2.48 | 0.46 |
| 3:C:3090[B]:ASN:HB3 | 3:L:2973[B]:THR:N | 2.29 | 0.46 |
| 3:C:3104[A]:MET:HA | 3:C:3110[A]:THR:CG2 | 2.17 | 0.46 |
| 3:C:3151[A]:LEU:HB2 | 3:C:3175[A]:TYR:HE2 | 1.68 | 0.46 |
| 3:C:3151[B]:LEU:C | 3:L:3154[B]:PRO:CB | 2.88 | 0.46 |
| 3:C:3153[B]:LYS:C | 3:L:3173[B]:THR:C | 2.84 | 0.46 |
| 3:C:3283[A]:ILE:HB | 3:C:3305[A]:ILE:HD11 | 1.97 | 0.46 |
| 3:C:3284[A]:LYS:HD3 | 3:C:3284[A]:LYS:C | 2.32 | 0.46 |
| 3:C:3284[A]:LYS:CE | 3:C:3285[A]:VAL:H | 2.28 | 0.46 |
| 1:D:673:PHE:HB3 | 1:D:677:LEU:HD13 | 1.98 | 0.46 |
| 3:F:2961[A]:HIS:CD2 | 3:F:2988[A]:TRP:CZ3 | 2.96 | 0.46 |
| 3:F:2987[A]:HIS:O | 3:F:2991[A]:LEU:HB2 | 2.16 | 0.46 |
| 3:F:3014[A]:TRP:CD2 | 3:F:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:F:3251[B]:ASP:CB | 3:a:3251[B]:ASP:HB2 | 2.08 | 0.46 |
| 1:G:177:VAL:O | 1:G:181:PRO:HD3 | 2.15 | 0.46 |
| 1:G:1576:THR:H | 1:G:1581:GLU:CB | 2.28 | 0.46 |
| 2:H:2094:ARG:HE | 2:K:2094:ARG:HH21 | 1.63 | 0.46 |
| 3:I:2965[A]:LEU:HD13 | 3:I:2975[A]:PHE:O | 2.16 | 0.46 |
| 3:I:3153[B]:LYS:O | 3:R:3154[B]:PRO:HA | 2.15 | 0.46 |
| 3:I:3203[A]:HIS:O | 3:I:3206[A]:LYS:HB3 | 2.16 | 0.46 |
| 3:I:3264[B]:TYR:HD1 | 3:I:3265[B]:ASP:N | 2.14 | 0.46 |
| 1:J:1077:LEU:HB3 | 1:J:1103:PHE:CE1 | 2.51 | 0.46 |
| 1:J:1494:ARG:NH1 | 1:J:1494:ARG:HG3 | 2.30 | 0.46 |
| 3:L:2976[A]:ALA:O | 3:L:2978[A]:CYS:N | 2.46 | 0.46 |
| 3:L:2987[A]:HIS:O | 3:L:2991[A]:LEU:HB2 | 2.15 | 0.46 |
| 1:M:1315:GLY:HA3 | 1:M:1601:TRP:HB2 | 1.96 | 0.46 |
| 2:N:2550:THR:O | 2:N:2554:PRO:HD3 | 2.16 | 0.46 |
| 3:O:2965[B]:LEU:CD1 | 3:O:2974[B]:ALA:CA | 2.89 | 0.46 |
| 3:O:2969[B]:TYR:HB3 | 3:X:3158[B]:PHE:CE2 | 2.45 | 0.46 |
| 3:O:3004[A]:GLY:C | 3:O:3006[A]:LYS:N | 2.74 | 0.46 |
| 3:O:3116[A]:PHE:CD1 | 3:O:3116[A]:PHE:C | 2.94 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3209[B]:GLU:O | 3:O:3310[B]:GLY:C | 2.59 | 0.46 |
| 3:O:3254[B]:MET:C | 3:X:3160[B]:SER:C | 2.84 | 0.46 |
| 3:O:3264[B]:TYR:HD1 | 3:O:3265[B]:ASP:N | 2.14 | 0.46 |
| 1:P:64:THR:HG21 | 1:P:239:LEU:HB2 | 1.97 | 0.46 |
| 1:P:625:SER:HA | 1:P:630:PHE:CG | 2.51 | 0.46 |
| 2:Q:2180:TRP:HH2 | 2:Q:2297:HIS:O | 1.99 | 0.46 |
| 3:R:2952[A]:ALA:N | 3:R:2953[A]:GLY:CA | 2.71 | 0.46 |
| 3:R:2954[B]:TYR:CA | 3:R:2957[B]:ILE:HG22 | 2.43 | 0.46 |
| 3:R:3074[B]:GLU:OE2 | 3:R:3208[B]:GLN:HG2 | 2.15 | 0.46 |
| 3:R:3104[A]:MET:HA | 3:R:3110[A]:THR:CG2 | 2.17 | 0.46 |
| 3:R:3209[B]:GLU:O | 3:R:3310[B]:GLY:C | 2.59 | 0.46 |
| 3:R:3264[B]:TYR:HD1 | 3:R:3265[B]:ASP:N | 2.14 | 0.46 |
| 2:T:2644:LEU:HD11 | 2:T:2683:ILE:HD13 | 1.96 | 0.46 |
| 3:U:2949[B]:LYS:C | 3:U:2949[B]:LYS:HZ3 | 2.18 | 0.46 |
| 3:U:2968[B]:GLN:HG2 | 3:d:3258[B]:PHE:CE1 | 2.42 | 0.46 |
| 3:U:2970[A]:PRO:C | 3:U:2972[A]:GLY:N | 2.72 | 0.46 |
| 3:U:2981[A]:GLY:N | 3:U:3086[A]:GLU:OE1 | 2.45 | 0.46 |
| 3:U:3169[B]:LYS:O | 3:d:3149[B]:ASN:N | 2.42 | 0.46 |
| 3:U:3203[A]:HIS:O | 3:U:3206[A]:LYS:HB3 | 2.16 | 0.46 |
| 3:U:3283[B]:ILE:HB | 3:U:3305[B]:ILE:HD11 | 1.97 | 0.46 |
| 1:V:149:GLU:HG3 | 1:V:150:GLY:N | 2.29 | 0.46 |
| 1:V:514:TRP:CZ2 | 1:V:606:ILE:HD11 | 2.50 | 0.46 |
| 1:V:717:GLN:O | 1:V:720:VAL:HG22 | 2.15 | 0.46 |
| 2:W:2401:GLU:HG2 | 2:W:2402:GLY:H | 1.80 | 0.46 |
| 3:X:2949[B]:LYS:C | 3:X:2953[B]:GLY:N | 2.72 | 0.46 |
| 3:X:3004[A]:GLY:C | 3:X:3006[A]:LYS:N | 2.74 | 0.46 |
| 3:X:3079[B]:CYS:SG | 3:X:3146[B]:CYS:O | 2.74 | 0.46 |
| 3:X:3191[A]:ASN:ND2 | 3:X:3191[A]:ASN:N | 2.60 | 0.46 |
| 3:X:3263[B]:LEU:N | 3:X:3263[B]:LEU:CD1 | 2.79 | 0.46 |
| 3:X:3283[B]:ILE:HB | 3:X:3305[B]:ILE:HD11 | 1.97 | 0.46 |
| 1:Y:578:PHE:H | 1:Y:578:PHE:HD1 | 1.63 | 0.46 |
| 1:Y:1546:LYS:HB3 | 3:d:3001[B]:LYS:HZ2 | 1.76 | 0.46 |
| 2:Z:2109:ARG:NH1 | 2:Z:2169:HIS:O | 2.48 | 0.46 |
| 2:Z:2572:VAL:HG22 | 2:Z:2768:LEU:HD22 | 1.97 | 0.46 |
| 3:a:2976[A]:ALA:O | 3:a:2978[A]:CYS:N | 2.46 | 0.46 |
| 3:a:3171[B]:HIS:C | 3:a:3173[B]:THR:N | 2.73 | 0.46 |
| 3:a:3200[A]:LEU:CD2 | 3:a:3204[A]:LEU:CD1 | 2.93 | 0.46 |
| 3:a:3263[B]:LEU:N | 3:a:3263[B]:LEU:CD1 | 2.79 | 0.46 |
| 3:a:3265[A]:ASP:CG | 3:a:3267[A]:SER:HG | 2.13 | 0.46 |
| 3:a:3284[B]:LYS:CE | 3:a:3285[B]:VAL:H | 2.28 | 0.46 |
| 1:b:1195:ASP:O | 1:b:1196:ILE:HG22 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2987[B]:HIS:O | 3:d:2991[B]:LEU:HB2 | 2.16 | 0.46 |
| 3:d:2991[A]:LEU:HD23 | 3:d:3158[A]:PHE:CE1 | 2.48 | 0.46 |
| 3:d:3264[A]:TYR:HD1 | 3:d:3265[A]:ASP:N | 2.14 | 0.46 |
| 1:A:120:LYS:HB3 | 1:A:121:ASN:HA | 1.97 | 0.46 |
| 1:A:462:HIS:HA | 1:A:490:TRP:HH2 | 1.80 | 0.46 |
| 1:A:949:ASP:HB2 | 1:A:953:GLU:HB2 | 1.98 | 0.46 |
| 2:B:2158:TYR:O | 2:B:2161:GLN:HB3 | 2.15 | 0.46 |
| 2:B:2802:ASP:OD1 | 2:B:2906:ALA:N | 2.44 | 0.46 |
| 3:C:3148[B]:ILE:HG22 | 3:C:3152[B]:LYS:CE | 2.44 | 0.46 |
| 3:C:3200[B]:LEU:HD22 | 3:C:3204[B]:LEU:HD11 | 1.95 | 0.46 |
| 3:C:3298[B]:ASN:CA | 3:C:3299[B]:LEU:C | 2.85 | 0.46 |
| 1:D:447:MET:HA | 1:D:455:TYR:CB | 2.46 | 0.46 |
| 1:D:905:TRP:HE1 | 1:D:1083:PRO:HD2 | 1.81 | 0.46 |
| 2:E:2525:LYS:NZ | 2:E:2526:ARG:HH12 | 2.14 | 0.46 |
| 2:E:2715:ASP:HB3 | 2:E:2778:TYR:OH | 2.16 | 0.46 |
| 3:F:3284[B]:LYS:CE | 3:F:3285[B]:VAL:H | 2.29 | 0.46 |
| 1:G:548:ALA:O | 1:G:559:THR:HG22 | 2.15 | 0.46 |
| 1:G:999:LEU:HD12 | 1:G:1059:LEU:HD12 | 1.98 | 0.46 |
| 1:G:1166:THR:OG1 | 1:G:1168:GLN:OE1 | 2.30 | 0.46 |
| 1:G:1315:GLY:HA3 | 1:G:1601:TRP:HB2 | 1.98 | 0.46 |
| 2:H:2121:THR:O | 2:H:2124:SER:HB3 | 2.16 | 0.46 |
| 2:H:2286:HIS:NE2 | 2:H:2433:THR:HG22 | 2.31 | 0.46 |
| 1:J:22:LEU:HG | 1:J:122:VAL:HB | 1.97 | 0.46 |
| 3:L:2940[A]:ASN:O | 3:L:2944[A]:ALA:N | 2.48 | 0.46 |
| 3:L:2970[A]:PRO:C | 3:L:2972[A]:GLY:H | 2.23 | 0.46 |
| 3:L:3264[A]:TYR:HD1 | 3:L:3265[A]:ASP:N | 2.14 | 0.46 |
| 3:L:3281[A]:PHE:HE1 | 3:L:3305[A]:ILE:HG21 | 1.81 | 0.46 |
| 3:L:3284[A]:LYS:HD3 | 3:L:3285[A]:VAL:O | 2.16 | 0.46 |
| 1:M:1129:LEU:O | 1:M:1133:ILE:HG23 | 2.16 | 0.46 |
| 1:M:1189:ASP:HA | 2:Q:2809:LEU:HD12 | 1.96 | 0.46 |
| 1:M:1394:GLN:HG3 | 1:M:1433:TRP:HA | 1.98 | 0.46 |
| 1:M:1438:ASP:OD1 | 1:M:1439:VAL:N | 2.49 | 0.46 |
| 2:N:2116:SER:HA | 2:N:2121:THR:HG21 | 1.97 | 0.46 |
| 3:O:2940[B]:ASN:O | 3:O:2944[B]:ALA:N | 2.48 | 0.46 |
| 3:O:2965[A]:LEU:HD13 | 3:O:2975[A]:PHE:O | 2.16 | 0.46 |
| 3:O:2965[B]:LEU:HD13 | 3:O:2975[B]:PHE:O | 2.16 | 0.46 |
| 3:O:2987[B]:HIS:O | 3:O:2991[B]:LEU:HB2 | 2.16 | 0.46 |
| 3:O:3074[B]:GLU:OE2 | 3:O:3208[B]:GLN:HG2 | 2.15 | 0.46 |
| 3:O:3116[B]:PHE:C | 3:O:3116[B]:PHE:CD1 | 2.94 | 0.46 |
| 3:O:3125[B]:ARG:O | 3:O:3129[B]:ILE:HG13 | 2.14 | 0.46 |
| 3:O:3148[A]:ILE:HG22 | 3:O:3152[A]:LYS:CE | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3200[B]:LEU:HD22 | 3:O:3204[B]:LEU:HD11 | 1.95 | 0.46 |
| 2:Q:2568:HIS:HE1 | 2:Q:2742:MET:SD | 2.38 | 0.46 |
| 3:R:2938[B]:LEU:O | 3:R:2939[B]:ARG:C | 2.58 | 0.46 |
| 3:R:3283[A]:ILE:HB | 3:R:3305[A]:ILE:HD11 | 1.97 | 0.46 |
| 1:S:250:ASP:HA | 1:S:258:LYS:NZ | 2.31 | 0.46 |
| 1:S:780:GLU:C | 1:S:782:THR:H | 2.24 | 0.46 |
| 1:S:807:GLY:HA2 | 1:S:808:THR:HB | 1.97 | 0.46 |
| 1:S:931:TRP:CE3 | 1:S:991:LEU:HD13 | 2.51 | 0.46 |
| 3:U:2961[A]:HIS:HB2 | 3:U:2992[A]:TYR:HE2 | 1.81 | 0.46 |
| 3:U:2965[B]:LEU:HD22 | 3:U:2975[B]:PHE:O | 2.16 | 0.46 |
| 3:U:3074[A]:GLU:CD | 3:U:3212[A]:ARG:NH2 | 2.73 | 0.46 |
| 3:U:3116[B]:PHE:C | 3:U:3116[B]:PHE:CD1 | 2.94 | 0.46 |
| 3:U:3162[B]:ASP:OD1 | 3:d:3260[B]:ARG:HD2 | 2.16 | 0.46 |
| 3:U:3203[B]:HIS:O | 3:U:3206[B]:LYS:HB3 | 2.16 | 0.46 |
| 3:U:3225[B]:SER:C | 3:U:3290[B]:ILE:HG23 | 2.39 | 0.46 |
| 3:U:3298[A]:ASN:CA | 3:U:3299[A]:LEU:HB2 | 2.44 | 0.46 |
| 1:V:1260:ARG:HD2 | 1:V:1343:VAL:O | 2.16 | 0.46 |
| 1:V:1309:HIS:N | 1:V:1309:HIS:CD2 | 2.83 | 0.46 |
| 1:V:1390:ASP:HB2 | 1:V:1438:ASP:OD2 | 2.15 | 0.46 |
| 2:W:2327:GLU:H | 2:W:2327:GLU:HG3 | 1.57 | 0.46 |
| 3:X:2940[A]:ASN:O | 3:X:2944[A]:ALA:N | 2.48 | 0.46 |
| 3:X:2954[A]:TYR:CA | 3:X:2957[A]:ILE:HG22 | 2.43 | 0.46 |
| 3:X:3200[A]:LEU:CD2 | 3:X:3204[A]:LEU:CD1 | 2.93 | 0.46 |
| 3:X:3285[A]:VAL:CG2 | 3:X:3286[A]:THR:H | 2.27 | 0.46 |
| 3:X:3298[B]:ASN:CB | 3:X:3300[B]:LEU:CD2 | 2.61 | 0.46 |
| 1:Y:472:ASP:HA | 1:Y:473:ALA:HA | 1.67 | 0.46 |
| 1:Y:1546:LYS:HA | 3:d:3002[B]:ALA:HA | 1.60 | 0.46 |
| 1:Y:1656:ASP:N | 3:d:3006[B]:LYS:HD2 | 2.30 | 0.46 |
| 2:Z:2128:LEU:HD22 | 2:Z:2286:HIS:HB3 | 1.98 | 0.46 |
| 2:Z:2680:HIS:NE2 | 2:Z:2684:HIS:CD2 | 2.83 | 0.46 |
| 3:a:2949[A]:LYS:NZ | 3:a:2949[A]:LYS:C | 2.73 | 0.46 |
| 3:a:2965[B]:LEU:HD13 | 3:a:2975[B]:PHE:O | 2.16 | 0.46 |
| 3:a:3004[A]:GLY:C | 3:a:3006[A]:LYS:N | 2.74 | 0.46 |
| 3:a:3298[A]:ASN:CA | 3:a:3299[A]:LEU:HB2 | 2.45 | 0.46 |
| 2:c:2142:ALA:HA | 2:c:2143:CYS:HA | 1.76 | 0.46 |
| 2:c:2185:THR:HG23 | 2:c:2186:GLU:HG2 | 1.98 | 0.46 |
| 2:c:2726:LYS:HB2 | 2:c:2726:LYS:HE3 | 1.75 | 0.46 |
| 2:c:2863:ARG:HB2 | 2:c:2865:ILE:HG12 | 1.97 | 0.46 |
| 3:d:3299[B]:LEU:HB3 | 3:d:3300[B]:LEU:H | 1.53 | 0.46 |
| 4:9:1:NAG:O6 | 4:9:2:NAG:C1 | 2.63 | 0.46 |
| 1:A:183:HIS:CG | 1:A:344:LEU:HD21 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:234:ASN:O | 1:A:821:ILE:HA | 2.16 | 0.46 |
| 1:A:376:ASN:HB2 | 1:A:665:TYR:CG | 2.51 | 0.46 |
| 1:A:483:GLY:HA2 | 1:A:773:PHE:CZ | 2.51 | 0.46 |
| 1:A:980:TYR:CE1 | 1:A:1021:LEU:HD13 | 2.50 | 0.46 |
| 3:C:2965[A]:LEU:HD22 | 3:C:2975[A]:PHE:O | 2.15 | 0.46 |
| 3:C:2971[B]:ASP:OD2 | 3:L:3248[B]:LEU:HD21 | 2.16 | 0.46 |
| 3:C:3079[B]:CYS:SG | 3:C:3146[B]:CYS:O | 2.74 | 0.46 |
| 3:C:3143[A]:SER:OG | 3:C:3144[A]:ALA:N | 2.46 | 0.46 |
| 3:C:3209[A]:GLU:O | 3:C:3310[A]:GLY:C | 2.59 | 0.46 |
| 1:D:22:LEU:HD12 | 1:D:25:MET:HG2 | 1.97 | 0.46 |
| 1:D:398:ARG:HH21 | 1:D:663:GLU:CD | 2.23 | 0.46 |
| 2:E:2657:PHE:O | 2:E:2661:MET:HG2 | 2.15 | 0.46 |
| 2:E:2890:VAL:HG13 | 2:E:2891:LEU:C | 2.40 | 0.46 |
| 3:F:3137[B]:ARG:O | 3:F:3139[B]:LEU:HD22 | 2.16 | 0.46 |
| 1:G:23:ARG:HD3 | 1:G:120:LYS:HD3 | 1.97 | 0.46 |
| 1:G:444:GLU:O | 1:G:448:SER:OG | 2.13 | 0.46 |
| 1:G:597:VAL:HG23 | 1:G:598:GLN:H | 1.81 | 0.46 |
| 1:G:1166:THR:H | 1:G:1166:THR:HG1 | 1.34 | 0.46 |
| 1:G:1287:TYR:HA | 1:G:1290:ILE:HB | 1.98 | 0.46 |
| 2:H:2803:ARG:HH21 | 2:H:2805:PHE:HZ | 1.64 | 0.46 |
| 3:I:2961[B]:HIS:CD2 | 3:I:2988[B]:TRP:CZ3 | 2.96 | 0.46 |
| 3:I:2966[B]:SER:CA | 3:R:3255[B]:PRO:C | 2.89 | 0.46 |
| 3:I:2985[B]:PHE:CE2 | 3:I:2989[B]:HIS:CD2 | 3.04 | 0.46 |
| 3:I:2987[A]:HIS:O | 3:I:2991[A]:LEU:HB2 | 2.16 | 0.46 |
| 3:I:3079[B]:CYS:SG | 3:I:3146[B]:CYS:O | 2.74 | 0.46 |
| 3:I:3154[B]:PRO:N | 3:R:3173[B]:THR:C | 2.74 | 0.46 |
| 3:I:3191[A]:ASN:C | 3:I:3192[A]:PHE:O | 2.52 | 0.46 |
| 3:I:3209[A]:GLU:O | 3:I:3310[A]:GLY:C | 2.59 | 0.46 |
| 3:I:3225[A]:SER:C | 3:I:3290[A]:ILE:HG23 | 2.39 | 0.46 |
| 3:I:3284[B]:LYS:CE | 3:I:3285[B]:VAL:H | 2.29 | 0.46 |
| 3:I:3301[B]:PRO:HB2 | 3:I:3302[B]:SER:H | 1.33 | 0.46 |
| 1:J:1324:ARG:NH1 | 1:J:1519:TYR:HB3 | 2.31 | 0.46 |
| 3:L:3283[A]:ILE:HB | 3:L:3305[A]:ILE:HD11 | 1.97 | 0.46 |
| 1:M:525:SER:HA | 1:M:528:ALA:HB3 | 1.98 | 0.46 |
| 1:M:1206:HIS:CD2 | 1:M:1207:TYR:H | 2.34 | 0.46 |
| 1:M:1578:ILE:HA | 1:M:1579:GLY:HA2 | 1.64 | 0.46 |
| 2:N:2177:TYR:HB2 | 2:N:2300:ASN:HB2 | 1.98 | 0.46 |
| 2:N:2325:ALA:HA | 1:P:1649:THR:HG23 | 1.97 | 0.46 |
| 2:N:2638:ARG:HG2 | 2:N:2687:ILE:O | 2.15 | 0.46 |
| 2:N:2762:VAL:O | 2:N:2768:LEU:HD23 | 2.16 | 0.46 |
| 3:O:2961[A]:HIS:CD2 | 3:O:2988[A]:TRP:CZ3 | 2.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2961[B]:HIS:CD2 | 3:O:2988[B]:TRP:CZ3 | 2.96 | 0.46 |
| 3:O:2971[B]:ASP:CG | 3:X:3158[B]:PHE:CZ | 2.92 | 0.46 |
| 3:O:2976[B]:ALA:HB2 | 3:X:3156[B]:MET:HE2 | 1.98 | 0.46 |
| 3:O:3196[B]:THR:CB | 3:O:3199[B]:GLN:OE1 | 2.64 | 0.46 |
| 1:P:109:LEU:HD21 | 2:T:2635:TYR:HB2 | 1.98 | 0.46 |
| 3:R:2991[B]:LEU:HD23 | 3:R:3158[B]:PHE:CE1 | 2.48 | 0.46 |
| 3:R:3079[A]:CYS:SG | 3:R:3146[A]:CYS:O | 2.74 | 0.46 |
| 3:R:3284[B]:LYS:HD3 | 3:R:3285[B]:VAL:O | 2.16 | 0.46 |
| 1:S:1156:LEU:HB2 | 1:S:1176:TYR:CE1 | 2.51 | 0.46 |
| 3:U:2940[A]:ASN:O | 3:U:2944[A]:ALA:N | 2.48 | 0.46 |
| 3:U:2969[A]:TYR:CD2 | 3:U:2970[A]:PRO:N | 2.83 | 0.46 |
| 3:U:2975[B]:PHE:CZ | 3:d:3253[B]:GLU:HB2 | 2.51 | 0.46 |
| 3:U:2994[A]:LYS:O | 3:U:2997[A]:GLU:N | 2.49 | 0.46 |
| 3:U:3161[B]:GLU:H | 3:U:3161[B]:GLU:CD | 2.19 | 0.46 |
| 3:U:3196[A]:THR:CB | 3:U:3199[A]:GLN:OE1 | 2.64 | 0.46 |
| 3:U:3263[B]:LEU:N | 3:U:3263[B]:LEU:CD1 | 2.79 | 0.46 |
| 3:U:3285[B]:VAL:CG2 | 3:U:3286[B]:THR:H | 2.27 | 0.46 |
| 1:V:854:LEU:HG | 1:V:959:PHE:CE2 | 2.51 | 0.46 |
| 2:W:2089:ARG:HD3 | 2:W:2163:GLU:OE2 | 2.16 | 0.46 |
| 2:W:2885:SER:OG | 2:W:2886:VAL:N | 2.47 | 0.46 |
| 3:X:2949[A]:LYS:C | 3:X:2953[A]:GLY:N | 2.72 | 0.46 |
| 3:X:2969[A]:TYR:CD2 | 3:X:2970[A]:PRO:N | 2.83 | 0.46 |
| 3:X:2981[A]:GLY:N | 3:X:3086[A]:GLU:OE1 | 2.45 | 0.46 |
| 3:X:3137[B]:ARG:O | 3:X:3139[B]:LEU:HD22 | 2.16 | 0.46 |
| 3:X:3196[A]:THR:CB | 3:X:3199[A]:GLN:OE1 | 2.64 | 0.46 |
| 3:X:3263[A]:LEU:CD1 | 3:X:3263[A]:LEU:N | 2.79 | 0.46 |
| 3:X:3284[B]:LYS:CE | 3:X:3285[B]:VAL:H | 2.28 | 0.46 |
| 1:Y:669:LYS:HB2 | 1:Y:670:PRO:HD3 | 1.98 | 0.46 |
| 3:a:2970[B]:PRO:C | 3:a:2972[B]:GLY:H | 2.23 | 0.46 |
| 3:a:2985[B]:PHE:CE2 | 3:a:2989[B]:HIS:CD2 | 3.04 | 0.46 |
| 3:a:2987[A]:HIS:O | 3:a:2991[A]:LEU:HB2 | 2.15 | 0.46 |
| 3:a:3079[B]:CYS:SG | 3:a:3146[B]:CYS:O | 2.74 | 0.46 |
| 3:a:3283[A]:ILE:HB | 3:a:3305[A]:ILE:HD11 | 1.97 | 0.46 |
| 1:b:1636:ASN:ND2 | 4:QA:1:NAG:C7 | 2.79 | 0.46 |
| 2:c:2115:SER:OG | 2:c:2116:SER:N | 2.48 | 0.46 |
| 2:c:2302:ASP:O | 2:c:2306:VAL:HG23 | 2.16 | 0.46 |
| 3:d:2994[A]:LYS:O | 3:d:2997[A]:GLU:N | 2.49 | 0.46 |
| 3:d:3074[A]:GLU:CD | 3:d:3212[A]:ARG:NH2 | 2.73 | 0.46 |
| 3:d:3263[B]:LEU:N | 3:d:3263[B]:LEU:CD1 | 2.79 | 0.46 |
| 2:B:2126:HIS:O | 2:B:2143:CYS:HB3 | 2.16 | 0.46 |
| 2:B:2218:SER:HB2 | 2:B:2221:THR:HG23 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2888:GLY:N | 2:B:2889:ALA:HA | 2.31 | 0.46 |
| 3:C:2994[B]:LYS:O | 3:C:2997[B]:GLU:N | 2.49 | 0.46 |
| 3:C:3196[A]:THR:CB | 3:C:3199[A]:GLN:OE1 | 2.64 | 0.46 |
| 1:D:956:PRO:HD2 | 1:D:957:ASN:HA | 1.97 | 0.46 |
| 1:D:1433:TRP:HE3 | 1:D:1433:TRP:N | 2.14 | 0.46 |
| 2:E:2639:GLU:OE1 | 2:E:2690:HIS:HB2 | 2.16 | 0.46 |
| 2:E:2805:PHE:CE1 | 2:E:2855:ASP:HB3 | 2.51 | 0.46 |
| 2:E:2822:LYS:HG3 | 2:E:2830:GLN:C | 2.41 | 0.46 |
| 3:F:2965[B]:LEU:HD13 | 3:F:2975[B]:PHE:O | 2.16 | 0.46 |
| 3:F:2968[B]:GLN:O | 3:a:2980[B]:HIS:N | 2.40 | 0.46 |
| 3:F:2970[A]:PRO:C | 3:F:2972[A]:GLY:H | 2.23 | 0.46 |
| 3:F:2973[B]:THR:HG21 | 3:a:3107[B]:LEU:N | 2.31 | 0.46 |
| 3:F:2985[B]:PHE:CE2 | 3:F:2989[B]:HIS:CD2 | 3.04 | 0.46 |
| 3:F:2994[B]:LYS:O | 3:F:2997[B]:GLU:N | 2.49 | 0.46 |
| 3:F:3203[B]:HIS:O | 3:F:3206[B]:LYS:HB3 | 2.16 | 0.46 |
| 3:F:3293[B]:LYS:CD | 3:F:3293[B]:LYS:C | 2.86 | 0.46 |
| 1:G:53:SER:O | 1:G:55:ILE:HG13 | 2.16 | 0.46 |
| 1:G:792:MET:HB2 | 1:G:793:PHE:CD1 | 2.51 | 0.46 |
| 1:G:877:HIS:CE1 | 1:G:905:TRP:HZ3 | 2.34 | 0.46 |
| 2:H:2800:LYS:C | 3:I:3023[A]:ILE:HD13 | 2.41 | 0.46 |
| 2:H:2870:LEU:HD11 | 2:H:2901:LEU:HD23 | 1.97 | 0.46 |
| 3:I:3014[A]:TRP:CD2 | 3:I:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:I:3135[A]:LYS:HB2 | 3:I:3141[A]:TYR:CD1 | 2.51 | 0.46 |
| 3:I:3157[B]:PRO:CD | 3:R:2982[B]:MET:CE | 2.93 | 0.46 |
| 1:J:730:PHE:CE2 | 1:J:780:GLU:HB3 | 2.51 | 0.46 |
| 1:J:913:PHE:HE2 | 1:J:1042:PHE:CD1 | 2.33 | 0.46 |
| 1:J:1494:ARG:HG3 | 1:J:1494:ARG:HH11 | 1.80 | 0.46 |
| 2:K:2115:SER:OG | 2:K:2116:SER:N | 2.49 | 0.46 |
| 3:L:2970[B]:PRO:C | 3:L:2972[B]:GLY:N | 2.72 | 0.46 |
| 3:L:2985[A]:PHE:CE2 | 3:L:2989[A]:HIS:CD2 | 3.04 | 0.46 |
| 1:M:854:LEU:HD23 | 1:M:941:LEU:HD21 | 1.98 | 0.46 |
| 2:N:2625:LEU:HD13 | 2:N:2626:ARG:HB2 | 1.98 | 0.46 |
| 2:N:2743:ALA:HB1 | 1:P:1210:LYS:HG3 | 1.98 | 0.46 |
| 2:N:2866:PRO:HA | 2:N:2867:PRO:HD3 | 1.78 | 0.46 |
| 3:O:3014[A]:TRP:CG | 3:O:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:O:3025[A]:VAL:CG2 | 3:O:3047[A]:ARG:NH1 | 2.73 | 0.46 |
| 3:O:3137[B]:ARG:O | 3:O:3139[B]:LEU:HD22 | 2.16 | 0.46 |
| 3:O:3230[B]:PHE:H | 3:O:3243[B]:GLY:HA3 | 1.79 | 0.46 |
| 3:O:3255[B]:PRO:HB3 | 3:X:3161[B]:GLU:CA | 2.46 | 0.46 |
| 3:O:3283[B]:ILE:HB | 3:O:3305[B]:ILE:HD11 | 1.97 | 0.46 |
| 1:P:239:LEU:H | 1:P:239:LEU:HD12 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:636:GLN:OE1 | 1:P:639:ARG:NH1 | 2.48 | 0.46 |
| 2:Q:2545:SER:CA | 2:Q:2546:LEU:HB3 | 2.44 | 0.46 |
| 3:R:2940[B]:ASN:O | 3:R:2944[B]:ALA:N | 2.48 | 0.46 |
| 3:R:2965[A]:LEU:HD22 | 3:R:2975[A]:PHE:O | 2.15 | 0.46 |
| 3:R:3023[B]:ILE:O | 3:R:3026[B]:THR:OG1 | 2.34 | 0.46 |
| 3:R:3185[B]:TYR:CE2 | 3:R:3187[B]:TYR:HE2 | 2.31 | 0.46 |
| 3:R:3196[A]:THR:CB | 3:R:3199[A]:GLN:OE1 | 2.64 | 0.46 |
| 3:R:3283[B]:ILE:HB | 3:R:3305[B]:ILE:HD11 | 1.97 | 0.46 |
| 3:U:2952[A]:ALA:HB1 | 3:U:2957[A]:ILE:H | 1.79 | 0.46 |
| 3:U:2991[B]:LEU:HD23 | 3:U:3158[B]:PHE:CE1 | 2.48 | 0.46 |
| 3:U:3074[A]:GLU:OE2 | 3:U:3208[A]:GLN:HG2 | 2.15 | 0.46 |
| 3:U:3106[B]:THR:O | 3:U:3106[B]:THR:HG23 | 2.16 | 0.46 |
| 3:U:3116[A]:PHE:CD1 | 3:U:3116[A]:PHE:C | 2.94 | 0.46 |
| 3:U:3200[B]:LEU:HD22 | 3:U:3204[B]:LEU:HD11 | 1.95 | 0.46 |
| 3:U:3220[B]:ARG:CG | 3:d:2973[B]:THR:HA | 2.43 | 0.46 |
| 1:V:780:GLU:O | 1:V:781:ILE:HG12 | 2.14 | 0.46 |
| 1:V:902:PHE:CD2 | 1:V:1012:GLU:HB2 | 2.50 | 0.46 |
| 1:V:1321:HIS:ND1 | 1:V:1513:PRO:HB3 | 2.31 | 0.46 |
| 3:X:2970[A]:PRO:C | 3:X:2972[A]:GLY:N | 2.72 | 0.46 |
| 3:X:2985[A]:PHE:CE2 | 3:X:2989[A]:HIS:NE2 | 2.83 | 0.46 |
| 3:X:3137[A]:ARG:O | 3:X:3139[A]:LEU:HD22 | 2.16 | 0.46 |
| 3:X:3191[A]:ASN:C | 3:X:3192[A]:PHE:O | 2.52 | 0.46 |
| 3:X:3281[B]:PHE:HE1 | 3:X:3305[B]:ILE:HG21 | 1.81 | 0.46 |
| 3:a:2994[A]:LYS:O | 3:a:2997[A]:GLU:N | 2.49 | 0.46 |
| 3:a:2994[B]:LYS:O | 3:a:2997[B]:GLU:N | 2.49 | 0.46 |
| 3:a:3023[B]:ILE:O | 3:a:3026[B]:THR:OG1 | 2.34 | 0.46 |
| 1:b:22:LEU:O | 1:b:26:GLN:HB2 | 2.16 | 0.46 |
| 1:b:434:GLU:O | 1:b:438:GLU:HG3 | 2.16 | 0.46 |
| 1:b:930:ASP:OD1 | 1:b:1051:ARG:NH2 | 2.48 | 0.46 |
| 1:b:947:TYR:CE1 | 1:b:956:PRO:HD2 | 2.51 | 0.46 |
| 1:b:1300:CYS:HB3 | 1:b:1494:ARG:NH1 | 2.30 | 0.46 |
| 2:c:2549:PRO:CD | 2:c:2554:PRO:HB3 | 2.37 | 0.46 |
| 2:c:2631:TYR:H | 2:c:2631:TYR:HD1 | 1.64 | 0.46 |
| 3:d:2970[A]:PRO:C | 3:d:2972[A]:GLY:H | 2.23 | 0.46 |
| 3:d:2991[B]:LEU:HD23 | 3:d:3158[B]:PHE:CE1 | 2.48 | 0.46 |
| 3:d:3171[B]:HIS:C | 3:d:3173[B]:THR:N | 2.73 | 0.46 |
| 3:d:3203[B]:HIS:O | 3:d:3206[B]:LYS:HB3 | 2.16 | 0.46 |
| 3:d:3263[A]:LEU:CD1 | 3:d:3263[A]:LEU:N | 2.79 | 0.46 |
| 3:d:3283[B]:ILE:HB | 3:d:3305[B]:ILE:HD11 | 1.97 | 0.46 |
| 5:l:3:BMA:H3 | 5:l:4:MAN:H2 | 1.54 | 0.46 |
| 1:A:321:LEU:HB2 | 1:A:338:ALA:HB2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:747:PHE:HE1 | 1:A:756:PHE:HD2 | 1.64 | 0.46 |
| 1:A:832:LYS:O | 1:A:832:LYS:HG3 | 2.15 | 0.46 |
| 1:A:912:ASN:HD21 | 1:A:1091:ASN:ND2 | 2.12 | 0.46 |
| 1:A:956:PRO:HB2 | 1:A:957:ASN:C | 2.40 | 0.46 |
| 1:A:1225:VAL:HG12 | 1:A:1226:THR:H | 1.80 | 0.46 |
| 1:A:1423:TYR:OH | 1:A:1461:VAL:HG13 | 2.16 | 0.46 |
| 2:B:2394:VAL:H | 2:B:2448:THR:CG2 | 2.20 | 0.46 |
| 2:B:2609:ALA:HA | 2:B:2625:LEU:HD23 | 1.97 | 0.46 |
| 3:C:2970[A]:PRO:C | 3:C:2972[A]:GLY:H | 2.23 | 0.46 |
| 3:C:2994[A]:LYS:O | 3:C:2997[A]:GLU:N | 2.49 | 0.46 |
| 3:C:3014[A]:TRP:CG | 3:C:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:C:3284[A]:LYS:HD3 | 3:C:3285[A]:VAL:O | 2.16 | 0.46 |
| 1:D:904:HIS:HB3 | 1:D:1105:VAL:HG21 | 1.96 | 0.46 |
| 2:E:2627:GLY:HA3 | 2:E:2703:PHE:O | 2.16 | 0.46 |
| 3:F:3116[B]:PHE:C | 3:F:3116[B]:PHE:CD1 | 2.94 | 0.46 |
| 3:F:3150[B]:LYS:HZ3 | 3:a:3160[B]:SER:HB2 | 1.69 | 0.46 |
| 3:F:3169[B]:LYS:HA | 3:a:3150[B]:LYS:HA | 1.92 | 0.46 |
| 3:F:3209[A]:GLU:O | 3:F:3310[A]:GLY:C | 2.59 | 0.46 |
| 3:F:3263[B]:LEU:N | 3:F:3263[B]:LEU:CD1 | 2.79 | 0.46 |
| 1:G:742:ALA:HA | 1:G:805:VAL:HG23 | 1.97 | 0.46 |
| 1:G:1026:GLU:OE1 | 1:G:1028:VAL:N | 2.49 | 0.46 |
| 1:G:1325:LEU:O | 1:G:1328:SER:HB3 | 2.16 | 0.46 |
| 1:G:1636:ASN:HB2 | 1:G:1639:LYS:HD3 | 1.98 | 0.46 |
| 2:H:2128:LEU:HB2 | 2:H:2286:HIS:HB3 | 1.98 | 0.46 |
| 2:H:2695:MET:HE2 | 2:H:2695:MET:HA | 1.98 | 0.46 |
| 3:I:2987[B]:HIS:O | 3:I:2991[B]:LEU:HB2 | 2.15 | 0.46 |
| 3:I:2994[B]:LYS:O | 3:I:2997[B]:GLU:N | 2.49 | 0.46 |
| 3:I:3024[A]:LEU:CD1 | 3:I:3024[A]:LEU:C | 2.85 | 0.46 |
| 3:I:3024[B]:LEU:CD1 | 3:I:3024[B]:LEU:C | 2.85 | 0.46 |
| 3:I:3116[A]:PHE:CD1 | 3:I:3116[A]:PHE:C | 2.94 | 0.46 |
| 3:I:3191[B]:ASN:ND2 | 3:I:3191[B]:ASN:N | 2.60 | 0.46 |
| 3:I:3251[B]:ASP:HB3 | 3:I:3252[B]:TYR:CD1 | 2.40 | 0.46 |
| 3:I:3263[B]:LEU:N | 3:I:3263[B]:LEU:CD1 | 2.79 | 0.46 |
| 1:J:480:CYS:HA | 1:J:490:TRP:CE2 | 2.51 | 0.46 |
| 1:J:880:THR:HB | 1:J:882:TRP:CZ2 | 2.50 | 0.46 |
| 3:L:2948[A]:ASP:CB | 3:L:2949[A]:LYS:HA | 2.16 | 0.46 |
| 3:L:3004[B]:GLY:C | 3:L:3006[B]:LYS:N | 2.74 | 0.46 |
| 3:L:3023[A]:ILE:O | 3:L:3026[A]:THR:OG1 | 2.34 | 0.46 |
| 3:L:3116[A]:PHE:C | 3:L:3116[A]:PHE:CD1 | 2.94 | 0.46 |
| 3:L:3137[A]:ARG:HB3 | 3:L:3139[A]:LEU:HD21 | 1.97 | 0.46 |
| 1:M:589:GLN:HG2 | 1:M:594:ASP:CB | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:618:MET:HE3 | 1:M:618:MET:HB3 | 1.67 | 0.46 |
| 1:M:935:ILE:HD11 | 1:M:980:TYR:HD2 | 1.80 | 0.46 |
| 1:P:329:ARG:HH22 | 1:S:1574:VAL:H | 1.63 | 0.46 |
| 1:P:376:ASN:HB2 | 1:P:665:TYR:CE1 | 2.51 | 0.46 |
| 2:Q:2115:SER:OG | 2:Q:2116:SER:N | 2.49 | 0.46 |
| 3:R:2985[A]:PHE:CE2 | 3:R:2989[A]:HIS:CD2 | 3.04 | 0.46 |
| 3:R:3074[A]:GLU:CD | 3:R:3212[A]:ARG:NH2 | 2.73 | 0.46 |
| 3:R:3106[B]:THR:O | 3:R:3106[B]:THR:HG23 | 2.16 | 0.46 |
| 3:R:3182[A]:GLN:H | 3:R:3182[A]:GLN:HG2 | 1.56 | 0.46 |
| 3:R:3196[A]:THR:CA | 3:R:3199[A]:GLN:HB2 | 2.43 | 0.46 |
| 3:R:3196[B]:THR:CB | 3:R:3199[B]:GLN:OE1 | 2.64 | 0.46 |
| 3:R:3285[B]:VAL:CG2 | 3:R:3286[B]:THR:N | 2.73 | 0.46 |
| 1:S:61:GLY:N | 1:S:176:GLU:OE2 | 2.43 | 0.46 |
| 1:S:664:VAL:O | 1:S:689:PRO:HD2 | 2.16 | 0.46 |
| 1:S:801:ASP:OD1 | 1:S:801:ASP:N | 2.48 | 0.46 |
| 3:U:2970[B]:PRO:C | 3:U:2972[B]:GLY:N | 2.72 | 0.46 |
| 3:U:3004[B]:GLY:C | 3:U:3006[B]:LYS:N | 2.74 | 0.46 |
| 3:U:3014[B]:TRP:CG | 3:U:3092[B]:ILE:CD1 | 2.98 | 0.46 |
| 3:U:3209[B]:GLU:O | 3:U:3310[B]:GLY:C | 2.59 | 0.46 |
| 3:U:3263[A]:LEU:N | 3:U:3263[A]:LEU:CD1 | 2.79 | 0.46 |
| 3:U:3283[B]:ILE:C | 3:U:3283[B]:ILE:CD1 | 2.85 | 0.46 |
| 3:U:3284[A]:LYS:CE | 3:U:3285[A]:VAL:H | 2.28 | 0.46 |
| 1:V:48:LYS:HE3 | 1:V:54:THR:HG22 | 1.97 | 0.46 |
| 1:V:1316:MET:HB3 | 1:V:1318:VAL:HG22 | 1.97 | 0.46 |
| 1:V:1498:ASN:ND2 | 1:V:1500:THR:O | 2.49 | 0.46 |
| 2:W:2568:HIS:HD2 | 2:W:2718:TRP:CH2 | 2.34 | 0.46 |
| 2:W:2740:ASP:OD1 | 2:W:2740:ASP:N | 2.49 | 0.46 |
| 3:X:2965[B]:LEU:HD13 | 3:X:2975[B]:PHE:O | 2.16 | 0.46 |
| 3:X:2994[A]:LYS:O | 3:X:2997[A]:GLU:N | 2.49 | 0.46 |
| 3:X:3134[A]:GLN:O | 3:X:3136[A]:TYR:N | 2.49 | 0.46 |
| 3:X:3283[A]:ILE:HB | 3:X:3305[A]:ILE:HD11 | 1.97 | 0.46 |
| 1:Y:92:TRP:O | 1:Y:212:ASN:ND2 | 2.49 | 0.46 |
| 2:Z:2128:LEU:O | 2:Z:2130:PRO:HD3 | 2.16 | 0.46 |
| 2:Z:2783:PHE:HB3 | 2:Z:2791:LEU:HD21 | 1.97 | 0.46 |
| 3:a:2938[A]:LEU:O | 3:a:2939[A]:ARG:C | 2.58 | 0.46 |
| 3:a:2965[A]:LEU:HD22 | 3:a:2975[A]:PHE:O | 2.15 | 0.46 |
| 3:a:2965[B]:LEU:HD22 | 3:a:2975[B]:PHE:O | 2.15 | 0.46 |
| 3:a:2987[B]:HIS:O | 3:a:2991[B]:LEU:HB2 | 2.16 | 0.46 |
| 3:a:3014[A]:TRP:CD2 | 3:a:3092[A]:ILE:CD1 | 2.98 | 0.46 |
| 3:a:3074[B]:GLU:OE2 | 3:a:3208[B]:GLN:HG2 | 2.15 | 0.46 |
| 3:a:3191[A]:ASN:C | 3:a:3192[A]:PHE:O | 2.52 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3196[B]:THR:CA | 3:a:3199[B]:GLN:HB2 | 2.43 | 0.46 |
| 3:a:3196[B]:THR:CB | 3:a:3199[B]:GLN:OE1 | 2.64 | 0.46 |
| 3:a:3301[A]:PRO:HB2 | 3:a:3302[A]:SER:H | 1.33 | 0.46 |
| 2:c:2802:ASP:OD2 | 2:c:2903:TYR:OH | 2.28 | 0.46 |
| 2:c:2890:VAL:HG23 | 2:c:2891:LEU:C | 2.40 | 0.46 |
| 3:d:2969[B]:TYR:CD2 | 3:d:2971[B]:ASP:N | 2.73 | 0.46 |
| 3:d:2994[B]:LYS:O | 3:d:2997[B]:GLU:N | 2.49 | 0.46 |
| 3:d:3135[B]:LYS:HB2 | 3:d:3141[B]:TYR:CD1 | 2.51 | 0.46 |
| 3:d:3137[B]:ARG:HB3 | 3:d:3139[B]:LEU:HD21 | 1.97 | 0.46 |
| 3:d:3285[A]:VAL:CG2 | 3:d:3286[A]:THR:H | 2.27 | 0.46 |
| 3:d:3298[B]:ASN:CA | 3:d:3299[B]:LEU:HB2 | 2.44 | 0.46 |
| 8:0:1:NAG:H62 | 8:0:2:NAG:HN2 | 1.75 | 0.46 |
| 1:A:1145:THR:HG22 | 1:A:1193:LYS:HG2 | 1.97 | 0.45 |
| 2:B:2145:LEU:HG | 2:B:2148:MET:SD | 2.55 | 0.45 |
| 3:C:2932[A]:PRO:CA | 3:C:2935[A]:ILE:CD1 | 2.85 | 0.45 |
| 3:C:2954[B]:TYR:CA | 3:C:2957[B]:ILE:HG22 | 2.43 | 0.45 |
| 3:C:3004[A]:GLY:C | 3:C:3006[A]:LYS:N | 2.74 | 0.45 |
| 3:C:3116[A]:PHE:CD1 | 3:C:3116[A]:PHE:C | 2.94 | 0.45 |
| 3:C:3116[B]:PHE:CD1 | 3:C:3116[B]:PHE:C | 2.94 | 0.45 |
| 3:C:3119[B]:HIS:O | 3:C:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 3:C:3204[B]:LEU:CD1 | 3:C:3204[B]:LEU:N | 2.80 | 0.45 |
| 3:C:3263[B]:LEU:CD1 | 3:C:3263[B]:LEU:N | 2.79 | 0.45 |
| 1:D:465:PRO:HD2 | 1:D:467:LYS:HZ1 | 1.79 | 0.45 |
| 1:D:522:ALA:HA | 1:D:568:PHE:CZ | 2.51 | 0.45 |
| 1:D:784:ALA:O | 1:D:788:LEU:HG | 2.16 | 0.45 |
| 1:D:1391:ARG:NH1 | 1:D:1451:ASP:OD1 | 2.49 | 0.45 |
| 2:E:2403:PHE:CZ | 2:E:2428:VAL:HG21 | 2.51 | 0.45 |
| 3:F:2937[A]:ASN:CB | 3:F:3006[A]:LYS:CE | 2.85 | 0.45 |
| 3:F:3135[A]:LYS:HG3 | 3:F:3141[A]:TYR:HE1 | 1.29 | 0.45 |
| 3:F:3137[A]:ARG:HB3 | 3:F:3139[A]:LEU:HD21 | 1.97 | 0.45 |
| 3:F:3162[B]:ASP:C | 3:a:3147[B]:GLU:OE1 | 2.59 | 0.45 |
| 3:F:3264[A]:TYR:HD1 | 3:F:3265[A]:ASP:N | 2.14 | 0.45 |
| 1:G:22:LEU:HD23 | 1:G:123:PHE:CE1 | 2.51 | 0.45 |
| 1:G:1026:GLU:OE2 | 1:G:1028:VAL:HG12 | 2.15 | 0.45 |
| 1:G:1301:PRO:HA | 1:G:1308:VAL:HA | 1.99 | 0.45 |
| 2:H:2217:ILE:HD11 | 2:H:2287:TYR:HE1 | 1.81 | 0.45 |
| 2:H:2625:LEU:O | 2:H:2638:ARG:NH2 | 2.49 | 0.45 |
| 2:H:2663:MET:HG3 | 2:H:2675:GLN:HB2 | 1.98 | 0.45 |
| 2:H:2822:LYS:HD2 | 2:H:2831:GLU:HA | 1.97 | 0.45 |
| 3:I:3196[B]:THR:CB | 3:I:3199[B]:GLN:OE1 | 2.64 | 0.45 |
| 3:I:3256[B]:TRP:NE1 | 3:R:2965[B]:LEU:HD13 | 2.29 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:494:VAL:HG23 | 1:J:671:PHE:HZ | 1.81 | 0.45 |
| 1:J:901:THR:HG23 | 1:J:1077:LEU:HD12 | 1.97 | 0.45 |
| 1:J:949:ASP:CB | 1:J:953:GLU:HB2 | 2.44 | 0.45 |
| 1:J:1578:ILE:HA | 1:J:1579:GLY:HA2 | 1.59 | 0.45 |
| 3:L:2961[B]:HIS:CD2 | 3:L:2988[B]:TRP:CZ3 | 2.97 | 0.45 |
| 3:L:2987[B]:HIS:O | 3:L:2991[B]:LEU:HB2 | 2.15 | 0.45 |
| 3:L:3137[B]:ARG:HB3 | 3:L:3139[B]:LEU:HD21 | 1.97 | 0.45 |
| 3:L:3242[A]:GLY:C | 3:L:3243[A]:GLY:O | 2.58 | 0.45 |
| 3:L:3264[B]:TYR:HD1 | 3:L:3265[B]:ASP:N | 2.14 | 0.45 |
| 1:M:1145:THR:OG1 | 1:M:1233:SER:HB3 | 2.16 | 0.45 |
| 2:N:2110:MET:HE1 | 2:N:2122:ILE:HD12 | 1.98 | 0.45 |
| 2:N:2778:TYR:HB2 | 2:N:2781:LEU:HD12 | 1.97 | 0.45 |
| 3:O:3004[B]:GLY:C | 3:O:3006[B]:LYS:N | 2.74 | 0.45 |
| 3:O:3004[B]:GLY:O | 3:O:3006[B]:LYS:N | 2.44 | 0.45 |
| 3:O:3079[A]:CYS:SG | 3:O:3146[A]:CYS:O | 2.74 | 0.45 |
| 3:O:3191[B]:ASN:ND2 | 3:O:3191[B]:ASN:N | 2.60 | 0.45 |
| 3:O:3196[A]:THR:CB | 3:O:3199[A]:GLN:OE1 | 2.64 | 0.45 |
| 3:O:3263[B]:LEU:CD1 | 3:O:3263[B]:LEU:N | 2.79 | 0.45 |
| 1:P:40:TYR:CE2 | 1:P:75:GLN:HG2 | 2.50 | 0.45 |
| 1:P:76:PHE:CD2 | 1:P:89:ILE:HG21 | 2.51 | 0.45 |
| 1:P:262:LYS:NZ | 1:P:795:GLU:OE1 | 2.49 | 0.45 |
| 1:P:897:HIS:CD2 | 1:P:899:MET:HE1 | 2.51 | 0.45 |
| 1:P:1241:GLY:HA2 | 1:P:1252:PRO:HB3 | 1.97 | 0.45 |
| 3:R:2951[B]:ASP:CG | 3:R:2952[B]:ALA:N | 2.74 | 0.45 |
| 3:R:2994[A]:LYS:O | 3:R:2997[A]:GLU:N | 2.49 | 0.45 |
| 3:R:3074[B]:GLU:CD | 3:R:3212[B]:ARG:NH2 | 2.73 | 0.45 |
| 3:R:3119[A]:HIS:O | 3:R:3122[A]:ASN:HB3 | 2.17 | 0.45 |
| 3:R:3134[A]:GLN:O | 3:R:3136[A]:TYR:N | 2.49 | 0.45 |
| 3:R:3263[A]:LEU:N | 3:R:3263[A]:LEU:CD1 | 2.79 | 0.45 |
| 1:S:308:LEU:O | 1:S:772:ARG:NH2 | 2.50 | 0.45 |
| 1:S:961:SER:HB3 | 1:S:972:SER:O | 2.16 | 0.45 |
| 1:S:1171:LYS:HG2 | 1:S:1173:GLY:H | 1.81 | 0.45 |
| 2:T:2867:PRO:HG2 | 3:U:2932[A]:PRO:CG | 2.45 | 0.45 |
| 2:T:2887:ASP:OD1 | 2:T:2887:ASP:N | 2.48 | 0.45 |
| 3:U:2969[B]:TYR:CD2 | 3:U:2970[B]:PRO:N | 2.83 | 0.45 |
| 3:U:2969[B]:TYR:CA | 3:d:2981[B]:GLY:HA3 | 2.39 | 0.45 |
| 3:U:2985[B]:PHE:CE2 | 3:U:2989[B]:HIS:CD2 | 3.04 | 0.45 |
| 3:U:2987[A]:HIS:O | 3:U:2991[A]:LEU:HB2 | 2.16 | 0.45 |
| 3:U:3087[B]:MET:HA | 3:U:3090[B]:ASN:OD1 | 2.17 | 0.45 |
| 3:U:3134[A]:GLN:O | 3:U:3136[A]:TYR:N | 2.49 | 0.45 |
| 3:U:3134[B]:GLN:O | 3:U:3136[B]:TYR:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3264[B]:TYR:HD1 | 3:U:3265[B]:ASP:N | 2.14 | 0.45 |
| 2:W:2723:GLU:HG2 | 2:W:2788:ILE:CD1 | 2.46 | 0.45 |
| 3:X:2937[A]:ASN:CB | 3:X:3006[A]:LYS:CE | 2.86 | 0.45 |
| 3:X:2951[A]:ASP:C | 3:X:2956[A]:LYS:HZ1 | 2.13 | 0.45 |
| 3:X:3014[A]:TRP:CG | 3:X:3092[A]:ILE:CD1 | 2.98 | 0.45 |
| 3:X:3014[A]:TRP:CD2 | 3:X:3092[A]:ILE:CD1 | 2.98 | 0.45 |
| 3:X:3116[B]:PHE:CD1 | 3:X:3116[B]:PHE:C | 2.94 | 0.45 |
| 3:X:3119[A]:HIS:O | 3:X:3122[A]:ASN:HB3 | 2.16 | 0.45 |
| 3:X:3134[B]:GLN:O | 3:X:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:X:3137[A]:ARG:HD3 | 3:X:3137[A]:ARG:HA | 1.71 | 0.45 |
| 3:X:3196[A]:THR:N | 3:X:3199[A]:GLN:CB | 2.65 | 0.45 |
| 3:X:3281[A]:PHE:HE1 | 3:X:3305[A]:ILE:HG21 | 1.81 | 0.45 |
| 3:a:3116[A]:PHE:CD1 | 3:a:3116[A]:PHE:C | 2.94 | 0.45 |
| 3:a:3209[B]:GLU:O | 3:a:3310[B]:GLY:C | 2.59 | 0.45 |
| 3:a:3293[A]:LYS:HB2 | 3:a:3294[A]:SER:CA | 2.41 | 0.45 |
| 1:b:418:ASP:C | 1:b:420:SER:HA | 2.41 | 0.45 |
| 1:b:468:CYS:SG | 1:b:669:LYS:HB3 | 2.56 | 0.45 |
| 2:c:2867:PRO:HG2 | 3:d:2932[A]:PRO:O | 2.16 | 0.45 |
| 3:d:2961[B]:HIS:HB2 | 3:d:2992[B]:TYR:HE2 | 1.81 | 0.45 |
| 3:d:2987[A]:HIS:O | 3:d:2991[A]:LEU:HB2 | 2.16 | 0.45 |
| 3:d:3196[A]:THR:CB | 3:d:3199[A]:GLN:OE1 | 2.64 | 0.45 |
| 1:A:428:ILE:HD12 | 1:A:514:TRP:HB3 | 1.99 | 0.45 |
| 1:A:1211:TYR:OH | 2:E:2739:LEU:HD12 | 2.16 | 0.45 |
| 2:B:2462:PHE:CE1 | 2:B:2486:ILE:HD13 | 2.51 | 0.45 |
| 3:C:2965[B]:LEU:HD13 | 3:C:2975[B]:PHE:O | 2.16 | 0.45 |
| 3:C:2973[B]:THR:HG22 | 3:L:3249[B]:GLY:N | 2.31 | 0.45 |
| 3:C:3256[B]:TRP:NE1 | 3:L:2975[B]:PHE:O | 2.49 | 0.45 |
| 1:D:28:ASP:HB3 | 1:D:33:GLY:HA2 | 1.98 | 0.45 |
| 1:D:613:SER:HA | 1:D:805:VAL:HG12 | 1.97 | 0.45 |
| 1:D:962:GLY:HA2 | 1:D:971:THR:HB | 1.97 | 0.45 |
| 1:D:1313:LEU:HD13 | 1:D:1322:TRP:CD1 | 2.51 | 0.45 |
| 2:E:2737:CYS:O | 2:E:2739:LEU:HD23 | 2.15 | 0.45 |
| 3:F:2971[B]:ASP:CG | 3:a:3248[B]:LEU:HD21 | 2.40 | 0.45 |
| 3:F:3148[A]:ILE:O | 3:F:3148[A]:ILE:HG22 | 2.17 | 0.45 |
| 3:F:3252[B]:TYR:C | 3:a:2976[B]:ALA:CB | 2.88 | 0.45 |
| 1:G:1302:SER:HA | 1:G:1303:GLU:HA | 1.68 | 0.45 |
| 1:G:1331:GLU:OE1 | 1:G:1342:ALA:HB1 | 2.16 | 0.45 |
| 2:H:2114:ARG:HG3 | 2:K:2526:ARG:HE | 1.81 | 0.45 |
| 2:H:2500:ILE:HD11 | 2:H:2775:GLY:O | 2.16 | 0.45 |
| 3:I:2965[B]:LEU:HD22 | 3:I:2975[B]:PHE:O | 2.15 | 0.45 |
| 3:I:2985[A]:PHE:CE2 | 3:I:2989[A]:HIS:CD2 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2992[B]:TYR:HE2 | 3:R:2969[B]:TYR:HE1 | 1.62 | 0.45 |
| 3:I:3134[B]:GLN:O | 3:I:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:I:3137[B]:ARG:O | 3:I:3139[B]:LEU:HD22 | 2.16 | 0.45 |
| 3:I:3151[B]:LEU:CB | 3:I:3175[B]:TYR:CD2 | 2.93 | 0.45 |
| 3:I:3209[B]:GLU:O | 3:I:3310[B]:GLY:C | 2.59 | 0.45 |
| 1:J:1424:GLU:O | 1:J:1427:HIS:HB3 | 2.16 | 0.45 |
| 2:K:2329:MET:HA | 2:K:2354:PRO:HG2 | 1.96 | 0.45 |
| 3:L:2961[B]:HIS:HB2 | 3:L:2992[B]:TYR:HE2 | 1.81 | 0.45 |
| 3:L:2965[B]:LEU:HD22 | 3:L:2975[B]:PHE:O | 2.15 | 0.45 |
| 3:L:3137[B]:ARG:O | 3:L:3139[B]:LEU:HD22 | 2.16 | 0.45 |
| 3:L:3196[B]:THR:CB | 3:L:3199[B]:GLN:OE1 | 2.64 | 0.45 |
| 3:L:3209[A]:GLU:O | 3:L:3310[A]:GLY:C | 2.59 | 0.45 |
| 2:N:2244:PHE:HE2 | 2:N:2374:ASN:HD22 | 1.64 | 0.45 |
| 3:O:2956[A]:LYS:O | 3:O:2959[A]:SER:OG | 2.33 | 0.45 |
| 3:O:2965[B]:LEU:HD22 | 3:O:2975[B]:PHE:O | 2.15 | 0.45 |
| 3:O:2985[B]:PHE:CE2 | 3:O:2989[B]:HIS:CD2 | 3.04 | 0.45 |
| 3:O:3137[B]:ARG:HB3 | 3:O:3139[B]:LEU:HD21 | 1.97 | 0.45 |
| 3:O:3242[B]:GLY:C | 3:O:3243[B]:GLY:O | 2.58 | 0.45 |
| 3:O:3244[A]:THR:H | 3:O:3264[A]:TYR:HE2 | 1.65 | 0.45 |
| 3:O:3301[B]:PRO:HB2 | 3:O:3302[B]:SER:H | 1.33 | 0.45 |
| 1:P:899:MET:HE2 | 1:P:1012:GLU:OE2 | 2.16 | 0.45 |
| 1:P:931:TRP:CZ3 | 1:P:995:ILE:HD11 | 2.51 | 0.45 |
| 2:Q:2888:GLY:HA2 | 2:Q:2889:ALA:HA | 1.70 | 0.45 |
| 3:R:2994[B]:LYS:O | 3:R:2997[B]:GLU:N | 2.49 | 0.45 |
| 3:R:3171[A]:HIS:C | 3:R:3173[A]:THR:N | 2.73 | 0.45 |
| 3:R:3176[B]:LYS:C | 3:R:3177[B]:SER:HG | 2.09 | 0.45 |
| 3:R:3191[B]:ASN:ND2 | 3:R:3191[B]:ASN:N | 2.60 | 0.45 |
| 1:S:731:ALA:HB2 | 1:S:781:ILE:HD12 | 1.99 | 0.45 |
| 3:U:3135[A]:LYS:HB2 | 3:U:3141[A]:TYR:CD1 | 2.51 | 0.45 |
| 3:U:3158[B]:PHE:HB2 | 3:d:3149[B]:ASN:HB2 | 1.97 | 0.45 |
| 3:U:3255[B]:PRO:CD | 3:d:3253[B]:GLU:N | 2.78 | 0.45 |
| 1:V:133:LYS:HD2 | 1:V:134:VAL:HG22 | 1.98 | 0.45 |
| 1:V:428:ILE:HD12 | 1:V:514:TRP:HB3 | 1.97 | 0.45 |
| 1:V:688:VAL:HA | 1:V:689:PRO:HD3 | 1.74 | 0.45 |
| 1:V:896:HIS:HB2 | 1:V:905:TRP:CD1 | 2.52 | 0.45 |
| 2:W:2340:ALA:HB1 | 2:W:2341:PRO:CD | 2.42 | 0.45 |
| 3:X:3047[B]:ARG:NH2 | 3:X:3113[B]:ASP:OD1 | 2.43 | 0.45 |
| 3:X:3135[B]:LYS:HB2 | 3:X:3141[B]:TYR:CD1 | 2.51 | 0.45 |
| 3:X:3171[A]:HIS:C | 3:X:3173[A]:THR:N | 2.73 | 0.45 |
| 1:Y:25:MET:HA | 1:Y:83:HIS:CD2 | 2.51 | 0.45 |
| 1:Y:950:ALA:HA | 1:Y:951:ASN:HA | 1.55 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:2606:LEU:HD13 | 2:Z:2706:ILE:HG13 | 1.96 | 0.45 |
| 3:a:3148[A]:ILE:O | 3:a:3148[A]:ILE:HG22 | 2.17 | 0.45 |
| 3:a:3264[A]:TYR:HD1 | 3:a:3265[A]:ASP:N | 2.14 | 0.45 |
| 1:b:490:TRP:HE1 | 1:b:670:PRO:HD2 | 1.80 | 0.45 |
| 3:d:3074[A]:GLU:OE2 | 3:d:3208[A]:GLN:HG2 | 2.15 | 0.45 |
| 3:d:3196[B]:THR:CB | 3:d:3199[B]:GLN:OE1 | 2.64 | 0.45 |
| 2:B:2610:ASP:OD1 | 2:B:2610:ASP:N | 2.49 | 0.45 |
| 3:C:2970[A]:PRO:C | 3:C:2972[A]:GLY:N | 2.72 | 0.45 |
| 3:C:2973[B]:THR:HG22 | 3:L:3248[B]:LEU:C | 2.39 | 0.45 |
| 3:C:3134[B]:GLN:O | 3:C:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:C:3155[B]:MET:C | 3:L:3153[B]:LYS:HE3 | 2.40 | 0.45 |
| 3:C:3196[B]:THR:CB | 3:C:3199[B]:GLN:OE1 | 2.64 | 0.45 |
| 3:C:3264[A]:TYR:HD1 | 3:C:3265[A]:ASP:N | 2.14 | 0.45 |
| 1:D:17:ASN:HD21 | 1:D:86:THR:N | 2.11 | 0.45 |
| 1:D:176:GLU:O | 1:D:180:ASN:ND2 | 2.49 | 0.45 |
| 1:D:304:ALA:HB1 | 1:D:306:PHE:HE1 | 1.82 | 0.45 |
| 1:D:732:GLY:HA2 | 1:D:777:TYR:O | 2.16 | 0.45 |
| 1:D:1167:ASP:OD1 | 1:D:1167:ASP:N | 2.45 | 0.45 |
| 1:D:1562:ILE:C | 1:D:1564:ALA:H | 2.23 | 0.45 |
| 2:E:2274:LEU:HD23 | 2:E:2274:LEU:HA | 1.77 | 0.45 |
| 2:E:2344:LEU:HA | 2:E:2345:ASN:O | 2.17 | 0.45 |
| 2:E:2672:PHE:CZ | 2:E:2718:TRP:HA | 2.52 | 0.45 |
| 3:F:2969[A]:TYR:CD2 | 3:F:2970[A]:PRO:N | 2.83 | 0.45 |
| 3:F:3079[B]:CYS:SG | 3:F:3146[B]:CYS:O | 2.73 | 0.45 |
| 3:F:3106[A]:THR:O | 3:F:3106[A]:THR:HG23 | 2.16 | 0.45 |
| 3:F:3116[A]:PHE:CD1 | 3:F:3116[A]:PHE:C | 2.94 | 0.45 |
| 3:F:3120[B]:HIS:NE2 | 3:a:2969[B]:TYR:CD2 | 2.65 | 0.45 |
| 3:F:3150[B]:LYS:HZ2 | 3:a:3160[B]:SER:CB | 1.99 | 0.45 |
| 3:F:3196[A]:THR:CB | 3:F:3199[A]:GLN:OE1 | 2.64 | 0.45 |
| 3:F:3242[B]:GLY:C | 3:F:3243[B]:GLY:O | 2.58 | 0.45 |
| 3:F:3263[A]:LEU:N | 3:F:3263[A]:LEU:CD1 | 2.79 | 0.45 |
| 3:F:3284[A]:LYS:HD3 | 3:F:3285[A]:VAL:O | 2.16 | 0.45 |
| 1:G:883:CYS:HB3 | 1:G:884:PRO:CD | 2.47 | 0.45 |
| 1:G:1169:LYS:HE3 | 1:G:1169:LYS:HB2 | 1.70 | 0.45 |
| 1:G:1189:ASP:HB2 | 2:K:2851:ASN:OD1 | 2.16 | 0.45 |
| 2:H:2625:LEU:HD13 | 2:H:2626:ARG:N | 2.30 | 0.45 |
| 3:I:2931[A]:THR:HG1 | 3:I:2934[A]:GLU:CD | 2.04 | 0.45 |
| 3:I:2949[A]:LYS:C | 3:I:2953[A]:GLY:N | 2.73 | 0.45 |
| 3:I:2974[B]:ALA:CA | 3:R:3248[B]:LEU:C | 2.87 | 0.45 |
| 3:I:2991[B]:LEU:HD23 | 3:I:3158[B]:PHE:CE1 | 2.48 | 0.45 |
| 3:I:3025[B]:VAL:CG2 | 3:I:3047[B]:ARG:NH1 | 2.73 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3087[A]:MET:HA | 3:I:3090[A]:ASN:OD1 | 2.17 | 0.45 |
| 3:I:3153[B]:LYS:CD | 3:R:3155[B]:MET:HB3 | 2.33 | 0.45 |
| 3:I:3204[A]:LEU:CD1 | 3:I:3204[A]:LEU:N | 2.80 | 0.45 |
| 3:I:3253[B]:GLU:HB2 | 3:R:2965[B]:LEU:HD22 | 1.42 | 0.45 |
| 3:I:3284[A]:LYS:CE | 3:I:3285[A]:VAL:H | 2.28 | 0.45 |
| 1:J:961:SER:HB2 | 1:J:972:SER:O | 2.16 | 0.45 |
| 1:J:1445:LEU:HD13 | 1:J:1594:GLY:HA2 | 1.99 | 0.45 |
| 2:K:2180:TRP:HB2 | 2:K:2243:LEU:HD13 | 1.98 | 0.45 |
| 2:K:2561:HIS:HA | 2:K:2562:GLY:HA2 | 1.71 | 0.45 |
| 2:K:2783:PHE:HB3 | 2:K:2791:LEU:HD21 | 1.98 | 0.45 |
| 3:L:2994[B]:LYS:O | 3:L:2997[B]:GLU:N | 2.49 | 0.45 |
| 3:L:3074[B]:GLU:CD | 3:L:3212[B]:ARG:NH2 | 2.73 | 0.45 |
| 3:L:3116[B]:PHE:CD1 | 3:L:3116[B]:PHE:C | 2.94 | 0.45 |
| 3:L:3134[A]:GLN:O | 3:L:3136[A]:TYR:N | 2.50 | 0.45 |
| 3:L:3135[B]:LYS:HB2 | 3:L:3141[B]:TYR:CD1 | 2.52 | 0.45 |
| 3:L:3143[A]:SER:OG | 3:L:3144[A]:ALA:N | 2.47 | 0.45 |
| 3:L:3204[A]:LEU:CD1 | 3:L:3204[A]:LEU:N | 2.80 | 0.45 |
| 3:L:3209[B]:GLU:O | 3:L:3310[B]:GLY:C | 2.59 | 0.45 |
| 1:M:573:LYS:NZ | 1:M:780:GLU:O | 2.49 | 0.45 |
| 1:M:931:TRP:CZ3 | 1:M:995:ILE:HD11 | 2.52 | 0.45 |
| 1:M:1279:LYS:O | 1:M:1283:ASP:N | 2.45 | 0.45 |
| 1:M:1280:GLN:HG2 | 1:M:1337:ARG:HH11 | 1.80 | 0.45 |
| 3:O:2994[B]:LYS:O | 3:O:2997[B]:GLU:N | 2.49 | 0.45 |
| 3:O:3087[A]:MET:HA | 3:O:3090[A]:ASN:OD1 | 2.17 | 0.45 |
| 3:O:3146[B]:CYS:HA | 3:O:3147[B]:GLU:HA | 1.70 | 0.45 |
| 3:O:3156[B]:MET:SD | 3:X:3173[B]:THR:CG2 | 3.05 | 0.45 |
| 3:O:3228[B]:VAL:CG2 | 3:O:3245[B]:PHE:CE1 | 2.97 | 0.45 |
| 1:P:944:GLU:O | 1:P:957:ASN:ND2 | 2.48 | 0.45 |
| 1:P:1575:PRO:HA | 1:P:1581:GLU:O | 2.17 | 0.45 |
| 2:Q:2142:ALA:HA | 2:Q:2143:CYS:HA | 1.71 | 0.45 |
| 3:R:2965[B]:LEU:HD13 | 3:R:2975[B]:PHE:O | 2.16 | 0.45 |
| 3:R:2985[B]:PHE:CE2 | 3:R:2989[B]:HIS:CD2 | 3.04 | 0.45 |
| 3:R:3148[B]:ILE:O | 3:R:3148[B]:ILE:HG22 | 2.17 | 0.45 |
| 1:S:353:ASN:HD22 | 1:S:772:ARG:HH22 | 1.64 | 0.45 |
| 1:S:1017:HIS:C | 1:S:1021:LEU:HG | 2.41 | 0.45 |
| 2:T:2225:ARG:HB2 | 2:T:2274:LEU:O | 2.17 | 0.45 |
| 2:T:2822:LYS:HE2 | 2:T:2882:GLU:OE1 | 2.16 | 0.45 |
| 3:U:3086[B]:GLU:OE1 | 3:d:2970[B]:PRO:HG2 | 2.17 | 0.45 |
| 1:V:452:ILE:HD11 | 1:V:676:PRO:O | 2.15 | 0.45 |
| 1:V:938:LEU:HD23 | 1:V:1041:ILE:HD12 | 1.97 | 0.45 |
| 2:W:2181:THR:HB | 2:W:2374:ASN:H | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W:2800:LYS:HB3 | 3:X:3023[A]:ILE:CD1 | 2.46 | 0.45 |
| 3:X:2937[B]:ASN:CB | 3:X:3006[B]:LYS:CE | 2.86 | 0.45 |
| 3:X:2965[A]:LEU:HD13 | 3:X:2975[A]:PHE:O | 2.16 | 0.45 |
| 3:X:3013[B]:ASP:CG | 3:X:3015[B]:THR:HG1 | 2.23 | 0.45 |
| 3:X:3106[B]:THR:O | 3:X:3106[B]:THR:HG23 | 2.17 | 0.45 |
| 3:X:3285[B]:VAL:CG2 | 3:X:3286[B]:THR:H | 2.27 | 0.45 |
| 1:Y:236:GLY:HA2 | 1:Y:819:ILE:HG13 | 1.98 | 0.45 |
| 1:Y:516:TRP:HD1 | 1:Y:579:LEU:HB3 | 1.82 | 0.45 |
| 1:Y:885:SER:HA | 1:Y:888:ALA:H | 1.80 | 0.45 |
| 1:Y:1427:HIS:CD2 | 1:Y:1457:HIS:HE1 | 2.33 | 0.45 |
| 1:Y:1596:GLU:O | 1:Y:1597:THR:HG22 | 2.16 | 0.45 |
| 2:Z:2819:VAL:HG22 | 2:Z:2883:ILE:HG22 | 1.99 | 0.45 |
| 3:a:3134[A]:GLN:O | 3:a:3136[A]:TYR:N | 2.49 | 0.45 |
| 3:a:3196[A]:THR:CB | 3:a:3199[A]:GLN:OE1 | 2.64 | 0.45 |
| 3:a:3200[A]:LEU:HD22 | 3:a:3204[A]:LEU:HD11 | 1.95 | 0.45 |
| 3:a:3200[B]:LEU:CD2 | 3:a:3204[B]:LEU:CD1 | 2.93 | 0.45 |
| 1:b:227:ARG:HA | 1:b:227:ARG:NH1 | 2.30 | 0.45 |
| 1:b:402:THR:HG23 | 1:b:659:CYS:HA | 1.98 | 0.45 |
| 3:d:2949[A]:LYS:NZ | 3:d:2949[A]:LYS:C | 2.73 | 0.45 |
| 3:d:2976[B]:ALA:O | 3:d:2978[B]:CYS:N | 2.46 | 0.45 |
| 3:d:3004[B]:GLY:C | 3:d:3006[B]:LYS:N | 2.74 | 0.45 |
| 3:d:3087[B]:MET:HA | 3:d:3090[B]:ASN:OD1 | 2.17 | 0.45 |
| 3:d:3106[B]:THR:O | 3:d:3106[B]:THR:HG23 | 2.16 | 0.45 |
| 3:d:3148[A]:ILE:O | 3:d:3148[A]:ILE:HG22 | 2.17 | 0.45 |
| 3:d:3209[A]:GLU:O | 3:d:3310[A]:GLY:C | 2.59 | 0.45 |
| 1:A:277:ASP:OD1 | 1:A:277:ASP:N | 2.24 | 0.45 |
| 1:A:364:ASP:O | 1:A:368:SER:OG | 2.31 | 0.45 |
| 1:A:601:VAL:HG11 | 1:A:777:TYR:CG | 2.51 | 0.45 |
| 1:A:943:LEU:HD13 | 1:A:944:GLU:H | 1.82 | 0.45 |
| 1:A:1000:GLU:HG2 | 1:A:1133:ILE:HB | 1.99 | 0.45 |
| 1:A:1403:LEU:O | 1:A:1407:THR:OG1 | 2.35 | 0.45 |
| 1:A:1422:HIS:NE2 | 1:A:1608:ARG:HB2 | 2.32 | 0.45 |
| 2:B:2738:ALA:HB1 | 2:B:2740:ASP:OD1 | 2.17 | 0.45 |
| 3:C:2966[B]:SER:CB | 3:L:2982[B]:MET:CE | 2.93 | 0.45 |
| 3:C:2976[B]:ALA:H | 3:L:3253[B]:GLU:CA | 2.30 | 0.45 |
| 3:C:3014[B]:TRP:CD2 | 3:C:3092[B]:ILE:CD1 | 2.98 | 0.45 |
| 3:C:3074[A]:GLU:OE2 | 3:C:3208[A]:GLN:HG2 | 2.15 | 0.45 |
| 3:C:3074[B]:GLU:OE2 | 3:C:3208[B]:GLN:HG2 | 2.15 | 0.45 |
| 3:C:3147[B]:GLU:CG | 3:L:3161[B]:GLU:N | 2.79 | 0.45 |
| 3:C:3250[B]:GLY:H | 3:L:3252[B]:TYR:HB3 | 1.49 | 0.45 |
| 3:C:3263[A]:LEU:N | 3:C:3263[A]:LEU:CD1 | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1412:GLU:OE2 | 1:D:1552:ARG:NH1 | 2.40 | 0.45 |
| 2:E:2121:THR:O | 2:E:2124:SER:OG | 2.31 | 0.45 |
| 3:F:2965[B]:LEU:HD22 | 3:F:2975[B]:PHE:O | 2.15 | 0.45 |
| 3:F:2994[A]:LYS:O | 3:F:2997[A]:GLU:N | 2.49 | 0.45 |
| 3:F:3013[A]:ASP:CG | 3:F:3015[A]:THR:HG1 | 2.21 | 0.45 |
| 3:F:3134[A]:GLN:O | 3:F:3136[A]:TYR:N | 2.50 | 0.45 |
| 3:F:3137[A]:ARG:O | 3:F:3139[A]:LEU:HD22 | 2.16 | 0.45 |
| 3:F:3146[A]:CYS:HA | 3:F:3147[A]:GLU:HA | 1.70 | 0.45 |
| 3:F:3169[B]:LYS:HG2 | 3:a:3151[B]:LEU:H | 1.80 | 0.45 |
| 3:F:3196[B]:THR:CB | 3:F:3199[B]:GLN:OE1 | 2.64 | 0.45 |
| 3:F:3244[B]:THR:H | 3:F:3264[B]:TYR:HE2 | 1.65 | 0.45 |
| 3:F:3283[A]:ILE:HB | 3:F:3305[A]:ILE:HD11 | 1.97 | 0.45 |
| 1:G:95:THR:O | 1:G:153:ASN:ND2 | 2.50 | 0.45 |
| 1:G:304:ALA:HB3 | 1:G:360:HIS:HB3 | 1.99 | 0.45 |
| 1:G:415:VAL:HG11 | 1:G:697:ALA:N | 2.32 | 0.45 |
| 1:G:902:PHE:CD1 | 1:G:1012:GLU:HB2 | 2.52 | 0.45 |
| 2:H:2572:VAL:HG22 | 2:H:2768:LEU:CD2 | 2.46 | 0.45 |
| 3:I:2951[B]:ASP:CG | 3:I:2952[B]:ALA:N | 2.74 | 0.45 |
| 3:I:2971[B]:ASP:C | 3:R:3090[B]:ASN:HA | 2.36 | 0.45 |
| 3:I:3023[B]:ILE:O | 3:I:3026[B]:THR:OG1 | 2.34 | 0.45 |
| 3:I:3119[B]:HIS:O | 3:I:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 3:I:3156[B]:MET:H | 3:R:2979[B]:GLN:HE21 | 1.63 | 0.45 |
| 3:I:3284[A]:LYS:HD3 | 3:I:3285[A]:VAL:O | 2.16 | 0.45 |
| 3:L:3047[B]:ARG:NH2 | 3:L:3113[B]:ASP:OD1 | 2.43 | 0.45 |
| 3:L:3079[A]:CYS:SG | 3:L:3146[A]:CYS:O | 2.74 | 0.45 |
| 3:L:3203[A]:HIS:O | 3:L:3206[A]:LYS:HB3 | 2.15 | 0.45 |
| 3:L:3242[B]:GLY:C | 3:L:3243[B]:GLY:O | 2.58 | 0.45 |
| 3:L:3244[B]:THR:H | 3:L:3264[B]:TYR:HE2 | 1.65 | 0.45 |
| 1:M:306:PHE:CE2 | 1:M:399:PRO:HG3 | 2.52 | 0.45 |
| 1:M:443:MET:HE1 | 1:M:455:TYR:CE1 | 2.51 | 0.45 |
| 1:M:695:TYR:HB3 | 1:M:696:GLN:HG3 | 1.99 | 0.45 |
| 2:N:2579:GLU:CD | 2:N:2582:ARG:HH12 | 2.24 | 0.45 |
| 2:N:2872:GLU:O | 1:P:1078:ARG:NH1 | 2.43 | 0.45 |
| 3:O:3134[B]:GLN:O | 3:O:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:O:3204[A]:LEU:CD1 | 3:O:3204[A]:LEU:N | 2.80 | 0.45 |
| 3:O:3264[A]:TYR:HD1 | 3:O:3265[A]:ASP:N | 2.14 | 0.45 |
| 3:O:3281[B]:PHE:HE1 | 3:O:3305[B]:ILE:HG21 | 1.81 | 0.45 |
| 1:P:398:ARG:HH21 | 1:P:663:GLU:CD | 2.23 | 0.45 |
| 1:P:730:PHE:CD1 | 1:P:780:GLU:HA | 2.52 | 0.45 |
| 1:P:1427:HIS:HD2 | 1:P:1457:HIS:HE1 | 1.63 | 0.45 |
| 2:Q:2402:GLY:HA3 | 2:Q:2403:PHE:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q:2732:HIS:CD2 | 2:Q:2732:HIS:H | 2.35 | 0.45 |
| 3:R:2970[B]:PRO:C | 3:R:2972[B]:GLY:N | 2.72 | 0.45 |
| 3:R:3004[A]:GLY:C | 3:R:3006[A]:LYS:N | 2.74 | 0.45 |
| 3:R:3116[A]:PHE:C | 3:R:3116[A]:PHE:CD1 | 2.94 | 0.45 |
| 3:R:3134[B]:GLN:O | 3:R:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:R:3137[B]:ARG:O | 3:R:3139[B]:LEU:HD22 | 2.16 | 0.45 |
| 3:R:3204[B]:LEU:CD1 | 3:R:3204[B]:LEU:N | 2.80 | 0.45 |
| 3:R:3264[A]:TYR:HD1 | 3:R:3265[A]:ASP:N | 2.14 | 0.45 |
| 1:S:622:HIS:HE1 | 1:S:767:LYS:H | 1.64 | 0.45 |
| 1:S:1012:GLU:O | 1:S:1015:HIS:N | 2.50 | 0.45 |
| 2:T:2236:ALA:HB3 | 2:T:2239:LYS:HB3 | 1.98 | 0.45 |
| 2:T:2706:ILE:O | 2:T:2710:HIS:N | 2.44 | 0.45 |
| 3:U:2949[A]:LYS:C | 3:U:2953[A]:GLY:N | 2.73 | 0.45 |
| 3:U:2965[A]:LEU:HD13 | 3:U:2975[A]:PHE:O | 2.16 | 0.45 |
| 3:U:2994[B]:LYS:O | 3:U:2997[B]:GLU:N | 2.49 | 0.45 |
| 3:U:3132[B]:ALA:HB3 | 3:U:3197[B]:ILE:HD13 | 1.98 | 0.45 |
| 3:U:3244[A]:THR:H | 3:U:3264[A]:TYR:HE2 | 1.65 | 0.45 |
| 1:V:424:PHE:CZ | 1:V:1125:SER:HB2 | 2.52 | 0.45 |
| 1:V:830:ASN:HB3 | 1:V:831:VAL:HA | 1.98 | 0.45 |
| 1:V:1372:ILE:HD12 | 1:Y:1438:ASP:HB2 | 1.99 | 0.45 |
| 3:X:3087[B]:MET:HA | 3:X:3090[B]:ASN:OD1 | 2.17 | 0.45 |
| 3:X:3204[A]:LEU:CD1 | 3:X:3204[A]:LEU:N | 2.80 | 0.45 |
| 3:X:3264[A]:TYR:HD1 | 3:X:3265[A]:ASP:N | 2.14 | 0.45 |
| 1:Y:86:THR:HB | 1:Y:87:LEU:HD12 | 1.98 | 0.45 |
| 1:Y:483:GLY:HA3 | 1:Y:771:TRP:CE3 | 2.52 | 0.45 |
| 1:Y:515:ASP:OD1 | 1:Y:517:THR:OG1 | 2.25 | 0.45 |
| 1:Y:931:TRP:CG | 1:Y:1018:ILE:HD11 | 2.51 | 0.45 |
| 1:Y:1019:HIS:NE2 | 1:Y:1046:HIS:HE1 | 2.12 | 0.45 |
| 1:Y:1612:THR:C | 3:d:3186[B]:GLU:HB2 | 2.40 | 0.45 |
| 3:a:2937[B]:ASN:CB | 3:a:3006[B]:LYS:CE | 2.86 | 0.45 |
| 3:a:2961[B]:HIS:CD2 | 3:a:2988[B]:TRP:CZ3 | 2.96 | 0.45 |
| 3:a:3116[B]:PHE:CD1 | 3:a:3116[B]:PHE:C | 2.94 | 0.45 |
| 3:a:3137[B]:ARG:O | 3:a:3139[B]:LEU:HD22 | 2.16 | 0.45 |
| 3:a:3285[B]:VAL:CG2 | 3:a:3286[B]:THR:H | 2.27 | 0.45 |
| 3:a:3293[B]:LYS:HB2 | 3:a:3294[B]:SER:CA | 2.41 | 0.45 |
| 1:b:520:PHE:CD1 | 1:b:520:PHE:N | 2.84 | 0.45 |
| 2:c:2477:PRO:O | 2:c:2480:LEU:HD22 | 2.16 | 0.45 |
| 3:d:3196[B]:THR:O | 3:d:3200[B]:LEU:N | 2.43 | 0.45 |
| 3:d:3200[A]:LEU:CD2 | 3:d:3204[A]:LEU:CD1 | 2.93 | 0.45 |
| 3:d:3283[A]:ILE:HB | 3:d:3305[A]:ILE:HD11 | 1.97 | 0.45 |
| 3:d:3298[A]:ASN:CA | 3:d:3299[A]:LEU:HB2 | 2.44 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2572:VAL:HG22 | 2:B:2768:LEU:CD2 | 2.46 | 0.45 |
| 2:B:2702:SER:HA | 2:B:2707:PHE:CD2 | 2.52 | 0.45 |
| 3:C:2949[B]:LYS:NZ | 3:C:2949[B]:LYS:C | 2.73 | 0.45 |
| 3:C:2952[B]:ALA:N | 3:C:2953[B]:GLY:CA | 2.71 | 0.45 |
| 3:C:2964[B]:PRO:CA | 3:L:3255[B]:PRO:HB3 | 2.47 | 0.45 |
| 3:C:2985[A]:PHE:CE2 | 3:C:2989[A]:HIS:CD2 | 3.04 | 0.45 |
| 3:C:3037[A]:TYR:C | 3:C:3038[A]:ILE:HG13 | 2.42 | 0.45 |
| 3:C:3137[A]:ARG:HB3 | 3:C:3139[A]:LEU:HD21 | 1.97 | 0.45 |
| 3:C:3173[A]:THR:HG22 | 3:C:3174[A]:GLY:H | 1.67 | 0.45 |
| 1:D:465:PRO:HD2 | 1:D:467:LYS:HZ3 | 1.81 | 0.45 |
| 1:D:587:PHE:HE2 | 1:D:643:ILE:HB | 1.81 | 0.45 |
| 1:D:760:ILE:HG21 | 1:D:777:TYR:HE2 | 1.82 | 0.45 |
| 1:D:834:ASP:OD1 | 1:D:834:ASP:N | 2.48 | 0.45 |
| 1:D:1470:GLU:OE2 | 1:D:1473:ARG:NH1 | 2.50 | 0.45 |
| 1:D:1562:ILE:HG13 | 1:D:1564:ALA:O | 2.15 | 0.45 |
| 3:F:2938[A]:LEU:O | 3:F:2939[A]:ARG:C | 2.58 | 0.45 |
| 3:F:2956[B]:LYS:O | 3:F:2959[B]:SER:OG | 2.33 | 0.45 |
| 3:F:2957[B]:ILE:HA | 3:F:2960[B]:PHE:HE1 | 1.64 | 0.45 |
| 3:F:2961[B]:HIS:HB2 | 3:F:2992[B]:TYR:HE2 | 1.81 | 0.45 |
| 3:F:2983[B]:VAL:HG23 | 3:a:3160[B]:SER:HG | 1.76 | 0.45 |
| 3:F:3134[B]:GLN:O | 3:F:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:F:3148[B]:ILE:O | 3:F:3148[B]:ILE:HG22 | 2.17 | 0.45 |
| 3:F:3173[B]:THR:HA | 3:a:3154[B]:PRO:CA | 2.46 | 0.45 |
| 3:F:3281[B]:PHE:HE1 | 3:F:3305[B]:ILE:HG21 | 1.81 | 0.45 |
| 1:G:728:ARG:HE | 1:G:730:PHE:HZ | 1.65 | 0.45 |
| 1:G:1142:VAL:HG12 | 1:G:1143:ALA:N | 2.32 | 0.45 |
| 2:H:2657:PHE:CD1 | 2:H:2783:PHE:HE2 | 2.35 | 0.45 |
| 3:I:3135[B]:LYS:HB2 | 3:I:3141[B]:TYR:CD1 | 2.51 | 0.45 |
| 2:K:2286:HIS:CD2 | 2:K:2433:THR:HG22 | 2.52 | 0.45 |
| 3:L:2939[A]:ARG:HG3 | 3:L:2939[A]:ARG:NH1 | 2.28 | 0.45 |
| 3:L:3037[A]:TYR:C | 3:L:3038[A]:ILE:HG13 | 2.42 | 0.45 |
| 3:L:3119[A]:HIS:O | 3:L:3122[A]:ASN:HB3 | 2.17 | 0.45 |
| 3:L:3263[A]:LEU:N | 3:L:3263[A]:LEU:CD1 | 2.79 | 0.45 |
| 3:L:3281[B]:PHE:HE1 | 3:L:3305[B]:ILE:HG21 | 1.81 | 0.45 |
| 1:M:140:ASP:OD1 | 1:M:141:ALA:N | 2.50 | 0.45 |
| 1:M:516:TRP:HH2 | 1:M:637:VAL:HG23 | 1.80 | 0.45 |
| 2:N:2132:CYS:H | 2:N:2142:ALA:HB2 | 1.80 | 0.45 |
| 3:O:2937[B]:ASN:CB | 3:O:3006[B]:LYS:CE | 2.86 | 0.45 |
| 3:O:3037[A]:TYR:C | 3:O:3038[A]:ILE:HG13 | 2.42 | 0.45 |
| 3:R:2969[A]:TYR:CD2 | 3:R:2970[A]:PRO:N | 2.83 | 0.45 |
| 3:R:3004[B]:GLY:C | 3:R:3006[B]:LYS:N | 2.74 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3087[B]:MET:HA | 3:R:3090[B]:ASN:OD1 | 2.17 | 0.45 |
| 3:R:3096[A]:VAL:HG11 | 3:R:3115[A]:LEU:HD12 | 1.89 | 0.45 |
| 3:R:3284[B]:LYS:CE | 3:R:3285[B]:VAL:H | 2.29 | 0.45 |
| 1:S:398:ARG:NH2 | 1:S:663:GLU:OE1 | 2.49 | 0.45 |
| 1:S:614:GLU:HA | 1:S:615:PRO:HD3 | 1.87 | 0.45 |
| 1:S:903:PRO:HG2 | 1:S:904:HIS:CD2 | 2.52 | 0.45 |
| 1:S:1415:ASP:OD1 | 1:S:1416:PHE:N | 2.48 | 0.45 |
| 2:T:2628:HIS:HB2 | 2:T:2635:TYR:CE2 | 2.52 | 0.45 |
| 3:U:2965[B]:LEU:HD13 | 3:U:2975[B]:PHE:O | 2.16 | 0.45 |
| 3:U:3119[B]:HIS:O | 3:U:3122[B]:ASN:HB3 | 2.16 | 0.45 |
| 3:U:3137[A]:ARG:O | 3:U:3139[A]:LEU:HD22 | 2.16 | 0.45 |
| 3:U:3283[A]:ILE:HB | 3:U:3305[A]:ILE:HD11 | 1.97 | 0.45 |
| 1:V:59:LEU:HD13 | 1:V:68:TRP:CD1 | 2.51 | 0.45 |
| 1:V:1243:PHE:CD2 | 1:V:1249:TRP:HD1 | 2.34 | 0.45 |
| 1:V:1599:MET:HG3 | 1:V:1600:PRO:HD2 | 1.97 | 0.45 |
| 2:W:2866:PRO:HB2 | 2:W:2868:GLU:HG3 | 1.98 | 0.45 |
| 1:Y:949:ASP:OD1 | 1:Y:950:ALA:N | 2.49 | 0.45 |
| 1:Y:1077:LEU:HD23 | 1:Y:1103:PHE:HE1 | 1.82 | 0.45 |
| 2:Z:2568:HIS:CD2 | 2:Z:2718:TRP:CH2 | 3.05 | 0.45 |
| 2:Z:2568:HIS:HD2 | 2:Z:2718:TRP:CH2 | 2.35 | 0.45 |
| 2:Z:2568:HIS:HE1 | 2:Z:2742:MET:SD | 2.40 | 0.45 |
| 3:a:2965[A]:LEU:HD13 | 3:a:2975[A]:PHE:O | 2.16 | 0.45 |
| 3:a:3004[B]:GLY:C | 3:a:3006[B]:LYS:N | 2.74 | 0.45 |
| 1:b:664:VAL:HG12 | 1:b:690:THR:HG22 | 1.97 | 0.45 |
| 1:b:1642:GLN:N | 1:b:1642:GLN:OE1 | 2.50 | 0.45 |
| 3:d:3087[A]:MET:HA | 3:d:3090[A]:ASN:OD1 | 2.17 | 0.45 |
| 3:d:3264[B]:TYR:HD1 | 3:d:3265[B]:ASP:N | 2.14 | 0.45 |
| 3:d:3281[B]:PHE:HE1 | 3:d:3305[B]:ILE:HG21 | 1.81 | 0.45 |
| 3:d:3284[A]:LYS:CE | 3:d:3285[A]:VAL:H | 2.29 | 0.45 |
| 1:A:567:LEU:CB | 1:A:571:PRO:HG2 | 2.43 | 0.45 |
| 2:B:2114:ARG:HG3 | 2:E:2526:ARG:HH21 | 1.81 | 0.45 |
| 2:B:2382:GLU:O | 2:B:2386:ARG:HG3 | 2.17 | 0.45 |
| 2:B:2805:PHE:CE1 | 2:B:2855:ASP:HB3 | 2.51 | 0.45 |
| 3:C:3004[B]:GLY:O | 3:C:3006[B]:LYS:N | 2.44 | 0.45 |
| 3:C:3014[B]:TRP:CG | 3:C:3092[B]:ILE:CD1 | 2.98 | 0.45 |
| 3:C:3148[A]:ILE:O | 3:C:3148[A]:ILE:HG22 | 2.17 | 0.45 |
| 3:C:3155[B]:MET:SD | 3:L:3154[B]:PRO:N | 2.88 | 0.45 |
| 3:C:3156[B]:MET:CB | 3:L:2982[B]:MET:HB2 | 2.22 | 0.45 |
| 3:C:3163[B]:ASN:HD21 | 3:L:3149[B]:ASN:HB2 | 1.45 | 0.45 |
| 3:C:3191[A]:ASN:C | 3:C:3192[A]:PHE:O | 2.52 | 0.45 |
| 3:C:3222[B]:ILE:CD1 | 3:C:3223[B]:GLY:N | 2.73 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3223[B]:GLY:N | 3:L:2963[B]:MET:HE1 | 2.10 | 0.45 |
| 3:C:3253[B]:GLU:CB | 3:L:2976[B]:ALA:H | 1.90 | 0.45 |
| 3:C:3306[A]:LEU:C | 3:C:3306[A]:LEU:CD1 | 2.86 | 0.45 |
| 3:F:3119[A]:HIS:O | 3:F:3122[A]:ASN:HB3 | 2.17 | 0.45 |
| 3:F:3150[B]:LYS:CE | 3:a:3163[B]:ASN:HB3 | 2.42 | 0.45 |
| 3:F:3203[A]:HIS:O | 3:F:3206[A]:LYS:HB3 | 2.16 | 0.45 |
| 3:F:3244[A]:THR:H | 3:F:3264[A]:TYR:HE2 | 1.65 | 0.45 |
| 3:F:3255[B]:PRO:CB | 3:a:2964[B]:PRO:CD | 2.94 | 0.45 |
| 3:I:2952[B]:ALA:N | 3:I:2953[B]:GLY:HA2 | 2.06 | 0.45 |
| 3:I:2962[B]:GLY:N | 3:R:3255[B]:PRO:HD3 | 2.32 | 0.45 |
| 3:I:2971[B]:ASP:C | 3:R:3248[B]:LEU:HD22 | 2.42 | 0.45 |
| 3:I:2979[A]:GLN:HB2 | 3:I:2988[A]:TRP:CD1 | 2.52 | 0.45 |
| 3:I:3087[B]:MET:HA | 3:I:3090[B]:ASN:OD1 | 2.17 | 0.45 |
| 3:I:3119[A]:HIS:O | 3:I:3122[A]:ASN:HB3 | 2.17 | 0.45 |
| 3:I:3134[A]:GLN:O | 3:I:3136[A]:TYR:N | 2.49 | 0.45 |
| 1:J:92:TRP:CZ3 | 1:J:102:PRO:HD3 | 2.51 | 0.45 |
| 3:L:2949[B]:LYS:NZ | 3:L:2949[B]:LYS:C | 2.73 | 0.45 |
| 3:L:2971[A]:ASP:CG | 3:L:2973[A]:THR:HG1 | 2.13 | 0.45 |
| 3:L:3134[B]:GLN:O | 3:L:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:L:3137[A]:ARG:O | 3:L:3139[A]:LEU:HD22 | 2.16 | 0.45 |
| 3:L:3283[B]:ILE:HB | 3:L:3305[B]:ILE:HD11 | 1.97 | 0.45 |
| 1:M:991:LEU:O | 1:M:995:ILE:HG13 | 2.17 | 0.45 |
| 1:M:1166:THR:N | 1:M:1167:ASP:HA | 2.32 | 0.45 |
| 1:M:1321:HIS:HE1 | 1:M:1489:MET:HE1 | 1.82 | 0.45 |
| 2:N:2128:LEU:HD22 | 2:N:2287:TYR:CE1 | 2.51 | 0.45 |
| 3:O:2951[A]:ASP:C | 3:O:2956[A]:LYS:HZ1 | 2.12 | 0.45 |
| 3:O:2969[B]:TYR:CD2 | 3:O:2970[B]:PRO:N | 2.83 | 0.45 |
| 3:O:3119[B]:HIS:O | 3:O:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 1:P:398:ARG:NH2 | 1:P:663:GLU:OE1 | 2.42 | 0.45 |
| 1:P:1075:GLU:H | 1:P:1075:GLU:HG3 | 1.35 | 0.45 |
| 1:P:1082:SER:HB3 | 1:P:1083:PRO:HD3 | 1.98 | 0.45 |
| 1:P:1400:ASN:HD22 | 1:P:1433:TRP:HZ3 | 1.64 | 0.45 |
| 1:P:1423:TYR:OH | 1:P:1461:VAL:O | 2.28 | 0.45 |
| 3:R:2948[B]:ASP:CB | 3:R:2949[B]:LYS:HA | 2.16 | 0.45 |
| 3:R:3209[A]:GLU:O | 3:R:3310[A]:GLY:C | 2.59 | 0.45 |
| 1:S:284:MET:HE1 | 1:S:292:LEU:HD22 | 1.99 | 0.45 |
| 1:S:730:PHE:O | 1:S:820:VAL:HA | 2.17 | 0.45 |
| 1:S:877:HIS:ND1 | 1:S:1036:SER:OG | 2.49 | 0.45 |
| 1:S:1029:SER:OG | 1:S:1030:MET:N | 2.49 | 0.45 |
| 1:S:1153:LYS:H | 1:S:1153:LYS:HG2 | 1.50 | 0.45 |
| 2:T:2217:ILE:HG22 | 2:T:2218:SER:H | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:2823:ILE:O | 2:T:2823:ILE:HG13 | 2.16 | 0.45 |
| 3:U:2965[A]:LEU:HD22 | 3:U:2975[A]:PHE:O | 2.15 | 0.45 |
| 3:U:2969[B]:TYR:CB | 3:d:3256[B]:TRP:NE1 | 2.80 | 0.45 |
| 3:U:2979[A]:GLN:HB2 | 3:U:2988[A]:TRP:CD1 | 2.52 | 0.45 |
| 3:U:3024[B]:LEU:CD1 | 3:U:3024[B]:LEU:C | 2.85 | 0.45 |
| 3:U:3171[B]:HIS:C | 3:d:3152[B]:LYS:NZ | 2.74 | 0.45 |
| 3:U:3180[B]:TYR:CB | 3:U:3183[B]:LEU:CD2 | 2.90 | 0.45 |
| 3:U:3196[B]:THR:CB | 3:U:3199[B]:GLN:OE1 | 2.64 | 0.45 |
| 3:U:3200[A]:LEU:CD2 | 3:U:3204[A]:LEU:CD1 | 2.93 | 0.45 |
| 3:U:3230[B]:PHE:H | 3:U:3243[B]:GLY:HA3 | 1.79 | 0.45 |
| 3:U:3244[B]:THR:H | 3:U:3264[B]:TYR:HE2 | 1.65 | 0.45 |
| 3:U:3273[B]:LEU:C | 3:U:3275[B]:LEU:HD12 | 2.42 | 0.45 |
| 1:V:308:LEU:HG | 1:V:343:ILE:HD11 | 1.98 | 0.45 |
| 2:W:2412:GLN:HG2 | 2:W:2422:GLU:HA | 1.99 | 0.45 |
| 3:X:2979[A]:GLN:HB2 | 3:X:2988[A]:TRP:CD1 | 2.52 | 0.45 |
| 3:X:2986[A]:PRO:CB | 3:X:3127[A]:TRP:CE3 | 3.00 | 0.45 |
| 3:X:3244[A]:THR:H | 3:X:3264[A]:TYR:HE2 | 1.65 | 0.45 |
| 1:Y:277:ASP:OD1 | 1:Y:278:ASP:N | 2.50 | 0.45 |
| 1:Y:991:LEU:HD12 | 1:Y:991:LEU:HA | 1.69 | 0.45 |
| 1:Y:1473:ARG:HG3 | 1:Y:1479:TYR:CG | 2.51 | 0.45 |
| 1:Y:1604:ASP:OD1 | 1:Y:1605:ARG:NH1 | 2.50 | 0.45 |
| 1:Y:1650:ILE:HG13 | 2:c:2327:GLU:HG2 | 1.99 | 0.45 |
| 2:Z:2156:ARG:HH22 | 2:Z:2309:GLN:HE22 | 1.65 | 0.45 |
| 2:Z:2472:ASN:N | 2:Z:2473:GLY:HA2 | 2.31 | 0.45 |
| 3:a:2956[A]:LYS:O | 3:a:2959[A]:SER:OG | 2.33 | 0.45 |
| 3:a:3037[A]:TYR:C | 3:a:3038[A]:ILE:HG13 | 2.42 | 0.45 |
| 3:a:3037[B]:TYR:C | 3:a:3038[B]:ILE:HG13 | 2.42 | 0.45 |
| 3:a:3106[A]:THR:O | 3:a:3106[A]:THR:HG23 | 2.16 | 0.45 |
| 3:a:3183[A]:LEU:H | 3:a:3184[A]:ASN:CA | 2.22 | 0.45 |
| 3:a:3200[B]:LEU:HD22 | 3:a:3204[B]:LEU:HD11 | 1.95 | 0.45 |
| 3:a:3204[B]:LEU:CD1 | 3:a:3204[B]:LEU:N | 2.80 | 0.45 |
| 3:a:3225[B]:SER:C | 3:a:3290[B]:ILE:HG23 | 2.39 | 0.45 |
| 3:a:3263[A]:LEU:N | 3:a:3263[A]:LEU:CD1 | 2.79 | 0.45 |
| 1:b:452:ILE:HD11 | 1:b:676:PRO:O | 2.16 | 0.45 |
| 1:b:1001:GLN:CD | 1:b:1001:GLN:H | 2.24 | 0.45 |
| 1:b:1528:ASP:N | 1:b:1528:ASP:OD1 | 2.49 | 0.45 |
| 3:d:3004[A]:GLY:C | 3:d:3006[A]:LYS:N | 2.74 | 0.45 |
| 3:d:3014[B]:TRP:CG | 3:d:3092[B]:ILE:CD1 | 2.98 | 0.45 |
| 3:d:3024[A]:LEU:CD1 | 3:d:3024[A]:LEU:C | 2.85 | 0.45 |
| 3:d:3025[A]:VAL:CG2 | 3:d:3047[A]:ARG:NH1 | 2.73 | 0.45 |
| 3:d:3037[B]:TYR:C | 3:d:3038[B]:ILE:HG13 | 2.42 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3101[B]:PRO:O | 3:d:3109[B]:TYR:HD2 | 2.00 | 0.45 |
| 3:d:3116[B]:PHE:CD1 | 3:d:3116[B]:PHE:C | 2.94 | 0.45 |
| 3:d:3132[A]:ALA:HB3 | 3:d:3197[A]:ILE:HD13 | 1.98 | 0.45 |
| 3:d:3244[A]:THR:H | 3:d:3264[A]:TYR:HE2 | 1.65 | 0.45 |
| 4:q:1:NAG:H4 | 4:q:2:NAG:N2 | 2.31 | 0.45 |
| 1:A:19:GLN:HG2 | 1:A:110:PHE:CD2 | 2.52 | 0.45 |
| 1:A:470:ARG:O | 1:A:472:ASP:N | 2.45 | 0.45 |
| 1:A:729:VAL:HG22 | 1:A:781:ILE:O | 2.17 | 0.45 |
| 1:A:958:PRO:O | 1:A:959:PHE:HB2 | 2.15 | 0.45 |
| 2:B:2638:ARG:NH2 | 2:B:2706:ILE:HG13 | 2.32 | 0.45 |
| 3:C:3101[A]:PRO:O | 3:C:3109[A]:TYR:HD2 | 2.00 | 0.45 |
| 3:C:3152[B]:LYS:N | 3:L:3172[B]:SER:HB2 | 2.32 | 0.45 |
| 3:C:3204[A]:LEU:CD1 | 3:C:3204[A]:LEU:N | 2.79 | 0.45 |
| 3:C:3209[B]:GLU:O | 3:C:3310[B]:GLY:C | 2.59 | 0.45 |
| 1:D:464:LEU:HD13 | 1:D:622:HIS:CD2 | 2.51 | 0.45 |
| 1:D:905:TRP:CD1 | 1:D:1084:PHE:HE2 | 2.35 | 0.45 |
| 3:F:2937[B]:ASN:CB | 3:F:3006[B]:LYS:CE | 2.85 | 0.45 |
| 3:F:2986[A]:PRO:CB | 3:F:3127[A]:TRP:CE3 | 3.00 | 0.45 |
| 3:F:3023[B]:ILE:HA | 3:F:3026[B]:THR:HG1 | 1.82 | 0.45 |
| 3:F:3087[B]:MET:HA | 3:F:3090[B]:ASN:OD1 | 2.17 | 0.45 |
| 3:F:3104[A]:MET:HA | 3:F:3110[A]:THR:CG2 | 2.17 | 0.45 |
| 3:F:3132[A]:ALA:HB3 | 3:F:3197[A]:ILE:HD13 | 1.98 | 0.45 |
| 3:F:3156[B]:MET:HG2 | 3:a:2979[B]:GLN:NE2 | 2.24 | 0.45 |
| 1:G:7:VAL:HG23 | 1:G:91:TYR:O | 2.16 | 0.45 |
| 1:G:1604:ASP:OD1 | 1:G:1605:ARG:NH1 | 2.49 | 0.45 |
| 3:I:2951[A]:ASP:CG | 3:I:2952[A]:ALA:N | 2.74 | 0.45 |
| 3:I:2965[B]:LEU:CD1 | 3:I:2974[B]:ALA:CA | 2.89 | 0.45 |
| 3:I:2976[A]:ALA:O | 3:I:2978[A]:CYS:N | 2.46 | 0.45 |
| 3:I:3037[A]:TYR:C | 3:I:3038[A]:ILE:HG13 | 2.42 | 0.45 |
| 3:I:3150[B]:LYS:HG3 | 3:R:3163[B]:ASN:CB | 2.46 | 0.45 |
| 3:I:3163[B]:ASN:HB3 | 3:R:3149[B]:ASN:ND2 | 2.30 | 0.45 |
| 3:I:3255[B]:PRO:CB | 3:R:2959[B]:SER:C | 2.69 | 0.45 |
| 1:J:93:ASP:HA | 1:J:212:ASN:ND2 | 2.31 | 0.45 |
| 1:J:977:GLU:HG2 | 1:J:1021:LEU:O | 2.17 | 0.45 |
| 1:J:1143:ALA:HA | 1:J:1195:ASP:HA | 1.99 | 0.45 |
| 2:K:2147:GLY:HA3 | 2:K:2437:TRP:CE3 | 2.51 | 0.45 |
| 2:K:2360:TYR:HB2 | 2:K:2366:TYR:CE1 | 2.52 | 0.45 |
| 3:L:2965[A]:LEU:HD13 | 3:L:2975[A]:PHE:O | 2.16 | 0.45 |
| 3:L:2979[A]:GLN:HB2 | 3:L:2988[A]:TRP:CD1 | 2.52 | 0.45 |
| 3:L:3034[B]:HIS:HB3 | 3:L:3035[B]:HIS:CE1 | 2.50 | 0.45 |
| 3:L:3185[B]:TYR:CE2 | 3:L:3187[B]:TYR:HE2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:63:PRO:HA | 1:M:172:GLU:HG3 | 1.97 | 0.45 |
| 1:M:904:HIS:O | 1:M:907:ARG:HB3 | 2.17 | 0.45 |
| 1:M:1260:ARG:HD3 | 1:M:1331:GLU:OE1 | 2.16 | 0.45 |
| 1:M:1571:TYR:HE2 | 1:M:1631:GLU:HB3 | 1.81 | 0.45 |
| 2:N:2128:LEU:HB3 | 2:N:2129:PRO:HD3 | 1.98 | 0.45 |
| 2:N:2569:TRP:O | 2:N:2572:VAL:HG23 | 2.16 | 0.45 |
| 3:O:3191[A]:ASN:ND2 | 3:O:3191[A]:ASN:N | 2.60 | 0.45 |
| 2:Q:2606:LEU:HD13 | 2:Q:2706:ILE:HG13 | 1.98 | 0.45 |
| 3:R:2989[A]:HIS:C | 3:R:2991[A]:LEU:N | 2.75 | 0.45 |
| 3:R:3037[A]:TYR:C | 3:R:3038[A]:ILE:HG13 | 2.42 | 0.45 |
| 3:R:3119[B]:HIS:O | 3:R:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 1:S:593:CYS:O | 1:S:597:VAL:HG22 | 2.17 | 0.45 |
| 1:S:601:VAL:HG11 | 1:S:777:TYR:CD1 | 2.52 | 0.45 |
| 1:S:601:VAL:HG11 | 1:S:777:TYR:CG | 2.51 | 0.45 |
| 1:S:897:HIS:C | 1:S:899:MET:HA | 2.42 | 0.45 |
| 1:S:1271:MET:HG2 | 1:S:1358:LEU:HD13 | 1.99 | 0.45 |
| 1:S:1307:MET:HE3 | 1:S:1307:MET:HB2 | 1.81 | 0.45 |
| 1:S:1325:LEU:HG | 1:S:1516:VAL:HG11 | 1.99 | 0.45 |
| 2:T:2186:GLU:HA | 2:T:2232:PHE:HE1 | 1.82 | 0.45 |
| 2:T:2561:HIS:HB3 | 2:T:2677:GLU:OE2 | 2.17 | 0.45 |
| 3:U:2946[A]:GLN:CD | 3:U:2947[A]:ALA:N | 2.72 | 0.45 |
| 3:U:2989[B]:HIS:C | 3:U:2991[B]:LEU:N | 2.75 | 0.45 |
| 3:U:3204[A]:LEU:CD1 | 3:U:3204[A]:LEU:N | 2.80 | 0.45 |
| 1:V:495:VAL:HG12 | 1:V:511:VAL:HG11 | 1.99 | 0.45 |
| 1:V:1562:ILE:HD11 | 1:V:1645:PHE:CZ | 2.52 | 0.45 |
| 2:W:2128:LEU:HD13 | 2:W:2286:HIS:CG | 2.52 | 0.45 |
| 3:X:2985[A]:PHE:CE2 | 3:X:2989[A]:HIS:CD2 | 3.04 | 0.45 |
| 3:X:2985[B]:PHE:CE2 | 3:X:2989[B]:HIS:CD2 | 3.04 | 0.45 |
| 3:X:3200[B]:LEU:CD2 | 3:X:3204[B]:LEU:CD1 | 2.93 | 0.45 |
| 1:Y:53:SER:O | 1:Y:55:ILE:HG13 | 2.17 | 0.45 |
| 1:Y:469:PRO:O | 1:Y:673:PHE:HZ | 2.00 | 0.45 |
| 1:Y:1423:TYR:OH | 1:Y:1461:VAL:HG12 | 2.16 | 0.45 |
| 1:Y:1619:GLY:H | 3:d:3190[B]:LEU:HG | 1.82 | 0.45 |
| 2:Z:2889:ALA:HB3 | 2:Z:2890:VAL:C | 2.41 | 0.45 |
| 3:a:3014[A]:TRP:CG | 3:a:3092[A]:ILE:CD1 | 2.98 | 0.45 |
| 3:a:3087[A]:MET:HA | 3:a:3090[A]:ASN:OD1 | 2.17 | 0.45 |
| 3:a:3087[B]:MET:HA | 3:a:3090[B]:ASN:OD1 | 2.17 | 0.45 |
| 3:a:3171[A]:HIS:C | 3:a:3173[A]:THR:N | 2.73 | 0.45 |
| 3:a:3204[A]:LEU:CD1 | 3:a:3204[A]:LEU:N | 2.80 | 0.45 |
| 3:a:3225[A]:SER:C | 3:a:3290[A]:ILE:HG23 | 2.39 | 0.45 |
| 3:a:3244[B]:THR:H | 3:a:3264[B]:TYR:HE2 | 1.65 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:c:2561:HIS:HB3 | 2:c:2677:GLU:OE2 | 2.16 | 0.45 |
| 3:d:2932[A]:PRO:CA | 3:d:2935[A]:ILE:CD1 | 2.85 | 0.45 |
| 3:d:2938[A]:LEU:O | 3:d:2939[A]:ARG:C | 2.58 | 0.45 |
| 3:d:2981[A]:GLY:N | 3:d:3086[A]:GLU:OE1 | 2.45 | 0.45 |
| 3:d:2985[A]:PHE:CE2 | 3:d:2989[A]:HIS:CD2 | 3.04 | 0.45 |
| 3:d:3134[B]:GLN:O | 3:d:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:d:3135[A]:LYS:HB2 | 3:d:3141[A]:TYR:CD1 | 2.51 | 0.45 |
| 3:d:3137[B]:ARG:O | 3:d:3139[B]:LEU:HD22 | 2.16 | 0.45 |
| 3:d:3203[A]:HIS:O | 3:d:3206[A]:LYS:HB3 | 2.16 | 0.45 |
| 3:d:3209[B]:GLU:O | 3:d:3310[B]:GLY:C | 2.59 | 0.45 |
| 3:d:3229[A]:ASN:O | 3:d:3286[A]:THR:N | 2.50 | 0.45 |
| 4:j:1:NAG:C6 | 4:j:2:NAG:HN2 | 2.01 | 0.45 |
| 6:r:1:NAG:C4 | 6:r:2:NAG:O7 | 2.62 | 0.45 |
| 1:A:163:LEU:HD21 | 1:A:219:LEU:HD13 | 1.97 | 0.45 |
| 1:A:407:GLN:OE1 | 1:A:407:GLN:N | 2.39 | 0.45 |
| 1:A:647:LEU:O | 1:A:651:ARG:HB2 | 2.17 | 0.45 |
| 2:B:2715:ASP:HB3 | 2:B:2778:TYR:OH | 2.16 | 0.45 |
| 3:C:3019[A]:HIS:CD2 | 3:C:3020[A]:SER:H | 2.35 | 0.45 |
| 3:C:3034[A]:HIS:HB3 | 3:C:3035[A]:HIS:CE1 | 2.50 | 0.45 |
| 3:C:3089[B]:HIS:C | 3:L:2971[B]:ASP:HA | 2.42 | 0.45 |
| 3:C:3134[A]:GLN:O | 3:C:3136[A]:TYR:N | 2.49 | 0.45 |
| 3:C:3153[B]:LYS:HE3 | 3:L:3158[B]:PHE:HB2 | 1.98 | 0.45 |
| 3:C:3174[B]:GLY:N | 3:L:3154[B]:PRO:N | 2.64 | 0.45 |
| 3:C:3242[A]:GLY:C | 3:C:3243[A]:GLY:O | 2.58 | 0.45 |
| 3:C:3264[B]:TYR:HD1 | 3:C:3265[B]:ASP:N | 2.14 | 0.45 |
| 1:D:838:ARG:NH1 | 1:D:915:ASN:OD1 | 2.50 | 0.45 |
| 1:D:1161:ILE:HD11 | 1:D:1196:ILE:CD1 | 2.42 | 0.45 |
| 1:D:1493:MET:HG2 | 1:D:1511:SER:O | 2.16 | 0.45 |
| 3:F:2969[A]:TYR:CD2 | 3:F:2970[A]:PRO:CG | 3.00 | 0.45 |
| 3:F:2975[B]:PHE:CZ | 3:a:2961[B]:HIS:CD2 | 3.04 | 0.45 |
| 3:F:2981[A]:GLY:N | 3:F:3086[A]:GLU:OE1 | 2.45 | 0.45 |
| 3:F:3014[B]:TRP:CD2 | 3:F:3092[B]:ILE:CD1 | 2.98 | 0.45 |
| 3:F:3119[B]:HIS:O | 3:F:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 3:F:3149[B]:ASN:HD22 | 3:a:3163[B]:ASN:C | 2.25 | 0.45 |
| 3:F:3259[B]:ASP:H | 3:a:3162[B]:ASP:CG | 2.24 | 0.45 |
| 1:G:126:GLY:HA3 | 1:G:127:GLU:HA | 1.72 | 0.45 |
| 2:H:2575:LEU:HD23 | 2:H:2575:LEU:HA | 1.82 | 0.45 |
| 2:H:2870:LEU:O | 1:J:1078:ARG:NH1 | 2.49 | 0.45 |
| 3:I:2965[B]:LEU:HD13 | 3:I:2975[B]:PHE:O | 2.16 | 0.45 |
| 3:I:2994[A]:LYS:O | 3:I:2997[A]:GLU:N | 2.49 | 0.45 |
| 3:I:3038[B]:ILE:HG23 | 3:I:3040[B]:VAL:HG22 | 1.90 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3044[A]:LYS:H | 3:I:3044[A]:LYS:HG2 | 1.65 | 0.45 |
| 3:I:3094[B]:SER:HG | 3:I:3227[B]:ASP:CG | 2.25 | 0.45 |
| 3:I:3132[B]:ALA:HB3 | 3:I:3197[B]:ILE:HD13 | 1.99 | 0.45 |
| 3:I:3148[B]:ILE:O | 3:I:3148[B]:ILE:HG22 | 2.17 | 0.45 |
| 3:I:3230[A]:PHE:H | 3:I:3243[A]:GLY:HA3 | 1.79 | 0.45 |
| 3:I:3251[B]:ASP:CG | 3:R:3108[B]:HIS:CE1 | 2.94 | 0.45 |
| 3:I:3263[A]:LEU:CD1 | 3:I:3263[A]:LEU:N | 2.79 | 0.45 |
| 1:J:906:HIS:CD2 | 1:J:1046:HIS:CE1 | 3.05 | 0.45 |
| 1:J:1421:VAL:HG23 | 1:J:1422:HIS:HD1 | 1.82 | 0.45 |
| 3:L:2952[B]:ALA:CB | 3:L:2953[B]:GLY:CA | 2.82 | 0.45 |
| 3:L:2970[B]:PRO:C | 3:L:2972[B]:GLY:H | 2.23 | 0.45 |
| 3:L:2986[A]:PRO:CB | 3:L:3127[A]:TRP:CE3 | 3.00 | 0.45 |
| 3:L:3101[A]:PRO:O | 3:L:3109[A]:TYR:HD2 | 2.00 | 0.45 |
| 3:L:3106[B]:THR:O | 3:L:3106[B]:THR:HG23 | 2.17 | 0.45 |
| 3:L:3132[A]:ALA:HB3 | 3:L:3197[A]:ILE:HD13 | 1.99 | 0.45 |
| 3:L:3244[A]:THR:H | 3:L:3264[A]:TYR:HE2 | 1.64 | 0.45 |
| 1:M:896:HIS:HB2 | 1:M:905:TRP:CD1 | 2.52 | 0.45 |
| 1:M:1378:PHE:O | 1:M:1391:ARG:NH1 | 2.50 | 0.45 |
| 1:M:1627:ARG:NH2 | 1:M:1629:GLU:OE1 | 2.50 | 0.45 |
| 2:N:2156:ARG:HD2 | 2:N:2357:VAL:HG12 | 1.99 | 0.45 |
| 2:N:2275:GLY:HA3 | 2:N:2283:ASN:HB2 | 1.98 | 0.45 |
| 3:O:2969[A]:TYR:CD2 | 3:O:2970[A]:PRO:CG | 3.00 | 0.45 |
| 3:O:3106[A]:THR:O | 3:O:3106[A]:THR:HG23 | 2.16 | 0.45 |
| 3:O:3137[A]:ARG:O | 3:O:3139[A]:LEU:HD22 | 2.16 | 0.45 |
| 3:O:3263[A]:LEU:N | 3:O:3263[A]:LEU:CD1 | 2.79 | 0.45 |
| 3:O:3306[A]:LEU:C | 3:O:3306[A]:LEU:CD1 | 2.85 | 0.45 |
| 1:P:156:LEU:O | 1:P:160:LEU:HB2 | 2.17 | 0.45 |
| 1:P:613:SER:HA | 1:P:805:VAL:O | 2.16 | 0.45 |
| 2:Q:2830:GLN:H | 2:Q:2863:ARG:HH22 | 1.64 | 0.45 |
| 3:R:3132[A]:ALA:HB3 | 3:R:3197[A]:ILE:HD13 | 1.99 | 0.45 |
| 3:R:3203[A]:HIS:O | 3:R:3206[A]:LYS:HB3 | 2.16 | 0.45 |
| 3:R:3273[B]:LEU:C | 3:R:3275[B]:LEU:HD12 | 2.42 | 0.45 |
| 1:S:899:MET:HE2 | 1:S:1012:GLU:CD | 2.41 | 0.45 |
| 2:T:2274:LEU:HD23 | 2:T:2274:LEU:HA | 1.78 | 0.45 |
| 3:U:2975[B]:PHE:CE1 | 3:d:3256[B]:TRP:HD1 | 2.19 | 0.45 |
| 3:U:2985[A]:PHE:CE2 | 3:U:2989[A]:HIS:CD2 | 3.04 | 0.45 |
| 3:U:3154[B]:PRO:HD3 | 3:d:3151[B]:LEU:HA | 1.99 | 0.45 |
| 3:U:3180[A]:TYR:CA | 3:U:3183[A]:LEU:CD2 | 2.95 | 0.45 |
| 3:U:3255[B]:PRO:C | 3:d:2975[B]:PHE:CA | 2.90 | 0.45 |
| 1:V:607:HIS:CE1 | 1:V:634:HIS:HE1 | 2.35 | 0.45 |
| 1:V:717:GLN:O | 1:V:721:GLU:HG3 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:958:PRO:O | 1:V:959:PHE:HB2 | 2.17 | 0.45 |
| 1:V:1166:THR:HB | 1:V:1167:ASP:C | 2.42 | 0.45 |
| 2:W:2361:LYS:HD2 | 2:W:2362:GLN:HG3 | 1.98 | 0.45 |
| 2:W:2564:PRO:HA | 2:W:2673:GLU:HG3 | 1.99 | 0.45 |
| 3:X:2970[A]:PRO:C | 3:X:2972[A]:GLY:H | 2.23 | 0.45 |
| 3:X:3241[A]:PHE:CZ | 3:X:3243[A]:GLY:O | 2.70 | 0.45 |
| 1:Y:784:ALA:O | 1:Y:788:LEU:HB2 | 2.16 | 0.45 |
| 1:Y:843:VAL:HG13 | 1:Y:927:PRO:HB2 | 1.99 | 0.45 |
| 1:Y:885:SER:HB3 | 1:Y:886:PRO:HA | 1.99 | 0.45 |
| 1:Y:1286:ARG:HD2 | 1:Y:1286:ARG:HA | 1.66 | 0.45 |
| 1:Y:1296:VAL:HG11 | 1:Y:1447:TYR:CE1 | 2.51 | 0.45 |
| 2:Z:2359:ASN:HB3 | 2:Z:2361:LYS:HZ2 | 1.82 | 0.45 |
| 3:a:2985[A]:PHE:CE2 | 3:a:2989[A]:HIS:CD2 | 3.04 | 0.45 |
| 3:a:3074[A]:GLU:OE2 | 3:a:3208[A]:GLN:HG2 | 2.15 | 0.45 |
| 3:a:3132[B]:ALA:HB3 | 3:a:3197[B]:ILE:HD13 | 1.98 | 0.45 |
| 1:b:266:LEU:HD12 | 1:b:272:LEU:HD11 | 1.98 | 0.45 |
| 1:b:999:LEU:O | 1:b:1063:ARG:NH2 | 2.45 | 0.45 |
| 2:c:2251:LEU:HA | 2:c:2308:TRP:HD1 | 1.82 | 0.45 |
| 3:d:2965[B]:LEU:HD13 | 3:d:2975[B]:PHE:O | 2.16 | 0.45 |
| 3:d:2969[B]:TYR:CD2 | 3:d:2970[B]:PRO:CG | 3.00 | 0.45 |
| 3:d:3106[A]:THR:O | 3:d:3106[A]:THR:HG23 | 2.17 | 0.45 |
| 3:d:3119[B]:HIS:O | 3:d:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 3:d:3132[B]:ALA:HB3 | 3:d:3197[B]:ILE:HD13 | 1.98 | 0.45 |
| 3:d:3134[A]:GLN:O | 3:d:3136[A]:TYR:N | 2.49 | 0.45 |
| 3:d:3242[A]:GLY:C | 3:d:3243[A]:GLY:O | 2.58 | 0.45 |
| 4:v:1:NAG:C6 | 4:v:2:NAG:C1 | 2.94 | 0.45 |
| 1:A:177:VAL:O | 1:A:181:PRO:HD3 | 2.16 | 0.45 |
| 1:A:304:ALA:HB1 | 1:A:306:PHE:CE1 | 2.48 | 0.45 |
| 1:A:460:GLU:CB | 1:A:465:PRO:HG2 | 2.44 | 0.45 |
| 3:C:2948[B]:ASP:CB | 3:C:2949[B]:LYS:CA | 2.78 | 0.45 |
| 3:C:2959[B]:SER:O | 3:L:3255[B]:PRO:HD2 | 2.16 | 0.45 |
| 3:C:3038[B]:ILE:HG23 | 3:C:3040[B]:VAL:HG22 | 1.90 | 0.45 |
| 3:C:3203[B]:HIS:O | 3:C:3206[B]:LYS:HB3 | 2.16 | 0.45 |
| 3:C:3241[B]:PHE:CZ | 3:C:3243[B]:GLY:O | 2.70 | 0.45 |
| 1:D:513:TYR:OH | 1:D:704:ASP:OD1 | 2.28 | 0.45 |
| 1:D:953:GLU:OE2 | 1:D:956:PRO:HG3 | 2.17 | 0.45 |
| 1:D:1033:LEU:HA | 1:D:1036:SER:HB3 | 1.98 | 0.45 |
| 1:D:1091:ASN:HA | 1:D:1092:PRO:HD3 | 1.82 | 0.45 |
| 2:E:2465:LYS:HB2 | 2:E:2465:LYS:HE3 | 1.67 | 0.45 |
| 3:F:2965[A]:LEU:HD13 | 3:F:2975[A]:PHE:O | 2.16 | 0.45 |
| 3:F:3025[A]:VAL:CG2 | 3:F:3047[A]:ARG:NH1 | 2.73 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:456:GLN:O | 1:G:460:GLU:HG3 | 2.16 | 0.45 |
| 1:G:618:MET:HE2 | 1:G:618:MET:HB3 | 1.60 | 0.45 |
| 1:G:1019:HIS:CE1 | 1:G:1046:HIS:HE1 | 2.35 | 0.45 |
| 1:G:1150:GLY:N | 1:G:1186:TRP:O | 2.46 | 0.45 |
| 3:I:2976[B]:ALA:HB3 | 3:R:2976[B]:ALA:H | 1.81 | 0.45 |
| 3:I:3037[B]:TYR:C | 3:I:3038[B]:ILE:HG13 | 2.42 | 0.45 |
| 3:I:3101[B]:PRO:O | 3:I:3109[B]:TYR:HD2 | 2.00 | 0.45 |
| 3:I:3108[B]:HIS:CE1 | 3:R:3252[B]:TYR:CG | 3.05 | 0.45 |
| 3:I:3133[B]:LEU:O | 3:I:3136[B]:TYR:HB3 | 2.17 | 0.45 |
| 3:I:3137[B]:ARG:HB3 | 3:I:3139[B]:LEU:HD21 | 1.97 | 0.45 |
| 3:I:3141[B]:TYR:CD2 | 3:I:3141[B]:TYR:C | 2.86 | 0.45 |
| 3:I:3152[B]:LYS:HB2 | 3:R:3172[B]:SER:H | 0.33 | 0.45 |
| 3:I:3180[A]:TYR:CA | 3:I:3183[A]:LEU:CD2 | 2.95 | 0.45 |
| 1:J:193:SER:C | 1:J:195:SER:H | 2.25 | 0.45 |
| 1:J:567:LEU:HD23 | 1:J:571:PRO:CG | 2.47 | 0.45 |
| 1:J:639:ARG:HB2 | 1:J:703:TYR:CE1 | 2.52 | 0.45 |
| 1:J:832:LYS:HA | 1:J:833:PHE:HA | 1.57 | 0.45 |
| 1:J:905:TRP:HE1 | 1:J:1083:PRO:HD2 | 1.82 | 0.45 |
| 1:J:1075:GLU:OE2 | 1:J:1076:ILE:HG13 | 2.17 | 0.45 |
| 1:J:1427:HIS:CE1 | 1:J:1457:HIS:HE1 | 2.35 | 0.45 |
| 1:J:1530:LEU:HD23 | 1:J:1530:LEU:HA | 1.78 | 0.45 |
| 3:L:2985[B]:PHE:CE2 | 3:L:2989[B]:HIS:CD2 | 3.04 | 0.45 |
| 3:L:3014[A]:TRP:CG | 3:L:3092[A]:ILE:CD1 | 2.98 | 0.45 |
| 3:L:3101[B]:PRO:O | 3:L:3109[B]:TYR:HD2 | 2.00 | 0.45 |
| 3:L:3185[B]:TYR:HE2 | 3:L:3187[B]:TYR:CD2 | 2.35 | 0.45 |
| 3:L:3263[B]:LEU:N | 3:L:3263[B]:LEU:CD1 | 2.79 | 0.45 |
| 1:M:2:LEU:O | 1:M:275:ALA:N | 2.47 | 0.45 |
| 1:M:294:LYS:HA | 1:M:297:ARG:CD | 2.46 | 0.45 |
| 1:M:483:GLY:HA2 | 1:M:773:PHE:CE1 | 2.52 | 0.45 |
| 3:O:3132[B]:ALA:HB3 | 3:O:3197[B]:ILE:HD13 | 1.99 | 0.45 |
| 3:O:3204[B]:LEU:CD1 | 3:O:3204[B]:LEU:N | 2.79 | 0.45 |
| 3:O:3273[A]:LEU:C | 3:O:3275[A]:LEU:HD12 | 2.42 | 0.45 |
| 1:P:838:ARG:NH1 | 1:P:915:ASN:OD1 | 2.31 | 0.45 |
| 1:P:1638:SER:C | 4:6:1:NAG:H82 | 2.42 | 0.45 |
| 3:R:2986[B]:PRO:CB | 3:R:3127[B]:TRP:CE3 | 3.00 | 0.45 |
| 3:R:3037[B]:TYR:C | 3:R:3038[B]:ILE:HG13 | 2.42 | 0.45 |
| 3:R:3101[A]:PRO:O | 3:R:3109[A]:TYR:HD2 | 2.00 | 0.45 |
| 3:R:3116[B]:PHE:CD1 | 3:R:3116[B]:PHE:C | 2.94 | 0.45 |
| 3:R:3137[A]:ARG:O | 3:R:3139[A]:LEU:HD22 | 2.16 | 0.45 |
| 3:R:3137[B]:ARG:HB3 | 3:R:3139[B]:LEU:HD21 | 1.97 | 0.45 |
| 3:R:3196[A]:THR:N | 3:R:3199[A]:GLN:CB | 2.65 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3241[A]:PHE:CZ | 3:R:3243[A]:GLY:O | 2.70 | 0.45 |
| 3:R:3263[B]:LEU:N | 3:R:3263[B]:LEU:CD1 | 2.79 | 0.45 |
| 3:R:3285[A]:VAL:CG2 | 3:R:3286[A]:THR:H | 2.27 | 0.45 |
| 3:R:3301[A]:PRO:HB2 | 3:R:3302[A]:SER:H | 1.33 | 0.45 |
| 1:S:1101:VAL:HG11 | 2:W:2873:HIS:HD2 | 1.81 | 0.45 |
| 1:S:1423:TYR:OH | 1:S:1461:VAL:HG12 | 2.17 | 0.45 |
| 1:S:1489:MET:HA | 1:S:1513:PRO:HB2 | 1.98 | 0.45 |
| 2:T:2546:LEU:N | 2:T:2557:ALA:HA | 2.26 | 0.45 |
| 3:U:3037[B]:TYR:C | 3:U:3038[B]:ILE:HG13 | 2.42 | 0.45 |
| 3:U:3209[A]:GLU:O | 3:U:3310[A]:GLY:C | 2.59 | 0.45 |
| 3:U:3281[B]:PHE:HE1 | 3:U:3305[B]:ILE:HG21 | 1.81 | 0.45 |
| 1:V:107:HIS:O | 1:V:121:ASN:ND2 | 2.50 | 0.45 |
| 1:V:1300:CYS:HB3 | 1:V:1494:ARG:NH1 | 2.32 | 0.45 |
| 3:X:3019[B]:HIS:CD2 | 3:X:3020[B]:SER:H | 2.35 | 0.45 |
| 3:X:3023[B]:ILE:O | 3:X:3026[B]:THR:OG1 | 2.34 | 0.45 |
| 3:X:3024[B]:LEU:CD1 | 3:X:3024[B]:LEU:C | 2.85 | 0.45 |
| 3:X:3037[B]:TYR:C | 3:X:3038[B]:ILE:HG13 | 2.42 | 0.45 |
| 3:X:3101[A]:PRO:O | 3:X:3109[A]:TYR:HD2 | 2.00 | 0.45 |
| 3:X:3119[B]:HIS:O | 3:X:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 3:X:3204[B]:LEU:CD1 | 3:X:3204[B]:LEU:N | 2.80 | 0.45 |
| 3:X:3241[B]:PHE:CE2 | 3:X:3243[B]:GLY:O | 2.70 | 0.45 |
| 3:X:3242[B]:GLY:C | 3:X:3243[B]:GLY:O | 2.58 | 0.45 |
| 3:X:3264[B]:TYR:HD1 | 3:X:3265[B]:ASP:N | 2.14 | 0.45 |
| 1:Y:140:ASP:OD2 | 1:Y:142:ARG:NE | 2.38 | 0.45 |
| 1:Y:490:TRP:HE1 | 1:Y:670:PRO:CD | 2.29 | 0.45 |
| 2:Z:2161:GLN:NE2 | 2:Z:2348:THR:HG21 | 2.32 | 0.45 |
| 3:a:2956[B]:LYS:O | 3:a:2959[B]:SER:OG | 2.33 | 0.45 |
| 3:a:2981[B]:GLY:N | 3:a:3086[B]:GLU:OE1 | 2.45 | 0.45 |
| 3:a:2986[A]:PRO:CB | 3:a:3127[A]:TRP:CE3 | 3.00 | 0.45 |
| 3:a:3101[B]:PRO:O | 3:a:3109[B]:TYR:HD2 | 2.00 | 0.45 |
| 3:a:3119[B]:HIS:O | 3:a:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 3:a:3134[B]:GLN:O | 3:a:3136[B]:TYR:N | 2.49 | 0.45 |
| 3:a:3183[A]:LEU:N | 3:a:3184[A]:ASN:CA | 2.80 | 0.45 |
| 3:a:3241[A]:PHE:CZ | 3:a:3243[A]:GLY:O | 2.70 | 0.45 |
| 1:b:301:ARG:HD2 | 1:b:361:GLU:OE2 | 2.17 | 0.45 |
| 1:b:329:ARG:C | 1:b:331:SER:H | 2.24 | 0.45 |
| 1:b:403:TYR:HD2 | 1:b:658:TYR:CD1 | 2.35 | 0.45 |
| 1:b:1015:HIS:CD2 | 1:b:1045:HIS:HE1 | 2.35 | 0.45 |
| 1:b:1143:ALA:HB3 | 1:b:1235:ILE:HG23 | 1.99 | 0.45 |
| 1:b:1221:THR:OG1 | 1:b:1222:GLY:N | 2.49 | 0.45 |
| 2:c:2608:ASP:O | 2:c:2622:ASN:ND2 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2932[B]:PRO:CA | 3:d:2935[B]:ILE:CD1 | 2.85 | 0.45 |
| 3:d:2956[A]:LYS:O | 3:d:2959[A]:SER:OG | 2.33 | 0.45 |
| 3:d:2986[A]:PRO:CB | 3:d:3127[A]:TRP:CE3 | 3.00 | 0.45 |
| 3:d:3074[B]:GLU:CD | 3:d:3212[B]:ARG:NH2 | 2.73 | 0.45 |
| 3:d:3204[A]:LEU:CD1 | 3:d:3204[A]:LEU:N | 2.80 | 0.45 |
| 4:m:1:NAG:C3 | 4:m:2:NAG:HN2 | 2.27 | 0.45 |
| 1:A:192:HIS:O | 1:A:193:SER:OG | 2.30 | 0.45 |
| 1:A:389:THR:HA | 2:Z:2136:THR:HB | 1.99 | 0.45 |
| 1:A:447:MET:HA | 1:A:455:TYR:CB | 2.46 | 0.45 |
| 1:A:792:MET:HE3 | 1:A:822:PHE:CE2 | 2.52 | 0.45 |
| 1:A:1359:ILE:HG22 | 1:A:1377:PHE:HB3 | 1.99 | 0.45 |
| 3:C:2951[A]:ASP:CG | 3:C:2952[A]:ALA:N | 2.74 | 0.45 |
| 3:C:2969[B]:TYR:CE2 | 3:L:3120[B]:HIS:CD2 | 2.88 | 0.45 |
| 3:C:2979[A]:GLN:HB2 | 3:C:2988[A]:TRP:CD1 | 2.52 | 0.45 |
| 3:C:2986[B]:PRO:CB | 3:C:3127[B]:TRP:CE3 | 3.00 | 0.45 |
| 3:C:3013[B]:ASP:CG | 3:C:3015[B]:THR:HG1 | 2.24 | 0.45 |
| 3:C:3019[B]:HIS:CD2 | 3:C:3020[B]:SER:H | 2.35 | 0.45 |
| 3:C:3047[B]:ARG:NH2 | 3:C:3113[B]:ASP:OD1 | 2.43 | 0.45 |
| 3:C:3135[A]:LYS:HB2 | 3:C:3141[A]:TYR:CD1 | 2.51 | 0.45 |
| 3:C:3172[B]:SER:CB | 3:L:3152[B]:LYS:CA | 2.95 | 0.45 |
| 3:C:3172[B]:SER:OG | 3:L:3149[B]:ASN:C | 2.60 | 0.45 |
| 3:C:3180[B]:TYR:CA | 3:C:3183[B]:LEU:CD2 | 2.95 | 0.45 |
| 3:C:3241[B]:PHE:CE2 | 3:C:3243[B]:GLY:O | 2.70 | 0.45 |
| 3:C:3249[B]:GLY:N | 3:L:2973[B]:THR:HG22 | 2.32 | 0.45 |
| 1:D:618:MET:HE3 | 1:D:618:MET:HB3 | 1.89 | 0.45 |
| 1:D:638:ASP:HB3 | 1:D:703:TYR:OH | 2.17 | 0.45 |
| 1:D:1300:CYS:HB3 | 1:D:1494:ARG:NH1 | 2.32 | 0.45 |
| 1:D:1301:PRO:O | 1:D:1494:ARG:NH2 | 2.50 | 0.45 |
| 2:E:2130:PRO:HG2 | 2:E:2140:ARG:HD2 | 1.98 | 0.45 |
| 2:E:2213:HIS:CD2 | 2:E:2222:MET:HG2 | 2.52 | 0.45 |
| 3:F:2938[B]:LEU:O | 3:F:2939[B]:ARG:C | 2.58 | 0.45 |
| 3:F:3037[A]:TYR:C | 3:F:3038[A]:ILE:HG13 | 2.42 | 0.45 |
| 3:F:3037[B]:TYR:C | 3:F:3038[B]:ILE:HG13 | 2.42 | 0.45 |
| 3:F:3241[B]:PHE:CE2 | 3:F:3243[B]:GLY:O | 2.70 | 0.45 |
| 1:G:184:TYR:CE1 | 1:G:386:ILE:HG12 | 2.52 | 0.45 |
| 1:G:712:SER:O | 1:G:716:LEU:N | 2.40 | 0.45 |
| 1:G:982:LYS:N | 1:G:983:PRO:CD | 2.80 | 0.45 |
| 1:G:1475:ARG:NE | 1:G:1541:GLU:OE2 | 2.30 | 0.45 |
| 2:H:2825:ILE:HG23 | 2:H:2826:GLU:H | 1.81 | 0.45 |
| 3:I:2932[B]:PRO:CA | 3:I:2935[B]:ILE:CD1 | 2.85 | 0.45 |
| 3:I:2956[B]:LYS:O | 3:I:2959[B]:SER:OG | 2.33 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2977[B]:CYS:HB3 | 3:R:2982[B]:MET:CE | 2.42 | 0.45 |
| 3:I:3004[A]:GLY:C | 3:I:3006[A]:LYS:N | 2.74 | 0.45 |
| 3:I:3014[B]:TRP:CG | 3:I:3092[B]:ILE:CD1 | 2.98 | 0.45 |
| 3:I:3161[B]:GLU:C | 3:R:3147[B]:GLU:HG2 | 2.29 | 0.45 |
| 3:I:3242[A]:GLY:C | 3:I:3243[A]:GLY:O | 2.58 | 0.45 |
| 1:J:732:GLY:HA2 | 1:J:777:TYR:O | 2.17 | 0.45 |
| 2:K:2822:LYS:HG2 | 2:K:2831:GLU:H | 1.81 | 0.45 |
| 3:L:2938[B]:LEU:O | 3:L:2939[B]:ARG:C | 2.58 | 0.45 |
| 3:L:2969[A]:TYR:CD2 | 3:L:2970[A]:PRO:CG | 3.00 | 0.45 |
| 3:L:3114[B]:PRO:CD | 3:L:3115[B]:LEU:N | 2.72 | 0.45 |
| 3:L:3119[B]:HIS:O | 3:L:3122[B]:ASN:HB3 | 2.17 | 0.45 |
| 3:L:3132[B]:ALA:HB3 | 3:L:3197[B]:ILE:HD13 | 1.99 | 0.45 |
| 1:M:321:LEU:HD11 | 1:M:377:TYR:CD1 | 2.52 | 0.45 |
| 1:M:735:LEU:HB2 | 1:M:773:PHE:HD2 | 1.82 | 0.45 |
| 2:N:2327:GLU:H | 2:N:2327:GLU:HG3 | 1.40 | 0.45 |
| 3:O:2986[B]:PRO:CB | 3:O:3127[B]:TRP:CE3 | 3.00 | 0.45 |
| 3:O:2994[A]:LYS:O | 3:O:2997[A]:GLU:N | 2.49 | 0.45 |
| 3:O:3093[B]:HIS:HD2 | 3:O:3248[B]:LEU:CD2 | 2.30 | 0.45 |
| 3:O:3157[B]:PRO:HA | 3:X:3150[B]:LYS:CA | 2.47 | 0.45 |
| 3:O:3182[B]:GLN:H | 3:O:3182[B]:GLN:HG2 | 1.56 | 0.45 |
| 3:O:3225[A]:SER:C | 3:O:3290[A]:ILE:HG23 | 2.39 | 0.45 |
| 3:O:3241[B]:PHE:CE2 | 3:O:3243[B]:GLY:O | 2.70 | 0.45 |
| 3:O:3266[B]:ILE:O | 3:O:3269[B]:SER:HB2 | 2.17 | 0.45 |
| 1:P:931:TRP:NE1 | 1:P:1048:ASN:HD22 | 2.15 | 0.45 |
| 2:Q:2451:LEU:HD11 | 2:Q:2462:PHE:CZ | 2.51 | 0.45 |
| 2:Q:2500:ILE:HD11 | 2:Q:2776:TYR:HA | 1.99 | 0.45 |
| 2:Q:2522:SER:O | 2:Q:2526:ARG:HG2 | 2.16 | 0.45 |
| 2:Q:2791:LEU:HD23 | 2:Q:2791:LEU:HA | 1.85 | 0.45 |
| 3:R:3146[A]:CYS:HA | 3:R:3147[A]:GLU:HA | 1.70 | 0.45 |
| 3:R:3171[B]:HIS:C | 3:R:3173[B]:THR:N | 2.73 | 0.45 |
| 3:R:3183[A]:LEU:N | 3:R:3184[A]:ASN:CA | 2.80 | 0.45 |
| 3:R:3200[A]:LEU:CD2 | 3:R:3204[A]:LEU:CD1 | 2.93 | 0.45 |
| 3:R:3241[B]:PHE:CZ | 3:R:3243[B]:GLY:O | 2.70 | 0.45 |
| 2:T:2890:VAL:HG23 | 2:T:2891:LEU:C | 2.42 | 0.45 |
| 3:U:3023[B]:ILE:HA | 3:U:3026[B]:THR:HG1 | 1.81 | 0.45 |
| 3:U:3027[A]:GLU:CD | 3:U:3027[A]:GLU:C | 2.85 | 0.45 |
| 3:U:3106[A]:THR:O | 3:U:3106[A]:THR:HG23 | 2.17 | 0.45 |
| 3:U:3119[A]:HIS:O | 3:U:3122[A]:ASN:HB3 | 2.17 | 0.45 |
| 3:U:3133[A]:LEU:O | 3:U:3136[A]:TYR:HB3 | 2.17 | 0.45 |
| 3:U:3137[B]:ARG:HB3 | 3:U:3139[B]:LEU:HD21 | 1.97 | 0.45 |
| 3:U:3204[B]:LEU:CD1 | 3:U:3204[B]:LEU:N | 2.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3273[A]:LEU:C | 3:U:3275[A]:LEU:HD12 | 2.42 | 0.45 |
| 3:U:3301[A]:PRO:HB2 | 3:U:3302[A]:SER:H | 1.33 | 0.45 |
| 1:V:901:THR:HG22 | 1:V:904:HIS:HB2 | 1.99 | 0.45 |
| 1:V:907:ARG:CZ | 1:V:1108:TYR:HB3 | 2.47 | 0.45 |
| 2:W:2556:TYR:CE1 | 2:W:2844:MET:HG3 | 2.52 | 0.45 |
| 3:X:2951[A]:ASP:CG | 3:X:2952[A]:ALA:N | 2.74 | 0.45 |
| 3:X:3135[A]:LYS:HB2 | 3:X:3141[A]:TYR:CD1 | 2.51 | 0.45 |
| 3:X:3148[A]:ILE:O | 3:X:3148[A]:ILE:HG22 | 2.17 | 0.45 |
| 1:Y:134:VAL:HG12 | 1:Y:135:THR:H | 1.82 | 0.45 |
| 1:Y:142:ARG:HH22 | 1:Y:316:ASN:ND2 | 2.14 | 0.45 |
| 1:Y:516:TRP:CD1 | 1:Y:579:LEU:HB3 | 2.52 | 0.45 |
| 1:Y:684:ARG:HB3 | 1:Y:684:ARG:NH1 | 2.32 | 0.45 |
| 1:Y:1007:PHE:CE1 | 1:Y:1011:TYR:HB2 | 2.51 | 0.45 |
| 1:Y:1506:LEU:H | 1:Y:1506:LEU:HG | 1.39 | 0.45 |
| 2:Z:2181:THR:HB | 2:Z:2374:ASN:H | 1.82 | 0.45 |
| 2:Z:2278:GLU:O | 2:Z:2281:SER:OG | 2.32 | 0.45 |
| 2:Z:2739:LEU:HG | 1:b:1234:VAL:O | 2.17 | 0.45 |
| 3:a:2949[B]:LYS:NZ | 3:a:2949[B]:LYS:C | 2.73 | 0.45 |
| 3:a:2979[A]:GLN:HB2 | 3:a:2988[A]:TRP:CD1 | 2.52 | 0.45 |
| 3:a:2979[B]:GLN:HB2 | 3:a:2988[B]:TRP:CD1 | 2.52 | 0.45 |
| 3:a:3027[B]:GLU:CD | 3:a:3027[B]:GLU:C | 2.85 | 0.45 |
| 3:a:3133[B]:LEU:O | 3:a:3136[B]:TYR:HB3 | 2.17 | 0.45 |
| 3:a:3180[A]:TYR:CA | 3:a:3183[A]:LEU:CD2 | 2.95 | 0.45 |
| 3:a:3185[A]:TYR:HE2 | 3:a:3187[A]:TYR:CD2 | 2.35 | 0.45 |
| 3:a:3242[B]:GLY:C | 3:a:3243[B]:GLY:O | 2.58 | 0.45 |
| 1:b:108:PRO:HA | 1:b:124:TYR:CG | 2.52 | 0.45 |
| 1:b:810:LEU:HD12 | 1:b:810:LEU:HA | 1.88 | 0.45 |
| 1:b:836:GLN:H | 1:b:836:GLN:HG3 | 1.60 | 0.45 |
| 1:b:987:LYS:HE2 | 1:b:987:LYS:N | 2.31 | 0.45 |
| 1:b:1059:LEU:HD13 | 1:b:1063:ARG:HH21 | 1.82 | 0.45 |
| 3:d:3019[B]:HIS:CD2 | 3:d:3020[B]:SER:H | 2.35 | 0.45 |
| 3:d:3038[A]:ILE:HG23 | 3:d:3040[A]:VAL:HG22 | 1.90 | 0.45 |
| 3:d:3093[A]:HIS:HD2 | 3:d:3248[A]:LEU:CD2 | 2.30 | 0.45 |
| 3:d:3101[A]:PRO:O | 3:d:3109[A]:TYR:HD2 | 2.00 | 0.45 |
| 3:d:3180[B]:TYR:CA | 3:d:3183[B]:LEU:CD2 | 2.95 | 0.45 |
| 3:d:3196[A]:THR:N | 3:d:3199[A]:GLN:CB | 2.65 | 0.45 |
| 3:d:3241[A]:PHE:CE2 | 3:d:3243[A]:GLY:O | 2.70 | 0.45 |
| 3:d:3244[B]:THR:H | 3:d:3264[B]:TYR:HE2 | 1.65 | 0.45 |
| 2:B:2370:MET:HE1 | 2:E:2094:ARG:NH1 | 2.32 | 0.44 |
| 2:B:2448:THR:OG1 | 2:B:2449:ASP:N | 2.49 | 0.44 |
| 2:B:2630:LYS:HA | 2:B:2630:LYS:HD2 | 1.77 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2901:LEU:H | 1:D:1075:GLU:HG3 | 1.81 | 0.44 |
| 3:C:2938[B]:LEU:O | 3:C:2939[B]:ARG:C | 2.58 | 0.44 |
| 3:C:2961[B]:HIS:HB2 | 3:C:2992[B]:TYR:HE2 | 1.80 | 0.44 |
| 3:C:2986[A]:PRO:CB | 3:C:3127[A]:TRP:CE3 | 3.00 | 0.44 |
| 3:C:2989[A]:HIS:CD2 | 9:L:3401[A]:CUO:O1 | 2.70 | 0.44 |
| 3:C:3087[A]:MET:HA | 3:C:3090[A]:ASN:OD1 | 2.17 | 0.44 |
| 3:C:3119[A]:HIS:O | 3:C:3122[A]:ASN:HB3 | 2.17 | 0.44 |
| 3:C:3225[B]:SER:C | 3:C:3290[B]:ILE:HG23 | 2.39 | 0.44 |
| 3:C:3229[A]:ASN:O | 3:C:3286[A]:THR:N | 2.50 | 0.44 |
| 3:C:3255[B]:PRO:HD3 | 3:L:2961[B]:HIS:C | 2.42 | 0.44 |
| 1:D:901:THR:HG22 | 1:D:904:HIS:HD2 | 1.82 | 0.44 |
| 1:D:905:TRP:HZ2 | 1:D:1083:PRO:HG2 | 1.82 | 0.44 |
| 1:D:906:HIS:HD2 | 1:D:1046:HIS:CD2 | 2.35 | 0.44 |
| 1:D:1393:THR:HG22 | 1:D:1434:LEU:HD12 | 1.99 | 0.44 |
| 2:E:2128:LEU:HD23 | 2:E:2216:PHE:HZ | 1.80 | 0.44 |
| 3:F:3027[A]:GLU:CD | 3:F:3027[A]:GLU:C | 2.85 | 0.44 |
| 3:F:3204[A]:LEU:CD1 | 3:F:3204[A]:LEU:N | 2.80 | 0.44 |
| 3:F:3241[B]:PHE:CZ | 3:F:3243[B]:GLY:O | 2.70 | 0.44 |
| 3:F:3253[B]:GLU:HA | 3:a:2976[B]:ALA:H | 1.74 | 0.44 |
| 1:G:411:ASP:OD1 | 1:G:411:ASP:N | 2.49 | 0.44 |
| 1:G:1075:GLU:H | 1:G:1075:GLU:HG3 | 1.38 | 0.44 |
| 1:G:1302:SER:H | 1:G:1494:ARG:HH22 | 1.64 | 0.44 |
| 2:H:2854:MET:HE3 | 2:H:2854:MET:HB2 | 1.94 | 0.44 |
| 3:I:2932[A]:PRO:CA | 3:I:2935[A]:ILE:CD1 | 2.85 | 0.44 |
| 3:I:3106[A]:THR:O | 3:I:3106[A]:THR:HG23 | 2.16 | 0.44 |
| 3:I:3137[A]:ARG:O | 3:I:3139[A]:LEU:HD22 | 2.16 | 0.44 |
| 3:I:3150[B]:LYS:O | 3:R:3172[B]:SER:HB2 | 2.15 | 0.44 |
| 3:I:3150[B]:LYS:HD3 | 3:R:3160[B]:SER:N | 1.89 | 0.44 |
| 3:I:3162[B]:ASP:OD1 | 3:R:2983[B]:VAL:HG22 | 2.17 | 0.44 |
| 3:I:3241[B]:PHE:CZ | 3:I:3243[B]:GLY:O | 2.70 | 0.44 |
| 3:I:3244[B]:THR:H | 3:I:3264[B]:TYR:HE2 | 1.65 | 0.44 |
| 3:I:3253[B]:GLU:HA | 3:R:3252[B]:TYR:O | 2.17 | 0.44 |
| 3:I:3266[B]:ILE:O | 3:I:3269[B]:SER:HB2 | 2.17 | 0.44 |
| 1:J:23:ARG:HD3 | 1:J:120:LYS:HD3 | 1.99 | 0.44 |
| 1:J:452:ILE:HD11 | 1:J:679:ASN:HD21 | 1.82 | 0.44 |
| 1:J:957:ASN:N | 1:J:958:PRO:HA | 2.32 | 0.44 |
| 1:J:1321:HIS:CD2 | 1:J:1465:TRP:HH2 | 2.35 | 0.44 |
| 2:K:2541:GLY:O | 2:K:2545:SER:OG | 2.28 | 0.44 |
| 3:L:2951[B]:ASP:CG | 3:L:2952[B]:ALA:N | 2.74 | 0.44 |
| 3:L:2986[B]:PRO:CB | 3:L:3127[B]:TRP:CE3 | 3.00 | 0.44 |
| 3:L:2989[B]:HIS:O | 3:L:2990[B]:ARG:C | 2.61 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3004[A]:GLY:O | 3:L:3006[A]:LYS:N | 2.44 | 0.44 |
| 3:L:3023[A]:ILE:HA | 3:L:3026[A]:THR:HG1 | 1.82 | 0.44 |
| 3:L:3196[A]:THR:CB | 3:L:3199[A]:GLN:OE1 | 2.64 | 0.44 |
| 3:L:3273[B]:LEU:C | 3:L:3275[B]:LEU:HD12 | 2.42 | 0.44 |
| 1:M:148:GLN:O | 1:M:149:GLU:HG2 | 2.17 | 0.44 |
| 1:M:1636:ASN:OD1 | 4:1:1:NAG:H82 | 2.17 | 0.44 |
| 3:O:2949[B]:LYS:NZ | 3:O:2949[B]:LYS:C | 2.73 | 0.44 |
| 3:O:2985[A]:PHE:CE2 | 3:O:2989[A]:HIS:CD2 | 3.04 | 0.44 |
| 3:O:3019[B]:HIS:CD2 | 3:O:3020[B]:SER:H | 2.35 | 0.44 |
| 3:O:3106[B]:THR:O | 3:O:3106[B]:THR:HG23 | 2.16 | 0.44 |
| 3:O:3133[A]:LEU:O | 3:O:3136[A]:TYR:HB3 | 2.17 | 0.44 |
| 3:O:3134[A]:GLN:O | 3:O:3136[A]:TYR:N | 2.49 | 0.44 |
| 3:O:3137[B]:ARG:HA | 3:O:3137[B]:ARG:HD3 | 1.71 | 0.44 |
| 3:O:3157[B]:PRO:CA | 3:X:3152[B]:LYS:N | 2.80 | 0.44 |
| 3:O:3241[B]:PHE:CZ | 3:O:3243[B]:GLY:O | 2.70 | 0.44 |
| 3:O:3273[B]:LEU:C | 3:O:3275[B]:LEU:HD12 | 2.42 | 0.44 |
| 1:P:300:ALA:HB2 | 1:P:406:PRO:HD3 | 2.00 | 0.44 |
| 1:P:1149:GLU:HG3 | 1:P:1187:LYS:HE2 | 2.00 | 0.44 |
| 1:P:1321:HIS:CD2 | 1:P:1465:TRP:CH2 | 3.01 | 0.44 |
| 3:R:2979[B]:GLN:HB2 | 3:R:2988[B]:TRP:CD1 | 2.52 | 0.44 |
| 3:R:3038[A]:ILE:HG23 | 3:R:3040[A]:VAL:HG22 | 1.90 | 0.44 |
| 3:R:3241[A]:PHE:CE2 | 3:R:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:R:3266[B]:ILE:O | 3:R:3269[B]:SER:HB2 | 2.18 | 0.44 |
| 1:S:472:ASP:HA | 1:S:473:ALA:HA | 1.69 | 0.44 |
| 1:S:957:ASN:N | 1:S:958:PRO:HA | 2.33 | 0.44 |
| 2:T:2252:GLU:HA | 2:T:2385:ILE:HD13 | 1.99 | 0.44 |
| 2:T:2884:LYS:HB3 | 2:T:2889:ALA:O | 2.17 | 0.44 |
| 3:U:2938[A]:LEU:O | 3:U:2939[A]:ARG:C | 2.58 | 0.44 |
| 3:U:3185[A]:TYR:HE2 | 3:U:3187[A]:TYR:CD2 | 2.35 | 0.44 |
| 3:U:3299[A]:LEU:O | 3:U:3300[A]:LEU:C | 2.60 | 0.44 |
| 2:W:2823:ILE:HG13 | 2:W:2830:GLN:NE2 | 2.23 | 0.44 |
| 3:X:2989[A]:HIS:C | 3:X:2991[A]:LEU:N | 2.75 | 0.44 |
| 3:X:2989[B]:HIS:CD2 | 9:X:3401[B]:CUO:O1 | 2.70 | 0.44 |
| 3:X:2994[B]:LYS:O | 3:X:2997[B]:GLU:N | 2.49 | 0.44 |
| 3:X:3019[A]:HIS:CD2 | 3:X:3020[A]:SER:H | 2.35 | 0.44 |
| 3:X:3087[A]:MET:HA | 3:X:3090[A]:ASN:OD1 | 2.17 | 0.44 |
| 3:X:3093[A]:HIS:HD2 | 3:X:3248[A]:LEU:CD2 | 2.31 | 0.44 |
| 3:X:3116[A]:PHE:CD1 | 3:X:3116[A]:PHE:C | 2.94 | 0.44 |
| 3:X:3182[A]:GLN:C | 3:X:3183[A]:LEU:CD1 | 2.91 | 0.44 |
| 3:X:3229[B]:ASN:O | 3:X:3286[B]:THR:N | 2.50 | 0.44 |
| 3:X:3241[A]:PHE:CE2 | 3:X:3243[A]:GLY:O | 2.70 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:1156:LEU:HB2 | 1:Y:1176:TYR:CE1 | 2.52 | 0.44 |
| 1:Y:1349:VAL:HG13 | 1:Y:1404:TYR:HA | 2.00 | 0.44 |
| 2:Z:2340:ALA:HB1 | 2:Z:2341:PRO:CD | 2.47 | 0.44 |
| 2:Z:2739:LEU:HD11 | 1:b:1236:TYR:HB2 | 1.98 | 0.44 |
| 3:a:2951[B]:ASP:CG | 3:a:2952[B]:ALA:N | 2.74 | 0.44 |
| 3:a:3101[A]:PRO:O | 3:a:3109[A]:TYR:HD2 | 2.00 | 0.44 |
| 3:a:3137[A]:ARG:HD3 | 3:a:3137[A]:ARG:HA | 1.71 | 0.44 |
| 3:a:3273[B]:LEU:C | 3:a:3275[B]:LEU:HD12 | 2.42 | 0.44 |
| 3:a:3281[A]:PHE:HE1 | 3:a:3305[A]:ILE:HG21 | 1.81 | 0.44 |
| 1:b:38:SER:HB3 | 1:b:202:TYR:CD1 | 2.52 | 0.44 |
| 3:d:2970[A]:PRO:C | 3:d:2972[A]:GLY:N | 2.72 | 0.44 |
| 3:d:2979[B]:GLN:HB2 | 3:d:2988[B]:TRP:CD1 | 2.52 | 0.44 |
| 3:d:3185[B]:TYR:HE2 | 3:d:3187[B]:TYR:CD2 | 2.35 | 0.44 |
| 3:d:3200[B]:LEU:CD2 | 3:d:3204[B]:LEU:HD11 | 2.48 | 0.44 |
| 3:d:3273[B]:LEU:C | 3:d:3275[B]:LEU:HD12 | 2.42 | 0.44 |
| 1:A:17:ASN:OD1 | 1:A:18:LEU:N | 2.50 | 0.44 |
| 1:A:133:LYS:HG3 | 1:A:134:VAL:N | 2.32 | 0.44 |
| 1:A:593:CYS:O | 1:A:597:VAL:HG23 | 2.17 | 0.44 |
| 2:B:2135:PRO:HG3 | 2:B:2342:TYR:CE2 | 2.52 | 0.44 |
| 3:C:2988[B]:TRP:CD1 | 3:C:3158[B]:PHE:CE2 | 3.06 | 0.44 |
| 3:C:3014[A]:TRP:CH2 | 3:C:3123[A]:THR:HG23 | 2.53 | 0.44 |
| 3:C:3133[B]:LEU:O | 3:C:3136[B]:TYR:HB3 | 2.17 | 0.44 |
| 3:C:3200[A]:LEU:CD2 | 3:C:3204[A]:LEU:CD1 | 2.93 | 0.44 |
| 3:C:3241[A]:PHE:CZ | 3:C:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:C:3252[B]:TYR:HB3 | 3:L:3253[B]:GLU:CG | 2.47 | 0.44 |
| 3:C:3256[B]:TRP:CZ2 | 3:L:2965[B]:LEU:HG | 2.49 | 0.44 |
| 3:C:3266[A]:ILE:O | 3:C:3269[A]:SER:HB2 | 2.17 | 0.44 |
| 1:D:170:HIS:O | 1:D:173:VAL:HG22 | 2.17 | 0.44 |
| 1:D:748:VAL:HG22 | 1:D:781:ILE:HD11 | 1.99 | 0.44 |
| 1:D:957:ASN:CB | 1:D:960:PHE:HB2 | 2.47 | 0.44 |
| 3:F:2964[B]:PRO:CB | 3:a:3255[B]:PRO:HB3 | 2.39 | 0.44 |
| 3:F:2989[B]:HIS:O | 3:F:2990[B]:ARG:C | 2.61 | 0.44 |
| 3:F:3014[B]:TRP:CH2 | 3:F:3123[B]:THR:HG23 | 2.53 | 0.44 |
| 3:F:3019[B]:HIS:CD2 | 3:F:3020[B]:SER:H | 2.36 | 0.44 |
| 3:F:3156[B]:MET:O | 3:a:3153[B]:LYS:NZ | 2.50 | 0.44 |
| 3:F:3241[A]:PHE:CE2 | 3:F:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:F:3241[A]:PHE:CZ | 3:F:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:F:3273[A]:LEU:C | 3:F:3275[A]:LEU:HD12 | 2.42 | 0.44 |
| 3:F:3293[A]:LYS:HB2 | 3:F:3294[A]:SER:CA | 2.41 | 0.44 |
| 1:G:1000:GLU:OE1 | 1:G:1141:ARG:NH2 | 2.50 | 0.44 |
| 1:G:1324:ARG:NH1 | 1:G:1516:VAL:O | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2970[A]:PRO:C | 3:I:2972[A]:GLY:N | 2.72 | 0.44 |
| 3:I:2992[B]:TYR:CE2 | 3:R:2969[B]:TYR:CE1 | 3.05 | 0.44 |
| 3:I:3027[B]:GLU:CD | 3:I:3027[B]:GLU:C | 2.86 | 0.44 |
| 3:I:3183[A]:LEU:N | 3:I:3184[A]:ASN:HA | 2.12 | 0.44 |
| 3:I:3229[B]:ASN:O | 3:I:3286[B]:THR:N | 2.50 | 0.44 |
| 1:J:247:PHE:O | 1:J:252:ASN:ND2 | 2.37 | 0.44 |
| 1:J:906:HIS:HA | 1:J:909:ILE:HG22 | 1.99 | 0.44 |
| 1:J:932:THR:O | 1:J:989:THR:OG1 | 2.32 | 0.44 |
| 1:J:1160:PHE:HB3 | 1:J:1171:LYS:HA | 1.98 | 0.44 |
| 3:L:2994[A]:LYS:O | 3:L:2997[A]:GLU:N | 2.49 | 0.44 |
| 3:L:3004[A]:GLY:C | 3:L:3006[A]:LYS:N | 2.74 | 0.44 |
| 3:L:3087[A]:MET:HA | 3:L:3090[A]:ASN:OD1 | 2.17 | 0.44 |
| 3:L:3135[A]:LYS:HB2 | 3:L:3141[A]:TYR:CD1 | 2.51 | 0.44 |
| 3:L:3200[A]:LEU:CD2 | 3:L:3204[A]:LEU:HD11 | 2.48 | 0.44 |
| 3:L:3204[B]:LEU:CD1 | 3:L:3204[B]:LEU:N | 2.80 | 0.44 |
| 1:M:956:PRO:HD2 | 1:M:957:ASN:O | 2.17 | 0.44 |
| 1:M:1240:ILE:HD12 | 1:M:1247:ARG:HG3 | 2.00 | 0.44 |
| 2:N:2502:LEU:HB3 | 2:Q:2168:ARG:HA | 1.99 | 0.44 |
| 3:O:2963[B]:MET:CE | 3:X:2969[B]:TYR:N | 2.81 | 0.44 |
| 3:O:2967[B]:CYS:CB | 3:X:3155[B]:MET:CG | 2.82 | 0.44 |
| 3:O:2974[B]:ALA:N | 3:X:2977[B]:CYS:O | 2.46 | 0.44 |
| 3:O:2989[A]:HIS:CD2 | 9:O:3401[A]:CUO:O1 | 2.71 | 0.44 |
| 3:O:2989[B]:HIS:CD2 | 9:O:3401[B]:CUO:O1 | 2.70 | 0.44 |
| 3:O:3087[B]:MET:HA | 3:O:3090[B]:ASN:OD1 | 2.17 | 0.44 |
| 3:O:3132[A]:ALA:HB3 | 3:O:3197[A]:ILE:HD13 | 1.99 | 0.44 |
| 3:O:3180[A]:TYR:CB | 3:O:3183[A]:LEU:CD2 | 2.89 | 0.44 |
| 3:O:3298[A]:ASN:CA | 3:O:3299[A]:LEU:HB2 | 2.44 | 0.44 |
| 1:P:842:ASN:HB3 | 1:P:928:TYR:CE1 | 2.52 | 0.44 |
| 2:Q:2270:ILE:HB | 2:Q:2297:HIS:CD2 | 2.53 | 0.44 |
| 2:Q:2635:TYR:HB2 | 1:S:109:LEU:HD21 | 1.99 | 0.44 |
| 2:Q:2765:PRO:HA | 2:Q:2768:LEU:HD12 | 1.98 | 0.44 |
| 3:R:2979[A]:GLN:HB2 | 3:R:2988[A]:TRP:CD1 | 2.52 | 0.44 |
| 3:R:3014[B]:TRP:CG | 3:R:3092[B]:ILE:CD1 | 2.98 | 0.44 |
| 3:R:3027[A]:GLU:CD | 3:R:3027[A]:GLU:C | 2.85 | 0.44 |
| 3:R:3093[A]:HIS:HB2 | 3:R:3248[A]:LEU:CD1 | 2.48 | 0.44 |
| 3:R:3180[B]:TYR:CA | 3:R:3183[B]:LEU:CD2 | 2.95 | 0.44 |
| 3:R:3182[A]:GLN:C | 3:R:3183[A]:LEU:CD1 | 2.91 | 0.44 |
| 3:R:3200[B]:LEU:CD2 | 3:R:3204[B]:LEU:CD1 | 2.93 | 0.44 |
| 1:S:7:VAL:HG23 | 1:S:91:TYR:C | 2.43 | 0.44 |
| 1:S:385:ALA:HB2 | 1:S:391:MET:SD | 2.57 | 0.44 |
| 1:S:1315:GLY:HA3 | 1:S:1601:TRP:CG | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:2571:ARG:NH1 | 2:T:2771:TYR:HB3 | 2.32 | 0.44 |
| 3:U:2956[B]:LYS:O | 3:U:2959[B]:SER:OG | 2.33 | 0.44 |
| 3:U:2961[B]:HIS:HB2 | 3:U:2992[B]:TYR:HE2 | 1.81 | 0.44 |
| 3:U:3037[A]:TYR:C | 3:U:3038[A]:ILE:HG13 | 2.42 | 0.44 |
| 3:U:3163[B]:ASN:HB3 | 3:d:3147[B]:GLU:OE2 | 2.17 | 0.44 |
| 3:U:3171[A]:HIS:C | 3:U:3173[A]:THR:N | 2.73 | 0.44 |
| 3:U:3229[A]:ASN:O | 3:U:3286[A]:THR:N | 2.50 | 0.44 |
| 1:V:71:LEU:HD22 | 1:V:266:LEU:HD21 | 1.99 | 0.44 |
| 1:V:991:LEU:O | 1:V:995:ILE:HG13 | 2.18 | 0.44 |
| 2:W:2644:LEU:HD22 | 2:W:2687:ILE:HG22 | 1.99 | 0.44 |
| 3:X:3148[B]:ILE:HG22 | 3:X:3148[B]:ILE:O | 2.17 | 0.44 |
| 3:X:3149[B]:ASN:N | 3:X:3149[B]:ASN:OD1 | 2.51 | 0.44 |
| 3:X:3161[B]:GLU:CD | 3:X:3161[B]:GLU:H | 2.19 | 0.44 |
| 3:X:3182[B]:GLN:C | 3:X:3183[B]:LEU:CD1 | 2.91 | 0.44 |
| 3:X:3244[B]:THR:H | 3:X:3264[B]:TYR:HE2 | 1.65 | 0.44 |
| 3:X:3266[B]:ILE:O | 3:X:3269[B]:SER:HB2 | 2.17 | 0.44 |
| 1:Y:183:HIS:O | 1:Y:195:SER:HA | 2.17 | 0.44 |
| 1:Y:1134:ASN:HB2 | 1:Y:1253:ILE:HD12 | 2.00 | 0.44 |
| 1:Y:1290:ILE:HD13 | 1:Y:1329:LEU:HG | 1.99 | 0.44 |
| 3:a:2981[A]:GLY:N | 3:a:3086[A]:GLU:OE1 | 2.45 | 0.44 |
| 3:a:3104[B]:MET:SD | 3:a:3110[B]:THR:CG2 | 3.06 | 0.44 |
| 3:a:3149[A]:ASN:OD1 | 3:a:3149[A]:ASN:N | 2.51 | 0.44 |
| 3:a:3229[B]:ASN:O | 3:a:3286[B]:THR:N | 2.50 | 0.44 |
| 3:a:3241[B]:PHE:CE2 | 3:a:3243[B]:GLY:O | 2.70 | 0.44 |
| 3:a:3273[A]:LEU:C | 3:a:3275[A]:LEU:HD12 | 2.42 | 0.44 |
| 3:a:3284[B]:LYS:HD3 | 3:a:3285[B]:VAL:O | 2.16 | 0.44 |
| 1:b:40:TYR:CD1 | 1:b:246:PRO:HG2 | 2.52 | 0.44 |
| 2:c:2345:ASN:HB3 | 2:c:2348:THR:HB | 1.98 | 0.44 |
| 2:c:2723:GLU:HG2 | 2:c:2788:ILE:CD1 | 2.47 | 0.44 |
| 3:d:2986[B]:PRO:CB | 3:d:3127[B]:TRP:CE3 | 3.00 | 0.44 |
| 3:d:3027[A]:GLU:CD | 3:d:3027[A]:GLU:C | 2.85 | 0.44 |
| 3:d:3037[A]:TYR:C | 3:d:3038[A]:ILE:HG13 | 2.42 | 0.44 |
| 3:d:3093[A]:HIS:HB2 | 3:d:3248[A]:LEU:CD1 | 2.48 | 0.44 |
| 3:d:3182[B]:GLN:C | 3:d:3183[B]:LEU:CD1 | 2.90 | 0.44 |
| 3:d:3241[B]:PHE:CE2 | 3:d:3243[B]:GLY:O | 2.70 | 0.44 |
| 3:d:3273[A]:LEU:C | 3:d:3275[A]:LEU:HD12 | 2.42 | 0.44 |
| 3:d:3284[B]:LYS:CD | 3:d:3284[B]:LYS:C | 2.86 | 0.44 |
| 1:A:40:TYR:CG | 1:A:246:PRO:HG2 | 2.52 | 0.44 |
| 1:A:117:LYS:H | 1:A:117:LYS:HG2 | 1.33 | 0.44 |
| 1:A:173:VAL:HG12 | 1:A:354:PHE:CD1 | 2.53 | 0.44 |
| 1:A:1209:ASP:HA | 2:E:2743:ALA:HB1 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1211:TYR:OH | 2:E:2739:LEU:HB2 | 2.18 | 0.44 |
| 1:A:1305:GLY:HA3 | 1:A:1306:THR:HA | 1.60 | 0.44 |
| 2:B:2244:PHE:HD1 | 2:B:2373:MET:HE2 | 1.81 | 0.44 |
| 3:C:2982[B]:MET:HB2 | 3:L:3156[B]:MET:CB | 2.09 | 0.44 |
| 3:C:3037[B]:TYR:C | 3:C:3038[B]:ILE:HG13 | 2.42 | 0.44 |
| 3:C:3132[B]:ALA:HB3 | 3:C:3197[B]:ILE:HD13 | 1.99 | 0.44 |
| 3:C:3133[A]:LEU:O | 3:C:3136[A]:TYR:HB3 | 2.17 | 0.44 |
| 3:C:3154[B]:PRO:O | 3:L:3155[B]:MET:CE | 2.64 | 0.44 |
| 3:C:3182[A]:GLN:C | 3:C:3183[A]:LEU:CD1 | 2.90 | 0.44 |
| 1:D:670:PRO:HD2 | 1:D:671:PHE:CD1 | 2.53 | 0.44 |
| 2:E:2147:GLY:N | 2:E:2264:GLU:OE2 | 2.48 | 0.44 |
| 2:E:2573:TYR:CE2 | 2:E:2707:PHE:HE2 | 2.33 | 0.44 |
| 3:F:3180[A]:TYR:CB | 3:F:3183[A]:LEU:CD2 | 2.90 | 0.44 |
| 3:F:3182[B]:GLN:C | 3:F:3183[B]:LEU:CD1 | 2.90 | 0.44 |
| 3:F:3191[B]:ASN:ND2 | 3:F:3191[B]:ASN:N | 2.60 | 0.44 |
| 3:F:3229[A]:ASN:O | 3:F:3286[A]:THR:N | 2.50 | 0.44 |
| 3:F:3232[A]:VAL:HG21 | 3:F:3273[A]:LEU:HD11 | 2.00 | 0.44 |
| 3:F:3252[B]:TYR:C | 3:a:3252[B]:TYR:O | 2.60 | 0.44 |
| 1:G:562:GLN:HG2 | 1:G:563:ILE:N | 2.33 | 0.44 |
| 1:G:784:ALA:O | 1:G:788:LEU:HB2 | 2.17 | 0.44 |
| 1:G:1581:GLU:HG3 | 1:G:1582:ASN:N | 2.31 | 0.44 |
| 2:H:2286:HIS:CD2 | 2:H:2433:THR:HG22 | 2.51 | 0.44 |
| 2:H:2450:ILE:O | 2:H:2454:MET:HG3 | 2.17 | 0.44 |
| 3:I:2938[A]:LEU:O | 3:I:2939[A]:ARG:C | 2.58 | 0.44 |
| 3:I:2981[B]:GLY:CA | 3:R:2966[B]:SER:O | 2.65 | 0.44 |
| 3:I:2986[A]:PRO:CB | 3:I:3127[A]:TRP:CE3 | 3.00 | 0.44 |
| 3:I:3074[A]:GLU:CD | 3:I:3212[A]:ARG:NH2 | 2.73 | 0.44 |
| 3:I:3074[B]:GLU:CD | 3:I:3212[B]:ARG:NH2 | 2.73 | 0.44 |
| 3:I:3116[B]:PHE:C | 3:I:3116[B]:PHE:CD1 | 2.94 | 0.44 |
| 3:I:3137[A]:ARG:HA | 3:I:3137[A]:ARG:HD3 | 1.72 | 0.44 |
| 3:I:3150[B]:LYS:HB2 | 3:R:3169[B]:LYS:HE3 | 1.99 | 0.44 |
| 3:I:3174[B]:GLY:H | 3:R:3154[B]:PRO:CB | 2.02 | 0.44 |
| 1:J:876:PHE:H | 1:J:876:PHE:HD1 | 1.65 | 0.44 |
| 1:J:1315:GLY:HA3 | 1:J:1601:TRP:CG | 2.53 | 0.44 |
| 2:K:2821:LEU:HD11 | 2:K:2879:LEU:HD23 | 1.98 | 0.44 |
| 3:L:2989[B]:HIS:C | 3:L:2991[B]:LEU:N | 2.75 | 0.44 |
| 3:L:2991[B]:LEU:HD23 | 3:L:3158[B]:PHE:CE1 | 2.47 | 0.44 |
| 3:L:3013[B]:ASP:CG | 3:L:3015[B]:THR:HG1 | 2.23 | 0.44 |
| 3:L:3019[B]:HIS:CD2 | 3:L:3020[B]:SER:H | 2.35 | 0.44 |
| 3:L:3087[B]:MET:HA | 3:L:3090[B]:ASN:OD1 | 2.17 | 0.44 |
| 3:L:3171[A]:HIS:C | 3:L:3173[A]:THR:N | 2.73 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:883:CYS:HB3 | 1:M:884:PRO:CD | 2.47 | 0.44 |
| 1:M:1240:ILE:HG22 | 1:M:1250:ILE:HG21 | 1.99 | 0.44 |
| 1:M:1348:TRP:CG | 1:M:1430:ILE:HD11 | 2.51 | 0.44 |
| 2:N:2161:GLN:NE2 | 2:N:2348:THR:HG21 | 2.33 | 0.44 |
| 3:O:2969[B]:TYR:CA | 3:X:2991[B]:LEU:HD22 | 2.36 | 0.44 |
| 3:O:3024[A]:LEU:CD1 | 3:O:3024[A]:LEU:C | 2.85 | 0.44 |
| 3:O:3101[A]:PRO:O | 3:O:3109[A]:TYR:HD2 | 2.00 | 0.44 |
| 3:O:3157[B]:PRO:O | 3:X:3149[B]:ASN:CA | 2.57 | 0.44 |
| 3:O:3159[B]:SER:HB2 | 3:X:3152[B]:LYS:HG2 | 1.12 | 0.44 |
| 3:O:3241[A]:PHE:CZ | 3:O:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:O:3255[B]:PRO:CB | 3:X:3161[B]:GLU:HA | 2.48 | 0.44 |
| 1:P:450:LYS:CE | 1:P:451:SER:H | 2.30 | 0.44 |
| 1:P:729:VAL:HG11 | 1:P:785:LEU:HD12 | 1.99 | 0.44 |
| 1:P:1209:ASP:O | 1:P:1211:TYR:HD2 | 2.00 | 0.44 |
| 3:R:2961[A]:HIS:CD2 | 3:R:2988[A]:TRP:CZ3 | 2.96 | 0.44 |
| 3:R:2986[A]:PRO:CB | 3:R:3127[A]:TRP:CE3 | 3.00 | 0.44 |
| 3:R:3019[B]:HIS:CD2 | 3:R:3020[B]:SER:H | 2.35 | 0.44 |
| 3:R:3024[A]:LEU:CD1 | 3:R:3024[A]:LEU:C | 2.85 | 0.44 |
| 3:R:3218[B]:LEU:HD12 | 3:R:3218[B]:LEU:HA | 1.78 | 0.44 |
| 1:S:729:VAL:HG23 | 1:S:820:VAL:HG13 | 1.99 | 0.44 |
| 1:S:899:MET:HE2 | 1:S:1012:GLU:OE2 | 2.17 | 0.44 |
| 1:S:1575:PRO:HA | 1:S:1581:GLU:O | 2.18 | 0.44 |
| 2:T:2161:GLN:NE2 | 2:T:2348:THR:HG21 | 2.32 | 0.44 |
| 2:T:2317:LEU:HB3 | 2:T:2318:PRO:HD2 | 2.00 | 0.44 |
| 3:U:3024[A]:LEU:CD1 | 3:U:3024[A]:LEU:C | 2.85 | 0.44 |
| 3:U:3087[A]:MET:HA | 3:U:3090[A]:ASN:OD1 | 2.17 | 0.44 |
| 3:U:3132[A]:ALA:HB3 | 3:U:3197[A]:ILE:HD13 | 1.98 | 0.44 |
| 3:U:3133[B]:LEU:O | 3:U:3136[B]:TYR:HB3 | 2.17 | 0.44 |
| 3:U:3137[B]:ARG:O | 3:U:3139[B]:LEU:HD22 | 2.16 | 0.44 |
| 3:U:3230[B]:PHE:CB | 3:U:3242[B]:GLY:C | 2.91 | 0.44 |
| 3:U:3241[A]:PHE:CZ | 3:U:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:U:3241[B]:PHE:CZ | 3:U:3243[B]:GLY:O | 2.70 | 0.44 |
| 3:U:3242[B]:GLY:C | 3:U:3243[B]:GLY:O | 2.58 | 0.44 |
| 3:U:3254[B]:MET:CB | 3:d:3254[B]:MET:HB3 | 2.25 | 0.44 |
| 3:U:3301[B]:PRO:HB2 | 3:U:3302[B]:SER:H | 1.33 | 0.44 |
| 1:V:111:ILE:HG23 | 2:Z:2637:VAL:HG11 | 1.99 | 0.44 |
| 1:V:1086:LEU:HD13 | 1:V:1090:ILE:HG21 | 1.98 | 0.44 |
| 2:W:2722:GLN:NE2 | 2:W:2769:PHE:O | 2.33 | 0.44 |
| 3:X:2969[A]:TYR:CD2 | 3:X:2970[A]:PRO:CG | 3.00 | 0.44 |
| 3:X:2986[B]:PRO:CB | 3:X:3127[B]:TRP:CE3 | 3.00 | 0.44 |
| 3:X:3027[B]:GLU:CD | 3:X:3027[B]:GLU:C | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3037[A]:TYR:C | 3:X:3038[A]:ILE:HG13 | 2.42 | 0.44 |
| 3:X:3133[A]:LEU:O | 3:X:3136[A]:TYR:HB3 | 2.17 | 0.44 |
| 3:X:3200[B]:LEU:CD2 | 3:X:3204[B]:LEU:HD11 | 2.47 | 0.44 |
| 1:Y:654:PRO:HB2 | 1:Y:658:TYR:HE2 | 1.82 | 0.44 |
| 1:Y:1156:LEU:HB2 | 1:Y:1176:TYR:HE1 | 1.83 | 0.44 |
| 1:Y:1616:LYS:HG2 | 3:d:3186[B]:GLU:HB3 | 1.66 | 0.44 |
| 2:Z:2142:ALA:HB3 | 2:Z:2434:GLU:HA | 1.99 | 0.44 |
| 2:Z:2627:GLY:HA3 | 2:Z:2703:PHE:O | 2.17 | 0.44 |
| 2:Z:2782:ASN:HB2 | 2:Z:2786:MET:O | 2.17 | 0.44 |
| 2:Z:2866:PRO:HB3 | 3:a:2933[A]:SER:CB | 2.47 | 0.44 |
| 3:a:2969[A]:TYR:CD2 | 3:a:2970[A]:PRO:CG | 3.00 | 0.44 |
| 3:a:2986[B]:PRO:CB | 3:a:3127[B]:TRP:CE3 | 3.00 | 0.44 |
| 3:a:3028[B]:PRO:HG2 | 3:a:3029[B]:LYS:HG3 | 2.00 | 0.44 |
| 3:a:3093[B]:HIS:HB2 | 3:a:3248[B]:LEU:CD1 | 2.48 | 0.44 |
| 3:a:3093[B]:HIS:HD2 | 3:a:3248[B]:LEU:CD2 | 2.31 | 0.44 |
| 3:a:3283[A]:ILE:C | 3:a:3283[A]:ILE:CD1 | 2.85 | 0.44 |
| 3:a:3298[B]:ASN:CA | 3:a:3299[B]:LEU:HB2 | 2.44 | 0.44 |
| 1:b:953:GLU:HG2 | 1:b:954:ALA:N | 2.32 | 0.44 |
| 3:d:2989[B]:HIS:O | 3:d:2990[B]:ARG:C | 2.61 | 0.44 |
| 3:d:3093[B]:HIS:HB2 | 3:d:3248[B]:LEU:CD1 | 2.47 | 0.44 |
| 3:d:3182[A]:GLN:C | 3:d:3183[A]:LEU:CD1 | 2.91 | 0.44 |
| 1:A:903:PRO:HG2 | 1:A:904:HIS:CD2 | 2.53 | 0.44 |
| 1:A:974:ALA:HB1 | 1:A:1022:VAL:HG22 | 2.00 | 0.44 |
| 2:B:2155:HIS:CD2 | 2:B:2298:HIS:CE1 | 3.05 | 0.44 |
| 2:B:2739:LEU:HD12 | 1:D:1211:TYR:OH | 2.17 | 0.44 |
| 3:C:2951[B]:ASP:CG | 3:C:2952[B]:ALA:N | 2.74 | 0.44 |
| 3:C:2965[B]:LEU:HB2 | 3:L:3222[B]:ILE:N | 2.31 | 0.44 |
| 3:C:3074[B]:GLU:CD | 3:C:3212[B]:ARG:NH2 | 2.73 | 0.44 |
| 3:C:3137[A]:ARG:O | 3:C:3139[A]:LEU:HD22 | 2.16 | 0.44 |
| 3:C:3146[B]:CYS:HA | 3:C:3147[B]:GLU:HA | 1.70 | 0.44 |
| 3:C:3161[B]:GLU:N | 3:L:2983[B]:VAL:CG2 | 2.41 | 0.44 |
| 3:C:3182[B]:GLN:C | 3:C:3183[B]:LEU:CD1 | 2.91 | 0.44 |
| 3:C:3200[A]:LEU:CD2 | 3:C:3204[A]:LEU:HD11 | 2.48 | 0.44 |
| 3:C:3241[A]:PHE:CE2 | 3:C:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:C:3242[B]:GLY:C | 3:C:3243[B]:GLY:O | 2.58 | 0.44 |
| 1:D:350:MET:O | 1:D:352:TRP:HD1 | 2.00 | 0.44 |
| 1:D:516:TRP:CD1 | 1:D:579:LEU:HD13 | 2.53 | 0.44 |
| 1:D:1494:ARG:HH11 | 1:D:1494:ARG:CG | 2.16 | 0.44 |
| 2:E:2631:TYR:HD1 | 2:E:2631:TYR:H | 1.64 | 0.44 |
| 3:F:3023[B]:ILE:O | 3:F:3026[B]:THR:OG1 | 2.34 | 0.44 |
| 3:F:3087[A]:MET:HA | 3:F:3090[A]:ASN:OD1 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3104[B]:MET:HA | 3:F:3110[B]:THR:CG2 | 2.17 | 0.44 |
| 3:F:3133[B]:LEU:O | 3:F:3136[B]:TYR:HB3 | 2.17 | 0.44 |
| 3:F:3157[B]:PRO:HD2 | 3:a:3153[B]:LYS:HZ2 | 1.81 | 0.44 |
| 3:F:3200[A]:LEU:CD2 | 3:F:3204[A]:LEU:CD1 | 2.93 | 0.44 |
| 3:F:3218[B]:LEU:HD12 | 3:F:3218[B]:LEU:HA | 1.78 | 0.44 |
| 3:F:3225[B]:SER:C | 3:F:3290[B]:ILE:HG23 | 2.39 | 0.44 |
| 3:F:3273[B]:LEU:C | 3:F:3275[B]:LEU:HD12 | 2.42 | 0.44 |
| 1:G:1055:THR:HA | 1:G:1119:LEU:HD13 | 1.99 | 0.44 |
| 2:H:2424:SER:HB3 | 2:H:2445:MET:HG2 | 1.99 | 0.44 |
| 2:H:2527:LEU:HD22 | 2:H:2581:MET:HG3 | 2.00 | 0.44 |
| 2:H:2680:HIS:CD2 | 2:H:2684:HIS:HD2 | 2.36 | 0.44 |
| 3:I:2946[A]:GLN:CD | 3:I:2947[A]:ALA:N | 2.72 | 0.44 |
| 3:I:2989[A]:HIS:O | 3:I:2990[A]:ARG:C | 2.61 | 0.44 |
| 3:I:3014[A]:TRP:CG | 3:I:3092[A]:ILE:CD1 | 2.98 | 0.44 |
| 3:I:3014[A]:TRP:CH2 | 3:I:3123[A]:THR:HG23 | 2.53 | 0.44 |
| 3:I:3023[B]:ILE:HA | 3:I:3026[B]:THR:HG1 | 1.83 | 0.44 |
| 3:I:3137[A]:ARG:HB3 | 3:I:3139[A]:LEU:HD21 | 1.97 | 0.44 |
| 3:I:3147[B]:GLU:CD | 3:R:3163[B]:ASN:O | 2.61 | 0.44 |
| 3:I:3169[B]:LYS:O | 3:R:3152[B]:LYS:CA | 2.62 | 0.44 |
| 3:I:3180[B]:TYR:CB | 3:I:3183[B]:LEU:CD2 | 2.89 | 0.44 |
| 3:I:3185[A]:TYR:HE2 | 3:I:3187[A]:TYR:CD2 | 2.35 | 0.44 |
| 3:I:3191[B]:ASN:C | 3:I:3192[B]:PHE:O | 2.52 | 0.44 |
| 3:I:3196[A]:THR:CB | 3:I:3199[A]:GLN:OE1 | 2.64 | 0.44 |
| 3:I:3200[A]:LEU:CD2 | 3:I:3204[A]:LEU:CD1 | 2.93 | 0.44 |
| 1:J:119:LYS:HB2 | 1:J:120:LYS:CA | 2.48 | 0.44 |
| 1:J:931:TRP:CD1 | 1:J:1048:ASN:HD22 | 2.36 | 0.44 |
| 1:J:1629:GLU:HG3 | 1:J:1630:MET:N | 2.33 | 0.44 |
| 2:K:2390:GLN:O | 2:K:2491:PRO:HB3 | 2.18 | 0.44 |
| 2:K:2602:LEU:HG | 2:K:2603:PRO:HD2 | 2.00 | 0.44 |
| 3:L:2949[A]:LYS:NZ | 3:L:2949[A]:LYS:C | 2.73 | 0.44 |
| 3:L:2988[B]:TRP:CD1 | 3:L:3158[B]:PHE:CE2 | 3.06 | 0.44 |
| 3:L:3074[A]:GLU:CD | 3:L:3212[A]:ARG:NH2 | 2.73 | 0.44 |
| 3:L:3230[A]:PHE:CB | 3:L:3242[A]:GLY:C | 2.91 | 0.44 |
| 3:L:3266[A]:ILE:O | 3:L:3269[A]:SER:HB2 | 2.17 | 0.44 |
| 3:L:3273[A]:LEU:C | 3:L:3275[A]:LEU:HD12 | 2.42 | 0.44 |
| 1:M:930:ASP:OD1 | 1:M:1051:ARG:NH2 | 2.51 | 0.44 |
| 1:M:1649:THR:HA | 2:Q:2327:GLU:HG2 | 2.00 | 0.44 |
| 2:N:2797:LYS:HA | 2:N:2800:LYS:HD3 | 1.98 | 0.44 |
| 3:O:2956[B]:LYS:O | 3:O:2959[B]:SER:OG | 2.33 | 0.44 |
| 3:O:3093[A]:HIS:HD2 | 3:O:3248[A]:LEU:CD2 | 2.30 | 0.44 |
| 3:O:3135[B]:LYS:HB2 | 3:O:3141[B]:TYR:CD1 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3230[B]:PHE:CB | 3:O:3242[B]:GLY:C | 2.91 | 0.44 |
| 3:O:3300[A]:LEU:HD23 | 3:O:3300[A]:LEU:H | 1.83 | 0.44 |
| 1:P:567:LEU:HB2 | 1:P:571:PRO:CA | 2.46 | 0.44 |
| 1:P:745:ASP:HB2 | 1:P:801:ASP:OD1 | 2.16 | 0.44 |
| 1:P:962:GLY:HA2 | 1:P:971:THR:HB | 1.99 | 0.44 |
| 1:P:1013:ILE:HG21 | 1:P:1192:TYR:CD1 | 2.53 | 0.44 |
| 3:R:2988[B]:TRP:CD1 | 3:R:3158[B]:PHE:CE2 | 3.06 | 0.44 |
| 3:R:3031[B]:ASN:HA | 3:R:3032[B]:PRO:HD2 | 1.87 | 0.44 |
| 3:R:3047[A]:ARG:NH2 | 3:R:3113[A]:ASP:OD1 | 2.43 | 0.44 |
| 3:R:3106[A]:THR:O | 3:R:3106[A]:THR:HG23 | 2.16 | 0.44 |
| 3:R:3182[B]:GLN:C | 3:R:3183[B]:LEU:CD1 | 2.91 | 0.44 |
| 3:R:3284[A]:LYS:CE | 3:R:3285[A]:VAL:H | 2.29 | 0.44 |
| 1:S:400:ILE:HG23 | 1:S:663:GLU:HG2 | 1.99 | 0.44 |
| 1:S:739:GLN:OE1 | 1:S:739:GLN:N | 2.51 | 0.44 |
| 1:S:1485:ALA:O | 1:S:1489:MET:HG2 | 2.18 | 0.44 |
| 2:T:2132:CYS:HB2 | 2:T:2142:ALA:HB1 | 1.99 | 0.44 |
| 2:T:2550:THR:O | 2:T:2553:ALA:N | 2.27 | 0.44 |
| 2:T:2799:LYS:HA | 2:T:2803:ARG:NH1 | 2.32 | 0.44 |
| 3:U:2938[B]:LEU:O | 3:U:2939[B]:ARG:C | 2.58 | 0.44 |
| 3:U:2980[B]:HIS:HB2 | 3:d:2969[B]:TYR:OH | 2.17 | 0.44 |
| 3:U:2988[B]:TRP:CD1 | 3:U:3158[B]:PHE:CE2 | 3.06 | 0.44 |
| 3:U:3004[A]:GLY:C | 3:U:3006[A]:LYS:N | 2.74 | 0.44 |
| 3:U:3200[A]:LEU:CD2 | 3:U:3204[A]:LEU:HD11 | 2.48 | 0.44 |
| 3:U:3225[A]:SER:C | 3:U:3290[A]:ILE:HG23 | 2.39 | 0.44 |
| 1:V:639:ARG:HB2 | 1:V:703:TYR:CE1 | 2.52 | 0.44 |
| 2:W:2124:SER:HB2 | 2:W:2129:PRO:HG2 | 2.00 | 0.44 |
| 2:W:2745:PRO:HA | 2:W:2764:THR:HA | 1.99 | 0.44 |
| 3:X:2931[A]:THR:O | 3:X:2934[A]:GLU:HG3 | 2.18 | 0.44 |
| 3:X:3093[A]:HIS:HB2 | 3:X:3248[A]:LEU:CD1 | 2.48 | 0.44 |
| 3:X:3171[B]:HIS:C | 3:X:3173[B]:THR:N | 2.73 | 0.44 |
| 3:X:3183[A]:LEU:H | 3:X:3184[A]:ASN:CA | 2.21 | 0.44 |
| 3:X:3222[B]:ILE:CD1 | 3:X:3223[B]:GLY:N | 2.73 | 0.44 |
| 3:X:3293[B]:LYS:HB2 | 3:X:3294[B]:SER:CA | 2.41 | 0.44 |
| 1:Y:638:ASP:O | 1:Y:641:TRP:HB3 | 2.18 | 0.44 |
| 1:Y:999:LEU:HB3 | 1:Y:1133:ILE:HD11 | 2.00 | 0.44 |
| 2:Z:2234:GLN:HG3 | 2:Z:2235:PRO:HD2 | 1.99 | 0.44 |
| 2:Z:2866:PRO:CG | 3:a:2933[A]:SER:OG | 2.65 | 0.44 |
| 3:a:2989[A]:HIS:O | 3:a:2990[A]:ARG:C | 2.61 | 0.44 |
| 3:a:3014[A]:TRP:CH2 | 3:a:3123[A]:THR:HG23 | 2.53 | 0.44 |
| 3:a:3019[A]:HIS:CD2 | 3:a:3020[A]:SER:H | 2.35 | 0.44 |
| 3:a:3019[B]:HIS:CD2 | 3:a:3020[B]:SER:H | 2.35 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3093[A]:HIS:HD2 | 3:a:3248[A]:LEU:CD2 | 2.30 | 0.44 |
| 3:a:3104[A]:MET:SD | 3:a:3110[A]:THR:CG2 | 3.06 | 0.44 |
| 3:a:3137[B]:ARG:HD3 | 3:a:3137[B]:ARG:HA | 1.72 | 0.44 |
| 3:a:3182[B]:GLN:C | 3:a:3183[B]:LEU:CD1 | 2.91 | 0.44 |
| 3:a:3218[A]:LEU:HD12 | 3:a:3218[A]:LEU:HA | 1.78 | 0.44 |
| 3:a:3229[A]:ASN:O | 3:a:3286[A]:THR:N | 2.50 | 0.44 |
| 3:a:3299[A]:LEU:O | 3:a:3300[A]:LEU:C | 2.60 | 0.44 |
| 1:b:1427:HIS:NE2 | 1:b:1431:HIS:CD2 | 2.84 | 0.44 |
| 3:d:2951[A]:ASP:CG | 3:d:2952[A]:ALA:N | 2.74 | 0.44 |
| 3:d:2961[A]:HIS:HB2 | 3:d:2992[A]:TYR:HE2 | 1.80 | 0.44 |
| 3:d:3014[B]:TRP:CH2 | 3:d:3123[B]:THR:HG23 | 2.53 | 0.44 |
| 3:d:3019[A]:HIS:CD2 | 3:d:3020[A]:SER:H | 2.35 | 0.44 |
| 3:d:3116[A]:PHE:CD1 | 3:d:3116[A]:PHE:C | 2.94 | 0.44 |
| 3:d:3119[A]:HIS:O | 3:d:3122[A]:ASN:HB3 | 2.17 | 0.44 |
| 3:d:3230[B]:PHE:CB | 3:d:3242[B]:GLY:C | 2.91 | 0.44 |
| 3:d:3283[A]:ILE:C | 3:d:3283[A]:ILE:CD1 | 2.85 | 0.44 |
| 3:d:3293[B]:LYS:HB2 | 3:d:3294[B]:SER:CA | 2.41 | 0.44 |
| 1:A:1145:THR:HB | 1:A:1191:PRO:CB | 2.47 | 0.44 |
| 1:A:1260:ARG:HD3 | 1:A:1331:GLU:OE1 | 2.17 | 0.44 |
| 1:A:1622:GLN:HG2 | 1:A:1652:PHE:CD1 | 2.53 | 0.44 |
| 2:B:2814:LYS:HE3 | 2:B:2843:GLU:HB3 | 1.99 | 0.44 |
| 3:C:2931[B]:THR:O | 3:C:2934[B]:GLU:HG3 | 2.18 | 0.44 |
| 3:C:2989[A]:HIS:C | 3:C:2991[A]:LEU:N | 2.75 | 0.44 |
| 3:C:3025[B]:VAL:CG2 | 3:C:3047[B]:ARG:NH1 | 2.73 | 0.44 |
| 3:C:3171[A]:HIS:C | 3:C:3173[A]:THR:N | 2.73 | 0.44 |
| 3:C:3218[A]:LEU:HD12 | 3:C:3218[A]:LEU:HA | 1.78 | 0.44 |
| 3:C:3229[B]:ASN:O | 3:C:3286[B]:THR:N | 2.50 | 0.44 |
| 3:C:3244[A]:THR:H | 3:C:3264[A]:TYR:HE2 | 1.65 | 0.44 |
| 3:C:3254[B]:MET:HE2 | 3:L:2977[B]:CYS:HB3 | 1.02 | 0.44 |
| 1:D:464:LEU:HD13 | 1:D:622:HIS:CG | 2.52 | 0.44 |
| 1:D:999:LEU:HD12 | 1:D:1056:TRP:HD1 | 1.82 | 0.44 |
| 2:E:2329:MET:HA | 2:E:2354:PRO:HG2 | 2.00 | 0.44 |
| 2:E:2389:ARG:HG2 | 2:E:2393:ARG:HH22 | 1.82 | 0.44 |
| 3:F:2979[B]:GLN:HB2 | 3:F:2988[B]:TRP:CD1 | 2.52 | 0.44 |
| 3:F:2989[A]:HIS:CD2 | 9:a:3401[A]:CUO:O1 | 2.71 | 0.44 |
| 3:F:3242[A]:GLY:C | 3:F:3243[A]:GLY:O | 2.58 | 0.44 |
| 3:F:3248[B]:LEU:HB3 | 3:a:2973[B]:THR:C | 2.24 | 0.44 |
| 3:F:3266[A]:ILE:O | 3:F:3269[A]:SER:HB2 | 2.17 | 0.44 |
| 1:G:946:GLU:HG2 | 1:G:955:LYS:HB3 | 1.99 | 0.44 |
| 1:G:961:SER:HB3 | 1:G:974:ALA:HB3 | 2.00 | 0.44 |
| 1:G:1245:GLU:N | 1:G:1245:GLU:OE1 | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2989[A]:HIS:CD2 | 9:R:3401[A]:CUO:O1 | 2.71 | 0.44 |
| 3:I:3019[A]:HIS:CD2 | 3:I:3020[A]:SER:H | 2.35 | 0.44 |
| 3:I:3101[A]:PRO:O | 3:I:3109[A]:TYR:HD2 | 2.00 | 0.44 |
| 3:I:3106[B]:THR:O | 3:I:3106[B]:THR:HG23 | 2.17 | 0.44 |
| 3:I:3160[B]:SER:O | 3:R:3147[B]:GLU:HG3 | 2.18 | 0.44 |
| 3:I:3163[B]:ASN:HD22 | 3:R:3150[B]:LYS:HG3 | 0.59 | 0.44 |
| 3:I:3241[B]:PHE:CE2 | 3:I:3243[B]:GLY:O | 2.70 | 0.44 |
| 2:K:2114:ARG:HA | 2:K:2114:ARG:HD3 | 1.82 | 0.44 |
| 3:L:3013[A]:ASP:CG | 3:L:3015[A]:THR:HG1 | 2.24 | 0.44 |
| 3:L:3106[A]:THR:O | 3:L:3106[A]:THR:HG23 | 2.16 | 0.44 |
| 3:L:3182[A]:GLN:C | 3:L:3183[A]:LEU:CD1 | 2.90 | 0.44 |
| 3:L:3182[B]:GLN:C | 3:L:3183[B]:LEU:CD1 | 2.91 | 0.44 |
| 3:L:3241[A]:PHE:CE2 | 3:L:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:L:3241[B]:PHE:CZ | 3:L:3243[B]:GLY:O | 2.70 | 0.44 |
| 3:L:3293[A]:LYS:HB2 | 3:L:3294[A]:SER:CA | 2.41 | 0.44 |
| 1:M:669:LYS:HA | 1:M:669:LYS:HD2 | 1.63 | 0.44 |
| 2:N:2361:LYS:HD2 | 2:N:2362:GLN:N | 2.32 | 0.44 |
| 2:N:2472:ASN:N | 2:N:2473:GLY:HA2 | 2.33 | 0.44 |
| 3:O:2972[B]:GLY:HA3 | 3:X:2985[B]:PHE:O | 2.18 | 0.44 |
| 3:O:3104[A]:MET:SD | 3:O:3110[A]:THR:CG2 | 3.06 | 0.44 |
| 3:O:3180[B]:TYR:CA | 3:O:3183[B]:LEU:CD2 | 2.95 | 0.44 |
| 3:O:3230[A]:PHE:CB | 3:O:3242[A]:GLY:C | 2.91 | 0.44 |
| 3:O:3285[B]:VAL:CG2 | 3:O:3286[B]:THR:H | 2.27 | 0.44 |
| 1:P:788:LEU:HB3 | 1:P:790:VAL:HG23 | 1.99 | 0.44 |
| 1:P:1091:ASN:HA | 1:P:1092:PRO:HD3 | 1.61 | 0.44 |
| 1:P:1279:LYS:HE3 | 1:P:1376:PRO:HG3 | 2.00 | 0.44 |
| 1:P:1528:ASP:OD1 | 1:P:1528:ASP:N | 2.48 | 0.44 |
| 2:Q:2800:LYS:HB3 | 3:R:3023[A]:ILE:HD13 | 1.99 | 0.44 |
| 3:R:2940[A]:ASN:O | 3:R:2943[A]:ALA:HB3 | 2.18 | 0.44 |
| 3:R:3014[A]:TRP:CH2 | 3:R:3123[A]:THR:HG23 | 2.53 | 0.44 |
| 3:R:3019[A]:HIS:CD2 | 3:R:3020[A]:SER:H | 2.35 | 0.44 |
| 3:R:3093[A]:HIS:HD2 | 3:R:3248[A]:LEU:CD2 | 2.30 | 0.44 |
| 3:R:3093[B]:HIS:HD2 | 3:R:3248[B]:LEU:CD2 | 2.31 | 0.44 |
| 3:R:3133[B]:LEU:O | 3:R:3136[B]:TYR:HB3 | 2.18 | 0.44 |
| 3:R:3204[A]:LEU:CD1 | 3:R:3204[A]:LEU:N | 2.80 | 0.44 |
| 3:R:3230[B]:PHE:CB | 3:R:3242[B]:GLY:C | 2.91 | 0.44 |
| 3:R:3244[A]:THR:H | 3:R:3264[A]:TYR:HE2 | 1.65 | 0.44 |
| 3:R:3266[A]:ILE:O | 3:R:3269[A]:SER:HB2 | 2.17 | 0.44 |
| 1:S:22:LEU:HD12 | 1:S:25:MET:HG2 | 1.98 | 0.44 |
| 1:S:633:HIS:C | 1:S:633:HIS:ND1 | 2.75 | 0.44 |
| 1:S:903:PRO:HG3 | 1:S:1004:PHE:HZ | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1195:ASP:HA | 1:S:1196:ILE:HG22 | 1.98 | 0.44 |
| 1:S:1335:LEU:HD23 | 1:S:1339:SER:HA | 1.99 | 0.44 |
| 1:S:1634:ALA:HB2 | 1:S:1639:LYS:NZ | 2.33 | 0.44 |
| 2:T:2873:HIS:ND1 | 1:V:1101:VAL:HG21 | 2.32 | 0.44 |
| 3:U:2963[B]:MET:SD | 3:U:2963[B]:MET:C | 3.01 | 0.44 |
| 3:U:2975[B]:PHE:CG | 3:d:3256[B]:TRP:CB | 3.00 | 0.44 |
| 3:U:2979[B]:GLN:HB2 | 3:U:2988[B]:TRP:CD1 | 2.52 | 0.44 |
| 3:U:2986[A]:PRO:CB | 3:U:3127[A]:TRP:CE3 | 3.00 | 0.44 |
| 3:U:3023[B]:ILE:O | 3:U:3026[B]:THR:OG1 | 2.34 | 0.44 |
| 3:U:3148[A]:ILE:O | 3:U:3148[A]:ILE:HG22 | 2.17 | 0.44 |
| 3:U:3182[B]:GLN:C | 3:U:3183[B]:LEU:CD1 | 2.91 | 0.44 |
| 3:U:3230[A]:PHE:CB | 3:U:3242[A]:GLY:C | 2.91 | 0.44 |
| 1:V:1324:ARG:NH1 | 1:V:1516:VAL:O | 2.50 | 0.44 |
| 1:V:1587:ALA:HA | 1:V:1614:GLU:HG2 | 1.99 | 0.44 |
| 3:X:2956[B]:LYS:O | 3:X:2959[B]:SER:OG | 2.33 | 0.44 |
| 3:X:3028[B]:PRO:HG2 | 3:X:3029[B]:LYS:HG3 | 2.00 | 0.44 |
| 3:X:3146[A]:CYS:HA | 3:X:3147[A]:GLU:HA | 1.70 | 0.44 |
| 3:X:3146[B]:CYS:HA | 3:X:3147[B]:GLU:HA | 1.70 | 0.44 |
| 3:X:3196[B]:THR:CB | 3:X:3199[B]:GLN:OE1 | 2.64 | 0.44 |
| 3:X:3200[A]:LEU:CD2 | 3:X:3204[A]:LEU:HD11 | 2.48 | 0.44 |
| 1:Y:1158:GLU:HB2 | 1:Y:1171:LYS:HE3 | 2.00 | 0.44 |
| 2:Z:2107:LEU:HA | 2:Z:2110:MET:HG2 | 1.98 | 0.44 |
| 2:Z:2244:PHE:HA | 2:Z:2373:MET:HE1 | 1.99 | 0.44 |
| 2:Z:2310:GLU:HG3 | 2:Z:2371:LEU:HD13 | 1.99 | 0.44 |
| 2:Z:2824:CYS:HB3 | 2:Z:2826:GLU:O | 2.17 | 0.44 |
| 3:a:2979[A]:GLN:HG2 | 3:a:3155[A]:MET:HE2 | 1.85 | 0.44 |
| 3:a:2988[B]:TRP:CD1 | 3:a:3158[B]:PHE:CE2 | 3.06 | 0.44 |
| 3:a:2989[A]:HIS:C | 3:a:2991[A]:LEU:N | 2.75 | 0.44 |
| 3:a:3038[B]:ILE:HG23 | 3:a:3040[B]:VAL:HG22 | 1.90 | 0.44 |
| 3:a:3074[A]:GLU:CD | 3:a:3212[A]:ARG:NH2 | 2.73 | 0.44 |
| 3:a:3244[A]:THR:H | 3:a:3264[A]:TYR:HE2 | 1.65 | 0.44 |
| 3:a:3266[A]:ILE:O | 3:a:3269[A]:SER:HB2 | 2.17 | 0.44 |
| 2:c:2361:LYS:H | 2:c:2361:LYS:HG3 | 1.53 | 0.44 |
| 2:c:2539:ILE:O | 2:c:2573:TYR:OH | 2.21 | 0.44 |
| 3:d:2952[A]:ALA:CB | 3:d:2953[A]:GLY:CA | 2.82 | 0.44 |
| 3:d:2963[B]:MET:SD | 3:d:2963[B]:MET:C | 3.01 | 0.44 |
| 3:d:3133[A]:LEU:O | 3:d:3136[A]:TYR:HB3 | 2.17 | 0.44 |
| 3:d:3137[A]:ARG:O | 3:d:3139[A]:LEU:HD22 | 2.16 | 0.44 |
| 3:d:3204[B]:LEU:CD1 | 3:d:3204[B]:LEU:N | 2.80 | 0.44 |
| 3:d:3241[A]:PHE:CZ | 3:d:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:d:3242[B]:GLY:C | 3:d:3243[B]:GLY:O | 2.58 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3266[B]:ILE:O | 3:d:3269[B]:SER:HB2 | 2.17 | 0.44 |
| 2:B:2089:ARG:HB3 | 2:B:2175:VAL:O | 2.18 | 0.44 |
| 2:B:2745:PRO:HB2 | 2:B:2750:ILE:HD12 | 1.99 | 0.44 |
| 2:B:2791:LEU:HD23 | 2:B:2791:LEU:HA | 1.84 | 0.44 |
| 3:C:3087[B]:MET:HA | 3:C:3090[B]:ASN:OD1 | 2.17 | 0.44 |
| 3:C:3106[A]:THR:O | 3:C:3106[A]:THR:HG23 | 2.17 | 0.44 |
| 3:C:3137[B]:ARG:O | 3:C:3139[B]:LEU:HD22 | 2.16 | 0.44 |
| 3:C:3230[B]:PHE:CB | 3:C:3242[B]:GLY:C | 2.91 | 0.44 |
| 3:C:3273[A]:LEU:C | 3:C:3275[A]:LEU:HD12 | 2.42 | 0.44 |
| 3:C:3299[A]:LEU:HB3 | 3:C:3300[A]:LEU:H | 1.54 | 0.44 |
| 3:C:3300[B]:LEU:HD23 | 3:C:3300[B]:LEU:H | 1.83 | 0.44 |
| 9:C:3401[A]:CUO:O1 | 3:L:2989[A]:HIS:CD2 | 2.70 | 0.44 |
| 1:D:737:GLY:HA2 | 1:D:771:TRP:CZ2 | 2.52 | 0.44 |
| 1:D:991:LEU:HD22 | 1:D:991:LEU:H | 1.82 | 0.44 |
| 2:E:2554:PRO:HA | 2:E:2555:GLU:HB3 | 1.98 | 0.44 |
| 3:F:2986[B]:PRO:CB | 3:F:3127[B]:TRP:CE3 | 3.00 | 0.44 |
| 3:F:3093[B]:HIS:HB2 | 3:F:3248[B]:LEU:CD1 | 2.48 | 0.44 |
| 3:F:3185[B]:TYR:HE2 | 3:F:3187[B]:TYR:CD2 | 2.35 | 0.44 |
| 3:F:3252[B]:TYR:CG | 3:a:3108[B]:HIS:CE1 | 3.06 | 0.44 |
| 3:F:3300[B]:LEU:HD23 | 3:F:3300[B]:LEU:H | 1.83 | 0.44 |
| 1:G:392:PRO:O | 1:G:395:THR:OG1 | 2.31 | 0.44 |
| 1:G:1172:ALA:CB | 1:G:1196:ILE:HG13 | 2.48 | 0.44 |
| 1:G:1470:GLU:HG2 | 1:G:1537:ILE:CD1 | 2.46 | 0.44 |
| 2:H:2107:LEU:O | 2:H:2111:GLN:HB2 | 2.18 | 0.44 |
| 2:H:2133:PRO:HG2 | 2:H:2140:ARG:HA | 1.99 | 0.44 |
| 2:H:2849:ASP:HB3 | 2:H:2850:ARG:NH1 | 2.33 | 0.44 |
| 3:I:2969[A]:TYR:CD2 | 3:I:2970[A]:PRO:CG | 3.00 | 0.44 |
| 3:I:3241[A]:PHE:CZ | 3:I:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:I:3273[A]:LEU:C | 3:I:3275[A]:LEU:HD12 | 2.42 | 0.44 |
| 3:I:3273[B]:LEU:C | 3:I:3275[B]:LEU:HD12 | 2.42 | 0.44 |
| 1:J:270:GLU:OE1 | 1:J:270:GLU:N | 2.47 | 0.44 |
| 1:J:464:LEU:HD22 | 1:J:622:HIS:CG | 2.52 | 0.44 |
| 1:J:875:ALA:HA | 1:J:1038:PHE:CZ | 2.52 | 0.44 |
| 1:J:1315:GLY:HA3 | 1:J:1601:TRP:CB | 2.48 | 0.44 |
| 2:K:2327:GLU:H | 2:K:2327:GLU:HG3 | 1.45 | 0.44 |
| 2:K:2663:MET:HG3 | 2:K:2675:GLN:HB2 | 1.98 | 0.44 |
| 3:L:2979[B]:GLN:HB2 | 3:L:2988[B]:TRP:CD1 | 2.52 | 0.44 |
| 3:L:2988[A]:TRP:CD1 | 3:L:3158[A]:PHE:CE2 | 3.06 | 0.44 |
| 3:L:2989[A]:HIS:O | 3:L:2990[A]:ARG:C | 2.61 | 0.44 |
| 3:L:3019[A]:HIS:CD2 | 3:L:3020[A]:SER:H | 2.36 | 0.44 |
| 3:L:3104[A]:MET:SD | 3:L:3110[A]:THR:CG2 | 3.06 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3104[B]:MET:SD | 3:L:3110[B]:THR:CG2 | 3.06 | 0.44 |
| 3:L:3148[A]:ILE:O | 3:L:3148[A]:ILE:HG22 | 2.17 | 0.44 |
| 3:L:3241[A]:PHE:CZ | 3:L:3243[A]:GLY:O | 2.70 | 0.44 |
| 1:M:108:PRO:HA | 1:M:124:TYR:CG | 2.52 | 0.44 |
| 1:M:472:ASP:HA | 1:M:473:ALA:HA | 1.70 | 0.44 |
| 2:N:2562:GLY:H | 2:N:2846:TRP:CB | 2.30 | 0.44 |
| 3:O:2938[A]:LEU:O | 3:O:2939[A]:ARG:C | 2.58 | 0.44 |
| 3:O:2951[B]:ASP:CG | 3:O:2952[B]:ALA:N | 2.74 | 0.44 |
| 3:O:2979[B]:GLN:HB2 | 3:O:2988[B]:TRP:CD1 | 2.52 | 0.44 |
| 3:O:3027[A]:GLU:CD | 3:O:3027[A]:GLU:C | 2.85 | 0.44 |
| 3:O:3093[B]:HIS:HB2 | 3:O:3248[B]:LEU:CD1 | 2.48 | 0.44 |
| 3:O:3094[B]:SER:HG | 3:O:3227[B]:ASP:CG | 2.25 | 0.44 |
| 3:O:3156[B]:MET:SD | 3:X:3173[B]:THR:HG22 | 2.57 | 0.44 |
| 3:O:3244[B]:THR:H | 3:O:3264[B]:TYR:HE2 | 1.65 | 0.44 |
| 1:P:140:ASP:OD1 | 1:P:142:ARG:NE | 2.34 | 0.44 |
| 1:P:448:SER:O | 1:P:450:LYS:HG2 | 2.18 | 0.44 |
| 1:P:587:PHE:HA | 1:P:644:TRP:HD1 | 1.83 | 0.44 |
| 1:P:736:MET:HG2 | 1:P:772:ARG:HD2 | 2.00 | 0.44 |
| 1:P:1156:LEU:HB2 | 1:P:1176:TYR:CE1 | 2.53 | 0.44 |
| 1:P:1411:PHE:HB3 | 1:P:1544:LEU:HD21 | 1.99 | 0.44 |
| 2:Q:2879:LEU:HA | 2:Q:2879:LEU:HD12 | 1.77 | 0.44 |
| 3:R:2946[A]:GLN:CD | 3:R:2947[A]:ALA:N | 2.72 | 0.44 |
| 3:R:2948[B]:ASP:CB | 3:R:2949[B]:LYS:CA | 2.78 | 0.44 |
| 3:R:2969[A]:TYR:CD2 | 3:R:2970[A]:PRO:CG | 3.00 | 0.44 |
| 3:R:3023[B]:ILE:HA | 3:R:3026[B]:THR:HG1 | 1.82 | 0.44 |
| 3:R:3027[B]:GLU:CD | 3:R:3027[B]:GLU:C | 2.85 | 0.44 |
| 3:R:3087[A]:MET:HA | 3:R:3090[A]:ASN:OD1 | 2.17 | 0.44 |
| 3:R:3133[A]:LEU:O | 3:R:3136[A]:TYR:HB3 | 2.18 | 0.44 |
| 3:R:3241[B]:PHE:CE2 | 3:R:3243[B]:GLY:O | 2.71 | 0.44 |
| 1:S:7:VAL:HG21 | 1:S:208:LEU:HD23 | 2.00 | 0.44 |
| 1:S:627:ASP:HA | 1:S:628:PRO:HD3 | 1.86 | 0.44 |
| 1:S:858:MET:HE1 | 1:S:870:TYR:CE1 | 2.52 | 0.44 |
| 1:S:1236:TYR:HB3 | 2:W:2736:TYR:HB3 | 1.99 | 0.44 |
| 2:T:2128:LEU:O | 2:T:2130:PRO:HD3 | 2.18 | 0.44 |
| 2:T:2186:GLU:HA | 2:T:2232:PHE:CE1 | 2.53 | 0.44 |
| 2:T:2526:ARG:HE | 2:W:2114:ARG:HG3 | 1.82 | 0.44 |
| 2:T:2840:GLY:O | 2:T:2843:GLU:HB2 | 2.17 | 0.44 |
| 3:U:2969[B]:TYR:CD2 | 3:U:2970[B]:PRO:CG | 3.00 | 0.44 |
| 3:U:2975[B]:PHE:HA | 3:d:3255[B]:PRO:HA | 1.33 | 0.44 |
| 3:U:2976[B]:ALA:O | 3:U:2978[B]:CYS:N | 2.46 | 0.44 |
| 3:U:2989[B]:HIS:O | 3:U:2990[B]:ARG:C | 2.61 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3028[B]:PRO:HG2 | 3:U:3029[B]:LYS:HG3 | 2.00 | 0.44 |
| 3:U:3093[A]:HIS:HB2 | 3:U:3248[A]:LEU:CD1 | 2.48 | 0.44 |
| 3:U:3101[A]:PRO:O | 3:U:3109[A]:TYR:HD2 | 2.00 | 0.44 |
| 3:U:3101[B]:PRO:O | 3:U:3109[B]:TYR:HD2 | 2.00 | 0.44 |
| 3:U:3171[B]:HIS:C | 3:U:3173[B]:THR:N | 2.73 | 0.44 |
| 3:U:3182[A]:GLN:C | 3:U:3183[A]:LEU:CD1 | 2.91 | 0.44 |
| 3:U:3254[B]:MET:HB3 | 3:d:3255[B]:PRO:N | 2.31 | 0.44 |
| 3:U:3306[A]:LEU:C | 3:U:3306[A]:LEU:CD1 | 2.86 | 0.44 |
| 1:V:437:TYR:CE1 | 1:V:535:PRO:HD2 | 2.53 | 0.44 |
| 1:V:931:TRP:CB | 1:V:1018:ILE:HD11 | 2.47 | 0.44 |
| 1:V:956:PRO:HD2 | 1:V:957:ASN:O | 2.18 | 0.44 |
| 2:W:2286:HIS:NE2 | 2:W:2433:THR:HG22 | 2.32 | 0.44 |
| 2:W:2373:MET:HB3 | 2:W:2381:LEU:HD11 | 2.00 | 0.44 |
| 3:X:2938[A]:LEU:O | 3:X:2939[A]:ARG:C | 2.58 | 0.44 |
| 3:X:2989[A]:HIS:O | 3:X:2990[A]:ARG:C | 2.61 | 0.44 |
| 3:X:3004[B]:GLY:C | 3:X:3006[B]:LYS:N | 2.73 | 0.44 |
| 3:X:3241[B]:PHE:CZ | 3:X:3243[B]:GLY:O | 2.70 | 0.44 |
| 3:X:3273[A]:LEU:C | 3:X:3275[A]:LEU:HD12 | 2.42 | 0.44 |
| 1:Y:147:SER:O | 1:Y:149:GLU:N | 2.49 | 0.44 |
| 1:Y:262:LYS:NZ | 1:Y:795:GLU:OE1 | 2.50 | 0.44 |
| 1:Y:492:ARG:NH2 | 1:Y:641:TRP:CE2 | 2.85 | 0.44 |
| 1:Y:817:PRO:HA | 1:Y:818:PRO:HD3 | 1.87 | 0.44 |
| 1:Y:987:LYS:H | 1:Y:987:LYS:HG2 | 1.51 | 0.44 |
| 1:Y:1655:SER:CB | 3:d:3007[B]:ILE:HG23 | 2.34 | 0.44 |
| 3:a:2951[A]:ASP:CG | 3:a:2952[A]:ALA:N | 2.74 | 0.44 |
| 3:a:2963[A]:MET:SD | 3:a:2963[A]:MET:C | 3.01 | 0.44 |
| 3:a:2991[A]:LEU:HD23 | 3:a:3158[A]:PHE:CE1 | 2.48 | 0.44 |
| 3:a:3034[A]:HIS:HB3 | 3:a:3035[A]:HIS:CE1 | 2.50 | 0.44 |
| 3:a:3132[A]:ALA:HB3 | 3:a:3197[A]:ILE:HD13 | 1.99 | 0.44 |
| 3:a:3135[B]:LYS:HB2 | 3:a:3141[B]:TYR:CD1 | 2.51 | 0.44 |
| 3:a:3161[A]:GLU:H | 3:a:3161[A]:GLU:CD | 2.19 | 0.44 |
| 3:a:3230[A]:PHE:CB | 3:a:3242[A]:GLY:C | 2.91 | 0.44 |
| 3:a:3264[B]:TYR:HD1 | 3:a:3265[B]:ASP:N | 2.14 | 0.44 |
| 3:a:3300[A]:LEU:HD23 | 3:a:3300[A]:LEU:H | 1.83 | 0.44 |
| 1:b:725:SER:HB2 | 1:b:827:ALA:HB2 | 1.98 | 0.44 |
| 3:d:2931[A]:THR:O | 3:d:2934[A]:GLU:HG3 | 2.18 | 0.44 |
| 3:d:2949[B]:LYS:NZ | 3:d:2949[B]:LYS:C | 2.73 | 0.44 |
| 3:d:2952[B]:ALA:CA | 3:d:2956[B]:LYS:CB | 2.89 | 0.44 |
| 3:d:2969[A]:TYR:CD2 | 3:d:2970[A]:PRO:CG | 3.00 | 0.44 |
| 3:d:2985[B]:PHE:CE2 | 3:d:2989[B]:HIS:CD2 | 3.04 | 0.44 |
| 3:d:2989[B]:HIS:C | 3:d:2991[B]:LEU:N | 2.75 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3180[A]:TYR:CA | 3:d:3183[A]:LEU:CD2 | 2.95 | 0.44 |
| 3:d:3180[A]:TYR:CB | 3:d:3183[A]:LEU:CD2 | 2.90 | 0.44 |
| 6:NA:1:NAG:H61 | 6:NA:2:NAG:N2 | 2.24 | 0.44 |
| 1:A:76:PHE:HD2 | 1:A:89:ILE:HD13 | 1.83 | 0.44 |
| 1:A:457:ALA:O | 1:A:460:GLU:HB2 | 2.17 | 0.44 |
| 1:A:855:ARG:HH21 | 1:A:941:LEU:HA | 1.83 | 0.44 |
| 1:A:1026:GLU:C | 1:A:1028:VAL:H | 2.26 | 0.44 |
| 1:A:1163:ALA:HB2 | 1:A:1205:LEU:HD21 | 1.99 | 0.44 |
| 1:A:1315:GLY:HA3 | 1:A:1601:TRP:CB | 2.48 | 0.44 |
| 1:A:1643:LYS:HA | 1:A:1643:LYS:HD2 | 1.76 | 0.44 |
| 2:B:2782:ASN:HB2 | 2:B:2786:MET:O | 2.18 | 0.44 |
| 2:B:2907:LYS:HB3 | 2:B:2907:LYS:HE2 | 1.66 | 0.44 |
| 3:C:2974[B]:ALA:O | 3:L:3249[B]:GLY:HA2 | 2.18 | 0.44 |
| 3:C:3014[B]:TRP:CH2 | 3:C:3123[B]:THR:HG23 | 2.53 | 0.44 |
| 3:C:3101[B]:PRO:O | 3:C:3109[B]:TYR:HD2 | 2.00 | 0.44 |
| 3:C:3293[A]:LYS:CB | 3:C:3294[A]:SER:CA | 2.96 | 0.44 |
| 1:D:120:LYS:HA | 1:D:120:LYS:HD2 | 1.72 | 0.44 |
| 1:D:610:THR:HB | 1:D:629:MET:HE1 | 1.99 | 0.44 |
| 1:D:1166:THR:CB | 1:D:1168:GLN:HG3 | 2.48 | 0.44 |
| 2:E:2651:GLN:NE2 | 2:E:2652:LYS:HG3 | 2.33 | 0.44 |
| 3:F:2931[A]:THR:O | 3:F:2934[A]:GLU:HG3 | 2.18 | 0.44 |
| 3:F:2931[B]:THR:O | 3:F:2934[B]:GLU:HG3 | 2.18 | 0.44 |
| 3:F:2963[B]:MET:SD | 3:F:2963[B]:MET:C | 3.01 | 0.44 |
| 3:F:2989[A]:HIS:C | 3:F:2991[A]:LEU:N | 2.75 | 0.44 |
| 3:F:3023[A]:ILE:O | 3:F:3026[A]:THR:OG1 | 2.34 | 0.44 |
| 3:F:3093[B]:HIS:HD2 | 3:F:3248[B]:LEU:CD2 | 2.31 | 0.44 |
| 3:F:3106[B]:THR:O | 3:F:3106[B]:THR:HG23 | 2.16 | 0.44 |
| 3:F:3135[A]:LYS:HB2 | 3:F:3141[A]:TYR:CD1 | 2.52 | 0.44 |
| 3:F:3200[B]:LEU:CD2 | 3:F:3204[B]:LEU:HD11 | 2.47 | 0.44 |
| 1:G:127:GLU:HG2 | 1:G:135:THR:N | 2.31 | 0.44 |
| 2:H:2132:CYS:O | 2:H:2334:LYS:HD3 | 2.18 | 0.44 |
| 2:H:2133:PRO:HG3 | 2:H:2141:HIS:CE1 | 2.53 | 0.44 |
| 3:I:2940[A]:ASN:O | 3:I:2943[A]:ALA:HB3 | 2.18 | 0.44 |
| 3:I:2963[A]:MET:SD | 3:I:2963[A]:MET:C | 3.01 | 0.44 |
| 3:I:2979[B]:GLN:HB2 | 3:I:2988[B]:TRP:CD1 | 2.52 | 0.44 |
| 3:I:2989[A]:HIS:C | 3:I:2991[A]:LEU:N | 2.75 | 0.44 |
| 3:I:3104[A]:MET:SD | 3:I:3110[A]:THR:CG2 | 3.06 | 0.44 |
| 3:I:3204[B]:LEU:CD1 | 3:I:3204[B]:LEU:N | 2.80 | 0.44 |
| 3:I:3230[A]:PHE:CB | 3:I:3242[A]:GLY:C | 2.91 | 0.44 |
| 3:I:3284[B]:LYS:CD | 3:I:3284[B]:LYS:C | 2.86 | 0.44 |
| 3:I:3298[B]:ASN:CA | 3:I:3299[B]:LEU:HB2 | 2.44 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1498:ASN:ND2 | 1:J:1500:THR:O | 2.51 | 0.44 |
| 2:K:2158:TYR:HE2 | 2:K:2294:PHE:CE1 | 2.35 | 0.44 |
| 2:K:2265:ILE:HD12 | 2:K:2443:TYR:CG | 2.53 | 0.44 |
| 2:K:2283:ASN:O | 2:K:2283:ASN:ND2 | 2.51 | 0.44 |
| 3:L:2963[B]:MET:SD | 3:L:2963[B]:MET:C | 3.01 | 0.44 |
| 3:L:3028[B]:PRO:HG2 | 3:L:3029[B]:LYS:HG3 | 2.00 | 0.44 |
| 3:L:3093[A]:HIS:HB2 | 3:L:3248[A]:LEU:CD1 | 2.48 | 0.44 |
| 3:L:3133[A]:LEU:O | 3:L:3136[A]:TYR:HB3 | 2.17 | 0.44 |
| 3:L:3148[B]:ILE:O | 3:L:3148[B]:ILE:HG22 | 2.17 | 0.44 |
| 3:L:3180[A]:TYR:CA | 3:L:3183[A]:LEU:CD2 | 2.95 | 0.44 |
| 3:L:3266[B]:ILE:O | 3:L:3269[B]:SER:HB2 | 2.18 | 0.44 |
| 3:L:3293[B]:LYS:CD | 3:L:3293[B]:LYS:C | 2.86 | 0.44 |
| 1:M:567:LEU:HD12 | 1:M:567:LEU:HA | 1.89 | 0.44 |
| 1:M:1614:GLU:OE1 | 1:M:1614:GLU:N | 2.50 | 0.44 |
| 2:N:2504:ARG:HD3 | 2:N:2775:GLY:O | 2.17 | 0.44 |
| 3:O:2963[B]:MET:SD | 3:O:2963[B]:MET:C | 3.01 | 0.44 |
| 3:O:2971[B]:ASP:OD2 | 3:X:3158[B]:PHE:HZ | 2.00 | 0.44 |
| 3:O:2977[B]:CYS:SG | 3:X:3154[B]:PRO:O | 2.67 | 0.44 |
| 3:O:3027[B]:GLU:CD | 3:O:3027[B]:GLU:C | 2.85 | 0.44 |
| 3:O:3119[A]:HIS:O | 3:O:3122[A]:ASN:HB3 | 2.17 | 0.44 |
| 3:O:3229[B]:ASN:O | 3:O:3286[B]:THR:N | 2.50 | 0.44 |
| 3:O:3300[B]:LEU:HD23 | 3:O:3300[B]:LEU:H | 1.83 | 0.44 |
| 1:P:746:LEU:HD21 | 1:P:781:ILE:HD11 | 1.99 | 0.44 |
| 1:P:1073:ALA:O | 1:P:1077:LEU:HB2 | 2.18 | 0.44 |
| 1:P:1078:ARG:HB2 | 1:P:1078:ARG:HH11 | 1.82 | 0.44 |
| 2:Q:2107:LEU:HD22 | 2:Q:2209:PHE:CE2 | 2.53 | 0.44 |
| 2:Q:2568:HIS:HD2 | 2:Q:2718:TRP:CH2 | 2.35 | 0.44 |
| 3:R:2931[A]:THR:O | 3:R:2934[A]:GLU:HG3 | 2.18 | 0.44 |
| 3:R:2951[B]:ASP:OD2 | 3:R:2952[B]:ALA:CB | 2.66 | 0.44 |
| 3:R:2963[A]:MET:SD | 3:R:2963[A]:MET:C | 3.01 | 0.44 |
| 3:R:2989[A]:HIS:O | 3:R:2990[A]:ARG:C | 2.61 | 0.44 |
| 3:R:3135[A]:LYS:HB2 | 3:R:3141[A]:TYR:CD1 | 2.52 | 0.44 |
| 3:R:3148[A]:ILE:O | 3:R:3148[A]:ILE:HG22 | 2.17 | 0.44 |
| 3:R:3200[A]:LEU:CD2 | 3:R:3204[A]:LEU:HD11 | 2.48 | 0.44 |
| 3:R:3229[B]:ASN:O | 3:R:3286[B]:THR:N | 2.50 | 0.44 |
| 3:R:3230[A]:PHE:CB | 3:R:3242[A]:GLY:C | 2.91 | 0.44 |
| 3:R:3293[A]:LYS:CB | 3:R:3294[A]:SER:CA | 2.96 | 0.44 |
| 1:S:1082:SER:O | 1:S:1086:LEU:HD23 | 2.18 | 0.44 |
| 3:U:2937[B]:ASN:CB | 3:U:3006[B]:LYS:CE | 2.86 | 0.44 |
| 3:U:2986[B]:PRO:CB | 3:U:3127[B]:TRP:CE3 | 3.00 | 0.44 |
| 3:U:2988[A]:TRP:CD1 | 3:U:3158[A]:PHE:CE2 | 3.06 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3014[A]:TRP:CH2 | 3:U:3123[A]:THR:HG23 | 2.53 | 0.44 |
| 3:U:3027[B]:GLU:CD | 3:U:3027[B]:GLU:C | 2.85 | 0.44 |
| 3:U:3241[A]:PHE:CE2 | 3:U:3243[A]:GLY:O | 2.70 | 0.44 |
| 3:U:3266[A]:ILE:O | 3:U:3269[A]:SER:HB2 | 2.18 | 0.44 |
| 3:U:3266[B]:ILE:O | 3:U:3269[B]:SER:HB2 | 2.17 | 0.44 |
| 1:V:329:ARG:NH2 | 1:Y:1584:GLY:HA2 | 2.33 | 0.44 |
| 1:V:1249:TRP:CZ2 | 1:V:1537:ILE:HD12 | 2.53 | 0.44 |
| 2:W:2446:GLU:HG2 | 2:W:2448:THR:HG23 | 2.00 | 0.44 |
| 2:W:2854:MET:HE3 | 2:W:2854:MET:HB2 | 1.84 | 0.44 |
| 3:X:2938[B]:LEU:O | 3:X:2939[B]:ARG:C | 2.58 | 0.44 |
| 3:X:2988[A]:TRP:CD1 | 3:X:3158[A]:PHE:CE2 | 3.06 | 0.44 |
| 3:X:3014[B]:TRP:CH2 | 3:X:3123[B]:THR:HG23 | 2.53 | 0.44 |
| 3:X:3306[A]:LEU:C | 3:X:3306[A]:LEU:CD1 | 2.86 | 0.44 |
| 1:Y:490:TRP:HE1 | 1:Y:670:PRO:HD2 | 1.82 | 0.44 |
| 1:Y:1325:LEU:HD11 | 1:Y:1511:SER:HA | 2.00 | 0.44 |
| 1:Y:1636:ASN:HB3 | 1:Y:1638:SER:O | 2.16 | 0.44 |
| 3:a:2948[B]:ASP:HB3 | 3:a:2949[B]:LYS:C | 2.43 | 0.44 |
| 3:a:2963[B]:MET:C | 3:a:2963[B]:MET:SD | 3.01 | 0.44 |
| 3:a:3119[A]:HIS:O | 3:a:3122[A]:ASN:HB3 | 2.17 | 0.44 |
| 3:a:3182[A]:GLN:C | 3:a:3183[A]:LEU:CD1 | 2.91 | 0.44 |
| 3:a:3200[A]:LEU:CD2 | 3:a:3204[A]:LEU:HD11 | 2.48 | 0.44 |
| 3:a:3200[B]:LEU:CD2 | 3:a:3204[B]:LEU:HD11 | 2.48 | 0.44 |
| 3:a:3232[B]:VAL:HG21 | 3:a:3273[B]:LEU:HD11 | 2.00 | 0.44 |
| 1:b:238:ASN:OD1 | 1:b:238:ASN:N | 2.38 | 0.44 |
| 1:b:832:LYS:HD2 | 1:b:832:LYS:HA | 1.67 | 0.44 |
| 2:c:2431:GLY:O | 2:c:2434:GLU:HG2 | 2.16 | 0.44 |
| 2:c:2640:ILE:H | 2:c:2640:ILE:HG12 | 1.55 | 0.44 |
| 2:c:2716:ARG:HB2 | 2:c:2778:TYR:CE1 | 2.52 | 0.44 |
| 3:d:2979[A]:GLN:HB2 | 3:d:2988[A]:TRP:CD1 | 2.52 | 0.44 |
| 3:d:2989[B]:HIS:CD2 | 9:d:3401[B]:CUO:O1 | 2.70 | 0.44 |
| 3:d:3013[A]:ASP:CG | 3:d:3015[A]:THR:HG1 | 2.24 | 0.44 |
| 3:d:3028[A]:PRO:HG2 | 3:d:3029[A]:LYS:HG3 | 2.00 | 0.44 |
| 3:d:3185[B]:TYR:CE2 | 3:d:3187[B]:TYR:HE2 | 2.31 | 0.44 |
| 3:d:3196[B]:THR:N | 3:d:3199[B]:GLN:CB | 2.65 | 0.44 |
| 3:d:3241[B]:PHE:CZ | 3:d:3243[B]:GLY:O | 2.70 | 0.44 |
| 1:A:643:ILE:HD13 | 1:A:708:PHE:HB2 | 1.99 | 0.44 |
| 1:A:817:PRO:HA | 1:A:818:PRO:HD3 | 1.78 | 0.44 |
| 1:A:1412:GLU:OE2 | 1:A:1552:ARG:NH1 | 2.51 | 0.44 |
| 2:B:2780:HIS:HD2 | 2:B:2782:ASN:ND2 | 2.15 | 0.44 |
| 3:C:2931[A]:THR:O | 3:C:2934[A]:GLU:HG3 | 2.18 | 0.44 |
| 3:C:2969[A]:TYR:CD2 | 3:C:2970[A]:PRO:CG | 3.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2988[A]:TRP:CD1 | 3:C:3158[A]:PHE:CE2 | 3.06 | 0.44 |
| 3:C:3093[A]:HIS:HB2 | 3:C:3248[A]:LEU:CD1 | 2.48 | 0.44 |
| 3:C:3133[B]:LEU:HD12 | 3:C:3133[B]:LEU:HA | 1.86 | 0.44 |
| 3:C:3230[A]:PHE:CB | 3:C:3242[A]:GLY:C | 2.91 | 0.44 |
| 3:C:3244[B]:THR:H | 3:C:3264[B]:TYR:HE2 | 1.65 | 0.44 |
| 1:D:23:ARG:HD3 | 1:D:120:LYS:HG2 | 2.00 | 0.44 |
| 1:D:320:LYS:HD3 | 1:D:337:ASP:HB3 | 2.00 | 0.44 |
| 1:D:1231:VAL:HG22 | 1:D:1231:VAL:O | 2.18 | 0.44 |
| 1:D:1286:ARG:NH2 | 1:D:1333:GLU:OE2 | 2.49 | 0.44 |
| 2:E:2180:TRP:CD1 | 2:E:2247:ILE:HD11 | 2.53 | 0.44 |
| 2:E:2345:ASN:HA | 2:E:2346:PRO:HD2 | 1.86 | 0.44 |
| 2:E:2680:HIS:CD2 | 2:E:2684:HIS:HD2 | 2.35 | 0.44 |
| 2:E:2723:GLU:HG2 | 2:E:2788:ILE:CD1 | 2.47 | 0.44 |
| 3:F:2933[A]:SER:CA | 3:F:2936[A]:GLU:HB3 | 2.48 | 0.44 |
| 3:F:2964[B]:PRO:CA | 3:a:3221[B]:ALA:HB3 | 2.48 | 0.44 |
| 3:F:2979[A]:GLN:HB2 | 3:F:2988[A]:TRP:CD1 | 2.52 | 0.44 |
| 3:F:3047[A]:ARG:NH2 | 3:F:3113[A]:ASP:OD1 | 2.43 | 0.44 |
| 3:F:3074[A]:GLU:CD | 3:F:3212[A]:ARG:NH2 | 2.73 | 0.44 |
| 3:F:3101[A]:PRO:O | 3:F:3109[A]:TYR:HD2 | 2.00 | 0.44 |
| 3:F:3133[A]:LEU:O | 3:F:3136[A]:TYR:HB3 | 2.17 | 0.44 |
| 3:F:3204[B]:LEU:CD1 | 3:F:3204[B]:LEU:N | 2.80 | 0.44 |
| 3:F:3222[B]:ILE:CD1 | 3:F:3223[B]:GLY:N | 2.73 | 0.44 |
| 3:F:3230[A]:PHE:CB | 3:F:3242[A]:GLY:C | 2.91 | 0.44 |
| 3:F:3281[A]:PHE:HE1 | 3:F:3305[A]:ILE:HG21 | 1.81 | 0.44 |
| 9:F:3401[A]:CUO:O1 | 3:a:2989[A]:HIS:CD2 | 2.70 | 0.44 |
| 1:G:62:MET:HE2 | 1:G:62:MET:HB3 | 1.88 | 0.44 |
| 1:G:470:ARG:HD2 | 1:G:470:ARG:HA | 1.80 | 0.44 |
| 1:G:566:ARG:HA | 1:G:567:LEU:HB2 | 2.00 | 0.44 |
| 1:G:710:GLY:H | 1:G:711:LEU:HD12 | 1.82 | 0.44 |
| 1:G:1145:THR:HB | 1:G:1191:PRO:HB2 | 1.99 | 0.44 |
| 1:G:1324:ARG:NE | 1:G:1462:ASP:OD1 | 2.42 | 0.44 |
| 1:G:1536:SER:O | 1:G:1539:GLN:HG2 | 2.18 | 0.44 |
| 3:I:2931[A]:THR:O | 3:I:2934[A]:GLU:HG3 | 2.18 | 0.44 |
| 3:I:2973[B]:THR:HG21 | 3:R:3106[B]:THR:O | 2.18 | 0.44 |
| 3:I:2988[A]:TRP:CD1 | 3:I:3158[A]:PHE:CE2 | 3.06 | 0.44 |
| 3:I:3182[A]:GLN:C | 3:I:3183[A]:LEU:CD1 | 2.91 | 0.44 |
| 3:I:3230[B]:PHE:CB | 3:I:3242[B]:GLY:C | 2.91 | 0.44 |
| 3:I:3241[A]:PHE:CE2 | 3:I:3243[A]:GLY:O | 2.71 | 0.44 |
| 3:I:3281[B]:PHE:HE1 | 3:I:3305[B]:ILE:HG21 | 1.81 | 0.44 |
| 1:J:2:LEU:HD12 | 1:J:2:LEU:HA | 1.88 | 0.44 |
| 1:J:1552:ARG:HB2 | 1:J:1653:VAL:HG22 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2574:LEU:HD12 | 2:K:2574:LEU:HA | 1.85 | 0.44 |
| 3:L:2937[B]:ASN:CB | 3:L:3006[B]:LYS:CE | 2.86 | 0.44 |
| 3:L:2940[A]:ASN:O | 3:L:2943[A]:ALA:HB3 | 2.18 | 0.44 |
| 3:L:3014[A]:TRP:CH2 | 3:L:3123[A]:THR:HG23 | 2.53 | 0.44 |
| 3:L:3014[B]:TRP:CH2 | 3:L:3123[B]:THR:HG23 | 2.53 | 0.44 |
| 3:L:3034[A]:HIS:HB3 | 3:L:3035[A]:HIS:CE1 | 2.50 | 0.44 |
| 3:L:3200[B]:LEU:CD2 | 3:L:3204[B]:LEU:HD11 | 2.48 | 0.44 |
| 1:M:173:VAL:HG23 | 1:M:174:GLN:HG2 | 1.99 | 0.44 |
| 1:M:1030:MET:HA | 1:M:1036:SER:HA | 2.00 | 0.44 |
| 1:M:1093:ASP:HB2 | 1:M:1096:THR:OG1 | 2.17 | 0.44 |
| 1:M:1331:GLU:HB2 | 1:M:1343:VAL:HG23 | 1.99 | 0.44 |
| 2:N:2263:PHE:HE1 | 2:N:2304:LEU:HB3 | 1.82 | 0.44 |
| 2:N:2554:PRO:HA | 2:N:2555:GLU:HB3 | 2.00 | 0.44 |
| 2:N:2627:GLY:HA3 | 2:N:2703:PHE:O | 2.18 | 0.44 |
| 3:O:2931[B]:THR:O | 3:O:2934[B]:GLU:HG3 | 2.18 | 0.44 |
| 3:O:2974[B]:ALA:HA | 3:X:2979[B]:GLN:OE1 | 2.17 | 0.44 |
| 3:O:2988[A]:TRP:CD1 | 3:O:3158[A]:PHE:CE2 | 3.06 | 0.44 |
| 3:O:3133[B]:LEU:O | 3:O:3136[B]:TYR:HB3 | 2.17 | 0.44 |
| 3:O:3161[A]:GLU:H | 3:O:3161[A]:GLU:CD | 2.19 | 0.44 |
| 3:O:3200[B]:LEU:CD2 | 3:O:3204[B]:LEU:HD11 | 2.48 | 0.44 |
| 3:O:3266[A]:ILE:O | 3:O:3269[A]:SER:HB2 | 2.18 | 0.44 |
| 1:P:781:ILE:HG22 | 1:P:781:ILE:O | 2.18 | 0.44 |
| 1:P:870:TYR:OH | 1:P:963:ALA:HB1 | 2.18 | 0.44 |
| 1:P:1274:LEU:HD21 | 1:P:1344:PRO:HD3 | 1.99 | 0.44 |
| 2:Q:2327:GLU:H | 2:Q:2327:GLU:HG3 | 1.44 | 0.44 |
| 2:Q:2799:LYS:HA | 2:Q:2803:ARG:NH1 | 2.33 | 0.44 |
| 3:R:2987[B]:HIS:O | 3:R:2991[B]:LEU:HB2 | 2.16 | 0.44 |
| 3:R:3101[B]:PRO:O | 3:R:3109[B]:TYR:HD2 | 2.00 | 0.44 |
| 1:S:516:TRP:HH2 | 1:S:637:VAL:HG22 | 1.82 | 0.44 |
| 1:S:905:TRP:CZ3 | 1:S:909:ILE:HG13 | 2.53 | 0.44 |
| 1:S:980:TYR:CE2 | 1:S:1021:LEU:HD13 | 2.53 | 0.44 |
| 2:T:2873:HIS:CD2 | 2:T:2873:HIS:H | 2.36 | 0.44 |
| 3:U:2951[A]:ASP:CG | 3:U:2952[A]:ALA:N | 2.74 | 0.44 |
| 3:U:2989[A]:HIS:O | 3:U:2990[A]:ARG:C | 2.61 | 0.44 |
| 3:U:3019[B]:HIS:CD2 | 3:U:3020[B]:SER:H | 2.35 | 0.44 |
| 1:V:282:ASN:OD1 | 1:V:282:ASN:N | 2.49 | 0.44 |
| 3:X:2933[A]:SER:CA | 3:X:2936[A]:GLU:HB3 | 2.48 | 0.44 |
| 3:X:2985[B]:PHE:HE2 | 3:X:2989[B]:HIS:HE2 | 1.66 | 0.44 |
| 3:X:3044[A]:LYS:H | 3:X:3044[A]:LYS:HG2 | 1.64 | 0.44 |
| 2:Z:2134:ASN:ND2 | 2:Z:2137:ALA:HB2 | 2.33 | 0.44 |
| 2:Z:2539:ILE:O | 2:Z:2573:TYR:OH | 2.23 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:2695:MET:HE1 | 2:Z:2707:PHE:HB2 | 2.00 | 0.44 |
| 2:Z:2844:MET:O | 2:Z:2846:TRP:HD1 | 2.01 | 0.44 |
| 3:a:2988[A]:TRP:HE3 | 3:a:2989[A]:HIS:CE1 | 2.25 | 0.44 |
| 3:a:2988[A]:TRP:CD1 | 3:a:3158[A]:PHE:CE2 | 3.06 | 0.44 |
| 3:a:3133[A]:LEU:O | 3:a:3136[A]:TYR:HB3 | 2.17 | 0.44 |
| 3:a:3137[A]:ARG:O | 3:a:3139[A]:LEU:HD22 | 2.16 | 0.44 |
| 1:b:139:VAL:HG11 | 1:b:144:TYR:OH | 2.18 | 0.44 |
| 1:b:597:VAL:HG12 | 1:b:773:PHE:CD1 | 2.52 | 0.44 |
| 1:b:668:MET:HE2 | 1:b:668:MET:HA | 2.00 | 0.44 |
| 2:c:2286:HIS:CD2 | 2:c:2433:THR:HG22 | 2.53 | 0.44 |
| 3:d:2931[B]:THR:O | 3:d:2934[B]:GLU:HG3 | 2.18 | 0.44 |
| 3:d:2981[B]:GLY:N | 3:d:3086[B]:GLU:OE1 | 2.45 | 0.44 |
| 3:d:3133[B]:LEU:O | 3:d:3136[B]:TYR:HB3 | 2.17 | 0.44 |
| 3:d:3137[A]:ARG:HB3 | 3:d:3139[A]:LEU:HD21 | 1.97 | 0.44 |
| 3:d:3299[B]:LEU:O | 3:d:3300[B]:LEU:C | 2.60 | 0.44 |
| 1:A:282:ASN:N | 1:A:282:ASN:OD1 | 2.51 | 0.44 |
| 1:A:1258:ARG:NH2 | 1:A:1332:ASP:OD1 | 2.50 | 0.44 |
| 1:A:1482:ALA:HB2 | 1:A:1517:PHE:HZ | 1.83 | 0.44 |
| 3:C:2948[A]:ASP:HB3 | 3:C:2949[A]:LYS:C | 2.43 | 0.44 |
| 3:C:2951[A]:ASP:OD2 | 3:C:2952[A]:ALA:CB | 2.66 | 0.44 |
| 3:C:2989[A]:HIS:O | 3:C:2990[A]:ARG:C | 2.61 | 0.44 |
| 3:C:3023[A]:ILE:O | 3:C:3026[A]:THR:OG1 | 2.34 | 0.44 |
| 3:C:3132[A]:ALA:HB3 | 3:C:3197[A]:ILE:HD13 | 1.99 | 0.44 |
| 3:C:3147[A]:GLU:CG | 3:C:3149[A]:ASN:ND2 | 2.73 | 0.44 |
| 3:C:3155[B]:MET:HG2 | 3:L:3153[B]:LYS:O | 2.15 | 0.44 |
| 3:C:3161[A]:GLU:N | 3:C:3161[A]:GLU:CD | 2.73 | 0.44 |
| 3:C:3172[B]:SER:OG | 3:L:3150[B]:LYS:N | 2.49 | 0.44 |
| 3:C:3293[A]:LYS:CD | 3:C:3293[A]:LYS:C | 2.86 | 0.44 |
| 1:D:35:GLN:HG3 | 1:D:129:LYS:HB2 | 2.00 | 0.44 |
| 1:D:226:HIS:HA | 1:D:227:ARG:HA | 1.55 | 0.44 |
| 1:D:353:ASN:HD22 | 1:D:772:ARG:HH22 | 1.66 | 0.44 |
| 1:D:446:PHE:CZ | 1:D:455:TYR:HA | 2.53 | 0.44 |
| 1:D:527:LEU:O | 1:D:561:ARG:NH1 | 2.51 | 0.44 |
| 1:D:836:GLN:O | 1:D:1113:HIS:HB3 | 2.18 | 0.44 |
| 1:D:843:VAL:HG22 | 1:D:928:TYR:O | 2.18 | 0.44 |
| 1:D:995:ILE:O | 1:D:999:LEU:HD22 | 2.18 | 0.44 |
| 2:E:2415:PRO:HD2 | 2:E:2418:GLY:O | 2.17 | 0.44 |
| 2:E:2663:MET:HE1 | 2:E:2717:LEU:HD13 | 2.00 | 0.44 |
| 3:F:2937[A]:ASN:CG | 3:F:3006[A]:LYS:HD3 | 2.43 | 0.44 |
| 3:F:2965[B]:LEU:O | 3:a:3221[B]:ALA:CB | 2.53 | 0.44 |
| 3:F:2977[B]:CYS:SG | 3:a:2982[B]:MET:CE | 2.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2995[B]:GLN:CG | 3:F:3168[B]:THR:HG21 | 2.48 | 0.44 |
| 3:F:3034[B]:HIS:HB3 | 3:F:3035[B]:HIS:CE1 | 2.50 | 0.44 |
| 3:F:3137[B]:ARG:HD3 | 3:F:3137[B]:ARG:HA | 1.72 | 0.44 |
| 3:F:3149[B]:ASN:HD22 | 3:a:3163[B]:ASN:CA | 2.29 | 0.44 |
| 3:F:3182[A]:GLN:C | 3:F:3183[A]:LEU:CD1 | 2.91 | 0.44 |
| 3:F:3223[B]:GLY:N | 3:a:2963[B]:MET:HE1 | 2.32 | 0.44 |
| 3:F:3230[B]:PHE:CB | 3:F:3242[B]:GLY:C | 2.91 | 0.44 |
| 3:F:3251[B]:ASP:C | 3:a:3251[B]:ASP:CB | 2.76 | 0.44 |
| 1:G:105:VAL:HB | 1:G:137:ARG:NH1 | 2.32 | 0.44 |
| 1:G:434:GLU:H | 1:G:434:GLU:HG3 | 1.55 | 0.44 |
| 1:G:949:ASP:HB2 | 1:G:953:GLU:HB2 | 2.00 | 0.44 |
| 2:H:2128:LEU:O | 2:H:2130:PRO:HD3 | 2.18 | 0.44 |
| 3:I:2938[B]:LEU:O | 3:I:2939[B]:ARG:C | 2.58 | 0.44 |
| 3:I:2970[B]:PRO:C | 3:I:2972[B]:GLY:N | 2.72 | 0.44 |
| 3:I:2971[B]:ASP:O | 3:R:3090[B]:ASN:CB | 2.66 | 0.44 |
| 3:I:3093[A]:HIS:HB2 | 3:I:3248[A]:LEU:CD1 | 2.48 | 0.44 |
| 3:I:3093[A]:HIS:HD2 | 3:I:3248[A]:LEU:CD2 | 2.30 | 0.44 |
| 3:I:3155[B]:MET:CB | 3:R:3153[B]:LYS:HB3 | 2.47 | 0.44 |
| 3:I:3163[B]:ASN:O | 3:R:3147[B]:GLU:OE2 | 2.36 | 0.44 |
| 3:I:3171[A]:HIS:C | 3:I:3173[A]:THR:N | 2.73 | 0.44 |
| 3:I:3200[B]:LEU:CD2 | 3:I:3204[B]:LEU:HD11 | 2.48 | 0.44 |
| 3:I:3266[A]:ILE:O | 3:I:3269[A]:SER:HB2 | 2.18 | 0.44 |
| 9:I:3401[A]:CUO:O1 | 3:R:2989[A]:HIS:CD2 | 2.70 | 0.44 |
| 1:J:293:LEU:O | 1:J:296:ARG:HG2 | 2.18 | 0.44 |
| 1:J:590:ASP:CG | 1:J:653:LYS:HZ1 | 2.26 | 0.44 |
| 1:J:840:ARG:HD3 | 1:J:926:LEU:O | 2.17 | 0.44 |
| 1:J:1347:ASP:HA | 1:J:1460:ASN:ND2 | 2.33 | 0.44 |
| 3:L:3025[A]:VAL:CG2 | 3:L:3047[A]:ARG:NH1 | 2.73 | 0.44 |
| 3:L:3027[A]:GLU:CD | 3:L:3027[A]:GLU:C | 2.85 | 0.44 |
| 3:L:3037[B]:TYR:C | 3:L:3038[B]:ILE:HG13 | 2.42 | 0.44 |
| 3:L:3241[B]:PHE:CE2 | 3:L:3243[B]:GLY:O | 2.70 | 0.44 |
| 1:M:873:VAL:HA | 1:M:876:PHE:HE1 | 1.80 | 0.44 |
| 1:M:1212:HIS:CD2 | 1:M:1212:HIS:N | 2.86 | 0.44 |
| 3:O:2933[B]:SER:CA | 3:O:2936[B]:GLU:HB3 | 2.48 | 0.44 |
| 3:O:2940[A]:ASN:O | 3:O:2943[A]:ALA:HB3 | 2.18 | 0.44 |
| 3:O:2951[B]:ASP:OD2 | 3:O:2952[B]:ALA:CB | 2.66 | 0.44 |
| 3:O:3148[A]:ILE:O | 3:O:3148[A]:ILE:HG22 | 2.17 | 0.44 |
| 3:O:3148[B]:ILE:O | 3:O:3148[B]:ILE:HG22 | 2.17 | 0.44 |
| 3:O:3182[A]:GLN:C | 3:O:3183[A]:LEU:CD1 | 2.91 | 0.44 |
| 1:P:979:LEU:HD23 | 1:P:980:TYR:CD1 | 2.52 | 0.44 |
| 1:P:1639:LYS:HD2 | 1:S:472:ASP:CB | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q:2830:GLN:H | 2:Q:2863:ARG:NH2 | 2.15 | 0.44 |
| 3:R:2963[B]:MET:C | 3:R:2963[B]:MET:SD | 3.01 | 0.44 |
| 3:R:2988[A]:TRP:CD1 | 3:R:3158[A]:PHE:CE2 | 3.06 | 0.44 |
| 3:R:3013[B]:ASP:CG | 3:R:3015[B]:THR:HG1 | 2.24 | 0.44 |
| 3:R:3023[A]:ILE:HA | 3:R:3026[A]:THR:HG1 | 1.82 | 0.44 |
| 3:R:3149[B]:ASN:OD1 | 3:R:3149[B]:ASN:N | 2.51 | 0.44 |
| 3:R:3273[A]:LEU:C | 3:R:3275[A]:LEU:HD12 | 2.42 | 0.44 |
| 3:R:3284[A]:LYS:CD | 3:R:3284[A]:LYS:C | 2.86 | 0.44 |
| 1:S:318:ARG:HB2 | 1:S:382:GLU:HB2 | 1.98 | 0.44 |
| 1:S:464:LEU:HD22 | 1:S:622:HIS:CG | 2.53 | 0.44 |
| 1:S:1160:PHE:HB3 | 1:S:1171:LYS:HA | 2.00 | 0.44 |
| 1:S:1390:ASP:HB2 | 1:S:1438:ASP:OD2 | 2.17 | 0.44 |
| 1:S:1622:GLN:H | 1:S:1622:GLN:HG3 | 1.47 | 0.44 |
| 2:T:2239:LYS:HG2 | 2:T:2240:GLN:N | 2.33 | 0.44 |
| 2:T:2877:ILE:HB | 1:V:1078:ARG:HH21 | 1.82 | 0.44 |
| 3:U:2969[A]:TYR:CD2 | 3:U:2970[A]:PRO:CG | 3.00 | 0.44 |
| 3:U:3014[B]:TRP:CH2 | 3:U:3123[B]:THR:HG23 | 2.53 | 0.44 |
| 3:U:3093[A]:HIS:HD2 | 3:U:3248[A]:LEU:CD2 | 2.31 | 0.44 |
| 3:U:3104[B]:MET:SD | 3:U:3110[B]:THR:CG2 | 3.06 | 0.44 |
| 3:U:3148[B]:ILE:O | 3:U:3148[B]:ILE:HG22 | 2.17 | 0.44 |
| 3:U:3183[A]:LEU:N | 3:U:3184[A]:ASN:CA | 2.80 | 0.44 |
| 3:U:3217[B]:PHE:CD2 | 3:U:3300[B]:LEU:HD12 | 2.53 | 0.44 |
| 3:U:3281[A]:PHE:HE1 | 3:U:3305[A]:ILE:HG21 | 1.81 | 0.44 |
| 3:U:3284[B]:LYS:CE | 3:U:3284[B]:LYS:CA | 2.85 | 0.44 |
| 3:U:3298[B]:ASN:CA | 3:U:3299[B]:LEU:HB2 | 2.44 | 0.44 |
| 1:V:464:LEU:HG | 1:V:465:PRO:HA | 1.99 | 0.44 |
| 2:W:2765:PRO:HA | 2:W:2768:LEU:HD11 | 2.00 | 0.44 |
| 2:W:2868:GLU:CD | 3:X:2932[A]:PRO:O | 2.61 | 0.44 |
| 3:X:2989[A]:HIS:CD2 | 9:X:3401[A]:CUO:O1 | 2.70 | 0.44 |
| 3:X:3001[B]:LYS:H | 3:X:3003[B]:LYS:HG3 | 1.83 | 0.44 |
| 3:X:3093[B]:HIS:HB2 | 3:X:3248[B]:LEU:CD1 | 2.47 | 0.44 |
| 3:X:3141[B]:TYR:CD2 | 3:X:3141[B]:TYR:C | 2.86 | 0.44 |
| 3:X:3229[A]:ASN:O | 3:X:3286[A]:THR:N | 2.50 | 0.44 |
| 3:X:3273[B]:LEU:C | 3:X:3275[B]:LEU:HD12 | 2.42 | 0.44 |
| 1:Y:114:THR:O | 1:Y:116:LYS:HG3 | 2.18 | 0.44 |
| 2:Z:2803:ARG:HH21 | 2:Z:2805:PHE:HZ | 1.66 | 0.44 |
| 2:Z:2867:PRO:CD | 3:a:2932[A]:PRO:HB2 | 2.46 | 0.44 |
| 3:a:3241[A]:PHE:CE2 | 3:a:3243[A]:GLY:O | 2.71 | 0.44 |
| 1:b:376:ASN:HB2 | 1:b:665:TYR:CG | 2.52 | 0.44 |
| 1:b:480:CYS:SG | 1:b:621:LEU:HD11 | 2.58 | 0.44 |
| 1:b:905:TRP:CD1 | 1:b:1084:PHE:HE2 | 2.35 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2963[A]:MET:SD | 3:d:2963[A]:MET:C | 3.01 | 0.44 |
| 3:d:2965[B]:LEU:CG | 3:d:2974[B]:ALA:CB | 2.85 | 0.44 |
| 3:d:3027[B]:GLU:CD | 3:d:3027[B]:GLU:C | 2.85 | 0.44 |
| 3:d:3028[B]:PRO:HG2 | 3:d:3029[B]:LYS:HG3 | 2.00 | 0.44 |
| 2:B:2549:PRO:HA | 2:B:2550:THR:HG23 | 1.99 | 0.43 |
| 2:B:2680:HIS:CD2 | 2:B:2684:HIS:CD2 | 3.06 | 0.43 |
| 3:C:2937[B]:ASN:CG | 3:C:3006[B]:LYS:HD3 | 2.43 | 0.43 |
| 3:C:2975[B]:PHE:CA | 3:L:3253[B]:GLU:HB2 | 2.46 | 0.43 |
| 3:C:2989[B]:HIS:C | 3:C:2991[B]:LEU:N | 2.75 | 0.43 |
| 3:C:3028[B]:PRO:HG2 | 3:C:3029[B]:LYS:HG3 | 2.00 | 0.43 |
| 3:C:3194[A]:GLY:C | 3:C:3195[A]:MET:CG | 2.90 | 0.43 |
| 3:C:3217[A]:PHE:CD2 | 3:C:3300[A]:LEU:HD12 | 2.53 | 0.43 |
| 3:C:3273[B]:LEU:C | 3:C:3275[B]:LEU:HD12 | 2.42 | 0.43 |
| 1:D:717:GLN:O | 1:D:720:VAL:HG22 | 2.18 | 0.43 |
| 1:D:997:SER:O | 1:D:1000:GLU:HB2 | 2.18 | 0.43 |
| 1:D:1390:ASP:HB3 | 1:G:1372:ILE:CD1 | 2.49 | 0.43 |
| 3:F:2981[B]:GLY:HA3 | 3:a:2967[B]:CYS:HA | 1.36 | 0.43 |
| 3:F:2982[B]:MET:CG | 3:a:3156[B]:MET:CB | 2.93 | 0.43 |
| 3:F:3019[A]:HIS:CD2 | 3:F:3020[A]:SER:H | 2.35 | 0.43 |
| 3:F:3093[A]:HIS:HD2 | 3:F:3248[A]:LEU:CD2 | 2.31 | 0.43 |
| 3:F:3094[B]:SER:HG | 3:F:3227[B]:ASP:CG | 2.25 | 0.43 |
| 3:F:3101[B]:PRO:O | 3:F:3109[B]:TYR:HD2 | 2.00 | 0.43 |
| 3:F:3150[B]:LYS:CE | 3:a:3163[B]:ASN:HB2 | 2.23 | 0.43 |
| 3:F:3156[B]:MET:CG | 3:a:2982[B]:MET:HG3 | 2.48 | 0.43 |
| 3:F:3276[B]:ASP:C | 3:F:3278[B]:HIS:N | 2.75 | 0.43 |
| 1:G:387:ASN:HD21 | 4:o:1:NAG:C6 | 2.31 | 0.43 |
| 1:G:419:THR:HA | 1:G:420:SER:HA | 1.65 | 0.43 |
| 1:G:464:LEU:HD22 | 1:G:622:HIS:HB3 | 1.99 | 0.43 |
| 1:G:494:VAL:HG13 | 1:G:631:TRP:HZ3 | 1.82 | 0.43 |
| 1:G:704:ASP:N | 1:G:704:ASP:OD1 | 2.50 | 0.43 |
| 1:G:717:GLN:HA | 1:G:720:VAL:HG22 | 1.99 | 0.43 |
| 1:G:939:PRO:O | 1:G:943:LEU:HG | 2.17 | 0.43 |
| 1:G:979:LEU:HB3 | 1:G:980:TYR:CG | 2.52 | 0.43 |
| 2:H:2339:GLY:HA2 | 2:H:2349:THR:HG21 | 2.00 | 0.43 |
| 2:H:2370:MET:HE3 | 2:H:2370:MET:HB2 | 1.78 | 0.43 |
| 2:H:2780:HIS:CE1 | 2:H:2782:ASN:HD21 | 2.35 | 0.43 |
| 3:I:2931[B]:THR:O | 3:I:2934[B]:GLU:HG3 | 2.18 | 0.43 |
| 3:I:2986[B]:PRO:CB | 3:I:3127[B]:TRP:CE3 | 3.00 | 0.43 |
| 3:I:3019[B]:HIS:CD2 | 3:I:3020[B]:SER:H | 2.35 | 0.43 |
| 3:I:3047[A]:ARG:NH2 | 3:I:3113[A]:ASP:OD1 | 2.43 | 0.43 |
| 3:I:3133[A]:LEU:O | 3:I:3136[A]:TYR:HB3 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3232[A]:VAL:HG21 | 3:I:3273[A]:LEU:HD11 | 2.00 | 0.43 |
| 2:K:2130:PRO:HB2 | 2:K:2142:ALA:HB3 | 2.00 | 0.43 |
| 3:L:2933[A]:SER:CA | 3:L:2936[A]:GLU:HB3 | 2.48 | 0.43 |
| 3:L:2963[A]:MET:SD | 3:L:2963[A]:MET:C | 3.01 | 0.43 |
| 3:L:3229[A]:ASN:O | 3:L:3286[A]:THR:N | 2.50 | 0.43 |
| 1:M:882:TRP:HE1 | 1:M:1090:ILE:HD13 | 1.83 | 0.43 |
| 2:N:2628:HIS:HB2 | 2:N:2635:TYR:CE2 | 2.53 | 0.43 |
| 2:N:2866:PRO:HB2 | 2:N:2868:GLU:OE2 | 2.18 | 0.43 |
| 3:O:2951[A]:ASP:OD2 | 3:O:2952[A]:ALA:CB | 2.66 | 0.43 |
| 3:O:2963[A]:MET:C | 3:O:2963[A]:MET:SD | 3.01 | 0.43 |
| 3:O:2968[B]:GLN:HB3 | 3:X:2979[B]:GLN:CG | 2.48 | 0.43 |
| 3:O:2975[B]:PHE:HD1 | 3:X:3156[B]:MET:O | 2.00 | 0.43 |
| 3:O:2979[A]:GLN:HB2 | 3:O:2988[A]:TRP:CD1 | 2.52 | 0.43 |
| 3:O:3014[B]:TRP:CH2 | 3:O:3123[B]:THR:HG23 | 2.53 | 0.43 |
| 3:O:3217[B]:PHE:CD2 | 3:O:3300[B]:LEU:HD12 | 2.53 | 0.43 |
| 1:P:728:ARG:HD2 | 1:P:780:GLU:OE2 | 2.18 | 0.43 |
| 1:P:733:PHE:CZ | 1:P:746:LEU:HD22 | 2.53 | 0.43 |
| 1:P:899:MET:HB3 | 1:P:1012:GLU:OE1 | 2.18 | 0.43 |
| 3:R:3044[A]:LYS:H | 3:R:3044[A]:LYS:HG2 | 1.65 | 0.43 |
| 3:R:3104[B]:MET:SD | 3:R:3110[B]:THR:CG2 | 3.06 | 0.43 |
| 3:R:3141[B]:TYR:CD2 | 3:R:3141[B]:TYR:C | 2.85 | 0.43 |
| 3:R:3200[B]:LEU:CD2 | 3:R:3204[B]:LEU:HD11 | 2.48 | 0.43 |
| 1:S:21:SER:HB2 | 1:S:83:HIS:O | 2.18 | 0.43 |
| 1:S:482:HIS:CE1 | 1:S:621:LEU:HD11 | 2.53 | 0.43 |
| 2:T:2644:LEU:HD22 | 2:T:2687:ILE:HG22 | 2.00 | 0.43 |
| 3:U:3160[B]:SER:O | 3:d:3147[B]:GLU:CG | 2.38 | 0.43 |
| 3:U:3241[B]:PHE:CE2 | 3:U:3243[B]:GLY:O | 2.70 | 0.43 |
| 1:V:988:TYR:O | 1:V:992:ALA:HB3 | 2.18 | 0.43 |
| 2:W:2156:ARG:HD2 | 2:W:2357:VAL:HG12 | 1.99 | 0.43 |
| 2:W:2267:HIS:CD2 | 2:W:2297:HIS:HE1 | 2.29 | 0.43 |
| 2:W:2472:ASN:N | 2:W:2472:ASN:OD1 | 2.48 | 0.43 |
| 2:W:2746:MET:HE2 | 2:W:2746:MET:HB2 | 1.91 | 0.43 |
| 2:W:2870:LEU:HA | 2:W:2877:ILE:HD11 | 1.99 | 0.43 |
| 3:X:2940[A]:ASN:O | 3:X:2943[A]:ALA:HB3 | 2.18 | 0.43 |
| 3:X:2948[A]:ASP:HB3 | 3:X:2949[A]:LYS:C | 2.43 | 0.43 |
| 3:X:2963[A]:MET:SD | 3:X:2963[A]:MET:C | 3.01 | 0.43 |
| 3:X:2965[A]:LEU:CG | 3:X:2974[A]:ALA:CB | 2.85 | 0.43 |
| 3:X:3027[A]:GLU:CD | 3:X:3027[A]:GLU:C | 2.85 | 0.43 |
| 3:X:3028[A]:PRO:HG2 | 3:X:3029[A]:LYS:HG3 | 2.00 | 0.43 |
| 3:X:3133[B]:LEU:O | 3:X:3136[B]:TYR:HB3 | 2.17 | 0.43 |
| 3:X:3180[A]:TYR:CA | 3:X:3183[A]:LEU:CD2 | 2.95 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3183[A]:LEU:N | 3:X:3184[A]:ASN:CA | 2.80 | 0.43 |
| 3:X:3230[A]:PHE:CB | 3:X:3242[A]:GLY:C | 2.91 | 0.43 |
| 3:X:3299[B]:LEU:O | 3:X:3300[B]:LEU:C | 2.60 | 0.43 |
| 1:Y:567:LEU:N | 1:Y:568:PHE:CA | 2.77 | 0.43 |
| 1:Y:1171:LYS:HG2 | 1:Y:1173:GLY:H | 1.83 | 0.43 |
| 2:Z:2303:ARG:NH2 | 2:Z:2372:GLU:O | 2.51 | 0.43 |
| 2:Z:2551:PRO:HA | 2:Z:2552:GLU:HA | 1.49 | 0.43 |
| 3:a:3194[B]:GLY:C | 3:a:3195[B]:MET:CG | 2.91 | 0.43 |
| 3:a:3217[A]:PHE:CD2 | 3:a:3300[A]:LEU:HD12 | 2.53 | 0.43 |
| 3:a:3293[A]:LYS:CD | 3:a:3293[A]:LYS:C | 2.86 | 0.43 |
| 2:c:2469:VAL:HG12 | 2:c:2475:GLU:HA | 2.00 | 0.43 |
| 3:d:2940[B]:ASN:O | 3:d:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:d:3047[B]:ARG:NH2 | 3:d:3113[B]:ASP:OD1 | 2.43 | 0.43 |
| 1:A:1210:LYS:HG2 | 2:E:2744:PHE:CD2 | 2.53 | 0.43 |
| 3:C:3024[A]:LEU:CD1 | 3:C:3024[A]:LEU:C | 2.85 | 0.43 |
| 3:C:3185[A]:TYR:HE2 | 3:C:3187[A]:TYR:CD2 | 2.35 | 0.43 |
| 3:C:3200[B]:LEU:CD2 | 3:C:3204[B]:LEU:HD11 | 2.48 | 0.43 |
| 3:C:3253[B]:GLU:OE1 | 3:L:2975[B]:PHE:C | 2.61 | 0.43 |
| 3:C:3266[B]:ILE:O | 3:C:3269[B]:SER:HB2 | 2.17 | 0.43 |
| 1:D:480:CYS:SG | 1:D:621:LEU:HD11 | 2.58 | 0.43 |
| 1:D:572:SER:HA | 1:D:573:LYS:HA | 1.42 | 0.43 |
| 1:D:588:GLU:HG3 | 1:D:724:LYS:HD2 | 1.99 | 0.43 |
| 1:D:893:ALA:HB2 | 1:D:1182:ASN:HB2 | 1.99 | 0.43 |
| 3:F:2951[A]:ASP:OD2 | 3:F:2952[A]:ALA:CB | 2.66 | 0.43 |
| 3:F:2970[B]:PRO:HD2 | 3:a:2989[B]:HIS:CE1 | 2.43 | 0.43 |
| 3:F:2976[A]:ALA:O | 3:F:2978[A]:CYS:N | 2.46 | 0.43 |
| 3:F:2991[A]:LEU:HD23 | 3:F:3158[A]:PHE:CE1 | 2.48 | 0.43 |
| 3:F:3014[A]:TRP:CH2 | 3:F:3123[A]:THR:HG23 | 2.53 | 0.43 |
| 3:F:3027[B]:GLU:CD | 3:F:3027[B]:GLU:C | 2.85 | 0.43 |
| 3:F:3093[A]:HIS:HB2 | 3:F:3248[A]:LEU:CD1 | 2.48 | 0.43 |
| 3:F:3131[B]:GLN:HE21 | 3:F:3131[B]:GLN:HB3 | 1.66 | 0.43 |
| 3:F:3217[A]:PHE:CD2 | 3:F:3300[A]:LEU:HD12 | 2.53 | 0.43 |
| 3:F:3266[B]:ILE:O | 3:F:3269[B]:SER:HB2 | 2.18 | 0.43 |
| 1:G:22:LEU:HD23 | 1:G:123:PHE:HE1 | 1.83 | 0.43 |
| 1:G:84:GLY:HA2 | 1:G:85:SER:C | 2.43 | 0.43 |
| 1:G:125:SER:OG | 1:G:125:SER:O | 2.31 | 0.43 |
| 1:G:1262:ASN:OD1 | 1:G:1263:LEU:N | 2.52 | 0.43 |
| 1:G:1346:TRP:O | 1:G:1460:ASN:ND2 | 2.51 | 0.43 |
| 2:H:2381:LEU:HD23 | 2:H:2381:LEU:HA | 1.84 | 0.43 |
| 2:H:2679:ILE:O | 2:H:2682:SER:HB3 | 2.18 | 0.43 |
| 3:I:2963[B]:MET:SD | 3:I:2963[B]:MET:C | 3.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2988[B]:TRP:CD1 | 3:I:3158[B]:PHE:CE2 | 3.06 | 0.43 |
| 3:I:3086[B]:GLU:HG3 | 3:R:2968[B]:GLN:HG3 | 1.47 | 0.43 |
| 3:I:3093[B]:HIS:HB2 | 3:I:3248[B]:LEU:CD1 | 2.48 | 0.43 |
| 3:I:3104[B]:MET:SD | 3:I:3110[B]:THR:CG2 | 3.06 | 0.43 |
| 3:I:3132[A]:ALA:HB3 | 3:I:3197[A]:ILE:HD13 | 1.98 | 0.43 |
| 3:I:3200[A]:LEU:CD2 | 3:I:3204[A]:LEU:HD11 | 2.48 | 0.43 |
| 3:I:3223[B]:GLY:CA | 3:R:2963[B]:MET:CE | 2.80 | 0.43 |
| 3:I:3293[A]:LYS:CB | 3:I:3294[A]:SER:CA | 2.96 | 0.43 |
| 1:J:98:MET:O | 1:J:144:TYR:HB3 | 2.18 | 0.43 |
| 1:J:237:LEU:HB2 | 1:J:820:VAL:HB | 2.00 | 0.43 |
| 1:J:918:ARG:HD3 | 1:J:924:GLY:O | 2.18 | 0.43 |
| 1:J:1230:LEU:H | 1:J:1230:LEU:HD23 | 1.83 | 0.43 |
| 1:J:1390:ASP:HB2 | 1:J:1438:ASP:OD2 | 2.18 | 0.43 |
| 1:J:1438:ASP:OD1 | 1:J:1439:VAL:N | 2.50 | 0.43 |
| 1:J:1519:TYR:OH | 1:J:1530:LEU:HD11 | 2.18 | 0.43 |
| 2:K:2089:ARG:HD2 | 2:K:2175:VAL:O | 2.18 | 0.43 |
| 2:K:2198:ASP:O | 2:K:2202:GLY:N | 2.50 | 0.43 |
| 2:K:2403:PHE:CD2 | 2:K:2476:LEU:HD13 | 2.52 | 0.43 |
| 2:K:2826:GLU:HB3 | 2:K:2827:ALA:H | 1.51 | 0.43 |
| 3:L:2937[B]:ASN:CG | 3:L:3006[B]:LYS:HD3 | 2.43 | 0.43 |
| 3:L:2991[A]:LEU:HD23 | 3:L:3158[A]:PHE:CE1 | 2.48 | 0.43 |
| 3:L:3217[B]:PHE:CD2 | 3:L:3300[B]:LEU:HD12 | 2.53 | 0.43 |
| 3:L:3285[B]:VAL:CG2 | 3:L:3286[B]:THR:H | 2.27 | 0.43 |
| 1:M:935:ILE:HD11 | 1:M:980:TYR:CD2 | 2.53 | 0.43 |
| 1:M:1161:ILE:O | 1:M:1203:MET:HE1 | 2.18 | 0.43 |
| 1:M:1427:HIS:CE1 | 1:M:1457:HIS:HE1 | 2.35 | 0.43 |
| 3:O:2971[B]:ASP:C | 3:X:2988[B]:TRP:CE3 | 2.96 | 0.43 |
| 3:O:2995[A]:GLN:CG | 3:O:3168[A]:THR:HG21 | 2.48 | 0.43 |
| 3:O:3034[B]:HIS:HB3 | 3:O:3035[B]:HIS:CE1 | 2.50 | 0.43 |
| 3:O:3093[A]:HIS:HB2 | 3:O:3248[A]:LEU:CD1 | 2.48 | 0.43 |
| 3:O:3182[B]:GLN:C | 3:O:3183[B]:LEU:CD1 | 2.91 | 0.43 |
| 1:P:387:ASN:ND2 | 6:3:1:NAG:C7 | 2.79 | 0.43 |
| 1:P:977:GLU:HG3 | 1:P:978:ALA:H | 1.83 | 0.43 |
| 1:P:1271:MET:HE1 | 1:P:1357:ARG:NH1 | 2.32 | 0.43 |
| 1:P:1578:ILE:HA | 1:P:1579:GLY:HA2 | 1.58 | 0.43 |
| 2:Q:2370:MET:HB2 | 2:Q:2370:MET:HE3 | 1.60 | 0.43 |
| 3:R:2952[A]:ALA:CA | 3:R:2956[A]:LYS:CB | 2.89 | 0.43 |
| 3:R:3001[B]:LYS:H | 3:R:3003[B]:LYS:HG3 | 1.83 | 0.43 |
| 3:R:3013[A]:ASP:CG | 3:R:3015[A]:THR:HG1 | 2.25 | 0.43 |
| 3:R:3149[A]:ASN:OD1 | 3:R:3149[A]:ASN:N | 2.51 | 0.43 |
| 1:S:1296:VAL:HG13 | 1:S:1384:PHE:HZ | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:2572:VAL:HG13 | 2:T:2768:LEU:HD23 | 1.99 | 0.43 |
| 2:T:2627:GLY:HA3 | 2:T:2703:PHE:O | 2.18 | 0.43 |
| 3:U:2931[A]:THR:O | 3:U:2934[A]:GLU:HG3 | 2.18 | 0.43 |
| 3:U:2973[B]:THR:CG2 | 3:d:3222[B]:ILE:O | 2.65 | 0.43 |
| 3:U:2989[A]:HIS:CD2 | 9:U:3401[A]:CUO:O1 | 2.71 | 0.43 |
| 3:U:2989[A]:HIS:C | 3:U:2991[A]:LEU:N | 2.75 | 0.43 |
| 3:U:2989[B]:HIS:CD2 | 9:U:3401[B]:CUO:O1 | 2.71 | 0.43 |
| 3:U:3096[B]:VAL:CG1 | 3:U:3115[B]:LEU:CD1 | 2.86 | 0.43 |
| 3:U:3149[B]:ASN:OD1 | 3:U:3149[B]:ASN:N | 2.51 | 0.43 |
| 3:U:3217[A]:PHE:CD2 | 3:U:3300[A]:LEU:HD12 | 2.53 | 0.43 |
| 3:U:3242[A]:GLY:C | 3:U:3243[A]:GLY:O | 2.58 | 0.43 |
| 1:V:385:ALA:HB2 | 1:V:391:MET:SD | 2.58 | 0.43 |
| 1:V:447:MET:HE2 | 1:V:447:MET:HB3 | 1.90 | 0.43 |
| 1:V:1286:ARG:HD2 | 1:V:1286:ARG:HA | 1.74 | 0.43 |
| 2:W:2237:LEU:H | 2:W:2237:LEU:HD13 | 1.82 | 0.43 |
| 3:X:2963[B]:MET:SD | 3:X:2963[B]:MET:C | 3.01 | 0.43 |
| 3:X:2979[B]:GLN:HB2 | 3:X:2988[B]:TRP:CD1 | 2.52 | 0.43 |
| 3:X:3096[A]:VAL:CG1 | 3:X:3115[A]:LEU:CD1 | 2.86 | 0.43 |
| 3:X:3101[B]:PRO:O | 3:X:3109[B]:TYR:HD2 | 2.00 | 0.43 |
| 3:X:3104[A]:MET:SD | 3:X:3110[A]:THR:CG2 | 3.06 | 0.43 |
| 3:X:3104[B]:MET:SD | 3:X:3110[B]:THR:CG2 | 3.06 | 0.43 |
| 3:X:3132[A]:ALA:HB3 | 3:X:3197[A]:ILE:HD13 | 1.99 | 0.43 |
| 2:Z:2226:GLU:OE1 | 2:Z:2277:LYS:HG2 | 2.17 | 0.43 |
| 3:a:3094[B]:SER:HG | 3:a:3227[B]:ASP:CG | 2.25 | 0.43 |
| 1:b:464:LEU:HD22 | 1:b:622:HIS:CD2 | 2.54 | 0.43 |
| 1:b:1005:CYS:O | 1:b:1009:VAL:HG23 | 2.18 | 0.43 |
| 1:b:1317:PRO:HA | 1:b:1420:GLU:HG3 | 2.01 | 0.43 |
| 2:c:2369:ASP:OD1 | 2:c:2370:MET:N | 2.51 | 0.43 |
| 3:d:2940[A]:ASN:O | 3:d:2943[A]:ALA:HB3 | 2.18 | 0.43 |
| 3:d:2989[A]:HIS:CD2 | 9:d:3401[A]:CUO:O1 | 2.70 | 0.43 |
| 3:d:3104[A]:MET:SD | 3:d:3110[A]:THR:CG2 | 3.06 | 0.43 |
| 3:d:3306[A]:LEU:C | 3:d:3306[A]:LEU:CD1 | 2.86 | 0.43 |
| 1:A:206:PHE:HE1 | 9:A:5001:CUO:O2 | 2.01 | 0.43 |
| 1:A:806:ASN:OD1 | 1:A:807:GLY:N | 2.51 | 0.43 |
| 1:A:1161:ILE:HB | 1:A:1203:MET:HE3 | 1.99 | 0.43 |
| 1:A:1325:LEU:O | 1:A:1328:SER:HB3 | 2.17 | 0.43 |
| 2:B:2553:ALA:N | 2:B:2554:PRO:CD | 2.81 | 0.43 |
| 3:C:2940[A]:ASN:O | 3:C:2943[A]:ALA:HB3 | 2.18 | 0.43 |
| 3:C:2948[A]:ASP:CB | 3:C:2949[A]:LYS:CA | 2.78 | 0.43 |
| 3:C:2963[A]:MET:SD | 3:C:2963[A]:MET:C | 3.01 | 0.43 |
| 3:C:2963[B]:MET:C | 3:C:2963[B]:MET:SD | 3.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3104[A]:MET:SD | 3:C:3110[A]:THR:CG2 | 3.06 | 0.43 |
| 1:D:322:CYS:HA | 1:D:333:ASN:O | 2.18 | 0.43 |
| 1:D:456:GLN:HG2 | 1:D:551:GLU:CB | 2.48 | 0.43 |
| 1:D:816:PRO:HA | 1:D:817:PRO:HD3 | 1.89 | 0.43 |
| 1:D:975:PRO:HB2 | 1:D:1024:GLY:HA3 | 2.00 | 0.43 |
| 2:E:2370:MET:HE3 | 2:E:2370:MET:HB2 | 1.76 | 0.43 |
| 3:F:2946[A]:GLN:CD | 3:F:2947[A]:ALA:N | 2.72 | 0.43 |
| 3:F:2949[A]:LYS:C | 3:F:2949[A]:LYS:HZ3 | 2.14 | 0.43 |
| 3:F:2951[A]:ASP:CG | 3:F:2952[A]:ALA:N | 2.74 | 0.43 |
| 3:F:2988[A]:TRP:CD1 | 3:F:3158[A]:PHE:CE2 | 3.06 | 0.43 |
| 3:F:2988[B]:TRP:CD1 | 3:F:3158[B]:PHE:CE2 | 3.06 | 0.43 |
| 3:F:3107[B]:LEU:HD21 | 3:a:2975[B]:PHE:HA | 1.99 | 0.43 |
| 3:F:3148[B]:ILE:HG22 | 3:F:3152[B]:LYS:HE3 | 2.01 | 0.43 |
| 3:F:3180[A]:TYR:CA | 3:F:3183[A]:LEU:CD2 | 2.95 | 0.43 |
| 3:F:3200[A]:LEU:CD2 | 3:F:3204[A]:LEU:HD11 | 2.48 | 0.43 |
| 3:F:3232[B]:VAL:HG21 | 3:F:3273[B]:LEU:HD11 | 2.00 | 0.43 |
| 3:F:3276[A]:ASP:C | 3:F:3278[A]:HIS:N | 2.75 | 0.43 |
| 1:G:14:GLU:O | 1:G:17:ASN:ND2 | 2.48 | 0.43 |
| 1:G:353:ASN:HB3 | 1:G:772:ARG:NH2 | 2.33 | 0.43 |
| 1:G:630:PHE:CE2 | 1:G:634:HIS:CE1 | 3.06 | 0.43 |
| 1:G:1148:LEU:HB2 | 1:G:1188:PHE:HD2 | 1.83 | 0.43 |
| 2:H:2666:GLN:HG3 | 2:H:2671:ASP:O | 2.18 | 0.43 |
| 3:I:2937[B]:ASN:CG | 3:I:3006[B]:LYS:HD3 | 2.43 | 0.43 |
| 3:I:2960[B]:PHE:C | 3:R:3255[B]:PRO:CD | 2.88 | 0.43 |
| 3:I:2965[B]:LEU:HG | 3:R:3249[B]:GLY:HA3 | 1.98 | 0.43 |
| 3:I:3023[A]:ILE:O | 3:I:3026[A]:THR:OG1 | 2.34 | 0.43 |
| 3:I:3034[B]:HIS:HB3 | 3:I:3035[B]:HIS:CE1 | 2.50 | 0.43 |
| 3:I:3148[A]:ILE:O | 3:I:3148[A]:ILE:HG22 | 2.17 | 0.43 |
| 3:I:3152[B]:LYS:O | 3:R:3171[B]:HIS:C | 2.59 | 0.43 |
| 3:I:3182[B]:GLN:C | 3:I:3183[B]:LEU:CD1 | 2.91 | 0.43 |
| 3:I:3217[B]:PHE:CD2 | 3:I:3300[B]:LEU:HD12 | 2.53 | 0.43 |
| 3:I:3232[B]:VAL:HG21 | 3:I:3273[B]:LEU:HD11 | 2.00 | 0.43 |
| 1:J:954:ALA:O | 1:J:956:PRO:HD3 | 2.18 | 0.43 |
| 1:J:1010:GLN:HE22 | 1:J:1193:LYS:H | 1.66 | 0.43 |
| 2:K:2341:PRO:HG2 | 2:K:2342:TYR:CD2 | 2.53 | 0.43 |
| 3:L:3229[B]:ASN:O | 3:L:3286[B]:THR:N | 2.50 | 0.43 |
| 3:L:3232[B]:VAL:HG21 | 3:L:3273[B]:LEU:HD11 | 2.00 | 0.43 |
| 1:M:187:GLY:HA3 | 1:M:195:SER:HB3 | 1.99 | 0.43 |
| 1:M:891:LYS:HB2 | 1:M:892:TYR:CD2 | 2.53 | 0.43 |
| 1:M:906:HIS:HA | 1:M:909:ILE:HB | 2.00 | 0.43 |
| 2:N:2168:ARG:O | 2:Q:2503:ASN:HB3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2940[B]:ASN:O | 3:O:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:O:2968[B]:GLN:CD | 3:X:2984[B]:THR:CB | 2.91 | 0.43 |
| 3:O:2986[A]:PRO:CB | 3:O:3127[A]:TRP:CE3 | 3.00 | 0.43 |
| 3:O:2995[B]:GLN:CG | 3:O:3168[B]:THR:HG21 | 2.48 | 0.43 |
| 3:O:3019[A]:HIS:CD2 | 3:O:3020[A]:SER:H | 2.35 | 0.43 |
| 3:O:3028[B]:PRO:HG2 | 3:O:3029[B]:LYS:HG3 | 2.00 | 0.43 |
| 3:O:3037[B]:TYR:C | 3:O:3038[B]:ILE:HG13 | 2.42 | 0.43 |
| 3:O:3217[A]:PHE:CD2 | 3:O:3300[A]:LEU:HD12 | 2.53 | 0.43 |
| 1:P:415:VAL:HB | 1:P:697:ALA:HB2 | 1.99 | 0.43 |
| 1:P:568:PHE:CD1 | 1:P:568:PHE:N | 2.85 | 0.43 |
| 1:P:1427:HIS:CD2 | 1:P:1457:HIS:HE1 | 2.37 | 0.43 |
| 2:Q:2249:LEU:HD11 | 2:Q:2395:PHE:HE2 | 1.83 | 0.43 |
| 2:Q:2561:HIS:HB3 | 2:Q:2677:GLU:OE2 | 2.18 | 0.43 |
| 3:R:3025[B]:VAL:CG2 | 3:R:3047[B]:ARG:NH1 | 2.73 | 0.43 |
| 3:R:3298[A]:ASN:CB | 3:R:3300[A]:LEU:CD2 | 2.61 | 0.43 |
| 3:R:3306[A]:LEU:C | 3:R:3306[A]:LEU:CD1 | 2.86 | 0.43 |
| 1:S:515:ASP:O | 1:S:518:LYS:HG2 | 2.17 | 0.43 |
| 1:S:1074:ILE:O | 1:S:1078:ARG:HG2 | 2.18 | 0.43 |
| 1:S:1195:ASP:HA | 1:S:1196:ILE:CG2 | 2.49 | 0.43 |
| 3:U:2948[A]:ASP:HB3 | 3:U:2949[A]:LYS:C | 2.43 | 0.43 |
| 3:U:2956[A]:LYS:O | 3:U:2959[A]:SER:OG | 2.33 | 0.43 |
| 3:U:2991[A]:LEU:HD23 | 3:U:3158[A]:PHE:CE1 | 2.47 | 0.43 |
| 3:U:3148[A]:ILE:HG22 | 3:U:3152[A]:LYS:HE3 | 2.01 | 0.43 |
| 3:U:3169[B]:LYS:HD3 | 3:d:3145[B]:ASN:O | 2.18 | 0.43 |
| 3:U:3194[A]:GLY:C | 3:U:3195[A]:MET:CG | 2.91 | 0.43 |
| 3:U:3200[B]:LEU:CD2 | 3:U:3204[B]:LEU:HD11 | 2.48 | 0.43 |
| 1:V:452:ILE:HD12 | 1:V:1367:SER:CB | 2.48 | 0.43 |
| 1:V:1156:LEU:HD11 | 1:V:1174:GLU:HG3 | 2.00 | 0.43 |
| 1:V:1512:ARG:HA | 1:V:1513:PRO:HD3 | 1.86 | 0.43 |
| 2:W:2345:ASN:HA | 2:W:2346:PRO:HD2 | 1.71 | 0.43 |
| 3:X:3014[A]:TRP:CH2 | 3:X:3123[A]:THR:HG23 | 2.52 | 0.43 |
| 3:X:3093[B]:HIS:HD2 | 3:X:3248[B]:LEU:CD2 | 2.31 | 0.43 |
| 3:X:3106[A]:THR:O | 3:X:3106[A]:THR:HG23 | 2.17 | 0.43 |
| 3:X:3276[B]:ASP:C | 3:X:3278[B]:HIS:N | 2.75 | 0.43 |
| 1:Y:603:HIS:O | 1:Y:606:ILE:HG22 | 2.19 | 0.43 |
| 2:Z:2500:ILE:HD11 | 2:Z:2776:TYR:HA | 1.99 | 0.43 |
| 3:a:2971[B]:ASP:CG | 9:a:3401[B]:CUO:O2 | 2.61 | 0.43 |
| 3:a:2989[B]:HIS:O | 3:a:2990[B]:ARG:C | 2.61 | 0.43 |
| 3:a:3137[A]:ARG:HB3 | 3:a:3139[A]:LEU:HD21 | 1.97 | 0.43 |
| 3:a:3242[A]:GLY:C | 3:a:3243[A]:GLY:O | 2.58 | 0.43 |
| 3:a:3299[A]:LEU:HB3 | 3:a:3300[A]:LEU:H | 1.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:119:LYS:HB2 | 1:b:120:LYS:CA | 2.48 | 0.43 |
| 1:b:157:GLU:OE2 | 1:b:296:ARG:NH2 | 2.51 | 0.43 |
| 1:b:322:CYS:HA | 1:b:333:ASN:O | 2.18 | 0.43 |
| 1:b:419:THR:N | 1:b:420:SER:HA | 2.33 | 0.43 |
| 1:b:1156:LEU:HD11 | 1:b:1174:GLU:HB2 | 2.00 | 0.43 |
| 3:d:2933[A]:SER:CA | 3:d:2936[A]:GLU:HB3 | 2.48 | 0.43 |
| 3:d:2933[B]:SER:CA | 3:d:2936[B]:GLU:HB3 | 2.48 | 0.43 |
| 3:d:3131[A]:GLN:HE21 | 3:d:3131[A]:GLN:HB3 | 1.66 | 0.43 |
| 3:d:3191[B]:ASN:ND2 | 3:d:3191[B]:ASN:N | 2.60 | 0.43 |
| 5:FA:3:BMA:O4 | 5:FA:4:MAN:H2 | 2.17 | 0.43 |
| 1:A:229:LEU:HB3 | 1:A:230:PRO:HD2 | 1.99 | 0.43 |
| 2:B:2163:GLU:HG3 | 2:B:2175:VAL:HG23 | 2.00 | 0.43 |
| 3:C:2989[B]:HIS:O | 3:C:2990[B]:ARG:C | 2.61 | 0.43 |
| 3:C:3001[B]:LYS:N | 3:C:3003[B]:LYS:HG3 | 2.34 | 0.43 |
| 3:C:3028[A]:PRO:HG2 | 3:C:3029[A]:LYS:HG3 | 2.00 | 0.43 |
| 3:C:3093[B]:HIS:HB2 | 3:C:3248[B]:LEU:CD1 | 2.48 | 0.43 |
| 3:C:3104[B]:MET:SD | 3:C:3110[B]:THR:CG2 | 3.06 | 0.43 |
| 3:C:3149[A]:ASN:OD1 | 3:C:3149[A]:ASN:N | 2.51 | 0.43 |
| 3:C:3163[B]:ASN:HD22 | 3:L:3149[B]:ASN:HB2 | 1.48 | 0.43 |
| 1:D:45:ALA:HB1 | 1:D:55:ILE:C | 2.43 | 0.43 |
| 1:D:71:LEU:HD22 | 1:D:266:LEU:HD21 | 1.99 | 0.43 |
| 1:D:547:LYS:HD2 | 1:D:558:HIS:HB3 | 1.99 | 0.43 |
| 1:D:564:ASP:OD1 | 1:D:564:ASP:N | 2.49 | 0.43 |
| 1:D:1060:GLN:OE1 | 1:D:1063:ARG:NH1 | 2.51 | 0.43 |
| 1:D:1210:LYS:O | 1:D:1210:LYS:HD2 | 2.18 | 0.43 |
| 3:F:2940[A]:ASN:O | 3:F:2943[A]:ALA:HB3 | 2.18 | 0.43 |
| 3:F:2940[B]:ASN:O | 3:F:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:F:2989[A]:HIS:O | 3:F:2990[A]:ARG:C | 2.61 | 0.43 |
| 3:F:3001[B]:LYS:H | 3:F:3003[B]:LYS:HG3 | 1.83 | 0.43 |
| 3:F:3001[B]:LYS:N | 3:F:3003[B]:LYS:HG3 | 2.34 | 0.43 |
| 3:F:3149[A]:ASN:OD1 | 3:F:3149[A]:ASN:N | 2.51 | 0.43 |
| 3:F:3185[B]:TYR:CE2 | 3:F:3187[B]:TYR:HE2 | 2.31 | 0.43 |
| 3:F:3217[B]:PHE:CD2 | 3:F:3300[B]:LEU:HD12 | 2.53 | 0.43 |
| 1:G:1356:PRO:HD2 | 1:G:1359:ILE:HD11 | 2.01 | 0.43 |
| 2:H:2156:ARG:O | 2:H:2160:VAL:HG13 | 2.17 | 0.43 |
| 3:I:2933[B]:SER:CA | 3:I:2936[B]:GLU:HB3 | 2.48 | 0.43 |
| 3:I:3013[B]:ASP:CG | 3:I:3015[B]:THR:HG1 | 2.24 | 0.43 |
| 3:I:3014[B]:TRP:CH2 | 3:I:3123[B]:THR:HG23 | 2.53 | 0.43 |
| 3:I:3120[B]:HIS:HD2 | 3:R:2969[B]:TYR:CE2 | 2.21 | 0.43 |
| 3:I:3161[B]:GLU:C | 3:R:3147[B]:GLU:CG | 2.60 | 0.43 |
| 3:I:3244[A]:THR:H | 3:I:3264[A]:TYR:HE2 | 1.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3251[B]:ASP:CG | 3:R:3108[B]:HIS:HE1 | 2.26 | 0.43 |
| 3:I:3255[B]:PRO:CB | 3:R:2964[B]:PRO:CA | 2.95 | 0.43 |
| 3:I:3299[A]:LEU:O | 3:I:3300[A]:LEU:C | 2.60 | 0.43 |
| 1:J:108:PRO:HB3 | 1:J:124:TYR:CE2 | 2.53 | 0.43 |
| 1:J:462:HIS:HA | 1:J:490:TRP:CH2 | 2.52 | 0.43 |
| 1:J:638:ASP:HB3 | 1:J:703:TYR:OH | 2.18 | 0.43 |
| 1:J:979:LEU:HD12 | 1:J:1021:LEU:HD22 | 2.01 | 0.43 |
| 1:J:1271:MET:HG2 | 1:J:1358:LEU:HD13 | 2.00 | 0.43 |
| 3:L:2931[B]:THR:O | 3:L:2934[B]:GLU:HG3 | 2.18 | 0.43 |
| 3:L:2933[B]:SER:CA | 3:L:2936[B]:GLU:HB3 | 2.48 | 0.43 |
| 3:L:3027[B]:GLU:CD | 3:L:3027[B]:GLU:C | 2.85 | 0.43 |
| 3:L:3133[B]:LEU:O | 3:L:3136[B]:TYR:HB3 | 2.17 | 0.43 |
| 3:L:3161[A]:GLU:H | 3:L:3161[A]:GLU:CD | 2.19 | 0.43 |
| 3:L:3230[B]:PHE:CB | 3:L:3242[B]:GLY:C | 2.91 | 0.43 |
| 3:L:3232[A]:VAL:HG21 | 3:L:3273[A]:LEU:HD11 | 2.00 | 0.43 |
| 3:L:3267[B]:SER:H | 3:L:3267[B]:SER:HG | 1.32 | 0.43 |
| 3:L:3298[A]:ASN:CA | 3:L:3299[A]:LEU:HB2 | 2.44 | 0.43 |
| 1:M:450:LYS:HD3 | 1:M:1338:GLY:O | 2.18 | 0.43 |
| 1:M:1250:ILE:O | 1:M:1473:ARG:NH2 | 2.51 | 0.43 |
| 2:N:2132:CYS:HB2 | 2:N:2142:ALA:HB1 | 2.00 | 0.43 |
| 2:N:2247:ILE:HG12 | 2:N:2266:VAL:HG11 | 1.99 | 0.43 |
| 2:N:2462:PHE:CE2 | 2:N:2486:ILE:HD13 | 2.53 | 0.43 |
| 3:O:3104[B]:MET:SD | 3:O:3110[B]:THR:CG2 | 3.06 | 0.43 |
| 3:O:3183[B]:LEU:N | 3:O:3184[B]:ASN:CA | 2.80 | 0.43 |
| 3:O:3241[A]:PHE:CE2 | 3:O:3243[A]:GLY:O | 2.70 | 0.43 |
| 3:O:3245[A]:PHE:CD1 | 3:O:3245[A]:PHE:C | 2.97 | 0.43 |
| 3:O:3252[B]:TYR:HB3 | 3:X:3156[B]:MET:CG | 2.49 | 0.43 |
| 1:P:603:HIS:O | 1:P:606:ILE:HG22 | 2.19 | 0.43 |
| 2:Q:2156:ARG:O | 2:Q:2160:VAL:HG13 | 2.18 | 0.43 |
| 2:Q:2545:SER:HB2 | 2:Q:2547:MET:HG2 | 1.99 | 0.43 |
| 2:Q:2549:PRO:HA | 2:Q:2550:THR:HA | 1.49 | 0.43 |
| 2:Q:2567:MET:HE3 | 2:Q:2718:TRP:HB2 | 1.99 | 0.43 |
| 3:R:2949[B]:LYS:NZ | 3:R:2949[B]:LYS:C | 2.73 | 0.43 |
| 3:R:2961[A]:HIS:HB2 | 3:R:2992[A]:TYR:HE2 | 1.81 | 0.43 |
| 3:R:3001[B]:LYS:N | 3:R:3003[B]:LYS:HG3 | 2.34 | 0.43 |
| 3:R:3180[A]:TYR:CA | 3:R:3183[A]:LEU:CD2 | 2.95 | 0.43 |
| 3:R:3222[B]:ILE:CD1 | 3:R:3223[B]:GLY:N | 2.73 | 0.43 |
| 3:R:3242[A]:GLY:C | 3:R:3243[A]:GLY:O | 2.58 | 0.43 |
| 3:R:3244[B]:THR:H | 3:R:3264[B]:TYR:HE2 | 1.65 | 0.43 |
| 3:R:3293[B]:LYS:CB | 3:R:3294[B]:SER:CA | 2.96 | 0.43 |
| 1:S:450:LYS:HE2 | 1:S:450:LYS:N | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1380:GLY:HA3 | 1:S:1450:TYR:O | 2.19 | 0.43 |
| 1:S:1422:HIS:NE2 | 1:S:1608:ARG:HB2 | 2.34 | 0.43 |
| 2:T:2488:ARG:O | 1:V:1483:ASN:HB3 | 2.18 | 0.43 |
| 3:U:2940[B]:ASN:O | 3:U:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:U:3152[B]:LYS:CD | 3:d:3173[B]:THR:OG1 | 2.61 | 0.43 |
| 3:U:3180[B]:TYR:CA | 3:U:3183[B]:LEU:CD2 | 2.95 | 0.43 |
| 3:U:3196[B]:THR:N | 3:U:3199[B]:GLN:CB | 2.64 | 0.43 |
| 3:U:3285[A]:VAL:CG2 | 3:U:3286[A]:THR:H | 2.27 | 0.43 |
| 1:V:499:GLU:HG3 | 1:V:511:VAL:H | 1.83 | 0.43 |
| 2:W:2799:LYS:HA | 2:W:2803:ARG:NH1 | 2.34 | 0.43 |
| 3:X:2940[B]:ASN:O | 3:X:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:X:2951[A]:ASP:OD2 | 3:X:2952[A]:ALA:CB | 2.66 | 0.43 |
| 3:X:3132[B]:ALA:HB3 | 3:X:3197[B]:ILE:HD13 | 1.99 | 0.43 |
| 3:X:3141[A]:TYR:CD2 | 3:X:3141[A]:TYR:C | 2.85 | 0.43 |
| 3:X:3266[A]:ILE:O | 3:X:3269[A]:SER:HB2 | 2.18 | 0.43 |
| 1:Y:797:THR:HG22 | 1:Y:798:LEU:H | 1.83 | 0.43 |
| 1:Y:961:SER:HB2 | 1:Y:972:SER:O | 2.18 | 0.43 |
| 2:Z:2129:PRO:O | 2:Z:2131:LEU:HD23 | 2.18 | 0.43 |
| 2:Z:2156:ARG:O | 2:Z:2160:VAL:HG13 | 2.18 | 0.43 |
| 3:a:2932[B]:PRO:CA | 3:a:2935[B]:ILE:CD1 | 2.85 | 0.43 |
| 3:a:2940[A]:ASN:O | 3:a:2943[A]:ALA:HB3 | 2.18 | 0.43 |
| 3:a:2991[B]:LEU:HD23 | 3:a:3158[B]:PHE:CE1 | 2.47 | 0.43 |
| 3:a:3106[B]:THR:O | 3:a:3106[B]:THR:HG23 | 2.17 | 0.43 |
| 3:a:3196[B]:THR:N | 3:a:3199[B]:GLN:CB | 2.64 | 0.43 |
| 3:a:3241[B]:PHE:CZ | 3:a:3243[B]:GLY:O | 2.70 | 0.43 |
| 3:a:3266[B]:ILE:O | 3:a:3269[B]:SER:HB2 | 2.17 | 0.43 |
| 3:a:3293[B]:LYS:CB | 3:a:3294[B]:SER:CA | 2.96 | 0.43 |
| 1:b:497:GLN:NE2 | 1:b:683:THR:OG1 | 2.50 | 0.43 |
| 1:b:991:LEU:HD21 | 1:b:1017:HIS:CG | 2.54 | 0.43 |
| 1:b:1004:PHE:HE1 | 1:b:1053:TRP:CZ3 | 2.37 | 0.43 |
| 1:b:1067:TYR:N | 1:b:1067:TYR:CD1 | 2.84 | 0.43 |
| 3:d:2937[A]:ASN:CG | 3:d:3006[A]:LYS:HD3 | 2.44 | 0.43 |
| 3:d:2988[A]:TRP:CD1 | 3:d:3158[A]:PHE:CE2 | 3.06 | 0.43 |
| 3:d:3183[A]:LEU:N | 3:d:3184[A]:ASN:CA | 2.80 | 0.43 |
| 1:A:329:ARG:HA | 1:b:1584:GLY:H | 1.83 | 0.43 |
| 1:A:451:SER:HB3 | 1:A:1273:SER:HA | 1.99 | 0.43 |
| 1:A:695:TYR:N | 1:A:695:TYR:CD1 | 2.87 | 0.43 |
| 1:A:732:GLY:HA2 | 1:A:777:TYR:O | 2.18 | 0.43 |
| 2:B:2522:SER:O | 2:B:2526:ARG:HG2 | 2.18 | 0.43 |
| 2:B:2799:LYS:HA | 2:B:2803:ARG:HH12 | 1.83 | 0.43 |
| 2:B:2823:ILE:HG22 | 2:B:2879:LEU:HD12 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2940[B]:ASN:O | 3:C:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:C:2963[B]:MET:CE | 3:L:3223[B]:GLY:H | 2.08 | 0.43 |
| 3:C:2979[B]:GLN:HB2 | 3:C:2988[B]:TRP:CD1 | 2.52 | 0.43 |
| 3:C:3001[A]:LYS:N | 3:C:3003[A]:LYS:HG3 | 2.34 | 0.43 |
| 3:C:3027[B]:GLU:CD | 3:C:3027[B]:GLU:C | 2.85 | 0.43 |
| 3:C:3135[B]:LYS:HB2 | 3:C:3141[B]:TYR:CD1 | 2.52 | 0.43 |
| 3:C:3148[B]:ILE:HG22 | 3:C:3152[B]:LYS:HE3 | 2.01 | 0.43 |
| 3:C:3153[B]:LYS:HZ3 | 3:L:2988[B]:TRP:HD1 | 1.44 | 0.43 |
| 3:C:3161[B]:GLU:OE1 | 3:L:3079[B]:CYS:HA | 2.18 | 0.43 |
| 3:C:3249[B]:GLY:C | 3:L:3252[B]:TYR:CD2 | 2.62 | 0.43 |
| 1:D:138:ALA:O | 1:D:188:GLY:HA3 | 2.19 | 0.43 |
| 1:D:563:ILE:HD12 | 1:D:613:SER:OG | 2.18 | 0.43 |
| 1:D:957:ASN:HB3 | 1:D:960:PHE:HB2 | 2.00 | 0.43 |
| 1:D:987:LYS:HB3 | 1:D:988:TYR:HD1 | 1.84 | 0.43 |
| 2:E:2546:LEU:HG | 2:E:2842:THR:HG21 | 2.00 | 0.43 |
| 3:F:2951[B]:ASP:OD2 | 3:F:2952[B]:ALA:CB | 2.66 | 0.43 |
| 3:F:2971[A]:ASP:CG | 3:F:2973[A]:THR:HG1 | 2.14 | 0.43 |
| 3:F:3001[A]:LYS:N | 3:F:3003[A]:LYS:HG3 | 2.34 | 0.43 |
| 3:F:3023[A]:ILE:HA | 3:F:3026[A]:THR:HG1 | 1.84 | 0.43 |
| 3:F:3132[B]:ALA:HB3 | 3:F:3197[B]:ILE:HD13 | 1.98 | 0.43 |
| 3:F:3135[B]:LYS:HB2 | 3:F:3141[B]:TYR:CD1 | 2.52 | 0.43 |
| 3:F:3228[A]:VAL:CG2 | 3:F:3245[A]:PHE:CD2 | 3.02 | 0.43 |
| 3:F:3259[B]:ASP:N | 3:a:3162[B]:ASP:HB3 | 2.33 | 0.43 |
| 3:F:3299[B]:LEU:O | 3:F:3300[B]:LEU:C | 2.60 | 0.43 |
| 1:G:226:HIS:HA | 1:G:227:ARG:HB2 | 2.00 | 0.43 |
| 1:G:732:GLY:HA2 | 1:G:777:TYR:O | 2.18 | 0.43 |
| 2:H:2179:ASP:HB3 | 2:H:2303:ARG:NH1 | 2.33 | 0.43 |
| 3:I:2995[A]:GLN:CG | 3:I:3168[A]:THR:HG21 | 2.48 | 0.43 |
| 3:I:3001[B]:LYS:H | 3:I:3003[B]:LYS:HG3 | 1.83 | 0.43 |
| 3:I:3027[A]:GLU:CD | 3:I:3027[A]:GLU:C | 2.85 | 0.43 |
| 3:I:3148[A]:ILE:HG22 | 3:I:3152[A]:LYS:HE3 | 2.01 | 0.43 |
| 3:I:3293[A]:LYS:CD | 3:I:3293[A]:LYS:C | 2.86 | 0.43 |
| 1:J:206:PHE:O | 1:J:209:HIS:HB3 | 2.19 | 0.43 |
| 1:J:294:LYS:HA | 1:J:297:ARG:HD2 | 2.00 | 0.43 |
| 2:K:2644:LEU:H | 2:K:2644:LEU:HD23 | 1.84 | 0.43 |
| 3:L:3001[B]:LYS:N | 3:L:3003[B]:LYS:HG3 | 2.34 | 0.43 |
| 3:L:3028[A]:PRO:HG2 | 3:L:3029[A]:LYS:HG3 | 2.00 | 0.43 |
| 3:L:3245[B]:PHE:CD1 | 3:L:3245[B]:PHE:C | 2.97 | 0.43 |
| 1:M:293:LEU:O | 1:M:297:ARG:HG3 | 2.18 | 0.43 |
| 1:M:480:CYS:HA | 1:M:490:TRP:CE2 | 2.53 | 0.43 |
| 1:M:566:ARG:O | 1:M:609:TRP:NE1 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1247:ARG:HD3 | 1:M:1247:ARG:HA | 1.78 | 0.43 |
| 1:M:1621:ASN:HB3 | 1:M:1624:SER:H | 1.83 | 0.43 |
| 3:O:2989[B]:HIS:C | 3:O:2991[B]:LEU:N | 2.75 | 0.43 |
| 3:O:3001[B]:LYS:N | 3:O:3003[B]:LYS:HG3 | 2.34 | 0.43 |
| 3:O:3047[A]:ARG:NH2 | 3:O:3113[A]:ASP:OD1 | 2.43 | 0.43 |
| 3:O:3192[A]:PHE:HD2 | 3:O:3192[A]:PHE:HA | 1.77 | 0.43 |
| 3:O:3218[B]:LEU:HD13 | 3:O:3261[B]:LEU:HD23 | 2.01 | 0.43 |
| 1:P:17:ASN:OD1 | 1:P:85:SER:N | 2.52 | 0.43 |
| 1:P:947:TYR:HE1 | 1:P:956:PRO:HG2 | 1.83 | 0.43 |
| 1:P:1427:HIS:HD2 | 1:P:1457:HIS:CE1 | 2.36 | 0.43 |
| 2:Q:2089:ARG:HB2 | 2:Q:2368:TYR:CD1 | 2.54 | 0.43 |
| 3:R:2931[B]:THR:O | 3:R:2934[B]:GLU:HG3 | 2.18 | 0.43 |
| 3:R:2995[B]:GLN:CG | 3:R:3168[B]:THR:HG21 | 2.48 | 0.43 |
| 3:R:3001[A]:LYS:N | 3:R:3003[A]:LYS:HG3 | 2.34 | 0.43 |
| 3:R:3194[B]:GLY:C | 3:R:3195[B]:MET:CG | 2.90 | 0.43 |
| 3:R:3228[A]:VAL:CG2 | 3:R:3245[A]:PHE:CD2 | 3.02 | 0.43 |
| 3:R:3229[A]:ASN:O | 3:R:3286[A]:THR:N | 2.50 | 0.43 |
| 1:S:89:ILE:H | 1:S:89:ILE:HG12 | 1.63 | 0.43 |
| 1:S:1075:GLU:HG2 | 2:W:2900:SER:HA | 2.01 | 0.43 |
| 2:T:2207:ASN:HA | 2:T:2208:PRO:HD2 | 1.84 | 0.43 |
| 2:T:2525:LYS:HE3 | 2:T:2526:ARG:HH12 | 1.83 | 0.43 |
| 3:U:2940[A]:ASN:O | 3:U:2943[A]:ALA:HB3 | 2.18 | 0.43 |
| 3:U:2972[B]:GLY:C | 3:d:3247[B]:VAL:HG11 | 2.40 | 0.43 |
| 3:U:3001[B]:LYS:H | 3:U:3003[B]:LYS:HG3 | 1.83 | 0.43 |
| 3:U:3019[A]:HIS:CD2 | 3:U:3020[A]:SER:H | 2.35 | 0.43 |
| 3:U:3162[B]:ASP:OD1 | 3:d:3260[B]:ARG:CD | 2.66 | 0.43 |
| 3:U:3293[B]:LYS:CB | 3:U:3294[B]:SER:CA | 2.96 | 0.43 |
| 1:V:376:ASN:HB3 | 1:V:665:TYR:CE1 | 2.52 | 0.43 |
| 1:V:1171:LYS:HG2 | 1:V:1173:GLY:H | 1.83 | 0.43 |
| 1:V:1397:LEU:HA | 1:V:1433:TRP:HD1 | 1.84 | 0.43 |
| 1:V:1467:ILE:HD13 | 1:V:1532:PHE:HB2 | 2.00 | 0.43 |
| 2:W:2480:LEU:HD21 | 4:HA:2:NAG:H83 | 2.00 | 0.43 |
| 2:W:2641:GLN:HB3 | 2:W:2643:GLU:OE1 | 2.18 | 0.43 |
| 2:W:2726:LYS:HB2 | 2:W:2726:LYS:HE3 | 1.64 | 0.43 |
| 3:X:2937[A]:ASN:CG | 3:X:3006[A]:LYS:HD3 | 2.43 | 0.43 |
| 3:X:2948[B]:ASP:HB3 | 3:X:2949[B]:LYS:C | 2.43 | 0.43 |
| 3:X:2989[B]:HIS:O | 3:X:2990[B]:ARG:C | 2.61 | 0.43 |
| 3:X:3074[B]:GLU:CD | 3:X:3212[B]:ARG:NH2 | 2.73 | 0.43 |
| 3:X:3218[B]:LEU:HD13 | 3:X:3261[B]:LEU:HD23 | 2.01 | 0.43 |
| 1:Y:7:VAL:HG21 | 1:Y:208:LEU:HD23 | 1.99 | 0.43 |
| 1:Y:26:GLN:CD | 1:Y:122:VAL:HG13 | 2.43 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:357:PRO:HB3 | 1:Y:774:ASP:HB2 | 2.00 | 0.43 |
| 1:Y:448:SER:HA | 1:Y:449:ASP:HA | 1.54 | 0.43 |
| 1:Y:641:TRP:CD1 | 1:Y:641:TRP:C | 2.97 | 0.43 |
| 2:Z:2327:GLU:HG2 | 1:b:1650:ILE:H | 1.84 | 0.43 |
| 2:Z:2472:ASN:CG | 4:MA:1:NAG:H82 | 2.42 | 0.43 |
| 2:Z:2549:PRO:HA | 2:Z:2550:THR:HA | 1.41 | 0.43 |
| 2:Z:2734:LYS:HG2 | 2:Z:2735:ALA:H | 1.82 | 0.43 |
| 3:a:2931[A]:THR:O | 3:a:2934[A]:GLU:HG3 | 2.18 | 0.43 |
| 3:a:2946[B]:GLN:CD | 3:a:2947[B]:ALA:N | 2.72 | 0.43 |
| 3:a:3001[A]:LYS:H | 3:a:3003[A]:LYS:HG3 | 1.83 | 0.43 |
| 3:a:3001[B]:LYS:N | 3:a:3003[B]:LYS:HG3 | 2.34 | 0.43 |
| 3:a:3027[A]:GLU:CD | 3:a:3027[A]:GLU:C | 2.86 | 0.43 |
| 3:a:3228[A]:VAL:CG2 | 3:a:3245[A]:PHE:CD2 | 3.02 | 0.43 |
| 3:a:3228[B]:VAL:CG2 | 3:a:3245[B]:PHE:CD2 | 3.02 | 0.43 |
| 3:a:3276[B]:ASP:C | 3:a:3278[B]:HIS:N | 2.75 | 0.43 |
| 1:b:197:LEU:HB3 | 1:b:344:LEU:HD21 | 2.01 | 0.43 |
| 1:b:450:LYS:HD2 | 1:b:450:LYS:HA | 1.72 | 0.43 |
| 1:b:905:TRP:HZ2 | 1:b:1083:PRO:HG2 | 1.84 | 0.43 |
| 2:c:2267:HIS:HD2 | 2:c:2297:HIS:CE1 | 2.18 | 0.43 |
| 3:d:2988[B]:TRP:CD1 | 3:d:3158[B]:PHE:CE2 | 3.06 | 0.43 |
| 3:d:3183[B]:LEU:H | 3:d:3184[B]:ASN:CA | 2.21 | 0.43 |
| 1:A:1303:GLU:H | 1:A:1303:GLU:CD | 2.17 | 0.43 |
| 2:B:2446:GLU:HG2 | 2:B:2448:THR:HG23 | 2.01 | 0.43 |
| 2:B:2502:LEU:O | 2:B:2505:ILE:HG12 | 2.19 | 0.43 |
| 3:C:3106[B]:THR:O | 3:C:3106[B]:THR:HG23 | 2.17 | 0.43 |
| 3:C:3228[A]:VAL:CG2 | 3:C:3245[A]:PHE:CD2 | 3.02 | 0.43 |
| 3:C:3256[B]:TRP:HZ2 | 3:L:2965[B]:LEU:HG | 1.81 | 0.43 |
| 1:D:270:GLU:N | 1:D:270:GLU:OE1 | 2.51 | 0.43 |
| 1:D:1296:VAL:HG11 | 1:D:1447:TYR:CE1 | 2.53 | 0.43 |
| 3:F:2980[B]:HIS:CB | 3:a:2968[B]:GLN:CG | 2.50 | 0.43 |
| 3:F:3028[B]:PRO:HG2 | 3:F:3029[B]:LYS:HG3 | 2.00 | 0.43 |
| 3:F:3104[B]:MET:SD | 3:F:3110[B]:THR:CG2 | 3.06 | 0.43 |
| 3:F:3150[B]:LYS:HA | 3:a:3172[B]:SER:HB3 | 2.01 | 0.43 |
| 3:F:3163[B]:ASN:HB3 | 3:a:3149[B]:ASN:ND2 | 2.33 | 0.43 |
| 3:F:3218[B]:LEU:HD13 | 3:F:3261[B]:LEU:HD23 | 2.01 | 0.43 |
| 3:F:3299[A]:LEU:O | 3:F:3300[A]:LEU:C | 2.60 | 0.43 |
| 1:G:122:VAL:HG23 | 1:G:123:PHE:CD1 | 2.54 | 0.43 |
| 1:G:728:ARG:HD2 | 1:G:780:GLU:OE2 | 2.17 | 0.43 |
| 1:G:1411:PHE:HB3 | 1:G:1544:LEU:HD21 | 2.00 | 0.43 |
| 2:H:2549:PRO:HA | 2:H:2550:THR:HA | 1.39 | 0.43 |
| 2:H:2803:ARG:HE | 2:H:2805:PHE:HZ | 1.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:2814:LYS:HD2 | 2:H:2814:LYS:HA | 1.87 | 0.43 |
| 3:I:2949[A]:LYS:C | 3:I:2949[A]:LYS:HZ3 | 2.15 | 0.43 |
| 3:I:2965[B]:LEU:CA | 3:R:3221[B]:ALA:CB | 2.86 | 0.43 |
| 3:I:2979[B]:GLN:NE2 | 3:I:3155[B]:MET:HE3 | 2.19 | 0.43 |
| 3:I:2985[B]:PHE:HE2 | 3:R:2968[B]:GLN:C | 2.26 | 0.43 |
| 3:I:2989[B]:HIS:O | 3:I:2990[B]:ARG:C | 2.61 | 0.43 |
| 3:I:3028[A]:PRO:HG2 | 3:I:3029[A]:LYS:HG3 | 2.00 | 0.43 |
| 3:I:3083[B]:ILE:HD11 | 3:I:3260[B]:ARG:CG | 2.49 | 0.43 |
| 3:I:3108[B]:HIS:CE1 | 3:R:3252[B]:TYR:CD1 | 3.06 | 0.43 |
| 3:I:3120[B]:HIS:HA | 3:I:3123[B]:THR:HG1 | 1.82 | 0.43 |
| 3:I:3131[A]:GLN:HE21 | 3:I:3131[A]:GLN:HB3 | 1.66 | 0.43 |
| 3:I:3148[B]:ILE:HG22 | 3:I:3152[B]:LYS:HE3 | 2.01 | 0.43 |
| 3:I:3159[B]:SER:C | 3:R:3150[B]:LYS:CG | 2.90 | 0.43 |
| 3:I:3242[B]:GLY:C | 3:I:3243[B]:GLY:O | 2.58 | 0.43 |
| 1:J:66:PRO:O | 1:J:70:ARG:HB3 | 2.18 | 0.43 |
| 1:J:159:VAL:HG11 | 1:J:216:HIS:CE1 | 2.54 | 0.43 |
| 1:J:1622:GLN:HG2 | 1:J:1652:PHE:CD1 | 2.54 | 0.43 |
| 3:L:2961[A]:HIS:HB2 | 3:L:2992[A]:TYR:HE2 | 1.81 | 0.43 |
| 3:L:3183[A]:LEU:N | 3:L:3184[A]:ASN:CA | 2.80 | 0.43 |
| 3:L:3293[A]:LYS:CB | 3:L:3294[A]:SER:CA | 2.96 | 0.43 |
| 1:M:956:PRO:HB2 | 1:M:957:ASN:C | 2.43 | 0.43 |
| 2:N:2089:ARG:HB3 | 2:N:2175:VAL:O | 2.19 | 0.43 |
| 3:O:2965[B]:LEU:HD23 | 3:X:3156[B]:MET:HE3 | 2.00 | 0.43 |
| 3:O:2972[B]:GLY:C | 3:X:2979[B]:GLN:HB3 | 2.40 | 0.43 |
| 3:O:3014[A]:TRP:CH2 | 3:O:3123[A]:THR:HG23 | 2.53 | 0.43 |
| 3:O:3023[A]:ILE:O | 3:O:3026[A]:THR:OG1 | 2.34 | 0.43 |
| 3:O:3023[B]:ILE:HA | 3:O:3026[B]:THR:HG1 | 1.82 | 0.43 |
| 3:O:3180[B]:TYR:CB | 3:O:3183[B]:LEU:CD2 | 2.90 | 0.43 |
| 3:O:3183[A]:LEU:N | 3:O:3184[A]:ASN:CA | 2.80 | 0.43 |
| 1:P:321:LEU:HD11 | 1:P:377:TYR:CD2 | 2.54 | 0.43 |
| 1:P:729:VAL:O | 1:P:780:GLU:O | 2.36 | 0.43 |
| 3:R:2956[A]:LYS:O | 3:R:2959[A]:SER:OG | 2.33 | 0.43 |
| 3:R:3028[A]:PRO:HG2 | 3:R:3029[A]:LYS:HG3 | 2.00 | 0.43 |
| 3:R:3242[B]:GLY:C | 3:R:3243[B]:GLY:O | 2.58 | 0.43 |
| 3:R:3276[B]:ASP:C | 3:R:3278[B]:HIS:N | 2.75 | 0.43 |
| 1:S:1248:ARG:O | 1:S:1250:ILE:HG13 | 2.19 | 0.43 |
| 2:T:2271:HIS:O | 2:T:2283:ASN:HB3 | 2.19 | 0.43 |
| 2:T:2858:ASP:O | 2:T:2862:LYS:HG2 | 2.18 | 0.43 |
| 3:U:2931[B]:THR:O | 3:U:2934[B]:GLU:HG3 | 2.18 | 0.43 |
| 3:U:2951[B]:ASP:CG | 3:U:2952[B]:ALA:N | 2.74 | 0.43 |
| 3:U:2952[B]:ALA:CB | 3:U:2953[B]:GLY:CA | 2.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2969[B]:TYR:CE1 | 3:d:2980[B]:HIS:ND1 | 2.86 | 0.43 |
| 3:U:2970[B]:PRO:CA | 3:d:3086[B]:GLU:HG2 | 2.48 | 0.43 |
| 3:U:3093[B]:HIS:HD2 | 3:U:3248[B]:LEU:CD2 | 2.31 | 0.43 |
| 3:U:3267[B]:SER:H | 3:U:3267[B]:SER:HG | 1.26 | 0.43 |
| 1:V:883:CYS:HA | 1:V:884:PRO:HA | 1.70 | 0.43 |
| 1:V:1455:PHE:CE1 | 1:V:1456:LEU:HD12 | 2.53 | 0.43 |
| 2:W:2161:GLN:NE2 | 2:W:2348:THR:HG21 | 2.33 | 0.43 |
| 3:X:2951[B]:ASP:CG | 3:X:2952[B]:ALA:N | 2.74 | 0.43 |
| 3:X:3001[B]:LYS:N | 3:X:3003[B]:LYS:HG3 | 2.34 | 0.43 |
| 3:X:3183[B]:LEU:H | 3:X:3184[B]:ASN:CA | 2.22 | 0.43 |
| 3:X:3185[A]:TYR:HE2 | 3:X:3187[A]:TYR:CD2 | 2.35 | 0.43 |
| 3:X:3217[A]:PHE:CD2 | 3:X:3300[A]:LEU:HD12 | 2.53 | 0.43 |
| 3:X:3218[A]:LEU:HD13 | 3:X:3261[A]:LEU:HD23 | 2.01 | 0.43 |
| 1:Y:100:GLN:NE2 | 1:Y:103:GLU:OE1 | 2.47 | 0.43 |
| 1:Y:308:LEU:O | 1:Y:772:ARG:NH2 | 2.51 | 0.43 |
| 1:Y:708:PHE:HB3 | 1:Y:716:LEU:HD22 | 2.01 | 0.43 |
| 1:Y:999:LEU:HD12 | 1:Y:1056:TRP:HD1 | 1.82 | 0.43 |
| 1:Y:1179:GLY:HA2 | 1:Y:1183:GLU:OE1 | 2.19 | 0.43 |
| 2:Z:2470:ALA:HB2 | 2:Z:2476:LEU:HD21 | 2.00 | 0.43 |
| 2:Z:2738:ALA:HA | 1:b:1234:VAL:H | 1.82 | 0.43 |
| 3:a:2937[A]:ASN:CG | 3:a:3006[A]:LYS:HD3 | 2.43 | 0.43 |
| 3:a:2940[B]:ASN:O | 3:a:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:a:2961[A]:HIS:HB2 | 3:a:2992[A]:TYR:HE2 | 1.81 | 0.43 |
| 3:a:2961[B]:HIS:HB2 | 3:a:2992[B]:TYR:HE2 | 1.81 | 0.43 |
| 3:a:2988[B]:TRP:CZ3 | 3:a:2989[B]:HIS:CE1 | 3.07 | 0.43 |
| 3:a:3183[B]:LEU:N | 3:a:3184[B]:ASN:CA | 2.80 | 0.43 |
| 3:a:3217[B]:PHE:CD2 | 3:a:3300[B]:LEU:HD12 | 2.53 | 0.43 |
| 3:a:3232[A]:VAL:HG21 | 3:a:3273[A]:LEU:HD11 | 2.00 | 0.43 |
| 1:b:136:ALA:HB3 | 1:b:190:PHE:CE2 | 2.53 | 0.43 |
| 1:b:244:MET:HG3 | 1:b:261:SER:O | 2.18 | 0.43 |
| 1:b:293:LEU:O | 1:b:296:ARG:HG2 | 2.18 | 0.43 |
| 1:b:610:THR:HB | 1:b:629:MET:HE1 | 2.01 | 0.43 |
| 2:c:2505:ILE:HD11 | 2:c:2779:ASP:HA | 2.01 | 0.43 |
| 2:c:2811:HIS:HB3 | 2:c:2847:HIS:HD2 | 1.82 | 0.43 |
| 3:d:3001[A]:LYS:H | 3:d:3003[A]:LYS:HG3 | 1.83 | 0.43 |
| 3:d:3200[A]:LEU:CD2 | 3:d:3204[A]:LEU:HD11 | 2.48 | 0.43 |
| 3:d:3217[A]:PHE:CD2 | 3:d:3300[A]:LEU:HD12 | 2.53 | 0.43 |
| 3:d:3266[A]:ILE:O | 3:d:3269[A]:SER:HB2 | 2.17 | 0.43 |
| 1:A:830:ASN:HB3 | 1:A:832:LYS:H | 1.82 | 0.43 |
| 1:A:831:VAL:HG12 | 1:A:831:VAL:O | 2.18 | 0.43 |
| 1:A:1114:TYR:HE2 | 1:A:1116:TYR:CE2 | 2.37 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1318:VAL:HA | 1:A:1321:HIS:ND1 | 2.33 | 0.43 |
| 2:B:2302:ASP:HB3 | 2:B:2368:TYR:OH | 2.18 | 0.43 |
| 2:B:2648:ALA:HA | 2:B:2654:SER:HB2 | 2.00 | 0.43 |
| 3:C:3083[A]:ILE:HD11 | 3:C:3260[A]:ARG:CG | 2.49 | 0.43 |
| 3:C:3293[B]:LYS:CB | 3:C:3294[B]:SER:CA | 2.96 | 0.43 |
| 1:D:448:SER:HA | 1:D:449:ASP:HA | 1.40 | 0.43 |
| 1:D:449:ASP:HB2 | 1:D:1280:GLN:HE22 | 1.82 | 0.43 |
| 1:D:460:GLU:OE2 | 1:D:1368:ARG:NH2 | 2.51 | 0.43 |
| 1:D:1286:ARG:NE | 1:D:1333:GLU:OE1 | 2.51 | 0.43 |
| 1:D:1362:ALA:HA | 1:D:1378:PHE:CG | 2.54 | 0.43 |
| 2:E:2666:GLN:OE1 | 2:E:2671:ASP:HB3 | 2.19 | 0.43 |
| 2:E:2840:GLY:O | 2:E:2843:GLU:HB2 | 2.19 | 0.43 |
| 2:E:2848:PHE:HD1 | 2:E:2848:PHE:HA | 1.70 | 0.43 |
| 3:F:2948[B]:ASP:HB3 | 3:F:2949[B]:LYS:C | 2.43 | 0.43 |
| 3:F:2963[A]:MET:SD | 3:F:2963[A]:MET:C | 3.01 | 0.43 |
| 3:F:2967[B]:CYS:N | 3:a:3256[B]:TRP:HD1 | 1.90 | 0.43 |
| 3:F:3024[A]:LEU:CD1 | 3:F:3024[A]:LEU:C | 2.85 | 0.43 |
| 3:F:3083[A]:ILE:HD11 | 3:F:3260[A]:ARG:CG | 2.49 | 0.43 |
| 3:F:3107[B]:LEU:HD12 | 3:a:2973[B]:THR:HB | 2.01 | 0.43 |
| 3:F:3245[A]:PHE:CD1 | 3:F:3245[A]:PHE:C | 2.97 | 0.43 |
| 3:F:3285[B]:VAL:CG2 | 3:F:3286[B]:THR:H | 2.27 | 0.43 |
| 1:G:37:ILE:O | 1:G:40:TYR:HB2 | 2.19 | 0.43 |
| 1:G:590:ASP:HB3 | 1:G:653:LYS:NZ | 2.33 | 0.43 |
| 1:G:816:PRO:HA | 1:G:817:PRO:HD3 | 1.92 | 0.43 |
| 1:G:926:LEU:HD11 | 1:G:1043:MET:HB3 | 2.01 | 0.43 |
| 1:G:946:GLU:HG2 | 1:G:955:LYS:HD3 | 2.01 | 0.43 |
| 1:G:988:TYR:HB3 | 1:G:992:ALA:HB3 | 2.00 | 0.43 |
| 1:G:1147:MET:HB3 | 1:G:1230:LEU:HD11 | 2.01 | 0.43 |
| 1:G:1247:ARG:HA | 1:G:1247:ARG:HD3 | 1.85 | 0.43 |
| 1:G:1315:GLY:HA3 | 1:G:1601:TRP:CG | 2.53 | 0.43 |
| 2:H:2356:ASP:O | 2:H:2363:ASN:ND2 | 2.51 | 0.43 |
| 2:H:2571:ARG:HG3 | 2:H:2715:ASP:OD1 | 2.19 | 0.43 |
| 2:H:2782:ASN:O | 2:H:2782:ASN:ND2 | 2.50 | 0.43 |
| 3:I:2940[B]:ASN:O | 3:I:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:I:2948[A]:ASP:HB3 | 3:I:2949[A]:LYS:C | 2.44 | 0.43 |
| 3:I:2948[B]:ASP:HB3 | 3:I:2949[B]:LYS:C | 2.43 | 0.43 |
| 3:I:2951[B]:ASP:OD2 | 3:I:2952[B]:ALA:CB | 2.66 | 0.43 |
| 3:I:3013[B]:ASP:CA | 3:I:3122[B]:ASN:ND2 | 2.74 | 0.43 |
| 3:I:3093[B]:HIS:HD2 | 3:I:3248[B]:LEU:CD2 | 2.31 | 0.43 |
| 3:I:3151[B]:LEU:H | 3:R:3169[B]:LYS:CG | 2.19 | 0.43 |
| 3:I:3217[A]:PHE:CD2 | 3:I:3300[A]:LEU:HD12 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:3218[B]:LEU:HD13 | 3:I:3261[B]:LEU:HD23 | 2.01 | 0.43 |
| 3:I:3293[B]:LYS:CB | 3:I:3294[B]:SER:CA | 2.96 | 0.43 |
| 1:J:409:PHE:O | 1:J:654:PRO:HG3 | 2.18 | 0.43 |
| 1:J:982:LYS:N | 1:J:983:PRO:CD | 2.81 | 0.43 |
| 1:J:1094:ALA:O | 1:J:1097:ARG:HB3 | 2.18 | 0.43 |
| 1:J:1286:ARG:O | 1:J:1289:GLU:HB3 | 2.18 | 0.43 |
| 1:J:1528:ASP:OD1 | 1:J:1528:ASP:N | 2.51 | 0.43 |
| 3:L:2948[B]:ASP:HB3 | 3:L:2949[B]:LYS:C | 2.43 | 0.43 |
| 3:L:2951[B]:ASP:OD2 | 3:L:2952[B]:ALA:CB | 2.66 | 0.43 |
| 3:L:2989[A]:HIS:C | 3:L:2991[A]:LEU:N | 2.75 | 0.43 |
| 3:L:3182[A]:GLN:H | 3:L:3182[A]:GLN:HG2 | 1.56 | 0.43 |
| 1:M:417:MET:HE2 | 1:M:417:MET:HA | 2.01 | 0.43 |
| 1:M:573:LYS:HB3 | 1:M:574:GLY:HA2 | 2.01 | 0.43 |
| 1:M:945:ALA:O | 1:M:957:ASN:ND2 | 2.51 | 0.43 |
| 2:N:2477:PRO:O | 2:N:2479:SER:N | 2.51 | 0.43 |
| 2:N:2861:LYS:HE3 | 3:O:2936[A]:GLU:OE1 | 2.19 | 0.43 |
| 3:O:3083[B]:ILE:HD11 | 3:O:3260[B]:ARG:CG | 2.49 | 0.43 |
| 3:O:3196[A]:THR:N | 3:O:3199[A]:GLN:CB | 2.65 | 0.43 |
| 1:P:552:PHE:HZ | 1:P:623:TYR:HE1 | 1.65 | 0.43 |
| 1:P:1144:VAL:N | 1:P:1194:SER:O | 2.49 | 0.43 |
| 1:P:1219:ASP:N | 1:P:1223:ALA:O | 2.38 | 0.43 |
| 1:P:1321:HIS:HD2 | 1:P:1465:TRP:HH2 | 1.64 | 0.43 |
| 1:P:1638:SER:HA | 1:P:1639:LYS:HA | 1.62 | 0.43 |
| 2:Q:2252:GLU:HG3 | 2:Q:2385:ILE:HG23 | 2.00 | 0.43 |
| 3:R:2933[B]:SER:CA | 3:R:2936[B]:GLU:HB3 | 2.48 | 0.43 |
| 3:R:2940[B]:ASN:O | 3:R:2943[B]:ALA:HB3 | 2.18 | 0.43 |
| 3:R:2948[A]:ASP:HB3 | 3:R:2949[A]:LYS:C | 2.43 | 0.43 |
| 3:R:2989[B]:HIS:C | 3:R:2991[B]:LEU:N | 2.75 | 0.43 |
| 3:R:3148[B]:ILE:HG22 | 3:R:3152[B]:LYS:HE3 | 2.01 | 0.43 |
| 3:R:3218[A]:LEU:HD13 | 3:R:3261[A]:LEU:HD23 | 2.01 | 0.43 |
| 1:S:135:THR:HG22 | 1:S:192:HIS:HB3 | 2.00 | 0.43 |
| 1:S:1299:GLN:O | 1:S:1301:PRO:HD3 | 2.19 | 0.43 |
| 3:U:2969[B]:TYR:O | 3:d:3086[B]:GLU:OE1 | 2.37 | 0.43 |
| 3:U:3135[B]:LYS:HB2 | 3:U:3141[B]:TYR:CD1 | 2.51 | 0.43 |
| 3:U:3148[B]:ILE:HG22 | 3:U:3152[B]:LYS:HE3 | 2.01 | 0.43 |
| 3:U:3218[A]:LEU:HD12 | 3:U:3218[A]:LEU:HA | 1.78 | 0.43 |
| 3:U:3252[B]:TYR:CZ | 3:d:3222[B]:ILE:HD13 | 2.42 | 0.43 |
| 1:V:228:GLY:H | 1:V:229:LEU:HG | 1.83 | 0.43 |
| 2:W:2116:SER:HA | 2:W:2121:THR:HG21 | 2.01 | 0.43 |
| 2:W:2246:ASN:HB3 | 2:W:2266:VAL:HG22 | 2.01 | 0.43 |
| 2:W:2312:GLN:HB2 | 2:W:2319:ALA:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2988[B]:TRP:CD1 | 3:X:3158[B]:PHE:CE2 | 3.06 | 0.43 |
| 3:X:2995[B]:GLN:CG | 3:X:3168[B]:THR:HG21 | 2.48 | 0.43 |
| 3:X:3001[A]:LYS:H | 3:X:3003[A]:LYS:HG3 | 1.83 | 0.43 |
| 3:X:3149[A]:ASN:OD1 | 3:X:3149[A]:ASN:N | 2.51 | 0.43 |
| 3:X:3293[B]:LYS:CB | 3:X:3294[B]:SER:CA | 2.96 | 0.43 |
| 1:Y:195:SER:HB2 | 1:Y:386:ILE:HD11 | 2.00 | 0.43 |
| 1:Y:514:TRP:CZ3 | 1:Y:606:ILE:HD11 | 2.53 | 0.43 |
| 1:Y:931:TRP:CB | 1:Y:1018:ILE:HD11 | 2.48 | 0.43 |
| 1:Y:1018:ILE:HD12 | 1:Y:1045:HIS:HD2 | 1.84 | 0.43 |
| 1:Y:1025:THR:HG23 | 1:Y:1221:THR:HA | 2.01 | 0.43 |
| 1:Y:1245:GLU:HB3 | 2:c:2730:LEU:HA | 1.99 | 0.43 |
| 1:Y:1401:ARG:HH11 | 1:Y:1401:ARG:HB3 | 1.84 | 0.43 |
| 1:Y:1427:HIS:HD2 | 1:Y:1457:HIS:HE1 | 1.67 | 0.43 |
| 1:Y:1599:MET:SD | 1:Y:1600:PRO:HD2 | 2.59 | 0.43 |
| 2:Z:2562:GLY:H | 2:Z:2846:TRP:CB | 2.31 | 0.43 |
| 3:a:2931[B]:THR:O | 3:a:2934[B]:GLU:HG3 | 2.18 | 0.43 |
| 3:a:2951[B]:ASP:OD2 | 3:a:2952[B]:ALA:CB | 2.66 | 0.43 |
| 3:a:3048[B]:ASP:HB3 | 3:a:3099[B]:PRO:HD2 | 2.01 | 0.43 |
| 3:a:3093[A]:HIS:HB2 | 3:a:3248[A]:LEU:CD1 | 2.48 | 0.43 |
| 3:a:3148[B]:ILE:O | 3:a:3148[B]:ILE:HG22 | 2.17 | 0.43 |
| 3:a:3245[B]:PHE:CD1 | 3:a:3245[B]:PHE:C | 2.97 | 0.43 |
| 1:b:61:GLY:N | 1:b:176:GLU:OE2 | 2.48 | 0.43 |
| 1:b:149:GLU:HG3 | 1:b:150:GLY:N | 2.34 | 0.43 |
| 1:b:896:HIS:HB2 | 1:b:905:TRP:CG | 2.54 | 0.43 |
| 1:b:928:TYR:HB2 | 1:b:1048:ASN:HB2 | 2.00 | 0.43 |
| 1:b:1030:MET:HA | 1:b:1036:SER:HA | 2.00 | 0.43 |
| 2:c:2551:PRO:HA | 2:c:2552:GLU:HA | 1.73 | 0.43 |
| 3:d:3001[B]:LYS:H | 3:d:3003[B]:LYS:HG3 | 1.83 | 0.43 |
| 3:d:3025[B]:VAL:CG2 | 3:d:3047[B]:ARG:NH1 | 2.73 | 0.43 |
| 3:d:3083[A]:ILE:HD11 | 3:d:3260[A]:ARG:CG | 2.49 | 0.43 |
| 3:d:3104[B]:MET:HA | 3:d:3110[B]:THR:CG2 | 2.17 | 0.43 |
| 3:d:3148[A]:ILE:HG22 | 3:d:3152[A]:LYS:HE3 | 2.01 | 0.43 |
| 6:3:1:NAG:O3 | 6:3:2:NAG:N2 | 2.51 | 0.43 |
| 1:A:150:GLY:HA2 | 1:A:151:GLN:C | 2.42 | 0.43 |
| 1:A:183:HIS:CD2 | 1:A:344:LEU:HD21 | 2.54 | 0.43 |
| 1:A:535:PRO:HG3 | 1:A:985:PHE:CE1 | 2.53 | 0.43 |
| 1:A:784:ALA:O | 1:A:788:LEU:HB2 | 2.18 | 0.43 |
| 1:A:838:ARG:HD3 | 1:A:1114:TYR:HB3 | 2.00 | 0.43 |
| 1:A:854:LEU:HG | 1:A:959:PHE:CE2 | 2.53 | 0.43 |
| 1:A:899:MET:HB3 | 1:A:1012:GLU:OE1 | 2.19 | 0.43 |
| 1:A:1638:SER:HA | 1:A:1639:LYS:HA | 1.74 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2346:PRO:O | 2:B:2349:THR:OG1 | 2.33 | 0.43 |
| 2:B:2361:LYS:H | 2:B:2361:LYS:HG3 | 1.53 | 0.43 |
| 3:C:2972[B]:GLY:HA3 | 3:L:3086[B]:GLU:O | 2.19 | 0.43 |
| 3:C:3083[B]:ILE:HD11 | 3:C:3260[B]:ARG:CG | 2.49 | 0.43 |
| 3:C:3093[A]:HIS:HD2 | 3:C:3248[A]:LEU:CD2 | 2.31 | 0.43 |
| 3:C:3172[B]:SER:CB | 3:L:3152[B]:LYS:CB | 2.96 | 0.43 |
| 3:C:3180[A]:TYR:CB | 3:C:3183[A]:LEU:CD2 | 2.89 | 0.43 |
| 3:C:3183[B]:LEU:N | 3:C:3184[B]:ASN:CA | 2.80 | 0.43 |
| 3:C:3217[B]:PHE:CD2 | 3:C:3300[B]:LEU:HD12 | 2.53 | 0.43 |
| 3:C:3284[A]:LYS:CE | 3:C:3284[A]:LYS:CA | 2.86 | 0.43 |
| 1:D:132:ASN:HA | 1:D:133:LYS:HA | 1.86 | 0.43 |
| 1:D:361:GLU:HG2 | 1:D:363:THR:HG22 | 2.00 | 0.43 |
| 1:D:754:GLU:CD | 1:D:799:ARG:HH21 | 2.26 | 0.43 |
| 2:E:2244:PHE:HA | 2:E:2373:MET:HE1 | 2.01 | 0.43 |
| 2:E:2270:ILE:HB | 2:E:2297:HIS:CD2 | 2.54 | 0.43 |
| 2:E:2830:GLN:N | 2:E:2830:GLN:OE1 | 2.52 | 0.43 |
| 3:F:2933[B]:SER:CA | 3:F:2936[B]:GLU:HB3 | 2.48 | 0.43 |
| 3:F:2965[A]:LEU:CG | 3:F:2974[A]:ALA:CB | 2.85 | 0.43 |
| 3:F:2988[A]:TRP:CZ3 | 3:F:2989[A]:HIS:CE1 | 3.07 | 0.43 |
| 3:F:3147[B]:GLU:HG3 | 3:a:3160[B]:SER:C | 2.43 | 0.43 |
| 3:F:3148[A]:ILE:HG22 | 3:F:3152[A]:LYS:HE3 | 2.01 | 0.43 |
| 3:F:3155[B]:MET:SD | 3:a:3153[B]:LYS:HG2 | 2.59 | 0.43 |
| 1:G:1369:THR:HB | 1:G:1371:GLN:HG2 | 2.01 | 0.43 |
| 2:H:2808:PHE:HZ | 2:H:2821:LEU:HD13 | 1.83 | 0.43 |
| 3:I:3001[A]:LYS:H | 3:I:3003[A]:LYS:HG3 | 1.83 | 0.43 |
| 3:I:3001[A]:LYS:N | 3:I:3003[A]:LYS:HG3 | 2.34 | 0.43 |
| 3:I:3149[A]:ASN:OD1 | 3:I:3149[A]:ASN:N | 2.51 | 0.43 |
| 3:I:3173[B]:THR:HA | 3:R:3154[B]:PRO:CA | 2.48 | 0.43 |
| 3:I:3228[B]:VAL:CG2 | 3:I:3245[B]:PHE:CD2 | 3.02 | 0.43 |
| 1:J:1315:GLY:HA3 | 1:J:1601:TRP:HB2 | 2.00 | 0.43 |
| 2:K:2403:PHE:CE2 | 2:K:2476:LEU:HD13 | 2.54 | 0.43 |
| 3:L:2949[B]:LYS:C | 3:L:2949[B]:LYS:HZ3 | 2.13 | 0.43 |
| 3:L:3023[B]:ILE:HA | 3:L:3026[B]:THR:HG1 | 1.82 | 0.43 |
| 3:L:3180[A]:TYR:CB | 3:L:3183[A]:LEU:CD2 | 2.89 | 0.43 |
| 3:L:3218[A]:LEU:HD13 | 3:L:3261[A]:LEU:HD23 | 2.01 | 0.43 |
| 1:M:17:ASN:ND2 | 1:M:86:THR:H | 2.10 | 0.43 |
| 1:M:494:VAL:HG13 | 1:M:631:TRP:CZ3 | 2.54 | 0.43 |
| 1:M:1166:THR:HB | 1:M:1167:ASP:C | 2.44 | 0.43 |
| 2:N:2117:ASP:OD1 | 2:N:2168:ARG:NH2 | 2.52 | 0.43 |
| 2:N:2231:LEU:HD12 | 2:N:2273:TRP:HE3 | 1.83 | 0.43 |
| 2:N:2286:HIS:NE2 | 2:N:2433:THR:HG22 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:2311:LEU:O | 2:N:2315:ARG:HG3 | 2.19 | 0.43 |
| 3:O:2976[B]:ALA:O | 3:O:2978[B]:CYS:N | 2.46 | 0.43 |
| 3:O:2988[B]:TRP:CZ3 | 3:O:2989[B]:HIS:CE1 | 3.07 | 0.43 |
| 3:O:3028[A]:PRO:HG2 | 3:O:3029[A]:LYS:HG3 | 2.00 | 0.43 |
| 3:O:3185[A]:TYR:HE2 | 3:O:3187[A]:TYR:CD2 | 2.35 | 0.43 |
| 3:O:3200[A]:LEU:CD2 | 3:O:3204[A]:LEU:HD11 | 2.48 | 0.43 |
| 3:O:3293[A]:LYS:CB | 3:O:3294[A]:SER:CA | 2.96 | 0.43 |
| 1:P:195:SER:HB2 | 1:P:386:ILE:HD11 | 2.00 | 0.43 |
| 1:P:669:LYS:HB2 | 1:P:670:PRO:HD3 | 2.01 | 0.43 |
| 1:P:977:GLU:HB3 | 1:P:979:LEU:HD21 | 2.00 | 0.43 |
| 1:P:1329:LEU:HB2 | 1:P:1507:THR:HG21 | 2.01 | 0.43 |
| 2:Q:2596:THR:HG21 | 2:Q:2783:PHE:CZ | 2.53 | 0.43 |
| 2:Q:2695:MET:HE3 | 2:Q:2706:ILE:HG23 | 2.01 | 0.43 |
| 3:R:2951[A]:ASP:OD2 | 3:R:2952[A]:ALA:CB | 2.66 | 0.43 |
| 3:R:3044[B]:LYS:H | 3:R:3044[B]:LYS:HG2 | 1.64 | 0.43 |
| 3:R:3047[B]:ARG:NH2 | 3:R:3113[B]:ASP:OD1 | 2.43 | 0.43 |
| 3:R:3217[B]:PHE:CD2 | 3:R:3300[B]:LEU:HD12 | 2.53 | 0.43 |
| 3:R:3245[A]:PHE:CD1 | 3:R:3245[A]:PHE:C | 2.97 | 0.43 |
| 1:S:926:LEU:HA | 1:S:927:PRO:HD3 | 1.81 | 0.43 |
| 1:S:1394:GLN:HB2 | 1:S:1433:TRP:CB | 2.48 | 0.43 |
| 3:U:2933[A]:SER:CA | 3:U:2936[A]:GLU:HB3 | 2.48 | 0.43 |
| 3:U:2937[A]:ASN:CG | 3:U:3006[A]:LYS:HD3 | 2.43 | 0.43 |
| 3:U:2963[A]:MET:SD | 3:U:2963[A]:MET:C | 3.01 | 0.43 |
| 3:U:3001[B]:LYS:N | 3:U:3003[B]:LYS:HG3 | 2.34 | 0.43 |
| 3:U:3047[B]:ARG:NH2 | 3:U:3113[B]:ASP:OD1 | 2.43 | 0.43 |
| 3:U:3083[B]:ILE:HD11 | 3:U:3260[B]:ARG:CG | 2.49 | 0.43 |
| 3:U:3146[B]:CYS:HA | 3:U:3147[B]:GLU:HA | 1.70 | 0.43 |
| 3:U:3170[B]:ALA:CA | 3:d:3148[B]:ILE:CB | 2.96 | 0.43 |
| 3:U:3228[A]:VAL:CG2 | 3:U:3245[A]:PHE:CD2 | 3.02 | 0.43 |
| 3:U:3228[B]:VAL:CG2 | 3:U:3245[B]:PHE:CD2 | 3.02 | 0.43 |
| 1:V:226:HIS:O | 1:V:227:ARG:HG2 | 2.19 | 0.43 |
| 1:V:562:GLN:HG2 | 1:V:614:GLU:HG3 | 2.00 | 0.43 |
| 1:V:1559:LEU:HD21 | 1:V:1590:PHE:HE1 | 1.83 | 0.43 |
| 2:W:2275:GLY:HA3 | 2:W:2283:ASN:H | 1.84 | 0.43 |
| 2:W:2840:GLY:O | 2:W:2843:GLU:HB2 | 2.19 | 0.43 |
| 3:X:3023[A]:ILE:O | 3:X:3026[A]:THR:OG1 | 2.34 | 0.43 |
| 3:X:3228[A]:VAL:CG2 | 3:X:3245[A]:PHE:CD2 | 3.02 | 0.43 |
| 3:X:3284[A]:LYS:CE | 3:X:3284[A]:LYS:CA | 2.85 | 0.43 |
| 1:Y:63:PRO:HA | 1:Y:172:GLU:HG3 | 2.00 | 0.43 |
| 1:Y:1108:TYR:HB2 | 1:Y:1114:TYR:CE1 | 2.54 | 0.43 |
| 1:Y:1313:LEU:HD13 | 1:Y:1322:TRP:CD1 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:2390:GLN:O | 2:Z:2491:PRO:HB3 | 2.18 | 0.43 |
| 2:Z:2515:ARG:HD2 | 2:c:2168:ARG:CZ | 2.49 | 0.43 |
| 2:Z:2547:MET:O | 2:Z:2751:TRP:HH2 | 2.02 | 0.43 |
| 3:a:2933[A]:SER:CA | 3:a:2936[A]:GLU:HB3 | 2.48 | 0.43 |
| 3:a:2938[B]:LEU:O | 3:a:2939[B]:ARG:C | 2.58 | 0.43 |
| 3:a:2961[B]:HIS:NE2 | 3:a:2980[B]:HIS:CE1 | 2.73 | 0.43 |
| 3:a:2965[B]:LEU:CD1 | 3:a:2974[B]:ALA:CA | 2.89 | 0.43 |
| 3:a:3001[B]:LYS:H | 3:a:3003[B]:LYS:HG3 | 1.83 | 0.43 |
| 3:a:3083[B]:ILE:HD11 | 3:a:3260[B]:ARG:CG | 2.49 | 0.43 |
| 3:a:3281[B]:PHE:HE1 | 3:a:3305[B]:ILE:HG21 | 1.81 | 0.43 |
| 1:b:190:PHE:HD1 | 1:b:191:THR:N | 2.17 | 0.43 |
| 1:b:1260:ARG:HD2 | 1:b:1343:VAL:O | 2.18 | 0.43 |
| 1:b:1321:HIS:HD2 | 1:b:1465:TRP:CH2 | 2.36 | 0.43 |
| 3:d:2948[B]:ASP:HB3 | 3:d:2949[B]:LYS:C | 2.43 | 0.43 |
| 3:d:2965[A]:LEU:CD1 | 3:d:2974[A]:ALA:CA | 2.89 | 0.43 |
| 3:d:3013[B]:ASP:CG | 3:d:3015[B]:THR:HG1 | 2.26 | 0.43 |
| 3:d:3148[B]:ILE:HG22 | 3:d:3148[B]:ILE:O | 2.17 | 0.43 |
| 3:d:3149[A]:ASN:OD1 | 3:d:3149[A]:ASN:N | 2.50 | 0.43 |
| 3:d:3217[B]:PHE:CD2 | 3:d:3300[B]:LEU:HD12 | 2.53 | 0.43 |
| 3:d:3218[A]:LEU:HD13 | 3:d:3261[A]:LEU:HD23 | 2.01 | 0.43 |
| 3:d:3230[A]:PHE:CB | 3:d:3242[A]:GLY:C | 2.91 | 0.43 |
| 6:LA:1:NAG:H62 | 6:LA:2:NAG:C8 | 2.48 | 0.43 |
| 1:A:177:VAL:HG11 | 1:A:358:TYR:CE1 | 2.54 | 0.43 |
| 1:A:398:ARG:HA | 1:A:399:PRO:HD3 | 1.87 | 0.43 |
| 1:A:641:TRP:HZ2 | 1:A:693:TYR:HD1 | 1.65 | 0.43 |
| 1:A:904:HIS:HE1 | 1:A:1106:PHE:CZ | 2.37 | 0.43 |
| 1:A:1022:VAL:O | 1:A:1029:SER:OG | 2.34 | 0.43 |
| 3:C:2969[B]:TYR:CG | 3:L:2989[B]:HIS:NE2 | 2.87 | 0.43 |
| 3:C:3245[A]:PHE:CD1 | 3:C:3245[A]:PHE:C | 2.97 | 0.43 |
| 1:D:956:PRO:CD | 1:D:957:ASN:HA | 2.48 | 0.43 |
| 1:D:1427:HIS:HD2 | 1:D:1457:HIS:HE2 | 1.66 | 0.43 |
| 2:E:2240:GLN:HG2 | 2:E:2244:PHE:CD1 | 2.53 | 0.43 |
| 3:F:2995[A]:GLN:CG | 3:F:3168[A]:THR:HG21 | 2.48 | 0.43 |
| 3:F:3083[B]:ILE:HD11 | 3:F:3260[B]:ARG:CG | 2.49 | 0.43 |
| 3:F:3171[B]:HIS:C | 3:F:3173[B]:THR:N | 2.73 | 0.43 |
| 3:F:3183[B]:LEU:N | 3:F:3184[B]:ASN:CA | 2.80 | 0.43 |
| 3:F:3228[B]:VAL:CG2 | 3:F:3245[B]:PHE:CD2 | 3.02 | 0.43 |
| 3:F:3294[A]:SER:O | 3:F:3294[A]:SER:OG | 2.34 | 0.43 |
| 1:G:260:ASN:OD1 | 1:G:260:ASN:N | 2.50 | 0.43 |
| 1:G:425:ARG:NE | 1:G:499:GLU:OE2 | 2.51 | 0.43 |
| 1:G:1028:VAL:HA | 1:G:1035:TYR:CD2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1078:ARG:NH2 | 2:K:2875:SER:O | 2.33 | 0.43 |
| 1:G:1146:PHE:CE2 | 1:G:1175:PHE:HE1 | 2.37 | 0.43 |
| 1:G:1158:GLU:HG2 | 1:G:1174:GLU:HB3 | 2.01 | 0.43 |
| 2:H:2156:ARG:HD2 | 2:H:2357:VAL:HG12 | 2.01 | 0.43 |
| 3:I:2951[A]:ASP:OD2 | 3:I:2952[A]:ALA:CB | 2.66 | 0.43 |
| 3:I:3169[B]:LYS:NZ | 3:R:3149[B]:ASN:ND2 | 2.66 | 0.43 |
| 3:I:3174[B]:GLY:HA3 | 3:R:3154[B]:PRO:HB2 | 1.96 | 0.43 |
| 3:I:3194[B]:GLY:C | 3:I:3195[B]:MET:CG | 2.90 | 0.43 |
| 3:I:3255[B]:PRO:HB3 | 3:R:2964[B]:PRO:N | 2.33 | 0.43 |
| 3:I:3256[B]:TRP:N | 3:R:2965[B]:LEU:C | 2.77 | 0.43 |
| 3:I:3299[B]:LEU:HB3 | 3:I:3300[B]:LEU:H | 1.53 | 0.43 |
| 1:J:121:ASN:ND2 | 1:J:124:TYR:H | 2.16 | 0.43 |
| 1:J:922:TRP:CD1 | 1:J:924:GLY:H | 2.37 | 0.43 |
| 1:J:1146:PHE:HZ | 1:J:1159:TYR:CG | 2.36 | 0.43 |
| 1:J:1303:GLU:HA | 1:J:1304:ASP:HA | 1.80 | 0.43 |
| 3:L:2951[A]:ASP:OD2 | 3:L:2952[A]:ALA:CB | 2.66 | 0.43 |
| 3:L:3001[A]:LYS:N | 3:L:3003[A]:LYS:HG3 | 2.34 | 0.43 |
| 3:L:3093[B]:HIS:HB2 | 3:L:3248[B]:LEU:CD1 | 2.48 | 0.43 |
| 3:L:3148[A]:ILE:HG22 | 3:L:3152[A]:LYS:HE3 | 2.01 | 0.43 |
| 3:L:3148[B]:ILE:HG22 | 3:L:3152[B]:LYS:HE3 | 2.01 | 0.43 |
| 3:L:3217[A]:PHE:CD2 | 3:L:3300[A]:LEU:HD12 | 2.53 | 0.43 |
| 3:L:3228[B]:VAL:CG2 | 3:L:3245[B]:PHE:CD2 | 3.02 | 0.43 |
| 3:L:3300[B]:LEU:HD23 | 3:L:3300[B]:LEU:H | 1.83 | 0.43 |
| 3:O:2931[A]:THR:O | 3:O:2934[A]:GLU:HG3 | 2.18 | 0.43 |
| 3:O:2948[A]:ASP:HB3 | 3:O:2949[A]:LYS:C | 2.43 | 0.43 |
| 3:O:2948[B]:ASP:HB3 | 3:O:2949[B]:LYS:C | 2.43 | 0.43 |
| 3:O:2968[B]:GLN:C | 3:X:2988[B]:TRP:N | 2.77 | 0.43 |
| 3:O:2989[A]:HIS:C | 3:O:2991[A]:LEU:N | 2.75 | 0.43 |
| 3:O:3031[A]:ASN:HA | 3:O:3032[A]:PRO:HD2 | 1.87 | 0.43 |
| 3:O:3149[B]:ASN:OD1 | 3:O:3149[B]:ASN:N | 2.51 | 0.43 |
| 3:O:3242[A]:GLY:C | 3:O:3243[A]:GLY:O | 2.58 | 0.43 |
| 3:O:3284[B]:LYS:CE | 3:O:3284[B]:LYS:CA | 2.85 | 0.43 |
| 1:P:278:ASP:O | 1:P:279:LEU:HG | 2.19 | 0.43 |
| 2:Q:2603:PRO:HG2 | 2:Q:2606:LEU:HD12 | 2.00 | 0.43 |
| 2:Q:2808:PHE:CZ | 2:Q:2899:PRO:HG3 | 2.54 | 0.43 |
| 2:Q:2890:VAL:H | 2:Q:2891:LEU:HA | 1.81 | 0.43 |
| 3:R:2956[B]:LYS:O | 3:R:2959[B]:SER:OG | 2.33 | 0.43 |
| 3:R:3013[B]:ASP:CA | 3:R:3122[B]:ASN:ND2 | 2.73 | 0.43 |
| 3:R:3048[B]:ASP:HB3 | 3:R:3099[B]:PRO:HD2 | 2.01 | 0.43 |
| 3:R:3104[A]:MET:SD | 3:R:3110[A]:THR:CG2 | 3.06 | 0.43 |
| 2:T:2722:GLN:NE2 | 2:T:2769:PHE:O | 2.45 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2951[B]:ASP:OD2 | 3:U:2952[B]:ALA:CB | 2.66 | 0.43 |
| 3:U:2988[A]:TRP:CZ3 | 3:U:2989[A]:HIS:CE1 | 3.07 | 0.43 |
| 3:U:2995[A]:GLN:CG | 3:U:3168[A]:THR:HG21 | 2.48 | 0.43 |
| 3:U:3001[A]:LYS:H | 3:U:3003[A]:LYS:HG3 | 1.83 | 0.43 |
| 3:U:3093[B]:HIS:HB2 | 3:U:3248[B]:LEU:CD1 | 2.48 | 0.43 |
| 3:U:3245[A]:PHE:C | 3:U:3245[A]:PHE:CD1 | 2.97 | 0.43 |
| 1:V:7:VAL:HG23 | 1:V:91:TYR:O | 2.19 | 0.43 |
| 1:V:943:LEU:HD12 | 1:V:944:GLU:N | 2.33 | 0.43 |
| 1:V:1274:LEU:HD11 | 1:V:1334:LEU:HD21 | 2.00 | 0.43 |
| 1:V:1581:GLU:HG3 | 1:V:1582:ASN:H | 1.84 | 0.43 |
| 2:W:2244:PHE:CE1 | 2:W:2248:ILE:HG13 | 2.53 | 0.43 |
| 3:X:2932[A]:PRO:CA | 3:X:2935[A]:ILE:CD1 | 2.85 | 0.43 |
| 3:X:2933[B]:SER:CA | 3:X:2936[B]:GLU:HB3 | 2.48 | 0.43 |
| 3:X:2951[B]:ASP:OD2 | 3:X:2952[B]:ALA:CB | 2.66 | 0.43 |
| 3:X:3228[B]:VAL:CG2 | 3:X:3245[B]:PHE:CD2 | 3.02 | 0.43 |
| 1:Y:564:ASP:HA | 1:Y:609:TRP:O | 2.19 | 0.43 |
| 2:Z:2257:CYS:N | 2:Z:2324:CYS:SG | 2.91 | 0.43 |
| 3:a:2933[B]:SER:CA | 3:a:2936[B]:GLU:HB3 | 2.48 | 0.43 |
| 3:a:3014[B]:TRP:CH2 | 3:a:3123[B]:THR:HG23 | 2.53 | 0.43 |
| 3:a:3023[A]:ILE:O | 3:a:3026[A]:THR:OG1 | 2.34 | 0.43 |
| 3:a:3028[A]:PRO:HG2 | 3:a:3029[A]:LYS:HG3 | 2.00 | 0.43 |
| 3:a:3133[A]:LEU:HD12 | 3:a:3133[A]:LEU:HA | 1.86 | 0.43 |
| 3:a:3299[B]:LEU:O | 3:a:3300[B]:LEU:C | 2.60 | 0.43 |
| 1:b:120:LYS:N | 1:b:121:ASN:HA | 2.34 | 0.43 |
| 1:b:407:GLN:HA | 1:b:408:GLY:HA2 | 1.79 | 0.43 |
| 1:b:516:TRP:NE1 | 1:b:636:GLN:HG2 | 2.34 | 0.43 |
| 1:b:946:GLU:HA | 1:b:955:LYS:HB3 | 2.01 | 0.43 |
| 2:c:2131:LEU:HD12 | 2:c:2335:PRO:HB3 | 2.01 | 0.43 |
| 2:c:2569:TRP:O | 2:c:2572:VAL:HG23 | 2.19 | 0.43 |
| 3:d:2951[B]:ASP:OD2 | 3:d:2952[B]:ALA:CB | 2.66 | 0.43 |
| 3:d:3014[A]:TRP:CH2 | 3:d:3123[A]:THR:HG23 | 2.53 | 0.43 |
| 3:d:3047[A]:ARG:NH2 | 3:d:3113[A]:ASP:OD1 | 2.43 | 0.43 |
| 3:d:3228[A]:VAL:CG2 | 3:d:3245[A]:PHE:CD2 | 3.02 | 0.43 |
| 3:d:3232[A]:VAL:HG21 | 3:d:3273[A]:LEU:HD11 | 2.00 | 0.43 |
| 1:A:1152:LYS:HD2 | 1:A:1152:LYS:N | 2.34 | 0.43 |
| 1:A:1286:ARG:HA | 1:A:1286:ARG:HD2 | 1.58 | 0.43 |
| 1:A:1417:CYS:N | 1:A:1484:CYS:SG | 2.92 | 0.43 |
| 2:B:2094:ARG:NH2 | 2:E:2094:ARG:HH21 | 2.15 | 0.43 |
| 2:B:2114:ARG:HG3 | 2:E:2526:ARG:HE | 1.83 | 0.43 |
| 2:B:2244:PHE:CD1 | 2:B:2373:MET:HE2 | 2.54 | 0.43 |
| 2:B:2549:PRO:HA | 2:B:2550:THR:HA | 1.89 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2716:ARG:NH2 | 2:B:2780:HIS:O | 2.44 | 0.43 |
| 3:C:2974[B]:ALA:C | 3:L:3253[B]:GLU:OE1 | 2.62 | 0.43 |
| 3:C:2979[A]:GLN:HA | 3:C:2979[A]:GLN:OE1 | 2.19 | 0.43 |
| 3:C:3001[B]:LYS:H | 3:C:3003[B]:LYS:HG3 | 1.83 | 0.43 |
| 3:C:3048[B]:ASP:HB3 | 3:C:3099[B]:PRO:HD2 | 2.01 | 0.43 |
| 3:C:3229[B]:ASN:N | 3:C:3286[B]:THR:O | 2.52 | 0.43 |
| 1:D:801:ASP:OD1 | 1:D:801:ASP:N | 2.49 | 0.43 |
| 2:E:2435:MET:HA | 2:E:2436:PRO:HD3 | 1.91 | 0.43 |
| 2:E:2807:GLY:O | 2:E:2899:PRO:HA | 2.18 | 0.43 |
| 3:F:2956[A]:LYS:O | 3:F:2959[A]:SER:OG | 2.33 | 0.43 |
| 3:F:2961[B]:HIS:CB | 3:a:2975[B]:PHE:HZ | 2.31 | 0.43 |
| 3:F:2988[B]:TRP:CZ3 | 3:F:2989[B]:HIS:CE1 | 3.07 | 0.43 |
| 3:F:2989[B]:HIS:C | 3:F:2991[B]:LEU:N | 2.75 | 0.43 |
| 1:G:483:GLY:HA3 | 1:G:771:TRP:CE3 | 2.54 | 0.43 |
| 1:G:499:GLU:HG3 | 1:G:511:VAL:H | 1.83 | 0.43 |
| 1:G:1161:ILE:HG13 | 1:G:1196:ILE:HD11 | 2.01 | 0.43 |
| 2:H:2226:GLU:CD | 2:H:2277:LYS:HD2 | 2.44 | 0.43 |
| 2:H:2266:VAL:O | 2:H:2269:SER:OG | 2.24 | 0.43 |
| 3:I:3150[B]:LYS:O | 3:R:3159[B]:SER:OG | 2.36 | 0.43 |
| 3:I:3229[A]:ASN:O | 3:I:3286[A]:THR:N | 2.50 | 0.43 |
| 3:I:3255[B]:PRO:HD3 | 3:R:2962[B]:GLY:N | 2.34 | 0.43 |
| 3:I:3299[B]:LEU:O | 3:I:3300[B]:LEU:C | 2.60 | 0.43 |
| 1:J:473:ALA:HB2 | 1:M:1639:LYS:HG3 | 2.01 | 0.43 |
| 3:L:3083[A]:ILE:HD11 | 3:L:3260[A]:ARG:CG | 2.49 | 0.43 |
| 3:L:3093[A]:HIS:HD2 | 3:L:3248[A]:LEU:CD2 | 2.31 | 0.43 |
| 3:L:3218[B]:LEU:HD13 | 3:L:3261[B]:LEU:HD23 | 2.01 | 0.43 |
| 3:L:3293[B]:LYS:CB | 3:L:3294[B]:SER:CA | 2.96 | 0.43 |
| 1:M:70:ARG:HB2 | 1:M:214:GLU:CD | 2.44 | 0.43 |
| 1:M:633:HIS:C | 1:M:633:HIS:ND1 | 2.75 | 0.43 |
| 1:M:877:HIS:HB3 | 1:M:1034:GLU:HA | 2.01 | 0.43 |
| 2:N:2280:TYR:HD1 | 2:N:2287:TYR:CD1 | 2.37 | 0.43 |
| 2:N:2740:ASP:OD1 | 2:N:2740:ASP:N | 2.51 | 0.43 |
| 2:N:2854:MET:HE3 | 2:N:2854:MET:HB2 | 1.92 | 0.43 |
| 3:O:2988[B]:TRP:CD1 | 3:O:3158[B]:PHE:CE2 | 3.06 | 0.43 |
| 3:O:2989[B]:HIS:O | 3:O:2990[B]:ARG:C | 2.61 | 0.43 |
| 3:O:3171[A]:HIS:C | 3:O:3173[A]:THR:N | 2.73 | 0.43 |
| 3:O:3301[A]:PRO:HB2 | 3:O:3302[A]:SER:H | 1.33 | 0.43 |
| 1:P:117:LYS:HG3 | 2:T:2634:THR:OG1 | 2.18 | 0.43 |
| 1:P:605:SER:HA | 1:P:761:ALA:HB3 | 2.01 | 0.43 |
| 1:P:622:HIS:HE1 | 1:P:767:LYS:H | 1.63 | 0.43 |
| 1:P:1209:ASP:O | 1:P:1211:TYR:HB3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:2937[B]:ASN:CG | 3:R:3006[B]:LYS:HD3 | 2.43 | 0.43 |
| 3:R:2976[B]:ALA:O | 3:R:2978[B]:CYS:N | 2.46 | 0.43 |
| 3:R:3083[B]:ILE:HD11 | 3:R:3260[B]:ARG:CG | 2.49 | 0.43 |
| 3:R:3135[B]:LYS:HB2 | 3:R:3141[B]:TYR:CD1 | 2.51 | 0.43 |
| 3:R:3183[B]:LEU:N | 3:R:3184[B]:ASN:CA | 2.80 | 0.43 |
| 1:S:543:ASN:HA | 1:S:544:PRO:HD3 | 1.86 | 0.43 |
| 1:S:803:LYS:HA | 1:S:809:ALA:HA | 2.00 | 0.43 |
| 1:S:804:ASP:C | 1:S:807:GLY:H | 2.26 | 0.43 |
| 1:S:931:TRP:HE3 | 1:S:991:LEU:HD13 | 1.83 | 0.43 |
| 2:T:2109:ARG:O | 2:T:2113:ASP:N | 2.51 | 0.43 |
| 2:T:2130:PRO:CB | 2:T:2142:ALA:HB3 | 2.49 | 0.43 |
| 2:T:2336:PHE:HB3 | 2:T:2348:THR:HG22 | 2.00 | 0.43 |
| 2:T:2390:GLN:O | 2:T:2491:PRO:HB3 | 2.19 | 0.43 |
| 2:T:2559:CYS:SG | 2:T:2560:LEU:N | 2.91 | 0.43 |
| 2:T:2568:HIS:CD2 | 2:T:2718:TRP:HH2 | 2.36 | 0.43 |
| 2:T:2684:HIS:CE1 | 2:T:2711:HIS:HE1 | 2.37 | 0.43 |
| 3:U:2933[B]:SER:CA | 3:U:2936[B]:GLU:HB3 | 2.48 | 0.43 |
| 3:U:2948[B]:ASP:HB3 | 3:U:2949[B]:LYS:C | 2.43 | 0.43 |
| 3:U:2951[A]:ASP:OD2 | 3:U:2952[A]:ALA:CB | 2.66 | 0.43 |
| 3:U:3023[A]:ILE:HA | 3:U:3026[A]:THR:HG1 | 1.82 | 0.43 |
| 3:U:3220[B]:ARG:HH11 | 3:d:2974[B]:ALA:HB2 | 1.83 | 0.43 |
| 1:V:435:GLU:HB3 | 1:V:509:ILE:HD11 | 2.01 | 0.43 |
| 2:W:2275:GLY:HA3 | 2:W:2283:ASN:HB2 | 2.01 | 0.43 |
| 2:W:2830:GLN:HE21 | 2:W:2830:GLN:H | 1.67 | 0.43 |
| 3:X:2971[A]:ASP:CG | 3:X:2973[A]:THR:HG1 | 2.12 | 0.43 |
| 3:X:2979[A]:GLN:HG2 | 3:X:3155[A]:MET:HE2 | 1.85 | 0.43 |
| 3:X:2988[B]:TRP:CZ3 | 3:X:2989[B]:HIS:CE1 | 3.07 | 0.43 |
| 3:X:3013[A]:ASP:CA | 3:X:3122[A]:ASN:ND2 | 2.73 | 0.43 |
| 3:X:3047[A]:ARG:NH2 | 3:X:3113[A]:ASP:OD1 | 2.43 | 0.43 |
| 3:X:3194[B]:GLY:C | 3:X:3195[B]:MET:CG | 2.90 | 0.43 |
| 3:X:3230[B]:PHE:CB | 3:X:3242[B]:GLY:C | 2.91 | 0.43 |
| 1:Y:744:VAL:HG12 | 1:Y:802:ILE:HG23 | 2.01 | 0.43 |
| 1:Y:1059:LEU:O | 1:Y:1063:ARG:N | 2.50 | 0.43 |
| 1:Y:1407:THR:HG22 | 1:Y:1426:LEU:HD21 | 2.01 | 0.43 |
| 2:Z:2329:MET:HE2 | 2:Z:2358:PHE:HE2 | 1.83 | 0.43 |
| 3:a:2995[B]:GLN:CG | 3:a:3168[B]:THR:HG21 | 2.48 | 0.43 |
| 3:a:3230[B]:PHE:CB | 3:a:3242[B]:GLY:C | 2.91 | 0.43 |
| 3:a:3293[A]:LYS:CB | 3:a:3294[A]:SER:CA | 2.96 | 0.43 |
| 1:b:235:CYS:SG | 1:b:819:ILE:HD11 | 2.59 | 0.43 |
| 1:b:732:GLY:HA2 | 1:b:777:TYR:O | 2.19 | 0.43 |
| 2:c:2244:PHE:HZ | 2:c:2376:MET:HE1 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3034[A]:HIS:HB3 | 3:d:3035[A]:HIS:CE1 | 2.50 | 0.43 |
| 3:d:3083[B]:ILE:HD11 | 3:d:3260[B]:ARG:CG | 2.49 | 0.43 |
| 3:d:3131[B]:GLN:HE21 | 3:d:3131[B]:GLN:HB3 | 1.66 | 0.43 |
| 2:B:2884:LYS:HG3 | 2:B:2891:LEU:HG | 2.01 | 0.42 |
| 3:C:2933[A]:SER:CA | 3:C:2936[A]:GLU:HB3 | 2.48 | 0.42 |
| 3:C:3090[B]:ASN:HA | 3:L:2971[B]:ASP:HB2 | 2.01 | 0.42 |
| 3:C:3150[B]:LYS:N | 3:L:3158[B]:PHE:O | 2.42 | 0.42 |
| 3:C:3153[B]:LYS:CD | 3:L:2988[B]:TRP:HD1 | 2.29 | 0.42 |
| 3:C:3218[A]:LEU:HD13 | 3:C:3261[A]:LEU:HD23 | 2.01 | 0.42 |
| 3:C:3245[B]:PHE:CD1 | 3:C:3245[B]:PHE:C | 2.97 | 0.42 |
| 1:D:905:TRP:HE1 | 1:D:1083:PRO:CD | 2.32 | 0.42 |
| 1:D:1155:LEU:HD11 | 1:D:1228:LEU:HD11 | 2.00 | 0.42 |
| 1:D:1578:ILE:HA | 1:D:1579:GLY:HA2 | 1.63 | 0.42 |
| 1:D:1616:LYS:HA | 1:D:1616:LYS:HD3 | 1.90 | 0.42 |
| 2:E:2446:GLU:HG2 | 2:E:2448:THR:HG23 | 2.01 | 0.42 |
| 2:E:2866:PRO:HA | 2:E:2867:PRO:HD3 | 1.65 | 0.42 |
| 3:F:2938[B]:LEU:HD12 | 3:F:2938[B]:LEU:HA | 1.85 | 0.42 |
| 3:F:2948[A]:ASP:HB3 | 3:F:2949[A]:LYS:C | 2.43 | 0.42 |
| 3:F:3174[B]:GLY:N | 3:a:3154[B]:PRO:N | 2.66 | 0.42 |
| 3:F:3185[A]:TYR:HE2 | 3:F:3187[A]:TYR:CD2 | 2.35 | 0.42 |
| 3:F:3293[A]:LYS:CB | 3:F:3294[A]:SER:CA | 2.96 | 0.42 |
| 1:G:449:ASP:HB2 | 1:G:1338:GLY:HA3 | 1.99 | 0.42 |
| 1:G:979:LEU:HD23 | 1:G:1021:LEU:HD22 | 2.01 | 0.42 |
| 1:G:1500:THR:HA | 1:G:1501:ALA:HA | 1.76 | 0.42 |
| 2:H:2252:GLU:HA | 2:H:2385:ILE:HD13 | 2.01 | 0.42 |
| 2:H:2304:LEU:HA | 2:H:2304:LEU:HD12 | 1.76 | 0.42 |
| 3:I:2965[B]:LEU:O | 3:R:3221[B]:ALA:HB2 | 2.19 | 0.42 |
| 3:I:2969[B]:TYR:CE2 | 3:I:2970[B]:PRO:CG | 2.86 | 0.42 |
| 3:I:2979[B]:GLN:CD | 3:I:3155[B]:MET:CE | 2.92 | 0.42 |
| 3:I:3001[B]:LYS:N | 3:I:3003[B]:LYS:HG3 | 2.34 | 0.42 |
| 3:I:3028[B]:PRO:HG2 | 3:I:3029[B]:LYS:HG3 | 2.00 | 0.42 |
| 3:I:3108[B]:HIS:HE1 | 3:R:3251[B]:ASP:CB | 2.32 | 0.42 |
| 3:I:3149[B]:ASN:OD1 | 3:I:3149[B]:ASN:N | 2.50 | 0.42 |
| 3:I:3152[B]:LYS:HB2 | 3:R:3171[B]:HIS:CA | 2.49 | 0.42 |
| 3:I:3155[B]:MET:CG | 3:R:3153[B]:LYS:HG2 | 2.49 | 0.42 |
| 3:I:3165[B]:ASN:O | 3:R:3149[B]:ASN:CB | 2.42 | 0.42 |
| 1:J:1323:HIS:CD2 | 1:J:1458:HIS:CE1 | 3.07 | 0.42 |
| 3:L:2931[A]:THR:O | 3:L:2934[A]:GLU:HG3 | 2.18 | 0.42 |
| 3:L:2979[B]:GLN:CD | 3:L:3155[B]:MET:CE | 2.92 | 0.42 |
| 3:L:3276[A]:ASP:C | 3:L:3278[A]:HIS:N | 2.75 | 0.42 |
| 3:L:3299[B]:LEU:HB3 | 3:L:3300[B]:LEU:H | 1.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:868:THR:HG23 | 1:M:919:ARG:NE | 2.34 | 0.42 |
| 3:O:3001[A]:LYS:H | 3:O:3003[A]:LYS:HG3 | 1.83 | 0.42 |
| 3:O:3013[B]:ASP:CG | 3:O:3015[B]:THR:HG1 | 2.26 | 0.42 |
| 3:O:3083[A]:ILE:HD11 | 3:O:3260[A]:ARG:CG | 2.49 | 0.42 |
| 3:O:3148[B]:ILE:HG22 | 3:O:3152[B]:LYS:HE3 | 2.01 | 0.42 |
| 3:O:3171[B]:HIS:C | 3:O:3173[B]:THR:N | 2.73 | 0.42 |
| 3:O:3229[A]:ASN:O | 3:O:3286[A]:THR:N | 2.50 | 0.42 |
| 3:O:3245[B]:PHE:CD1 | 3:O:3245[B]:PHE:C | 2.97 | 0.42 |
| 1:P:838:ARG:HD2 | 1:P:914:GLU:CD | 2.44 | 0.42 |
| 1:P:929:TRP:CZ3 | 1:P:935:ILE:HD12 | 2.54 | 0.42 |
| 1:P:999:LEU:HD21 | 1:P:1121:LEU:HD22 | 1.99 | 0.42 |
| 1:P:1243:PHE:HD2 | 1:P:1474:TYR:HA | 1.84 | 0.42 |
| 2:Q:2758:THR:O | 2:Q:2762:VAL:HG22 | 2.19 | 0.42 |
| 3:R:2932[A]:PRO:CA | 3:R:2935[A]:ILE:CD1 | 2.85 | 0.42 |
| 3:R:2948[B]:ASP:HB3 | 3:R:2949[B]:LYS:C | 2.43 | 0.42 |
| 3:R:3028[B]:PRO:HG2 | 3:R:3029[B]:LYS:HG3 | 2.00 | 0.42 |
| 3:R:3132[B]:ALA:HB3 | 3:R:3197[B]:ILE:HD13 | 1.99 | 0.42 |
| 3:R:3301[B]:PRO:HB2 | 3:R:3302[B]:SER:H | 1.33 | 0.42 |
| 1:S:488:PRO:HB2 | 1:S:641:TRP:CE3 | 2.53 | 0.42 |
| 1:S:741:SER:OG | 1:S:763:LEU:HA | 2.19 | 0.42 |
| 1:S:896:HIS:HB2 | 1:S:905:TRP:CD1 | 2.54 | 0.42 |
| 2:T:2497:GLU:HB2 | 2:T:2498:VAL:HA | 2.00 | 0.42 |
| 2:T:2726:LYS:HE3 | 2:T:2726:LYS:HB2 | 1.71 | 0.42 |
| 3:U:2988[B]:TRP:CZ3 | 3:U:2989[B]:HIS:CE1 | 3.07 | 0.42 |
| 3:U:3038[B]:ILE:HG23 | 3:U:3040[B]:VAL:HG22 | 1.90 | 0.42 |
| 3:U:3218[B]:LEU:HD13 | 3:U:3261[B]:LEU:HD23 | 2.01 | 0.42 |
| 1:V:7:VAL:HG21 | 1:V:208:LEU:HD23 | 2.00 | 0.42 |
| 1:V:424:PHE:CE1 | 1:V:1125:SER:HB2 | 2.54 | 0.42 |
| 1:V:754:GLU:CD | 1:V:799:ARG:HH21 | 2.23 | 0.42 |
| 1:V:980:TYR:CD2 | 1:V:1021:LEU:HD13 | 2.54 | 0.42 |
| 1:V:1328:SER:HB2 | 1:V:1523:LEU:HD13 | 2.00 | 0.42 |
| 1:V:1539:GLN:O | 1:V:1542:ARG:HB3 | 2.19 | 0.42 |
| 1:V:1549:GLY:O | 1:V:1655:SER:HB2 | 2.18 | 0.42 |
| 2:W:2386:ARG:HB3 | 2:W:2496:LEU:HD21 | 2.01 | 0.42 |
| 3:X:3048[A]:ASP:HB3 | 3:X:3099[A]:PRO:HD2 | 2.01 | 0.42 |
| 3:X:3094[A]:SER:HG | 3:X:3227[A]:ASP:CG | 2.27 | 0.42 |
| 3:X:3148[A]:ILE:HG22 | 3:X:3152[A]:LYS:HE3 | 2.01 | 0.42 |
| 3:X:3217[B]:PHE:CD2 | 3:X:3300[B]:LEU:HD12 | 2.53 | 0.42 |
| 1:Y:137:ARG:HA | 1:Y:193:SER:OG | 2.18 | 0.42 |
| 1:Y:1382:ILE:N | 1:Y:1387:ALA:O | 2.38 | 0.42 |
| 1:Y:1616:LYS:C | 3:d:3187[B]:TYR:CB | 2.65 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:2795:ILE:O | 2:Z:2798:GLN:HG2 | 2.19 | 0.42 |
| 2:Z:2820:HIS:HB2 | 2:Z:2882:GLU:HG3 | 2.01 | 0.42 |
| 3:a:2951[A]:ASP:OD2 | 3:a:2952[A]:ALA:CB | 2.66 | 0.42 |
| 3:a:2951[A]:ASP:C | 3:a:2956[A]:LYS:HZ1 | 2.19 | 0.42 |
| 3:a:2979[A]:GLN:HA | 3:a:2979[A]:GLN:OE1 | 2.19 | 0.42 |
| 3:a:3083[A]:ILE:HD11 | 3:a:3260[A]:ARG:CG | 2.49 | 0.42 |
| 3:a:3182[B]:GLN:H | 3:a:3182[B]:GLN:HG2 | 1.56 | 0.42 |
| 1:b:398:ARG:HA | 1:b:399:PRO:HD3 | 1.86 | 0.42 |
| 1:b:745:ASP:HB2 | 1:b:801:ASP:OD1 | 2.18 | 0.42 |
| 1:b:868:THR:HG23 | 1:b:919:ARG:HH21 | 1.84 | 0.42 |
| 1:b:1243:PHE:O | 1:b:1476:LYS:HD3 | 2.19 | 0.42 |
| 2:c:2132:CYS:O | 2:c:2334:LYS:HD3 | 2.19 | 0.42 |
| 2:c:2189:GLY:HA2 | 2:c:2192:THR:HG22 | 2.01 | 0.42 |
| 3:d:2979[B]:GLN:CD | 3:d:3155[B]:MET:CE | 2.92 | 0.42 |
| 3:d:2988[A]:TRP:CZ3 | 3:d:2989[A]:HIS:CE1 | 3.07 | 0.42 |
| 1:A:995:ILE:HG22 | 1:A:999:LEU:HD22 | 2.00 | 0.42 |
| 1:A:1553:ILE:HD11 | 1:A:1622:GLN:HG3 | 2.01 | 0.42 |
| 3:C:2938[A]:LEU:HD12 | 3:C:2938[A]:LEU:HA | 1.85 | 0.42 |
| 3:C:2951[B]:ASP:OD2 | 3:C:2952[B]:ALA:CB | 2.66 | 0.42 |
| 3:C:2967[B]:CYS:SG | 3:L:2982[B]:MET:N | 2.89 | 0.42 |
| 3:C:2988[A]:TRP:CZ3 | 3:C:2989[A]:HIS:CE1 | 3.07 | 0.42 |
| 3:C:3023[B]:ILE:HA | 3:C:3026[B]:THR:HG1 | 1.83 | 0.42 |
| 3:C:3086[B]:GLU:HG2 | 3:L:2968[B]:GLN:NE2 | 2.34 | 0.42 |
| 3:C:3131[B]:GLN:HE21 | 3:C:3131[B]:GLN:HB3 | 1.66 | 0.42 |
| 3:C:3153[B]:LYS:CD | 3:L:3155[B]:MET:HE2 | 2.49 | 0.42 |
| 3:C:3228[B]:VAL:CG2 | 3:C:3245[B]:PHE:CD2 | 3.02 | 0.42 |
| 3:C:3299[B]:LEU:O | 3:C:3300[B]:LEU:C | 2.60 | 0.42 |
| 1:D:447:MET:HE1 | 1:D:544:PRO:O | 2.19 | 0.42 |
| 1:D:468:CYS:SG | 1:D:669:LYS:HB3 | 2.59 | 0.42 |
| 3:F:2969[B]:TYR:HD2 | 3:a:3093[B]:HIS:NE2 | 2.15 | 0.42 |
| 3:F:2971[B]:ASP:N | 9:F:3401[B]:CUO:CU1 | 1.40 | 0.42 |
| 3:F:3137[A]:ARG:HD3 | 3:F:3137[A]:ARG:HA | 1.71 | 0.42 |
| 3:F:3154[B]:PRO:CG | 3:a:3155[B]:MET:CG | 2.84 | 0.42 |
| 3:F:3196[B]:THR:OG1 | 3:F:3199[B]:GLN:OE1 | 2.38 | 0.42 |
| 3:F:3218[A]:LEU:HD13 | 3:F:3261[A]:LEU:HD23 | 2.01 | 0.42 |
| 3:F:3232[B]:VAL:HG21 | 3:F:3273[B]:LEU:CD1 | 2.49 | 0.42 |
| 3:F:3299[B]:LEU:HB3 | 3:F:3300[B]:LEU:H | 1.54 | 0.42 |
| 1:G:40:TYR:CE2 | 1:G:75:GLN:HG2 | 2.54 | 0.42 |
| 1:G:323:ILE:HA | 1:G:324:PRO:HD3 | 1.92 | 0.42 |
| 1:G:449:ASP:OD2 | 1:G:1280:GLN:NE2 | 2.51 | 0.42 |
| 1:G:767:LYS:HE2 | 1:G:767:LYS:HB3 | 1.94 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:929:TRP:CZ3 | 1:G:935:ILE:HD12 | 2.53 | 0.42 |
| 1:G:1582:ASN:HB3 | 1:G:1583:CYS:CB | 2.37 | 0.42 |
| 2:H:2457:LYS:NZ | 1:J:1206:HIS:HB3 | 2.34 | 0.42 |
| 2:H:2470:ALA:HB2 | 2:H:2476:LEU:HD11 | 2.00 | 0.42 |
| 2:H:2647:LEU:HD12 | 2:H:2647:LEU:HA | 1.81 | 0.42 |
| 3:I:2961[B]:HIS:HB2 | 3:I:2992[B]:TYR:HE2 | 1.81 | 0.42 |
| 3:I:2976[B]:ALA:O | 3:I:2978[B]:CYS:N | 2.46 | 0.42 |
| 3:I:3281[A]:PHE:HE1 | 3:I:3305[A]:ILE:HG21 | 1.81 | 0.42 |
| 1:J:219:LEU:O | 1:J:223:LEU:HB2 | 2.19 | 0.42 |
| 1:J:285:THR:HG22 | 1:J:287:GLU:H | 1.83 | 0.42 |
| 1:J:567:LEU:HD13 | 1:J:567:LEU:HA | 1.79 | 0.42 |
| 1:J:634:HIS:HA | 1:J:637:VAL:CG2 | 2.49 | 0.42 |
| 1:J:689:PRO:HA | 1:J:692:VAL:HG23 | 2.01 | 0.42 |
| 1:J:1263:LEU:HD11 | 1:J:1358:LEU:HD22 | 2.01 | 0.42 |
| 1:J:1298:ALA:O | 4:v:2:NAG:H62 | 2.19 | 0.42 |
| 2:K:2128:LEU:HD12 | 2:K:2128:LEU:HA | 1.78 | 0.42 |
| 2:K:2822:LYS:HB3 | 2:K:2829:CYS:HB3 | 2.01 | 0.42 |
| 3:L:2938[A]:LEU:O | 3:L:2939[A]:ARG:C | 2.58 | 0.42 |
| 3:L:2979[B]:GLN:HA | 3:L:2979[B]:GLN:OE1 | 2.19 | 0.42 |
| 3:L:2988[A]:TRP:CZ3 | 3:L:2989[A]:HIS:CE1 | 3.07 | 0.42 |
| 3:L:2995[A]:GLN:CG | 3:L:3168[A]:THR:HG21 | 2.48 | 0.42 |
| 3:L:3096[B]:VAL:CG1 | 3:L:3115[B]:LEU:CD1 | 2.86 | 0.42 |
| 3:L:3149[A]:ASN:OD1 | 3:L:3149[A]:ASN:N | 2.51 | 0.42 |
| 3:L:3301[B]:PRO:HB2 | 3:L:3302[B]:SER:H | 1.33 | 0.42 |
| 1:M:597:VAL:O | 1:M:601:VAL:HG13 | 2.19 | 0.42 |
| 1:M:893:ALA:HB2 | 1:M:1182:ASN:HB2 | 2.01 | 0.42 |
| 1:M:1424:GLU:O | 1:M:1427:HIS:HB3 | 2.19 | 0.42 |
| 2:N:2180:TRP:CH2 | 2:N:2300:ASN:HB3 | 2.55 | 0.42 |
| 2:N:2744:PHE:HA | 2:N:2745:PRO:HD3 | 1.87 | 0.42 |
| 2:N:2874:ASP:O | 2:N:2876:LYS:HG3 | 2.19 | 0.42 |
| 3:O:3160[B]:SER:HG | 3:X:3150[B]:LYS:HB2 | 1.81 | 0.42 |
| 3:O:3228[B]:VAL:CG2 | 3:O:3245[B]:PHE:CD2 | 3.02 | 0.42 |
| 1:P:145:GLN:OE1 | 1:P:151:GLN:HG3 | 2.19 | 0.42 |
| 1:P:607:HIS:NE2 | 1:P:634:HIS:CE1 | 2.88 | 0.42 |
| 1:P:1473:ARG:HG3 | 1:P:1479:TYR:CG | 2.55 | 0.42 |
| 2:Q:2128:LEU:HD22 | 2:Q:2287:TYR:CE1 | 2.55 | 0.42 |
| 3:R:2988[A]:TRP:CZ3 | 3:R:2989[A]:HIS:CE1 | 3.07 | 0.42 |
| 3:R:2995[A]:GLN:CG | 3:R:3168[A]:THR:HG21 | 2.49 | 0.42 |
| 3:R:3182[B]:GLN:H | 3:R:3182[B]:GLN:HG2 | 1.56 | 0.42 |
| 3:R:3185[B]:TYR:HE2 | 3:R:3187[B]:TYR:CD2 | 2.35 | 0.42 |
| 3:R:3191[A]:ASN:C | 3:R:3192[A]:PHE:O | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3196[B]:THR:OG1 | 3:R:3199[B]:GLN:OE1 | 2.37 | 0.42 |
| 3:R:3281[B]:PHE:HE1 | 3:R:3305[B]:ILE:HG21 | 1.81 | 0.42 |
| 1:S:361:GLU:HG2 | 1:S:363:THR:HG22 | 2.01 | 0.42 |
| 1:S:516:TRP:HD1 | 1:S:579:LEU:HB3 | 1.84 | 0.42 |
| 1:S:1382:ILE:HD13 | 1:S:1447:TYR:HD2 | 1.84 | 0.42 |
| 1:S:1398:PHE:HA | 1:S:1399:GLY:HA2 | 1.53 | 0.42 |
| 2:T:2576:HIS:CD2 | 2:T:2759:THR:HG21 | 2.54 | 0.42 |
| 3:U:2937[B]:ASN:CG | 3:U:3006[B]:LYS:HD3 | 2.43 | 0.42 |
| 3:U:2979[A]:GLN:CD | 3:U:3155[A]:MET:CE | 2.92 | 0.42 |
| 3:U:3083[A]:ILE:HD11 | 3:U:3260[A]:ARG:CG | 2.49 | 0.42 |
| 3:U:3232[B]:VAL:HG21 | 3:U:3273[B]:LEU:CD1 | 2.49 | 0.42 |
| 3:U:3299[B]:LEU:HB3 | 3:U:3300[B]:LEU:H | 1.54 | 0.42 |
| 3:U:3300[A]:LEU:HD23 | 3:U:3300[A]:LEU:H | 1.83 | 0.42 |
| 1:V:25:MET:HE2 | 1:V:34:TYR:HA | 2.01 | 0.42 |
| 1:V:80:LEU:HD12 | 1:V:80:LEU:HA | 1.81 | 0.42 |
| 1:V:109:LEU:HD13 | 2:Z:2626:ARG:NH1 | 2.34 | 0.42 |
| 1:V:163:LEU:HB3 | 1:V:293:LEU:HD21 | 2.00 | 0.42 |
| 3:X:2969[A]:TYR:CD2 | 3:X:2971[A]:ASP:CG | 2.97 | 0.42 |
| 3:X:3038[B]:ILE:HG23 | 3:X:3040[B]:VAL:HG22 | 1.90 | 0.42 |
| 3:X:3196[A]:THR:OG1 | 3:X:3199[A]:GLN:OE1 | 2.38 | 0.42 |
| 3:X:3293[A]:LYS:CD | 3:X:3293[A]:LYS:C | 2.85 | 0.42 |
| 1:Y:450:LYS:H | 1:Y:450:LYS:HG3 | 1.54 | 0.42 |
| 1:Y:1190:ARG:HA | 1:Y:1191:PRO:HD3 | 1.92 | 0.42 |
| 2:Z:2521:MET:HE3 | 2:Z:2605:LEU:HD12 | 2.01 | 0.42 |
| 2:Z:2542:TYR:HB2 | 2:Z:2573:TYR:CE1 | 2.51 | 0.42 |
| 2:Z:2561:HIS:ND1 | 2:Z:2561:HIS:N | 2.67 | 0.42 |
| 3:a:2937[B]:ASN:CG | 3:a:3006[B]:LYS:HD3 | 2.44 | 0.42 |
| 3:a:3001[A]:LYS:N | 3:a:3003[A]:LYS:HG3 | 2.34 | 0.42 |
| 3:a:3148[B]:ILE:HG22 | 3:a:3152[B]:LYS:HE3 | 2.01 | 0.42 |
| 3:a:3218[B]:LEU:HD13 | 3:a:3261[B]:LEU:HD23 | 2.01 | 0.42 |
| 3:a:3245[A]:PHE:CD1 | 3:a:3245[A]:PHE:C | 2.97 | 0.42 |
| 3:a:3267[A]:SER:HG | 3:a:3267[A]:SER:H | 1.42 | 0.42 |
| 1:b:531:THR:HG22 | 1:b:542:PRO:HA | 2.01 | 0.42 |
| 1:b:1329:LEU:HB2 | 1:b:1507:THR:HG21 | 2.01 | 0.42 |
| 3:d:2951[A]:ASP:OD2 | 3:d:2952[A]:ALA:CB | 2.66 | 0.42 |
| 3:d:3001[A]:LYS:N | 3:d:3003[A]:LYS:HG3 | 2.34 | 0.42 |
| 3:d:3048[A]:ASP:HB3 | 3:d:3099[A]:PRO:HD2 | 2.01 | 0.42 |
| 1:A:81:VAL:C | 1:A:83:HIS:N | 2.77 | 0.42 |
| 1:A:496:MET:O | 1:A:500:ASN:ND2 | 2.50 | 0.42 |
| 1:A:843:VAL:HG13 | 1:A:927:PRO:HB2 | 1.99 | 0.42 |
| 1:A:905:TRP:CZ3 | 1:A:909:ILE:HG13 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1158:GLU:HG2 | 1:A:1216:ARG:O | 2.19 | 0.42 |
| 1:A:1321:HIS:O | 1:A:1324:ARG:HB3 | 2.19 | 0.42 |
| 1:A:1633:THR:HA | 1:A:1639:LYS:O | 2.19 | 0.42 |
| 2:B:2107:LEU:O | 2:B:2111:GLN:HB2 | 2.19 | 0.42 |
| 2:B:2181:THR:HB | 2:B:2373:MET:SD | 2.59 | 0.42 |
| 2:B:2505:ILE:HD12 | 2:B:2507:ARG:HH21 | 1.84 | 0.42 |
| 2:B:2643:GLU:O | 2:B:2647:LEU:N | 2.46 | 0.42 |
| 2:B:2884:LYS:HD2 | 2:B:2889:ALA:HB3 | 2.02 | 0.42 |
| 3:C:2956[A]:LYS:O | 3:C:2959[A]:SER:OG | 2.33 | 0.42 |
| 3:C:2959[B]:SER:C | 3:L:3255[B]:PRO:HB2 | 2.33 | 0.42 |
| 3:C:2979[B]:GLN:HA | 3:C:2979[B]:GLN:OE1 | 2.19 | 0.42 |
| 3:C:3149[B]:ASN:HD21 | 3:L:3163[B]:ASN:HB3 | 1.82 | 0.42 |
| 3:C:3174[B]:GLY:N | 3:L:3154[B]:PRO:HB3 | 2.30 | 0.42 |
| 3:C:3232[A]:VAL:HG21 | 3:C:3273[A]:LEU:CD1 | 2.50 | 0.42 |
| 3:C:3284[A]:LYS:CD | 3:C:3284[A]:LYS:C | 2.86 | 0.42 |
| 1:D:931:TRP:CZ3 | 1:D:995:ILE:HD11 | 2.54 | 0.42 |
| 1:D:1385:GLU:OE1 | 1:D:1440:HIS:HE1 | 2.02 | 0.42 |
| 2:E:2549:PRO:HA | 2:E:2550:THR:HA | 1.56 | 0.42 |
| 2:E:2660:VAL:HG11 | 2:E:2783:PHE:CE1 | 2.54 | 0.42 |
| 3:F:2951[B]:ASP:C | 3:F:2956[B]:LYS:HZ1 | 2.13 | 0.42 |
| 3:F:2972[B]:GLY:HA3 | 3:a:3090[B]:ASN:CG | 2.44 | 0.42 |
| 3:F:2979[A]:GLN:CD | 3:F:3155[A]:MET:CE | 2.92 | 0.42 |
| 3:F:2985[B]:PHE:HD2 | 3:a:2968[B]:GLN:O | 2.02 | 0.42 |
| 3:F:3104[A]:MET:SD | 3:F:3110[A]:THR:CG2 | 3.06 | 0.42 |
| 1:G:497:GLN:CG | 1:G:683:THR:HG21 | 2.50 | 0.42 |
| 1:G:736:MET:HG3 | 1:G:772:ARG:HD2 | 2.00 | 0.42 |
| 1:G:945:ALA:C | 1:G:957:ASN:HD22 | 2.27 | 0.42 |
| 1:G:1321:HIS:HE1 | 1:G:1489:MET:SD | 2.42 | 0.42 |
| 3:I:2937[A]:ASN:CG | 3:I:3006[A]:LYS:HD3 | 2.43 | 0.42 |
| 3:I:3038[A]:ILE:HG23 | 3:I:3040[A]:VAL:HG22 | 1.89 | 0.42 |
| 3:I:3228[A]:VAL:CG2 | 3:I:3245[A]:PHE:CD2 | 3.02 | 0.42 |
| 3:I:3245[A]:PHE:CD1 | 3:I:3245[A]:PHE:C | 2.97 | 0.42 |
| 3:I:3255[B]:PRO:CB | 3:R:2959[B]:SER:HA | 2.46 | 0.42 |
| 1:J:179:HIS:HD2 | 1:J:209:HIS:HE2 | 1.67 | 0.42 |
| 1:J:227:ARG:HH22 | 1:J:297:ARG:HH22 | 1.67 | 0.42 |
| 1:J:514:TRP:CZ2 | 1:J:606:ILE:HD11 | 2.54 | 0.42 |
| 1:J:545:PHE:O | 1:J:561:ARG:NH2 | 2.52 | 0.42 |
| 1:J:804:ASP:OD2 | 4:u:1:NAG:O6 | 2.37 | 0.42 |
| 1:J:902:PHE:N | 1:J:903:PRO:HD2 | 2.34 | 0.42 |
| 1:J:1002:GLU:HG3 | 1:J:1003:ASP:N | 2.34 | 0.42 |
| 1:J:1355:LEU:HB2 | 1:J:1360:ASN:CG | 2.44 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2180:TRP:NE1 | 2:K:2300:ASN:HD22 | 2.17 | 0.42 |
| 2:K:2536:PHE:HE1 | 2:K:2708:TYR:HE2 | 1.67 | 0.42 |
| 2:K:2545:SER:HB3 | 2:K:2547:MET:HB3 | 2.01 | 0.42 |
| 3:L:2940[B]:ASN:O | 3:L:2943[B]:ALA:HB3 | 2.18 | 0.42 |
| 3:L:3096[A]:VAL:CG1 | 3:L:3115[A]:LEU:CD1 | 2.86 | 0.42 |
| 3:L:3185[A]:TYR:CE2 | 3:L:3187[A]:TYR:HE2 | 2.31 | 0.42 |
| 3:L:3228[A]:VAL:CG2 | 3:L:3245[A]:PHE:CD2 | 3.02 | 0.42 |
| 1:M:797:THR:HG22 | 1:M:798:LEU:H | 1.84 | 0.42 |
| 1:M:1077:LEU:HB3 | 1:M:1103:PHE:CE1 | 2.53 | 0.42 |
| 1:M:1435:GLY:O | 1:M:1441:SER:OG | 2.29 | 0.42 |
| 2:N:2126:HIS:O | 2:N:2143:CYS:HB3 | 2.20 | 0.42 |
| 2:N:2844:MET:O | 2:N:2846:TRP:HD1 | 2.03 | 0.42 |
| 3:O:2971[B]:ASP:OD2 | 3:X:3158[B]:PHE:CZ | 2.73 | 0.42 |
| 3:O:2979[A]:GLN:CD | 3:O:3155[A]:MET:CE | 2.92 | 0.42 |
| 3:O:3001[A]:LYS:N | 3:O:3003[A]:LYS:HG3 | 2.34 | 0.42 |
| 3:O:3013[A]:ASP:CA | 3:O:3122[A]:ASN:ND2 | 2.74 | 0.42 |
| 3:O:3276[B]:ASP:C | 3:O:3278[B]:HIS:N | 2.75 | 0.42 |
| 3:O:3293[A]:LYS:CD | 3:O:3293[A]:LYS:C | 2.86 | 0.42 |
| 1:P:554:LYS:HA | 1:P:554:LYS:HD3 | 1.76 | 0.42 |
| 1:P:566:ARG:HH22 | 1:P:803:LYS:CD | 2.31 | 0.42 |
| 1:P:816:PRO:HA | 1:P:817:PRO:HD3 | 1.87 | 0.42 |
| 1:P:865:LYS:HA | 1:P:865:LYS:HD2 | 1.80 | 0.42 |
| 1:P:1001:GLN:HG3 | 1:P:1007:PHE:HA | 2.00 | 0.42 |
| 1:P:1438:ASP:HB3 | 1:P:1441:SER:HB3 | 2.01 | 0.42 |
| 2:Q:2579:GLU:HG2 | 2:Q:2756:ASN:HD22 | 1.84 | 0.42 |
| 3:R:2979[B]:GLN:HA | 3:R:2979[B]:GLN:OE1 | 2.19 | 0.42 |
| 3:R:2988[B]:TRP:CZ3 | 3:R:2989[B]:HIS:CE1 | 3.07 | 0.42 |
| 3:R:3148[A]:ILE:HG22 | 3:R:3152[A]:LYS:HE3 | 2.01 | 0.42 |
| 1:S:554:LYS:HA | 1:S:554:LYS:HD2 | 1.63 | 0.42 |
| 1:S:585:LEU:O | 1:S:588:GLU:HB3 | 2.19 | 0.42 |
| 1:S:1081:MET:O | 1:S:1085:SER:HB3 | 2.20 | 0.42 |
| 1:S:1491:GLN:HA | 1:S:1492:PRO:HD3 | 1.90 | 0.42 |
| 2:T:2402:GLY:HA3 | 2:T:2403:PHE:HB2 | 2.02 | 0.42 |
| 2:T:2551:PRO:HA | 2:T:2552:GLU:HA | 1.51 | 0.42 |
| 3:U:2969[A]:TYR:CD2 | 3:U:2971[A]:ASP:CG | 2.98 | 0.42 |
| 3:U:2973[B]:THR:CA | 3:d:3247[B]:VAL:CG1 | 2.97 | 0.42 |
| 3:U:2976[A]:ALA:O | 3:U:2978[A]:CYS:N | 2.46 | 0.42 |
| 3:U:3048[B]:ASP:HB3 | 3:U:3099[B]:PRO:HD2 | 2.01 | 0.42 |
| 3:U:3104[A]:MET:SD | 3:U:3110[A]:THR:CG2 | 3.06 | 0.42 |
| 3:U:3196[B]:THR:OG1 | 3:U:3199[B]:GLN:OE1 | 2.38 | 0.42 |
| 3:U:3229[B]:ASN:O | 3:U:3286[B]:THR:N | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:302:ALA:H | 1:V:363:THR:HB | 1.84 | 0.42 |
| 2:W:2825:ILE:HG23 | 2:W:2826:GLU:H | 1.83 | 0.42 |
| 3:X:2931[B]:THR:O | 3:X:2934[B]:GLU:HG3 | 2.18 | 0.42 |
| 3:X:2965[B]:LEU:CG | 3:X:2974[B]:ALA:CB | 2.85 | 0.42 |
| 3:X:2988[A]:TRP:CZ3 | 3:X:2989[A]:HIS:CE1 | 3.07 | 0.42 |
| 3:X:3180[B]:TYR:CB | 3:X:3183[B]:LEU:CD2 | 2.90 | 0.42 |
| 3:X:3196[B]:THR:OG1 | 3:X:3199[B]:GLN:OE1 | 2.38 | 0.42 |
| 3:X:3232[B]:VAL:HG21 | 3:X:3273[B]:LEU:CD1 | 2.50 | 0.42 |
| 3:X:3232[B]:VAL:HG21 | 3:X:3273[B]:LEU:HD11 | 2.00 | 0.42 |
| 1:Y:37:ILE:O | 1:Y:72:TYR:OH | 2.30 | 0.42 |
| 1:Y:516:TRP:CD1 | 1:Y:579:LEU:HD13 | 2.54 | 0.42 |
| 1:Y:568:PHE:CE2 | 1:Y:609:TRP:HD1 | 2.37 | 0.42 |
| 1:Y:637:VAL:HA | 1:Y:640:LEU:HD12 | 2.01 | 0.42 |
| 1:Y:801:ASP:N | 1:Y:801:ASP:OD1 | 2.52 | 0.42 |
| 1:Y:1018:ILE:O | 1:Y:1022:VAL:HG12 | 2.19 | 0.42 |
| 3:a:2948[A]:ASP:HB3 | 3:a:2949[A]:LYS:C | 2.43 | 0.42 |
| 3:a:3180[B]:TYR:CA | 3:a:3183[B]:LEU:CD2 | 2.95 | 0.42 |
| 3:a:3232[A]:VAL:HG21 | 3:a:3273[A]:LEU:CD1 | 2.49 | 0.42 |
| 1:b:516:TRP:CG | 1:b:606:ILE:HD12 | 2.54 | 0.42 |
| 1:b:980:TYR:HE2 | 1:b:1021:LEU:HB3 | 1.84 | 0.42 |
| 1:b:1144:VAL:HG11 | 1:b:1196:ILE:HD12 | 2.01 | 0.42 |
| 1:b:1170:MET:SD | 1:b:1199:VAL:HG23 | 2.60 | 0.42 |
| 3:d:2949[A]:LYS:C | 3:d:2949[A]:LYS:HZ3 | 2.17 | 0.42 |
| 3:d:2951[B]:ASP:CG | 3:d:2952[B]:ALA:N | 2.74 | 0.42 |
| 3:d:2988[B]:TRP:CZ3 | 3:d:2989[B]:HIS:CE1 | 3.07 | 0.42 |
| 3:d:3228[B]:VAL:CG2 | 3:d:3245[B]:PHE:CD2 | 3.02 | 0.42 |
| 1:A:177:VAL:HG11 | 1:A:358:TYR:CZ | 2.54 | 0.42 |
| 1:A:792:MET:HE3 | 1:A:822:PHE:HE2 | 1.83 | 0.42 |
| 1:A:909:ILE:HG12 | 1:A:1084:PHE:HZ | 1.85 | 0.42 |
| 1:A:1518:ASP:OD2 | 1:A:1521:ASN:HB2 | 2.19 | 0.42 |
| 2:B:2336:PHE:HA | 2:B:2343:ASN:ND2 | 2.34 | 0.42 |
| 2:B:2904:ALA:HA | 2:B:2905:PRO:HD2 | 1.95 | 0.42 |
| 3:C:2948[B]:ASP:HB3 | 3:C:2949[B]:LYS:C | 2.44 | 0.42 |
| 3:C:2952[B]:ALA:CA | 3:C:2956[B]:LYS:CB | 2.89 | 0.42 |
| 3:C:2965[B]:LEU:CG | 3:C:2974[B]:ALA:CB | 2.85 | 0.42 |
| 3:C:3001[A]:LYS:H | 3:C:3003[A]:LYS:HG3 | 1.83 | 0.42 |
| 3:C:3025[A]:VAL:CG2 | 3:C:3047[A]:ARG:NH1 | 2.73 | 0.42 |
| 3:C:3148[B]:ILE:O | 3:C:3148[B]:ILE:HG22 | 2.17 | 0.42 |
| 3:C:3172[B]:SER:CA | 3:L:3149[B]:ASN:O | 2.66 | 0.42 |
| 3:C:3183[A]:LEU:N | 3:C:3184[A]:ASN:CA | 2.80 | 0.42 |
| 3:C:3196[B]:THR:OG1 | 3:C:3199[B]:GLN:OE1 | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3299[B]:LEU:HB3 | 3:C:3300[B]:LEU:H | 1.54 | 0.42 |
| 1:D:398:ARG:HA | 1:D:399:PRO:HD3 | 1.90 | 0.42 |
| 2:E:2814:LYS:HD3 | 2:E:2814:LYS:HA | 1.83 | 0.42 |
| 2:E:2879:LEU:HG | 2:E:2901:LEU:HD11 | 2.02 | 0.42 |
| 3:F:2937[B]:ASN:CG | 3:F:3006[B]:LYS:HD3 | 2.44 | 0.42 |
| 3:F:3001[A]:LYS:H | 3:F:3003[A]:LYS:HG3 | 1.83 | 0.42 |
| 3:F:3211[B]:ASP:OD1 | 3:F:3211[B]:ASP:N | 2.28 | 0.42 |
| 3:F:3218[A]:LEU:HD12 | 3:F:3218[A]:LEU:HA | 1.78 | 0.42 |
| 3:F:3255[B]:PRO:CA | 3:a:2965[B]:LEU:C | 2.92 | 0.42 |
| 1:G:107:HIS:CE1 | 1:G:109:LEU:HB2 | 2.54 | 0.42 |
| 1:G:572:SER:HA | 1:G:573:LYS:HA | 1.54 | 0.42 |
| 1:G:1137:LYS:HA | 1:G:1141:ARG:NH1 | 2.35 | 0.42 |
| 2:H:2317:LEU:HB3 | 2:H:2318:PRO:HD2 | 2.00 | 0.42 |
| 2:H:2402:GLY:HA3 | 2:H:2403:PHE:CD1 | 2.54 | 0.42 |
| 2:H:2651:GLN:HE21 | 2:H:2652:LYS:HD3 | 1.84 | 0.42 |
| 3:I:2952[A]:ALA:N | 3:I:2953[A]:GLY:CA | 2.71 | 0.42 |
| 3:I:3153[B]:LYS:CB | 3:R:3158[B]:PHE:CB | 2.76 | 0.42 |
| 3:I:3174[B]:GLY:N | 3:R:3154[B]:PRO:CD | 2.78 | 0.42 |
| 3:I:3183[A]:LEU:N | 3:I:3184[A]:ASN:CA | 2.80 | 0.42 |
| 3:I:3276[A]:ASP:C | 3:I:3278[A]:HIS:N | 2.75 | 0.42 |
| 1:J:95:THR:HB | 1:J:156:LEU:HD13 | 2.01 | 0.42 |
| 1:J:403:TYR:O | 1:J:658:TYR:HB3 | 2.20 | 0.42 |
| 1:J:904:HIS:O | 1:J:907:ARG:HB3 | 2.19 | 0.42 |
| 1:J:1206:HIS:CE1 | 1:J:1209:ASP:HB2 | 2.54 | 0.42 |
| 2:K:2156:ARG:HD2 | 2:K:2357:VAL:HG12 | 2.01 | 0.42 |
| 3:L:2937[A]:ASN:CG | 3:L:3006[A]:LYS:HD3 | 2.43 | 0.42 |
| 3:L:2969[A]:TYR:CD2 | 3:L:2971[A]:ASP:CG | 2.98 | 0.42 |
| 1:M:133:LYS:HB3 | 1:M:134:VAL:H | 1.48 | 0.42 |
| 1:M:518:LYS:O | 1:M:520:PHE:HD1 | 2.01 | 0.42 |
| 1:M:982:LYS:N | 1:M:983:PRO:HD3 | 2.34 | 0.42 |
| 1:M:1195:ASP:OD1 | 1:M:1197:THR:OG1 | 2.24 | 0.42 |
| 1:M:1210:LYS:CA | 1:M:1211:TYR:HB2 | 2.46 | 0.42 |
| 1:M:1486:LEU:HD12 | 2:Q:2486:ILE:HG22 | 2.02 | 0.42 |
| 3:O:2969[A]:TYR:CD2 | 3:O:2971[A]:ASP:CG | 2.97 | 0.42 |
| 3:O:2979[B]:GLN:HA | 3:O:2979[B]:GLN:OE1 | 2.20 | 0.42 |
| 3:O:2989[A]:HIS:O | 3:O:2990[A]:ARG:C | 2.61 | 0.42 |
| 3:O:3135[A]:LYS:HB2 | 3:O:3141[A]:TYR:CD1 | 2.51 | 0.42 |
| 1:P:897:HIS:HD2 | 1:P:899:MET:HE1 | 1.84 | 0.42 |
| 1:P:1039:ASP:OD1 | 1:P:1041:ILE:HG12 | 2.18 | 0.42 |
| 2:Q:2637:VAL:HG11 | 1:S:111:ILE:HG23 | 2.02 | 0.42 |
| 3:R:2969[A]:TYR:CD2 | 3:R:2971[A]:ASP:CG | 2.98 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:R:3245[B]:PHE:CD1 | 3:R:3245[B]:PHE:C | 2.97 | 0.42 |
| 2:T:2179:ASP:HB3 | 2:T:2303:ARG:HH12 | 1.85 | 0.42 |
| 3:U:2974[B]:ALA:HB2 | 3:d:3220[B]:ARG:HD2 | 2.01 | 0.42 |
| 3:U:3133[A]:LEU:HD12 | 3:U:3133[A]:LEU:HA | 1.86 | 0.42 |
| 3:U:3185[A]:TYR:CE2 | 3:U:3187[A]:TYR:HE2 | 2.31 | 0.42 |
| 3:U:3232[A]:VAL:HG21 | 3:U:3273[A]:LEU:CD1 | 2.50 | 0.42 |
| 1:V:426:LYS:HE3 | 1:V:435:GLU:OE2 | 2.19 | 0.42 |
| 1:V:464:LEU:HD22 | 1:V:622:HIS:HB3 | 2.02 | 0.42 |
| 1:V:760:ILE:HG21 | 1:V:777:TYR:CE2 | 2.52 | 0.42 |
| 1:V:1034:GLU:HB2 | 1:V:1180:SER:OG | 2.20 | 0.42 |
| 1:V:1528:ASP:OD1 | 1:V:1528:ASP:N | 2.53 | 0.42 |
| 2:W:2641:GLN:HA | 2:W:2642:PRO:HD3 | 1.85 | 0.42 |
| 3:X:2979[A]:GLN:HA | 3:X:2979[A]:GLN:OE1 | 2.19 | 0.42 |
| 3:X:3180[A]:TYR:CB | 3:X:3183[A]:LEU:CD2 | 2.90 | 0.42 |
| 3:X:3299[A]:LEU:O | 3:X:3300[A]:LEU:C | 2.60 | 0.42 |
| 1:Y:142:ARG:O | 1:Y:145:GLN:HG2 | 2.18 | 0.42 |
| 1:Y:170:HIS:O | 1:Y:174:GLN:HG3 | 2.19 | 0.42 |
| 1:Y:282:ASN:OD1 | 1:Y:282:ASN:N | 2.52 | 0.42 |
| 2:Z:2797:LYS:HA | 2:Z:2800:LYS:HD3 | 2.02 | 0.42 |
| 3:a:2979[B]:GLN:CD | 3:a:3155[B]:MET:CE | 2.92 | 0.42 |
| 3:a:2989[B]:HIS:C | 3:a:2991[B]:LEU:N | 2.75 | 0.42 |
| 3:a:3013[A]:ASP:CG | 3:a:3015[A]:THR:HG1 | 2.23 | 0.42 |
| 1:b:15:ILE:HG23 | 1:b:104:LEU:HD21 | 2.01 | 0.42 |
| 1:b:365:THR:O | 1:b:369:LEU:HG | 2.19 | 0.42 |
| 1:b:899:MET:HB3 | 1:b:1012:GLU:OE1 | 2.19 | 0.42 |
| 1:b:1125:SER:O | 1:b:1129:LEU:HB2 | 2.19 | 0.42 |
| 1:b:1315:GLY:HA3 | 1:b:1601:TRP:CG | 2.55 | 0.42 |
| 2:c:2856:ILE:HG22 | 2:c:2859:VAL:HB | 2.01 | 0.42 |
| 3:d:2948[A]:ASP:HB3 | 3:d:2949[A]:LYS:C | 2.43 | 0.42 |
| 3:d:2989[A]:HIS:O | 3:d:2990[A]:ARG:C | 2.61 | 0.42 |
| 3:d:3023[B]:ILE:HA | 3:d:3026[B]:THR:HG1 | 1.84 | 0.42 |
| 3:d:3023[B]:ILE:C | 3:d:3026[B]:THR:HG1 | 2.27 | 0.42 |
| 3:d:3104[B]:MET:SD | 3:d:3110[B]:THR:CG2 | 3.06 | 0.42 |
| 3:d:3245[A]:PHE:CD1 | 3:d:3245[A]:PHE:C | 2.97 | 0.42 |
| 4:q:1:NAG:C4 | 4:q:2:NAG:N2 | 2.80 | 0.42 |
| 1:A:882:TRP:CD1 | 1:A:1086:LEU:HD13 | 2.54 | 0.42 |
| 1:A:977:GLU:OE1 | 1:A:978:ALA:N | 2.49 | 0.42 |
| 2:B:2128:LEU:O | 2:B:2130:PRO:HD3 | 2.20 | 0.42 |
| 2:B:2854:MET:HE3 | 2:B:2854:MET:HB2 | 1.80 | 0.42 |
| 3:C:2969[B]:TYR:CD2 | 3:C:2971[B]:ASP:CG | 2.98 | 0.42 |
| 3:C:2969[B]:TYR:HH | 3:L:3120[B]:HIS:CD2 | 2.26 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3133[B]:LEU:HD13 | 3:C:3197[B]:ILE:HG23 | 2.02 | 0.42 |
| 3:C:3156[B]:MET:C | 3:L:3153[B]:LYS:NZ | 2.72 | 0.42 |
| 1:D:109:LEU:HG | 1:D:119:LYS:HB3 | 2.01 | 0.42 |
| 1:D:177:VAL:HG11 | 1:D:358:TYR:CZ | 2.55 | 0.42 |
| 1:D:851:MET:HE1 | 1:D:940:ALA:HB3 | 2.01 | 0.42 |
| 1:D:956:PRO:HB2 | 1:D:957:ASN:C | 2.44 | 0.42 |
| 1:D:1575:PRO:HA | 1:D:1581:GLU:O | 2.20 | 0.42 |
| 2:E:2092:VAL:HG23 | 2:E:2177:TYR:O | 2.20 | 0.42 |
| 2:E:2128:LEU:O | 2:E:2130:PRO:HD3 | 2.19 | 0.42 |
| 3:F:2977[B]:CYS:HB3 | 3:a:2982[B]:MET:HE3 | 1.97 | 0.42 |
| 3:F:2979[A]:GLN:HA | 3:F:2979[A]:GLN:OE1 | 2.19 | 0.42 |
| 3:F:3024[B]:LEU:CD1 | 3:F:3024[B]:LEU:C | 2.85 | 0.42 |
| 3:F:3028[A]:PRO:HG2 | 3:F:3029[A]:LYS:HG3 | 2.00 | 0.42 |
| 3:F:3048[A]:ASP:HB3 | 3:F:3099[A]:PRO:HD2 | 2.01 | 0.42 |
| 3:F:3222[A]:ILE:CD1 | 3:F:3223[A]:GLY:N | 2.73 | 0.42 |
| 3:F:3245[B]:PHE:CD1 | 3:F:3245[B]:PHE:C | 2.97 | 0.42 |
| 3:F:3299[A]:LEU:HB3 | 3:F:3300[A]:LEU:H | 1.54 | 0.42 |
| 1:G:516:TRP:CD1 | 1:G:579:LEU:HD13 | 2.54 | 0.42 |
| 1:G:603:HIS:O | 1:G:606:ILE:HG22 | 2.19 | 0.42 |
| 1:G:673:PHE:HB3 | 1:G:677:LEU:HB2 | 2.01 | 0.42 |
| 1:G:858:MET:HG3 | 1:G:959:PHE:CZ | 2.54 | 0.42 |
| 1:G:1275:ARG:HH22 | 1:G:1357:ARG:HH11 | 1.65 | 0.42 |
| 1:G:1323:HIS:CD2 | 1:G:1458:HIS:CE1 | 3.07 | 0.42 |
| 2:H:2132:CYS:CB | 2:H:2143:CYS:HA | 2.47 | 0.42 |
| 2:H:2234:GLN:HG3 | 2:H:2235:PRO:HD2 | 2.02 | 0.42 |
| 2:H:2573:TYR:HE2 | 2:H:2707:PHE:CE2 | 2.37 | 0.42 |
| 3:I:2969[A]:TYR:CD2 | 3:I:2971[A]:ASP:CG | 2.97 | 0.42 |
| 3:I:2979[A]:GLN:CD | 3:I:3155[A]:MET:CE | 2.92 | 0.42 |
| 3:I:3141[A]:TYR:CD2 | 3:I:3141[A]:TYR:C | 2.86 | 0.42 |
| 3:I:3300[A]:LEU:HD23 | 3:I:3300[A]:LEU:H | 1.83 | 0.42 |
| 1:J:704:ASP:OD1 | 1:J:704:ASP:N | 2.51 | 0.42 |
| 1:J:714:ARG:HH11 | 1:J:837:HIS:CE1 | 2.37 | 0.42 |
| 1:J:740:THR:HG21 | 4:u:1:NAG:O6 | 2.20 | 0.42 |
| 1:J:907:ARG:HD3 | 1:J:1050:ASP:OD1 | 2.19 | 0.42 |
| 1:J:1156:LEU:HB2 | 1:J:1176:TYR:CE1 | 2.55 | 0.42 |
| 1:J:1196:ILE:O | 1:J:1199:VAL:HG13 | 2.20 | 0.42 |
| 2:K:2504:ARG:HD2 | 2:K:2775:GLY:O | 2.20 | 0.42 |
| 2:K:2545:SER:O | 2:K:2558:CYS:N | 2.48 | 0.42 |
| 3:L:3133[B]:LEU:HD12 | 3:L:3133[B]:LEU:HA | 1.85 | 0.42 |
| 3:L:3151[A]:LEU:CB | 3:L:3175[A]:TYR:CE2 | 2.86 | 0.42 |
| 3:L:3245[A]:PHE:CD1 | 3:L:3245[A]:PHE:C | 2.97 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:447:MET:HE2 | 1:M:447:MET:HB3 | 1.86 | 0.42 |
| 1:M:535:PRO:O | 1:M:538:LYS:HE3 | 2.19 | 0.42 |
| 1:M:1308:VAL:HG11 | 8:0:2:NAG:O6 | 2.19 | 0.42 |
| 1:M:1473:ARG:HG3 | 1:M:1479:TYR:CG | 2.54 | 0.42 |
| 2:N:2178:TRP:CZ3 | 2:N:2188:PRO:HD3 | 2.55 | 0.42 |
| 2:N:2870:LEU:HA | 2:N:2877:ILE:HD11 | 2.00 | 0.42 |
| 3:O:2937[A]:ASN:CG | 3:O:3006[A]:LYS:HD3 | 2.43 | 0.42 |
| 3:O:2937[B]:ASN:CG | 3:O:3006[B]:LYS:HD3 | 2.43 | 0.42 |
| 3:O:2938[B]:LEU:O | 3:O:2939[B]:ARG:C | 2.58 | 0.42 |
| 3:O:2946[B]:GLN:CD | 3:O:2947[B]:ALA:N | 2.72 | 0.42 |
| 3:O:2951[A]:ASP:CG | 3:O:2952[A]:ALA:N | 2.74 | 0.42 |
| 3:O:2961[A]:HIS:HB2 | 3:O:2992[A]:TYR:HE2 | 1.80 | 0.42 |
| 3:O:3048[B]:ASP:HB3 | 3:O:3099[B]:PRO:HD2 | 2.01 | 0.42 |
| 3:O:3154[B]:PRO:HD2 | 3:X:3176[B]:LYS:HE2 | 1.86 | 0.42 |
| 3:O:3232[B]:VAL:HG21 | 3:O:3273[B]:LEU:CD1 | 2.50 | 0.42 |
| 1:P:77:GLU:O | 1:P:81:VAL:HG23 | 2.19 | 0.42 |
| 1:P:450:LYS:HZ1 | 1:P:1273:SER:CB | 2.29 | 0.42 |
| 1:P:1319:PHE:CE2 | 1:P:1424:GLU:HG3 | 2.55 | 0.42 |
| 2:Q:2562:GLY:H | 2:Q:2846:TRP:HB2 | 1.85 | 0.42 |
| 2:Q:2783:PHE:HB2 | 2:Q:2791:LEU:HD11 | 2.02 | 0.42 |
| 2:Q:2808:PHE:CE2 | 2:Q:2899:PRO:HG3 | 2.54 | 0.42 |
| 2:Q:2889:ALA:H | 2:Q:2890:VAL:HA | 1.82 | 0.42 |
| 3:R:2938[A]:LEU:O | 3:R:2939[A]:ARG:C | 2.58 | 0.42 |
| 3:R:2989[B]:HIS:O | 3:R:2990[B]:ARG:C | 2.61 | 0.42 |
| 3:R:3083[A]:ILE:HD11 | 3:R:3260[A]:ARG:CG | 2.49 | 0.42 |
| 3:R:3093[B]:HIS:HB2 | 3:R:3248[B]:LEU:CD1 | 2.48 | 0.42 |
| 3:R:3217[A]:PHE:CD2 | 3:R:3300[A]:LEU:HD12 | 2.53 | 0.42 |
| 1:S:401:VAL:HG23 | 1:S:661:ASN:HB3 | 2.00 | 0.42 |
| 1:S:633:HIS:O | 1:S:636:GLN:HB3 | 2.19 | 0.42 |
| 1:S:980:TYR:CZ | 1:S:1021:LEU:HD22 | 2.54 | 0.42 |
| 2:T:2606:LEU:HD22 | 2:T:2706:ILE:HG12 | 2.02 | 0.42 |
| 2:T:2731:PRO:HB3 | 2:T:2734:LYS:HG3 | 1.99 | 0.42 |
| 2:T:2819:VAL:HG13 | 2:T:2883:ILE:HG12 | 2.02 | 0.42 |
| 3:U:3082[B]:GLU:OE2 | 3:d:2970[B]:PRO:CB | 2.67 | 0.42 |
| 3:U:3245[B]:PHE:CD1 | 3:U:3245[B]:PHE:C | 2.97 | 0.42 |
| 1:V:904:HIS:HE1 | 1:V:1106:PHE:CZ | 2.37 | 0.42 |
| 1:V:975:PRO:HG2 | 1:V:1024:GLY:H | 1.84 | 0.42 |
| 2:W:2252:GLU:CD | 2:W:2393:ARG:HH12 | 2.26 | 0.42 |
| 2:W:2670:CYS:N | 2:W:2737:CYS:SG | 2.93 | 0.42 |
| 2:W:2830:GLN:HG2 | 2:W:2863:ARG:CZ | 2.50 | 0.42 |
| 3:X:2995[A]:GLN:CG | 3:X:3168[A]:THR:HG21 | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3034[B]:HIS:HB3 | 3:X:3035[B]:HIS:CE1 | 2.50 | 0.42 |
| 3:X:3041[B]:ALA:O | 3:X:3042[B]:ASP:HB2 | 2.20 | 0.42 |
| 3:X:3083[B]:ILE:HD11 | 3:X:3260[B]:ARG:CG | 2.49 | 0.42 |
| 3:X:3133[A]:LEU:HD13 | 3:X:3197[A]:ILE:HG23 | 2.02 | 0.42 |
| 3:X:3293[A]:LYS:CB | 3:X:3294[A]:SER:CA | 2.96 | 0.42 |
| 1:Y:48:LYS:HE3 | 1:Y:54:THR:HG22 | 2.02 | 0.42 |
| 1:Y:1263:LEU:HD11 | 1:Y:1358:LEU:HD22 | 2.01 | 0.42 |
| 2:Z:2431:GLY:O | 2:Z:2434:GLU:HG2 | 2.19 | 0.42 |
| 2:Z:2647:LEU:HD12 | 2:Z:2647:LEU:HA | 1.75 | 0.42 |
| 2:Z:2874:ASP:HA | 2:Z:2875:SER:C | 2.45 | 0.42 |
| 3:a:2969[B]:TYR:CD2 | 3:a:2971[B]:ASP:CG | 2.97 | 0.42 |
| 3:a:3023[B]:ILE:HA | 3:a:3026[B]:THR:HG1 | 1.82 | 0.42 |
| 1:b:19:GLN:HG3 | 1:b:122:VAL:HG22 | 2.02 | 0.42 |
| 1:b:1137:LYS:HA | 1:b:1141:ARG:NH1 | 2.34 | 0.42 |
| 2:c:2400:LEU:HB2 | 2:c:2439:PHE:HD2 | 1.84 | 0.42 |
| 3:d:2969[B]:TYR:CD2 | 3:d:2971[B]:ASP:CG | 2.98 | 0.42 |
| 3:d:2976[A]:ALA:O | 3:d:2978[A]:CYS:N | 2.46 | 0.42 |
| 3:d:2979[A]:GLN:HA | 3:d:2979[A]:GLN:OE1 | 2.19 | 0.42 |
| 3:d:2979[A]:GLN:CD | 3:d:3155[A]:MET:CE | 2.92 | 0.42 |
| 3:d:2995[A]:GLN:O | 3:d:2996[A]:MET:C | 2.63 | 0.42 |
| 3:d:3093[B]:HIS:HD2 | 3:d:3248[B]:LEU:CD2 | 2.31 | 0.42 |
| 3:d:3218[B]:LEU:HD13 | 3:d:3261[B]:LEU:HD23 | 2.01 | 0.42 |
| 3:d:3232[A]:VAL:HG21 | 3:d:3273[A]:LEU:CD1 | 2.50 | 0.42 |
| 3:d:3232[B]:VAL:HG21 | 3:d:3273[B]:LEU:CD1 | 2.50 | 0.42 |
| 1:A:561:ARG:NH2 | 1:A:629:MET:HB2 | 2.35 | 0.42 |
| 1:A:899:MET:HE2 | 1:A:1186:TRP:CE2 | 2.55 | 0.42 |
| 1:A:979:LEU:CD2 | 1:A:1021:LEU:HD22 | 2.50 | 0.42 |
| 1:A:1140:ASN:OD1 | 1:A:1239:GLY:N | 2.52 | 0.42 |
| 2:B:2581:MET:HE2 | 2:B:2581:MET:HB3 | 1.78 | 0.42 |
| 3:C:2937[A]:ASN:CG | 3:C:3006[A]:LYS:HD3 | 2.44 | 0.42 |
| 3:C:2965[B]:LEU:HB2 | 3:L:3221[B]:ALA:HA | 0.84 | 0.42 |
| 3:C:2966[B]:SER:HB2 | 3:C:2977[B]:CYS:H | 1.85 | 0.42 |
| 3:C:2969[B]:TYR:CD2 | 3:C:2971[B]:ASP:N | 2.73 | 0.42 |
| 3:C:3148[A]:ILE:HG22 | 3:C:3152[A]:LYS:HE3 | 2.01 | 0.42 |
| 3:C:3152[B]:LYS:CG | 3:L:3172[B]:SER:OG | 2.66 | 0.42 |
| 3:C:3172[B]:SER:OG | 3:L:3152[B]:LYS:HB2 | 2.11 | 0.42 |
| 3:C:3196[A]:THR:OG1 | 3:C:3199[A]:GLN:OE1 | 2.38 | 0.42 |
| 1:D:1438:ASP:OD1 | 1:D:1439:VAL:N | 2.52 | 0.42 |
| 2:E:2403:PHE:N | 2:E:2403:PHE:CD1 | 2.85 | 0.42 |
| 2:E:2544:GLY:HA3 | 2:E:2699:MET:O | 2.18 | 0.42 |
| 2:E:2550:THR:N | 2:E:2554:PRO:HD3 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:2568:HIS:HE1 | 2:E:2742:MET:SD | 2.43 | 0.42 |
| 3:F:2975[B]:PHE:HE1 | 3:a:3107[B]:LEU:HG | 1.81 | 0.42 |
| 3:F:2982[B]:MET:HE2 | 3:a:2966[B]:SER:CA | 2.49 | 0.42 |
| 3:F:3028[A]:PRO:HG2 | 3:F:3029[A]:LYS:HG2 | 2.02 | 0.42 |
| 3:F:3146[A]:CYS:O | 3:F:3146[A]:CYS:SG | 2.78 | 0.42 |
| 3:F:3151[B]:LEU:O | 3:a:3154[B]:PRO:CB | 2.67 | 0.42 |
| 3:F:3191[A]:ASN:ND2 | 3:F:3191[A]:ASN:N | 2.60 | 0.42 |
| 1:G:127:GLU:HG2 | 1:G:135:THR:HG23 | 2.02 | 0.42 |
| 1:G:304:ALA:HB1 | 1:G:306:PHE:CE1 | 2.51 | 0.42 |
| 2:H:2746:MET:HG3 | 2:H:2765:PRO:HD3 | 2.02 | 0.42 |
| 2:H:2808:PHE:HB3 | 2:H:2810:LEU:HD21 | 2.01 | 0.42 |
| 2:H:2888:GLY:HA2 | 2:H:2889:ALA:HA | 1.86 | 0.42 |
| 3:I:2969[B]:TYR:CD2 | 3:I:2971[B]:ASP:CG | 2.98 | 0.42 |
| 3:I:2983[B]:VAL:CG2 | 3:R:3162[B]:ASP:N | 2.65 | 0.42 |
| 3:I:2985[B]:PHE:CE2 | 3:R:2969[B]:TYR:O | 2.73 | 0.42 |
| 3:I:3090[B]:ASN:HB3 | 3:R:2971[B]:ASP:O | 2.20 | 0.42 |
| 3:I:3146[A]:CYS:O | 3:I:3146[A]:CYS:SG | 2.78 | 0.42 |
| 3:I:3196[B]:THR:OG1 | 3:I:3199[B]:GLN:OE1 | 2.37 | 0.42 |
| 3:I:3218[B]:LEU:HD12 | 3:I:3218[B]:LEU:HA | 1.78 | 0.42 |
| 1:J:468:CYS:HB2 | 1:J:477:VAL:O | 2.20 | 0.42 |
| 1:J:1034:GLU:CB | 1:J:1182:ASN:HD21 | 2.33 | 0.42 |
| 2:K:2667:GLU:HB3 | 2:K:2730:LEU:CD2 | 2.50 | 0.42 |
| 2:K:2805:PHE:HB2 | 2:K:2902:ILE:CG1 | 2.50 | 0.42 |
| 3:L:2979[A]:GLN:HA | 3:L:2979[A]:GLN:OE1 | 2.19 | 0.42 |
| 3:L:3171[A]:HIS:O | 3:L:3172[A]:SER:C | 2.63 | 0.42 |
| 1:M:17:ASN:O | 1:M:21:SER:OG | 2.35 | 0.42 |
| 1:M:282:ASN:OD1 | 1:M:282:ASN:N | 2.51 | 0.42 |
| 1:M:843:VAL:HG22 | 1:M:928:TYR:O | 2.20 | 0.42 |
| 1:M:1146:PHE:HZ | 1:M:1159:TYR:CG | 2.38 | 0.42 |
| 1:M:1427:HIS:HE1 | 1:M:1458:HIS:CD2 | 2.38 | 0.42 |
| 2:N:2168:ARG:CZ | 2:Q:2515:ARG:HD2 | 2.49 | 0.42 |
| 2:N:2664:PHE:HB3 | 2:N:2795:ILE:HD11 | 2.01 | 0.42 |
| 3:O:2970[B]:PRO:HD2 | 3:X:2991[B]:LEU:HD22 | 2.01 | 0.42 |
| 3:O:3023[B]:ILE:O | 3:O:3026[B]:THR:OG1 | 2.34 | 0.42 |
| 3:O:3024[B]:LEU:CD1 | 3:O:3024[B]:LEU:C | 2.85 | 0.42 |
| 3:O:3251[B]:ASP:HB2 | 3:X:2968[B]:GLN:CG | 2.49 | 0.42 |
| 2:Q:2562:GLY:H | 2:Q:2846:TRP:CB | 2.33 | 0.42 |
| 2:Q:2780:HIS:ND1 | 2:Q:2782:ASN:OD1 | 2.53 | 0.42 |
| 3:R:2937[A]:ASN:CG | 3:R:3006[A]:LYS:HD3 | 2.44 | 0.42 |
| 1:S:630:PHE:O | 1:S:633:HIS:HB3 | 2.19 | 0.42 |
| 1:S:647:LEU:HD13 | 1:S:651:ARG:NH2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:2181:THR:HB | 2:T:2373:MET:SD | 2.60 | 0.42 |
| 2:T:2884:LYS:HG2 | 2:T:2891:LEU:HB3 | 2.01 | 0.42 |
| 3:U:2979[B]:GLN:CD | 3:U:3155[B]:MET:CE | 2.92 | 0.42 |
| 3:U:3025[B]:VAL:CG2 | 3:U:3047[B]:ARG:NH1 | 2.73 | 0.42 |
| 3:U:3048[A]:ASP:HB3 | 3:U:3099[A]:PRO:HD2 | 2.01 | 0.42 |
| 3:U:3133[A]:LEU:HD13 | 3:U:3197[A]:ILE:HG23 | 2.02 | 0.42 |
| 3:U:3171[A]:HIS:O | 3:U:3172[A]:SER:C | 2.63 | 0.42 |
| 3:U:3183[B]:LEU:N | 3:U:3184[B]:ASN:CA | 2.80 | 0.42 |
| 3:U:3220[B]:ARG:CB | 3:d:2973[B]:THR:CG2 | 2.80 | 0.42 |
| 1:V:386:ILE:HD13 | 1:V:386:ILE:O | 2.20 | 0.42 |
| 1:V:387:ASN:OD1 | 1:V:387:ASN:N | 2.41 | 0.42 |
| 1:V:563:ILE:HG13 | 1:V:614:GLU:HG2 | 2.02 | 0.42 |
| 1:V:630:PHE:CE2 | 1:V:634:HIS:CE1 | 3.08 | 0.42 |
| 1:V:938:LEU:H | 1:V:938:LEU:HD12 | 1.85 | 0.42 |
| 1:V:1323:HIS:CD2 | 9:V:5004:CUO:O1 | 2.72 | 0.42 |
| 2:W:2275:GLY:HA2 | 2:W:2281:SER:HB2 | 2.01 | 0.42 |
| 2:W:2279:LEU:HD12 | 2:W:2284:HIS:HD2 | 1.84 | 0.42 |
| 3:X:2937[B]:ASN:CG | 3:X:3006[B]:LYS:HD3 | 2.43 | 0.42 |
| 1:Y:51:ASP:HA | 1:Y:52:GLY:HA3 | 1.70 | 0.42 |
| 1:Y:177:VAL:O | 1:Y:181:PRO:HD3 | 2.20 | 0.42 |
| 1:Y:668:MET:HA | 1:Y:668:MET:HE2 | 2.02 | 0.42 |
| 1:Y:880:THR:O | 1:Y:882:TRP:N | 2.51 | 0.42 |
| 1:Y:915:ASN:O | 1:Y:919:ARG:N | 2.31 | 0.42 |
| 1:Y:1327:VAL:O | 1:Y:1331:GLU:HB3 | 2.20 | 0.42 |
| 2:Z:2643:GLU:HA | 2:Z:2646:ALA:HB3 | 2.00 | 0.42 |
| 2:Z:2678:VAL:HG11 | 2:Z:2852:TYR:CE2 | 2.55 | 0.42 |
| 3:a:2952[B]:ALA:CA | 3:a:2956[B]:LYS:CB | 2.89 | 0.42 |
| 3:a:2971[B]:ASP:CG | 3:a:2973[B]:THR:HG1 | 2.10 | 0.42 |
| 3:a:3028[A]:PRO:HG2 | 3:a:3029[A]:LYS:HG2 | 2.02 | 0.42 |
| 3:a:3135[A]:LYS:HB2 | 3:a:3141[A]:TYR:CD1 | 2.52 | 0.42 |
| 1:b:543:ASN:HA | 1:b:544:PRO:HD3 | 1.81 | 0.42 |
| 2:c:2489:ILE:HA | 2:c:2490:PRO:HD3 | 1.87 | 0.42 |
| 3:d:2937[B]:ASN:CG | 3:d:3006[B]:LYS:HD3 | 2.43 | 0.42 |
| 3:d:3041[B]:ALA:O | 3:d:3042[B]:ASP:HB2 | 2.20 | 0.42 |
| 3:d:3133[B]:LEU:HD13 | 3:d:3197[B]:ILE:HG23 | 2.02 | 0.42 |
| 3:d:3293[B]:LYS:CB | 3:d:3294[B]:SER:CA | 2.96 | 0.42 |
| 1:A:1077:LEU:HB3 | 1:A:1103:PHE:CE1 | 2.55 | 0.42 |
| 1:A:1542:ARG:O | 1:A:1546:LYS:HG2 | 2.19 | 0.42 |
| 2:B:2718:TRP:HZ3 | 2:B:2721:TRP:CE3 | 2.37 | 0.42 |
| 3:C:2963[B]:MET:C | 3:L:3255[B]:PRO:HG3 | 2.45 | 0.42 |
| 3:C:2989[B]:HIS:NE2 | 3:L:2969[B]:TYR:CA | 2.81 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3155[B]:MET:O | 3:L:3150[B]:LYS:O | 2.37 | 0.42 |
| 3:C:3232[B]:VAL:HG21 | 3:C:3273[B]:LEU:CD1 | 2.50 | 0.42 |
| 1:D:21:SER:HB2 | 1:D:83:HIS:O | 2.19 | 0.42 |
| 1:D:276:PHE:HB2 | 1:D:279:LEU:HD23 | 2.02 | 0.42 |
| 1:D:682:LYS:O | 1:D:685:GLU:HB3 | 2.19 | 0.42 |
| 2:E:2116:SER:HA | 2:E:2121:THR:HG21 | 2.02 | 0.42 |
| 2:E:2333:LEU:HB3 | 2:E:2336:PHE:HD2 | 1.84 | 0.42 |
| 3:F:2932[A]:PRO:CA | 3:F:2935[A]:ILE:CD1 | 2.85 | 0.42 |
| 3:F:2969[A]:TYR:CD2 | 3:F:2971[A]:ASP:CG | 2.97 | 0.42 |
| 3:F:2969[B]:TYR:CD2 | 3:F:2971[B]:ASP:CG | 2.98 | 0.42 |
| 3:F:3034[A]:HIS:HB3 | 3:F:3035[A]:HIS:CE1 | 2.50 | 0.42 |
| 3:F:3196[A]:THR:OG1 | 3:F:3199[A]:GLN:OE1 | 2.38 | 0.42 |
| 3:F:3252[B]:TYR:O | 3:a:2976[B]:ALA:CB | 2.68 | 0.42 |
| 3:F:3252[B]:TYR:CD2 | 3:a:3108[B]:HIS:CE1 | 3.08 | 0.42 |
| 1:G:428:ILE:HG13 | 1:G:513:TYR:O | 2.20 | 0.42 |
| 1:G:483:GLY:HA2 | 1:G:773:PHE:CZ | 2.54 | 0.42 |
| 1:G:1028:VAL:HA | 1:G:1035:TYR:HD2 | 1.85 | 0.42 |
| 1:G:1245:GLU:HG2 | 2:K:2729:LYS:O | 2.20 | 0.42 |
| 1:G:1638:SER:OG | 1:G:1639:LYS:N | 2.53 | 0.42 |
| 2:H:2129:PRO:O | 2:H:2131:LEU:HD23 | 2.20 | 0.42 |
| 2:H:2667:GLU:HG2 | 2:H:2728:ARG:NH2 | 2.34 | 0.42 |
| 3:I:2933[A]:SER:CA | 3:I:2936[A]:GLU:HB3 | 2.48 | 0.42 |
| 3:I:2979[B]:GLN:HA | 3:I:2979[B]:GLN:OE1 | 2.20 | 0.42 |
| 3:I:2981[B]:GLY:C | 3:R:2966[B]:SER:O | 2.62 | 0.42 |
| 3:I:2982[B]:MET:HE1 | 3:R:3157[B]:PRO:HD3 | 2.00 | 0.42 |
| 3:I:2988[A]:TRP:CZ3 | 3:I:2989[A]:HIS:CE1 | 3.07 | 0.42 |
| 3:I:3023[A]:ILE:HA | 3:I:3026[A]:THR:HG1 | 1.83 | 0.42 |
| 3:I:3048[B]:ASP:HB3 | 3:I:3099[B]:PRO:HD2 | 2.01 | 0.42 |
| 3:I:3083[A]:ILE:HD11 | 3:I:3260[A]:ARG:CG | 2.49 | 0.42 |
| 3:I:3146[B]:CYS:O | 3:I:3146[B]:CYS:SG | 2.78 | 0.42 |
| 3:I:3245[B]:PHE:CD1 | 3:I:3245[B]:PHE:C | 2.97 | 0.42 |
| 1:J:499:GLU:HG3 | 1:J:511:VAL:H | 1.85 | 0.42 |
| 1:J:872:GLN:O | 1:J:875:ALA:HB3 | 2.19 | 0.42 |
| 1:J:1019:HIS:ND1 | 1:J:1030:MET:HE2 | 2.34 | 0.42 |
| 2:K:2758:THR:O | 2:K:2762:VAL:HG22 | 2.20 | 0.42 |
| 3:L:2939[A]:ARG:CB | 3:L:3032[A]:PRO:HG2 | 2.44 | 0.42 |
| 3:L:2948[A]:ASP:HB3 | 3:L:2949[A]:LYS:C | 2.43 | 0.42 |
| 3:L:3083[B]:ILE:HD11 | 3:L:3260[B]:ARG:CG | 2.49 | 0.42 |
| 3:L:3133[B]:LEU:HD13 | 3:L:3197[B]:ILE:HG23 | 2.02 | 0.42 |
| 3:L:3232[B]:VAL:HG21 | 3:L:3273[B]:LEU:CD1 | 2.50 | 0.42 |
| 1:M:187:GLY:HA2 | 1:M:193:SER:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:492:ARG:HG3 | 1:M:638:ASP:OD1 | 2.18 | 0.42 |
| 1:M:639:ARG:NH2 | 1:M:707:PHE:O | 2.53 | 0.42 |
| 1:M:870:TYR:HA | 1:M:873:VAL:HG12 | 2.02 | 0.42 |
| 1:M:1171:LYS:HG2 | 1:M:1173:GLY:H | 1.85 | 0.42 |
| 1:M:1243:PHE:O | 1:M:1476:LYS:HD3 | 2.19 | 0.42 |
| 3:O:2969[B]:TYR:CD2 | 3:O:2971[B]:ASP:CG | 2.98 | 0.42 |
| 3:O:2979[B]:GLN:CD | 3:O:3155[B]:MET:CE | 2.92 | 0.42 |
| 3:O:3001[B]:LYS:H | 3:O:3003[B]:LYS:HG3 | 1.83 | 0.42 |
| 3:O:3048[A]:ASP:HB3 | 3:O:3099[A]:PRO:HD2 | 2.01 | 0.42 |
| 3:O:3108[B]:HIS:CG | 3:X:2969[B]:TYR:O | 2.70 | 0.42 |
| 3:O:3133[B]:LEU:HD13 | 3:O:3197[B]:ILE:HG23 | 2.02 | 0.42 |
| 3:O:3157[B]:PRO:O | 3:X:3148[B]:ILE:C | 2.61 | 0.42 |
| 3:O:3159[B]:SER:CB | 3:X:3151[B]:LEU:HB2 | 2.42 | 0.42 |
| 3:O:3196[A]:THR:OG1 | 3:O:3199[A]:GLN:OE1 | 2.38 | 0.42 |
| 3:O:3228[A]:VAL:CG2 | 3:O:3245[A]:PHE:CD2 | 3.02 | 0.42 |
| 3:O:3229[A]:ASN:N | 3:O:3286[A]:THR:O | 2.52 | 0.42 |
| 3:O:3232[A]:VAL:HG21 | 3:O:3273[A]:LEU:CD1 | 2.49 | 0.42 |
| 3:O:3299[A]:LEU:O | 3:O:3300[A]:LEU:C | 2.60 | 0.42 |
| 1:P:131:GLU:OE2 | 1:P:192:HIS:HE1 | 2.02 | 0.42 |
| 1:P:929:TRP:CE3 | 1:P:939:PRO:HD3 | 2.54 | 0.42 |
| 1:P:1035:TYR:O | 1:P:1038:PHE:HD1 | 2.02 | 0.42 |
| 1:P:1086:LEU:HD13 | 1:P:1090:ILE:HD11 | 2.01 | 0.42 |
| 2:Q:2680:HIS:CE1 | 2:Q:2711:HIS:CE1 | 3.08 | 0.42 |
| 3:R:2946[B]:GLN:CD | 3:R:2947[B]:ALA:N | 2.72 | 0.42 |
| 3:R:2965[A]:LEU:CG | 3:R:2974[A]:ALA:CB | 2.85 | 0.42 |
| 3:R:2966[A]:SER:HB2 | 3:R:2977[A]:CYS:H | 1.85 | 0.42 |
| 3:R:3001[A]:LYS:H | 3:R:3003[A]:LYS:HG3 | 1.83 | 0.42 |
| 3:R:3014[B]:TRP:CH2 | 3:R:3123[B]:THR:HG23 | 2.53 | 0.42 |
| 3:R:3028[A]:PRO:HG2 | 3:R:3029[A]:LYS:HG2 | 2.02 | 0.42 |
| 3:R:3180[A]:TYR:CB | 3:R:3183[A]:LEU:CD2 | 2.90 | 0.42 |
| 3:R:3185[A]:TYR:HE2 | 3:R:3187[A]:TYR:CD2 | 2.36 | 0.42 |
| 1:S:446:PHE:CZ | 1:S:455:TYR:HA | 2.55 | 0.42 |
| 1:S:904:HIS:HB2 | 1:S:1081:MET:HE1 | 2.02 | 0.42 |
| 2:T:2234:GLN:HG3 | 2:T:2235:PRO:HD2 | 2.00 | 0.42 |
| 2:T:2442:LEU:HG | 1:V:1604:ASP:HB2 | 2.01 | 0.42 |
| 3:U:2946[B]:GLN:CD | 3:U:2947[B]:ALA:N | 2.72 | 0.42 |
| 3:U:2973[B]:THR:OG1 | 3:d:3249[B]:GLY:HA3 | 2.19 | 0.42 |
| 3:U:2979[A]:GLN:HA | 3:U:2979[A]:GLN:OE1 | 2.19 | 0.42 |
| 3:U:3156[B]:MET:HG2 | 3:d:3150[B]:LYS:HD3 | 1.48 | 0.42 |
| 3:U:3299[B]:LEU:O | 3:U:3300[B]:LEU:C | 2.60 | 0.42 |
| 1:V:452:ILE:HA | 1:V:1368:ARG:HD3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:995:ILE:O | 1:V:999:LEU:HD22 | 2.20 | 0.42 |
| 1:V:1392:ASP:H | 1:V:1435:GLY:HA2 | 1.85 | 0.42 |
| 2:W:2533:ASP:HB2 | 2:W:2755:PRO:HG3 | 2.01 | 0.42 |
| 2:W:2625:LEU:HD23 | 2:W:2625:LEU:H | 1.85 | 0.42 |
| 3:X:2966[B]:SER:HB2 | 3:X:2977[B]:CYS:H | 1.85 | 0.42 |
| 3:X:2979[B]:GLN:OE1 | 3:X:2979[B]:GLN:HA | 2.19 | 0.42 |
| 3:X:2989[B]:HIS:C | 3:X:2991[B]:LEU:N | 2.75 | 0.42 |
| 3:X:3146[B]:CYS:SG | 3:X:3146[B]:CYS:O | 2.78 | 0.42 |
| 3:X:3232[A]:VAL:HG21 | 3:X:3273[A]:LEU:CD1 | 2.50 | 0.42 |
| 3:X:3245[B]:PHE:CD1 | 3:X:3245[B]:PHE:C | 2.97 | 0.42 |
| 1:Y:217:PHE:O | 1:Y:220:TRP:HB3 | 2.19 | 0.42 |
| 1:Y:486:THR:HA | 1:Y:489:HIS:HD1 | 1.84 | 0.42 |
| 1:Y:1172:ALA:CB | 1:Y:1196:ILE:HG13 | 2.50 | 0.42 |
| 2:Z:2177:TYR:HB2 | 2:Z:2300:ASN:HB2 | 2.01 | 0.42 |
| 3:a:2979[A]:GLN:CD | 3:a:3155[A]:MET:CE | 2.92 | 0.42 |
| 3:a:2988[A]:TRP:CZ3 | 3:a:2989[A]:HIS:CE1 | 3.07 | 0.42 |
| 3:a:3148[A]:ILE:HG22 | 3:a:3152[A]:LYS:HE3 | 2.01 | 0.42 |
| 3:a:3276[A]:ASP:C | 3:a:3278[A]:HIS:N | 2.75 | 0.42 |
| 1:b:435:GLU:HB3 | 1:b:509:ILE:HD11 | 2.01 | 0.42 |
| 1:b:579:LEU:HD12 | 1:b:579:LEU:H | 1.84 | 0.42 |
| 1:b:639:ARG:HB2 | 1:b:703:TYR:CE2 | 2.55 | 0.42 |
| 1:b:949:ASP:H | 1:b:953:GLU:H | 1.68 | 0.42 |
| 1:b:977:GLU:HB3 | 1:b:979:LEU:CD2 | 2.49 | 0.42 |
| 1:b:979:LEU:HD23 | 1:b:980:TYR:CD2 | 2.55 | 0.42 |
| 1:b:989:THR:HG22 | 1:b:991:LEU:H | 1.84 | 0.42 |
| 1:b:1550:ARG:HD3 | 1:b:1550:ARG:HA | 1.72 | 0.42 |
| 2:c:2244:PHE:CZ | 2:c:2376:MET:HE1 | 2.55 | 0.42 |
| 2:c:2261:VAL:O | 2:c:2265:ILE:HG13 | 2.19 | 0.42 |
| 2:c:2791:LEU:HA | 2:c:2791:LEU:HD23 | 1.82 | 0.42 |
| 3:d:3041[A]:ALA:O | 3:d:3042[A]:ASP:HB2 | 2.20 | 0.42 |
| 3:d:3120[B]:HIS:HA | 3:d:3123[B]:THR:HG1 | 1.82 | 0.42 |
| 3:d:3146[A]:CYS:O | 3:d:3146[A]:CYS:SG | 2.78 | 0.42 |
| 3:d:3196[A]:THR:OG1 | 3:d:3199[A]:GLN:OE1 | 2.37 | 0.42 |
| 3:d:3232[B]:VAL:HG21 | 3:d:3273[B]:LEU:HD11 | 2.00 | 0.42 |
| 1:A:1023:GLY:HA2 | 1:A:1029:SER:HB3 | 2.00 | 0.42 |
| 1:A:1030:MET:HE2 | 1:A:1030:MET:HB3 | 1.98 | 0.42 |
| 1:A:1067:TYR:CD1 | 1:A:1067:TYR:N | 2.87 | 0.42 |
| 2:B:2089:ARG:HD2 | 2:B:2175:VAL:O | 2.20 | 0.42 |
| 2:B:2726:LYS:HB2 | 2:B:2726:LYS:HE3 | 1.84 | 0.42 |
| 2:B:2830:GLN:HB2 | 2:B:2863:ARG:NH2 | 2.33 | 0.42 |
| 3:C:2966[A]:SER:HB2 | 3:C:2977[A]:CYS:H | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:2988[B]:TRP:CZ3 | 3:C:2989[B]:HIS:CE1 | 3.07 | 0.42 |
| 3:C:3048[A]:ASP:HB3 | 3:C:3099[A]:PRO:HD2 | 2.01 | 0.42 |
| 3:C:3113[A]:ASP:OD2 | 3:C:3115[A]:LEU:HB2 | 2.20 | 0.42 |
| 3:C:3152[B]:LYS:CB | 3:L:3172[B]:SER:OG | 2.67 | 0.42 |
| 3:C:3218[B]:LEU:HD13 | 3:C:3261[B]:LEU:HD23 | 2.01 | 0.42 |
| 3:C:3252[B]:TYR:HB2 | 3:L:3253[B]:GLU:CB | 2.43 | 0.42 |
| 1:D:187:GLY:HA3 | 1:D:195:SER:HB3 | 2.02 | 0.42 |
| 1:D:205:LEU:HD23 | 1:D:205:LEU:HA | 1.88 | 0.42 |
| 1:D:597:VAL:O | 1:D:601:VAL:HG12 | 2.19 | 0.42 |
| 1:D:639:ARG:HB2 | 1:D:703:TYR:CE2 | 2.55 | 0.42 |
| 1:D:1319:PHE:CZ | 1:D:1424:GLU:HG3 | 2.55 | 0.42 |
| 1:D:1636:ASN:OD1 | 4:m:1:NAG:C7 | 2.67 | 0.42 |
| 2:E:2447:ILE:O | 2:E:2450:ILE:HG22 | 2.20 | 0.42 |
| 3:F:3154[B]:PRO:HD2 | 3:a:3155[B]:MET:HG3 | 1.85 | 0.42 |
| 3:F:3182[A]:GLN:H | 3:F:3182[A]:GLN:HG2 | 1.56 | 0.42 |
| 3:F:3293[B]:LYS:CG | 3:F:3294[B]:SER:CB | 2.98 | 0.42 |
| 1:G:105:VAL:CG1 | 1:G:123:PHE:HB3 | 2.48 | 0.42 |
| 1:G:127:GLU:OE2 | 1:G:134:VAL:HG13 | 2.19 | 0.42 |
| 1:G:212:ASN:O | 1:G:215:ARG:HB3 | 2.19 | 0.42 |
| 1:G:227:ARG:HA | 1:G:228:GLY:HA2 | 1.85 | 0.42 |
| 1:G:838:ARG:NH1 | 1:G:915:ASN:OD1 | 2.50 | 0.42 |
| 2:H:2302:ASP:OD2 | 2:H:2366:TYR:OH | 2.30 | 0.42 |
| 2:H:2303:ARG:NH2 | 2:H:2372:GLU:O | 2.53 | 0.42 |
| 2:H:2656:LEU:HD23 | 2:H:2656:LEU:HA | 1.81 | 0.42 |
| 3:I:2937[B]:ASN:CB | 3:I:3006[B]:LYS:CE | 2.86 | 0.42 |
| 3:I:2956[A]:LYS:O | 3:I:2959[A]:SER:OG | 2.33 | 0.42 |
| 3:I:2961[B]:HIS:ND1 | 3:R:2969[B]:TYR:CD1 | 2.72 | 0.42 |
| 3:I:3041[A]:ALA:O | 3:I:3042[A]:ASP:HB2 | 2.20 | 0.42 |
| 3:I:3041[B]:ALA:O | 3:I:3042[B]:ASP:HB2 | 2.20 | 0.42 |
| 3:I:3149[B]:ASN:HD22 | 3:R:3163[B]:ASN:CA | 2.31 | 0.42 |
| 3:I:3171[B]:HIS:O | 3:I:3172[B]:SER:C | 2.63 | 0.42 |
| 3:I:3196[A]:THR:OG1 | 3:I:3199[A]:GLN:OE1 | 2.38 | 0.42 |
| 1:J:1166:THR:N | 1:J:1167:ASP:HA | 2.34 | 0.42 |
| 1:J:1286:ARG:HA | 1:J:1286:ARG:HD3 | 1.82 | 0.42 |
| 1:J:1427:HIS:HD1 | 1:J:1461:VAL:HG21 | 1.85 | 0.42 |
| 2:K:2849:ASP:HB3 | 2:K:2850:ARG:NH1 | 2.34 | 0.42 |
| 2:K:2888:GLY:HA2 | 2:K:2889:ALA:HA | 1.83 | 0.42 |
| 2:K:2898:LYS:H | 2:K:2898:LYS:HG3 | 1.47 | 0.42 |
| 3:L:3001[A]:LYS:H | 3:L:3003[A]:LYS:HG3 | 1.83 | 0.42 |
| 3:L:3001[B]:LYS:H | 3:L:3003[B]:LYS:HG3 | 1.83 | 0.42 |
| 3:L:3146[A]:CYS:O | 3:L:3146[A]:CYS:SG | 2.78 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3183[B]:LEU:N | 3:L:3184[B]:ASN:CA | 2.80 | 0.42 |
| 1:M:415:VAL:CB | 1:M:697:ALA:HB2 | 2.50 | 0.42 |
| 1:M:1392:ASP:H | 1:M:1435:GLY:HA2 | 1.84 | 0.42 |
| 2:N:2235:PRO:HG2 | 2:Q:2097:LEU:HD12 | 2.02 | 0.42 |
| 2:N:2764:THR:HA | 2:N:2765:PRO:HD3 | 1.95 | 0.42 |
| 3:O:2961[B]:HIS:HB2 | 3:O:2992[B]:TYR:HE2 | 1.81 | 0.42 |
| 3:O:3041[B]:ALA:O | 3:O:3042[B]:ASP:HB2 | 2.20 | 0.42 |
| 3:O:3096[A]:VAL:CG1 | 3:O:3115[A]:LEU:CD1 | 2.86 | 0.42 |
| 3:O:3148[A]:ILE:HG22 | 3:O:3152[A]:LYS:HE3 | 2.01 | 0.42 |
| 3:O:3154[B]:PRO:HG3 | 3:X:3175[B]:TYR:CG | 2.51 | 0.42 |
| 3:O:3232[A]:VAL:HG21 | 3:O:3273[A]:LEU:HD11 | 2.00 | 0.42 |
| 3:O:3232[B]:VAL:HG21 | 3:O:3273[B]:LEU:HD11 | 2.00 | 0.42 |
| 3:O:3285[A]:VAL:CG2 | 3:O:3286[A]:THR:H | 2.27 | 0.42 |
| 1:P:353:ASN:HD22 | 1:P:772:ARG:NH2 | 2.17 | 0.42 |
| 1:P:416:ASN:ND2 | 1:P:416:ASN:H | 2.17 | 0.42 |
| 1:P:990:HIS:O | 1:P:991:LEU:HB2 | 2.20 | 0.42 |
| 1:P:1562:ILE:HG22 | 1:P:1563:LYS:N | 2.35 | 0.42 |
| 2:Q:2128:LEU:HB2 | 2:Q:2286:HIS:HB3 | 2.02 | 0.42 |
| 2:Q:2353:LYS:HB2 | 2:Q:2356:ASP:OD2 | 2.19 | 0.42 |
| 2:Q:2545:SER:HA | 2:Q:2546:LEU:CB | 2.49 | 0.42 |
| 2:Q:2811:HIS:HB3 | 2:Q:2847:HIS:CD2 | 2.54 | 0.42 |
| 3:R:3041[B]:ALA:O | 3:R:3042[B]:ASP:HB2 | 2.20 | 0.42 |
| 3:R:3299[B]:LEU:O | 3:R:3300[B]:LEU:C | 2.60 | 0.42 |
| 1:S:639:ARG:O | 1:S:643:ILE:HG13 | 2.20 | 0.42 |
| 2:T:2089:ARG:HD3 | 2:T:2163:GLU:OE2 | 2.20 | 0.42 |
| 2:T:2521:MET:HE3 | 2:T:2605:LEU:HD12 | 2.02 | 0.42 |
| 2:T:2556:TYR:HE1 | 2:T:2845:PRO:HD2 | 1.84 | 0.42 |
| 3:U:2969[B]:TYR:CD2 | 3:U:2971[B]:ASP:CG | 2.97 | 0.42 |
| 3:U:2975[B]:PHE:HE1 | 3:d:3253[B]:GLU:OE1 | 2.03 | 0.42 |
| 3:U:3028[A]:PRO:HG2 | 3:U:3029[A]:LYS:HG3 | 2.00 | 0.42 |
| 3:U:3044[A]:LYS:H | 3:U:3044[A]:LYS:HG2 | 1.64 | 0.42 |
| 3:U:3182[B]:GLN:H | 3:U:3182[B]:GLN:HG2 | 1.56 | 0.42 |
| 1:V:400:ILE:HD13 | 1:V:484:MET:HE1 | 2.02 | 0.42 |
| 1:V:1059:LEU:HD22 | 1:V:1063:ARG:HH21 | 1.85 | 0.42 |
| 1:V:1203:MET:HB2 | 1:V:1205:LEU:HB2 | 2.00 | 0.42 |
| 1:V:1562:ILE:HG22 | 1:V:1563:LYS:N | 2.35 | 0.42 |
| 2:W:2092:VAL:HG13 | 2:W:2190:LEU:HD23 | 2.01 | 0.42 |
| 3:X:2938[B]:LEU:HD12 | 3:X:2938[B]:LEU:HA | 1.85 | 0.42 |
| 3:X:3013[A]:ASP:CG | 3:X:3015[A]:THR:HG1 | 2.26 | 0.42 |
| 3:X:3133[A]:LEU:HD12 | 3:X:3133[A]:LEU:HA | 1.86 | 0.42 |
| 3:X:3200[A]:LEU:O | 3:X:3203[A]:HIS:HB3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3273[B]:LEU:HB2 | 3:X:3275[B]:LEU:CD1 | 2.34 | 0.42 |
| 1:Y:486:THR:HA | 1:Y:489:HIS:ND1 | 2.35 | 0.42 |
| 1:Y:1345:TYR:HB2 | 1:Y:1460:ASN:HB2 | 2.02 | 0.42 |
| 1:Y:1578:ILE:HA | 1:Y:1579:GLY:HA2 | 1.53 | 0.42 |
| 3:a:3137[B]:ARG:HB3 | 3:a:3139[B]:LEU:HD21 | 1.97 | 0.42 |
| 3:a:3232[B]:VAL:HG21 | 3:a:3273[B]:LEU:CD1 | 2.50 | 0.42 |
| 1:b:638:ASP:OD2 | 1:b:703:TYR:OH | 2.37 | 0.42 |
| 1:b:879:SER:O | 1:b:879:SER:OG | 2.26 | 0.42 |
| 2:c:2274:LEU:HD23 | 2:c:2274:LEU:HA | 1.91 | 0.42 |
| 2:c:2823:ILE:CD1 | 2:c:2856:ILE:HG21 | 2.50 | 0.42 |
| 3:d:2989[A]:HIS:C | 3:d:2991[A]:LEU:N | 2.75 | 0.42 |
| 1:A:80:LEU:HD12 | 1:A:80:LEU:HA | 1.92 | 0.42 |
| 1:A:566:ARG:HA | 1:A:567:LEU:HB2 | 2.02 | 0.42 |
| 1:A:956:PRO:HD2 | 1:A:957:ASN:O | 2.20 | 0.42 |
| 1:A:1142:VAL:O | 1:A:1195:ASP:HB2 | 2.19 | 0.42 |
| 2:B:2086:ASN:H | 2:B:2086:ASN:HD22 | 1.67 | 0.42 |
| 2:B:2121:THR:O | 2:B:2124:SER:HB3 | 2.20 | 0.42 |
| 2:B:2779:ASP:HA | 2:B:2780:HIS:HA | 1.66 | 0.42 |
| 3:C:2933[B]:SER:CA | 3:C:2936[B]:GLU:HB3 | 2.48 | 0.42 |
| 3:C:3154[B]:PRO:C | 3:L:3155[B]:MET:HG2 | 2.41 | 0.42 |
| 3:C:3161[A]:GLU:CD | 3:C:3161[A]:GLU:H | 2.19 | 0.42 |
| 3:C:3171[B]:HIS:O | 3:C:3172[B]:SER:C | 2.63 | 0.42 |
| 3:C:3182[A]:GLN:H | 3:C:3182[A]:GLN:HG2 | 1.56 | 0.42 |
| 1:D:319:ILE:O | 1:D:338:ALA:N | 2.51 | 0.42 |
| 1:D:716:LEU:O | 1:D:720:VAL:HG13 | 2.20 | 0.42 |
| 2:E:2257:CYS:O | 2:E:2261:VAL:HG23 | 2.20 | 0.42 |
| 2:E:2551:PRO:HA | 2:E:2552:GLU:HA | 1.60 | 0.42 |
| 3:F:3151[B]:LEU:H | 3:a:3169[B]:LYS:HG2 | 1.84 | 0.42 |
| 3:F:3171[B]:HIS:O | 3:F:3172[B]:SER:C | 2.63 | 0.42 |
| 3:F:3229[B]:ASN:O | 3:F:3286[B]:THR:N | 2.50 | 0.42 |
| 3:F:3251[B]:ASP:CG | 3:a:3251[B]:ASP:HB2 | 2.41 | 0.42 |
| 3:F:3293[B]:LYS:CB | 3:F:3294[B]:SER:CA | 2.96 | 0.42 |
| 1:G:43:GLU:HG3 | 1:G:44:PRO:HA | 2.02 | 0.42 |
| 1:G:832:LYS:HE2 | 1:G:832:LYS:HB3 | 1.77 | 0.42 |
| 1:G:858:MET:HG3 | 1:G:959:PHE:CE1 | 2.55 | 0.42 |
| 1:G:1078:ARG:NH1 | 2:K:2872:GLU:O | 2.43 | 0.42 |
| 1:G:1091:ASN:HA | 1:G:1092:PRO:HD3 | 1.79 | 0.42 |
| 1:G:1438:ASP:OD1 | 1:G:1439:VAL:N | 2.53 | 0.42 |
| 3:I:2985[B]:PHE:HE2 | 3:R:2969[B]:TYR:C | 2.27 | 0.42 |
| 3:I:2988[B]:TRP:CZ3 | 3:I:2989[B]:HIS:CE1 | 3.07 | 0.42 |
| 3:I:3183[B]:LEU:N | 3:I:3184[B]:ASN:CA | 2.80 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:84:GLY:CA | 1:J:85:SER:HB3 | 2.50 | 0.42 |
| 1:J:187:GLY:HA2 | 1:J:193:SER:HB2 | 2.02 | 0.42 |
| 1:J:843:VAL:HG22 | 1:J:929:TRP:HB3 | 2.02 | 0.42 |
| 1:J:1145:THR:OG1 | 1:J:1233:SER:HB3 | 2.20 | 0.42 |
| 1:J:1166:THR:HB | 1:J:1167:ASP:C | 2.45 | 0.42 |
| 1:J:1325:LEU:HG | 1:J:1516:VAL:HG11 | 2.02 | 0.42 |
| 2:K:2502:LEU:HD12 | 2:K:2502:LEU:HA | 1.85 | 0.42 |
| 2:K:2568:HIS:CB | 2:K:2746:MET:HE1 | 2.50 | 0.42 |
| 2:K:2805:PHE:HA | 2:K:2855:ASP:HA | 2.01 | 0.42 |
| 2:K:2808:PHE:HB3 | 2:K:2810:LEU:HD21 | 2.02 | 0.42 |
| 3:L:2969[B]:TYR:CD2 | 3:L:2971[B]:ASP:CG | 2.98 | 0.42 |
| 3:L:2988[B]:TRP:CZ3 | 3:L:2989[B]:HIS:CE1 | 3.07 | 0.42 |
| 3:L:2995[B]:GLN:CG | 3:L:3168[B]:THR:HG21 | 2.48 | 0.42 |
| 3:L:3028[B]:PRO:HG2 | 3:L:3029[B]:LYS:HG2 | 2.02 | 0.42 |
| 3:L:3041[B]:ALA:O | 3:L:3042[B]:ASP:HB2 | 2.20 | 0.42 |
| 3:L:3048[A]:ASP:HB3 | 3:L:3099[A]:PRO:HD2 | 2.01 | 0.42 |
| 3:L:3146[B]:CYS:O | 3:L:3146[B]:CYS:SG | 2.78 | 0.42 |
| 1:M:855:ARG:HD2 | 1:M:947:TYR:CG | 2.55 | 0.42 |
| 2:N:2565:THR:HG21 | 2:N:2741:GLN:HB3 | 2.02 | 0.42 |
| 3:O:2967[B]:CYS:CB | 3:X:3155[B]:MET:SD | 3.08 | 0.42 |
| 3:O:3096[B]:VAL:CG1 | 3:O:3115[B]:LEU:CD1 | 2.86 | 0.42 |
| 3:O:3113[B]:ASP:OD2 | 3:O:3115[B]:LEU:HB2 | 2.20 | 0.42 |
| 3:O:3133[A]:LEU:HD13 | 3:O:3197[A]:ILE:HG23 | 2.02 | 0.42 |
| 3:O:3185[B]:TYR:HE2 | 3:O:3187[B]:TYR:CD2 | 2.35 | 0.42 |
| 3:O:3293[B]:LYS:CB | 3:O:3294[B]:SER:CA | 2.96 | 0.42 |
| 1:P:62:MET:HE3 | 1:P:62:MET:HB3 | 1.71 | 0.42 |
| 1:P:73:LEU:HD11 | 1:P:210:HIS:O | 2.19 | 0.42 |
| 1:P:610:THR:HB | 1:P:629:MET:HE1 | 2.02 | 0.42 |
| 1:P:1400:ASN:OD1 | 1:P:1402:TYR:N | 2.52 | 0.42 |
| 2:Q:2244:PHE:HE2 | 2:Q:2374:ASN:HD22 | 1.66 | 0.42 |
| 2:Q:2251:LEU:HA | 2:Q:2308:TRP:HD1 | 1.85 | 0.42 |
| 3:R:3133[A]:LEU:HD13 | 3:R:3197[A]:ILE:HG23 | 2.02 | 0.42 |
| 3:R:3146[B]:CYS:O | 3:R:3146[B]:CYS:SG | 2.78 | 0.42 |
| 3:R:3200[A]:LEU:O | 3:R:3203[A]:HIS:HB3 | 2.20 | 0.42 |
| 1:S:116:LYS:O | 1:S:117:LYS:HD2 | 2.20 | 0.42 |
| 1:S:1347:ASP:HA | 1:S:1460:ASN:ND2 | 2.34 | 0.42 |
| 3:U:2975[B]:PHE:CZ | 3:d:3256[B]:TRP:CD1 | 3.06 | 0.42 |
| 3:U:3001[A]:LYS:N | 3:U:3003[A]:LYS:HG3 | 2.34 | 0.42 |
| 3:U:3169[B]:LYS:HE2 | 3:d:3146[B]:CYS:HB2 | 1.99 | 0.42 |
| 3:U:3196[A]:THR:N | 3:U:3199[A]:GLN:CB | 2.64 | 0.42 |
| 1:V:1248:ARG:HD2 | 1:V:1249:TRP:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:1567:ASP:OD1 | 1:V:1591:SER:OG | 2.33 | 0.42 |
| 2:W:2302:ASP:HB3 | 2:W:2368:TYR:OH | 2.20 | 0.42 |
| 2:W:2377:SER:HB3 | 2:W:2380:GLN:HG3 | 2.02 | 0.42 |
| 2:W:2500:ILE:HD11 | 2:W:2776:TYR:HA | 2.00 | 0.42 |
| 3:X:3001[A]:LYS:N | 3:X:3003[A]:LYS:HG3 | 2.34 | 0.42 |
| 3:X:3048[B]:ASP:HB3 | 3:X:3099[B]:PRO:HD2 | 2.01 | 0.42 |
| 3:X:3083[A]:ILE:HD11 | 3:X:3260[A]:ARG:CG | 2.49 | 0.42 |
| 3:X:3113[A]:ASP:OD2 | 3:X:3115[A]:LEU:HB2 | 2.20 | 0.42 |
| 3:X:3113[B]:ASP:OD2 | 3:X:3115[B]:LEU:HB2 | 2.20 | 0.42 |
| 3:X:3146[A]:CYS:O | 3:X:3146[A]:CYS:SG | 2.78 | 0.42 |
| 3:X:3148[A]:ILE:HD12 | 3:X:3175[A]:TYR:OH | 2.20 | 0.42 |
| 3:X:3200[B]:LEU:O | 3:X:3203[B]:HIS:HB3 | 2.20 | 0.42 |
| 3:X:3242[A]:GLY:C | 3:X:3243[A]:GLY:O | 2.58 | 0.42 |
| 3:X:3245[A]:PHE:CD1 | 3:X:3245[A]:PHE:C | 2.97 | 0.42 |
| 1:Y:73:LEU:HD11 | 1:Y:210:HIS:O | 2.20 | 0.42 |
| 1:Y:98:MET:HB3 | 1:Y:144:TYR:HD1 | 1.85 | 0.42 |
| 1:Y:718:ARG:HH21 | 1:Y:830:ASN:CG | 2.28 | 0.42 |
| 1:Y:956:PRO:C | 1:Y:958:PRO:HD2 | 2.45 | 0.42 |
| 2:Z:2142:ALA:N | 2:Z:2433:THR:O | 2.36 | 0.42 |
| 3:a:3113[B]:ASP:OD2 | 3:a:3115[B]:LEU:HB2 | 2.20 | 0.42 |
| 1:b:567:LEU:HB3 | 1:b:571:PRO:HD2 | 2.02 | 0.42 |
| 1:b:899:MET:HG3 | 1:b:1188:PHE:CZ | 2.55 | 0.42 |
| 2:c:2390:GLN:O | 2:c:2491:PRO:HB3 | 2.19 | 0.42 |
| 2:c:2628:HIS:CE1 | 2:c:2630:LYS:HA | 2.55 | 0.42 |
| 3:d:2966[A]:SER:HB2 | 3:d:2977[A]:CYS:H | 1.85 | 0.42 |
| 3:d:3222[A]:ILE:CD1 | 3:d:3223[A]:GLY:N | 2.73 | 0.42 |
| 3:d:3245[B]:PHE:C | 3:d:3245[B]:PHE:CD1 | 2.97 | 0.42 |
| 3:d:3301[B]:PRO:HB2 | 3:d:3302[B]:SER:H | 1.33 | 0.42 |
| 1:A:1279:LYS:HE3 | 1:A:1376:PRO:HG3 | 2.02 | 0.42 |
| 2:B:2326:ILE:HD11 | 1:D:1650:ILE:HG12 | 2.01 | 0.42 |
| 2:B:2606:LEU:HB3 | 2:B:2706:ILE:HD11 | 2.02 | 0.42 |
| 3:C:2969[A]:TYR:CD2 | 3:C:2971[A]:ASP:CG | 2.98 | 0.42 |
| 3:C:2995[B]:GLN:CG | 3:C:3168[B]:THR:HG21 | 2.48 | 0.42 |
| 3:C:3041[A]:ALA:O | 3:C:3042[A]:ASP:HB2 | 2.20 | 0.42 |
| 3:C:3161[B]:GLU:HA | 3:L:3147[B]:GLU:HG2 | 0.76 | 0.42 |
| 3:C:3196[A]:THR:HG21 | 1:D:416:ASN:HB2 | 2.01 | 0.42 |
| 3:C:3299[A]:LEU:O | 3:C:3300[A]:LEU:C | 2.60 | 0.42 |
| 1:D:128:ILE:HG22 | 1:D:134:VAL:HA | 2.01 | 0.42 |
| 1:D:593:CYS:O | 1:D:597:VAL:HG23 | 2.20 | 0.42 |
| 2:E:2830:GLN:HB2 | 2:E:2863:ARG:NH2 | 2.35 | 0.42 |
| 3:F:2979[B]:GLN:CD | 3:F:3155[B]:MET:CE | 2.92 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3133[B]:LEU:HD13 | 3:F:3197[B]:ILE:HG23 | 2.02 | 0.42 |
| 3:F:3255[B]:PRO:HG2 | 3:a:2959[B]:SER:HA | 2.01 | 0.42 |
| 1:G:904:HIS:O | 1:G:907:ARG:HB3 | 2.20 | 0.42 |
| 1:G:907:ARG:HD3 | 1:G:1050:ASP:OD1 | 2.20 | 0.42 |
| 1:G:907:ARG:NH1 | 1:G:1114:TYR:OH | 2.50 | 0.42 |
| 1:G:1231:VAL:O | 1:G:1233:SER:N | 2.53 | 0.42 |
| 1:G:1304:ASP:N | 1:G:1305:GLY:HA2 | 2.35 | 0.42 |
| 1:G:1328:SER:HB2 | 1:G:1523:LEU:HD13 | 2.01 | 0.42 |
| 3:I:2982[B]:MET:CB | 3:R:3156[B]:MET:HB3 | 2.50 | 0.42 |
| 3:I:3028[A]:PRO:HG2 | 3:I:3029[A]:LYS:HG2 | 2.02 | 0.42 |
| 3:I:3048[A]:ASP:HB3 | 3:I:3099[A]:PRO:HD2 | 2.01 | 0.42 |
| 3:I:3137[B]:ARG:HD3 | 3:I:3137[B]:ARG:HA | 1.72 | 0.42 |
| 3:I:3149[B]:ASN:HB2 | 3:R:3163[B]:ASN:HD21 | 0.46 | 0.42 |
| 3:I:3155[B]:MET:CG | 3:R:3154[B]:PRO:CD | 2.96 | 0.42 |
| 3:I:3200[B]:LEU:O | 3:I:3203[B]:HIS:HB3 | 2.20 | 0.42 |
| 3:I:3272[A]:HIS:CD2 | 1:J:1543:ILE:HD11 | 2.55 | 0.42 |
| 1:J:601:VAL:HG11 | 1:J:777:TYR:CG | 2.55 | 0.42 |
| 1:J:730:PHE:CD2 | 1:J:780:GLU:HB3 | 2.54 | 0.42 |
| 1:J:1150:GLY:HA2 | 1:J:1186:TRP:CE2 | 2.55 | 0.42 |
| 3:L:3148[B]:ILE:HD12 | 3:L:3175[B]:TYR:OH | 2.20 | 0.42 |
| 3:L:3180[B]:TYR:CA | 3:L:3183[B]:LEU:CD2 | 2.95 | 0.42 |
| 3:L:3196[A]:THR:OG1 | 3:L:3199[A]:GLN:OE1 | 2.37 | 0.42 |
| 3:L:3200[B]:LEU:O | 3:L:3203[B]:HIS:HB3 | 2.20 | 0.42 |
| 3:L:3294[B]:SER:O | 3:L:3294[B]:SER:OG | 2.34 | 0.42 |
| 1:M:1140:ASN:OD1 | 1:M:1239:GLY:N | 2.43 | 0.42 |
| 1:M:1369:THR:HB | 1:M:1371:GLN:HG2 | 2.00 | 0.42 |
| 1:M:1406:HIS:O | 1:M:1410:VAL:HG23 | 2.20 | 0.42 |
| 1:M:1639:LYS:HG2 | 1:M:1640:ILE:C | 2.45 | 0.42 |
| 2:N:2207:ASN:HA | 2:N:2208:PRO:HD2 | 1.92 | 0.42 |
| 3:O:2966[A]:SER:HB2 | 3:O:2977[A]:CYS:H | 1.85 | 0.42 |
| 3:O:2979[A]:GLN:OE1 | 3:O:2979[A]:GLN:HA | 2.19 | 0.42 |
| 3:O:2989[A]:HIS:NE2 | 9:O:3401[A]:CUO:O1 | 2.53 | 0.42 |
| 3:O:3146[A]:CYS:O | 3:O:3146[A]:CYS:SG | 2.78 | 0.42 |
| 3:O:3200[A]:LEU:O | 3:O:3203[A]:HIS:HB3 | 2.20 | 0.42 |
| 3:O:3218[A]:LEU:HD13 | 3:O:3261[A]:LEU:HD23 | 2.01 | 0.42 |
| 3:O:3222[B]:ILE:H | 3:X:3161[B]:GLU:HG2 | 1.85 | 0.42 |
| 3:O:3229[B]:ASN:N | 3:O:3286[B]:THR:O | 2.52 | 0.42 |
| 1:P:307:ARG:NH1 | 1:P:400:ILE:HD11 | 2.35 | 0.42 |
| 1:P:718:ARG:HD2 | 1:P:718:ARG:HA | 1.89 | 0.42 |
| 1:P:1077:LEU:HD12 | 1:P:1077:LEU:HA | 1.92 | 0.42 |
| 1:P:1178:LEU:HD12 | 1:P:1178:LEU:HA | 1.90 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:1346:TRP:CE3 | 1:P:1356:PRO:HG3 | 2.54 | 0.42 |
| 2:Q:2622:ASN:HA | 2:Q:2623:PRO:HD3 | 1.94 | 0.42 |
| 3:R:2969[B]:TYR:CD2 | 3:R:2971[B]:ASP:CG | 2.98 | 0.42 |
| 3:R:3171[B]:HIS:O | 3:R:3172[B]:SER:C | 2.63 | 0.42 |
| 3:R:3222[A]:ILE:CD1 | 3:R:3223[A]:GLY:N | 2.73 | 0.42 |
| 1:S:523:LEU:HA | 1:S:524:PRO:HD3 | 1.94 | 0.42 |
| 1:S:1007:PHE:CE1 | 1:S:1011:TYR:HB2 | 2.54 | 0.42 |
| 1:S:1275:ARG:HH12 | 1:S:1357:ARG:NH1 | 2.06 | 0.42 |
| 2:T:2201:THR:C | 2:T:2203:ILE:H | 2.24 | 0.42 |
| 3:U:2973[B]:THR:CG2 | 3:d:3222[B]:ILE:HG22 | 2.32 | 0.42 |
| 3:U:2979[B]:GLN:HA | 3:U:2979[B]:GLN:OE1 | 2.20 | 0.42 |
| 3:U:3028[B]:PRO:HG2 | 3:U:3029[B]:LYS:HG2 | 2.02 | 0.42 |
| 3:U:3149[A]:ASN:OD1 | 3:U:3149[A]:ASN:N | 2.51 | 0.42 |
| 3:U:3200[B]:LEU:O | 3:U:3203[B]:HIS:HB3 | 2.20 | 0.42 |
| 1:V:173:VAL:HG23 | 1:V:174:GLN:HG2 | 2.01 | 0.42 |
| 1:V:1406:HIS:HB3 | 1:V:1426:LEU:HD13 | 2.01 | 0.42 |
| 3:X:3025[B]:VAL:CG2 | 3:X:3047[B]:ARG:NH1 | 2.73 | 0.42 |
| 3:X:3133[B]:LEU:HD13 | 3:X:3197[B]:ILE:HG23 | 2.02 | 0.42 |
| 3:X:3151[A]:LEU:CB | 3:X:3175[A]:TYR:CE2 | 2.86 | 0.42 |
| 1:Y:494:VAL:CG2 | 1:Y:671:PHE:HZ | 2.33 | 0.42 |
| 1:Y:866:GLU:HG3 | 1:Y:867:VAL:N | 2.35 | 0.42 |
| 1:Y:891:LYS:HB2 | 1:Y:892:TYR:HA | 2.02 | 0.42 |
| 1:Y:1171:LYS:NZ | 1:Y:1174:GLU:OE2 | 2.50 | 0.42 |
| 1:Y:1228:LEU:HD22 | 1:Y:1228:LEU:O | 2.20 | 0.42 |
| 1:Y:1415:ASP:OD1 | 1:Y:1416:PHE:N | 2.53 | 0.42 |
| 1:Y:1650:ILE:HB | 2:c:2326:ILE:HG23 | 2.02 | 0.42 |
| 2:Z:2092:VAL:HG23 | 2:Z:2177:TYR:O | 2.20 | 0.42 |
| 2:Z:2145:LEU:HD22 | 2:Z:2154:TRP:CD1 | 2.55 | 0.42 |
| 2:Z:2876:LYS:NZ | 2:Z:2876:LYS:HB3 | 2.34 | 0.42 |
| 3:a:3013[B]:ASP:CA | 3:a:3122[B]:ASN:ND2 | 2.74 | 0.42 |
| 3:a:3028[B]:PRO:HG2 | 3:a:3029[B]:LYS:HG2 | 2.02 | 0.42 |
| 3:a:3133[A]:LEU:HD13 | 3:a:3197[A]:ILE:HG23 | 2.02 | 0.42 |
| 3:a:3133[B]:LEU:HD13 | 3:a:3197[B]:ILE:HG23 | 2.02 | 0.42 |
| 3:a:3218[A]:LEU:HD13 | 3:a:3261[A]:LEU:HD23 | 2.01 | 0.42 |
| 1:b:109:LEU:HD12 | 1:b:119:LYS:HB3 | 2.02 | 0.42 |
| 1:b:564:ASP:HA | 1:b:609:TRP:O | 2.19 | 0.42 |
| 1:b:897:HIS:C | 1:b:899:MET:HA | 2.45 | 0.42 |
| 1:b:1500:THR:HA | 1:b:1501:ALA:HA | 1.80 | 0.42 |
| 2:c:2327:GLU:H | 2:c:2327:GLU:HG3 | 1.50 | 0.42 |
| 2:c:2569:TRP:CZ2 | 2:c:2748:PRO:HG3 | 2.55 | 0.42 |
| 3:d:2937[A]:ASN:CB | 3:d:3006[A]:LYS:CE | 2.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2966[B]:SER:HB2 | 3:d:2977[B]:CYS:H | 1.85 | 0.42 |
| 3:d:3001[B]:LYS:N | 3:d:3003[B]:LYS:HG3 | 2.34 | 0.42 |
| 3:d:3148[B]:ILE:HD12 | 3:d:3175[B]:TYR:OH | 2.20 | 0.42 |
| 3:d:3276[A]:ASP:C | 3:d:3278[A]:HIS:N | 2.75 | 0.42 |
| 3:d:3293[B]:LYS:CD | 3:d:3293[B]:LYS:C | 2.86 | 0.42 |
| 1:A:480:CYS:SG | 1:A:621:LEU:HD11 | 2.59 | 0.41 |
| 1:A:816:PRO:HA | 1:A:817:PRO:HD3 | 1.95 | 0.41 |
| 2:B:2600:ASP:OD1 | 2:B:2601:ASN:N | 2.53 | 0.41 |
| 3:C:2959[B]:SER:O | 3:L:3255[B]:PRO:CD | 2.68 | 0.41 |
| 3:C:2995[A]:GLN:CG | 3:C:3168[A]:THR:HG21 | 2.48 | 0.41 |
| 3:C:3027[A]:GLU:CD | 3:C:3027[A]:GLU:C | 2.85 | 0.41 |
| 3:C:3067[B]:ARG:HA | 3:C:3067[B]:ARG:HD3 | 1.87 | 0.41 |
| 3:C:3158[B]:PHE:CG | 3:L:3153[B]:LYS:HE2 | 2.29 | 0.41 |
| 3:C:3182[B]:GLN:H | 3:C:3182[B]:GLN:HG2 | 1.56 | 0.41 |
| 3:C:3185[B]:TYR:CE2 | 3:C:3187[B]:TYR:HE2 | 2.31 | 0.41 |
| 3:C:3193[B]:HIS:ND1 | 3:C:3193[B]:HIS:N | 2.68 | 0.41 |
| 1:D:517:THR:HG21 | 1:D:708:PHE:HE1 | 1.85 | 0.41 |
| 1:D:671:PHE:O | 1:D:684:ARG:HG3 | 2.20 | 0.41 |
| 1:D:1156:LEU:HD13 | 1:D:1176:TYR:CE1 | 2.55 | 0.41 |
| 1:D:1211:TYR:OH | 1:D:1234:VAL:HB | 2.20 | 0.41 |
| 1:D:1564:ALA:HB1 | 4:m:1:NAG:C8 | 2.50 | 0.41 |
| 2:E:2180:TRP:CD1 | 2:E:2243:LEU:HD22 | 2.55 | 0.41 |
| 2:E:2400:LEU:HB2 | 2:E:2439:PHE:HD2 | 1.84 | 0.41 |
| 2:E:2644:LEU:HD13 | 2:E:2686:LEU:HB3 | 2.01 | 0.41 |
| 2:E:2667:GLU:HB3 | 2:E:2730:LEU:HD13 | 2.02 | 0.41 |
| 3:F:2965[B]:LEU:C | 3:a:3255[B]:PRO:C | 2.87 | 0.41 |
| 3:F:2975[B]:PHE:HZ | 3:a:2961[B]:HIS:CB | 2.33 | 0.41 |
| 3:F:3146[B]:CYS:HA | 3:F:3147[B]:GLU:HA | 1.70 | 0.41 |
| 1:G:1148:LEU:HD23 | 1:G:1229:LYS:HE2 | 2.01 | 0.41 |
| 3:I:2995[B]:GLN:CG | 3:I:3168[B]:THR:HG21 | 2.48 | 0.41 |
| 3:I:3185[B]:TYR:HE2 | 3:I:3187[B]:TYR:CD2 | 2.35 | 0.41 |
| 3:I:3232[B]:VAL:HG21 | 3:I:3273[B]:LEU:CD1 | 2.50 | 0.41 |
| 1:J:322:CYS:HA | 1:J:333:ASN:O | 2.20 | 0.41 |
| 1:J:464:LEU:HA | 1:J:464:LEU:HD12 | 1.85 | 0.41 |
| 1:J:566:ARG:HH22 | 1:J:803:LYS:NZ | 2.18 | 0.41 |
| 1:J:905:TRP:HB2 | 1:J:1081:MET:HE3 | 2.02 | 0.41 |
| 1:J:913:PHE:CD2 | 1:J:1043:MET:HG2 | 2.55 | 0.41 |
| 1:J:1148:LEU:HB2 | 1:J:1188:PHE:CD2 | 2.46 | 0.41 |
| 1:J:1494:ARG:HH11 | 1:J:1494:ARG:CG | 2.33 | 0.41 |
| 1:J:1562:ILE:HG13 | 1:J:1564:ALA:O | 2.20 | 0.41 |
| 2:K:2561:HIS:HB3 | 2:K:2677:GLU:OE2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2711:HIS:HA | 2:K:2714:VAL:HG22 | 2.01 | 0.41 |
| 3:L:2979[A]:GLN:CD | 3:L:3155[A]:MET:CE | 2.92 | 0.41 |
| 3:L:3200[A]:LEU:O | 3:L:3203[A]:HIS:HB3 | 2.20 | 0.41 |
| 3:L:3232[A]:VAL:HG21 | 3:L:3273[A]:LEU:CD1 | 2.50 | 0.41 |
| 1:M:84:GLY:HA2 | 1:M:85:SER:HB3 | 2.02 | 0.41 |
| 1:M:1484:CYS:O | 2:Q:2487:VAL:HG22 | 2.20 | 0.41 |
| 1:M:1485:ALA:O | 1:M:1489:MET:HG2 | 2.20 | 0.41 |
| 2:N:2778:TYR:HB2 | 2:N:2781:LEU:CD1 | 2.50 | 0.41 |
| 3:O:2988[A]:TRP:CZ3 | 3:O:2989[A]:HIS:CE1 | 3.07 | 0.41 |
| 3:O:3023[A]:ILE:HA | 3:O:3026[A]:THR:HG1 | 1.83 | 0.41 |
| 3:O:3149[A]:ASN:OD1 | 3:O:3149[A]:ASN:N | 2.51 | 0.41 |
| 3:O:3185[A]:TYR:CE2 | 3:O:3187[A]:TYR:HE2 | 2.31 | 0.41 |
| 1:P:40:TYR:HE2 | 1:P:75:GLN:HG2 | 1.85 | 0.41 |
| 1:P:71:LEU:HD13 | 1:P:266:LEU:HD21 | 2.01 | 0.41 |
| 1:P:107:HIS:HA | 1:P:108:PRO:HD3 | 1.89 | 0.41 |
| 1:P:468:CYS:HA | 1:P:469:PRO:C | 2.45 | 0.41 |
| 1:P:524:PRO:HD2 | 1:P:527:LEU:HD11 | 2.01 | 0.41 |
| 1:P:930:ASP:OD1 | 1:P:1051:ARG:NH2 | 2.53 | 0.41 |
| 2:Q:2261:VAL:HG21 | 2:Q:2441:ARG:HG3 | 2.01 | 0.41 |
| 2:Q:2398:PHE:HE1 | 2:Q:2466:THR:HG21 | 1.85 | 0.41 |
| 2:Q:2568:HIS:CD2 | 2:Q:2718:TRP:CH2 | 3.08 | 0.41 |
| 3:R:2952[B]:ALA:CA | 3:R:2956[B]:LYS:CB | 2.89 | 0.41 |
| 3:R:3048[A]:ASP:HB3 | 3:R:3099[A]:PRO:HD2 | 2.01 | 0.41 |
| 3:R:3133[B]:LEU:HD13 | 3:R:3197[B]:ILE:HG23 | 2.02 | 0.41 |
| 3:R:3171[A]:HIS:O | 3:R:3172[A]:SER:C | 2.63 | 0.41 |
| 3:R:3228[B]:VAL:CG2 | 3:R:3245[B]:PHE:CD2 | 3.02 | 0.41 |
| 3:R:3232[B]:VAL:HG21 | 3:R:3273[B]:LEU:CD1 | 2.49 | 0.41 |
| 3:R:3281[A]:PHE:CZ | 3:R:3305[A]:ILE:HG21 | 2.55 | 0.41 |
| 1:S:285:THR:HB | 1:S:288:GLU:H | 1.85 | 0.41 |
| 1:S:932:THR:O | 1:S:989:THR:OG1 | 2.37 | 0.41 |
| 1:S:1019:HIS:CE1 | 1:S:1046:HIS:CE1 | 3.08 | 0.41 |
| 1:S:1055:THR:HG21 | 1:S:1121:LEU:HD13 | 2.01 | 0.41 |
| 1:S:1263:LEU:HD11 | 1:S:1358:LEU:HD22 | 2.02 | 0.41 |
| 2:T:2104:ILE:O | 2:T:2108:LYS:HB2 | 2.20 | 0.41 |
| 3:U:2949[A]:LYS:C | 3:U:2949[A]:LYS:HZ3 | 2.18 | 0.41 |
| 3:U:2987[B]:HIS:CD2 | 3:U:3178[B]:PHE:CE1 | 3.08 | 0.41 |
| 3:U:2989[B]:HIS:NE2 | 9:U:3401[B]:CUO:O1 | 2.53 | 0.41 |
| 3:U:3041[B]:ALA:O | 3:U:3042[B]:ASP:HB2 | 2.20 | 0.41 |
| 3:U:3096[A]:VAL:CG1 | 3:U:3115[A]:LEU:CD1 | 2.86 | 0.41 |
| 3:U:3193[B]:HIS:ND1 | 3:U:3193[B]:HIS:N | 2.68 | 0.41 |
| 1:V:109:LEU:HD21 | 2:Z:2635:TYR:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:128:ILE:HG12 | 1:V:130:PHE:O | 2.20 | 0.41 |
| 1:V:664:VAL:HG12 | 1:V:690:THR:HG22 | 2.00 | 0.41 |
| 2:W:2191:LEU:HD13 | 2:W:2296:LEU:HD22 | 2.01 | 0.41 |
| 2:W:2381:LEU:HD23 | 2:W:2381:LEU:HA | 1.92 | 0.41 |
| 3:X:2969[B]:TYR:CD2 | 3:X:2971[B]:ASP:CG | 2.98 | 0.41 |
| 1:Y:843:VAL:CG1 | 1:Y:927:PRO:HB2 | 2.50 | 0.41 |
| 1:Y:1019:HIS:CE1 | 1:Y:1046:HIS:HE1 | 2.37 | 0.41 |
| 2:Z:2235:PRO:HG2 | 2:c:2097:LEU:HD12 | 2.02 | 0.41 |
| 3:a:3047[A]:ARG:NH2 | 3:a:3113[A]:ASP:OD1 | 2.43 | 0.41 |
| 3:a:3148[B]:ILE:HD12 | 3:a:3175[B]:TYR:OH | 2.20 | 0.41 |
| 3:a:3200[A]:LEU:O | 3:a:3203[A]:HIS:HB3 | 2.20 | 0.41 |
| 1:b:891:LYS:HB2 | 1:b:892:TYR:HB3 | 2.00 | 0.41 |
| 1:b:1180:SER:OG | 1:b:1181:GLU:N | 2.53 | 0.41 |
| 2:c:2336:PHE:HB3 | 2:c:2348:THR:HG22 | 2.02 | 0.41 |
| 3:d:2965[A]:LEU:CG | 3:d:2974[A]:ALA:CB | 2.85 | 0.41 |
| 3:d:2979[B]:GLN:HA | 3:d:2979[B]:GLN:OE1 | 2.19 | 0.41 |
| 3:d:2989[B]:HIS:NE2 | 9:d:3401[B]:CUO:O1 | 2.53 | 0.41 |
| 3:d:2995[B]:GLN:CG | 3:d:3168[B]:THR:HG21 | 2.48 | 0.41 |
| 3:d:3149[B]:ASN:OD1 | 3:d:3149[B]:ASN:N | 2.51 | 0.41 |
| 3:d:3183[B]:LEU:N | 3:d:3184[B]:ASN:CA | 2.80 | 0.41 |
| 3:d:3185[A]:TYR:HE2 | 3:d:3187[A]:TYR:CD2 | 2.35 | 0.41 |
| 1:A:119:LYS:CB | 1:A:120:LYS:HA | 2.34 | 0.41 |
| 1:A:139:VAL:HG11 | 1:A:144:TYR:CZ | 2.55 | 0.41 |
| 1:A:418:ASP:C | 1:A:420:SER:HA | 2.44 | 0.41 |
| 1:A:473:ALA:HB1 | 1:b:1639:LYS:HD2 | 2.02 | 0.41 |
| 1:A:718:ARG:HD3 | 1:A:834:ASP:OD2 | 2.19 | 0.41 |
| 1:A:1091:ASN:HA | 1:A:1092:PRO:HD3 | 1.76 | 0.41 |
| 1:A:1361:GLU:HG3 | 1:A:1363:THR:H | 1.85 | 0.41 |
| 3:C:2979[A]:GLN:CD | 3:C:3155[A]:MET:CE | 2.92 | 0.41 |
| 3:C:3146[B]:CYS:SG | 3:C:3146[B]:CYS:O | 2.78 | 0.41 |
| 3:C:3163[B]:ASN:O | 3:L:3147[B]:GLU:OE2 | 2.38 | 0.41 |
| 3:C:3171[B]:HIS:C | 3:L:3152[B]:LYS:CB | 2.82 | 0.41 |
| 3:C:3180[A]:TYR:CA | 3:C:3183[A]:LEU:CD2 | 2.95 | 0.41 |
| 3:C:3185[A]:TYR:CE2 | 3:C:3187[A]:TYR:HE2 | 2.31 | 0.41 |
| 3:C:3200[B]:LEU:O | 3:C:3203[B]:HIS:HB3 | 2.20 | 0.41 |
| 3:C:3222[A]:ILE:CD1 | 3:C:3223[A]:GLY:N | 2.73 | 0.41 |
| 9:C:3401[A]:CUO:O1 | 3:L:2989[A]:HIS:NE2 | 2.53 | 0.41 |
| 1:D:23:ARG:HD3 | 1:D:120:LYS:HD3 | 2.02 | 0.41 |
| 1:D:472:ASP:HA | 1:D:473:ALA:HA | 1.74 | 0.41 |
| 1:D:1634:ALA:HB1 | 4:m:1:NAG:O7 | 2.19 | 0.41 |
| 2:E:2107:LEU:HA | 2:E:2110:MET:HG2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:2597:MET:HE2 | 2:E:2598:PRO:HD2 | 2.02 | 0.41 |
| 2:E:2711:HIS:O | 2:E:2712:SER:C | 2.63 | 0.41 |
| 3:F:3041[A]:ALA:O | 3:F:3042[A]:ASP:HB2 | 2.20 | 0.41 |
| 3:F:3150[B]:LYS:NZ | 3:a:3162[B]:ASP:C | 2.77 | 0.41 |
| 3:F:3150[B]:LYS:HB2 | 3:a:3169[B]:LYS:HE3 | 2.02 | 0.41 |
| 3:F:3193[B]:HIS:ND1 | 3:F:3193[B]:HIS:N | 2.68 | 0.41 |
| 1:G:149:GLU:O | 1:G:151:GLN:N | 2.53 | 0.41 |
| 1:G:806:ASN:OD1 | 1:G:808:THR:HG22 | 2.20 | 0.41 |
| 1:G:1144:VAL:HG12 | 1:G:1194:SER:O | 2.19 | 0.41 |
| 1:G:1339:SER:HB3 | 1:G:1340:GLY:CA | 2.40 | 0.41 |
| 2:H:2406:SER:OG | 2:H:2430:GLY:N | 2.33 | 0.41 |
| 2:H:2521:MET:HE3 | 2:H:2605:LEU:HD12 | 2.01 | 0.41 |
| 2:H:2744:PHE:CZ | 1:J:1212:HIS:HB3 | 2.55 | 0.41 |
| 2:H:2800:LYS:HB3 | 3:I:3023[A]:ILE:HD13 | 2.02 | 0.41 |
| 3:I:3153[B]:LYS:HG2 | 3:R:3155[B]:MET:CG | 2.50 | 0.41 |
| 3:I:3259[B]:ASP:N | 3:R:3162[B]:ASP:CB | 2.77 | 0.41 |
| 3:I:3259[B]:ASP:H | 3:R:3162[B]:ASP:CG | 2.27 | 0.41 |
| 1:J:19:GLN:HG2 | 1:J:110:PHE:CD2 | 2.55 | 0.41 |
| 1:J:494:VAL:HG23 | 1:J:671:PHE:CZ | 2.56 | 0.41 |
| 1:J:946:GLU:HG2 | 1:J:955:LYS:HD3 | 2.01 | 0.41 |
| 2:K:2481:LEU:HA | 2:K:2482:PRO:HD3 | 1.94 | 0.41 |
| 2:K:2568:HIS:CD2 | 2:K:2718:TRP:CH2 | 3.08 | 0.41 |
| 3:L:3041[A]:ALA:O | 3:L:3042[A]:ASP:HB2 | 2.20 | 0.41 |
| 3:L:3048[B]:ASP:HB3 | 3:L:3099[B]:PRO:HD2 | 2.01 | 0.41 |
| 3:L:3161[B]:GLU:H | 3:L:3161[B]:GLU:CD | 2.19 | 0.41 |
| 3:L:3299[A]:LEU:HB3 | 3:L:3300[A]:LEU:H | 1.54 | 0.41 |
| 1:M:603:HIS:HD2 | 1:M:633:HIS:CE1 | 2.38 | 0.41 |
| 1:M:1636:ASN:HB2 | 1:M:1638:SER:O | 2.19 | 0.41 |
| 2:N:2155:HIS:O | 2:N:2159:VAL:HG23 | 2.21 | 0.41 |
| 3:O:2966[B]:SER:HB2 | 3:O:2977[B]:CYS:H | 1.85 | 0.41 |
| 3:O:3148[B]:ILE:HD12 | 3:O:3175[B]:TYR:OH | 2.20 | 0.41 |
| 3:O:3171[A]:HIS:O | 3:O:3172[A]:SER:C | 2.63 | 0.41 |
| 3:O:3200[B]:LEU:O | 3:O:3203[B]:HIS:HB3 | 2.20 | 0.41 |
| 1:P:64:THR:HG22 | 1:P:240:PHE:CE1 | 2.55 | 0.41 |
| 1:P:92:TRP:CE3 | 1:P:102:PRO:HD3 | 2.55 | 0.41 |
| 1:P:489:HIS:CD2 | 1:P:689:PRO:HB2 | 2.56 | 0.41 |
| 1:P:492:ARG:HD2 | 1:P:692:VAL:HG13 | 2.01 | 0.41 |
| 1:P:1324:ARG:NH1 | 1:P:1519:TYR:HB3 | 2.34 | 0.41 |
| 2:Q:2660:VAL:HG13 | 2:Q:2663:MET:HE2 | 2.02 | 0.41 |
| 3:R:2979[B]:GLN:CD | 3:R:3155[B]:MET:CE | 2.93 | 0.41 |
| 1:S:72:TYR:HD1 | 1:S:247:PHE:HZ | 1.67 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:305:ASN:HB3 | 1:S:400:ILE:HB | 2.02 | 0.41 |
| 1:S:714:ARG:NH1 | 1:S:1115:GLU:OE1 | 2.52 | 0.41 |
| 1:S:1166:THR:N | 1:S:1167:ASP:HA | 2.35 | 0.41 |
| 1:S:1312:CYS:HA | 1:S:1322:TRP:CE2 | 2.54 | 0.41 |
| 1:S:1438:ASP:HB3 | 1:S:1441:SER:HB3 | 2.01 | 0.41 |
| 2:T:2132:CYS:O | 2:T:2334:LYS:HD3 | 2.21 | 0.41 |
| 3:U:2970[B]:PRO:N | 3:d:2981[B]:GLY:N | 2.68 | 0.41 |
| 3:U:2975[B]:PHE:HD1 | 3:d:3221[B]:ALA:CB | 2.33 | 0.41 |
| 3:U:2980[B]:HIS:O | 3:d:2969[B]:TYR:HD1 | 1.92 | 0.41 |
| 3:U:3011[A]:TYR:CB | 3:U:3121[A]:SER:HB2 | 2.49 | 0.41 |
| 3:U:3133[B]:LEU:HD13 | 3:U:3197[B]:ILE:HG23 | 2.02 | 0.41 |
| 3:U:3148[A]:ILE:HD12 | 3:U:3175[A]:TYR:OH | 2.20 | 0.41 |
| 1:V:482:HIS:CE1 | 1:V:621:LEU:HD11 | 2.55 | 0.41 |
| 1:V:949:ASP:O | 1:V:952:GLY:N | 2.52 | 0.41 |
| 2:W:2553:ALA:N | 2:W:2554:PRO:CD | 2.84 | 0.41 |
| 3:X:2952[B]:ALA:CA | 3:X:2956[B]:LYS:CB | 2.89 | 0.41 |
| 3:X:2987[B]:HIS:CD2 | 3:X:3178[B]:PHE:CE1 | 3.08 | 0.41 |
| 3:X:2988[A]:TRP:HE3 | 3:X:2989[A]:HIS:CE1 | 2.25 | 0.41 |
| 3:X:3028[A]:PRO:HG2 | 3:X:3029[A]:LYS:HG2 | 2.02 | 0.41 |
| 3:X:3171[A]:HIS:O | 3:X:3172[A]:SER:C | 2.63 | 0.41 |
| 3:X:3194[A]:GLY:C | 3:X:3195[A]:MET:CG | 2.90 | 0.41 |
| 3:X:3281[A]:PHE:CZ | 3:X:3305[A]:ILE:HG21 | 2.55 | 0.41 |
| 3:X:3284[A]:LYS:CD | 3:X:3284[A]:LYS:C | 2.86 | 0.41 |
| 3:X:3299[A]:LEU:HB3 | 3:X:3300[A]:LEU:H | 1.54 | 0.41 |
| 3:X:3301[A]:PRO:HB2 | 3:X:3302[A]:SER:H | 1.33 | 0.41 |
| 1:Y:1319:PHE:CE2 | 1:Y:1424:GLU:HG3 | 2.55 | 0.41 |
| 1:Y:1489:MET:HB3 | 1:Y:1514:ASN:ND2 | 2.36 | 0.41 |
| 2:Z:2327:GLU:HG2 | 1:b:1649:THR:HA | 2.02 | 0.41 |
| 2:Z:2469:VAL:HG12 | 2:Z:2475:GLU:HG2 | 2.02 | 0.41 |
| 3:a:3048[A]:ASP:HB3 | 3:a:3099[A]:PRO:HD2 | 2.01 | 0.41 |
| 3:a:3084[B]:GLN:HE21 | 3:a:3084[B]:GLN:HB3 | 1.71 | 0.41 |
| 1:b:51:ASP:HA | 1:b:52:GLY:HA2 | 1.62 | 0.41 |
| 1:b:882:TRP:CD1 | 1:b:1086:LEU:HD13 | 2.55 | 0.41 |
| 1:b:1070:ALA:HB3 | 1:b:1077:LEU:HD21 | 2.01 | 0.41 |
| 2:c:2858:ASP:O | 2:c:2862:LYS:HG2 | 2.20 | 0.41 |
| 3:d:2969[A]:TYR:CD2 | 3:d:2971[A]:ASP:CG | 2.98 | 0.41 |
| 3:d:3133[A]:LEU:HD13 | 3:d:3197[A]:ILE:HG23 | 2.02 | 0.41 |
| 3:d:3230[A]:PHE:HB2 | 3:d:3242[A]:GLY:C | 2.45 | 0.41 |
| 3:d:3281[A]:PHE:HE1 | 3:d:3305[A]:ILE:HG21 | 1.81 | 0.41 |
| 1:A:1010:GLN:H | 1:A:1010:GLN:HG2 | 1.67 | 0.41 |
| 2:B:2191:LEU:HD12 | 2:B:2191:LEU:HA | 1.87 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2406:SER:O | 2:B:2471:HIS:HB2 | 2.20 | 0.41 |
| 3:C:2949[A]:LYS:NZ | 3:C:2949[A]:LYS:C | 2.73 | 0.41 |
| 3:C:3028[A]:PRO:HG2 | 3:C:3029[A]:LYS:HG2 | 2.02 | 0.41 |
| 3:C:3146[A]:CYS:HA | 3:C:3147[A]:GLU:HA | 1.70 | 0.41 |
| 1:D:40:TYR:CD1 | 1:D:246:PRO:HG2 | 2.54 | 0.41 |
| 1:D:282:ASN:OD1 | 1:D:282:ASN:N | 2.53 | 0.41 |
| 1:D:601:VAL:HG11 | 1:D:777:TYR:CG | 2.56 | 0.41 |
| 1:D:1023:GLY:HA2 | 1:D:1029:SER:OG | 2.21 | 0.41 |
| 1:D:1248:ARG:HG3 | 1:D:1249:TRP:H | 1.85 | 0.41 |
| 1:D:1260:ARG:HD2 | 1:D:1343:VAL:O | 2.21 | 0.41 |
| 2:E:2089:ARG:HD3 | 2:E:2163:GLU:OE2 | 2.20 | 0.41 |
| 2:E:2304:LEU:HD12 | 2:E:2304:LEU:HA | 1.89 | 0.41 |
| 2:E:2554:PRO:CB | 2:E:2556:TYR:HB2 | 2.51 | 0.41 |
| 3:F:2931[A]:THR:HG1 | 3:F:2934[A]:GLU:CD | 2.04 | 0.41 |
| 3:F:3120[B]:HIS:HA | 3:F:3123[B]:THR:HG1 | 1.82 | 0.41 |
| 3:F:3148[B]:ILE:O | 3:a:3170[B]:ALA:N | 2.53 | 0.41 |
| 1:G:104:LEU:HD23 | 1:G:123:PHE:CE2 | 2.51 | 0.41 |
| 1:G:590:ASP:OD1 | 1:G:590:ASP:N | 2.54 | 0.41 |
| 1:G:938:LEU:HD11 | 1:G:976:THR:HG21 | 2.02 | 0.41 |
| 2:H:2089:ARG:HB2 | 2:H:2368:TYR:CD1 | 2.56 | 0.41 |
| 2:H:2157:LEU:O | 2:H:2160:VAL:HG22 | 2.20 | 0.41 |
| 2:H:2680:HIS:CD2 | 2:H:2684:HIS:CD2 | 3.08 | 0.41 |
| 3:I:2963[A]:MET:SD | 3:I:2963[A]:MET:O | 2.79 | 0.41 |
| 3:I:2968[B]:GLN:O | 3:R:2985[B]:PHE:CE2 | 2.74 | 0.41 |
| 3:I:2971[B]:ASP:O | 3:R:3093[B]:HIS:CB | 2.67 | 0.41 |
| 3:I:2979[A]:GLN:HA | 3:I:2979[A]:GLN:OE1 | 2.19 | 0.41 |
| 3:I:2989[A]:HIS:NE2 | 9:R:3401[A]:CUO:O1 | 2.53 | 0.41 |
| 3:I:2989[B]:HIS:C | 3:I:2991[B]:LEU:N | 2.75 | 0.41 |
| 3:I:2995[A]:GLN:O | 3:I:2996[A]:MET:C | 2.63 | 0.41 |
| 3:I:3148[A]:ILE:HD12 | 3:I:3175[A]:TYR:OH | 2.20 | 0.41 |
| 3:I:3200[A]:LEU:O | 3:I:3203[A]:HIS:HB3 | 2.20 | 0.41 |
| 3:I:3218[A]:LEU:HD13 | 3:I:3261[A]:LEU:HD23 | 2.01 | 0.41 |
| 1:J:464:LEU:HD22 | 1:J:622:HIS:CD2 | 2.54 | 0.41 |
| 1:J:728:ARG:HE | 1:J:730:PHE:HZ | 1.68 | 0.41 |
| 2:K:2361:LYS:HE2 | 2:K:2362:GLN:HG3 | 2.01 | 0.41 |
| 2:K:2575:LEU:HD23 | 2:K:2575:LEU:HA | 1.87 | 0.41 |
| 3:L:2931[A]:THR:HG1 | 3:L:2934[A]:GLU:CD | 2.04 | 0.41 |
| 3:L:2963[A]:MET:SD | 3:L:2963[A]:MET:O | 2.78 | 0.41 |
| 3:L:2963[B]:MET:SD | 3:L:2963[B]:MET:O | 2.79 | 0.41 |
| 3:L:3196[A]:THR:N | 3:L:3199[A]:GLN:CB | 2.65 | 0.41 |
| 3:L:3196[B]:THR:OG1 | 3:L:3199[B]:GLN:OE1 | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3281[B]:PHE:CZ | 3:L:3305[B]:ILE:HG21 | 2.55 | 0.41 |
| 1:M:164:GLU:OE2 | 1:M:301:ARG:NH2 | 2.53 | 0.41 |
| 1:M:705:THR:HG22 | 1:M:1118:THR:HG22 | 2.02 | 0.41 |
| 1:M:862:ALA:HA | 1:M:870:TYR:HD2 | 1.85 | 0.41 |
| 1:M:1458:HIS:CE1 | 9:M:2105:CUO:O1 | 2.74 | 0.41 |
| 2:N:2641:GLN:HA | 2:N:2642:PRO:HD3 | 1.87 | 0.41 |
| 3:O:3047[B]:ARG:NH2 | 3:O:3113[B]:ASP:OD1 | 2.43 | 0.41 |
| 3:O:3131[A]:GLN:HE21 | 3:O:3131[A]:GLN:HB3 | 1.66 | 0.41 |
| 3:O:3180[B]:TYR:HA | 3:O:3183[B]:LEU:CD2 | 2.51 | 0.41 |
| 1:P:150:GLY:HA2 | 1:P:151:GLN:HA | 1.77 | 0.41 |
| 1:P:177:VAL:HA | 1:P:180:ASN:ND2 | 2.35 | 0.41 |
| 1:P:450:LYS:HZ2 | 1:P:505:ARG:HH21 | 1.67 | 0.41 |
| 3:R:2979[A]:GLN:HA | 3:R:2979[A]:GLN:OE1 | 2.19 | 0.41 |
| 3:R:2987[A]:HIS:CD2 | 3:R:3178[A]:PHE:CE1 | 3.08 | 0.41 |
| 3:R:3041[A]:ALA:O | 3:R:3042[A]:ASP:HB2 | 2.20 | 0.41 |
| 3:R:3083[B]:ILE:HD11 | 3:R:3260[B]:ARG:HG3 | 2.03 | 0.41 |
| 3:R:3173[B]:THR:HG22 | 3:R:3174[B]:GLY:H | 1.67 | 0.41 |
| 3:R:3180[B]:TYR:CB | 3:R:3183[B]:LEU:CD2 | 2.90 | 0.41 |
| 3:R:3294[B]:SER:O | 3:R:3294[B]:SER:OG | 2.34 | 0.41 |
| 1:S:858:MET:HE1 | 1:S:870:TYR:CZ | 2.55 | 0.41 |
| 1:S:980:TYR:CE1 | 1:S:1021:LEU:HB3 | 2.55 | 0.41 |
| 1:S:1166:THR:OG1 | 1:S:1168:GLN:N | 2.52 | 0.41 |
| 2:T:2549:PRO:HA | 2:T:2550:THR:HA | 1.56 | 0.41 |
| 2:T:2575:LEU:HD11 | 2:T:2774:LEU:HB3 | 2.01 | 0.41 |
| 3:U:2963[A]:MET:SD | 3:U:2963[A]:MET:O | 2.79 | 0.41 |
| 3:U:3034[A]:HIS:HB3 | 3:U:3035[A]:HIS:CE1 | 2.50 | 0.41 |
| 3:U:3094[B]:SER:HG | 3:U:3227[B]:ASP:CG | 2.28 | 0.41 |
| 3:U:3169[B]:LYS:HG2 | 3:d:3148[B]:ILE:H | 0.62 | 0.41 |
| 3:U:3182[A]:GLN:H | 3:U:3182[A]:GLN:HG2 | 1.56 | 0.41 |
| 3:U:3200[A]:LEU:O | 3:U:3203[A]:HIS:HB3 | 2.20 | 0.41 |
| 3:U:3218[A]:LEU:HD13 | 3:U:3261[A]:LEU:HD23 | 2.01 | 0.41 |
| 3:U:3222[B]:ILE:CD1 | 3:U:3223[B]:GLY:N | 2.73 | 0.41 |
| 1:V:225:LYS:HE2 | 1:V:225:LYS:HB2 | 1.93 | 0.41 |
| 1:V:518:LYS:HE2 | 1:V:520:PHE:HB3 | 2.00 | 0.41 |
| 1:V:567:LEU:HB2 | 1:V:571:PRO:HD2 | 2.01 | 0.41 |
| 1:V:1249:TRP:HZ2 | 1:V:1537:ILE:HD12 | 1.85 | 0.41 |
| 1:V:1304:ASP:OD1 | 1:V:1306:THR:N | 2.53 | 0.41 |
| 1:V:1573:CYS:HB2 | 1:V:1627:ARG:CG | 2.49 | 0.41 |
| 2:W:2180:TRP:HH2 | 2:W:2297:HIS:O | 2.02 | 0.41 |
| 3:X:3185[B]:TYR:HE2 | 3:X:3187[B]:TYR:CD2 | 2.35 | 0.41 |
| 1:Y:859:ALA:HB2 | 1:Y:957:ASN:ND2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:898:GLY:HA2 | 1:Y:1186:TRP:CB | 2.44 | 0.41 |
| 2:Z:2638:ARG:HG2 | 2:Z:2687:ILE:O | 2.20 | 0.41 |
| 3:a:2969[A]:TYR:CD2 | 3:a:2971[A]:ASP:CG | 2.97 | 0.41 |
| 3:a:2995[A]:GLN:CG | 3:a:3168[A]:THR:HG21 | 2.48 | 0.41 |
| 3:a:3041[A]:ALA:O | 3:a:3042[A]:ASP:HB2 | 2.20 | 0.41 |
| 3:a:3196[B]:THR:OG1 | 3:a:3199[B]:GLN:OE1 | 2.37 | 0.41 |
| 3:a:3285[A]:VAL:CG2 | 3:a:3286[A]:THR:H | 2.27 | 0.41 |
| 1:b:59:LEU:HD23 | 1:b:64:THR:OG1 | 2.20 | 0.41 |
| 1:b:350:MET:O | 1:b:352:TRP:HD1 | 2.04 | 0.41 |
| 1:b:619:SER:HB2 | 1:b:805:VAL:HG11 | 2.02 | 0.41 |
| 1:b:843:VAL:HG21 | 1:b:1044:LEU:HD13 | 2.02 | 0.41 |
| 1:b:882:TRP:N | 1:b:894:CYS:SG | 2.94 | 0.41 |
| 1:b:907:ARG:HD3 | 1:b:1050:ASP:OD1 | 2.19 | 0.41 |
| 1:b:949:ASP:OD1 | 1:b:950:ALA:N | 2.51 | 0.41 |
| 1:b:1081:MET:HG2 | 1:b:1100:SER:O | 2.20 | 0.41 |
| 1:b:1166:THR:N | 1:b:1167:ASP:HA | 2.34 | 0.41 |
| 1:b:1361:GLU:HG3 | 1:b:1363:THR:H | 1.84 | 0.41 |
| 1:b:1492:PRO:HA | 1:b:1512:ARG:HA | 2.02 | 0.41 |
| 1:b:1614:GLU:OE1 | 1:b:1614:GLU:N | 2.53 | 0.41 |
| 2:c:2393:ARG:O | 2:c:2489:ILE:N | 2.42 | 0.41 |
| 2:c:2562:GLY:H | 2:c:2846:TRP:CB | 2.33 | 0.41 |
| 2:c:2571:ARG:NH1 | 2:c:2771:TYR:HB3 | 2.35 | 0.41 |
| 2:c:2656:LEU:HD23 | 2:c:2656:LEU:HA | 1.91 | 0.41 |
| 2:c:2762:VAL:O | 2:c:2768:LEU:HD23 | 2.20 | 0.41 |
| 3:d:3193[A]:HIS:ND1 | 3:d:3193[A]:HIS:N | 2.69 | 0.41 |
| 1:A:100:GLN:HA | 1:A:100:GLN:HE21 | 1.85 | 0.41 |
| 1:A:103:GLU:OE2 | 1:A:106:GLN:NE2 | 2.54 | 0.41 |
| 1:A:119:LYS:HA | 1:A:119:LYS:HD2 | 1.86 | 0.41 |
| 1:A:232:ARG:NE | 1:A:267:PHE:HE2 | 2.19 | 0.41 |
| 1:A:307:ARG:HH12 | 1:A:484:MET:HE1 | 1.86 | 0.41 |
| 1:A:328:LYS:NZ | 1:b:1631:GLU:OE1 | 2.42 | 0.41 |
| 1:A:331:SER:HB3 | 1:b:1582:ASN:O | 2.20 | 0.41 |
| 1:A:1180:SER:N | 1:A:1183:GLU:OE1 | 2.53 | 0.41 |
| 1:A:1322:TRP:HZ2 | 1:A:1495:PRO:HG3 | 1.85 | 0.41 |
| 1:A:1498:ASN:ND2 | 1:A:1500:THR:O | 2.54 | 0.41 |
| 3:C:2987[B]:HIS:CD2 | 3:C:3178[B]:PHE:CE1 | 3.08 | 0.41 |
| 3:C:3158[B]:PHE:HE2 | 3:L:3153[B]:LYS:HZ1 | 1.49 | 0.41 |
| 3:C:3232[B]:VAL:HG21 | 3:C:3273[B]:LEU:HD11 | 2.00 | 0.41 |
| 3:C:3252[B]:TYR:HB3 | 3:L:3253[B]:GLU:CD | 2.45 | 0.41 |
| 3:C:3276[A]:ASP:C | 3:C:3278[A]:HIS:N | 2.75 | 0.41 |
| 3:C:3281[A]:PHE:HE1 | 3:C:3305[A]:ILE:HG21 | 1.81 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3300[A]:LEU:HD23 | 3:C:3300[A]:LEU:H | 1.83 | 0.41 |
| 1:D:81:VAL:C | 1:D:83:HIS:N | 2.76 | 0.41 |
| 1:D:442:ALA:HB2 | 1:D:507:SER:HB3 | 2.01 | 0.41 |
| 1:D:1099:TYR:CD2 | 1:D:1112:PHE:HE1 | 2.39 | 0.41 |
| 1:D:1170:MET:SD | 1:D:1199:VAL:HG23 | 2.60 | 0.41 |
| 1:D:1275:ARG:HH21 | 1:D:1375:ASN:ND2 | 2.17 | 0.41 |
| 1:D:1319:PHE:CE2 | 1:D:1424:GLU:HG3 | 2.54 | 0.41 |
| 1:D:1562:ILE:CG2 | 1:D:1644:ILE:HG21 | 2.50 | 0.41 |
| 2:E:2240:GLN:HG3 | 2:E:2241:THR:N | 2.35 | 0.41 |
| 3:F:2969[B]:TYR:HE2 | 3:a:3120[B]:HIS:CD2 | 2.36 | 0.41 |
| 3:F:2979[A]:GLN:NE2 | 3:F:3155[A]:MET:HE3 | 2.19 | 0.41 |
| 3:F:3083[A]:ILE:HD11 | 3:F:3260[A]:ARG:HG3 | 2.03 | 0.41 |
| 3:F:3232[A]:VAL:HG21 | 3:F:3273[A]:LEU:CD1 | 2.50 | 0.41 |
| 3:F:3232[B]:VAL:CG2 | 3:F:3273[B]:LEU:CD1 | 2.98 | 0.41 |
| 9:F:3401[A]:CUO:O1 | 3:a:2989[A]:HIS:NE2 | 2.53 | 0.41 |
| 1:G:69:HIS:CD2 | 1:G:210:HIS:CE1 | 3.08 | 0.41 |
| 1:G:104:LEU:HB3 | 1:G:123:PHE:CD2 | 2.50 | 0.41 |
| 1:G:686:HIS:NE2 | 1:G:698:GLU:HB3 | 2.35 | 0.41 |
| 1:G:1018:ILE:HD12 | 1:G:1045:HIS:CD2 | 2.55 | 0.41 |
| 1:G:1280:GLN:HE21 | 1:G:1280:GLN:HB3 | 1.66 | 0.41 |
| 2:H:2502:LEU:HD12 | 2:H:2502:LEU:HA | 1.89 | 0.41 |
| 3:I:3232[A]:VAL:HG21 | 3:I:3273[A]:LEU:CD1 | 2.50 | 0.41 |
| 1:J:385:ALA:HB2 | 1:J:391:MET:SD | 2.60 | 0.41 |
| 2:K:2263:PHE:HE1 | 2:K:2304:LEU:HB3 | 1.85 | 0.41 |
| 2:K:2304:LEU:O | 2:K:2307:VAL:HB | 2.20 | 0.41 |
| 2:K:2536:PHE:HE1 | 2:K:2708:TYR:CE2 | 2.38 | 0.41 |
| 2:K:2549:PRO:HA | 2:K:2550:THR:HA | 1.48 | 0.41 |
| 3:L:2952[B]:ALA:CA | 3:L:2956[B]:LYS:CB | 2.89 | 0.41 |
| 3:L:2965[A]:LEU:CG | 3:L:2974[A]:ALA:CB | 2.85 | 0.41 |
| 3:L:3229[A]:ASN:N | 3:L:3286[A]:THR:O | 2.52 | 0.41 |
| 1:M:84:GLY:CA | 1:M:85:SER:HB3 | 2.50 | 0.41 |
| 1:M:132:ASN:HB2 | 1:M:133:LYS:HG2 | 2.02 | 0.41 |
| 1:M:200:THR:O | 1:M:206:PHE:HB2 | 2.20 | 0.41 |
| 1:M:419:THR:HA | 1:M:420:SER:HA | 1.60 | 0.41 |
| 1:M:979:LEU:CB | 1:M:980:TYR:HD1 | 2.33 | 0.41 |
| 1:M:1207:TYR:O | 1:M:1207:TYR:HD1 | 2.03 | 0.41 |
| 1:M:1256:ALA:HB1 | 1:M:1526:LYS:HB2 | 2.02 | 0.41 |
| 2:N:2107:LEU:O | 2:N:2111:GLN:HB2 | 2.20 | 0.41 |
| 2:N:2181:THR:HB | 2:N:2374:ASN:H | 1.86 | 0.41 |
| 2:N:2187:VAL:HG12 | 2:N:2188:PRO:HD2 | 2.02 | 0.41 |
| 2:N:2638:ARG:NH2 | 2:N:2706:ILE:HD11 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2952[B]:ALA:CA | 3:O:2956[B]:LYS:CB | 2.89 | 0.41 |
| 3:O:2963[B]:MET:SD | 3:O:2963[B]:MET:O | 2.79 | 0.41 |
| 3:O:2980[B]:HIS:HA | 3:O:2985[B]:PHE:HD2 | 1.86 | 0.41 |
| 3:O:3028[B]:PRO:HG2 | 3:O:3029[B]:LYS:HG2 | 2.02 | 0.41 |
| 3:O:3146[B]:CYS:O | 3:O:3146[B]:CYS:SG | 2.78 | 0.41 |
| 3:O:3148[A]:ILE:HD12 | 3:O:3175[A]:TYR:OH | 2.20 | 0.41 |
| 3:O:3161[B]:GLU:OE1 | 3:X:3144[B]:ALA:CB | 2.68 | 0.41 |
| 3:O:3196[B]:THR:OG1 | 3:O:3199[B]:GLN:OE1 | 2.37 | 0.41 |
| 3:O:3276[A]:ASP:C | 3:O:3278[A]:HIS:N | 2.75 | 0.41 |
| 1:P:1118:THR:HB | 1:P:1120:GLU:HG2 | 2.02 | 0.41 |
| 2:Q:2764:THR:HG22 | 2:Q:2766:SER:H | 1.84 | 0.41 |
| 2:Q:2823:ILE:HD12 | 2:Q:2860:LEU:HD21 | 2.03 | 0.41 |
| 2:Q:2829:CYS:C | 2:Q:2830:GLN:HG2 | 2.46 | 0.41 |
| 3:R:2963[B]:MET:SD | 3:R:2963[B]:MET:O | 2.79 | 0.41 |
| 3:R:3229[A]:ASN:N | 3:R:3286[A]:THR:O | 2.52 | 0.41 |
| 3:R:3232[A]:VAL:HG21 | 3:R:3273[A]:LEU:CD1 | 2.50 | 0.41 |
| 3:R:3300[B]:LEU:HD23 | 3:R:3300[B]:LEU:H | 1.83 | 0.41 |
| 1:S:407:GLN:HA | 1:S:408:GLY:HA2 | 1.68 | 0.41 |
| 1:S:834:ASP:HB2 | 1:S:837:HIS:HB3 | 2.02 | 0.41 |
| 1:S:977:GLU:HG3 | 1:S:978:ALA:H | 1.84 | 0.41 |
| 1:S:995:ILE:HG22 | 1:S:999:LEU:HD22 | 2.02 | 0.41 |
| 1:S:1248:ARG:HG3 | 1:S:1249:TRP:H | 1.86 | 0.41 |
| 1:S:1634:ALA:HB3 | 1:S:1639:LYS:HD3 | 2.02 | 0.41 |
| 2:T:2339:GLY:HA2 | 2:T:2349:THR:HG21 | 2.03 | 0.41 |
| 2:T:2866:PRO:HA | 2:T:2867:PRO:HD3 | 1.96 | 0.41 |
| 3:U:2963[B]:MET:SD | 3:U:2963[B]:MET:O | 2.79 | 0.41 |
| 3:U:2995[B]:GLN:CG | 3:U:3168[B]:THR:HG21 | 2.48 | 0.41 |
| 3:U:3013[B]:ASP:CA | 3:U:3122[B]:ASN:ND2 | 2.73 | 0.41 |
| 3:U:3137[A]:ARG:HD3 | 3:U:3137[A]:ARG:HA | 1.71 | 0.41 |
| 3:U:3146[A]:CYS:O | 3:U:3146[A]:CYS:SG | 2.78 | 0.41 |
| 3:U:3148[B]:ILE:HD12 | 3:U:3175[B]:TYR:OH | 2.20 | 0.41 |
| 3:U:3158[B]:PHE:O | 3:d:3149[B]:ASN:HB3 | 2.14 | 0.41 |
| 3:U:3196[A]:THR:OG1 | 3:U:3199[A]:GLN:OE1 | 2.38 | 0.41 |
| 1:V:407:GLN:HA | 1:V:408:GLY:HA2 | 1.73 | 0.41 |
| 1:V:480:CYS:HA | 1:V:490:TRP:CE2 | 2.54 | 0.41 |
| 1:V:547:LYS:HG2 | 1:V:558:HIS:HB3 | 2.02 | 0.41 |
| 1:V:587:PHE:HA | 1:V:644:TRP:HD1 | 1.86 | 0.41 |
| 1:V:879:SER:O | 1:V:879:SER:OG | 2.34 | 0.41 |
| 1:V:897:HIS:HB3 | 1:V:899:MET:CE | 2.48 | 0.41 |
| 1:V:1147:MET:HE2 | 1:V:1147:MET:HB2 | 1.79 | 0.41 |
| 1:V:1161:ILE:O | 1:V:1203:MET:HE1 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W:2092:VAL:HG23 | 2:W:2177:TYR:O | 2.19 | 0.41 |
| 2:W:2191:LEU:O | 2:W:2225:ARG:NH2 | 2.53 | 0.41 |
| 3:X:2946[A]:GLN:CD | 3:X:2947[A]:ALA:N | 2.72 | 0.41 |
| 3:X:3137[B]:ARG:HD3 | 3:X:3137[B]:ARG:HA | 1.71 | 0.41 |
| 3:X:3192[A]:PHE:HD2 | 3:X:3192[A]:PHE:HA | 1.77 | 0.41 |
| 3:X:3218[A]:LEU:HD12 | 3:X:3218[A]:LEU:HA | 1.78 | 0.41 |
| 1:Y:266:LEU:HD12 | 1:Y:266:LEU:HA | 1.90 | 0.41 |
| 2:Z:2398:PHE:CE1 | 2:Z:2484:ALA:HB2 | 2.55 | 0.41 |
| 2:Z:2575:LEU:HD23 | 2:Z:2575:LEU:HA | 1.94 | 0.41 |
| 2:Z:2745:PRO:HA | 2:Z:2764:THR:HA | 2.02 | 0.41 |
| 3:a:3113[A]:ASP:OD2 | 3:a:3115[A]:LEU:HB2 | 2.20 | 0.41 |
| 3:a:3200[B]:LEU:O | 3:a:3203[B]:HIS:HB3 | 2.20 | 0.41 |
| 1:b:77:GLU:O | 1:b:81:VAL:HG23 | 2.21 | 0.41 |
| 1:b:361:GLU:HG2 | 1:b:363:THR:HG22 | 2.02 | 0.41 |
| 1:b:494:VAL:HG13 | 1:b:631:TRP:HZ3 | 1.85 | 0.41 |
| 3:d:2995[A]:GLN:CG | 3:d:3168[A]:THR:HG21 | 2.48 | 0.41 |
| 3:d:3048[B]:ASP:HB3 | 3:d:3099[B]:PRO:HD2 | 2.01 | 0.41 |
| 3:d:3176[A]:LYS:C | 3:d:3177[A]:SER:HG | 2.13 | 0.41 |
| 1:A:70:ARG:HA | 1:A:214:GLU:CD | 2.43 | 0.41 |
| 1:A:1470:GLU:HG3 | 1:A:1530:LEU:HD12 | 2.02 | 0.41 |
| 1:A:1649:THR:HG22 | 2:E:2325:ALA:HA | 2.02 | 0.41 |
| 3:C:3146[A]:CYS:O | 3:C:3146[A]:CYS:SG | 2.78 | 0.41 |
| 3:C:3146[B]:CYS:C | 3:L:3161[B]:GLU:HG3 | 2.45 | 0.41 |
| 3:C:3148[B]:ILE:HD12 | 3:C:3175[B]:TYR:OH | 2.21 | 0.41 |
| 3:C:3151[B]:LEU:O | 3:L:3154[B]:PRO:CB | 2.61 | 0.41 |
| 3:C:3281[B]:PHE:CZ | 3:C:3305[B]:ILE:HG21 | 2.55 | 0.41 |
| 1:D:11:THR:HG22 | 1:D:13:ASP:H | 1.86 | 0.41 |
| 1:D:407:GLN:HA | 1:D:408:GLY:HA2 | 1.69 | 0.41 |
| 2:E:2725:GLN:OE1 | 2:E:2728:ARG:NH2 | 2.31 | 0.41 |
| 2:E:2858:ASP:O | 2:E:2862:LYS:HG2 | 2.20 | 0.41 |
| 3:F:2961[A]:HIS:HB2 | 3:F:2992[A]:TYR:HE2 | 1.80 | 0.41 |
| 3:F:2973[B]:THR:C | 3:a:3107[B]:LEU:HD12 | 2.45 | 0.41 |
| 3:F:2976[B]:ALA:O | 3:F:2978[B]:CYS:N | 2.46 | 0.41 |
| 3:F:3067[A]:ARG:HA | 3:F:3067[A]:ARG:HD3 | 1.87 | 0.41 |
| 3:F:3173[B]:THR:OG1 | 3:a:3152[B]:LYS:HA | 2.21 | 0.41 |
| 3:F:3298[A]:ASN:CA | 3:F:3299[A]:LEU:HB2 | 2.44 | 0.41 |
| 1:G:897:HIS:HB3 | 1:G:899:MET:SD | 2.61 | 0.41 |
| 1:G:1108:TYR:HB2 | 1:G:1114:TYR:CE1 | 2.55 | 0.41 |
| 1:G:1275:ARG:HH21 | 1:G:1375:ASN:ND2 | 2.18 | 0.41 |
| 1:G:1415:ASP:OD1 | 1:G:1484:CYS:HB2 | 2.19 | 0.41 |
| 2:H:2554:PRO:HB3 | 2:H:2556:TYR:HB2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2938[B]:LEU:HD12 | 3:I:2938[B]:LEU:HA | 1.85 | 0.41 |
| 3:I:2966[A]:SER:HB2 | 3:I:2977[A]:CYS:H | 1.85 | 0.41 |
| 3:I:2975[B]:PHE:CE2 | 3:R:2988[B]:TRP:CH2 | 3.04 | 0.41 |
| 3:I:2995[B]:GLN:O | 3:I:2996[B]:MET:C | 2.62 | 0.41 |
| 3:I:3180[A]:TYR:HA | 3:I:3183[A]:LEU:CD2 | 2.51 | 0.41 |
| 3:I:3276[B]:ASP:C | 3:I:3278[B]:HIS:N | 2.75 | 0.41 |
| 1:J:4:ARG:HD2 | 1:J:89:ILE:O | 2.20 | 0.41 |
| 1:J:212:ASN:O | 1:J:215:ARG:HB3 | 2.21 | 0.41 |
| 1:J:474:LEU:HD22 | 1:J:475:ASN:H | 1.85 | 0.41 |
| 1:J:543:ASN:HA | 1:J:544:PRO:HD3 | 1.87 | 0.41 |
| 1:J:604:ASN:O | 1:J:607:HIS:HB2 | 2.20 | 0.41 |
| 1:J:1289:GLU:O | 1:J:1292:SER:OG | 2.24 | 0.41 |
| 1:J:1482:ALA:HB3 | 1:J:1489:MET:HE3 | 2.03 | 0.41 |
| 2:K:2650:GLY:N | 2:K:2651:GLN:HA | 2.35 | 0.41 |
| 3:L:3010[B]:PRO:HG2 | 3:L:3118[B]:VAL:HG13 | 2.03 | 0.41 |
| 3:L:3133[A]:LEU:HD12 | 3:L:3133[A]:LEU:HA | 1.86 | 0.41 |
| 3:L:3133[A]:LEU:HD13 | 3:L:3197[A]:ILE:HG23 | 2.02 | 0.41 |
| 3:L:3185[A]:TYR:HD2 | 3:L:3186[A]:GLU:N | 2.19 | 0.41 |
| 3:L:3185[B]:TYR:HD2 | 3:L:3186[B]:GLU:N | 2.19 | 0.41 |
| 3:L:3230[B]:PHE:HB2 | 3:L:3242[B]:GLY:C | 2.45 | 0.41 |
| 1:M:294:LYS:O | 1:M:297:ARG:HB2 | 2.20 | 0.41 |
| 1:M:319:ILE:HG23 | 1:M:379:VAL:HG13 | 2.01 | 0.41 |
| 1:M:323:ILE:HA | 1:M:324:PRO:HD3 | 1.84 | 0.41 |
| 1:M:627:ASP:HA | 1:M:628:PRO:HD3 | 1.88 | 0.41 |
| 1:M:1301:PRO:HB3 | 1:M:1308:VAL:HG12 | 2.03 | 0.41 |
| 2:N:2089:ARG:HH11 | 2:N:2163:GLU:CD | 2.28 | 0.41 |
| 2:N:2454:MET:HB3 | 2:N:2456:LEU:HG | 2.03 | 0.41 |
| 3:O:2965[A]:LEU:CG | 3:O:2974[A]:ALA:CB | 2.85 | 0.41 |
| 3:O:3281[A]:PHE:CZ | 3:O:3305[A]:ILE:HG21 | 2.55 | 0.41 |
| 1:P:35:GLN:HE22 | 1:P:127:GLU:HG3 | 1.86 | 0.41 |
| 1:P:604:ASN:ND2 | 1:P:763:LEU:H | 2.19 | 0.41 |
| 1:P:1081:MET:HG2 | 1:P:1100:SER:O | 2.20 | 0.41 |
| 2:Q:2695:MET:HE1 | 2:Q:2707:PHE:HB2 | 2.03 | 0.41 |
| 2:Q:2858:ASP:O | 2:Q:2862:LYS:HG2 | 2.20 | 0.41 |
| 3:R:2933[A]:SER:CA | 3:R:2936[A]:GLU:HB3 | 2.48 | 0.41 |
| 3:R:2939[B]:ARG:CB | 3:R:3032[B]:PRO:HG2 | 2.44 | 0.41 |
| 3:R:3148[B]:ILE:HD12 | 3:R:3175[B]:TYR:OH | 2.20 | 0.41 |
| 3:R:3196[A]:THR:OG1 | 3:R:3199[A]:GLN:OE1 | 2.38 | 0.41 |
| 1:S:320:LYS:HB2 | 1:S:380:THR:HG23 | 2.01 | 0.41 |
| 1:S:486:THR:HA | 1:S:489:HIS:ND1 | 2.35 | 0.41 |
| 1:S:490:TRP:HE1 | 1:S:670:PRO:CD | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:2995[A]:GLN:O | 3:U:2996[A]:MET:C | 2.63 | 0.41 |
| 3:U:3023[A]:ILE:O | 3:U:3026[A]:THR:OG1 | 2.34 | 0.41 |
| 3:U:3113[A]:ASP:OD2 | 3:U:3115[A]:LEU:HB2 | 2.20 | 0.41 |
| 3:U:3113[B]:ASP:OD2 | 3:U:3115[B]:LEU:HB2 | 2.20 | 0.41 |
| 3:U:3229[B]:ASN:N | 3:U:3286[B]:THR:O | 2.52 | 0.41 |
| 3:U:3258[B]:PHE:CZ | 3:d:2969[B]:TYR:CD2 | 3.09 | 0.41 |
| 1:V:151:GLN:H | 1:V:151:GLN:HG3 | 1.54 | 0.41 |
| 1:V:1013:ILE:HG21 | 1:V:1192:TYR:CE1 | 2.54 | 0.41 |
| 1:V:1311:CYS:HB3 | 1:V:1495:PRO:HD3 | 2.01 | 0.41 |
| 2:W:2534:PHE:CE2 | 2:W:2755:PRO:HB3 | 2.55 | 0.41 |
| 3:X:2963[B]:MET:SD | 3:X:2963[B]:MET:O | 2.79 | 0.41 |
| 3:X:2989[A]:HIS:NE2 | 9:X:3401[A]:CUO:O1 | 2.54 | 0.41 |
| 3:X:3185[B]:TYR:CZ | 3:X:3187[B]:TYR:CE2 | 3.09 | 0.41 |
| 1:Y:94:TRP:NE1 | 1:Y:212:ASN:HD22 | 2.18 | 0.41 |
| 1:Y:893:ALA:HB2 | 1:Y:1182:ASN:HD22 | 1.85 | 0.41 |
| 1:Y:1458:HIS:HA | 1:Y:1461:VAL:HB | 2.01 | 0.41 |
| 1:Y:1568:VAL:HB | 1:Y:1632:LEU:HG | 2.02 | 0.41 |
| 2:Z:2360:TYR:HB2 | 2:Z:2366:TYR:CE1 | 2.55 | 0.41 |
| 2:Z:2392:ASP:OD2 | 2:Z:2488:ARG:NH2 | 2.49 | 0.41 |
| 3:a:2963[A]:MET:SD | 3:a:2963[A]:MET:O | 2.79 | 0.41 |
| 3:a:3013[B]:ASP:CG | 3:a:3015[B]:THR:HG1 | 2.25 | 0.41 |
| 3:a:3192[B]:PHE:HD2 | 3:a:3192[B]:PHE:HA | 1.77 | 0.41 |
| 1:b:118:ALA:HB1 | 1:b:119:LYS:CA | 2.46 | 0.41 |
| 1:b:387:ASN:OD1 | 1:b:387:ASN:N | 2.41 | 0.41 |
| 1:b:464:LEU:HD22 | 1:b:622:HIS:CG | 2.54 | 0.41 |
| 1:b:1321:HIS:CD2 | 1:b:1465:TRP:CH2 | 3.09 | 0.41 |
| 2:c:2720:ILE:HG12 | 2:c:2781:LEU:HG | 2.02 | 0.41 |
| 3:d:2963[A]:MET:SD | 3:d:2963[A]:MET:O | 2.79 | 0.41 |
| 3:d:2963[B]:MET:SD | 3:d:2963[B]:MET:O | 2.79 | 0.41 |
| 3:d:3028[A]:PRO:HG2 | 3:d:3029[A]:LYS:HG2 | 2.02 | 0.41 |
| 3:d:3113[A]:ASP:OD2 | 3:d:3115[A]:LEU:HB2 | 2.20 | 0.41 |
| 3:d:3180[B]:TYR:HA | 3:d:3183[B]:LEU:CD2 | 2.51 | 0.41 |
| 1:A:71:LEU:HA | 1:A:71:LEU:HD12 | 1.83 | 0.41 |
| 1:A:120:LYS:HB3 | 1:A:121:ASN:CA | 2.50 | 0.41 |
| 1:A:443:MET:HE1 | 1:A:455:TYR:CE1 | 2.56 | 0.41 |
| 1:A:451:SER:CB | 1:A:1273:SER:HA | 2.51 | 0.41 |
| 1:A:1033:LEU:H | 1:A:1180:SER:HB2 | 1.85 | 0.41 |
| 1:A:1090:ILE:H | 1:A:1090:ILE:HG12 | 1.60 | 0.41 |
| 2:B:2867:PRO:CG | 3:C:2932[A]:PRO:HG2 | 2.42 | 0.41 |
| 3:C:3028[B]:PRO:HG2 | 3:C:3029[B]:LYS:HG2 | 2.02 | 0.41 |
| 3:C:3113[B]:ASP:OD2 | 3:C:3115[B]:LEU:HB2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3200[A]:LEU:O | 3:C:3203[A]:HIS:HB3 | 2.20 | 0.41 |
| 1:D:1148:LEU:HD23 | 1:D:1229:LYS:HD2 | 2.02 | 0.41 |
| 1:D:1406:HIS:O | 1:D:1410:VAL:HG23 | 2.20 | 0.41 |
| 3:F:3146[B]:CYS:O | 3:F:3146[B]:CYS:SG | 2.78 | 0.41 |
| 3:F:3148[A]:ILE:HD12 | 3:F:3175[A]:TYR:OH | 2.20 | 0.41 |
| 3:F:3150[B]:LYS:NZ | 3:a:3162[B]:ASP:O | 2.42 | 0.41 |
| 3:F:3230[A]:PHE:HB2 | 3:F:3242[A]:GLY:C | 2.44 | 0.41 |
| 3:F:3248[B]:LEU:HB2 | 3:a:2972[B]:GLY:C | 2.37 | 0.41 |
| 3:F:3259[B]:ASP:HB3 | 3:a:3162[B]:ASP:HA | 2.03 | 0.41 |
| 3:F:3281[B]:PHE:CZ | 3:F:3305[B]:ILE:HG21 | 2.55 | 0.41 |
| 1:G:456:GLN:HG2 | 1:G:551:GLU:CB | 2.47 | 0.41 |
| 1:G:618:MET:SD | 1:G:629:MET:HE3 | 2.60 | 0.41 |
| 1:G:733:PHE:HZ | 1:G:746:LEU:HD13 | 1.86 | 0.41 |
| 1:G:891:LYS:HB2 | 1:G:892:TYR:HB3 | 2.01 | 0.41 |
| 1:G:1074:ILE:HG21 | 2:K:2870:LEU:HD22 | 2.02 | 0.41 |
| 1:G:1082:SER:OG | 1:G:1083:PRO:HD3 | 2.20 | 0.41 |
| 2:H:2110:MET:O | 2:H:2119:PHE:N | 2.52 | 0.41 |
| 3:I:2963[B]:MET:SD | 3:I:2963[B]:MET:O | 2.79 | 0.41 |
| 3:I:3094[A]:SER:HG | 3:I:3227[A]:ASP:CG | 2.28 | 0.41 |
| 3:I:3096[A]:VAL:CG1 | 3:I:3115[A]:LEU:CD1 | 2.86 | 0.41 |
| 3:I:3113[A]:ASP:OD2 | 3:I:3115[A]:LEU:HB2 | 2.20 | 0.41 |
| 3:I:3133[A]:LEU:HD13 | 3:I:3197[A]:ILE:HG23 | 2.02 | 0.41 |
| 3:I:3155[B]:MET:CA | 3:R:3153[B]:LYS:HD2 | 2.40 | 0.41 |
| 3:I:3196[A]:THR:N | 3:I:3199[A]:GLN:CB | 2.64 | 0.41 |
| 1:J:260:ASN:OD1 | 1:J:271:HIS:NE2 | 2.51 | 0.41 |
| 1:J:319:ILE:HG22 | 1:J:338:ALA:HB3 | 2.03 | 0.41 |
| 1:J:415:VAL:HG11 | 1:J:697:ALA:HB2 | 2.03 | 0.41 |
| 1:J:767:LYS:HE2 | 1:J:767:LYS:HB3 | 1.83 | 0.41 |
| 1:J:1018:ILE:HB | 1:J:1045:HIS:NE2 | 2.35 | 0.41 |
| 1:J:1182:ASN:HD22 | 1:J:1182:ASN:N | 2.09 | 0.41 |
| 2:K:2179:ASP:HB3 | 2:K:2303:ARG:NH1 | 2.35 | 0.41 |
| 2:K:2296:LEU:O | 2:K:2299:SER:HB3 | 2.20 | 0.41 |
| 3:L:3028[B]:PRO:HG2 | 3:L:3029[B]:LYS:N | 2.36 | 0.41 |
| 3:L:3299[A]:LEU:O | 3:L:3300[A]:LEU:C | 2.60 | 0.41 |
| 1:M:804:ASP:HB2 | 1:M:810:LEU:HD11 | 2.02 | 0.41 |
| 1:M:1207:TYR:O | 1:M:1207:TYR:CD1 | 2.74 | 0.41 |
| 1:M:1215:LEU:HD11 | 1:M:1228:LEU:HD21 | 2.03 | 0.41 |
| 1:M:1300:CYS:HB3 | 1:M:1494:ARG:NH1 | 2.34 | 0.41 |
| 2:N:2097:LEU:HD12 | 2:Q:2235:PRO:HG2 | 2.03 | 0.41 |
| 2:N:2421:TYR:HB2 | 2:N:2454:MET:HE3 | 2.03 | 0.41 |
| 2:N:2742:MET:HA | 2:N:2765:PRO:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:2963[B]:MET:HE2 | 3:X:2968[B]:GLN:C | 2.46 | 0.41 |
| 3:O:2995[B]:GLN:O | 3:O:2996[B]:MET:C | 2.63 | 0.41 |
| 3:O:3041[A]:ALA:O | 3:O:3042[A]:ASP:HB2 | 2.20 | 0.41 |
| 3:O:3185[B]:TYR:HD2 | 3:O:3186[B]:GLU:N | 2.19 | 0.41 |
| 1:P:1225:VAL:HG12 | 1:P:1226:THR:H | 1.85 | 0.41 |
| 1:P:1299:GLN:HB2 | 1:P:1311:CYS:SG | 2.60 | 0.41 |
| 2:Q:2451:LEU:HD23 | 2:Q:2451:LEU:HA | 1.87 | 0.41 |
| 2:Q:2561:HIS:HA | 2:Q:2562:GLY:HA2 | 1.80 | 0.41 |
| 3:R:2995[B]:GLN:O | 3:R:2996[B]:MET:C | 2.63 | 0.41 |
| 3:R:3024[B]:LEU:CD1 | 3:R:3024[B]:LEU:C | 2.85 | 0.41 |
| 3:R:3028[B]:PRO:HG2 | 3:R:3029[B]:LYS:HG2 | 2.02 | 0.41 |
| 3:R:3148[A]:ILE:HD12 | 3:R:3175[A]:TYR:OH | 2.20 | 0.41 |
| 1:S:41:HIS:O | 1:S:201:SER:OG | 2.27 | 0.41 |
| 1:S:241:HIS:CD2 | 1:S:795:GLU:HA | 2.56 | 0.41 |
| 2:T:2740:ASP:OD2 | 1:V:1232:THR:HA | 2.20 | 0.41 |
| 3:U:2931[B]:THR:HG1 | 3:U:2934[B]:GLU:CD | 2.04 | 0.41 |
| 3:U:2952[B]:ALA:CA | 3:U:2956[B]:LYS:CB | 2.89 | 0.41 |
| 3:U:3028[B]:PRO:HG2 | 3:U:3029[B]:LYS:N | 2.36 | 0.41 |
| 3:U:3041[A]:ALA:O | 3:U:3042[A]:ASP:HB2 | 2.20 | 0.41 |
| 3:U:3161[A]:GLU:H | 3:U:3161[A]:GLU:CD | 2.19 | 0.41 |
| 1:V:4:ARG:HD2 | 1:V:89:ILE:O | 2.20 | 0.41 |
| 1:V:319:ILE:HG22 | 1:V:338:ALA:HB3 | 2.02 | 0.41 |
| 1:V:669:LYS:HB2 | 1:V:670:PRO:HD3 | 2.03 | 0.41 |
| 1:V:1018:ILE:HB | 1:V:1045:HIS:NE2 | 2.36 | 0.41 |
| 2:W:2525:LYS:NZ | 2:W:2526:ARG:HH12 | 2.18 | 0.41 |
| 2:W:2656:LEU:HA | 2:W:2656:LEU:HD23 | 1.84 | 0.41 |
| 3:X:3010[B]:PRO:HG2 | 3:X:3118[B]:VAL:HG13 | 2.03 | 0.41 |
| 3:X:3182[B]:GLN:H | 3:X:3182[B]:GLN:HG2 | 1.56 | 0.41 |
| 3:X:3298[A]:ASN:CB | 3:X:3300[A]:LEU:CD2 | 2.61 | 0.41 |
| 1:Y:260:ASN:OD1 | 1:Y:271:HIS:NE2 | 2.49 | 0.41 |
| 1:Y:385:ALA:HB2 | 1:Y:391:MET:SD | 2.61 | 0.41 |
| 1:Y:474:LEU:HD12 | 1:Y:474:LEU:HA | 1.78 | 0.41 |
| 2:Z:2394:VAL:H | 2:Z:2448:THR:HB | 1.85 | 0.41 |
| 3:a:3171[B]:HIS:O | 3:a:3172[B]:SER:C | 2.63 | 0.41 |
| 3:a:3274[A]:ARG:NE | 3:a:3274[A]:ARG:CA | 2.84 | 0.41 |
| 1:b:112:ASP:N | 1:b:112:ASP:OD1 | 2.51 | 0.41 |
| 1:b:306:PHE:CE2 | 1:b:399:PRO:HG3 | 2.55 | 0.41 |
| 1:b:855:ARG:HD3 | 1:b:957:ASN:O | 2.20 | 0.41 |
| 1:b:1237:GLU:HA | 1:b:1238:PRO:HD2 | 1.88 | 0.41 |
| 1:b:1423:TYR:OH | 1:b:1461:VAL:O | 2.38 | 0.41 |
| 2:c:2404:GLY:HA2 | 2:c:2405:SER:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:c:2500:ILE:HD11 | 2:c:2504:ARG:HB3 | 2.02 | 0.41 |
| 2:c:2625:LEU:HA | 2:c:2638:ARG:NH1 | 2.26 | 0.41 |
| 3:d:3028[B]:PRO:HG2 | 3:d:3029[B]:LYS:N | 2.36 | 0.41 |
| 3:d:3096[B]:VAL:CG1 | 3:d:3115[B]:LEU:CD1 | 2.86 | 0.41 |
| 3:d:3148[B]:ILE:HG22 | 3:d:3152[B]:LYS:HE3 | 2.01 | 0.41 |
| 3:d:3281[A]:PHE:CZ | 3:d:3305[A]:ILE:HG21 | 2.55 | 0.41 |
| 3:d:3299[A]:LEU:O | 3:d:3300[A]:LEU:C | 2.60 | 0.41 |
| 1:A:293:LEU:O | 1:A:296:ARG:HG2 | 2.20 | 0.41 |
| 1:A:1319:PHE:HB3 | 1:A:1420:GLU:OE2 | 2.21 | 0.41 |
| 1:A:1647:ASN:HA | 1:A:1648:PRO:HD3 | 1.93 | 0.41 |
| 2:B:2469:VAL:HG12 | 2:B:2475:GLU:HG2 | 2.03 | 0.41 |
| 3:C:2969[B]:TYR:CE2 | 3:L:3093[B]:HIS:NE2 | 2.78 | 0.41 |
| 3:C:2989[A]:HIS:NE2 | 9:L:3401[A]:CUO:O1 | 2.54 | 0.41 |
| 3:C:3041[B]:ALA:O | 3:C:3042[B]:ASP:HB2 | 2.20 | 0.41 |
| 3:C:3171[A]:HIS:O | 3:C:3172[A]:SER:C | 2.63 | 0.41 |
| 3:C:3276[B]:ASP:C | 3:C:3278[B]:HIS:N | 2.75 | 0.41 |
| 1:D:425:ARG:HB2 | 1:D:703:TYR:CD2 | 2.55 | 0.41 |
| 1:D:622:HIS:HE1 | 1:D:766:SER:HB3 | 1.85 | 0.41 |
| 3:F:3180[B]:TYR:CA | 3:F:3183[B]:LEU:CD2 | 2.95 | 0.41 |
| 3:F:3200[A]:LEU:O | 3:F:3203[A]:HIS:HB3 | 2.20 | 0.41 |
| 1:G:614:GLU:O | 1:G:617:SER:OG | 2.28 | 0.41 |
| 1:G:905:TRP:HE1 | 1:G:1083:PRO:HD2 | 1.85 | 0.41 |
| 1:G:1576:THR:H | 1:G:1581:GLU:CG | 2.32 | 0.41 |
| 2:H:2765:PRO:HA | 2:H:2768:LEU:HD11 | 2.01 | 0.41 |
| 3:I:3013[A]:ASP:CG | 3:I:3015[A]:THR:HG1 | 2.24 | 0.41 |
| 3:I:3028[A]:PRO:HG2 | 3:I:3029[A]:LYS:N | 2.36 | 0.41 |
| 3:I:3155[A]:MET:HE2 | 3:I:3155[A]:MET:HB3 | 1.99 | 0.41 |
| 3:I:3185[B]:TYR:CE2 | 3:I:3187[B]:TYR:HE2 | 2.31 | 0.41 |
| 1:J:1312:CYS:HA | 1:J:1322:TRP:CE2 | 2.56 | 0.41 |
| 1:J:1599:MET:HA | 1:J:1600:PRO:HD2 | 1.93 | 0.41 |
| 2:K:2398:PHE:HE2 | 2:K:2466:THR:HG21 | 1.86 | 0.41 |
| 3:L:2966[B]:SER:HB2 | 3:L:2977[B]:CYS:H | 1.85 | 0.41 |
| 3:L:3028[A]:PRO:HG2 | 3:L:3029[A]:LYS:N | 2.36 | 0.41 |
| 3:L:3067[B]:ARG:HA | 3:L:3067[B]:ARG:HD3 | 1.87 | 0.41 |
| 3:L:3171[B]:HIS:C | 3:L:3173[B]:THR:N | 2.73 | 0.41 |
| 3:L:3180[A]:TYR:HA | 3:L:3183[A]:LEU:CD2 | 2.51 | 0.41 |
| 3:L:3185[A]:TYR:HE2 | 3:L:3187[A]:TYR:CD2 | 2.35 | 0.41 |
| 1:M:89:ILE:H | 1:M:89:ILE:HG12 | 1.69 | 0.41 |
| 1:M:436:GLU:O | 1:M:440:ARG:HB2 | 2.20 | 0.41 |
| 1:M:450:LYS:NZ | 1:M:505:ARG:HH21 | 2.18 | 0.41 |
| 1:M:548:ALA:HA | 1:M:549:PRO:HD3 | 1.94 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:597:VAL:HG23 | 1:M:598:GLN:H | 1.85 | 0.41 |
| 1:M:1146:PHE:CD2 | 1:M:1231:VAL:HG12 | 2.55 | 0.41 |
| 1:M:1156:LEU:HB2 | 1:M:1176:TYR:CE1 | 2.56 | 0.41 |
| 2:N:2515:ARG:HD2 | 2:Q:2168:ARG:NH2 | 2.36 | 0.41 |
| 3:O:2933[A]:SER:CA | 3:O:2936[A]:GLU:HB3 | 2.48 | 0.41 |
| 3:O:2989[B]:HIS:NE2 | 9:O:3401[B]:CUO:O1 | 2.53 | 0.41 |
| 3:O:3028[A]:PRO:HG2 | 3:O:3029[A]:LYS:HG2 | 2.02 | 0.41 |
| 3:O:3083[A]:ILE:HD11 | 3:O:3260[A]:ARG:HG3 | 2.03 | 0.41 |
| 3:O:3113[A]:ASP:OD2 | 3:O:3115[A]:LEU:HB2 | 2.20 | 0.41 |
| 3:O:3194[B]:GLY:C | 3:O:3195[B]:MET:CG | 2.90 | 0.41 |
| 3:O:3293[B]:LYS:CG | 3:O:3294[B]:SER:CB | 2.98 | 0.41 |
| 3:O:3299[B]:LEU:O | 3:O:3300[B]:LEU:C | 2.60 | 0.41 |
| 1:P:639:ARG:HB2 | 1:P:703:TYR:CE1 | 2.55 | 0.41 |
| 1:P:745:ASP:OD1 | 1:P:759:SER:OG | 2.31 | 0.41 |
| 1:P:975:PRO:HG3 | 1:P:1026:GLU:HG2 | 2.03 | 0.41 |
| 1:P:1560:HIS:HB3 | 1:P:1602:GLN:HG3 | 2.03 | 0.41 |
| 2:Q:2156:ARG:HD2 | 2:Q:2357:VAL:HG12 | 2.02 | 0.41 |
| 2:Q:2800:LYS:HB3 | 3:R:3023[A]:ILE:CD1 | 2.51 | 0.41 |
| 2:Q:2898:LYS:H | 2:Q:2898:LYS:HG3 | 1.43 | 0.41 |
| 3:R:3034[B]:HIS:HB3 | 3:R:3035[B]:HIS:CE1 | 2.50 | 0.41 |
| 3:R:3113[A]:ASP:OD2 | 3:R:3115[A]:LEU:HB2 | 2.20 | 0.41 |
| 3:R:3133[B]:LEU:HD12 | 3:R:3133[B]:LEU:HA | 1.86 | 0.41 |
| 3:R:3193[A]:HIS:ND1 | 3:R:3193[A]:HIS:N | 2.68 | 0.41 |
| 3:R:3232[B]:VAL:HG21 | 3:R:3273[B]:LEU:HD11 | 2.00 | 0.41 |
| 1:S:25:MET:HE2 | 1:S:34:TYR:HA | 2.02 | 0.41 |
| 1:S:285:THR:HG22 | 1:S:287:GLU:H | 1.85 | 0.41 |
| 1:S:817:PRO:HA | 1:S:818:PRO:HD3 | 1.87 | 0.41 |
| 1:S:1234:VAL:O | 2:W:2739:LEU:HG | 2.21 | 0.41 |
| 1:S:1339:SER:CB | 1:S:1340:GLY:HA2 | 2.51 | 0.41 |
| 2:T:2323:ASN:HB3 | 1:V:1652:PHE:O | 2.21 | 0.41 |
| 2:T:2345:ASN:HA | 2:T:2346:PRO:HD2 | 1.96 | 0.41 |
| 2:T:2648:ALA:HB2 | 2:T:2656:LEU:HD12 | 2.03 | 0.41 |
| 3:U:2966[A]:SER:HB2 | 3:U:2977[A]:CYS:H | 1.85 | 0.41 |
| 3:U:2989[A]:HIS:NE2 | 9:U:3401[A]:CUO:O1 | 2.53 | 0.41 |
| 3:U:3146[B]:CYS:O | 3:U:3146[B]:CYS:SG | 2.78 | 0.41 |
| 3:U:3185[B]:TYR:HD2 | 3:U:3186[B]:GLU:N | 2.19 | 0.41 |
| 3:U:3256[B]:TRP:CE3 | 3:d:2969[B]:TYR:CG | 3.05 | 0.41 |
| 1:V:40:TYR:HE2 | 1:V:75:GLN:HG2 | 1.85 | 0.41 |
| 1:V:95:THR:HG21 | 1:V:159:VAL:HG21 | 2.02 | 0.41 |
| 1:V:816:PRO:HA | 1:V:817:PRO:HD3 | 1.95 | 0.41 |
| 1:V:877:HIS:HE1 | 1:V:1042:PHE:CE2 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W:2622:ASN:HA | 2:W:2623:PRO:HD3 | 1.94 | 0.41 |
| 3:X:2989[B]:HIS:O | 3:X:2991[B]:LEU:N | 2.54 | 0.41 |
| 3:X:2995[B]:GLN:O | 3:X:2996[B]:MET:C | 2.63 | 0.41 |
| 3:X:3031[B]:ASN:HA | 3:X:3032[B]:PRO:HD2 | 1.87 | 0.41 |
| 3:X:3183[B]:LEU:N | 3:X:3184[B]:ASN:CA | 2.80 | 0.41 |
| 3:X:3193[A]:HIS:ND1 | 3:X:3193[A]:HIS:N | 2.68 | 0.41 |
| 1:Y:183:HIS:HE1 | 1:Y:206:PHE:HD1 | 1.69 | 0.41 |
| 1:Y:407:GLN:HA | 1:Y:408:GLY:HA2 | 1.78 | 0.41 |
| 1:Y:1229:LYS:HD3 | 1:Y:1230:LEU:N | 2.34 | 0.41 |
| 1:Y:1417:CYS:O | 1:Y:1421:VAL:HG22 | 2.20 | 0.41 |
| 2:Z:2133:PRO:HG2 | 2:Z:2140:ARG:HA | 2.03 | 0.41 |
| 2:Z:2779:ASP:HA | 2:Z:2780:HIS:HA | 1.73 | 0.41 |
| 3:a:2957[B]:ILE:HD11 | 3:a:2995[B]:GLN:C | 2.46 | 0.41 |
| 3:a:3028[B]:PRO:HG2 | 3:a:3029[B]:LYS:N | 2.36 | 0.41 |
| 3:a:3041[B]:ALA:O | 3:a:3042[B]:ASP:HB2 | 2.20 | 0.41 |
| 3:a:3146[B]:CYS:O | 3:a:3146[B]:CYS:SG | 2.78 | 0.41 |
| 3:a:3193[B]:HIS:ND1 | 3:a:3193[B]:HIS:N | 2.68 | 0.41 |
| 1:b:975:PRO:HG2 | 1:b:1024:GLY:CA | 2.51 | 0.41 |
| 2:c:2277:LYS:H | 2:c:2277:LYS:HE2 | 1.86 | 0.41 |
| 2:c:2552:GLU:HA | 2:c:2553:ALA:HA | 1.78 | 0.41 |
| 2:c:2610:ASP:OD1 | 2:c:2610:ASP:N | 2.54 | 0.41 |
| 3:d:2957[B]:ILE:HD11 | 3:d:2995[B]:GLN:C | 2.46 | 0.41 |
| 3:d:3010[B]:PRO:HG2 | 3:d:3118[B]:VAL:HG13 | 2.03 | 0.41 |
| 3:d:3096[A]:VAL:CG1 | 3:d:3115[A]:LEU:CD1 | 2.86 | 0.41 |
| 3:d:3148[A]:ILE:HD12 | 3:d:3175[A]:TYR:OH | 2.20 | 0.41 |
| 3:d:3171[A]:HIS:C | 3:d:3173[A]:THR:N | 2.73 | 0.41 |
| 3:d:3254[B]:MET:H | 3:d:3254[B]:MET:HG2 | 1.71 | 0.41 |
| 1:A:450:LYS:HG3 | 1:A:551:GLU:OE1 | 2.20 | 0.41 |
| 1:A:456:GLN:O | 1:A:460:GLU:HG3 | 2.21 | 0.41 |
| 1:A:747:PHE:CE1 | 1:A:756:PHE:HD2 | 2.38 | 0.41 |
| 1:A:901:THR:HG22 | 1:A:904:HIS:HB2 | 2.01 | 0.41 |
| 1:A:1560:HIS:HB3 | 1:A:1602:GLN:HG3 | 2.03 | 0.41 |
| 2:B:2824:CYS:HB3 | 2:B:2826:GLU:O | 2.20 | 0.41 |
| 2:B:2885:SER:OG | 2:B:2886:VAL:N | 2.54 | 0.41 |
| 3:C:3077[B]:ASP:HB3 | 3:C:3080[B]:ASP:OD2 | 2.21 | 0.41 |
| 3:C:3137[B]:ARG:HB3 | 3:C:3139[B]:LEU:HD21 | 1.97 | 0.41 |
| 3:C:3180[A]:TYR:HA | 3:C:3183[A]:LEU:CD2 | 2.51 | 0.41 |
| 3:C:3281[B]:PHE:HE1 | 3:C:3305[B]:ILE:HG21 | 1.81 | 0.41 |
| 1:D:514:TRP:HZ2 | 1:D:606:ILE:HD11 | 1.86 | 0.41 |
| 1:D:736:MET:HE2 | 1:D:816:PRO:HD3 | 2.03 | 0.41 |
| 1:D:829:ALA:HA | 1:D:830:ASN:C | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:2097:LEU:HD23 | 2:E:2097:LEU:HA | 1.92 | 0.41 |
| 2:E:2104:ILE:HG21 | 2:E:2196:TYR:CD2 | 2.56 | 0.41 |
| 2:E:2145:LEU:HD22 | 2:E:2154:TRP:CD1 | 2.56 | 0.41 |
| 3:F:2963[B]:MET:SD | 3:F:2963[B]:MET:O | 2.79 | 0.41 |
| 3:F:3152[B]:LYS:HB3 | 3:a:3172[B]:SER:N | 2.23 | 0.41 |
| 3:F:3180[A]:TYR:HA | 3:F:3183[A]:LEU:CD2 | 2.51 | 0.41 |
| 3:F:3274[B]:ARG:NE | 3:F:3274[B]:ARG:CA | 2.84 | 0.41 |
| 3:F:3300[A]:LEU:HD23 | 3:F:3300[A]:LEU:H | 1.83 | 0.41 |
| 1:G:41:HIS:HD2 | 1:G:68:TRP:CZ3 | 2.38 | 0.41 |
| 1:G:674:LYS:HE3 | 1:G:674:LYS:HB2 | 1.89 | 0.41 |
| 1:G:737:GLY:HA2 | 1:G:771:TRP:CZ2 | 2.55 | 0.41 |
| 2:H:2625:LEU:HD13 | 2:H:2626:ARG:HG2 | 2.01 | 0.41 |
| 2:H:2811:HIS:NE2 | 2:H:2896:LEU:HD22 | 2.36 | 0.41 |
| 3:I:2980[B]:HIS:HA | 3:I:2985[B]:PHE:HD2 | 1.86 | 0.41 |
| 3:I:3139[A]:LEU:CD2 | 3:I:3139[A]:LEU:H | 2.34 | 0.41 |
| 3:I:3180[B]:TYR:CA | 3:I:3183[B]:LEU:CD2 | 2.95 | 0.41 |
| 9:I:3401[A]:CUO:O1 | 3:R:2989[A]:HIS:NE2 | 2.54 | 0.41 |
| 1:J:306:PHE:CE2 | 1:J:399:PRO:HG3 | 2.56 | 0.41 |
| 1:J:705:THR:HG22 | 1:J:1118:THR:HG23 | 2.02 | 0.41 |
| 1:J:1252:PRO:HD3 | 1:J:1473:ARG:NH2 | 2.36 | 0.41 |
| 1:J:1647:ASN:HA | 1:J:1648:PRO:HD3 | 1.93 | 0.41 |
| 2:K:2562:GLY:H | 2:K:2846:TRP:CB | 2.34 | 0.41 |
| 2:K:2569:TRP:HZ2 | 2:K:2748:PRO:HG3 | 1.86 | 0.41 |
| 2:K:2677:GLU:O | 2:K:2680:HIS:HB3 | 2.20 | 0.41 |
| 3:L:3011[A]:TYR:CB | 3:L:3121[A]:SER:HB2 | 2.49 | 0.41 |
| 3:L:3024[B]:LEU:CD1 | 3:L:3024[B]:LEU:C | 2.85 | 0.41 |
| 3:L:3137[B]:ARG:HA | 3:L:3137[B]:ARG:HD3 | 1.71 | 0.41 |
| 3:L:3192[A]:PHE:HD2 | 3:L:3192[A]:PHE:HA | 1.77 | 0.41 |
| 3:L:3274[A]:ARG:NE | 3:L:3274[A]:ARG:CA | 2.84 | 0.41 |
| 3:L:3281[A]:PHE:CZ | 3:L:3305[A]:ILE:HG21 | 2.55 | 0.41 |
| 1:M:447:MET:HA | 1:M:455:TYR:CB | 2.50 | 0.41 |
| 2:N:2695:MET:HE2 | 2:N:2695:MET:HB2 | 1.87 | 0.41 |
| 3:O:2951[B]:ASP:CG | 3:O:2952[B]:ALA:H | 2.28 | 0.41 |
| 3:O:2968[B]:GLN:HB3 | 3:X:2979[B]:GLN:HG2 | 2.03 | 0.41 |
| 3:O:2989[B]:HIS:O | 3:O:2991[B]:LEU:N | 2.54 | 0.41 |
| 3:O:3028[A]:PRO:HG2 | 3:O:3029[A]:LYS:N | 2.36 | 0.41 |
| 3:O:3034[A]:HIS:HB3 | 3:O:3035[A]:HIS:CE1 | 2.50 | 0.41 |
| 3:O:3083[B]:ILE:HD11 | 3:O:3260[B]:ARG:HG3 | 2.03 | 0.41 |
| 3:O:3180[A]:TYR:HA | 3:O:3183[A]:LEU:CD2 | 2.51 | 0.41 |
| 3:O:3221[B]:ALA:HA | 3:X:3161[B]:GLU:HG2 | 1.21 | 0.41 |
| 3:O:3281[A]:PHE:HE1 | 3:O:3305[A]:ILE:HG21 | 1.81 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3281[B]:PHE:CZ | 3:O:3305[B]:ILE:HG21 | 2.56 | 0.41 |
| 1:P:187:GLY:HA2 | 1:P:193:SER:HB2 | 2.03 | 0.41 |
| 1:P:327:ASP:OD1 | 1:P:328:LYS:N | 2.54 | 0.41 |
| 1:P:732:GLY:HA2 | 1:P:777:TYR:O | 2.20 | 0.41 |
| 1:P:891:LYS:HB3 | 1:P:892:TYR:HD2 | 1.81 | 0.41 |
| 1:P:1077:LEU:O | 1:P:1102:PRO:HG2 | 2.21 | 0.41 |
| 1:P:1380:GLY:HA3 | 1:P:1450:TYR:O | 2.21 | 0.41 |
| 1:P:1562:ILE:HG22 | 1:P:1563:LYS:H | 1.85 | 0.41 |
| 2:Q:2377:SER:HB3 | 2:Q:2380:GLN:HG3 | 2.02 | 0.41 |
| 3:R:2957[B]:ILE:HD11 | 3:R:2995[B]:GLN:C | 2.46 | 0.41 |
| 3:R:2963[A]:MET:SD | 3:R:2963[A]:MET:O | 2.79 | 0.41 |
| 3:R:3139[B]:LEU:CD2 | 3:R:3139[B]:LEU:H | 2.34 | 0.41 |
| 1:S:120:LYS:H | 1:S:121:ASN:HA | 1.86 | 0.41 |
| 2:T:2527:LEU:HD22 | 2:T:2581:MET:HG2 | 2.02 | 0.41 |
| 3:U:2965[A]:LEU:CG | 3:U:2974[A]:ALA:CB | 2.85 | 0.41 |
| 3:U:2969[B]:TYR:CA | 3:d:2981[B]:GLY:CA | 2.97 | 0.41 |
| 3:U:3180[B]:TYR:HA | 3:U:3183[B]:LEU:CD2 | 2.51 | 0.41 |
| 3:U:3255[B]:PRO:CG | 3:d:3252[B]:TYR:HB3 | 2.51 | 0.41 |
| 3:U:3281[B]:PHE:CZ | 3:U:3305[B]:ILE:HG21 | 2.55 | 0.41 |
| 1:V:548:ALA:N | 1:V:559:THR:HG22 | 2.35 | 0.41 |
| 1:V:904:HIS:CD2 | 1:V:904:HIS:H | 2.38 | 0.41 |
| 3:X:2948[B]:ASP:HB2 | 3:X:2953[B]:GLY:HA3 | 1.99 | 0.41 |
| 3:X:2980[B]:HIS:HA | 3:X:2985[B]:PHE:HD2 | 1.86 | 0.41 |
| 3:X:2989[B]:HIS:NE2 | 9:X:3401[B]:CUO:O1 | 2.53 | 0.41 |
| 3:X:3028[B]:PRO:HG2 | 3:X:3029[B]:LYS:N | 2.36 | 0.41 |
| 3:X:3083[A]:ILE:HD11 | 3:X:3260[A]:ARG:HG3 | 2.03 | 0.41 |
| 1:Y:148:GLN:C | 1:Y:150:GLY:N | 2.78 | 0.41 |
| 1:Y:554:LYS:HD3 | 1:Y:554:LYS:HA | 1.79 | 0.41 |
| 1:Y:1401:ARG:NE | 3:d:3182[B]:GLN:OE1 | 2.53 | 0.41 |
| 1:Y:1621:ASN:HA | 3:d:3188[B]:ASP:CB | 2.51 | 0.41 |
| 2:Z:2602:LEU:HG | 2:Z:2603:PRO:HD2 | 2.02 | 0.41 |
| 2:Z:2716:ARG:O | 2:Z:2720:ILE:HG13 | 2.21 | 0.41 |
| 3:a:3089[A]:HIS:CE1 | 3:a:3119[A]:HIS:CE1 | 2.81 | 0.41 |
| 3:a:3146[A]:CYS:O | 3:a:3146[A]:CYS:SG | 2.78 | 0.41 |
| 3:a:3171[A]:HIS:O | 3:a:3172[A]:SER:C | 2.63 | 0.41 |
| 3:a:3180[B]:TYR:HA | 3:a:3183[B]:LEU:CD2 | 2.51 | 0.41 |
| 3:a:3193[A]:HIS:ND1 | 3:a:3193[A]:HIS:N | 2.69 | 0.41 |
| 1:b:1430:ILE:HD13 | 1:b:1457:HIS:CD2 | 2.56 | 0.41 |
| 1:b:1647:ASN:HA | 1:b:1648:PRO:HD3 | 1.96 | 0.41 |
| 2:c:2446:GLU:CG | 2:c:2448:THR:HG23 | 2.50 | 0.41 |
| 2:c:2670:CYS:HB3 | 2:c:2850:ARG:CZ | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:2970[B]:PRO:C | 3:d:2972[B]:GLY:H | 2.23 | 0.41 |
| 3:d:3200[B]:LEU:O | 3:d:3203[B]:HIS:HB3 | 2.20 | 0.41 |
| 3:d:3281[B]:PHE:CZ | 3:d:3305[B]:ILE:HG21 | 2.56 | 0.41 |
| 1:A:236:GLY:HA2 | 1:A:819:ILE:HB | 2.03 | 0.41 |
| 1:A:468:CYS:SG | 1:A:669:LYS:HB3 | 2.61 | 0.41 |
| 1:A:749:VAL:HB | 1:A:754:GLU:HB3 | 2.03 | 0.41 |
| 1:A:837:HIS:HA | 1:A:1113:HIS:O | 2.21 | 0.41 |
| 1:A:1059:LEU:HB3 | 1:A:1063:ARG:NH2 | 2.36 | 0.41 |
| 1:A:1075:GLU:H | 1:A:1075:GLU:HG3 | 1.61 | 0.41 |
| 2:B:2235:PRO:HB3 | 2:B:2240:GLN:CD | 2.46 | 0.41 |
| 2:B:2582:ARG:HG2 | 2:E:2109:ARG:HD3 | 2.02 | 0.41 |
| 3:C:2969[B]:TYR:CE2 | 3:L:3089[B]:HIS:NE2 | 2.86 | 0.41 |
| 3:C:2975[B]:PHE:CZ | 3:L:2961[B]:HIS:CD2 | 3.09 | 0.41 |
| 3:C:2976[A]:ALA:O | 3:C:2978[A]:CYS:N | 2.46 | 0.41 |
| 3:C:2979[A]:GLN:NE2 | 3:C:3155[A]:MET:HE3 | 2.19 | 0.41 |
| 3:C:2980[A]:HIS:HA | 3:C:2985[A]:PHE:HD2 | 1.86 | 0.41 |
| 3:C:2980[B]:HIS:HA | 3:C:2985[B]:PHE:HD2 | 1.86 | 0.41 |
| 3:C:2995[A]:GLN:O | 3:C:2996[A]:MET:C | 2.63 | 0.41 |
| 3:C:3028[A]:PRO:HG2 | 3:C:3029[A]:LYS:N | 2.36 | 0.41 |
| 3:C:3148[A]:ILE:HD12 | 3:C:3175[A]:TYR:OH | 2.20 | 0.41 |
| 3:C:3180[B]:TYR:HA | 3:C:3183[B]:LEU:CD2 | 2.51 | 0.41 |
| 3:C:3185[B]:TYR:HD2 | 3:C:3186[B]:GLU:N | 2.19 | 0.41 |
| 3:C:3192[B]:PHE:HD2 | 3:C:3192[B]:PHE:HA | 1.77 | 0.41 |
| 3:C:3232[B]:VAL:CG2 | 3:C:3273[B]:LEU:CD1 | 2.99 | 0.41 |
| 3:C:3298[B]:ASN:HA | 3:C:3300[B]:LEU:N | 2.36 | 0.41 |
| 1:D:588:GLU:OE2 | 1:D:728:ARG:NH1 | 2.53 | 0.41 |
| 1:D:946:GLU:CG | 1:D:955:LYS:HB3 | 2.51 | 0.41 |
| 1:D:1200:MET:HE1 | 1:D:1205:LEU:HD23 | 2.03 | 0.41 |
| 1:D:1278:PHE:HD2 | 1:D:1376:PRO:HB2 | 1.85 | 0.41 |
| 1:D:1528:ASP:OD1 | 1:D:1528:ASP:N | 2.53 | 0.41 |
| 1:D:1564:ALA:HB1 | 4:m:1:NAG:H81 | 2.03 | 0.41 |
| 2:E:2100:ILE:O | 2:E:2104:ILE:HG12 | 2.21 | 0.41 |
| 2:E:2132:CYS:HA | 2:E:2133:PRO:C | 2.46 | 0.41 |
| 2:E:2361:LYS:HD3 | 2:E:2367:GLU:HG2 | 2.03 | 0.41 |
| 2:E:2568:HIS:CD2 | 2:E:2718:TRP:CH2 | 3.08 | 0.41 |
| 2:E:2647:LEU:HD12 | 2:E:2647:LEU:HA | 1.64 | 0.41 |
| 3:F:3028[A]:PRO:HG2 | 3:F:3029[A]:LYS:N | 2.36 | 0.41 |
| 3:F:3113[B]:ASP:OD2 | 3:F:3115[B]:LEU:HB2 | 2.20 | 0.41 |
| 3:F:3133[A]:LEU:HD13 | 3:F:3197[A]:ILE:HG23 | 2.02 | 0.41 |
| 3:F:3139[A]:LEU:CD2 | 3:F:3139[A]:LEU:H | 2.34 | 0.41 |
| 3:F:3149[B]:ASN:HA | 3:a:3169[B]:LYS:H | 1.25 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:3153[B]:LYS:HE3 | 3:a:3155[B]:MET:O | 2.21 | 0.41 |
| 3:F:3158[B]:PHE:HB2 | 3:a:3153[B]:LYS:CG | 2.51 | 0.41 |
| 3:F:3172[B]:SER:HB3 | 3:a:3150[B]:LYS:C | 2.46 | 0.41 |
| 1:G:294:LYS:HA | 1:G:297:ARG:HD2 | 2.03 | 0.41 |
| 1:G:745:ASP:OD1 | 1:G:759:SER:OG | 2.37 | 0.41 |
| 1:G:792:MET:HB2 | 1:G:793:PHE:HD1 | 1.86 | 0.41 |
| 1:G:943:LEU:HD12 | 1:G:944:GLU:H | 1.86 | 0.41 |
| 1:G:977:GLU:OE1 | 1:G:978:ALA:N | 2.54 | 0.41 |
| 1:G:1002:GLU:HG3 | 1:G:1065:LYS:HD3 | 2.01 | 0.41 |
| 1:G:1037:ALA:HA | 1:G:1042:PHE:CG | 2.56 | 0.41 |
| 1:G:1081:MET:HG2 | 1:G:1100:SER:O | 2.21 | 0.41 |
| 1:G:1302:SER:CB | 1:G:1494:ARG:HH22 | 2.34 | 0.41 |
| 1:G:1319:PHE:CZ | 1:G:1424:GLU:HG3 | 2.55 | 0.41 |
| 2:H:2218:SER:HG | 2:H:2221:THR:HG1 | 1.60 | 0.41 |
| 2:H:2309:GLN:HG2 | 2:H:2319:ALA:HB1 | 2.02 | 0.41 |
| 2:H:2442:LEU:HG | 1:J:1604:ASP:HB2 | 2.02 | 0.41 |
| 2:H:2527:LEU:HG | 2:H:2536:PHE:HB2 | 2.03 | 0.41 |
| 2:H:2561:HIS:HA | 2:H:2562:GLY:HA2 | 1.83 | 0.41 |
| 2:H:2742:MET:HA | 2:H:2765:PRO:HB2 | 2.02 | 0.41 |
| 2:H:2816:SER:HB2 | 2:H:2886:VAL:HG21 | 2.03 | 0.41 |
| 3:I:2946[B]:GLN:CD | 3:I:2947[B]:ALA:N | 2.72 | 0.41 |
| 3:I:2954[B]:TYR:HA | 3:I:2957[B]:ILE:CG2 | 2.50 | 0.41 |
| 3:I:2965[A]:LEU:CG | 3:I:2974[A]:ALA:CB | 2.85 | 0.41 |
| 3:I:2982[B]:MET:SD | 3:R:3156[B]:MET:HB2 | 2.60 | 0.41 |
| 3:I:2987[B]:HIS:CD2 | 3:I:3178[B]:PHE:CE1 | 3.08 | 0.41 |
| 3:I:3096[B]:VAL:CG1 | 3:I:3115[B]:LEU:CD1 | 2.86 | 0.41 |
| 3:I:3148[B]:ILE:HD12 | 3:I:3175[B]:TYR:OH | 2.20 | 0.41 |
| 3:I:3153[B]:LYS:NZ | 3:R:3156[B]:MET:C | 2.79 | 0.41 |
| 3:I:3163[B]:ASN:ND2 | 3:R:3150[B]:LYS:CG | 2.37 | 0.41 |
| 3:I:3173[B]:THR:HG21 | 3:R:3173[B]:THR:HG1 | 1.77 | 0.41 |
| 3:I:3180[B]:TYR:HA | 3:I:3183[B]:LEU:CD2 | 2.51 | 0.41 |
| 3:I:3185[B]:TYR:HD2 | 3:I:3186[B]:GLU:N | 2.19 | 0.41 |
| 3:I:3281[A]:PHE:CZ | 3:I:3305[A]:ILE:HG21 | 2.55 | 0.41 |
| 1:J:51:ASP:HA | 1:J:52:GLY:HA2 | 1.66 | 0.41 |
| 1:J:418:ASP:OD1 | 1:J:418:ASP:N | 2.53 | 0.41 |
| 1:J:572:SER:OG | 1:J:574:GLY:HA3 | 2.21 | 0.41 |
| 1:J:876:PHE:CD2 | 1:J:1083:PRO:HB2 | 2.56 | 0.41 |
| 1:J:877:HIS:CE1 | 1:J:905:TRP:HZ3 | 2.39 | 0.41 |
| 1:J:1258:ARG:HG2 | 1:J:1335:LEU:HD11 | 2.01 | 0.41 |
| 1:J:1480:ASN:ND2 | 1:J:1518:ASP:HB3 | 2.34 | 0.41 |
| 1:J:1550:ARG:HD2 | 1:J:1551:ASP:H | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2130:PRO:CB | 2:K:2142:ALA:HB3 | 2.51 | 0.41 |
| 2:K:2305:TRP:HZ2 | 2:K:2358:PHE:CE1 | 2.39 | 0.41 |
| 2:K:2746:MET:HG2 | 2:K:2763:SER:O | 2.20 | 0.41 |
| 3:L:2951[A]:ASP:C | 3:L:2956[A]:LYS:HZ1 | 2.17 | 0.41 |
| 3:L:2957[B]:ILE:HD11 | 3:L:2995[B]:GLN:C | 2.46 | 0.41 |
| 3:L:2980[A]:HIS:HA | 3:L:2985[A]:PHE:HD2 | 1.86 | 0.41 |
| 3:L:2980[B]:HIS:HA | 3:L:2985[B]:PHE:HD2 | 1.86 | 0.41 |
| 3:L:3028[A]:PRO:HG2 | 3:L:3029[A]:LYS:HG2 | 2.02 | 0.41 |
| 3:L:3067[A]:ARG:HA | 3:L:3067[A]:ARG:HD3 | 1.87 | 0.41 |
| 3:L:3083[A]:ILE:HD11 | 3:L:3260[A]:ARG:HG3 | 2.03 | 0.41 |
| 3:L:3089[A]:HIS:HD1 | 3:L:3119[A]:HIS:HE1 | 1.65 | 0.41 |
| 3:L:3139[B]:LEU:CD2 | 3:L:3139[B]:LEU:H | 2.34 | 0.41 |
| 3:L:3194[B]:GLY:C | 3:L:3195[B]:MET:CG | 2.90 | 0.41 |
| 3:L:3196[B]:THR:N | 3:L:3199[B]:GLN:CB | 2.64 | 0.41 |
| 3:L:3218[A]:LEU:HD12 | 3:L:3218[A]:LEU:HA | 1.78 | 0.41 |
| 3:L:3218[B]:LEU:HD12 | 3:L:3218[B]:LEU:HA | 1.78 | 0.41 |
| 3:L:3230[A]:PHE:HB2 | 3:L:3242[A]:GLY:C | 2.44 | 0.41 |
| 1:M:67:MET:H | 1:M:67:MET:HG2 | 1.57 | 0.41 |
| 1:M:92:TRP:CE3 | 1:M:102:PRO:HD3 | 2.55 | 0.41 |
| 1:M:416:ASN:N | 1:M:416:ASN:HD22 | 2.17 | 0.41 |
| 1:M:629:MET:HE2 | 1:M:629:MET:HB3 | 1.96 | 0.41 |
| 1:M:988:TYR:HB3 | 1:M:992:ALA:HB3 | 2.02 | 0.41 |
| 1:M:1007:PHE:CE1 | 1:M:1011:TYR:HB2 | 2.55 | 0.41 |
| 1:M:1080:PRO:HB2 | 1:M:1085:SER:CB | 2.50 | 0.41 |
| 1:M:1156:LEU:HD13 | 1:M:1176:TYR:CE1 | 2.56 | 0.41 |
| 1:M:1528:ASP:OD1 | 1:M:1528:ASP:N | 2.54 | 0.41 |
| 2:N:2184:MET:HB2 | 2:N:2231:LEU:O | 2.20 | 0.41 |
| 2:N:2398:PHE:CE2 | 2:N:2484:ALA:HB2 | 2.56 | 0.41 |
| 2:N:2570:HIS:CD2 | 2:N:2711:HIS:CE1 | 3.09 | 0.41 |
| 2:N:2595:TRP:CD2 | 2:N:2683:ILE:HG13 | 2.56 | 0.41 |
| 2:N:2606:LEU:HD21 | 2:N:2709:VAL:HG21 | 2.03 | 0.41 |
| 3:O:2957[A]:ILE:HD11 | 3:O:2995[A]:GLN:C | 2.46 | 0.41 |
| 3:O:2970[B]:PRO:CG | 3:X:2991[B]:LEU:HD12 | 2.50 | 0.41 |
| 3:O:2989[A]:HIS:O | 3:O:2991[A]:LEU:N | 2.54 | 0.41 |
| 3:O:3031[B]:ASN:HA | 3:O:3032[B]:PRO:HD2 | 1.87 | 0.41 |
| 3:O:3084[A]:GLN:HE21 | 3:O:3084[A]:GLN:HB3 | 1.71 | 0.41 |
| 3:O:3106[B]:THR:CG2 | 3:X:2970[B]:PRO:O | 2.46 | 0.41 |
| 3:O:3139[B]:LEU:CD2 | 3:O:3139[B]:LEU:H | 2.34 | 0.41 |
| 3:O:3151[A]:LEU:HB2 | 3:O:3175[A]:TYR:HE2 | 1.68 | 0.41 |
| 3:O:3194[A]:GLY:C | 3:O:3195[A]:MET:CG | 2.91 | 0.41 |
| 3:O:3218[B]:LEU:HD12 | 3:O:3218[B]:LEU:HA | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:3223[B]:GLY:N | 3:X:3162[B]:ASP:OD1 | 2.53 | 0.41 |
| 3:O:3253[B]:GLU:OE1 | 3:X:3161[B]:GLU:CD | 2.44 | 0.41 |
| 1:P:16:LEU:HD12 | 1:P:113:PRO:HG2 | 2.02 | 0.41 |
| 1:P:119:LYS:H | 1:P:119:LYS:HG2 | 1.71 | 0.41 |
| 1:P:567:LEU:HB2 | 1:P:571:PRO:HB3 | 2.01 | 0.41 |
| 1:P:1573:CYS:HA | 1:P:1583:CYS:O | 2.21 | 0.41 |
| 2:Q:2134:ASN:OD1 | 2:Q:2137:ALA:HB2 | 2.20 | 0.41 |
| 2:Q:2471:HIS:O | 2:Q:2471:HIS:ND1 | 2.47 | 0.41 |
| 3:R:2980[B]:HIS:HA | 3:R:2985[B]:PHE:HD2 | 1.86 | 0.41 |
| 3:R:3010[A]:PRO:HG2 | 3:R:3118[A]:VAL:HG13 | 2.03 | 0.41 |
| 3:R:3023[A]:ILE:O | 3:R:3026[A]:THR:OG1 | 2.34 | 0.41 |
| 3:R:3028[A]:PRO:HG2 | 3:R:3029[A]:LYS:N | 2.36 | 0.41 |
| 3:R:3028[B]:PRO:HG2 | 3:R:3029[B]:LYS:N | 2.36 | 0.41 |
| 3:R:3113[B]:ASP:OD2 | 3:R:3115[B]:LEU:HB2 | 2.20 | 0.41 |
| 3:R:3146[A]:CYS:O | 3:R:3146[A]:CYS:SG | 2.78 | 0.41 |
| 3:R:3151[B]:LEU:CB | 3:R:3175[B]:TYR:CE2 | 2.85 | 0.41 |
| 3:R:3180[A]:TYR:HA | 3:R:3183[A]:LEU:CD2 | 2.51 | 0.41 |
| 3:R:3200[B]:LEU:O | 3:R:3203[B]:HIS:HB3 | 2.20 | 0.41 |
| 3:R:3218[B]:LEU:HD13 | 3:R:3261[B]:LEU:HD23 | 2.01 | 0.41 |
| 3:R:3265[A]:ASP:OD1 | 3:R:3266[A]:ILE:N | 2.54 | 0.41 |
| 1:S:664:VAL:HG12 | 1:S:690:THR:HG22 | 2.02 | 0.41 |
| 1:S:718:ARG:HD2 | 1:S:718:ARG:HA | 1.81 | 0.41 |
| 1:S:902:PHE:N | 1:S:903:PRO:HD2 | 2.36 | 0.41 |
| 1:S:913:PHE:O | 1:S:917:LEU:HB2 | 2.21 | 0.41 |
| 1:S:1057:GLN:NE2 | 1:S:1067:TYR:O | 2.43 | 0.41 |
| 1:S:1078:ARG:NH1 | 2:W:2872:GLU:O | 2.45 | 0.41 |
| 1:S:1086:LEU:HB3 | 1:S:1090:ILE:HD12 | 2.03 | 0.41 |
| 1:S:1348:TRP:CZ3 | 1:S:1460:ASN:HB3 | 2.56 | 0.41 |
| 1:S:1359:ILE:O | 1:S:1391:ARG:NH2 | 2.54 | 0.41 |
| 1:S:1426:LEU:O | 1:S:1429:THR:HB | 2.20 | 0.41 |
| 1:S:1487:PRO:O | 1:S:1491:GLN:NE2 | 2.52 | 0.41 |
| 2:T:2361:LYS:HD2 | 2:T:2362:GLN:H | 1.85 | 0.41 |
| 2:T:2381:LEU:HD23 | 2:T:2381:LEU:HA | 1.90 | 0.41 |
| 2:T:2481:LEU:HD23 | 2:T:2481:LEU:HA | 1.96 | 0.41 |
| 2:T:2679:ILE:O | 2:T:2682:SER:HB3 | 2.21 | 0.41 |
| 2:T:2749:PHE:HA | 2:T:2754:ASN:ND2 | 2.36 | 0.41 |
| 3:U:2969[B]:TYR:CZ | 3:d:2980[B]:HIS:CG | 3.08 | 0.41 |
| 3:U:2974[B]:ALA:N | 3:d:3222[B]:ILE:N | 2.58 | 0.41 |
| 3:U:3010[A]:PRO:HG2 | 3:U:3118[A]:VAL:HG13 | 2.03 | 0.41 |
| 3:U:3034[B]:HIS:HB3 | 3:U:3035[B]:HIS:CE1 | 2.50 | 0.41 |
| 3:U:3077[B]:ASP:HB3 | 3:U:3080[B]:ASP:OD2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:U:3134[A]:GLN:C | 3:U:3136[A]:TYR:N | 2.77 | 0.41 |
| 3:U:3193[A]:HIS:ND1 | 3:U:3193[A]:HIS:N | 2.69 | 0.41 |
| 3:U:3281[A]:PHE:CZ | 3:U:3305[A]:ILE:HG21 | 2.55 | 0.41 |
| 1:V:227:ARG:HA | 1:V:228:GLY:HA2 | 1.84 | 0.41 |
| 1:V:237:LEU:HA | 1:V:240:PHE:CD2 | 2.56 | 0.41 |
| 1:V:425:ARG:HD2 | 1:V:703:TYR:CE1 | 2.56 | 0.41 |
| 1:V:450:LYS:HZ2 | 1:V:451:SER:H | 1.66 | 0.41 |
| 1:V:468:CYS:HA | 1:V:469:PRO:C | 2.45 | 0.41 |
| 1:V:912:ASN:OD1 | 1:V:1096:THR:HG21 | 2.21 | 0.41 |
| 1:V:1008:GLU:HA | 1:V:1011:TYR:HB3 | 2.03 | 0.41 |
| 1:V:1145:THR:HB | 1:V:1191:PRO:HB2 | 2.03 | 0.41 |
| 1:V:1149:GLU:HG3 | 1:V:1187:LYS:HB3 | 2.02 | 0.41 |
| 1:V:1267:GLU:H | 1:V:1267:GLU:HG2 | 1.74 | 0.41 |
| 1:V:1492:PRO:HB2 | 1:V:1497:SER:HB3 | 2.03 | 0.41 |
| 2:W:2506:ARG:NH1 | 2:W:2778:TYR:OH | 2.51 | 0.41 |
| 2:W:2612:TYR:HB2 | 1:Y:138:ALA:HB1 | 2.02 | 0.41 |
| 2:W:2667:GLU:HB3 | 2:W:2730:LEU:HD13 | 2.03 | 0.41 |
| 2:W:2744:PHE:HA | 2:W:2745:PRO:HD3 | 1.84 | 0.41 |
| 2:W:2745:PRO:HB2 | 2:W:2750:ILE:HD12 | 2.03 | 0.41 |
| 3:X:2942[A]:LEU:CD1 | 3:X:3033[A]:PHE:CZ | 3.04 | 0.41 |
| 3:X:2963[A]:MET:SD | 3:X:2963[A]:MET:O | 2.79 | 0.41 |
| 3:X:2966[A]:SER:HB2 | 3:X:2977[A]:CYS:H | 1.85 | 0.41 |
| 3:X:2995[A]:GLN:O | 3:X:2996[A]:MET:C | 2.63 | 0.41 |
| 3:X:3010[A]:PRO:HG2 | 3:X:3118[A]:VAL:HG13 | 2.03 | 0.41 |
| 3:X:3023[A]:ILE:HA | 3:X:3026[A]:THR:HG1 | 1.82 | 0.41 |
| 3:X:3023[B]:ILE:HA | 3:X:3026[B]:THR:HG1 | 1.84 | 0.41 |
| 3:X:3067[B]:ARG:HA | 3:X:3067[B]:ARG:HD3 | 1.87 | 0.41 |
| 3:X:3180[A]:TYR:HA | 3:X:3183[A]:LEU:CD2 | 2.51 | 0.41 |
| 3:X:3265[A]:ASP:OD1 | 3:X:3266[A]:ILE:N | 2.54 | 0.41 |
| 1:Y:398:ARG:HA | 1:Y:399:PRO:HD3 | 1.91 | 0.41 |
| 1:Y:548:ALA:HA | 1:Y:549:PRO:HD3 | 1.97 | 0.41 |
| 1:Y:566:ARG:HH11 | 1:Y:803:LYS:HZ2 | 1.69 | 0.41 |
| 1:Y:806:ASN:ND2 | 1:Y:806:ASN:C | 2.72 | 0.41 |
| 1:Y:834:ASP:OD1 | 1:Y:834:ASP:N | 2.54 | 0.41 |
| 1:Y:899:MET:HB3 | 1:Y:1012:GLU:OE1 | 2.21 | 0.41 |
| 1:Y:913:PHE:O | 1:Y:917:LEU:HB2 | 2.20 | 0.41 |
| 1:Y:1300:CYS:SG | 1:Y:1494:ARG:HB3 | 2.61 | 0.41 |
| 1:Y:1301:PRO:HD2 | 5:KA:1:NAG:H83 | 2.02 | 0.41 |
| 1:Y:1403:LEU:HD21 | 1:Y:1429:THR:HG21 | 2.03 | 0.41 |
| 1:Y:1493:MET:HG2 | 1:Y:1511:SER:O | 2.21 | 0.41 |
| 1:Y:1573:CYS:HB2 | 1:Y:1627:ARG:HG2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:2122:ILE:O | 2:Z:2125:PHE:HB2 | 2.21 | 0.41 |
| 2:Z:2168:ARG:O | 2:c:2503:ASN:HB3 | 2.21 | 0.41 |
| 2:Z:2180:TRP:HB3 | 2:Z:2184:MET:HE2 | 2.02 | 0.41 |
| 2:Z:2724:LEU:O | 2:Z:2728:ARG:HG3 | 2.21 | 0.41 |
| 3:a:2957[A]:ILE:HD11 | 3:a:2995[A]:GLN:C | 2.46 | 0.41 |
| 3:a:2980[B]:HIS:HA | 3:a:2985[B]:PHE:HD2 | 1.86 | 0.41 |
| 3:a:3010[A]:PRO:HG2 | 3:a:3118[A]:VAL:HG13 | 2.03 | 0.41 |
| 3:a:3010[B]:PRO:HG2 | 3:a:3118[B]:VAL:HG13 | 2.03 | 0.41 |
| 3:a:3023[A]:ILE:HA | 3:a:3026[A]:THR:HG1 | 1.84 | 0.41 |
| 3:a:3025[A]:VAL:CG2 | 3:a:3047[A]:ARG:NH1 | 2.73 | 0.41 |
| 3:a:3155[A]:MET:HE2 | 3:a:3155[A]:MET:HB3 | 1.99 | 0.41 |
| 3:a:3185[B]:TYR:CZ | 3:a:3187[B]:TYR:CE2 | 3.09 | 0.41 |
| 3:a:3196[A]:THR:OG1 | 3:a:3199[A]:GLN:OE1 | 2.38 | 0.41 |
| 1:b:35:GLN:OE1 | 1:b:127:GLU:HG2 | 2.21 | 0.41 |
| 1:b:93:ASP:HA | 1:b:212:ASN:HD21 | 1.85 | 0.41 |
| 1:b:468:CYS:HA | 1:b:469:PRO:C | 2.46 | 0.41 |
| 1:b:740:THR:OG1 | 1:b:741:SER:N | 2.54 | 0.41 |
| 1:b:1002:GLU:HG3 | 1:b:1065:LYS:HD3 | 2.03 | 0.41 |
| 1:b:1017:HIS:ND1 | 1:b:1021:LEU:HD11 | 2.36 | 0.41 |
| 1:b:1109:LYS:H | 1:b:1109:LYS:HG3 | 1.57 | 0.41 |
| 1:b:1161:ILE:HG21 | 1:b:1200:MET:HE3 | 2.02 | 0.41 |
| 1:b:1228:LEU:HA | 1:b:1228:LEU:HD23 | 1.77 | 0.41 |
| 1:b:1481:GLU:HG2 | 1:b:1482:ALA:H | 1.86 | 0.41 |
| 2:c:2153:GLN:OE1 | 2:c:2153:GLN:N | 2.48 | 0.41 |
| 2:c:2490:PRO:HA | 2:c:2491:PRO:HD3 | 1.97 | 0.41 |
| 2:c:2521:MET:HE3 | 2:c:2605:LEU:HD12 | 2.03 | 0.41 |
| 2:c:2640:ILE:HD13 | 2:c:2687:ILE:O | 2.20 | 0.41 |
| 3:d:2942[B]:LEU:CD1 | 3:d:3033[B]:PHE:CZ | 3.04 | 0.41 |
| 3:d:3028[A]:PRO:HG2 | 3:d:3029[A]:LYS:N | 2.36 | 0.41 |
| 3:d:3028[B]:PRO:HG2 | 3:d:3029[B]:LYS:HG2 | 2.02 | 0.41 |
| 3:d:3113[B]:ASP:OD2 | 3:d:3115[B]:LEU:HB2 | 2.20 | 0.41 |
| 3:d:3134[B]:GLN:C | 3:d:3136[B]:TYR:N | 2.77 | 0.41 |
| 3:d:3196[B]:THR:OG1 | 3:d:3199[B]:GLN:OE1 | 2.38 | 0.41 |
| 3:d:3229[A]:ASN:N | 3:d:3286[A]:THR:O | 2.52 | 0.41 |
| 3:d:3229[B]:ASN:O | 3:d:3286[B]:THR:N | 2.50 | 0.41 |
| 3:d:3265[A]:ASP:OD1 | 3:d:3266[A]:ILE:N | 2.54 | 0.41 |
| 3:d:3276[B]:ASP:C | 3:d:3278[B]:HIS:N | 2.75 | 0.41 |
| 3:d:3284[A]:LYS:CD | 3:d:3284[A]:LYS:C | 2.86 | 0.41 |
| 6:k:1:NAG:O4 | 6:k:2:NAG:O7 | 2.39 | 0.41 |
| 1:A:40:TYR:CD1 | 1:A:246:PRO:HG2 | 2.56 | 0.41 |
| 1:A:203:ASP:HA | 1:A:204:PRO:HD2 | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1492:PRO:HB2 | 1:A:1497:SER:CB | 2.48 | 0.41 |
| 1:A:1508:PHE:CD1 | 1:A:1508:PHE:C | 2.99 | 0.41 |
| 3:C:2954[A]:TYR:HA | 3:C:2957[A]:ILE:CG2 | 2.50 | 0.41 |
| 3:C:2963[A]:MET:SD | 3:C:2963[A]:MET:O | 2.79 | 0.41 |
| 3:C:2995[B]:GLN:O | 3:C:2996[B]:MET:C | 2.63 | 0.41 |
| 3:C:3242[A]:GLY:O | 3:C:3243[A]:GLY:O | 2.39 | 0.41 |
| 3:C:3274[A]:ARG:NE | 3:C:3274[A]:ARG:CA | 2.84 | 0.41 |
| 1:D:59:LEU:HD13 | 1:D:68:TRP:CD1 | 2.56 | 0.41 |
| 1:D:225:LYS:HD2 | 1:D:231:THR:HG21 | 2.03 | 0.41 |
| 1:D:568:PHE:O | 1:D:569:LYS:HD2 | 2.20 | 0.41 |
| 1:D:587:PHE:O | 1:D:651:ARG:NH2 | 2.43 | 0.41 |
| 1:D:717:GLN:NE2 | 1:D:832:LYS:HE3 | 2.35 | 0.41 |
| 2:E:2582:ARG:HG2 | 2:E:2586:ALA:O | 2.20 | 0.41 |
| 2:E:2651:GLN:C | 2:E:2653:GLU:H | 2.27 | 0.41 |
| 2:E:2764:THR:HA | 2:E:2765:PRO:HD3 | 1.96 | 0.41 |
| 3:F:2952[B]:ALA:N | 3:F:2953[B]:GLY:CA | 2.71 | 0.41 |
| 3:F:2957[B]:ILE:HD11 | 3:F:2995[B]:GLN:C | 2.46 | 0.41 |
| 3:F:2966[A]:SER:HB2 | 3:F:2977[A]:CYS:H | 1.85 | 0.41 |
| 3:F:2966[B]:SER:HB3 | 3:a:2982[B]:MET:HE1 | 2.00 | 0.41 |
| 3:F:2972[B]:GLY:N | 3:a:3248[B]:LEU:HD22 | 2.35 | 0.41 |
| 3:F:3048[B]:ASP:HB3 | 3:F:3099[B]:PRO:HD2 | 2.01 | 0.41 |
| 3:F:3137[B]:ARG:HB3 | 3:F:3139[B]:LEU:HD21 | 1.97 | 0.41 |
| 3:F:3152[B]:LYS:HB3 | 3:a:3170[B]:ALA:O | 2.21 | 0.41 |
| 3:F:3229[A]:ASN:N | 3:F:3286[A]:THR:O | 2.52 | 0.41 |
| 3:F:3265[B]:ASP:OD1 | 3:F:3266[B]:ILE:N | 2.54 | 0.41 |
| 1:G:35:GLN:NE2 | 1:G:129:LYS:HB2 | 2.36 | 0.41 |
| 1:G:164:GLU:OE2 | 1:G:297:ARG:HG2 | 2.21 | 0.41 |
| 1:G:1033:LEU:HA | 1:G:1036:SER:OG | 2.21 | 0.41 |
| 1:G:1149:GLU:HG3 | 1:G:1187:LYS:HE2 | 2.03 | 0.41 |
| 1:G:1380:GLY:O | 1:G:1389:THR:HG23 | 2.21 | 0.41 |
| 3:I:2980[A]:HIS:HA | 3:I:2985[A]:PHE:HD2 | 1.86 | 0.41 |
| 3:I:2989[B]:HIS:O | 3:I:2991[B]:LEU:N | 2.54 | 0.41 |
| 3:I:2991[B]:LEU:CD2 | 3:R:3153[B]:LYS:HG3 | 2.51 | 0.41 |
| 3:I:3028[B]:PRO:HG2 | 3:I:3029[B]:LYS:HG2 | 2.02 | 0.41 |
| 3:I:3169[B]:LYS:C | 3:R:3152[B]:LYS:HB2 | 2.46 | 0.41 |
| 3:I:3193[A]:HIS:ND1 | 3:I:3193[A]:HIS:N | 2.69 | 0.41 |
| 3:I:3281[B]:PHE:CZ | 3:I:3305[B]:ILE:HG21 | 2.55 | 0.41 |
| 1:J:750:ALA:HA | 1:J:796:TYR:HB3 | 2.02 | 0.41 |
| 1:J:842:ASN:OD1 | 1:J:843:VAL:N | 2.54 | 0.41 |
| 1:J:891:LYS:HA | 1:J:892:TYR:HA | 1.92 | 0.41 |
| 1:J:1302:SER:HA | 1:J:1303:GLU:HA | 1.90 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2399:LEU:HA | 2:K:2399:LEU:HD12 | 1.87 | 0.41 |
| 2:K:2818:ASP:OD2 | 2:K:2820:HIS:NE2 | 2.54 | 0.41 |
| 3:L:2989[A]:HIS:O | 3:L:2991[A]:LEU:N | 2.54 | 0.41 |
| 3:L:3010[A]:PRO:HG2 | 3:L:3118[A]:VAL:HG13 | 2.03 | 0.41 |
| 3:L:3083[B]:ILE:HD11 | 3:L:3260[B]:ARG:HG3 | 2.03 | 0.41 |
| 3:L:3134[A]:GLN:C | 3:L:3136[A]:TYR:N | 2.77 | 0.41 |
| 3:L:3139[A]:LEU:CD2 | 3:L:3139[A]:LEU:H | 2.34 | 0.41 |
| 3:L:3242[A]:GLY:O | 3:L:3243[A]:GLY:O | 2.39 | 0.41 |
| 1:M:131:GLU:OE2 | 1:M:192:HIS:HE1 | 2.04 | 0.41 |
| 1:M:876:PHE:CE2 | 1:M:1083:PRO:HB2 | 2.56 | 0.41 |
| 2:N:2534:PHE:CD2 | 2:N:2755:PRO:HB3 | 2.56 | 0.41 |
| 3:O:2975[B]:PHE:CD2 | 3:X:3172[B]:SER:O | 2.74 | 0.41 |
| 3:O:3028[B]:PRO:HG2 | 3:O:3029[B]:LYS:N | 2.36 | 0.41 |
| 3:O:3160[B]:SER:OG | 3:X:3150[B]:LYS:HB3 | 2.15 | 0.41 |
| 3:O:3180[A]:TYR:CA | 3:O:3183[A]:LEU:CD2 | 2.95 | 0.41 |
| 3:O:3182[A]:GLN:H | 3:O:3182[A]:GLN:HG2 | 1.56 | 0.41 |
| 3:O:3284[B]:LYS:CD | 3:O:3284[B]:LYS:C | 2.86 | 0.41 |
| 1:P:197:LEU:HG | 1:P:345:GLY:C | 2.46 | 0.41 |
| 1:P:305:ASN:HB3 | 1:P:400:ILE:HB | 2.03 | 0.41 |
| 1:P:450:LYS:HD3 | 1:P:1338:GLY:O | 2.20 | 0.41 |
| 1:P:1086:LEU:HD12 | 1:P:1086:LEU:N | 2.36 | 0.41 |
| 3:R:2942[A]:LEU:CD1 | 3:R:3033[A]:PHE:CZ | 3.04 | 0.41 |
| 3:R:3193[B]:HIS:ND1 | 3:R:3193[B]:HIS:N | 2.68 | 0.41 |
| 1:S:188:GLY:O | 1:S:386:ILE:HD11 | 2.20 | 0.41 |
| 1:S:1258:ARG:HG2 | 1:S:1335:LEU:CD1 | 2.51 | 0.41 |
| 1:S:1319:PHE:CE2 | 1:S:1424:GLU:HG3 | 2.56 | 0.41 |
| 2:T:2132:CYS:HB2 | 2:T:2142:ALA:CB | 2.51 | 0.41 |
| 2:T:2568:HIS:HB2 | 2:T:2746:MET:HE1 | 2.02 | 0.41 |
| 2:T:2764:THR:HG22 | 2:T:2766:SER:H | 1.84 | 0.41 |
| 2:T:2889:ALA:H | 2:T:2890:VAL:HA | 1.84 | 0.41 |
| 3:U:2957[A]:ILE:HD11 | 3:U:2995[A]:GLN:C | 2.46 | 0.41 |
| 3:U:3134[B]:GLN:C | 3:U:3136[B]:TYR:N | 2.77 | 0.41 |
| 3:U:3232[B]:VAL:HG21 | 3:U:3273[B]:LEU:HD11 | 2.00 | 0.41 |
| 3:U:3298[B]:ASN:HA | 3:U:3300[B]:LEU:N | 2.36 | 0.41 |
| 1:V:570:GLN:HE21 | 1:V:570:GLN:HB2 | 1.54 | 0.41 |
| 1:V:1258:ARG:HD2 | 1:V:1524:HIS:O | 2.20 | 0.41 |
| 1:V:1350:GLU:HA | 1:V:1351:PRO:HD2 | 1.93 | 0.41 |
| 1:V:1410:VAL:HG22 | 1:V:1422:HIS:HB3 | 2.03 | 0.41 |
| 1:V:1571:TYR:HA | 1:V:1585:ASN:O | 2.21 | 0.41 |
| 2:W:2156:ARG:O | 2:W:2160:VAL:HG13 | 2.21 | 0.41 |
| 2:W:2373:MET:HE3 | 2:W:2374:ASN:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:2976[B]:ALA:O | 3:X:2978[B]:CYS:N | 2.46 | 0.41 |
| 3:X:2980[A]:HIS:HA | 3:X:2985[A]:PHE:HD2 | 1.86 | 0.41 |
| 3:X:2980[A]:HIS:ND1 | 3:X:2980[A]:HIS:N | 2.59 | 0.41 |
| 3:X:3025[A]:VAL:CG2 | 3:X:3047[A]:ARG:NH1 | 2.73 | 0.41 |
| 3:X:3041[A]:ALA:O | 3:X:3042[A]:ASP:HB2 | 2.20 | 0.41 |
| 3:X:3276[A]:ASP:C | 3:X:3278[A]:HIS:N | 2.75 | 0.41 |
| 3:X:3281[B]:PHE:CZ | 3:X:3305[B]:ILE:HG21 | 2.55 | 0.41 |
| 1:Y:69:HIS:NE2 | 9:Y:2102:CUO:O2 | 2.53 | 0.41 |
| 1:Y:589:GLN:HG2 | 1:Y:594:ASP:CB | 2.49 | 0.41 |
| 1:Y:704:ASP:OD1 | 1:Y:705:THR:N | 2.49 | 0.41 |
| 1:Y:907:ARG:NH1 | 1:Y:1114:TYR:OH | 2.54 | 0.41 |
| 1:Y:1195:ASP:O | 1:Y:1197:THR:N | 2.54 | 0.41 |
| 1:Y:1334:LEU:HD12 | 1:Y:1334:LEU:HA | 1.90 | 0.41 |
| 1:Y:1613:ASP:CG | 3:d:3185[B]:TYR:C | 2.89 | 0.41 |
| 1:Y:1622:GLN:H | 1:Y:1622:GLN:HG3 | 1.43 | 0.41 |
| 2:Z:2866:PRO:HB3 | 3:a:2933[A]:SER:N | 2.36 | 0.41 |
| 2:Z:2903:TYR:OH | 3:a:2932[A]:PRO:HD2 | 2.21 | 0.41 |
| 3:a:2930[B]:LEU:N | 3:a:2930[B]:LEU:HD13 | 2.36 | 0.41 |
| 3:a:2932[A]:PRO:CA | 3:a:2935[A]:ILE:CD1 | 2.85 | 0.41 |
| 3:a:2948[A]:ASP:HB2 | 3:a:2953[A]:GLY:HA3 | 1.99 | 0.41 |
| 3:a:2966[A]:SER:HB2 | 3:a:2977[A]:CYS:H | 1.85 | 0.41 |
| 3:a:3084[A]:GLN:HE21 | 3:a:3084[A]:GLN:HB3 | 1.71 | 0.41 |
| 3:a:3133[B]:LEU:HD12 | 3:a:3133[B]:LEU:HA | 1.86 | 0.41 |
| 3:a:3148[A]:ILE:HD12 | 3:a:3175[A]:TYR:OH | 2.20 | 0.41 |
| 1:b:447:MET:HA | 1:b:455:TYR:HB3 | 2.01 | 0.41 |
| 1:b:491:HIS:CD2 | 1:b:634:HIS:CE1 | 3.09 | 0.41 |
| 1:b:514:TRP:CZ2 | 1:b:606:ILE:HD11 | 2.56 | 0.41 |
| 1:b:535:PRO:O | 1:b:538:LYS:HE3 | 2.21 | 0.41 |
| 1:b:1401:ARG:H | 1:b:1401:ARG:HG3 | 1.55 | 0.41 |
| 1:b:1470:GLU:HB3 | 1:b:1537:ILE:HD13 | 2.03 | 0.41 |
| 2:c:2089:ARG:HB2 | 2:c:2368:TYR:CD1 | 2.56 | 0.41 |
| 2:c:2606:LEU:HD13 | 2:c:2706:ILE:HG23 | 2.03 | 0.41 |
| 3:d:2938[A]:LEU:HD12 | 3:d:2938[A]:LEU:HA | 1.85 | 0.41 |
| 3:d:2952[A]:ALA:CA | 3:d:2956[A]:LYS:CB | 2.89 | 0.41 |
| 3:d:2989[A]:HIS:O | 3:d:2991[A]:LEU:N | 2.54 | 0.41 |
| 3:d:3133[B]:LEU:HD12 | 3:d:3133[B]:LEU:HA | 1.86 | 0.41 |
| 3:d:3185[B]:TYR:HD2 | 3:d:3186[B]:GLU:N | 2.19 | 0.41 |
| 1:A:128:ILE:N | 1:A:133:LYS:O | 2.49 | 0.40 |
| 1:A:462:HIS:HA | 1:A:490:TRP:CH2 | 2.56 | 0.40 |
| 1:A:492:ARG:HH22 | 1:A:641:TRP:CD1 | 2.40 | 0.40 |
| 1:A:1400:ASN:HD22 | 1:A:1400:ASN:HA | 1.53 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1519:TYR:CE2 | 1:A:1520:GLN:HG3 | 2.56 | 0.40 |
| 1:A:1528:ASP:N | 1:A:1528:ASP:OD1 | 2.55 | 0.40 |
| 1:A:1565:SER:HB3 | 1:A:1594:GLY:H | 1.86 | 0.40 |
| 2:B:2647:LEU:O | 2:B:2654:SER:HB2 | 2.20 | 0.40 |
| 2:B:2687:ILE:HD11 | 2:B:2695:MET:HG2 | 2.04 | 0.40 |
| 3:C:2963[B]:MET:SD | 3:C:2963[B]:MET:O | 2.79 | 0.40 |
| 3:C:3010[B]:PRO:HG2 | 3:C:3118[B]:VAL:HG13 | 2.03 | 0.40 |
| 3:C:3023[B]:ILE:O | 3:C:3026[B]:THR:OG1 | 2.34 | 0.40 |
| 3:C:3133[A]:LEU:HD13 | 3:C:3197[A]:ILE:HG23 | 2.02 | 0.40 |
| 3:C:3183[B]:LEU:H | 3:C:3184[B]:ASN:CA | 2.22 | 0.40 |
| 1:D:7:VAL:HG21 | 1:D:208:LEU:HD23 | 2.03 | 0.40 |
| 1:D:753:ASN:HD22 | 1:D:753:ASN:C | 2.29 | 0.40 |
| 3:F:2931[A]:THR:O | 3:F:2934[A]:GLU:HB2 | 2.22 | 0.40 |
| 3:F:2975[B]:PHE:O | 3:a:3253[B]:GLU:CG | 2.65 | 0.40 |
| 3:F:2983[B]:VAL:CG2 | 3:a:3161[B]:GLU:HB2 | 2.49 | 0.40 |
| 3:F:3028[B]:PRO:HG2 | 3:F:3029[B]:LYS:HG2 | 2.02 | 0.40 |
| 3:F:3084[A]:GLN:HE21 | 3:F:3084[A]:GLN:HB3 | 1.71 | 0.40 |
| 3:F:3150[B]:LYS:C | 3:a:3172[B]:SER:HB3 | 2.46 | 0.40 |
| 3:F:3306[A]:LEU:C | 3:F:3306[A]:LEU:CD1 | 2.85 | 0.40 |
| 1:G:695:TYR:N | 1:G:695:TYR:HD1 | 2.19 | 0.40 |
| 1:G:1025:THR:HG23 | 1:G:1221:THR:HA | 2.02 | 0.40 |
| 1:G:1156:LEU:HB2 | 1:G:1176:TYR:CE1 | 2.55 | 0.40 |
| 1:G:1248:ARG:HG3 | 1:G:1249:TRP:N | 2.36 | 0.40 |
| 2:H:2107:LEU:HD22 | 2:H:2209:PHE:CE1 | 2.55 | 0.40 |
| 2:H:2145:LEU:HD12 | 2:H:2145:LEU:HA | 1.93 | 0.40 |
| 2:H:2311:LEU:HD23 | 2:H:2311:LEU:HA | 1.98 | 0.40 |
| 2:H:2568:HIS:HD2 | 2:H:2718:TRP:CH2 | 2.40 | 0.40 |
| 2:H:2590:VAL:HA | 2:H:2591:PRO:HD3 | 1.90 | 0.40 |
| 2:H:2901:LEU:H | 1:J:1075:GLU:HG3 | 1.86 | 0.40 |
| 3:I:2952[A]:ALA:CA | 3:I:2956[A]:LYS:CB | 2.89 | 0.40 |
| 3:I:2970[B]:PRO:CA | 3:R:2989[B]:HIS:HD2 | 2.29 | 0.40 |
| 3:I:3010[B]:PRO:HG2 | 3:I:3118[B]:VAL:HG13 | 2.03 | 0.40 |
| 3:I:3023[A]:ILE:C | 3:I:3025[A]:VAL:N | 2.79 | 0.40 |
| 3:I:3093[B]:HIS:NE2 | 3:R:2969[B]:TYR:CD2 | 2.90 | 0.40 |
| 3:I:3113[B]:ASP:OD2 | 3:I:3115[B]:LEU:HB2 | 2.20 | 0.40 |
| 3:I:3139[B]:LEU:CD2 | 3:I:3139[B]:LEU:H | 2.34 | 0.40 |
| 3:I:3153[B]:LYS:O | 3:R:3154[B]:PRO:CA | 2.68 | 0.40 |
| 3:I:3229[B]:ASN:N | 3:I:3286[B]:THR:O | 2.52 | 0.40 |
| 3:I:3265[B]:ASP:OD1 | 3:I:3266[B]:ILE:N | 2.54 | 0.40 |
| 3:I:3299[A]:LEU:HB3 | 3:I:3300[A]:LEU:H | 1.54 | 0.40 |
| 1:J:1051:ARG:HD2 | 1:J:1118:THR:O | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:2303:ARG:NH2 | 2:K:2372:GLU:O | 2.53 | 0.40 |
| 3:L:3031[B]:ASN:HA | 3:L:3032[B]:PRO:HD2 | 1.87 | 0.40 |
| 3:L:3113[A]:ASP:OD2 | 3:L:3115[A]:LEU:HB2 | 2.20 | 0.40 |
| 3:L:3113[B]:ASP:OD2 | 3:L:3115[B]:LEU:HB2 | 2.20 | 0.40 |
| 1:M:1339:SER:OG | 1:M:1340:GLY:HA2 | 2.21 | 0.40 |
| 2:N:2403:PHE:CZ | 2:N:2428:VAL:HG21 | 2.56 | 0.40 |
| 2:N:2622:ASN:HA | 2:N:2623:PRO:HD3 | 1.96 | 0.40 |
| 2:N:2651:GLN:C | 2:N:2653:GLU:H | 2.29 | 0.40 |
| 3:O:2963[A]:MET:SD | 3:O:2963[A]:MET:O | 2.79 | 0.40 |
| 3:O:2987[A]:HIS:CD2 | 3:O:3178[A]:PHE:CE1 | 3.08 | 0.40 |
| 3:O:2987[B]:HIS:CD2 | 3:O:3178[B]:PHE:CE1 | 3.08 | 0.40 |
| 3:O:2995[A]:GLN:O | 3:O:2996[A]:MET:C | 2.63 | 0.40 |
| 3:O:3010[B]:PRO:HG2 | 3:O:3118[B]:VAL:HG13 | 2.03 | 0.40 |
| 3:O:3139[A]:LEU:CD2 | 3:O:3139[A]:LEU:H | 2.34 | 0.40 |
| 1:P:424:PHE:HB2 | 1:P:1128:GLN:NE2 | 2.36 | 0.40 |
| 1:P:953:GLU:HG3 | 1:P:954:ALA:O | 2.21 | 0.40 |
| 1:P:1137:LYS:HA | 1:P:1141:ARG:NH1 | 2.36 | 0.40 |
| 1:P:1293:PHE:O | 1:P:1311:CYS:HB2 | 2.20 | 0.40 |
| 2:Q:2361:LYS:HD2 | 2:Q:2362:GLN:H | 1.85 | 0.40 |
| 2:Q:2470:ALA:HB2 | 2:Q:2476:LEU:HD21 | 2.02 | 0.40 |
| 3:R:2957[A]:ILE:HD11 | 3:R:2995[A]:GLN:C | 2.46 | 0.40 |
| 3:R:3180[B]:TYR:HA | 3:R:3183[B]:LEU:CD2 | 2.51 | 0.40 |
| 3:R:3230[A]:PHE:HB2 | 3:R:3242[A]:GLY:C | 2.45 | 0.40 |
| 3:R:3232[A]:VAL:HG21 | 3:R:3273[A]:LEU:HD11 | 2.00 | 0.40 |
| 3:R:3276[A]:ASP:C | 3:R:3278[A]:HIS:N | 2.75 | 0.40 |
| 3:R:3298[A]:ASN:HA | 3:R:3300[A]:LEU:N | 2.36 | 0.40 |
| 1:S:474:LEU:HD12 | 1:S:475:ASN:N | 2.36 | 0.40 |
| 1:S:909:ILE:HG12 | 1:S:1084:PHE:CZ | 2.50 | 0.40 |
| 1:S:1034:GLU:HG3 | 1:S:1182:ASN:HD21 | 1.86 | 0.40 |
| 2:T:2344:LEU:HA | 2:T:2344:LEU:HD13 | 1.89 | 0.40 |
| 2:T:2446:GLU:HG2 | 2:T:2448:THR:HG22 | 2.04 | 0.40 |
| 3:U:2957[B]:ILE:HD11 | 3:U:2995[B]:GLN:C | 2.46 | 0.40 |
| 3:U:2966[B]:SER:HB2 | 3:U:2977[B]:CYS:H | 1.85 | 0.40 |
| 3:U:2989[A]:HIS:O | 3:U:2991[A]:LEU:N | 2.54 | 0.40 |
| 3:U:2989[B]:HIS:O | 3:U:2991[B]:LEU:N | 2.54 | 0.40 |
| 3:U:3028[A]:PRO:HG2 | 3:U:3029[A]:LYS:HG2 | 2.02 | 0.40 |
| 3:U:3083[B]:ILE:CD1 | 3:U:3260[B]:ARG:HB2 | 2.52 | 0.40 |
| 3:U:3274[A]:ARG:NE | 3:U:3274[A]:ARG:CA | 2.84 | 0.40 |
| 1:V:78:GLN:HE21 | 1:V:256:ILE:HG21 | 1.85 | 0.40 |
| 1:V:1572:ILE:HD13 | 1:V:1615:LEU:HD23 | 2.02 | 0.40 |
| 3:X:2989[A]:HIS:O | 3:X:2991[A]:LEU:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3028[B]:PRO:HG2 | 3:X:3029[B]:LYS:HG2 | 2.02 | 0.40 |
| 3:X:3180[B]:TYR:HA | 3:X:3183[B]:LEU:CD2 | 2.51 | 0.40 |
| 1:Y:194:MET:HA | 1:Y:200:THR:CA | 2.48 | 0.40 |
| 1:Y:710:GLY:O | 1:Y:841:LYS:HE2 | 2.21 | 0.40 |
| 1:Y:1347:ASP:HA | 1:Y:1460:ASN:ND2 | 2.36 | 0.40 |
| 1:Y:1356:PRO:HD2 | 1:Y:1359:ILE:HD11 | 2.04 | 0.40 |
| 2:Z:2353:LYS:O | 2:Z:2357:VAL:HG23 | 2.21 | 0.40 |
| 3:a:2963[B]:MET:SD | 3:a:2963[B]:MET:O | 2.79 | 0.40 |
| 3:a:3013[A]:ASP:CA | 3:a:3122[A]:ASN:ND2 | 2.74 | 0.40 |
| 3:a:3028[A]:PRO:HG2 | 3:a:3029[A]:LYS:N | 2.36 | 0.40 |
| 3:a:3185[B]:TYR:HD2 | 3:a:3186[B]:GLU:N | 2.19 | 0.40 |
| 3:a:3281[B]:PHE:CZ | 3:a:3305[B]:ILE:HG21 | 2.56 | 0.40 |
| 3:a:3298[B]:ASN:HA | 3:a:3300[B]:LEU:N | 2.36 | 0.40 |
| 1:b:168:PHE:O | 1:b:172:GLU:N | 2.54 | 0.40 |
| 1:b:760:ILE:HG21 | 1:b:777:TYR:HE2 | 1.86 | 0.40 |
| 1:b:991:LEU:HD23 | 1:b:991:LEU:HA | 1.86 | 0.40 |
| 1:b:1480:ASN:CG | 1:b:1518:ASP:HB3 | 2.46 | 0.40 |
| 2:c:2179:ASP:HB3 | 2:c:2303:ARG:NH1 | 2.36 | 0.40 |
| 2:c:2849:ASP:OD2 | 2:c:2850:ARG:NH2 | 2.54 | 0.40 |
| 3:d:2931[B]:THR:O | 3:d:2934[B]:GLU:HB2 | 2.22 | 0.40 |
| 3:d:2987[A]:HIS:CD2 | 3:d:3178[A]:PHE:CE1 | 3.08 | 0.40 |
| 3:d:3044[B]:LYS:H | 3:d:3044[B]:LYS:HG2 | 1.65 | 0.40 |
| 3:d:3083[B]:ILE:HD11 | 3:d:3260[B]:ARG:HG3 | 2.03 | 0.40 |
| 3:d:3139[A]:LEU:CD2 | 3:d:3139[A]:LEU:H | 2.34 | 0.40 |
| 3:d:3139[B]:LEU:CD2 | 3:d:3139[B]:LEU:H | 2.34 | 0.40 |
| 3:d:3146[B]:CYS:O | 3:d:3146[B]:CYS:SG | 2.78 | 0.40 |
| 3:d:3232[B]:VAL:CG2 | 3:d:3273[B]:LEU:CD1 | 2.99 | 0.40 |
| 1:A:1030:MET:HE3 | 1:A:1036:SER:O | 2.21 | 0.40 |
| 1:A:1260:ARG:HD2 | 1:A:1343:VAL:O | 2.21 | 0.40 |
| 2:B:2528:LYS:NZ | 2:B:2626:ARG:O | 2.54 | 0.40 |
| 2:B:2547:MET:O | 2:B:2554:PRO:HG2 | 2.21 | 0.40 |
| 2:B:2556:TYR:CE1 | 2:B:2844:MET:HG3 | 2.57 | 0.40 |
| 2:B:2840:GLY:O | 2:B:2843:GLU:HB2 | 2.21 | 0.40 |
| 3:C:2957[A]:ILE:HD11 | 3:C:2995[A]:GLN:C | 2.46 | 0.40 |
| 3:C:2957[B]:ILE:HD11 | 3:C:2995[B]:GLN:C | 2.46 | 0.40 |
| 3:C:3013[A]:ASP:CA | 3:C:3122[A]:ASN:ND2 | 2.74 | 0.40 |
| 3:C:3185[B]:TYR:CZ | 3:C:3187[B]:TYR:CE2 | 3.09 | 0.40 |
| 3:C:3194[B]:GLY:C | 3:C:3195[B]:MET:CG | 2.90 | 0.40 |
| 3:C:3281[A]:PHE:CZ | 3:C:3305[A]:ILE:HG21 | 2.55 | 0.40 |
| 3:C:3298[A]:ASN:HA | 3:C:3300[A]:LEU:N | 2.36 | 0.40 |
| 1:D:177:VAL:O | 1:D:181:PRO:HD3 | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:278:ASP:O | 1:D:279:LEU:HG | 2.21 | 0.40 |
| 1:D:417:MET:HB3 | 1:D:418:ASP:H | 1.59 | 0.40 |
| 1:D:512:PRO:HG2 | 1:D:632:LEU:HD23 | 2.02 | 0.40 |
| 1:D:564:ASP:HA | 1:D:609:TRP:O | 2.21 | 0.40 |
| 1:D:639:ARG:O | 1:D:642:ALA:HB3 | 2.21 | 0.40 |
| 1:D:979:LEU:CB | 1:D:980:TYR:HA | 2.51 | 0.40 |
| 1:D:1016:ASN:HD22 | 1:D:1177:VAL:HA | 1.85 | 0.40 |
| 1:D:1037:ALA:HA | 1:D:1042:PHE:CD2 | 2.57 | 0.40 |
| 2:E:2403:PHE:HD2 | 2:E:2480:LEU:HG | 1.87 | 0.40 |
| 3:F:2942[A]:LEU:CD1 | 3:F:3033[A]:PHE:CZ | 3.04 | 0.40 |
| 3:F:2957[A]:ILE:HD11 | 3:F:2995[A]:GLN:C | 2.46 | 0.40 |
| 3:F:2961[B]:HIS:CG | 3:a:2975[B]:PHE:CE1 | 3.09 | 0.40 |
| 3:F:2963[A]:MET:SD | 3:F:2963[A]:MET:O | 2.79 | 0.40 |
| 3:F:2965[B]:LEU:CG | 3:F:2974[B]:ALA:CB | 2.85 | 0.40 |
| 3:F:2966[B]:SER:CB | 3:a:2982[B]:MET:HE2 | 2.49 | 0.40 |
| 3:F:2989[B]:HIS:O | 3:F:2991[B]:LEU:N | 2.54 | 0.40 |
| 3:F:3067[B]:ARG:HA | 3:F:3067[B]:ARG:HD3 | 1.87 | 0.40 |
| 3:F:3108[B]:HIS:CE1 | 3:a:3251[B]:ASP:CG | 2.87 | 0.40 |
| 3:F:3160[B]:SER:C | 3:a:3150[B]:LYS:NZ | 2.63 | 0.40 |
| 3:F:3306[B]:LEU:C | 3:F:3306[B]:LEU:CD1 | 2.86 | 0.40 |
| 1:G:930:ASP:HB3 | 1:G:933:ARG:HD2 | 2.03 | 0.40 |
| 1:G:1290:ILE:HD11 | 1:G:1333:GLU:HG3 | 2.03 | 0.40 |
| 1:G:1454:PHE:O | 1:G:1457:HIS:HB3 | 2.21 | 0.40 |
| 1:G:1512:ARG:O | 1:G:1516:VAL:HG23 | 2.21 | 0.40 |
| 2:H:2275:GLY:HA2 | 2:H:2281:SER:HB2 | 2.03 | 0.40 |
| 2:H:2398:PHE:HE2 | 2:H:2466:THR:HG21 | 1.86 | 0.40 |
| 2:H:2400:LEU:HD23 | 2:H:2400:LEU:HA | 1.85 | 0.40 |
| 2:H:2547:MET:C | 2:H:2554:PRO:HG3 | 2.46 | 0.40 |
| 2:H:2825:ILE:HG23 | 2:H:2826:GLU:N | 2.36 | 0.40 |
| 3:I:2965[B]:LEU:HD12 | 3:R:3256[B]:TRP:HE1 | 1.81 | 0.40 |
| 3:I:3083[A]:ILE:HD11 | 3:I:3260[A]:ARG:HG3 | 2.03 | 0.40 |
| 3:I:3083[B]:ILE:CD1 | 3:I:3260[B]:ARG:HB2 | 2.52 | 0.40 |
| 3:I:3185[A]:TYR:HD2 | 3:I:3186[A]:GLU:N | 2.19 | 0.40 |
| 3:I:3185[B]:TYR:CZ | 3:I:3187[B]:TYR:CE2 | 3.09 | 0.40 |
| 3:I:3193[B]:HIS:ND1 | 3:I:3193[B]:HIS:N | 2.69 | 0.40 |
| 3:I:3301[A]:PRO:HB2 | 3:I:3302[A]:SER:H | 1.33 | 0.40 |
| 1:J:148:GLN:O | 1:J:149:GLU:HB2 | 2.22 | 0.40 |
| 1:J:320:LYS:HZ3 | 1:J:337:ASP:HB3 | 1.85 | 0.40 |
| 1:J:639:ARG:O | 1:J:643:ILE:HG13 | 2.21 | 0.40 |
| 1:J:810:LEU:HD12 | 1:J:810:LEU:HA | 1.93 | 0.40 |
| 1:J:876:PHE:N | 1:J:876:PHE:CD1 | 2.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1081:MET:SD | 1:J:1102:PRO:HG3 | 2.62 | 0.40 |
| 2:K:2135:PRO:HG2 | 2:K:2342:TYR:CZ | 2.56 | 0.40 |
| 2:K:2224:THR:HG23 | 2:K:2278:GLU:HG3 | 2.04 | 0.40 |
| 2:K:2271:HIS:O | 2:K:2283:ASN:HB3 | 2.21 | 0.40 |
| 3:L:2938[B]:LEU:HD12 | 3:L:2938[B]:LEU:HA | 1.85 | 0.40 |
| 3:L:2951[A]:ASP:CG | 3:L:2952[A]:ALA:H | 2.28 | 0.40 |
| 3:L:2966[A]:SER:HB2 | 3:L:2977[A]:CYS:H | 1.85 | 0.40 |
| 3:L:3180[B]:TYR:HA | 3:L:3183[B]:LEU:CD2 | 2.51 | 0.40 |
| 3:L:3300[A]:LEU:HD23 | 3:L:3300[A]:LEU:H | 1.83 | 0.40 |
| 1:M:95:THR:O | 1:M:153:ASN:ND2 | 2.54 | 0.40 |
| 1:M:318:ARG:HB2 | 1:M:382:GLU:HB2 | 2.02 | 0.40 |
| 1:M:320:LYS:HB2 | 1:M:380:THR:HG23 | 2.02 | 0.40 |
| 1:M:324:PRO:HA | 1:M:332:ASP:OD2 | 2.21 | 0.40 |
| 1:M:747:PHE:HD1 | 1:M:756:PHE:HA | 1.87 | 0.40 |
| 1:M:876:PHE:CD2 | 1:M:1083:PRO:HB2 | 2.56 | 0.40 |
| 1:M:884:PRO:O | 1:M:888:ALA:HB2 | 2.22 | 0.40 |
| 1:M:1005:CYS:O | 1:M:1009:VAL:HG23 | 2.21 | 0.40 |
| 1:M:1019:HIS:CE1 | 1:M:1046:HIS:HE1 | 2.38 | 0.40 |
| 1:M:1091:ASN:HA | 1:M:1092:PRO:HD3 | 1.83 | 0.40 |
| 1:M:1390:ASP:HB2 | 1:M:1438:ASP:OD2 | 2.22 | 0.40 |
| 2:N:2235:PRO:HG3 | 2:N:2240:GLN:HE22 | 1.85 | 0.40 |
| 2:N:2668:ASP:HB3 | 2:N:2671:ASP:HB2 | 2.04 | 0.40 |
| 3:O:2980[A]:HIS:HA | 3:O:2985[A]:PHE:HD2 | 1.86 | 0.40 |
| 3:O:3112[B]:TYR:CZ | 3:X:2969[B]:TYR:CE1 | 3.09 | 0.40 |
| 3:O:3157[B]:PRO:CD | 3:X:3153[B]:LYS:CA | 2.99 | 0.40 |
| 3:O:3242[B]:GLY:O | 3:O:3243[B]:GLY:O | 2.39 | 0.40 |
| 1:P:450:LYS:HA | 1:P:450:LYS:HD2 | 1.71 | 0.40 |
| 1:P:1380:GLY:O | 1:P:1389:THR:HG23 | 2.22 | 0.40 |
| 1:P:1616:LYS:HA | 1:P:1616:LYS:HD3 | 1.89 | 0.40 |
| 2:Q:2891:LEU:HD12 | 2:Q:2891:LEU:H | 1.86 | 0.40 |
| 3:R:2989[A]:HIS:O | 3:R:2991[A]:LEU:N | 2.54 | 0.40 |
| 3:R:3242[B]:GLY:O | 3:R:3243[B]:GLY:O | 2.40 | 0.40 |
| 1:S:982:LYS:N | 1:S:983:PRO:CD | 2.84 | 0.40 |
| 2:T:2092:VAL:HG23 | 2:T:2177:TYR:O | 2.22 | 0.40 |
| 3:U:2931[B]:THR:O | 3:U:2934[B]:GLU:HB2 | 2.22 | 0.40 |
| 3:U:3185[A]:TYR:HD2 | 3:U:3186[A]:GLU:N | 2.19 | 0.40 |
| 3:U:3256[B]:TRP:CA | 3:d:2969[B]:TYR:N | 2.84 | 0.40 |
| 3:U:3276[B]:ASP:C | 3:U:3278[B]:HIS:N | 2.75 | 0.40 |
| 1:V:71:LEU:HB2 | 1:V:266:LEU:HD21 | 2.03 | 0.40 |
| 1:V:524:PRO:HD2 | 1:V:527:LEU:HD11 | 2.03 | 0.40 |
| 1:V:566:ARG:HH12 | 1:V:745:ASP:CG | 2.29 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:729:VAL:HG11 | 1:V:785:LEU:HD12 | 2.03 | 0.40 |
| 2:W:2184:MET:HB2 | 2:W:2231:LEU:O | 2.21 | 0.40 |
| 2:W:2684:HIS:HA | 2:W:2695:MET:HG3 | 2.03 | 0.40 |
| 3:X:2957[A]:ILE:HD11 | 3:X:2995[A]:GLN:C | 2.46 | 0.40 |
| 3:X:3023[B]:ILE:C | 3:X:3025[B]:VAL:N | 2.79 | 0.40 |
| 3:X:3044[B]:LYS:H | 3:X:3044[B]:LYS:HG2 | 1.65 | 0.40 |
| 3:X:3171[B]:HIS:O | 3:X:3172[B]:SER:C | 2.63 | 0.40 |
| 3:X:3176[B]:LYS:O | 3:X:3177[B]:SER:CB | 2.70 | 0.40 |
| 3:X:3180[B]:TYR:CA | 3:X:3183[B]:LEU:CD2 | 2.95 | 0.40 |
| 3:X:3191[B]:ASN:ND2 | 3:X:3191[B]:ASN:N | 2.60 | 0.40 |
| 1:Y:810:LEU:HD11 | 4:JA:1:NAG:O6 | 2.21 | 0.40 |
| 2:Z:2098:GLN:HE22 | 2:c:2374:ASN:ND2 | 2.19 | 0.40 |
| 2:Z:2771:TYR:HB2 | 2:Z:2776:TYR:CE1 | 2.56 | 0.40 |
| 2:Z:2819:VAL:HB | 2:Z:2835:ILE:HG23 | 2.03 | 0.40 |
| 3:a:2931[B]:THR:O | 3:a:2934[B]:GLU:HB2 | 2.22 | 0.40 |
| 3:a:2989[A]:HIS:O | 3:a:2991[A]:LEU:N | 2.54 | 0.40 |
| 3:a:2989[B]:HIS:O | 3:a:2991[B]:LEU:N | 2.54 | 0.40 |
| 3:a:3134[A]:GLN:C | 3:a:3136[A]:TYR:N | 2.77 | 0.40 |
| 3:a:3180[A]:TYR:HA | 3:a:3183[A]:LEU:CD2 | 2.51 | 0.40 |
| 3:a:3242[B]:GLY:O | 3:a:3243[B]:GLY:O | 2.40 | 0.40 |
| 3:a:3265[A]:ASP:OD1 | 3:a:3266[A]:ILE:N | 2.54 | 0.40 |
| 1:b:93:ASP:HA | 1:b:212:ASN:ND2 | 2.37 | 0.40 |
| 1:b:907:ARG:NH2 | 1:b:1106:PHE:O | 2.53 | 0.40 |
| 1:b:1304:ASP:OD2 | 1:b:1306:THR:HG23 | 2.22 | 0.40 |
| 2:c:2179:ASP:HA | 2:c:2300:ASN:ND2 | 2.35 | 0.40 |
| 2:c:2569:TRP:HE3 | 2:c:2570:HIS:ND1 | 2.18 | 0.40 |
| 2:c:2590:VAL:HA | 2:c:2591:PRO:HD3 | 1.90 | 0.40 |
| 3:d:2957[A]:ILE:HD11 | 3:d:2995[A]:GLN:C | 2.46 | 0.40 |
| 3:d:2980[B]:HIS:HA | 3:d:2985[B]:PHE:HD2 | 1.86 | 0.40 |
| 3:d:3083[A]:ILE:CD1 | 3:d:3260[A]:ARG:HB2 | 2.52 | 0.40 |
| 3:d:3094[A]:SER:HG | 3:d:3227[A]:ASP:CG | 2.28 | 0.40 |
| 3:d:3185[A]:TYR:CE2 | 3:d:3187[A]:TYR:HE2 | 2.31 | 0.40 |
| 3:d:3274[A]:ARG:NE | 3:d:3274[A]:ARG:CA | 2.84 | 0.40 |
| 3:d:3298[B]:ASN:HA | 3:d:3300[B]:LEU:N | 2.36 | 0.40 |
| 1:A:243:PRO:HB2 | 1:A:248:GLY:HA3 | 2.02 | 0.40 |
| 1:A:597:VAL:O | 1:A:601:VAL:HG12 | 2.21 | 0.40 |
| 1:A:745:ASP:OD1 | 1:A:759:SER:OG | 2.35 | 0.40 |
| 1:A:896:HIS:HB2 | 1:A:905:TRP:CD1 | 2.56 | 0.40 |
| 1:A:1001:GLN:HE21 | 1:A:1001:GLN:HB3 | 1.77 | 0.40 |
| 1:A:1390:ASP:HB3 | 1:b:1372:ILE:HD11 | 2.03 | 0.40 |
| 2:B:2145:LEU:HD12 | 2:B:2145:LEU:HA | 1.84 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2848:PHE:HD1 | 2:B:2848:PHE:HA | 1.76 | 0.40 |
| 3:C:2965[B]:LEU:HB3 | 3:L:3256[B]:TRP:CD2 | 2.11 | 0.40 |
| 3:C:2989[A]:HIS:O | 3:C:2991[A]:LEU:N | 2.54 | 0.40 |
| 3:C:3023[A]:ILE:HA | 3:C:3026[A]:THR:HG1 | 1.83 | 0.40 |
| 3:C:3139[A]:LEU:CD2 | 3:C:3139[A]:LEU:H | 2.34 | 0.40 |
| 3:C:3168[A]:THR:O | 3:C:3172[A]:SER:N | 2.55 | 0.40 |
| 3:C:3185[B]:TYR:C | 3:C:3185[B]:TYR:HD2 | 2.30 | 0.40 |
| 3:C:3265[A]:ASP:OD1 | 3:C:3266[A]:ILE:N | 2.54 | 0.40 |
| 1:D:3:ILE:O | 1:D:88:GLY:N | 2.48 | 0.40 |
| 1:D:450:LYS:O | 1:D:450:LYS:HD3 | 2.22 | 0.40 |
| 1:D:513:TYR:HB2 | 1:D:636:GLN:HB2 | 2.02 | 0.40 |
| 1:D:843:VAL:HG13 | 1:D:927:PRO:HB2 | 2.03 | 0.40 |
| 1:D:899:MET:HE2 | 1:D:1012:GLU:OE1 | 2.21 | 0.40 |
| 1:D:907:ARG:HD3 | 1:D:1050:ASP:OD1 | 2.22 | 0.40 |
| 1:D:1249:TRP:CZ2 | 1:D:1537:ILE:HD12 | 2.55 | 0.40 |
| 1:D:1470:GLU:HB3 | 1:D:1537:ILE:HD11 | 2.03 | 0.40 |
| 2:E:2122:ILE:HD11 | 2:E:2165:SER:OG | 2.21 | 0.40 |
| 3:F:2931[B]:THR:O | 3:F:2934[B]:GLU:HB2 | 2.22 | 0.40 |
| 3:F:2961[B]:HIS:O | 3:a:2975[B]:PHE:CE1 | 2.75 | 0.40 |
| 3:F:2980[B]:HIS:HB3 | 3:a:2968[B]:GLN:CG | 1.76 | 0.40 |
| 3:F:2987[B]:HIS:CD2 | 3:F:3178[B]:PHE:CE1 | 3.08 | 0.40 |
| 3:F:3010[B]:PRO:HG2 | 3:F:3118[B]:VAL:HG13 | 2.03 | 0.40 |
| 3:F:3041[B]:ALA:O | 3:F:3042[B]:ASP:HB2 | 2.20 | 0.40 |
| 3:F:3221[B]:ALA:HB2 | 3:a:2965[B]:LEU:O | 2.21 | 0.40 |
| 3:F:3298[A]:ASN:HA | 3:F:3300[A]:LEU:N | 2.37 | 0.40 |
| 3:F:3301[B]:PRO:HB2 | 3:F:3302[B]:SER:H | 1.33 | 0.40 |
| 1:G:1303:GLU:C | 1:G:1306:THR:H | 2.29 | 0.40 |
| 1:G:1408:LEU:HD23 | 1:G:1547:ASN:HD21 | 1.86 | 0.40 |
| 1:G:1473:ARG:HG3 | 1:G:1479:TYR:CG | 2.56 | 0.40 |
| 2:H:2089:ARG:HD3 | 2:H:2163:GLU:OE2 | 2.21 | 0.40 |
| 3:I:3011[B]:TYR:CB | 3:I:3121[B]:SER:HB2 | 2.49 | 0.40 |
| 3:I:3133[B]:LEU:HD13 | 3:I:3197[B]:ILE:HG23 | 2.02 | 0.40 |
| 3:I:3150[B]:LYS:CD | 3:R:3160[B]:SER:CA | 2.73 | 0.40 |
| 3:I:3163[B]:ASN:HD22 | 3:R:3149[B]:ASN:CG | 2.23 | 0.40 |
| 1:J:177:VAL:HG11 | 1:J:358:TYR:CZ | 2.56 | 0.40 |
| 1:J:321:LEU:HD11 | 1:J:377:TYR:CD1 | 2.55 | 0.40 |
| 1:J:902:PHE:CE2 | 1:J:1012:GLU:HG3 | 2.56 | 0.40 |
| 2:K:2117:ASP:OD2 | 2:K:2168:ARG:NH2 | 2.54 | 0.40 |
| 2:K:2244:PHE:CD1 | 2:K:2244:PHE:C | 2.99 | 0.40 |
| 2:K:2448:THR:OG1 | 2:K:2449:ASP:N | 2.55 | 0.40 |
| 3:L:2951[B]:ASP:CG | 3:L:2952[B]:ALA:H | 2.28 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:3176[A]:LYS:O | 3:L:3177[A]:SER:CB | 2.70 | 0.40 |
| 3:L:3222[A]:ILE:CD1 | 3:L:3223[A]:GLY:N | 2.73 | 0.40 |
| 1:M:398:ARG:HA | 1:M:399:PRO:HD3 | 1.85 | 0.40 |
| 1:M:651:ARG:HG3 | 1:M:717:GLN:HE22 | 1.87 | 0.40 |
| 1:M:979:LEU:HB3 | 1:M:980:TYR:CB | 2.52 | 0.40 |
| 1:M:1289:GLU:O | 1:M:1292:SER:OG | 2.34 | 0.40 |
| 1:M:1492:PRO:HA | 1:M:1512:ARG:HA | 2.02 | 0.40 |
| 2:N:2224:THR:HG23 | 2:N:2278:GLU:HB3 | 2.03 | 0.40 |
| 2:N:2527:LEU:HD11 | 2:N:2580:SER:HB3 | 2.03 | 0.40 |
| 3:O:3160[B]:SER:HB3 | 3:X:3149[B]:ASN:CG | 2.27 | 0.40 |
| 3:O:3265[B]:ASP:OD1 | 3:O:3266[B]:ILE:N | 2.54 | 0.40 |
| 1:P:754:GLU:OE2 | 1:P:799:ARG:NH2 | 2.53 | 0.40 |
| 3:R:2991[A]:LEU:O | 3:R:2994[A]:LYS:CB | 2.70 | 0.40 |
| 3:R:3083[B]:ILE:CD1 | 3:R:3260[B]:ARG:HB2 | 2.52 | 0.40 |
| 3:R:3211[A]:ASP:CB | 3:R:3309[A]:PRO:HA | 2.46 | 0.40 |
| 3:R:3274[B]:ARG:NE | 3:R:3274[B]:ARG:CA | 2.84 | 0.40 |
| 3:R:3299[A]:LEU:HB3 | 3:R:3300[A]:LEU:H | 1.54 | 0.40 |
| 1:S:307:ARG:HG2 | 1:S:774:ASP:HA | 2.04 | 0.40 |
| 1:S:403:TYR:HD2 | 1:S:658:TYR:CD1 | 2.39 | 0.40 |
| 1:S:843:VAL:HG22 | 1:S:928:TYR:O | 2.21 | 0.40 |
| 1:S:1384:PHE:CZ | 1:S:1385:GLU:HG3 | 2.56 | 0.40 |
| 1:S:1632:LEU:HD22 | 1:S:1644:ILE:HD11 | 2.02 | 0.40 |
| 2:T:2526:ARG:HB3 | 2:T:2584:HIS:CD2 | 2.57 | 0.40 |
| 2:T:2890:VAL:H | 2:T:2891:LEU:HA | 1.83 | 0.40 |
| 3:U:2951[A]:ASP:CG | 3:U:2952[A]:ALA:H | 2.28 | 0.40 |
| 3:U:2991[A]:LEU:O | 3:U:2994[A]:LYS:CB | 2.70 | 0.40 |
| 3:U:3083[B]:ILE:HD11 | 3:U:3260[B]:ARG:HG3 | 2.03 | 0.40 |
| 3:U:3137[B]:ARG:HD3 | 3:U:3137[B]:ARG:HA | 1.71 | 0.40 |
| 3:U:3171[B]:HIS:O | 3:U:3172[B]:SER:C | 2.63 | 0.40 |
| 1:V:215:ARG:NE | 1:V:279:LEU:HA | 2.35 | 0.40 |
| 1:V:1565:SER:HB3 | 1:V:1594:GLY:H | 1.86 | 0.40 |
| 2:W:2338:PHE:O | 2:W:2343:ASN:HB3 | 2.20 | 0.40 |
| 3:X:2954[B]:TYR:HA | 3:X:2957[B]:ILE:CG2 | 2.50 | 0.40 |
| 3:X:2957[B]:ILE:HD11 | 3:X:2995[B]:GLN:C | 2.46 | 0.40 |
| 3:X:2979[A]:GLN:CD | 3:X:3155[A]:MET:CE | 2.92 | 0.40 |
| 3:X:3131[B]:GLN:HE21 | 3:X:3131[B]:GLN:HB3 | 1.66 | 0.40 |
| 3:X:3185[B]:TYR:HD2 | 3:X:3186[B]:GLU:N | 2.19 | 0.40 |
| 1:Y:150:GLY:HA2 | 1:Y:151:GLN:C | 2.46 | 0.40 |
| 1:Y:1293:PHE:O | 1:Y:1311:CYS:HB2 | 2.22 | 0.40 |
| 2:Z:2553:ALA:N | 2:Z:2554:PRO:CD | 2.84 | 0.40 |
| 3:a:3083[B]:ILE:HD11 | 3:a:3260[B]:ARG:HG3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:a:3139[A]:LEU:CD2 | 3:a:3139[A]:LEU:H | 2.34 | 0.40 |
| 3:a:3176[A]:LYS:O | 3:a:3177[A]:SER:CB | 2.70 | 0.40 |
| 1:b:566:ARG:N | 1:b:567:LEU:HA | 2.36 | 0.40 |
| 1:b:904:HIS:HB3 | 1:b:1105:VAL:HG21 | 2.02 | 0.40 |
| 1:b:1321:HIS:ND1 | 1:b:1513:PRO:HB3 | 2.36 | 0.40 |
| 2:c:2426:PHE:HB3 | 2:c:2445:MET:HE1 | 2.04 | 0.40 |
| 2:c:2568:HIS:HD2 | 2:c:2718:TRP:CH2 | 2.38 | 0.40 |
| 2:c:2578:GLU:O | 2:c:2581:MET:HB2 | 2.22 | 0.40 |
| 2:c:2685:TYR:OH | 2:c:2818:ASP:OD1 | 2.30 | 0.40 |
| 3:d:3194[B]:GLY:C | 3:d:3195[B]:MET:CG | 2.91 | 0.40 |
| 3:d:3242[B]:GLY:O | 3:d:3243[B]:GLY:O | 2.40 | 0.40 |
| 1:A:83:HIS:O | 1:A:85:SER:HB3 | 2.21 | 0.40 |
| 1:A:489:HIS:CD2 | 1:A:689:PRO:HB3 | 2.57 | 0.40 |
| 1:A:695:TYR:N | 1:A:695:TYR:HD1 | 2.19 | 0.40 |
| 2:B:2214:ILE:HD13 | 2:B:2287:TYR:HD1 | 1.86 | 0.40 |
| 2:B:2502:LEU:HA | 2:B:2502:LEU:HD12 | 1.84 | 0.40 |
| 3:C:2946[B]:GLN:CD | 3:C:2947[B]:ALA:N | 2.72 | 0.40 |
| 3:C:3083[B]:ILE:HD11 | 3:C:3260[B]:ARG:HG3 | 2.03 | 0.40 |
| 3:C:3163[B]:ASN:N | 3:L:3147[B]:GLU:OE2 | 2.32 | 0.40 |
| 1:D:572:SER:HB2 | 1:D:578:PHE:HB2 | 2.03 | 0.40 |
| 1:D:627:ASP:HA | 1:D:628:PRO:HD3 | 1.95 | 0.40 |
| 1:D:1017:HIS:CD2 | 1:D:1176:TYR:HD2 | 2.39 | 0.40 |
| 2:E:2181:THR:HB | 2:E:2374:ASN:N | 2.36 | 0.40 |
| 2:E:2262:GLN:O | 2:E:2266:VAL:HG23 | 2.20 | 0.40 |
| 3:F:2963[B]:MET:C | 3:a:3255[B]:PRO:HG3 | 2.46 | 0.40 |
| 3:F:2980[A]:HIS:HA | 3:F:2985[A]:PHE:HD2 | 1.86 | 0.40 |
| 3:F:2989[A]:HIS:NE2 | 9:a:3401[A]:CUO:O1 | 2.54 | 0.40 |
| 3:F:3031[B]:ASN:HA | 3:F:3032[B]:PRO:HD2 | 1.87 | 0.40 |
| 3:F:3083[B]:ILE:HD11 | 3:F:3260[B]:ARG:HG3 | 2.03 | 0.40 |
| 3:F:3113[A]:ASP:OD2 | 3:F:3115[A]:LEU:HB2 | 2.20 | 0.40 |
| 3:F:3148[B]:ILE:HD12 | 3:F:3175[B]:TYR:OH | 2.20 | 0.40 |
| 3:F:3172[B]:SER:CB | 3:a:3150[B]:LYS:O | 2.68 | 0.40 |
| 3:F:3185[A]:TYR:HD2 | 3:F:3186[A]:GLU:N | 2.19 | 0.40 |
| 3:F:3193[A]:HIS:ND1 | 3:F:3193[A]:HIS:N | 2.68 | 0.40 |
| 3:F:3242[B]:GLY:O | 3:F:3243[B]:GLY:O | 2.40 | 0.40 |
| 3:F:3254[B]:MET:CA | 3:a:2966[B]:SER:OG | 2.67 | 0.40 |
| 3:F:3255[B]:PRO:HD3 | 3:a:2962[B]:GLY:C | 2.23 | 0.40 |
| 3:F:3281[A]:PHE:CZ | 3:F:3305[A]:ILE:HG21 | 2.55 | 0.40 |
| 1:G:398:ARG:HA | 1:G:399:PRO:HD3 | 1.93 | 0.40 |
| 1:G:597:VAL:HG12 | 1:G:773:PHE:CD1 | 2.57 | 0.40 |
| 2:H:2168:ARG:O | 2:K:2503:ASN:HB3 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:2931[A]:THR:O | 3:I:2934[A]:GLU:HB2 | 2.22 | 0.40 |
| 3:I:2951[B]:ASP:CG | 3:I:2952[B]:ALA:H | 2.28 | 0.40 |
| 3:I:2951[B]:ASP:C | 3:I:2956[B]:LYS:HZ1 | 2.15 | 0.40 |
| 3:I:2961[A]:HIS:HB2 | 3:I:2992[A]:TYR:HE2 | 1.80 | 0.40 |
| 3:I:3010[A]:PRO:HG2 | 3:I:3118[A]:VAL:HG13 | 2.03 | 0.40 |
| 3:I:3083[B]:ILE:HD11 | 3:I:3260[B]:ARG:HG3 | 2.03 | 0.40 |
| 3:I:3150[B]:LYS:CG | 3:R:3163[B]:ASN:ND2 | 2.52 | 0.40 |
| 3:I:3229[A]:ASN:N | 3:I:3286[A]:THR:O | 2.52 | 0.40 |
| 3:I:3265[A]:ASP:OD1 | 3:I:3266[A]:ILE:N | 2.54 | 0.40 |
| 3:I:3298[B]:ASN:HA | 3:I:3300[B]:LEU:N | 2.37 | 0.40 |
| 1:J:472:ASP:HA | 1:J:473:ALA:HA | 1.82 | 0.40 |
| 1:J:633:HIS:O | 1:J:636:GLN:HB3 | 2.21 | 0.40 |
| 1:J:872:GLN:NE2 | 1:J:1090:ILE:O | 2.47 | 0.40 |
| 2:K:2134:ASN:OD1 | 2:K:2137:ALA:HB2 | 2.21 | 0.40 |
| 2:K:2156:ARG:NH1 | 2:K:2360:TYR:HB3 | 2.36 | 0.40 |
| 2:K:2241:THR:HG23 | 2:K:2244:PHE:HB2 | 2.02 | 0.40 |
| 2:K:2381:LEU:O | 2:K:2385:ILE:HG13 | 2.21 | 0.40 |
| 3:L:2930[A]:LEU:N | 3:L:2930[A]:LEU:HD13 | 2.36 | 0.40 |
| 3:L:2938[A]:LEU:HD12 | 3:L:2938[A]:LEU:HA | 1.85 | 0.40 |
| 3:L:2989[B]:HIS:O | 3:L:2991[B]:LEU:N | 2.54 | 0.40 |
| 3:L:2991[B]:LEU:O | 3:L:2994[B]:LYS:CB | 2.70 | 0.40 |
| 3:L:3023[B]:ILE:O | 3:L:3026[B]:THR:OG1 | 2.34 | 0.40 |
| 3:L:3023[B]:ILE:C | 3:L:3025[B]:VAL:N | 2.79 | 0.40 |
| 3:L:3265[B]:ASP:OD1 | 3:L:3266[B]:ILE:N | 2.54 | 0.40 |
| 3:L:3301[A]:PRO:HB2 | 3:L:3302[A]:SER:H | 1.33 | 0.40 |
| 1:M:73:LEU:HD22 | 1:M:89:ILE:HD12 | 2.03 | 0.40 |
| 1:M:837:HIS:HA | 1:M:1113:HIS:O | 2.21 | 0.40 |
| 1:M:881:GLN:NE2 | 1:M:888:ALA:HB3 | 2.34 | 0.40 |
| 1:M:897:HIS:HB3 | 1:M:899:MET:CE | 2.51 | 0.40 |
| 1:M:1022:VAL:HG13 | 1:M:1030:MET:HB2 | 2.03 | 0.40 |
| 1:M:1296:VAL:N | 1:M:1446:ASP:O | 2.54 | 0.40 |
| 3:O:2931[B]:THR:O | 3:O:2934[B]:GLU:HB2 | 2.22 | 0.40 |
| 3:O:2967[B]:CYS:SG | 3:X:3150[B]:LYS:O | 2.79 | 0.40 |
| 3:O:3120[A]:HIS:HA | 3:O:3123[A]:THR:HG1 | 1.83 | 0.40 |
| 3:O:3185[A]:TYR:C | 3:O:3185[A]:TYR:HD2 | 2.30 | 0.40 |
| 3:O:3185[A]:TYR:HD2 | 3:O:3186[A]:GLU:N | 2.19 | 0.40 |
| 3:O:3193[A]:HIS:ND1 | 3:O:3193[A]:HIS:N | 2.68 | 0.40 |
| 3:O:3228[A]:VAL:CG2 | 3:O:3245[A]:PHE:CZ | 2.86 | 0.40 |
| 1:P:92:TRP:CZ3 | 1:P:102:PRO:HD3 | 2.56 | 0.40 |
| 1:P:514:TRP:CZ2 | 1:P:606:ILE:HD11 | 2.56 | 0.40 |
| 1:P:550:ILE:HG22 | 1:P:552:PHE:CE1 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:618:MET:HB3 | 1:P:618:MET:HE3 | 1.69 | 0.40 |
| 1:P:633:HIS:O | 1:P:636:GLN:HB3 | 2.21 | 0.40 |
| 1:P:991:LEU:HD21 | 1:P:1017:HIS:CG | 2.56 | 0.40 |
| 2:Q:2235:PRO:HG3 | 2:Q:2240:GLN:OE1 | 2.21 | 0.40 |
| 2:Q:2861:LYS:NZ | 3:R:2936[A]:GLU:OE1 | 2.52 | 0.40 |
| 3:R:2931[A]:THR:O | 3:R:2934[A]:GLU:HB2 | 2.22 | 0.40 |
| 3:R:3010[B]:PRO:HG2 | 3:R:3118[B]:VAL:HG13 | 2.03 | 0.40 |
| 3:R:3131[B]:GLN:HE21 | 3:R:3131[B]:GLN:HB3 | 1.66 | 0.40 |
| 3:R:3133[A]:LEU:HD12 | 3:R:3133[A]:LEU:HA | 1.86 | 0.40 |
| 3:R:3155[B]:MET:HB3 | 3:R:3155[B]:MET:HE2 | 1.99 | 0.40 |
| 3:R:3168[B]:THR:O | 3:R:3172[B]:SER:N | 2.55 | 0.40 |
| 3:R:3176[B]:LYS:O | 3:R:3177[B]:SER:CB | 2.70 | 0.40 |
| 1:S:717:GLN:O | 1:S:720:VAL:HG22 | 2.21 | 0.40 |
| 1:S:816:PRO:HA | 1:S:817:PRO:HD3 | 1.88 | 0.40 |
| 1:S:1348:TRP:CD2 | 1:S:1430:ILE:HD11 | 2.56 | 0.40 |
| 3:U:3180[A]:TYR:HA | 3:U:3183[A]:LEU:CD2 | 2.51 | 0.40 |
| 3:U:3298[A]:ASN:HA | 3:U:3300[A]:LEU:N | 2.36 | 0.40 |
| 1:V:279:LEU:HD12 | 1:V:279:LEU:O | 2.20 | 0.40 |
| 1:V:361:GLU:HG2 | 1:V:363:THR:HG22 | 2.03 | 0.40 |
| 1:V:573:LYS:HD2 | 1:V:573:LYS:HA | 1.93 | 0.40 |
| 1:V:1015:HIS:NE2 | 1:V:1019:HIS:CD2 | 2.89 | 0.40 |
| 1:V:1143:ALA:O | 1:V:1235:ILE:N | 2.52 | 0.40 |
| 1:V:1153:LYS:H | 1:V:1153:LYS:HG2 | 1.48 | 0.40 |
| 1:V:1300:CYS:SG | 1:V:1494:ARG:HD2 | 2.62 | 0.40 |
| 1:V:1622:GLN:H | 1:V:1622:GLN:HG3 | 1.45 | 0.40 |
| 2:W:2695:MET:SD | 2:W:2701:SER:HB2 | 2.61 | 0.40 |
| 3:X:2931[A]:THR:O | 3:X:2934[A]:GLU:HB2 | 2.22 | 0.40 |
| 3:X:3028[A]:PRO:HG2 | 3:X:3029[A]:LYS:N | 2.36 | 0.40 |
| 3:X:3148[B]:ILE:HD12 | 3:X:3175[B]:TYR:OH | 2.20 | 0.40 |
| 3:X:3265[B]:ASP:OD1 | 3:X:3266[B]:ILE:N | 2.54 | 0.40 |
| 1:Y:555:ALA:C | 1:Y:557:VAL:H | 2.28 | 0.40 |
| 1:Y:563:ILE:O | 1:Y:612:GLY:N | 2.54 | 0.40 |
| 1:Y:975:PRO:HG2 | 1:Y:1024:GLY:HA3 | 2.03 | 0.40 |
| 1:Y:1359:ILE:O | 1:Y:1391:ARG:NH2 | 2.53 | 0.40 |
| 2:Z:2465:LYS:HE2 | 2:Z:2467:LYS:HE3 | 2.04 | 0.40 |
| 3:a:3122[A]:ASN:O | 3:a:3126[A]:ILE:HG13 | 2.22 | 0.40 |
| 3:a:3146[B]:CYS:HA | 3:a:3147[B]:GLU:HA | 1.70 | 0.40 |
| 3:a:3176[B]:LYS:O | 3:a:3177[B]:SER:CB | 2.70 | 0.40 |
| 3:a:3265[B]:ASP:OD1 | 3:a:3266[B]:ILE:N | 2.54 | 0.40 |
| 3:a:3299[B]:LEU:HB3 | 3:a:3300[B]:LEU:H | 1.54 | 0.40 |
| 3:d:3034[B]:HIS:HB3 | 3:d:3035[B]:HIS:CE1 | 2.50 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:d:3122[B]:ASN:O | 3:d:3126[B]:ILE:HG13 | 2.22 | 0.40 |
| 3:d:3171[A]:HIS:O | 3:d:3172[A]:SER:C | 2.63 | 0.40 |
| 3:d:3176[B]:LYS:O | 3:d:3177[B]:SER:CB | 2.70 | 0.40 |
| 3:d:3180[A]:TYR:HA | 3:d:3183[A]:LEU:CD2 | 2.51 | 0.40 |
| 1:A:76:PHE:CE2 | 1:A:89:ILE:HG21 | 2.56 | 0.40 |
| 1:A:210:HIS:ND1 | 1:A:213:VAL:HG21 | 2.37 | 0.40 |
| 1:A:636:GLN:O | 1:A:640:LEU:HG | 2.21 | 0.40 |
| 2:B:2500:ILE:HG13 | 2:B:2501:PRO:CD | 2.50 | 0.40 |
| 2:B:2561:HIS:HA | 2:B:2562:GLY:HA2 | 1.85 | 0.40 |
| 3:C:2991[B]:LEU:O | 3:C:2994[B]:LYS:CB | 2.70 | 0.40 |
| 3:C:3139[B]:LEU:CD2 | 3:C:3139[B]:LEU:H | 2.34 | 0.40 |
| 3:C:3185[A]:TYR:HD2 | 3:C:3186[A]:GLU:N | 2.19 | 0.40 |
| 3:C:3185[A]:TYR:CZ | 3:C:3187[A]:TYR:CE2 | 3.09 | 0.40 |
| 3:C:3185[B]:TYR:HE2 | 3:C:3187[B]:TYR:CD2 | 2.35 | 0.40 |
| 3:C:3231[A]:ASP:CA | 3:C:3284[A]:LYS:O | 2.70 | 0.40 |
| 3:C:3298[A]:ASN:CA | 3:C:3299[A]:LEU:HB2 | 2.44 | 0.40 |
| 1:D:35:GLN:NE2 | 1:D:127:GLU:O | 2.52 | 0.40 |
| 1:D:434:GLU:H | 1:D:434:GLU:HG3 | 1.64 | 0.40 |
| 1:D:882:TRP:HB3 | 1:D:1086:LEU:HD11 | 2.03 | 0.40 |
| 2:E:2450:ILE:O | 2:E:2454:MET:HG3 | 2.21 | 0.40 |
| 3:F:3028[B]:PRO:HG2 | 3:F:3029[B]:LYS:N | 2.36 | 0.40 |
| 3:F:3083[B]:ILE:CD1 | 3:F:3260[B]:ARG:HB2 | 2.51 | 0.40 |
| 3:F:3139[B]:LEU:CD2 | 3:F:3139[B]:LEU:H | 2.34 | 0.40 |
| 3:F:3148[B]:ILE:HA | 3:a:3169[B]:LYS:HD3 | 1.70 | 0.40 |
| 3:F:3200[B]:LEU:O | 3:F:3203[B]:HIS:HB3 | 2.20 | 0.40 |
| 1:G:512:PRO:HG2 | 1:G:632:LEU:HD22 | 2.03 | 0.40 |
| 1:G:892:TYR:HB2 | 1:G:893:ALA:H | 1.70 | 0.40 |
| 1:G:1380:GLY:HA3 | 1:G:1450:TYR:O | 2.21 | 0.40 |
| 3:I:2930[B]:LEU:N | 3:I:2930[B]:LEU:HD13 | 2.36 | 0.40 |
| 3:I:2942[A]:LEU:CD1 | 3:I:3033[A]:PHE:CZ | 3.04 | 0.40 |
| 3:I:2968[B]:GLN:O | 3:R:2985[B]:PHE:HE2 | 2.04 | 0.40 |
| 3:I:2979[B]:GLN:O | 3:R:2967[B]:CYS:HB3 | 2.16 | 0.40 |
| 3:I:3028[B]:PRO:HG2 | 3:I:3029[B]:LYS:N | 2.36 | 0.40 |
| 3:I:3093[B]:HIS:CD2 | 3:R:2971[B]:ASP:O | 2.62 | 0.40 |
| 3:I:3133[B]:LEU:HD12 | 3:I:3133[B]:LEU:HA | 1.86 | 0.40 |
| 3:I:3171[A]:HIS:O | 3:I:3172[A]:SER:C | 2.63 | 0.40 |
| 3:I:3242[B]:GLY:O | 3:I:3243[B]:GLY:O | 2.40 | 0.40 |
| 3:I:3268[A]:LYS:HG2 | 1:J:1539:GLN:HE22 | 1.86 | 0.40 |
| 1:J:236:GLY:HA2 | 1:J:819:ILE:HB | 2.04 | 0.40 |
| 1:J:492:ARG:HG3 | 1:J:638:ASP:OD1 | 2.21 | 0.40 |
| 1:J:1091:ASN:HA | 1:J:1092:PRO:HD3 | 1.78 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1618:LEU:O | 1:J:1620:LEU:HD13 | 2.20 | 0.40 |
| 2:K:2800:LYS:O | 3:L:3023[A]:ILE:HD11 | 2.21 | 0.40 |
| 2:K:2814:LYS:HD3 | 2:K:2814:LYS:HA | 1.91 | 0.40 |
| 3:L:2931[A]:THR:O | 3:L:2934[A]:GLU:HB2 | 2.22 | 0.40 |
| 3:L:3122[B]:ASN:O | 3:L:3126[B]:ILE:HG13 | 2.22 | 0.40 |
| 3:L:3148[A]:ILE:HD12 | 3:L:3175[A]:TYR:OH | 2.20 | 0.40 |
| 3:L:3176[B]:LYS:O | 3:L:3177[B]:SER:CB | 2.70 | 0.40 |
| 3:L:3185[A]:TYR:C | 3:L:3185[A]:TYR:HD2 | 2.30 | 0.40 |
| 3:L:3185[B]:TYR:CZ | 3:L:3187[B]:TYR:CE2 | 3.09 | 0.40 |
| 3:L:3299[B]:LEU:O | 3:L:3300[B]:LEU:C | 2.60 | 0.40 |
| 1:M:425:ARG:HD2 | 1:M:703:TYR:CZ | 2.57 | 0.40 |
| 2:N:2500:ILE:HD11 | 2:N:2504:ARG:O | 2.21 | 0.40 |
| 3:O:3010[A]:PRO:HG2 | 3:O:3118[A]:VAL:HG13 | 2.03 | 0.40 |
| 3:O:3155[A]:MET:HE2 | 3:O:3155[A]:MET:HB3 | 1.99 | 0.40 |
| 3:O:3158[B]:PHE:HB2 | 3:X:3152[B]:LYS:HD2 | 0.94 | 0.40 |
| 3:O:3168[B]:THR:O | 3:O:3172[B]:SER:N | 2.55 | 0.40 |
| 3:O:3193[B]:HIS:ND1 | 3:O:3193[B]:HIS:N | 2.69 | 0.40 |
| 3:O:3298[B]:ASN:HA | 3:O:3300[B]:LEU:N | 2.37 | 0.40 |
| 1:P:449:ASP:HB3 | 1:P:1280:GLN:CD | 2.46 | 0.40 |
| 1:P:599:PHE:HZ | 1:P:637:VAL:O | 2.04 | 0.40 |
| 1:P:1002:GLU:HB2 | 1:P:1065:LYS:CD | 2.51 | 0.40 |
| 1:P:1055:THR:HA | 1:P:1119:LEU:HD13 | 2.02 | 0.40 |
| 1:P:1312:CYS:HA | 1:P:1322:TRP:CE2 | 2.56 | 0.40 |
| 1:P:1325:LEU:HG | 1:P:1516:VAL:HG11 | 2.03 | 0.40 |
| 2:Q:2457:LYS:HB2 | 2:Q:2457:LYS:HE2 | 1.92 | 0.40 |
| 3:R:2995[A]:GLN:O | 3:R:2996[A]:MET:C | 2.63 | 0.40 |
| 3:R:3265[B]:ASP:OD1 | 3:R:3266[B]:ILE:N | 2.54 | 0.40 |
| 1:S:73:LEU:HD11 | 1:S:210:HIS:O | 2.21 | 0.40 |
| 1:S:246:PRO:HB3 | 1:S:249:ARG:NE | 2.35 | 0.40 |
| 1:S:1557:PHE:HB3 | 1:S:1559:LEU:HD13 | 2.04 | 0.40 |
| 2:T:2816:SER:HB2 | 2:T:2886:VAL:CG2 | 2.51 | 0.40 |
| 2:T:2823:ILE:HD11 | 2:T:2863:ARG:HD3 | 2.04 | 0.40 |
| 3:U:2991[B]:LEU:O | 3:U:2994[B]:LYS:CB | 2.69 | 0.40 |
| 3:U:3013[A]:ASP:CG | 3:U:3015[A]:THR:HG1 | 2.28 | 0.40 |
| 3:U:3028[A]:PRO:HG2 | 3:U:3029[A]:LYS:N | 2.36 | 0.40 |
| 3:U:3139[A]:LEU:CD2 | 3:U:3139[A]:LEU:H | 2.34 | 0.40 |
| 3:U:3185[B]:TYR:HE2 | 3:U:3187[B]:TYR:CD2 | 2.35 | 0.40 |
| 3:U:3231[A]:ASP:CA | 3:U:3284[A]:LYS:O | 2.70 | 0.40 |
| 3:U:3293[B]:LYS:CG | 3:U:3294[B]:SER:CB | 2.98 | 0.40 |
| 1:V:109:LEU:HD12 | 1:V:109:LEU:HA | 1.92 | 0.40 |
| 1:V:999:LEU:HA | 1:V:1056:TRP:HD1 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:X:3139[A]:LEU:CD2 | 3:X:3139[A]:LEU:H | 2.34 | 0.40 |
| 3:X:3242[B]:GLY:O | 3:X:3243[B]:GLY:O | 2.40 | 0.40 |
| 3:X:3298[A]:ASN:HA | 3:X:3300[A]:LEU:N | 2.37 | 0.40 |
| 1:Y:43:GLU:HG3 | 1:Y:44:PRO:HA | 2.04 | 0.40 |
| 1:Y:978:ALA:HB1 | 1:Y:979:LEU:HD13 | 2.04 | 0.40 |
| 1:Y:1429:THR:HG23 | 1:Y:1433:TRP:CE2 | 2.56 | 0.40 |
| 1:Y:1647:ASN:HA | 1:Y:1648:PRO:HD3 | 1.98 | 0.40 |
| 2:Z:2116:SER:CA | 2:Z:2121:THR:HG21 | 2.52 | 0.40 |
| 2:Z:2304:LEU:HD12 | 2:Z:2304:LEU:HA | 1.95 | 0.40 |
| 2:Z:2502:LEU:HD12 | 2:Z:2502:LEU:HA | 1.85 | 0.40 |
| 2:Z:2764:THR:HG22 | 2:Z:2766:SER:H | 1.87 | 0.40 |
| 3:a:2980[A]:HIS:HA | 3:a:2985[A]:PHE:HD2 | 1.86 | 0.40 |
| 3:a:3139[B]:LEU:CD2 | 3:a:3139[B]:LEU:H | 2.34 | 0.40 |
| 3:a:3185[B]:TYR:HE2 | 3:a:3187[B]:TYR:CD2 | 2.35 | 0.40 |
| 3:a:3232[A]:VAL:CG2 | 3:a:3273[A]:LEU:CD1 | 2.98 | 0.40 |
| 1:b:525:SER:HA | 1:b:528:ALA:HB3 | 2.03 | 0.40 |
| 1:b:1294:HIS:HB2 | 1:b:1322:TRP:HH2 | 1.86 | 0.40 |
| 1:b:1311:CYS:HB3 | 1:b:1495:PRO:HD3 | 2.03 | 0.40 |
| 1:b:1316:MET:HE1 | 1:b:1599:MET:HE2 | 2.04 | 0.40 |
| 2:c:2303:ARG:NH2 | 2:c:2372:GLU:O | 2.55 | 0.40 |
| 2:c:2854:MET:HB2 | 2:c:2854:MET:HE3 | 1.81 | 0.40 |
| 2:c:2888:GLY:HA2 | 2:c:2889:ALA:HA | 1.75 | 0.40 |
| 3:d:2989[A]:HIS:NE2 | 9:d:3401[A]:CUO:O1 | 2.53 | 0.40 |
| 3:d:3168[B]:THR:O | 3:d:3172[B]:SER:N | 2.55 | 0.40 |
| 3:d:3185[A]:TYR:C | 3:d:3185[A]:TYR:HD2 | 2.30 | 0.40 |
| 3:d:3185[A]:TYR:HD2 | 3:d:3186[A]:GLU:N | 2.19 | 0.40 |
| 3:d:3222[B]:ILE:CD1 | 3:d:3223[B]:GLY:N | 2.73 | 0.40 |
| 3:d:3242[A]:GLY:O | 3:d:3243[A]:GLY:O | 2.40 | 0.40 |
| 3:d:3265[B]:ASP:OD1 | 3:d:3266[B]:ILE:N | 2.54 | 0.40 |
| 3:d:3298[A]:ASN:HA | 3:d:3300[A]:LEU:N | 2.36 | 0.40 |
| 6:DA:1:NAG:O4 | 6:DA:2:NAG:O7 | 2.39 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1:ASN:N | 1:b:887:ASP:OD1[1_455] | 2.19 | 0.01 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 1654/2000 (83%) | 1552 (94%) | 89 (5%) | 13 (1%) | 16 | 50 |
| 1 | D | 1654/2000 (83%) | 1541 (93%) | 100 (6%) | 13 (1%) | 16 | 50 |
| 1 | G | 1654/2000 (83%) | 1560 (94%) | 78 (5%) | 16 (1%) | 12 | 45 |
| 1 | J | 1654/2000 (83%) | 1537 (93%) | 103 (6%) | 14 (1%) | 16 | 50 |
| 1 | M | 1654/2000 (83%) | 1569 (95%) | 73 (4%) | 12 (1%) | 18 | 53 |
| 1 | P | 1654/2000 (83%) | 1562 (94%) | 78 (5%) | 14 (1%) | 16 | 50 |
| 1 | S | 1654/2000 (83%) | 1581 (96%) | 64 (4%) | 9 (0%) | 24 | 60 |
| 1 | V | 1654/2000 (83%) | 1570 (95%) | 68 (4%) | 16 (1%) | 12 | 45 |
| 1 | Y | 1654/2000 (83%) | 1580 (96%) | 66 (4%) | 8 (0%) | 24 | 60 |
| 1 | b | 1654/2000 (83%) | 1564 (95%) | 80 (5%) | 10 (1%) | 21 | 56 |
| 2 | B | 823/920 (90%) | 778 (94%) | 40 (5%) | 5 (1%) | 21 | 56 |
| 2 | E | 823/920 (90%) | 781 (95%) | 34 (4%) | 8 (1%) | 12 | 45 |
| 2 | H | 823/920 (90%) | 787 (96%) | 33 (4%) | 3 (0%) | 30 | 65 |
| 2 | K | 823/920 (90%) | 778 (94%) | 37 (4%) | 8 (1%) | 12 | 45 |
| 2 | N | 823/920 (90%) | 789 (96%) | 32 (4%) | 2 (0%) | 43 | 76 |
| 2 | Q | 823/920 (90%) | 787 (96%) | 32 (4%) | 4 (0%) | 24 | 60 |
| 2 | T | 823/920 (90%) | 794 (96%) | 22 (3%) | 7 (1%) | 14 | 48 |
| 2 | W | 823/920 (90%) | 791 (96%) | 28 (3%) | 4 (0%) | 24 | 60 |
| 2 | Z | 823/920 (90%) | 797 (97%) | 23 (3%) | 3 (0%) | 30 | 65 |
| 2 | c | 823/920 (90%) | 791 (96%) | 29 (4%) | 3 (0%) | 30 | 65 |
| 3 | C | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 | 50 |
| 3 | F | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 | 50 |
| 3 | I | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 | 50 |
| 3 | L | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 | 50 |
| 3 | O | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 | 50 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | R | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 50 |
| 3 | U | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 50 |
| 3 | X | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 50 |
| 3 | a | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 50 |
| 3 | d | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 16 50 |
| All | All | 31970/33140 (96%) | 30149 (94%) | 1589 (5%) | 232 (1%) | 18 53 |

All (232) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1196 | ILE |
| 1 | D | 695 | TYR |
| 1 | D | 1196 | ILE |
| 1 | G | 331 | SER |
| 1 | G | 1086 | LEU |
| 1 | J | 883 | CYS |
| 1 | M | 127 | GLU |
| 1 | M | 695 | TYR |
| 2 | N | 2340 | ALA |
| 1 | P | 781 | ILE |
| 1 | P | 1436 | GLY |
| 1 | S | 51 | ASP |
| 1 | S | 1196 | ILE |
| 2 | T | 2424 | SER |
| 2 | T | 2631 | TYR |
| 1 | V | 867 | VAL |
| 1 | Y | 148 | GLN |
| 2 | Z | 2340 | ALA |
| 1 | b | 134 | VAL |
| 1 | b | 331 | SER |
| 1 | b | 675 | SER |
| 1 | b | 1301 | PRO |
| 1 | A | 149 | GLU |
| 1 | A | 831 | VAL |
| 1 | A | 1436 | GLY |
| 2 | B | 2343 | ASN |
| 2 | B | 2404 | GLY |
| 3 | C | 3111[A] | SER |
| 3 | C | 3111[B] | SER |
| 3 | C | 3301[A] | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 3301[B] | PRO |
| 2 | E | 2340 | ALA |
| 2 | E | 2419 | ASP |
| 3 | F | 3111[A] | SER |
| 3 | F | 3111[B] | SER |
| 3 | F | 3301[A] | PRO |
| 3 | F | 3301[B] | PRO |
| 1 | G | 116 | LYS |
| 1 | G | 150 | GLY |
| 1 | G | 563 | ILE |
| 1 | G | 674 | LYS |
| 2 | H | 2340 | ALA |
| 3 | I | 3111[A] | SER |
| 3 | I | 3111[B] | SER |
| 3 | I | 3301[A] | PRO |
| 3 | I | 3301[B] | PRO |
| 1 | J | 84 | GLY |
| 1 | J | 952 | GLY |
| 1 | J | 1436 | GLY |
| 2 | K | 2738 | ALA |
| 2 | K | 2831 | GLU |
| 2 | K | 2877 | ILE |
| 2 | K | 2894 | ASN |
| 3 | L | 3111[A] | SER |
| 3 | L | 3111[B] | SER |
| 3 | L | 3301[A] | PRO |
| 3 | L | 3301[B] | PRO |
| 1 | M | 84 | GLY |
| 1 | M | 149 | GLU |
| 1 | M | 447 | MET |
| 1 | M | 1436 | GLY |
| 3 | O | 3111[A] | SER |
| 3 | O | 3111[B] | SER |
| 3 | O | 3301[A] | PRO |
| 3 | O | 3301[B] | PRO |
| 1 | P | 962 | GLY |
| 1 | P | 1484 | CYS |
| 1 | P | 1485 | ALA |
| 2 | Q | 2340 | ALA |
| 3 | R | 3111[A] | SER |
| 3 | R | 3111[B] | SER |
| 3 | R | 3301[A] | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | R | 3301[B] | PRO |
| 1 | S | 153 | ASN |
| 1 | S | 781 | ILE |
| 1 | S | 1232 | THR |
| 1 | S | 1436 | GLY |
| 2 | T | 2202 | GLY |
| 3 | U | 3111[A] | SER |
| 3 | U | 3111[B] | SER |
| 3 | U | 3301[A] | PRO |
| 3 | U | 3301[B] | PRO |
| 1 | V | 753 | ASN |
| 1 | V | 1436 | GLY |
| 1 | V | 1485 | ALA |
| 3 | X | 3111[A] | SER |
| 3 | X | 3111[B] | SER |
| 3 | X | 3301[A] | PRO |
| 3 | X | 3301[B] | PRO |
| 1 | Y | 611 | GLY |
| 1 | Y | 807 | GLY |
| 3 | a | 3111[A] | SER |
| 3 | a | 3111[B] | SER |
| 3 | a | 3301[A] | PRO |
| 3 | a | 3301[B] | PRO |
| 1 | b | 867 | VAL |
| 1 | b | 1485 | ALA |
| 2 | c | 2404 | GLY |
| 2 | c | 2461 | HIS |
| 3 | d | 3111[A] | SER |
| 3 | d | 3111[B] | SER |
| 3 | d | 3301[A] | PRO |
| 3 | d | 3301[B] | PRO |
| 1 | A | 333 | ASN |
| 2 | B | 2547 | MET |
| 1 | D | 134 | VAL |
| 1 | D | 417 | MET |
| 1 | D | 867 | VAL |
| 1 | D | 1484 | CYS |
| 1 | D | 1485 | ALA |
| 2 | E | 2779 | ASP |
| 1 | G | 867 | VAL |
| 1 | G | 1211 | TYR |
| 1 | G | 1436 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 2738 | ALA |
| 1 | M | 227 | ARG |
| 1 | M | 867 | VAL |
| 1 | P | 227 | ARG |
| 1 | P | 881 | GLN |
| 1 | S | 149 | GLU |
| 2 | T | 2461 | HIS |
| 1 | V | 781 | ILE |
| 1 | V | 834 | ASP |
| 1 | V | 1037 | ALA |
| 1 | V | 1232 | THR |
| 2 | W | 2344 | LEU |
| 2 | W | 2418 | GLY |
| 1 | Y | 153 | ASN |
| 1 | Y | 881 | GLN |
| 1 | Y | 1228 | LEU |
| 1 | A | 867 | VAL |
| 1 | A | 875 | ALA |
| 1 | A | 1232 | THR |
| 2 | B | 2738 | ALA |
| 3 | C | 3099[A] | PRO |
| 3 | C | 3099[B] | PRO |
| 1 | D | 884 | PRO |
| 1 | D | 956 | PRO |
| 1 | D | 1436 | GLY |
| 2 | E | 2344 | LEU |
| 2 | E | 2461 | HIS |
| 2 | E | 2548 | CYS |
| 3 | F | 3099[A] | PRO |
| 3 | F | 3099[B] | PRO |
| 1 | G | 153 | ASN |
| 3 | I | 3099[A] | PRO |
| 3 | I | 3099[B] | PRO |
| 1 | J | 555 | ALA |
| 1 | J | 867 | VAL |
| 1 | J | 1301 | PRO |
| 1 | J | 1582 | ASN |
| 2 | K | 2830 | GLN |
| 3 | L | 3099[A] | PRO |
| 3 | L | 3099[B] | PRO |
| 1 | M | 464 | LEU |
| 1 | M | 1211 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | O | 3099[A] | PRO |
| 3 | O | 3099[B] | PRO |
| 1 | P | 571 | PRO |
| 1 | P | 1036 | SER |
| 3 | R | 3099[A] | PRO |
| 3 | R | 3099[B] | PRO |
| 1 | S | 1301 | PRO |
| 3 | U | 3099[A] | PRO |
| 3 | U | 3099[B] | PRO |
| 1 | V | 116 | LYS |
| 1 | V | 330 | GLN |
| 1 | V | 1583 | CYS |
| 2 | W | 2461 | HIS |
| 3 | X | 3099[A] | PRO |
| 3 | X | 3099[B] | PRO |
| 3 | a | 3099[A] | PRO |
| 3 | a | 3099[B] | PRO |
| 1 | b | 962 | GLY |
| 3 | d | 3099[A] | PRO |
| 3 | d | 3099[B] | PRO |
| 1 | A | 464 | LEU |
| 2 | B | 2548 | CYS |
| 1 | G | 53 | SER |
| 1 | G | 983 | PRO |
| 2 | H | 2894 | ASN |
| 1 | J | 884 | PRO |
| 1 | J | 956 | PRO |
| 2 | Q | 2831 | GLU |
| 1 | S | 1432 | SER |
| 2 | T | 2738 | ALA |
| 1 | V | 570 | GLN |
| 2 | W | 2340 | ALA |
| 1 | Y | 884 | PRO |
| 1 | A | 956 | PRO |
| 2 | E | 2738 | ALA |
| 1 | G | 883 | CYS |
| 1 | G | 956 | PRO |
| 1 | J | 116 | LYS |
| 2 | K | 2340 | ALA |
| 1 | P | 884 | PRO |
| 2 | Q | 2738 | ALA |
| 2 | T | 2237 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | T | 2650 | GLY |
| 1 | V | 153 | ASN |
| 2 | Z | 2499 | ALA |
| 1 | D | 831 | VAL |
| 1 | G | 676 | PRO |
| 1 | P | 956 | PRO |
| 2 | Q | 2217 | ILE |
| 1 | V | 982 | LYS |
| 1 | b | 956 | PRO |
| 1 | b | 1196 | ILE |
| 1 | G | 1196 | ILE |
| 1 | J | 1196 | ILE |
| 1 | M | 982 | LYS |
| 1 | Y | 1196 | ILE |
| 1 | b | 52 | GLY |
| 1 | M | 126 | GLY |
| 1 | P | 867 | VAL |
| 1 | P | 982 | LYS |
| 1 | V | 1083 | PRO |
| 2 | Z | 2650 | GLY |
| 2 | c | 2549 | PRO |
| 1 | A | 921 | GLY |
| 1 | A | 1083 | PRO |
| 1 | A | 1301 | PRO |
| 1 | D | 464 | LEU |
| 2 | E | 2418 | GLY |
| 1 | J | 52 | GLY |
| 2 | K | 2415 | PRO |
| 1 | P | 1196 | ILE |
| 1 | J | 556 | GLY |
| 2 | K | 2339 | GLY |
| 1 | V | 1196 | ILE |
| 2 | N | 2477 | PRO |
| 1 | D | 571 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 1429/1738 (82%) | 1263 (88%) | 166 (12%) | 5 23 |
| 1 | D | 1429/1738 (82%) | 1249 (87%) | 180 (13%) | 4 20 |
| 1 | G | 1429/1738 (82%) | 1242 (87%) | 187 (13%) | 4 19 |
| 1 | J | 1429/1738 (82%) | 1246 (87%) | 183 (13%) | 4 19 |
| 1 | M | 1429/1738 (82%) | 1269 (89%) | 160 (11%) | 6 24 |
| 1 | P | 1429/1738 (82%) | 1245 (87%) | 184 (13%) | 4 19 |
| 1 | S | 1429/1738 (82%) | 1241 (87%) | 188 (13%) | 4 18 |
| 1 | V | 1429/1738 (82%) | 1249 (87%) | 180 (13%) | 4 20 |
| 1 | Y | 1429/1738 (82%) | 1243 (87%) | 186 (13%) | 4 19 |
| 1 | b | 1429/1738 (82%) | 1265 (88%) | 164 (12%) | 5 24 |
| 2 | B | 731/814 (90%) | 654 (90%) | 77 (10%) | 6 27 |
| 2 | E | 731/814 (90%) | 651 (89%) | 80 (11%) | 6 26 |
| 2 | H | 731/814 (90%) | 631 (86%) | 100 (14%) | 3 17 |
| 2 | K | 731/814 (90%) | 649 (89%) | 82 (11%) | 6 24 |
| 2 | N | 731/814 (90%) | 646 (88%) | 85 (12%) | 5 23 |
| 2 | Q | 731/814 (90%) | 650 (89%) | 81 (11%) | 6 25 |
| 2 | T | 731/814 (90%) | 653 (89%) | 78 (11%) | 6 26 |
| 2 | W | 731/814 (90%) | 655 (90%) | 76 (10%) | 7 28 |
| 2 | Z | 731/814 (90%) | 639 (87%) | 92 (13%) | 4 20 |
| 2 | c | 731/814 (90%) | 641 (88%) | 90 (12%) | 4 21 |
| 3 | C | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| 3 | F | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| 3 | I | 636/343 (185%) | 410 (64%) | 226 (36%) | 0 1 |
| 3 | L | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| 3 | O | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| 3 | R | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| 3 | U | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| 3 | X | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| 3 | a | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| 3 | d | 636/343 (185%) | 412 (65%) | 224 (35%) | 0 1 |
| All | All | 27960/28950 (97%) | 23099 (83%) | 4861 (17%) | 3 10 |

All (4861) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4 | ARG |
| 1 | A | 16 | LEU |
| 1 | A | 26 | GLN |
| 1 | A | 62 | MET |
| 1 | A | 67 | MET |
| 1 | A | 73 | LEU |
| 1 | A | 83 | HIS |
| 1 | A | 109 | LEU |
| 1 | A | 114 | THR |
| 1 | A | 117 | LYS |
| 1 | A | 127 | GLU |
| 1 | A | 133 | LYS |
| 1 | A | 134 | VAL |
| 1 | A | 140 | ASP |
| 1 | A | 149 | GLU |
| 1 | A | 151 | GLN |
| 1 | A | 163 | LEU |
| 1 | A | 174 | GLN |
| 1 | A | 179 | HIS |
| 1 | A | 185 | LEU |
| 1 | A | 205 | LEU |
| 1 | A | 210 | HIS |
| 1 | A | 219 | LEU |
| 1 | A | 235 | CYS |
| 1 | A | 238 | ASN |
| 1 | A | 239 | LEU |
| 1 | A | 245 | GLU |
| 1 | A | 249 | ARG |
| 1 | A | 266 | LEU |
| 1 | A | 277 | ASP |
| 1 | A | 279 | LEU |
| 1 | A | 285 | THR |
| 1 | A | 326 | GLU |
| 1 | A | 336 | ASN |
| 1 | A | 344 | LEU |
| 1 | A | 365 | THR |
| 1 | A | 367 | LEU |
| 1 | A | 368 | SER |
| 1 | A | 373 | LEU |
| 1 | A | 376 | ASN |
| 1 | A | 384 | THR |
| 1 | A | 386 | ILE |
| 1 | A | 417 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 430 | SER |
| 1 | A | 432 | THR |
| 1 | A | 434 | GLU |
| 1 | A | 452 | ILE |
| 1 | A | 456 | GLN |
| 1 | A | 494 | VAL |
| 1 | A | 497 | GLN |
| 1 | A | 509 | ILE |
| 1 | A | 511 | VAL |
| 1 | A | 515 | ASP |
| 1 | A | 516 | TRP |
| 1 | A | 527 | LEU |
| 1 | A | 554 | LYS |
| 1 | A | 557 | VAL |
| 1 | A | 568 | PHE |
| 1 | A | 570 | GLN |
| 1 | A | 572 | SER |
| 1 | A | 573 | LYS |
| 1 | A | 579 | LEU |
| 1 | A | 589 | GLN |
| 1 | A | 603 | HIS |
| 1 | A | 610 | THR |
| 1 | A | 624 | THR |
| 1 | A | 650 | GLN |
| 1 | A | 688 | VAL |
| 1 | A | 692 | VAL |
| 1 | A | 695 | TYR |
| 1 | A | 713 | ILE |
| 1 | A | 720 | VAL |
| 1 | A | 729 | VAL |
| 1 | A | 744 | VAL |
| 1 | A | 749 | VAL |
| 1 | A | 754 | GLU |
| 1 | A | 783 | ASP |
| 1 | A | 801 | ASP |
| 1 | A | 810 | LEU |
| 1 | A | 821 | ILE |
| 1 | A | 833 | PHE |
| 1 | A | 836 | GLN |
| 1 | A | 865 | LYS |
| 1 | A | 867 | VAL |
| 1 | A | 881 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 917 | LEU |
| 1 | A | 920 | ASN |
| 1 | A | 935 | ILE |
| 1 | A | 943 | LEU |
| 1 | A | 965 | ASP |
| 1 | A | 979 | LEU |
| 1 | A | 981 | GLU |
| 1 | A | 982 | LYS |
| 1 | A | 999 | LEU |
| 1 | A | 1001 | GLN |
| 1 | A | 1003 | ASP |
| 1 | A | 1013 | ILE |
| 1 | A | 1015 | HIS |
| 1 | A | 1017 | HIS |
| 1 | A | 1033 | LEU |
| 1 | A | 1067 | TYR |
| 1 | A | 1075 | GLU |
| 1 | A | 1077 | LEU |
| 1 | A | 1089 | ASP |
| 1 | A | 1090 | ILE |
| 1 | A | 1098 | GLU |
| 1 | A | 1126 | ILE |
| 1 | A | 1139 | LYS |
| 1 | A | 1144 | VAL |
| 1 | A | 1153 | LYS |
| 1 | A | 1155 | LEU |
| 1 | A | 1157 | VAL |
| 1 | A | 1160 | PHE |
| 1 | A | 1166 | THR |
| 1 | A | 1170 | MET |
| 1 | A | 1196 | ILE |
| 1 | A | 1200 | MET |
| 1 | A | 1210 | LYS |
| 1 | A | 1211 | TYR |
| 1 | A | 1213 | VAL |
| 1 | A | 1219 | ASP |
| 1 | A | 1221 | THR |
| 1 | A | 1225 | VAL |
| 1 | A | 1227 | ASP |
| 1 | A | 1229 | LYS |
| 1 | A | 1230 | LEU |
| 1 | A | 1245 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1248 | ARG |
| 1 | A | 1249 | TRP |
| 1 | A | 1258 | ARG |
| 1 | A | 1266 | PHE |
| 1 | A | 1280 | GLN |
| 1 | A | 1286 | ARG |
| 1 | A | 1302 | SER |
| 1 | A | 1303 | GLU |
| 1 | A | 1307 | MET |
| 1 | A | 1308 | VAL |
| 1 | A | 1325 | LEU |
| 1 | A | 1331 | GLU |
| 1 | A | 1354 | GLU |
| 1 | A | 1367 | SER |
| 1 | A | 1369 | THR |
| 1 | A | 1372 | ILE |
| 1 | A | 1396 | GLU |
| 1 | A | 1400 | ASN |
| 1 | A | 1407 | THR |
| 1 | A | 1408 | LEU |
| 1 | A | 1427 | HIS |
| 1 | A | 1430 | ILE |
| 1 | A | 1439 | VAL |
| 1 | A | 1441 | SER |
| 1 | A | 1461 | VAL |
| 1 | A | 1494 | ARG |
| 1 | A | 1509 | THR |
| 1 | A | 1516 | VAL |
| 1 | A | 1543 | ILE |
| 1 | A | 1563 | LYS |
| 1 | A | 1568 | VAL |
| 1 | A | 1581 | GLU |
| 1 | A | 1597 | THR |
| 1 | A | 1622 | GLN |
| 1 | A | 1632 | LEU |
| 1 | A | 1642 | GLN |
| 1 | A | 1643 | LYS |
| 1 | A | 1649 | THR |
| 1 | A | 1653 | VAL |
| 2 | B | 2084 | ARG |
| 2 | B | 2089 | ARG |
| 2 | B | 2104 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 2121 | THR |
| 2 | B | 2131 | LEU |
| 2 | B | 2132 | CYS |
| 2 | B | 2145 | LEU |
| 2 | B | 2160 | VAL |
| 2 | B | 2180 | TRP |
| 2 | B | 2184 | MET |
| 2 | B | 2185 | THR |
| 2 | B | 2187 | VAL |
| 2 | B | 2191 | LEU |
| 2 | B | 2205 | THR |
| 2 | B | 2216 | PHE |
| 2 | B | 2237 | LEU |
| 2 | B | 2240 | GLN |
| 2 | B | 2241 | THR |
| 2 | B | 2260 | GLU |
| 2 | B | 2267 | HIS |
| 2 | B | 2274 | LEU |
| 2 | B | 2285 | LEU |
| 2 | B | 2296 | LEU |
| 2 | B | 2326 | ILE |
| 2 | B | 2327 | GLU |
| 2 | B | 2328 | LEU |
| 2 | B | 2329 | MET |
| 2 | B | 2333 | LEU |
| 2 | B | 2334 | LYS |
| 2 | B | 2361 | LYS |
| 2 | B | 2394 | VAL |
| 2 | B | 2406 | SER |
| 2 | B | 2445 | MET |
| 2 | B | 2456 | LEU |
| 2 | B | 2478 | GLU |
| 2 | B | 2500 | ILE |
| 2 | B | 2507 | ARG |
| 2 | B | 2531 | GLU |
| 2 | B | 2546 | LEU |
| 2 | B | 2547 | MET |
| 2 | B | 2550 | THR |
| 2 | B | 2555 | GLU |
| 2 | B | 2556 | TYR |
| 2 | B | 2561 | HIS |
| 2 | B | 2572 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 2581 | MET |
| 2 | B | 2595 | TRP |
| 2 | B | 2597 | MET |
| 2 | B | 2616 | THR |
| 2 | B | 2617 | ASP |
| 2 | B | 2625 | LEU |
| 2 | B | 2644 | LEU |
| 2 | B | 2658 | LYS |
| 2 | B | 2662 | LEU |
| 2 | B | 2680 | HIS |
| 2 | B | 2718 | TRP |
| 2 | B | 2728 | ARG |
| 2 | B | 2750 | ILE |
| 2 | B | 2752 | GLU |
| 2 | B | 2758 | THR |
| 2 | B | 2769 | PHE |
| 2 | B | 2772 | LYS |
| 2 | B | 2798 | GLN |
| 2 | B | 2809 | LEU |
| 2 | B | 2814 | LYS |
| 2 | B | 2822 | LYS |
| 2 | B | 2825 | ILE |
| 2 | B | 2828 | ASP |
| 2 | B | 2838 | LEU |
| 2 | B | 2851 | ASN |
| 2 | B | 2876 | LYS |
| 2 | B | 2879 | LEU |
| 2 | B | 2883 | ILE |
| 2 | B | 2894 | ASN |
| 2 | B | 2898 | LYS |
| 2 | B | 2900 | SER |
| 2 | B | 2907 | LYS |
| 3 | C | 2929[A] | SER |
| 3 | C | 2929[B] | SER |
| 3 | C | 2930[A] | LEU |
| 3 | C | 2930[B] | LEU |
| 3 | C | 2931[A] | THR |
| 3 | C | 2931[B] | THR |
| 3 | C | 2933[A] | SER |
| 3 | C | 2933[B] | SER |
| 3 | C | 2935[A] | ILE |
| 3 | C | 2935[B] | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 2938[A] | LEU |
| 3 | C | 2938[B] | LEU |
| 3 | C | 2942[A] | LEU |
| 3 | C | 2942[B] | LEU |
| 3 | C | 2946[A] | GLN |
| 3 | C | 2946[B] | GLN |
| 3 | C | 2949[A] | LYS |
| 3 | C | 2949[B] | LYS |
| 3 | C | 2954[A] | TYR |
| 3 | C | 2954[B] | TYR |
| 3 | C | 2956[A] | LYS |
| 3 | C | 2956[B] | LYS |
| 3 | C | 2959[A] | SER |
| 3 | C | 2959[B] | SER |
| 3 | C | 2960[A] | PHE |
| 3 | C | 2960[B] | PHE |
| 3 | C | 2963[A] | MET |
| 3 | C | 2963[B] | MET |
| 3 | C | 2965[A] | LEU |
| 3 | C | 2965[B] | LEU |
| 3 | C | 2968[A] | GLN |
| 3 | C | 2968[B] | GLN |
| 3 | C | 2973[A] | THR |
| 3 | C | 2973[B] | THR |
| 3 | C | 2980[A] | HIS |
| 3 | C | 2980[B] | HIS |
| 3 | C | 2982[A] | MET |
| 3 | C | 2982[B] | MET |
| 3 | C | 2990[A] | ARG |
| 3 | C | 2990[B] | ARG |
| 3 | C | 2995[A] | GLN |
| 3 | C | 2995[B] | GLN |
| 3 | C | 2996[A] | MET |
| 3 | C | 2996[B] | MET |
| 3 | C | 2997[A] | GLU |
| 3 | C | 2997[B] | GLU |
| 3 | C | 3000[A] | LEU |
| 3 | C | 3000[B] | LEU |
| 3 | C | 3001[A] | LYS |
| 3 | C | 3001[B] | LYS |
| 3 | C | 3019[A] | HIS |
| 3 | C | 3019[B] | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 3021[A] | LEU |
| 3 | C | 3021[B] | LEU |
| 3 | C | 3023[A] | ILE |
| 3 | C | 3023[B] | ILE |
| 3 | C | 3024[A] | LEU |
| 3 | C | 3024[B] | LEU |
| 3 | C | 3026[A] | THR |
| 3 | C | 3026[B] | THR |
| 3 | C | 3029[A] | LYS |
| 3 | C | 3029[B] | LYS |
| 3 | C | 3040[A] | VAL |
| 3 | C | 3040[B] | VAL |
| 3 | C | 3042[A] | ASP |
| 3 | C | 3042[B] | ASP |
| 3 | C | 3044[A] | LYS |
| 3 | C | 3044[B] | LYS |
| 3 | C | 3048[A] | ASP |
| 3 | C | 3048[B] | ASP |
| 3 | C | 3050[A] | ARG |
| 3 | C | 3050[B] | ARG |
| 3 | C | 3063[A] | SER |
| 3 | C | 3063[B] | SER |
| 3 | C | 3067[A] | ARG |
| 3 | C | 3067[B] | ARG |
| 3 | C | 3077[A] | ASP |
| 3 | C | 3077[B] | ASP |
| 3 | C | 3081[A] | PHE |
| 3 | C | 3081[B] | PHE |
| 3 | C | 3096[A] | VAL |
| 3 | C | 3096[B] | VAL |
| 3 | C | 3105[A] | SER |
| 3 | C | 3105[B] | SER |
| 3 | C | 3107[A] | LEU |
| 3 | C | 3107[B] | LEU |
| 3 | C | 3110[A] | THR |
| 3 | C | 3110[B] | THR |
| 3 | C | 3111[A] | SER |
| 3 | C | 3111[B] | SER |
| 3 | C | 3115[A] | LEU |
| 3 | C | 3115[B] | LEU |
| 3 | C | 3123[A] | THR |
| 3 | C | 3123[B] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 3131[A] | GLN |
| 3 | C | 3131[B] | GLN |
| 3 | C | 3133[A] | LEU |
| 3 | C | 3133[B] | LEU |
| 3 | C | 3134[A] | GLN |
| 3 | C | 3134[B] | GLN |
| 3 | C | 3135[A] | LYS |
| 3 | C | 3135[B] | LYS |
| 3 | C | 3139[A] | LEU |
| 3 | C | 3139[B] | LEU |
| 3 | C | 3141[A] | TYR |
| 3 | C | 3141[B] | TYR |
| 3 | C | 3147[A] | GLU |
| 3 | C | 3147[B] | GLU |
| 3 | C | 3151[A] | LEU |
| 3 | C | 3151[B] | LEU |
| 3 | C | 3156[A] | MET |
| 3 | C | 3156[B] | MET |
| 3 | C | 3159[A] | SER |
| 3 | C | 3159[B] | SER |
| 3 | C | 3160[A] | SER |
| 3 | C | 3160[B] | SER |
| 3 | C | 3161[A] | GLU |
| 3 | C | 3161[B] | GLU |
| 3 | C | 3162[A] | ASP |
| 3 | C | 3162[B] | ASP |
| 3 | C | 3163[A] | ASN |
| 3 | C | 3163[B] | ASN |
| 3 | C | 3169[A] | LYS |
| 3 | C | 3169[B] | LYS |
| 3 | C | 3172[A] | SER |
| 3 | C | 3172[B] | SER |
| 3 | C | 3176[A] | LYS |
| 3 | C | 3176[B] | LYS |
| 3 | C | 3181[A] | GLN |
| 3 | C | 3181[B] | GLN |
| 3 | C | 3182[A] | GLN |
| 3 | C | 3182[B] | GLN |
| 3 | C | 3183[A] | LEU |
| 3 | C | 3183[B] | LEU |
| 3 | C | 3185[A] | TYR |
| 3 | C | 3185[B] | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 3186[A] | GLU |
| 3 | C | 3186[B] | GLU |
| 3 | C | 3188[A] | ASP |
| 3 | C | 3188[B] | ASP |
| 3 | C | 3191[A] | ASN |
| 3 | C | 3191[B] | ASN |
| 3 | C | 3192[A] | PHE |
| 3 | C | 3192[B] | PHE |
| 3 | C | 3193[A] | HIS |
| 3 | C | 3193[B] | HIS |
| 3 | C | 3195[A] | MET |
| 3 | C | 3195[B] | MET |
| 3 | C | 3196[A] | THR |
| 3 | C | 3196[B] | THR |
| 3 | C | 3200[A] | LEU |
| 3 | C | 3200[B] | LEU |
| 3 | C | 3201[A] | GLU |
| 3 | C | 3201[B] | GLU |
| 3 | C | 3204[A] | LEU |
| 3 | C | 3204[B] | LEU |
| 3 | C | 3205[A] | LYS |
| 3 | C | 3205[B] | LYS |
| 3 | C | 3210[A] | LYS |
| 3 | C | 3210[B] | LYS |
| 3 | C | 3211[A] | ASP |
| 3 | C | 3211[B] | ASP |
| 3 | C | 3212[A] | ARG |
| 3 | C | 3212[B] | ARG |
| 3 | C | 3218[A] | LEU |
| 3 | C | 3218[B] | LEU |
| 3 | C | 3220[A] | ARG |
| 3 | C | 3220[B] | ARG |
| 3 | C | 3222[A] | ILE |
| 3 | C | 3222[B] | ILE |
| 3 | C | 3224[A] | GLN |
| 3 | C | 3224[B] | GLN |
| 3 | C | 3225[A] | SER |
| 3 | C | 3225[B] | SER |
| 3 | C | 3230[A] | PHE |
| 3 | C | 3230[B] | PHE |
| 3 | C | 3244[A] | THR |
| 3 | C | 3244[B] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 3251[A] | ASP |
| 3 | C | 3251[B] | ASP |
| 3 | C | 3254[A] | MET |
| 3 | C | 3254[B] | MET |
| 3 | C | 3260[A] | ARG |
| 3 | C | 3260[B] | ARG |
| 3 | C | 3267[A] | SER |
| 3 | C | 3267[B] | SER |
| 3 | C | 3268[A] | LYS |
| 3 | C | 3268[B] | LYS |
| 3 | C | 3271[A] | VAL |
| 3 | C | 3271[B] | VAL |
| 3 | C | 3272[A] | HIS |
| 3 | C | 3272[B] | HIS |
| 3 | C | 3274[A] | ARG |
| 3 | C | 3274[B] | ARG |
| 3 | C | 3276[A] | ASP |
| 3 | C | 3276[B] | ASP |
| 3 | C | 3278[A] | HIS |
| 3 | C | 3278[B] | HIS |
| 3 | C | 3279[A] | ASP |
| 3 | C | 3279[B] | ASP |
| 3 | C | 3283[A] | ILE |
| 3 | C | 3283[B] | ILE |
| 3 | C | 3286[A] | THR |
| 3 | C | 3286[B] | THR |
| 3 | C | 3287[A] | ILE |
| 3 | C | 3287[B] | ILE |
| 3 | C | 3288[A] | MET |
| 3 | C | 3288[B] | MET |
| 3 | C | 3290[A] | ILE |
| 3 | C | 3290[B] | ILE |
| 3 | C | 3293[A] | LYS |
| 3 | C | 3293[B] | LYS |
| 3 | C | 3297[A] | PRO |
| 3 | C | 3297[B] | PRO |
| 3 | C | 3299[A] | LEU |
| 3 | C | 3299[B] | LEU |
| 3 | C | 3302[A] | SER |
| 3 | C | 3302[B] | SER |
| 3 | C | 3304[A] | THR |
| 3 | C | 3304[B] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 3306[A] | LEU |
| 3 | C | 3306[B] | LEU |
| 3 | C | 3308[A] | LYS |
| 3 | C | 3308[B] | LYS |
| 1 | D | 2 | LEU |
| 1 | D | 3 | ILE |
| 1 | D | 26 | GLN |
| 1 | D | 28 | ASP |
| 1 | D | 32 | SER |
| 1 | D | 55 | ILE |
| 1 | D | 62 | MET |
| 1 | D | 67 | MET |
| 1 | D | 70 | ARG |
| 1 | D | 83 | HIS |
| 1 | D | 96 | LYS |
| 1 | D | 110 | PHE |
| 1 | D | 119 | LYS |
| 1 | D | 128 | ILE |
| 1 | D | 132 | ASN |
| 1 | D | 133 | LYS |
| 1 | D | 134 | VAL |
| 1 | D | 135 | THR |
| 1 | D | 137 | ARG |
| 1 | D | 140 | ASP |
| 1 | D | 163 | LEU |
| 1 | D | 174 | GLN |
| 1 | D | 179 | HIS |
| 1 | D | 185 | LEU |
| 1 | D | 205 | LEU |
| 1 | D | 214 | GLU |
| 1 | D | 226 | HIS |
| 1 | D | 235 | CYS |
| 1 | D | 238 | ASN |
| 1 | D | 249 | ARG |
| 1 | D | 251 | THR |
| 1 | D | 261 | SER |
| 1 | D | 266 | LEU |
| 1 | D | 281 | LEU |
| 1 | D | 285 | THR |
| 1 | D | 289 | LEU |
| 1 | D | 296 | ARG |
| 1 | D | 297 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 325 | THR |
| 1 | D | 336 | ASN |
| 1 | D | 365 | THR |
| 1 | D | 371 | LEU |
| 1 | D | 384 | THR |
| 1 | D | 386 | ILE |
| 1 | D | 394 | GLN |
| 1 | D | 416 | ASN |
| 1 | D | 419 | THR |
| 1 | D | 423 | ARG |
| 1 | D | 449 | ASP |
| 1 | D | 450 | LYS |
| 1 | D | 456 | GLN |
| 1 | D | 499 | GLU |
| 1 | D | 509 | ILE |
| 1 | D | 511 | VAL |
| 1 | D | 515 | ASP |
| 1 | D | 527 | LEU |
| 1 | D | 557 | VAL |
| 1 | D | 560 | SER |
| 1 | D | 565 | GLU |
| 1 | D | 567 | LEU |
| 1 | D | 568 | PHE |
| 1 | D | 570 | GLN |
| 1 | D | 572 | SER |
| 1 | D | 573 | LYS |
| 1 | D | 579 | LEU |
| 1 | D | 589 | GLN |
| 1 | D | 603 | HIS |
| 1 | D | 606 | ILE |
| 1 | D | 609 | TRP |
| 1 | D | 633 | HIS |
| 1 | D | 674 | LYS |
| 1 | D | 677 | LEU |
| 1 | D | 692 | VAL |
| 1 | D | 695 | TYR |
| 1 | D | 729 | VAL |
| 1 | D | 736 | MET |
| 1 | D | 739 | GLN |
| 1 | D | 744 | VAL |
| 1 | D | 749 | VAL |
| 1 | D | 753 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 781 | ILE |
| 1 | D | 797 | THR |
| 1 | D | 808 | THR |
| 1 | D | 810 | LEU |
| 1 | D | 813 | THR |
| 1 | D | 830 | ASN |
| 1 | D | 835 | GLU |
| 1 | D | 836 | GLN |
| 1 | D | 842 | ASN |
| 1 | D | 851 | MET |
| 1 | D | 865 | LYS |
| 1 | D | 870 | TYR |
| 1 | D | 877 | HIS |
| 1 | D | 880 | THR |
| 1 | D | 891 | LYS |
| 1 | D | 896 | HIS |
| 1 | D | 901 | THR |
| 1 | D | 917 | LEU |
| 1 | D | 935 | ILE |
| 1 | D | 936 | ASP |
| 1 | D | 964 | ILE |
| 1 | D | 979 | LEU |
| 1 | D | 984 | ASP |
| 1 | D | 990 | HIS |
| 1 | D | 999 | LEU |
| 1 | D | 1001 | GLN |
| 1 | D | 1008 | GLU |
| 1 | D | 1013 | ILE |
| 1 | D | 1015 | HIS |
| 1 | D | 1017 | HIS |
| 1 | D | 1067 | TYR |
| 1 | D | 1075 | GLU |
| 1 | D | 1077 | LEU |
| 1 | D | 1078 | ARG |
| 1 | D | 1096 | THR |
| 1 | D | 1105 | VAL |
| 1 | D | 1118 | THR |
| 1 | D | 1122 | ASN |
| 1 | D | 1126 | ILE |
| 1 | D | 1133 | ILE |
| 1 | D | 1140 | ASN |
| 1 | D | 1153 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 1155 | LEU |
| 1 | D | 1156 | LEU |
| 1 | D | 1157 | VAL |
| 1 | D | 1160 | PHE |
| 1 | D | 1167 | ASP |
| 1 | D | 1174 | GLU |
| 1 | D | 1196 | ILE |
| 1 | D | 1200 | MET |
| 1 | D | 1206 | HIS |
| 1 | D | 1210 | LYS |
| 1 | D | 1221 | THR |
| 1 | D | 1225 | VAL |
| 1 | D | 1228 | LEU |
| 1 | D | 1230 | LEU |
| 1 | D | 1232 | THR |
| 1 | D | 1234 | VAL |
| 1 | D | 1242 | ASN |
| 1 | D | 1245 | GLU |
| 1 | D | 1249 | TRP |
| 1 | D | 1258 | ARG |
| 1 | D | 1260 | ARG |
| 1 | D | 1266 | PHE |
| 1 | D | 1283 | ASP |
| 1 | D | 1286 | ARG |
| 1 | D | 1302 | SER |
| 1 | D | 1304 | ASP |
| 1 | D | 1306 | THR |
| 1 | D | 1307 | MET |
| 1 | D | 1328 | SER |
| 1 | D | 1355 | LEU |
| 1 | D | 1369 | THR |
| 1 | D | 1394 | GLN |
| 1 | D | 1408 | LEU |
| 1 | D | 1427 | HIS |
| 1 | D | 1433 | TRP |
| 1 | D | 1439 | VAL |
| 1 | D | 1456 | LEU |
| 1 | D | 1478 | SER |
| 1 | D | 1480 | ASN |
| 1 | D | 1494 | ARG |
| 1 | D | 1505 | ARG |
| 1 | D | 1516 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 1542 | ARG |
| 1 | D | 1550 | ARG |
| 1 | D | 1563 | LYS |
| 1 | D | 1568 | VAL |
| 1 | D | 1598 | GLU |
| 1 | D | 1621 | ASN |
| 1 | D | 1622 | GLN |
| 1 | D | 1629 | GLU |
| 1 | D | 1632 | LEU |
| 1 | D | 1635 | VAL |
| 1 | D | 1636 | ASN |
| 1 | D | 1639 | LYS |
| 1 | D | 1641 | THR |
| 1 | D | 1643 | LYS |
| 1 | D | 1647 | ASN |
| 1 | D | 1650 | ILE |
| 2 | E | 2086 | ASN |
| 2 | E | 2089 | ARG |
| 2 | E | 2117 | ASP |
| 2 | E | 2145 | LEU |
| 2 | E | 2184 | MET |
| 2 | E | 2187 | VAL |
| 2 | E | 2191 | LEU |
| 2 | E | 2205 | THR |
| 2 | E | 2211 | HIS |
| 2 | E | 2220 | GLU |
| 2 | E | 2233 | GLU |
| 2 | E | 2237 | LEU |
| 2 | E | 2239 | LYS |
| 2 | E | 2254 | THR |
| 2 | E | 2260 | GLU |
| 2 | E | 2265 | ILE |
| 2 | E | 2267 | HIS |
| 2 | E | 2274 | LEU |
| 2 | E | 2277 | LYS |
| 2 | E | 2326 | ILE |
| 2 | E | 2328 | LEU |
| 2 | E | 2333 | LEU |
| 2 | E | 2344 | LEU |
| 2 | E | 2378 | ILE |
| 2 | E | 2394 | VAL |
| 2 | E | 2403 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 2435 | MET |
| 2 | E | 2445 | MET |
| 2 | E | 2457 | LYS |
| 2 | E | 2459 | ASP |
| 2 | E | 2474 | THR |
| 2 | E | 2480 | LEU |
| 2 | E | 2489 | ILE |
| 2 | E | 2496 | LEU |
| 2 | E | 2500 | ILE |
| 2 | E | 2533 | ASP |
| 2 | E | 2548 | CYS |
| 2 | E | 2555 | GLU |
| 2 | E | 2556 | TYR |
| 2 | E | 2561 | HIS |
| 2 | E | 2572 | VAL |
| 2 | E | 2579 | GLU |
| 2 | E | 2581 | MET |
| 2 | E | 2595 | TRP |
| 2 | E | 2597 | MET |
| 2 | E | 2600 | ASP |
| 2 | E | 2616 | THR |
| 2 | E | 2617 | ASP |
| 2 | E | 2630 | LYS |
| 2 | E | 2631 | TYR |
| 2 | E | 2647 | LEU |
| 2 | E | 2652 | LYS |
| 2 | E | 2653 | GLU |
| 2 | E | 2662 | LEU |
| 2 | E | 2680 | HIS |
| 2 | E | 2684 | HIS |
| 2 | E | 2686 | LEU |
| 2 | E | 2739 | LEU |
| 2 | E | 2742 | MET |
| 2 | E | 2758 | THR |
| 2 | E | 2769 | PHE |
| 2 | E | 2772 | LYS |
| 2 | E | 2780 | HIS |
| 2 | E | 2814 | LYS |
| 2 | E | 2816 | SER |
| 2 | E | 2824 | CYS |
| 2 | E | 2825 | ILE |
| 2 | E | 2826 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 2828 | ASP |
| 2 | E | 2838 | LEU |
| 2 | E | 2847 | HIS |
| 2 | E | 2848 | PHE |
| 2 | E | 2851 | ASN |
| 2 | E | 2858 | ASP |
| 2 | E | 2868 | GLU |
| 2 | E | 2876 | LYS |
| 2 | E | 2879 | LEU |
| 2 | E | 2883 | ILE |
| 2 | E | 2898 | LYS |
| 2 | E | 2901 | LEU |
| 3 | F | 2929[A] | SER |
| 3 | F | 2929[B] | SER |
| 3 | F | 2930[A] | LEU |
| 3 | F | 2930[B] | LEU |
| 3 | F | 2931[A] | THR |
| 3 | F | 2931[B] | THR |
| 3 | F | 2933[A] | SER |
| 3 | F | 2933[B] | SER |
| 3 | F | 2935[A] | ILE |
| 3 | F | 2935[B] | ILE |
| 3 | F | 2938[A] | LEU |
| 3 | F | 2938[B] | LEU |
| 3 | F | 2942[A] | LEU |
| 3 | F | 2942[B] | LEU |
| 3 | F | 2946[A] | GLN |
| 3 | F | 2946[B] | GLN |
| 3 | F | 2949[A] | LYS |
| 3 | F | 2949[B] | LYS |
| 3 | F | 2954[A] | TYR |
| 3 | F | 2954[B] | TYR |
| 3 | F | 2956[A] | LYS |
| 3 | F | 2956[B] | LYS |
| 3 | F | 2959[A] | SER |
| 3 | F | 2959[B] | SER |
| 3 | F | 2960[A] | PHE |
| 3 | F | 2960[B] | PHE |
| 3 | F | 2963[A] | MET |
| 3 | F | 2963[B] | MET |
| 3 | F | 2965[A] | LEU |
| 3 | F | 2965[B] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | F | 2968[A] | GLN |
| 3 | F | 2968[B] | GLN |
| 3 | F | 2973[A] | THR |
| 3 | F | 2973[B] | THR |
| 3 | F | 2980[A] | HIS |
| 3 | F | 2980[B] | HIS |
| 3 | F | 2982[A] | MET |
| 3 | F | 2982[B] | MET |
| 3 | F | 2990[A] | ARG |
| 3 | F | 2990[B] | ARG |
| 3 | F | 2995[A] | GLN |
| 3 | F | 2995[B] | GLN |
| 3 | F | 2996[A] | MET |
| 3 | F | 2996[B] | MET |
| 3 | F | 2997[A] | GLU |
| 3 | F | 2997[B] | GLU |
| 3 | F | 3000[A] | LEU |
| 3 | F | 3000[B] | LEU |
| 3 | F | 3001[A] | LYS |
| 3 | F | 3001[B] | LYS |
| 3 | F | 3019[A] | HIS |
| 3 | F | 3019[B] | HIS |
| 3 | F | 3021[A] | LEU |
| 3 | F | 3021[B] | LEU |
| 3 | F | 3023[A] | ILE |
| 3 | F | 3023[B] | ILE |
| 3 | F | 3024[A] | LEU |
| 3 | F | 3024[B] | LEU |
| 3 | F | 3026[A] | THR |
| 3 | F | 3026[B] | THR |
| 3 | F | 3029[A] | LYS |
| 3 | F | 3029[B] | LYS |
| 3 | F | 3040[A] | VAL |
| 3 | F | 3040[B] | VAL |
| 3 | F | 3042[A] | ASP |
| 3 | F | 3042[B] | ASP |
| 3 | F | 3044[A] | LYS |
| 3 | F | 3044[B] | LYS |
| 3 | F | 3048[A] | ASP |
| 3 | F | 3048[B] | ASP |
| 3 | F | 3050[A] | ARG |
| 3 | F | 3050[B] | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | F | 3063[A] | SER |
| 3 | F | 3063[B] | SER |
| 3 | F | 3067[A] | ARG |
| 3 | F | 3067[B] | ARG |
| 3 | F | 3077[A] | ASP |
| 3 | F | 3077[B] | ASP |
| 3 | F | 3081[A] | PHE |
| 3 | F | 3081[B] | PHE |
| 3 | F | 3096[A] | VAL |
| 3 | F | 3096[B] | VAL |
| 3 | F | 3105[A] | SER |
| 3 | F | 3105[B] | SER |
| 3 | F | 3107[A] | LEU |
| 3 | F | 3107[B] | LEU |
| 3 | F | 3110[A] | THR |
| 3 | F | 3110[B] | THR |
| 3 | F | 3111[A] | SER |
| 3 | F | 3111[B] | SER |
| 3 | F | 3115[A] | LEU |
| 3 | F | 3115[B] | LEU |
| 3 | F | 3123[A] | THR |
| 3 | F | 3123[B] | THR |
| 3 | F | 3131[A] | GLN |
| 3 | F | 3131[B] | GLN |
| 3 | F | 3133[A] | LEU |
| 3 | F | 3133[B] | LEU |
| 3 | F | 3134[A] | GLN |
| 3 | F | 3134[B] | GLN |
| 3 | F | 3135[A] | LYS |
| 3 | F | 3135[B] | LYS |
| 3 | F | 3139[A] | LEU |
| 3 | F | 3139[B] | LEU |
| 3 | F | 3141[A] | TYR |
| 3 | F | 3141[B] | TYR |
| 3 | F | 3147[A] | GLU |
| 3 | F | 3147[B] | GLU |
| 3 | F | 3151[A] | LEU |
| 3 | F | 3151[B] | LEU |
| 3 | F | 3156[A] | MET |
| 3 | F | 3156[B] | MET |
| 3 | F | 3159[A] | SER |
| 3 | F | 3159[B] | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | F | 3160[A] | SER |
| 3 | F | 3160[B] | SER |
| 3 | F | 3161[A] | GLU |
| 3 | F | 3161[B] | GLU |
| 3 | F | 3162[A] | ASP |
| 3 | F | 3162[B] | ASP |
| 3 | F | 3163[A] | ASN |
| 3 | F | 3163[B] | ASN |
| 3 | F | 3169[A] | LYS |
| 3 | F | 3169[B] | LYS |
| 3 | F | 3172[A] | SER |
| 3 | F | 3172[B] | SER |
| 3 | F | 3176[A] | LYS |
| 3 | F | 3176[B] | LYS |
| 3 | F | 3181[A] | GLN |
| 3 | F | 3181[B] | GLN |
| 3 | F | 3182[A] | GLN |
| 3 | F | 3182[B] | GLN |
| 3 | F | 3183[A] | LEU |
| 3 | F | 3183[B] | LEU |
| 3 | F | 3185[A] | TYR |
| 3 | F | 3185[B] | TYR |
| 3 | F | 3186[A] | GLU |
| 3 | F | 3186[B] | GLU |
| 3 | F | 3188[A] | ASP |
| 3 | F | 3188[B] | ASP |
| 3 | F | 3191[A] | ASN |
| 3 | F | 3191[B] | ASN |
| 3 | F | 3192[A] | PHE |
| 3 | F | 3192[B] | PHE |
| 3 | F | 3193[A] | HIS |
| 3 | F | 3193[B] | HIS |
| 3 | F | 3195[A] | MET |
| 3 | F | 3195[B] | MET |
| 3 | F | 3196[A] | THR |
| 3 | F | 3196[B] | THR |
| 3 | F | 3200[A] | LEU |
| 3 | F | 3200[B] | LEU |
| 3 | F | 3201[A] | GLU |
| 3 | F | 3201[B] | GLU |
| 3 | F | 3204[A] | LEU |
| 3 | F | 3204[B] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | F | 3205[A] | LYS |
| 3 | F | 3205[B] | LYS |
| 3 | F | 3210[A] | LYS |
| 3 | F | 3210[B] | LYS |
| 3 | F | 3211[A] | ASP |
| 3 | F | 3211[B] | ASP |
| 3 | F | 3212[A] | ARG |
| 3 | F | 3212[B] | ARG |
| 3 | F | 3218[A] | LEU |
| 3 | F | 3218[B] | LEU |
| 3 | F | 3220[A] | ARG |
| 3 | F | 3220[B] | ARG |
| 3 | F | 3222[A] | ILE |
| 3 | F | 3222[B] | ILE |
| 3 | F | 3224[A] | GLN |
| 3 | F | 3224[B] | GLN |
| 3 | F | 3225[A] | SER |
| 3 | F | 3225[B] | SER |
| 3 | F | 3230[A] | PHE |
| 3 | F | 3230[B] | PHE |
| 3 | F | 3244[A] | THR |
| 3 | F | 3244[B] | THR |
| 3 | F | 3251[A] | ASP |
| 3 | F | 3251[B] | ASP |
| 3 | F | 3254[A] | MET |
| 3 | F | 3254[B] | MET |
| 3 | F | 3260[A] | ARG |
| 3 | F | 3260[B] | ARG |
| 3 | F | 3267[A] | SER |
| 3 | F | 3267[B] | SER |
| 3 | F | 3268[A] | LYS |
| 3 | F | 3268[B] | LYS |
| 3 | F | 3271[A] | VAL |
| 3 | F | 3271[B] | VAL |
| 3 | F | 3272[A] | HIS |
| 3 | F | 3272[B] | HIS |
| 3 | F | 3274[A] | ARG |
| 3 | F | 3274[B] | ARG |
| 3 | F | 3276[A] | ASP |
| 3 | F | 3276[B] | ASP |
| 3 | F | 3278[A] | HIS |
| 3 | F | 3278[B] | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | F | 3279[A] | ASP |
| 3 | F | 3279[B] | ASP |
| 3 | F | 3283[A] | ILE |
| 3 | F | 3283[B] | ILE |
| 3 | F | 3286[A] | THR |
| 3 | F | 3286[B] | THR |
| 3 | F | 3287[A] | ILE |
| 3 | F | 3287[B] | ILE |
| 3 | F | 3288[A] | MET |
| 3 | F | 3288[B] | MET |
| 3 | F | 3290[A] | ILE |
| 3 | F | 3290[B] | ILE |
| 3 | F | 3293[A] | LYS |
| 3 | F | 3293[B] | LYS |
| 3 | F | 3297[A] | PRO |
| 3 | F | 3297[B] | PRO |
| 3 | F | 3299[A] | LEU |
| 3 | F | 3299[B] | LEU |
| 3 | F | 3302[A] | SER |
| 3 | F | 3302[B] | SER |
| 3 | F | 3304[A] | THR |
| 3 | F | 3304[B] | THR |
| 3 | F | 3306[A] | LEU |
| 3 | F | 3306[B] | LEU |
| 3 | F | 3308[A] | LYS |
| 3 | F | 3308[B] | LYS |
| 1 | G | 4 | ARG |
| 1 | G | 17 | ASN |
| 1 | G | 19 | GLN |
| 1 | G | 26 | GLN |
| 1 | G | 37 | ILE |
| 1 | G | 53 | SER |
| 1 | G | 62 | MET |
| 1 | G | 67 | MET |
| 1 | G | 70 | ARG |
| 1 | G | 83 | HIS |
| 1 | G | 89 | ILE |
| 1 | G | 116 | LYS |
| 1 | G | 119 | LYS |
| 1 | G | 128 | ILE |
| 1 | G | 131 | GLU |
| 1 | G | 132 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 134 | VAL |
| 1 | G | 148 | GLN |
| 1 | G | 163 | LEU |
| 1 | G | 166 | GLU |
| 1 | G | 182 | ILE |
| 1 | G | 185 | LEU |
| 1 | G | 191 | THR |
| 1 | G | 205 | LEU |
| 1 | G | 214 | GLU |
| 1 | G | 223 | LEU |
| 1 | G | 226 | HIS |
| 1 | G | 238 | ASN |
| 1 | G | 249 | ARG |
| 1 | G | 260 | ASN |
| 1 | G | 266 | LEU |
| 1 | G | 280 | SER |
| 1 | G | 281 | LEU |
| 1 | G | 285 | THR |
| 1 | G | 290 | GLU |
| 1 | G | 308 | LEU |
| 1 | G | 325 | THR |
| 1 | G | 330 | GLN |
| 1 | G | 331 | SER |
| 1 | G | 336 | ASN |
| 1 | G | 337 | ASP |
| 1 | G | 344 | LEU |
| 1 | G | 349 | GLU |
| 1 | G | 353 | ASN |
| 1 | G | 354 | PHE |
| 1 | G | 384 | THR |
| 1 | G | 386 | ILE |
| 1 | G | 387 | ASN |
| 1 | G | 395 | THR |
| 1 | G | 400 | ILE |
| 1 | G | 411 | ASP |
| 1 | G | 415 | VAL |
| 1 | G | 450 | LYS |
| 1 | G | 451 | SER |
| 1 | G | 456 | GLN |
| 1 | G | 472 | ASP |
| 1 | G | 474 | LEU |
| 1 | G | 476 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 494 | VAL |
| 1 | G | 497 | GLN |
| 1 | G | 509 | ILE |
| 1 | G | 515 | ASP |
| 1 | G | 540 | THR |
| 1 | G | 553 | LEU |
| 1 | G | 565 | GLU |
| 1 | G | 566 | ARG |
| 1 | G | 567 | LEU |
| 1 | G | 568 | PHE |
| 1 | G | 570 | GLN |
| 1 | G | 572 | SER |
| 1 | G | 579 | LEU |
| 1 | G | 584 | SER |
| 1 | G | 588 | GLU |
| 1 | G | 597 | VAL |
| 1 | G | 600 | GLU |
| 1 | G | 603 | HIS |
| 1 | G | 610 | THR |
| 1 | G | 618 | MET |
| 1 | G | 624 | THR |
| 1 | G | 674 | LYS |
| 1 | G | 675 | SER |
| 1 | G | 684 | ARG |
| 1 | G | 687 | SER |
| 1 | G | 692 | VAL |
| 1 | G | 695 | TYR |
| 1 | G | 722 | GLU |
| 1 | G | 727 | ASP |
| 1 | G | 744 | VAL |
| 1 | G | 749 | VAL |
| 1 | G | 753 | ASN |
| 1 | G | 762 | VAL |
| 1 | G | 783 | ASP |
| 1 | G | 788 | LEU |
| 1 | G | 797 | THR |
| 1 | G | 808 | THR |
| 1 | G | 821 | ILE |
| 1 | G | 832 | LYS |
| 1 | G | 834 | ASP |
| 1 | G | 838 | ARG |
| 1 | G | 842 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 856 | THR |
| 1 | G | 866 | GLU |
| 1 | G | 885 | SER |
| 1 | G | 894 | CYS |
| 1 | G | 896 | HIS |
| 1 | G | 901 | THR |
| 1 | G | 912 | ASN |
| 1 | G | 930 | ASP |
| 1 | G | 935 | ILE |
| 1 | G | 943 | LEU |
| 1 | G | 953 | GLU |
| 1 | G | 961 | SER |
| 1 | G | 965 | ASP |
| 1 | G | 973 | ARG |
| 1 | G | 977 | GLU |
| 1 | G | 979 | LEU |
| 1 | G | 987 | LYS |
| 1 | G | 999 | LEU |
| 1 | G | 1001 | GLN |
| 1 | G | 1012 | GLU |
| 1 | G | 1013 | ILE |
| 1 | G | 1015 | HIS |
| 1 | G | 1017 | HIS |
| 1 | G | 1026 | GLU |
| 1 | G | 1028 | VAL |
| 1 | G | 1075 | GLU |
| 1 | G | 1077 | LEU |
| 1 | G | 1078 | ARG |
| 1 | G | 1081 | MET |
| 1 | G | 1097 | ARG |
| 1 | G | 1105 | VAL |
| 1 | G | 1118 | THR |
| 1 | G | 1121 | LEU |
| 1 | G | 1126 | ILE |
| 1 | G | 1154 | SER |
| 1 | G | 1156 | LEU |
| 1 | G | 1157 | VAL |
| 1 | G | 1160 | PHE |
| 1 | G | 1166 | THR |
| 1 | G | 1174 | GLU |
| 1 | G | 1182 | ASN |
| 1 | G | 1183 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 1195 | ASP |
| 1 | G | 1199 | VAL |
| 1 | G | 1200 | MET |
| 1 | G | 1210 | LYS |
| 1 | G | 1213 | VAL |
| 1 | G | 1226 | THR |
| 1 | G | 1228 | LEU |
| 1 | G | 1230 | LEU |
| 1 | G | 1240 | ILE |
| 1 | G | 1245 | GLU |
| 1 | G | 1254 | THR |
| 1 | G | 1255 | SER |
| 1 | G | 1258 | ARG |
| 1 | G | 1260 | ARG |
| 1 | G | 1280 | GLN |
| 1 | G | 1303 | GLU |
| 1 | G | 1304 | ASP |
| 1 | G | 1339 | SER |
| 1 | G | 1354 | GLU |
| 1 | G | 1369 | THR |
| 1 | G | 1372 | ILE |
| 1 | G | 1381 | LYS |
| 1 | G | 1401 | ARG |
| 1 | G | 1427 | HIS |
| 1 | G | 1439 | VAL |
| 1 | G | 1441 | SER |
| 1 | G | 1456 | LEU |
| 1 | G | 1470 | GLU |
| 1 | G | 1471 | LEU |
| 1 | G | 1476 | LYS |
| 1 | G | 1478 | SER |
| 1 | G | 1494 | ARG |
| 1 | G | 1509 | THR |
| 1 | G | 1530 | LEU |
| 1 | G | 1543 | ILE |
| 1 | G | 1559 | LEU |
| 1 | G | 1563 | LYS |
| 1 | G | 1568 | VAL |
| 1 | G | 1578 | ILE |
| 1 | G | 1599 | MET |
| 1 | G | 1622 | GLN |
| 1 | G | 1632 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 1642 | GLN |
| 1 | G | 1643 | LYS |
| 1 | G | 1655 | SER |
| 2 | H | 2083 | VAL |
| 2 | H | 2086 | ASN |
| 2 | H | 2089 | ARG |
| 2 | H | 2131 | LEU |
| 2 | H | 2143 | CYS |
| 2 | H | 2145 | LEU |
| 2 | H | 2160 | VAL |
| 2 | H | 2168 | ARG |
| 2 | H | 2186 | GLU |
| 2 | H | 2187 | VAL |
| 2 | H | 2191 | LEU |
| 2 | H | 2203 | ILE |
| 2 | H | 2204 | GLU |
| 2 | H | 2205 | THR |
| 2 | H | 2224 | THR |
| 2 | H | 2226 | GLU |
| 2 | H | 2231 | LEU |
| 2 | H | 2237 | LEU |
| 2 | H | 2241 | THR |
| 2 | H | 2260 | GLU |
| 2 | H | 2267 | HIS |
| 2 | H | 2274 | LEU |
| 2 | H | 2277 | LYS |
| 2 | H | 2296 | LEU |
| 2 | H | 2327 | GLU |
| 2 | H | 2328 | LEU |
| 2 | H | 2333 | LEU |
| 2 | H | 2344 | LEU |
| 2 | H | 2345 | ASN |
| 2 | H | 2359 | ASN |
| 2 | H | 2361 | LYS |
| 2 | H | 2373 | MET |
| 2 | H | 2394 | VAL |
| 2 | H | 2445 | MET |
| 2 | H | 2456 | LEU |
| 2 | H | 2457 | LYS |
| 2 | H | 2469 | VAL |
| 2 | H | 2480 | LEU |
| 2 | H | 2497 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 2500 | ILE |
| 2 | H | 2505 | ILE |
| 2 | H | 2545 | SER |
| 2 | H | 2548 | CYS |
| 2 | H | 2556 | TYR |
| 2 | H | 2561 | HIS |
| 2 | H | 2571 | ARG |
| 2 | H | 2572 | VAL |
| 2 | H | 2575 | LEU |
| 2 | H | 2581 | MET |
| 2 | H | 2595 | TRP |
| 2 | H | 2597 | MET |
| 2 | H | 2600 | ASP |
| 2 | H | 2615 | TRP |
| 2 | H | 2616 | THR |
| 2 | H | 2625 | LEU |
| 2 | H | 2630 | LYS |
| 2 | H | 2631 | TYR |
| 2 | H | 2637 | VAL |
| 2 | H | 2644 | LEU |
| 2 | H | 2652 | LYS |
| 2 | H | 2653 | GLU |
| 2 | H | 2662 | LEU |
| 2 | H | 2680 | HIS |
| 2 | H | 2687 | ILE |
| 2 | H | 2739 | LEU |
| 2 | H | 2742 | MET |
| 2 | H | 2750 | ILE |
| 2 | H | 2758 | THR |
| 2 | H | 2768 | LEU |
| 2 | H | 2769 | PHE |
| 2 | H | 2774 | LEU |
| 2 | H | 2780 | HIS |
| 2 | H | 2781 | LEU |
| 2 | H | 2782 | ASN |
| 2 | H | 2788 | ILE |
| 2 | H | 2791 | LEU |
| 2 | H | 2794 | LEU |
| 2 | H | 2809 | LEU |
| 2 | H | 2822 | LYS |
| 2 | H | 2826 | GLU |
| 2 | H | 2831 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 2838 | LEU |
| 2 | H | 2842 | THR |
| 2 | H | 2844 | MET |
| 2 | H | 2848 | PHE |
| 2 | H | 2849 | ASP |
| 2 | H | 2851 | ASN |
| 2 | H | 2858 | ASP |
| 2 | H | 2864 | ASN |
| 2 | H | 2868 | GLU |
| 2 | H | 2876 | LYS |
| 2 | H | 2878 | ARG |
| 2 | H | 2881 | VAL |
| 2 | H | 2883 | ILE |
| 2 | H | 2884 | LYS |
| 2 | H | 2887 | ASP |
| 2 | H | 2890 | VAL |
| 2 | H | 2891 | LEU |
| 2 | H | 2898 | LYS |
| 2 | H | 2900 | SER |
| 3 | I | 2929[A] | SER |
| 3 | I | 2929[B] | SER |
| 3 | I | 2930[A] | LEU |
| 3 | I | 2930[B] | LEU |
| 3 | I | 2931[A] | THR |
| 3 | I | 2931[B] | THR |
| 3 | I | 2933[A] | SER |
| 3 | I | 2933[B] | SER |
| 3 | I | 2935[A] | ILE |
| 3 | I | 2935[B] | ILE |
| 3 | I | 2938[A] | LEU |
| 3 | I | 2938[B] | LEU |
| 3 | I | 2942[A] | LEU |
| 3 | I | 2942[B] | LEU |
| 3 | I | 2946[A] | GLN |
| 3 | I | 2946[B] | GLN |
| 3 | I | 2949[A] | LYS |
| 3 | I | 2949[B] | LYS |
| 3 | I | 2954[A] | TYR |
| 3 | I | 2954[B] | TYR |
| 3 | I | 2956[A] | LYS |
| 3 | I | 2956[B] | LYS |
| 3 | I | 2959[A] | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | I | 2959[B] | SER |
| 3 | I | 2960[A] | PHE |
| 3 | I | 2960[B] | PHE |
| 3 | I | 2963[A] | MET |
| 3 | I | 2963[B] | MET |
| 3 | I | 2965[A] | LEU |
| 3 | I | 2965[B] | LEU |
| 3 | I | 2968[A] | GLN |
| 3 | I | 2968[B] | GLN |
| 3 | I | 2973[A] | THR |
| 3 | I | 2973[B] | THR |
| 3 | I | 2980[A] | HIS |
| 3 | I | 2980[B] | HIS |
| 3 | I | 2982[A] | MET |
| 3 | I | 2982[B] | MET |
| 3 | I | 2990[A] | ARG |
| 3 | I | 2990[B] | ARG |
| 3 | I | 2995[A] | GLN |
| 3 | I | 2995[B] | GLN |
| 3 | I | 2996[A] | MET |
| 3 | I | 2996[B] | MET |
| 3 | I | 2997[A] | GLU |
| 3 | I | 2997[B] | GLU |
| 3 | I | 3000[A] | LEU |
| 3 | I | 3000[B] | LEU |
| 3 | I | 3001[A] | LYS |
| 3 | I | 3001[B] | LYS |
| 3 | I | 3019[A] | HIS |
| 3 | I | 3019[B] | HIS |
| 3 | I | 3021[A] | LEU |
| 3 | I | 3021[B] | LEU |
| 3 | I | 3023[A] | ILE |
| 3 | I | 3023[B] | ILE |
| 3 | I | 3024[A] | LEU |
| 3 | I | 3024[B] | LEU |
| 3 | I | 3026[A] | THR |
| 3 | I | 3026[B] | THR |
| 3 | I | 3029[A] | LYS |
| 3 | I | 3029[B] | LYS |
| 3 | I | 3040[A] | VAL |
| 3 | I | 3040[B] | VAL |
| 3 | I | 3042[A] | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | I | 3042[B] | ASP |
| 3 | I | 3044[A] | LYS |
| 3 | I | 3044[B] | LYS |
| 3 | I | 3048[A] | ASP |
| 3 | I | 3048[B] | ASP |
| 3 | I | 3050[A] | ARG |
| 3 | I | 3050[B] | ARG |
| 3 | I | 3063[A] | SER |
| 3 | I | 3063[B] | SER |
| 3 | I | 3067[A] | ARG |
| 3 | I | 3067[B] | ARG |
| 3 | I | 3077[A] | ASP |
| 3 | I | 3077[B] | ASP |
| 3 | I | 3081[A] | PHE |
| 3 | I | 3081[B] | PHE |
| 3 | I | 3096[A] | VAL |
| 3 | I | 3096[B] | VAL |
| 3 | I | 3105[A] | SER |
| 3 | I | 3105[B] | SER |
| 3 | I | 3107[A] | LEU |
| 3 | I | 3107[B] | LEU |
| 3 | I | 3110[A] | THR |
| 3 | I | 3110[B] | THR |
| 3 | I | 3111[A] | SER |
| 3 | I | 3111[B] | SER |
| 3 | I | 3115[A] | LEU |
| 3 | I | 3115[B] | LEU |
| 3 | I | 3123[A] | THR |
| 3 | I | 3123[B] | THR |
| 3 | I | 3131[A] | GLN |
| 3 | I | 3131[B] | GLN |
| 3 | I | 3133[A] | LEU |
| 3 | I | 3133[B] | LEU |
| 3 | I | 3134[A] | GLN |
| 3 | I | 3134[B] | GLN |
| 3 | I | 3135[A] | LYS |
| 3 | I | 3135[B] | LYS |
| 3 | I | 3139[A] | LEU |
| 3 | I | 3139[B] | LEU |
| 3 | I | 3141[A] | TYR |
| 3 | I | 3141[B] | TYR |
| 3 | I | 3147[A] | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | I | 3147[B] | GLU |
| 3 | I | 3151[A] | LEU |
| 3 | I | 3151[B] | LEU |
| 3 | I | 3152[A] | LYS |
| 3 | I | 3152[B] | LYS |
| 3 | I | 3156[A] | MET |
| 3 | I | 3156[B] | MET |
| 3 | I | 3159[A] | SER |
| 3 | I | 3159[B] | SER |
| 3 | I | 3160[A] | SER |
| 3 | I | 3160[B] | SER |
| 3 | I | 3161[A] | GLU |
| 3 | I | 3161[B] | GLU |
| 3 | I | 3162[A] | ASP |
| 3 | I | 3162[B] | ASP |
| 3 | I | 3163[A] | ASN |
| 3 | I | 3163[B] | ASN |
| 3 | I | 3169[A] | LYS |
| 3 | I | 3169[B] | LYS |
| 3 | I | 3172[A] | SER |
| 3 | I | 3172[B] | SER |
| 3 | I | 3176[A] | LYS |
| 3 | I | 3176[B] | LYS |
| 3 | I | 3181[A] | GLN |
| 3 | I | 3181[B] | GLN |
| 3 | I | 3182[A] | GLN |
| 3 | I | 3182[B] | GLN |
| 3 | I | 3183[A] | LEU |
| 3 | I | 3183[B] | LEU |
| 3 | I | 3185[A] | TYR |
| 3 | I | 3185[B] | TYR |
| 3 | I | 3186[A] | GLU |
| 3 | I | 3186[B] | GLU |
| 3 | I | 3188[A] | ASP |
| 3 | I | 3188[B] | ASP |
| 3 | I | 3191[A] | ASN |
| 3 | I | 3191[B] | ASN |
| 3 | I | 3192[A] | PHE |
| 3 | I | 3192[B] | PHE |
| 3 | I | 3193[A] | HIS |
| 3 | I | 3193[B] | HIS |
| 3 | I | 3195[A] | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | I | 3195[B] | MET |
| 3 | I | 3196[A] | THR |
| 3 | I | 3196[B] | THR |
| 3 | I | 3200[A] | LEU |
| 3 | I | 3200[B] | LEU |
| 3 | I | 3201[A] | GLU |
| 3 | I | 3201[B] | GLU |
| 3 | I | 3204[A] | LEU |
| 3 | I | 3204[B] | LEU |
| 3 | I | 3205[A] | LYS |
| 3 | I | 3205[B] | LYS |
| 3 | I | 3210[A] | LYS |
| 3 | I | 3210[B] | LYS |
| 3 | I | 3211[A] | ASP |
| 3 | I | 3211[B] | ASP |
| 3 | I | 3212[A] | ARG |
| 3 | I | 3212[B] | ARG |
| 3 | I | 3218[A] | LEU |
| 3 | I | 3218[B] | LEU |
| 3 | I | 3220[A] | ARG |
| 3 | I | 3220[B] | ARG |
| 3 | I | 3222[A] | ILE |
| 3 | I | 3222[B] | ILE |
| 3 | I | 3224[A] | GLN |
| 3 | I | 3224[B] | GLN |
| 3 | I | 3225[A] | SER |
| 3 | I | 3225[B] | SER |
| 3 | I | 3230[A] | PHE |
| 3 | I | 3230[B] | PHE |
| 3 | I | 3244[A] | THR |
| 3 | I | 3244[B] | THR |
| 3 | I | 3251[A] | ASP |
| 3 | I | 3251[B] | ASP |
| 3 | I | 3254[A] | MET |
| 3 | I | 3254[B] | MET |
| 3 | I | 3260[A] | ARG |
| 3 | I | 3260[B] | ARG |
| 3 | I | 3267[A] | SER |
| 3 | I | 3267[B] | SER |
| 3 | I | 3268[A] | LYS |
| 3 | I | 3268[B] | LYS |
| 3 | I | 3271[A] | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | I | 3271[B] | VAL |
| 3 | I | 3272[A] | HIS |
| 3 | I | 3272[B] | HIS |
| 3 | I | 3274[A] | ARG |
| 3 | I | 3274[B] | ARG |
| 3 | I | 3276[A] | ASP |
| 3 | I | 3276[B] | ASP |
| 3 | I | 3278[A] | HIS |
| 3 | I | 3278[B] | HIS |
| 3 | I | 3279[A] | ASP |
| 3 | I | 3279[B] | ASP |
| 3 | I | 3283[A] | ILE |
| 3 | I | 3283[B] | ILE |
| 3 | I | 3286[A] | THR |
| 3 | I | 3286[B] | THR |
| 3 | I | 3287[A] | ILE |
| 3 | I | 3287[B] | ILE |
| 3 | I | 3288[A] | MET |
| 3 | I | 3288[B] | MET |
| 3 | I | 3290[A] | ILE |
| 3 | I | 3290[B] | ILE |
| 3 | I | 3293[A] | LYS |
| 3 | I | 3293[B] | LYS |
| 3 | I | 3297[A] | PRO |
| 3 | I | 3297[B] | PRO |
| 3 | I | 3299[A] | LEU |
| 3 | I | 3299[B] | LEU |
| 3 | I | 3302[A] | SER |
| 3 | I | 3302[B] | SER |
| 3 | I | 3304[A] | THR |
| 3 | I | 3304[B] | THR |
| 3 | I | 3306[A] | LEU |
| 3 | I | 3306[B] | LEU |
| 3 | I | 3308[A] | LYS |
| 3 | I | 3308[B] | LYS |
| 1 | J | 2 | LEU |
| 1 | J | 4 | ARG |
| 1 | J | 17 | ASN |
| 1 | J | 19 | GLN |
| 1 | J | 22 | LEU |
| 1 | J | 25 | MET |
| 1 | J | 26 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 55 | ILE |
| 1 | J | 59 | LEU |
| 1 | J | 62 | MET |
| 1 | J | 67 | MET |
| 1 | J | 70 | ARG |
| 1 | J | 100 | GLN |
| 1 | J | 121 | ASN |
| 1 | J | 133 | LYS |
| 1 | J | 137 | ARG |
| 1 | J | 144 | TYR |
| 1 | J | 151 | GLN |
| 1 | J | 160 | LEU |
| 1 | J | 163 | LEU |
| 1 | J | 179 | HIS |
| 1 | J | 185 | LEU |
| 1 | J | 205 | LEU |
| 1 | J | 211 | SER |
| 1 | J | 214 | GLU |
| 1 | J | 219 | LEU |
| 1 | J | 223 | LEU |
| 1 | J | 225 | LYS |
| 1 | J | 227 | ARG |
| 1 | J | 235 | CYS |
| 1 | J | 237 | LEU |
| 1 | J | 238 | ASN |
| 1 | J | 239 | LEU |
| 1 | J | 249 | ARG |
| 1 | J | 266 | LEU |
| 1 | J | 279 | LEU |
| 1 | J | 281 | LEU |
| 1 | J | 289 | LEU |
| 1 | J | 290 | GLU |
| 1 | J | 308 | LEU |
| 1 | J | 329 | ARG |
| 1 | J | 330 | GLN |
| 1 | J | 332 | ASP |
| 1 | J | 336 | ASN |
| 1 | J | 376 | ASN |
| 1 | J | 384 | THR |
| 1 | J | 386 | ILE |
| 1 | J | 390 | LEU |
| 1 | J | 391 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 407 | GLN |
| 1 | J | 419 | THR |
| 1 | J | 420 | SER |
| 1 | J | 432 | THR |
| 1 | J | 433 | THR |
| 1 | J | 434 | GLU |
| 1 | J | 444 | GLU |
| 1 | J | 450 | LYS |
| 1 | J | 452 | ILE |
| 1 | J | 456 | GLN |
| 1 | J | 467 | LYS |
| 1 | J | 472 | ASP |
| 1 | J | 474 | LEU |
| 1 | J | 477 | VAL |
| 1 | J | 494 | VAL |
| 1 | J | 509 | ILE |
| 1 | J | 518 | LYS |
| 1 | J | 527 | LEU |
| 1 | J | 557 | VAL |
| 1 | J | 559 | THR |
| 1 | J | 560 | SER |
| 1 | J | 567 | LEU |
| 1 | J | 568 | PHE |
| 1 | J | 569 | LYS |
| 1 | J | 570 | GLN |
| 1 | J | 573 | LYS |
| 1 | J | 597 | VAL |
| 1 | J | 600 | GLU |
| 1 | J | 603 | HIS |
| 1 | J | 617 | SER |
| 1 | J | 633 | HIS |
| 1 | J | 669 | LYS |
| 1 | J | 675 | SER |
| 1 | J | 695 | TYR |
| 1 | J | 705 | THR |
| 1 | J | 712 | SER |
| 1 | J | 739 | GLN |
| 1 | J | 744 | VAL |
| 1 | J | 749 | VAL |
| 1 | J | 753 | ASN |
| 1 | J | 782 | THR |
| 1 | J | 797 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 806 | ASN |
| 1 | J | 810 | LEU |
| 1 | J | 832 | LYS |
| 1 | J | 844 | ASP |
| 1 | J | 871 | GLN |
| 1 | J | 881 | GLN |
| 1 | J | 894 | CYS |
| 1 | J | 901 | THR |
| 1 | J | 912 | ASN |
| 1 | J | 917 | LEU |
| 1 | J | 930 | ASP |
| 1 | J | 935 | ILE |
| 1 | J | 936 | ASP |
| 1 | J | 941 | LEU |
| 1 | J | 953 | GLU |
| 1 | J | 965 | ASP |
| 1 | J | 999 | LEU |
| 1 | J | 1001 | GLN |
| 1 | J | 1015 | HIS |
| 1 | J | 1017 | HIS |
| 1 | J | 1025 | THR |
| 1 | J | 1075 | GLU |
| 1 | J | 1077 | LEU |
| 1 | J | 1078 | ARG |
| 1 | J | 1090 | ILE |
| 1 | J | 1093 | ASP |
| 1 | J | 1105 | VAL |
| 1 | J | 1131 | ARG |
| 1 | J | 1142 | VAL |
| 1 | J | 1145 | THR |
| 1 | J | 1152 | LYS |
| 1 | J | 1157 | VAL |
| 1 | J | 1160 | PHE |
| 1 | J | 1167 | ASP |
| 1 | J | 1168 | GLN |
| 1 | J | 1182 | ASN |
| 1 | J | 1183 | GLU |
| 1 | J | 1199 | VAL |
| 1 | J | 1200 | MET |
| 1 | J | 1206 | HIS |
| 1 | J | 1210 | LYS |
| 1 | J | 1215 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 1221 | THR |
| 1 | J | 1228 | LEU |
| 1 | J | 1231 | VAL |
| 1 | J | 1233 | SER |
| 1 | J | 1249 | TRP |
| 1 | J | 1258 | ARG |
| 1 | J | 1260 | ARG |
| 1 | J | 1266 | PHE |
| 1 | J | 1280 | GLN |
| 1 | J | 1284 | GLU |
| 1 | J | 1286 | ARG |
| 1 | J | 1307 | MET |
| 1 | J | 1331 | GLU |
| 1 | J | 1339 | SER |
| 1 | J | 1341 | VAL |
| 1 | J | 1369 | THR |
| 1 | J | 1372 | ILE |
| 1 | J | 1393 | THR |
| 1 | J | 1396 | GLU |
| 1 | J | 1408 | LEU |
| 1 | J | 1430 | ILE |
| 1 | J | 1439 | VAL |
| 1 | J | 1441 | SER |
| 1 | J | 1458 | HIS |
| 1 | J | 1473 | ARG |
| 1 | J | 1478 | SER |
| 1 | J | 1494 | ARG |
| 1 | J | 1516 | VAL |
| 1 | J | 1541 | GLU |
| 1 | J | 1550 | ARG |
| 1 | J | 1553 | ILE |
| 1 | J | 1559 | LEU |
| 1 | J | 1562 | ILE |
| 1 | J | 1563 | LYS |
| 1 | J | 1567 | ASP |
| 1 | J | 1568 | VAL |
| 1 | J | 1580 | GLU |
| 1 | J | 1581 | GLU |
| 1 | J | 1583 | CYS |
| 1 | J | 1597 | THR |
| 1 | J | 1599 | MET |
| 1 | J | 1602 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 1620 | LEU |
| 1 | J | 1622 | GLN |
| 1 | J | 1629 | GLU |
| 1 | J | 1632 | LEU |
| 1 | J | 1633 | THR |
| 1 | J | 1639 | LYS |
| 1 | J | 1642 | GLN |
| 1 | J | 1644 | ILE |
| 2 | K | 2089 | ARG |
| 2 | K | 2092 | VAL |
| 2 | K | 2108 | LYS |
| 2 | K | 2117 | ASP |
| 2 | K | 2131 | LEU |
| 2 | K | 2145 | LEU |
| 2 | K | 2160 | VAL |
| 2 | K | 2180 | TRP |
| 2 | K | 2184 | MET |
| 2 | K | 2185 | THR |
| 2 | K | 2190 | LEU |
| 2 | K | 2205 | THR |
| 2 | K | 2211 | HIS |
| 2 | K | 2220 | GLU |
| 2 | K | 2222 | MET |
| 2 | K | 2237 | LEU |
| 2 | K | 2239 | LYS |
| 2 | K | 2248 | ILE |
| 2 | K | 2260 | GLU |
| 2 | K | 2267 | HIS |
| 2 | K | 2270 | ILE |
| 2 | K | 2274 | LEU |
| 2 | K | 2282 | LEU |
| 2 | K | 2283 | ASN |
| 2 | K | 2326 | ILE |
| 2 | K | 2327 | GLU |
| 2 | K | 2333 | LEU |
| 2 | K | 2344 | LEU |
| 2 | K | 2355 | SER |
| 2 | K | 2370 | MET |
| 2 | K | 2373 | MET |
| 2 | K | 2460 | SER |
| 2 | K | 2468 | ILE |
| 2 | K | 2480 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | K | 2489 | ILE |
| 2 | K | 2500 | ILE |
| 2 | K | 2502 | LEU |
| 2 | K | 2506 | ARG |
| 2 | K | 2507 | ARG |
| 2 | K | 2533 | ASP |
| 2 | K | 2546 | LEU |
| 2 | K | 2547 | MET |
| 2 | K | 2548 | CYS |
| 2 | K | 2561 | HIS |
| 2 | K | 2572 | VAL |
| 2 | K | 2579 | GLU |
| 2 | K | 2581 | MET |
| 2 | K | 2595 | TRP |
| 2 | K | 2597 | MET |
| 2 | K | 2600 | ASP |
| 2 | K | 2601 | ASN |
| 2 | K | 2616 | THR |
| 2 | K | 2620 | ILE |
| 2 | K | 2625 | LEU |
| 2 | K | 2653 | GLU |
| 2 | K | 2662 | LEU |
| 2 | K | 2714 | VAL |
| 2 | K | 2750 | ILE |
| 2 | K | 2758 | THR |
| 2 | K | 2769 | PHE |
| 2 | K | 2772 | LYS |
| 2 | K | 2780 | HIS |
| 2 | K | 2809 | LEU |
| 2 | K | 2826 | GLU |
| 2 | K | 2835 | ILE |
| 2 | K | 2848 | PHE |
| 2 | K | 2849 | ASP |
| 2 | K | 2860 | LEU |
| 2 | K | 2862 | LYS |
| 2 | K | 2868 | GLU |
| 2 | K | 2870 | LEU |
| 2 | K | 2875 | SER |
| 2 | K | 2879 | LEU |
| 2 | K | 2880 | GLU |
| 2 | K | 2881 | VAL |
| 2 | K | 2883 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | K | 2884 | LYS |
| 2 | K | 2891 | LEU |
| 2 | K | 2895 | SER |
| 2 | K | 2898 | LYS |
| 2 | K | 2900 | SER |
| 2 | K | 2902 | ILE |
| 3 | L | 2929[A] | SER |
| 3 | L | 2929[B] | SER |
| 3 | L | 2930[A] | LEU |
| 3 | L | 2930[B] | LEU |
| 3 | L | 2931[A] | THR |
| 3 | L | 2931[B] | THR |
| 3 | L | 2933[A] | SER |
| 3 | L | 2933[B] | SER |
| 3 | L | 2935[A] | ILE |
| 3 | L | 2935[B] | ILE |
| 3 | L | 2938[A] | LEU |
| 3 | L | 2938[B] | LEU |
| 3 | L | 2942[A] | LEU |
| 3 | L | 2942[B] | LEU |
| 3 | L | 2946[A] | GLN |
| 3 | L | 2946[B] | GLN |
| 3 | L | 2949[A] | LYS |
| 3 | L | 2949[B] | LYS |
| 3 | L | 2954[A] | TYR |
| 3 | L | 2954[B] | TYR |
| 3 | L | 2956[A] | LYS |
| 3 | L | 2956[B] | LYS |
| 3 | L | 2959[A] | SER |
| 3 | L | 2959[B] | SER |
| 3 | L | 2960[A] | PHE |
| 3 | L | 2960[B] | PHE |
| 3 | L | 2963[A] | MET |
| 3 | L | 2963[B] | MET |
| 3 | L | 2965[A] | LEU |
| 3 | L | 2965[B] | LEU |
| 3 | L | 2968[A] | GLN |
| 3 | L | 2968[B] | GLN |
| 3 | L | 2973[A] | THR |
| 3 | L | 2973[B] | THR |
| 3 | L | 2980[A] | HIS |
| 3 | L | 2980[B] | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | L | 2982[A] | MET |
| 3 | L | 2982[B] | MET |
| 3 | L | 2990[A] | ARG |
| 3 | L | 2990[B] | ARG |
| 3 | L | 2995[A] | GLN |
| 3 | L | 2995[B] | GLN |
| 3 | L | 2996[A] | MET |
| 3 | L | 2996[B] | MET |
| 3 | L | 2997[A] | GLU |
| 3 | L | 2997[B] | GLU |
| 3 | L | 3000[A] | LEU |
| 3 | L | 3000[B] | LEU |
| 3 | L | 3001[A] | LYS |
| 3 | L | 3001[B] | LYS |
| 3 | L | 3019[A] | HIS |
| 3 | L | 3019[B] | HIS |
| 3 | L | 3021[A] | LEU |
| 3 | L | 3021[B] | LEU |
| 3 | L | 3023[A] | ILE |
| 3 | L | 3023[B] | ILE |
| 3 | L | 3024[A] | LEU |
| 3 | L | 3024[B] | LEU |
| 3 | L | 3026[A] | THR |
| 3 | L | 3026[B] | THR |
| 3 | L | 3029[A] | LYS |
| 3 | L | 3029[B] | LYS |
| 3 | L | 3040[A] | VAL |
| 3 | L | 3040[B] | VAL |
| 3 | L | 3042[A] | ASP |
| 3 | L | 3042[B] | ASP |
| 3 | L | 3044[A] | LYS |
| 3 | L | 3044[B] | LYS |
| 3 | L | 3048[A] | ASP |
| 3 | L | 3048[B] | ASP |
| 3 | L | 3050[A] | ARG |
| 3 | L | 3050[B] | ARG |
| 3 | L | 3063[A] | SER |
| 3 | L | 3063[B] | SER |
| 3 | L | 3067[A] | ARG |
| 3 | L | 3067[B] | ARG |
| 3 | L | 3077[A] | ASP |
| 3 | L | 3077[B] | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | L | 3081[A] | PHE |
| 3 | L | 3081[B] | PHE |
| 3 | L | 3096[A] | VAL |
| 3 | L | 3096[B] | VAL |
| 3 | L | 3105[A] | SER |
| 3 | L | 3105[B] | SER |
| 3 | L | 3107[A] | LEU |
| 3 | L | 3107[B] | LEU |
| 3 | L | 3110[A] | THR |
| 3 | L | 3110[B] | THR |
| 3 | L | 3111[A] | SER |
| 3 | L | 3111[B] | SER |
| 3 | L | 3115[A] | LEU |
| 3 | L | 3115[B] | LEU |
| 3 | L | 3123[A] | THR |
| 3 | L | 3123[B] | THR |
| 3 | L | 3131[A] | GLN |
| 3 | L | 3131[B] | GLN |
| 3 | L | 3133[A] | LEU |
| 3 | L | 3133[B] | LEU |
| 3 | L | 3134[A] | GLN |
| 3 | L | 3134[B] | GLN |
| 3 | L | 3135[A] | LYS |
| 3 | L | 3135[B] | LYS |
| 3 | L | 3139[A] | LEU |
| 3 | L | 3139[B] | LEU |
| 3 | L | 3141[A] | TYR |
| 3 | L | 3141[B] | TYR |
| 3 | L | 3147[A] | GLU |
| 3 | L | 3147[B] | GLU |
| 3 | L | 3151[A] | LEU |
| 3 | L | 3151[B] | LEU |
| 3 | L | 3156[A] | MET |
| 3 | L | 3156[B] | MET |
| 3 | L | 3159[A] | SER |
| 3 | L | 3159[B] | SER |
| 3 | L | 3160[A] | SER |
| 3 | L | 3160[B] | SER |
| 3 | L | 3161[A] | GLU |
| 3 | L | 3161[B] | GLU |
| 3 | L | 3162[A] | ASP |
| 3 | L | 3162[B] | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | L | 3163[A] | ASN |
| 3 | L | 3163[B] | ASN |
| 3 | L | 3169[A] | LYS |
| 3 | L | 3169[B] | LYS |
| 3 | L | 3172[A] | SER |
| 3 | L | 3172[B] | SER |
| 3 | L | 3176[A] | LYS |
| 3 | L | 3176[B] | LYS |
| 3 | L | 3181[A] | GLN |
| 3 | L | 3181[B] | GLN |
| 3 | L | 3182[A] | GLN |
| 3 | L | 3182[B] | GLN |
| 3 | L | 3183[A] | LEU |
| 3 | L | 3183[B] | LEU |
| 3 | L | 3185[A] | TYR |
| 3 | L | 3185[B] | TYR |
| 3 | L | 3186[A] | GLU |
| 3 | L | 3186[B] | GLU |
| 3 | L | 3188[A] | ASP |
| 3 | L | 3188[B] | ASP |
| 3 | L | 3191[A] | ASN |
| 3 | L | 3191[B] | ASN |
| 3 | L | 3192[A] | PHE |
| 3 | L | 3192[B] | PHE |
| 3 | L | 3193[A] | HIS |
| 3 | L | 3193[B] | HIS |
| 3 | L | 3195[A] | MET |
| 3 | L | 3195[B] | MET |
| 3 | L | 3196[A] | THR |
| 3 | L | 3196[B] | THR |
| 3 | L | 3200[A] | LEU |
| 3 | L | 3200[B] | LEU |
| 3 | L | 3201[A] | GLU |
| 3 | L | 3201[B] | GLU |
| 3 | L | 3204[A] | LEU |
| 3 | L | 3204[B] | LEU |
| 3 | L | 3205[A] | LYS |
| 3 | L | 3205[B] | LYS |
| 3 | L | 3210[A] | LYS |
| 3 | L | 3210[B] | LYS |
| 3 | L | 3211[A] | ASP |
| 3 | L | 3211[B] | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | L | 3212[A] | ARG |
| 3 | L | 3212[B] | ARG |
| 3 | L | 3218[A] | LEU |
| 3 | L | 3218[B] | LEU |
| 3 | L | 3220[A] | ARG |
| 3 | L | 3220[B] | ARG |
| 3 | L | 3222[A] | ILE |
| 3 | L | 3222[B] | ILE |
| 3 | L | 3224[A] | GLN |
| 3 | L | 3224[B] | GLN |
| 3 | L | 3225[A] | SER |
| 3 | L | 3225[B] | SER |
| 3 | L | 3230[A] | PHE |
| 3 | L | 3230[B] | PHE |
| 3 | L | 3244[A] | THR |
| 3 | L | 3244[B] | THR |
| 3 | L | 3251[A] | ASP |
| 3 | L | 3251[B] | ASP |
| 3 | L | 3254[A] | MET |
| 3 | L | 3254[B] | MET |
| 3 | L | 3260[A] | ARG |
| 3 | L | 3260[B] | ARG |
| 3 | L | 3267[A] | SER |
| 3 | L | 3267[B] | SER |
| 3 | L | 3268[A] | LYS |
| 3 | L | 3268[B] | LYS |
| 3 | L | 3271[A] | VAL |
| 3 | L | 3271[B] | VAL |
| 3 | L | 3272[A] | HIS |
| 3 | L | 3272[B] | HIS |
| 3 | L | 3274[A] | ARG |
| 3 | L | 3274[B] | ARG |
| 3 | L | 3276[A] | ASP |
| 3 | L | 3276[B] | ASP |
| 3 | L | 3278[A] | HIS |
| 3 | L | 3278[B] | HIS |
| 3 | L | 3279[A] | ASP |
| 3 | L | 3279[B] | ASP |
| 3 | L | 3283[A] | ILE |
| 3 | L | 3283[B] | ILE |
| 3 | L | 3286[A] | THR |
| 3 | L | 3286[B] | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | L | 3287[A] | ILE |
| 3 | L | 3287[B] | ILE |
| 3 | L | 3288[A] | MET |
| 3 | L | 3288[B] | MET |
| 3 | L | 3290[A] | ILE |
| 3 | L | 3290[B] | ILE |
| 3 | L | 3293[A] | LYS |
| 3 | L | 3293[B] | LYS |
| 3 | L | 3297[A] | PRO |
| 3 | L | 3297[B] | PRO |
| 3 | L | 3299[A] | LEU |
| 3 | L | 3299[B] | LEU |
| 3 | L | 3302[A] | SER |
| 3 | L | 3302[B] | SER |
| 3 | L | 3304[A] | THR |
| 3 | L | 3304[B] | THR |
| 3 | L | 3306[A] | LEU |
| 3 | L | 3306[B] | LEU |
| 3 | L | 3308[A] | LYS |
| 3 | L | 3308[B] | LYS |
| 1 | M | 4 | ARG |
| 1 | M | 19 | GLN |
| 1 | M | 26 | GLN |
| 1 | M | 51 | ASP |
| 1 | M | 67 | MET |
| 1 | M | 70 | ARG |
| 1 | M | 89 | ILE |
| 1 | M | 100 | GLN |
| 1 | M | 104 | LEU |
| 1 | M | 109 | LEU |
| 1 | M | 114 | THR |
| 1 | M | 116 | LYS |
| 1 | M | 128 | ILE |
| 1 | M | 130 | PHE |
| 1 | M | 133 | LYS |
| 1 | M | 139 | VAL |
| 1 | M | 160 | LEU |
| 1 | M | 163 | LEU |
| 1 | M | 167 | ASP |
| 1 | M | 174 | GLN |
| 1 | M | 179 | HIS |
| 1 | M | 185 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 205 | LEU |
| 1 | M | 227 | ARG |
| 1 | M | 235 | CYS |
| 1 | M | 238 | ASN |
| 1 | M | 245 | GLU |
| 1 | M | 249 | ARG |
| 1 | M | 266 | LEU |
| 1 | M | 281 | LEU |
| 1 | M | 289 | LEU |
| 1 | M | 290 | GLU |
| 1 | M | 308 | LEU |
| 1 | M | 313 | THR |
| 1 | M | 329 | ARG |
| 1 | M | 330 | GLN |
| 1 | M | 336 | ASN |
| 1 | M | 365 | THR |
| 1 | M | 371 | LEU |
| 1 | M | 376 | ASN |
| 1 | M | 386 | ILE |
| 1 | M | 387 | ASN |
| 1 | M | 394 | GLN |
| 1 | M | 395 | THR |
| 1 | M | 407 | GLN |
| 1 | M | 424 | PHE |
| 1 | M | 448 | SER |
| 1 | M | 456 | GLN |
| 1 | M | 474 | LEU |
| 1 | M | 494 | VAL |
| 1 | M | 509 | ILE |
| 1 | M | 511 | VAL |
| 1 | M | 515 | ASP |
| 1 | M | 527 | LEU |
| 1 | M | 539 | GLU |
| 1 | M | 557 | VAL |
| 1 | M | 562 | GLN |
| 1 | M | 563 | ILE |
| 1 | M | 565 | GLU |
| 1 | M | 568 | PHE |
| 1 | M | 570 | GLN |
| 1 | M | 572 | SER |
| 1 | M | 589 | GLN |
| 1 | M | 597 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 601 | VAL |
| 1 | M | 603 | HIS |
| 1 | M | 606 | ILE |
| 1 | M | 618 | MET |
| 1 | M | 633 | HIS |
| 1 | M | 650 | GLN |
| 1 | M | 687 | SER |
| 1 | M | 688 | VAL |
| 1 | M | 695 | TYR |
| 1 | M | 705 | THR |
| 1 | M | 711 | LEU |
| 1 | M | 729 | VAL |
| 1 | M | 744 | VAL |
| 1 | M | 776 | VAL |
| 1 | M | 797 | THR |
| 1 | M | 808 | THR |
| 1 | M | 831 | VAL |
| 1 | M | 834 | ASP |
| 1 | M | 836 | GLN |
| 1 | M | 841 | LYS |
| 1 | M | 867 | VAL |
| 1 | M | 870 | TYR |
| 1 | M | 887 | ASP |
| 1 | M | 891 | LYS |
| 1 | M | 896 | HIS |
| 1 | M | 901 | THR |
| 1 | M | 909 | ILE |
| 1 | M | 913 | PHE |
| 1 | M | 930 | ASP |
| 1 | M | 935 | ILE |
| 1 | M | 938 | LEU |
| 1 | M | 943 | LEU |
| 1 | M | 964 | ILE |
| 1 | M | 965 | ASP |
| 1 | M | 980 | TYR |
| 1 | M | 999 | LEU |
| 1 | M | 1002 | GLU |
| 1 | M | 1013 | ILE |
| 1 | M | 1015 | HIS |
| 1 | M | 1017 | HIS |
| 1 | M | 1075 | GLU |
| 1 | M | 1077 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 1086 | LEU |
| 1 | M | 1098 | GLU |
| 1 | M | 1110 | LYS |
| 1 | M | 1126 | ILE |
| 1 | M | 1139 | LYS |
| 1 | M | 1157 | VAL |
| 1 | M | 1160 | PHE |
| 1 | M | 1164 | ASP |
| 1 | M | 1168 | GLN |
| 1 | M | 1169 | LYS |
| 1 | M | 1174 | GLU |
| 1 | M | 1182 | ASN |
| 1 | M | 1203 | MET |
| 1 | M | 1205 | LEU |
| 1 | M | 1207 | TYR |
| 1 | M | 1210 | LYS |
| 1 | M | 1211 | TYR |
| 1 | M | 1212 | HIS |
| 1 | M | 1213 | VAL |
| 1 | M | 1221 | THR |
| 1 | M | 1229 | LYS |
| 1 | M | 1230 | LEU |
| 1 | M | 1258 | ARG |
| 1 | M | 1260 | ARG |
| 1 | M | 1280 | GLN |
| 1 | M | 1286 | ARG |
| 1 | M | 1307 | MET |
| 1 | M | 1343 | VAL |
| 1 | M | 1357 | ARG |
| 1 | M | 1369 | THR |
| 1 | M | 1430 | ILE |
| 1 | M | 1439 | VAL |
| 1 | M | 1471 | LEU |
| 1 | M | 1473 | ARG |
| 1 | M | 1494 | ARG |
| 1 | M | 1509 | THR |
| 1 | M | 1516 | VAL |
| 1 | M | 1520 | GLN |
| 1 | M | 1537 | ILE |
| 1 | M | 1541 | GLU |
| 1 | M | 1550 | ARG |
| 1 | M | 1559 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 1567 | ASP |
| 1 | M | 1568 | VAL |
| 1 | M | 1580 | GLU |
| 1 | M | 1581 | GLU |
| 1 | M | 1597 | THR |
| 1 | M | 1632 | LEU |
| 1 | M | 1640 | ILE |
| 1 | M | 1642 | GLN |
| 1 | M | 1643 | LYS |
| 1 | M | 1649 | THR |
| 1 | M | 1653 | VAL |
| 1 | M | 1656 | ASP |
| 2 | N | 2089 | ARG |
| 2 | N | 2098 | GLN |
| 2 | N | 2104 | ILE |
| 2 | N | 2131 | LEU |
| 2 | N | 2132 | CYS |
| 2 | N | 2141 | HIS |
| 2 | N | 2145 | LEU |
| 2 | N | 2160 | VAL |
| 2 | N | 2185 | THR |
| 2 | N | 2187 | VAL |
| 2 | N | 2190 | LEU |
| 2 | N | 2191 | LEU |
| 2 | N | 2205 | THR |
| 2 | N | 2211 | HIS |
| 2 | N | 2221 | THR |
| 2 | N | 2222 | MET |
| 2 | N | 2231 | LEU |
| 2 | N | 2241 | THR |
| 2 | N | 2248 | ILE |
| 2 | N | 2260 | GLU |
| 2 | N | 2267 | HIS |
| 2 | N | 2327 | GLU |
| 2 | N | 2333 | LEU |
| 2 | N | 2344 | LEU |
| 2 | N | 2361 | LYS |
| 2 | N | 2432 | SER |
| 2 | N | 2445 | MET |
| 2 | N | 2456 | LEU |
| 2 | N | 2476 | LEU |
| 2 | N | 2479 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | N | 2500 | ILE |
| 2 | N | 2505 | ILE |
| 2 | N | 2507 | ARG |
| 2 | N | 2531 | GLU |
| 2 | N | 2552 | GLU |
| 2 | N | 2556 | TYR |
| 2 | N | 2561 | HIS |
| 2 | N | 2571 | ARG |
| 2 | N | 2572 | VAL |
| 2 | N | 2575 | LEU |
| 2 | N | 2579 | GLU |
| 2 | N | 2581 | MET |
| 2 | N | 2595 | TRP |
| 2 | N | 2597 | MET |
| 2 | N | 2616 | THR |
| 2 | N | 2621 | GLU |
| 2 | N | 2625 | LEU |
| 2 | N | 2631 | TYR |
| 2 | N | 2647 | LEU |
| 2 | N | 2649 | GLU |
| 2 | N | 2653 | GLU |
| 2 | N | 2654 | SER |
| 2 | N | 2662 | LEU |
| 2 | N | 2680 | HIS |
| 2 | N | 2723 | GLU |
| 2 | N | 2730 | LEU |
| 2 | N | 2750 | ILE |
| 2 | N | 2752 | GLU |
| 2 | N | 2758 | THR |
| 2 | N | 2760 | ARG |
| 2 | N | 2769 | PHE |
| 2 | N | 2772 | LYS |
| 2 | N | 2780 | HIS |
| 2 | N | 2809 | LEU |
| 2 | N | 2818 | ASP |
| 2 | N | 2826 | GLU |
| 2 | N | 2828 | ASP |
| 2 | N | 2830 | GLN |
| 2 | N | 2848 | PHE |
| 2 | N | 2851 | ASN |
| 2 | N | 2856 | ILE |
| 2 | N | 2868 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | N | 2870 | LEU |
| 2 | N | 2872 | GLU |
| 2 | N | 2873 | HIS |
| 2 | N | 2876 | LYS |
| 2 | N | 2877 | ILE |
| 2 | N | 2882 | GLU |
| 2 | N | 2886 | VAL |
| 2 | N | 2887 | ASP |
| 2 | N | 2890 | VAL |
| 2 | N | 2891 | LEU |
| 2 | N | 2898 | LYS |
| 2 | N | 2900 | SER |
| 2 | N | 2901 | LEU |
| 3 | O | 2929[A] | SER |
| 3 | O | 2929[B] | SER |
| 3 | O | 2930[A] | LEU |
| 3 | O | 2930[B] | LEU |
| 3 | O | 2931[A] | THR |
| 3 | O | 2931[B] | THR |
| 3 | O | 2933[A] | SER |
| 3 | O | 2933[B] | SER |
| 3 | O | 2935[A] | ILE |
| 3 | O | 2935[B] | ILE |
| 3 | O | 2938[A] | LEU |
| 3 | O | 2938[B] | LEU |
| 3 | O | 2942[A] | LEU |
| 3 | O | 2942[B] | LEU |
| 3 | O | 2946[A] | GLN |
| 3 | O | 2946[B] | GLN |
| 3 | O | 2949[A] | LYS |
| 3 | O | 2949[B] | LYS |
| 3 | O | 2954[A] | TYR |
| 3 | O | 2954[B] | TYR |
| 3 | O | 2956[A] | LYS |
| 3 | O | 2956[B] | LYS |
| 3 | O | 2959[A] | SER |
| 3 | O | 2959[B] | SER |
| 3 | O | 2960[A] | PHE |
| 3 | O | 2960[B] | PHE |
| 3 | O | 2963[A] | MET |
| 3 | O | 2963[B] | MET |
| 3 | O | 2965[A] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | O | 2965[B] | LEU |
| 3 | O | 2968[A] | GLN |
| 3 | O | 2968[B] | GLN |
| 3 | O | 2973[A] | THR |
| 3 | O | 2973[B] | THR |
| 3 | O | 2980[A] | HIS |
| 3 | O | 2980[B] | HIS |
| 3 | O | 2982[A] | MET |
| 3 | O | 2982[B] | MET |
| 3 | O | 2990[A] | ARG |
| 3 | O | 2990[B] | ARG |
| 3 | O | 2995[A] | GLN |
| 3 | O | 2995[B] | GLN |
| 3 | O | 2996[A] | MET |
| 3 | O | 2996[B] | MET |
| 3 | O | 2997[A] | GLU |
| 3 | O | 2997[B] | GLU |
| 3 | O | 3000[A] | LEU |
| 3 | O | 3000[B] | LEU |
| 3 | O | 3001[A] | LYS |
| 3 | O | 3001[B] | LYS |
| 3 | O | 3019[A] | HIS |
| 3 | O | 3019[B] | HIS |
| 3 | O | 3021[A] | LEU |
| 3 | O | 3021[B] | LEU |
| 3 | O | 3023[A] | ILE |
| 3 | O | 3023[B] | ILE |
| 3 | O | 3024[A] | LEU |
| 3 | O | 3024[B] | LEU |
| 3 | O | 3026[A] | THR |
| 3 | O | 3026[B] | THR |
| 3 | O | 3029[A] | LYS |
| 3 | O | 3029[B] | LYS |
| 3 | O | 3040[A] | VAL |
| 3 | O | 3040[B] | VAL |
| 3 | O | 3042[A] | ASP |
| 3 | O | 3042[B] | ASP |
| 3 | O | 3044[A] | LYS |
| 3 | O | 3044[B] | LYS |
| 3 | O | 3048[A] | ASP |
| 3 | O | 3048[B] | ASP |
| 3 | O | 3050[A] | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | O | 3050[B] | ARG |
| 3 | O | 3063[A] | SER |
| 3 | O | 3063[B] | SER |
| 3 | O | 3067[A] | ARG |
| 3 | O | 3067[B] | ARG |
| 3 | O | 3077[A] | ASP |
| 3 | O | 3077[B] | ASP |
| 3 | O | 3081[A] | PHE |
| 3 | O | 3081[B] | PHE |
| 3 | O | 3096[A] | VAL |
| 3 | O | 3096[B] | VAL |
| 3 | O | 3105[A] | SER |
| 3 | O | 3105[B] | SER |
| 3 | O | 3107[A] | LEU |
| 3 | O | 3107[B] | LEU |
| 3 | O | 3110[A] | THR |
| 3 | O | 3110[B] | THR |
| 3 | O | 3111[A] | SER |
| 3 | O | 3111[B] | SER |
| 3 | O | 3115[A] | LEU |
| 3 | O | 3115[B] | LEU |
| 3 | O | 3123[A] | THR |
| 3 | O | 3123[B] | THR |
| 3 | O | 3131[A] | GLN |
| 3 | O | 3131[B] | GLN |
| 3 | O | 3133[A] | LEU |
| 3 | O | 3133[B] | LEU |
| 3 | O | 3134[A] | GLN |
| 3 | O | 3134[B] | GLN |
| 3 | O | 3135[A] | LYS |
| 3 | O | 3135[B] | LYS |
| 3 | O | 3139[A] | LEU |
| 3 | O | 3139[B] | LEU |
| 3 | O | 3141[A] | TYR |
| 3 | O | 3141[B] | TYR |
| 3 | O | 3147[A] | GLU |
| 3 | O | 3147[B] | GLU |
| 3 | O | 3151[A] | LEU |
| 3 | O | 3151[B] | LEU |
| 3 | O | 3156[A] | MET |
| 3 | O | 3156[B] | MET |
| 3 | O | 3159[A] | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | O | 3159[B] | SER |
| 3 | O | 3160[A] | SER |
| 3 | O | 3160[B] | SER |
| 3 | O | 3161[A] | GLU |
| 3 | O | 3161[B] | GLU |
| 3 | O | 3162[A] | ASP |
| 3 | O | 3162[B] | ASP |
| 3 | O | 3163[A] | ASN |
| 3 | O | 3163[B] | ASN |
| 3 | O | 3169[A] | LYS |
| 3 | O | 3169[B] | LYS |
| 3 | O | 3172[A] | SER |
| 3 | O | 3172[B] | SER |
| 3 | O | 3176[A] | LYS |
| 3 | O | 3176[B] | LYS |
| 3 | O | 3181[A] | GLN |
| 3 | O | 3181[B] | GLN |
| 3 | O | 3182[A] | GLN |
| 3 | O | 3182[B] | GLN |
| 3 | O | 3183[A] | LEU |
| 3 | O | 3183[B] | LEU |
| 3 | O | 3185[A] | TYR |
| 3 | O | 3185[B] | TYR |
| 3 | O | 3186[A] | GLU |
| 3 | O | 3186[B] | GLU |
| 3 | O | 3188[A] | ASP |
| 3 | O | 3188[B] | ASP |
| 3 | O | 3191[A] | ASN |
| 3 | O | 3191[B] | ASN |
| 3 | O | 3192[A] | PHE |
| 3 | O | 3192[B] | PHE |
| 3 | O | 3193[A] | HIS |
| 3 | O | 3193[B] | HIS |
| 3 | O | 3195[A] | MET |
| 3 | O | 3195[B] | MET |
| 3 | O | 3196[A] | THR |
| 3 | O | 3196[B] | THR |
| 3 | O | 3200[A] | LEU |
| 3 | O | 3200[B] | LEU |
| 3 | O | 3201[A] | GLU |
| 3 | O | 3201[B] | GLU |
| 3 | O | 3204[A] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | O | 3204[B] | LEU |
| 3 | O | 3205[A] | LYS |
| 3 | O | 3205[B] | LYS |
| 3 | O | 3210[A] | LYS |
| 3 | O | 3210[B] | LYS |
| 3 | O | 3211[A] | ASP |
| 3 | O | 3211[B] | ASP |
| 3 | O | 3212[A] | ARG |
| 3 | O | 3212[B] | ARG |
| 3 | O | 3218[A] | LEU |
| 3 | O | 3218[B] | LEU |
| 3 | O | 3220[A] | ARG |
| 3 | O | 3220[B] | ARG |
| 3 | O | 3222[A] | ILE |
| 3 | O | 3222[B] | ILE |
| 3 | O | 3224[A] | GLN |
| 3 | O | 3224[B] | GLN |
| 3 | O | 3225[A] | SER |
| 3 | O | 3225[B] | SER |
| 3 | O | 3230[A] | PHE |
| 3 | O | 3230[B] | PHE |
| 3 | O | 3244[A] | THR |
| 3 | O | 3244[B] | THR |
| 3 | O | 3251[A] | ASP |
| 3 | O | 3251[B] | ASP |
| 3 | O | 3254[A] | MET |
| 3 | O | 3254[B] | MET |
| 3 | O | 3260[A] | ARG |
| 3 | O | 3260[B] | ARG |
| 3 | O | 3267[A] | SER |
| 3 | O | 3267[B] | SER |
| 3 | O | 3268[A] | LYS |
| 3 | O | 3268[B] | LYS |
| 3 | O | 3271[A] | VAL |
| 3 | O | 3271[B] | VAL |
| 3 | O | 3272[A] | HIS |
| 3 | O | 3272[B] | HIS |
| 3 | O | 3274[A] | ARG |
| 3 | O | 3274[B] | ARG |
| 3 | O | 3276[A] | ASP |
| 3 | O | 3276[B] | ASP |
| 3 | O | 3278[A] | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | O | 3278[B] | HIS |
| 3 | O | 3279[A] | ASP |
| 3 | O | 3279[B] | ASP |
| 3 | O | 3283[A] | ILE |
| 3 | O | 3283[B] | ILE |
| 3 | O | 3286[A] | THR |
| 3 | O | 3286[B] | THR |
| 3 | O | 3287[A] | ILE |
| 3 | O | 3287[B] | ILE |
| 3 | O | 3288[A] | MET |
| 3 | O | 3288[B] | MET |
| 3 | O | 3290[A] | ILE |
| 3 | O | 3290[B] | ILE |
| 3 | O | 3293[A] | LYS |
| 3 | O | 3293[B] | LYS |
| 3 | O | 3297[A] | PRO |
| 3 | O | 3297[B] | PRO |
| 3 | O | 3299[A] | LEU |
| 3 | O | 3299[B] | LEU |
| 3 | O | 3302[A] | SER |
| 3 | O | 3302[B] | SER |
| 3 | O | 3304[A] | THR |
| 3 | O | 3304[B] | THR |
| 3 | O | 3306[A] | LEU |
| 3 | O | 3306[B] | LEU |
| 3 | O | 3308[A] | LYS |
| 3 | O | 3308[B] | LYS |
| 1 | P | 2 | LEU |
| 1 | P | 4 | ARG |
| 1 | P | 17 | ASN |
| 1 | P | 19 | GLN |
| 1 | P | 23 | ARG |
| 1 | P | 28 | ASP |
| 1 | P | 37 | ILE |
| 1 | P | 51 | ASP |
| 1 | P | 62 | MET |
| 1 | P | 67 | MET |
| 1 | P | 70 | ARG |
| 1 | P | 83 | HIS |
| 1 | P | 104 | LEU |
| 1 | P | 109 | LEU |
| 1 | P | 114 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P | 116 | LYS |
| 1 | P | 119 | LYS |
| 1 | P | 120 | LYS |
| 1 | P | 133 | LYS |
| 1 | P | 151 | GLN |
| 1 | P | 152 | LYS |
| 1 | P | 160 | LEU |
| 1 | P | 179 | HIS |
| 1 | P | 185 | LEU |
| 1 | P | 205 | LEU |
| 1 | P | 214 | GLU |
| 1 | P | 223 | LEU |
| 1 | P | 239 | LEU |
| 1 | P | 249 | ARG |
| 1 | P | 266 | LEU |
| 1 | P | 281 | LEU |
| 1 | P | 289 | LEU |
| 1 | P | 308 | LEU |
| 1 | P | 325 | THR |
| 1 | P | 329 | ARG |
| 1 | P | 336 | ASN |
| 1 | P | 365 | THR |
| 1 | P | 371 | LEU |
| 1 | P | 376 | ASN |
| 1 | P | 386 | ILE |
| 1 | P | 407 | GLN |
| 1 | P | 411 | ASP |
| 1 | P | 418 | ASP |
| 1 | P | 420 | SER |
| 1 | P | 423 | ARG |
| 1 | P | 424 | PHE |
| 1 | P | 448 | SER |
| 1 | P | 449 | ASP |
| 1 | P | 450 | LYS |
| 1 | P | 452 | ILE |
| 1 | P | 464 | LEU |
| 1 | P | 474 | LEU |
| 1 | P | 494 | VAL |
| 1 | P | 499 | GLU |
| 1 | P | 504 | THR |
| 1 | P | 515 | ASP |
| 1 | P | 516 | TRP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P | 527 | LEU |
| 1 | P | 547 | LYS |
| 1 | P | 551 | GLU |
| 1 | P | 557 | VAL |
| 1 | P | 558 | HIS |
| 1 | P | 560 | SER |
| 1 | P | 562 | GLN |
| 1 | P | 565 | GLU |
| 1 | P | 568 | PHE |
| 1 | P | 575 | ASP |
| 1 | P | 576 | HIS |
| 1 | P | 579 | LEU |
| 1 | P | 583 | LEU |
| 1 | P | 584 | SER |
| 1 | P | 589 | GLN |
| 1 | P | 603 | HIS |
| 1 | P | 609 | TRP |
| 1 | P | 624 | THR |
| 1 | P | 633 | HIS |
| 1 | P | 674 | LYS |
| 1 | P | 692 | VAL |
| 1 | P | 729 | VAL |
| 1 | P | 734 | LEU |
| 1 | P | 736 | MET |
| 1 | P | 744 | VAL |
| 1 | P | 749 | VAL |
| 1 | P | 762 | VAL |
| 1 | P | 775 | ARG |
| 1 | P | 776 | VAL |
| 1 | P | 781 | ILE |
| 1 | P | 788 | LEU |
| 1 | P | 797 | THR |
| 1 | P | 810 | LEU |
| 1 | P | 832 | LYS |
| 1 | P | 834 | ASP |
| 1 | P | 841 | LYS |
| 1 | P | 847 | THR |
| 1 | P | 870 | TYR |
| 1 | P | 873 | VAL |
| 1 | P | 877 | HIS |
| 1 | P | 881 | GLN |
| 1 | P | 885 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P | 901 | THR |
| 1 | P | 909 | ILE |
| 1 | P | 917 | LEU |
| 1 | P | 930 | ASP |
| 1 | P | 935 | ILE |
| 1 | P | 955 | LYS |
| 1 | P | 961 | SER |
| 1 | P | 965 | ASP |
| 1 | P | 979 | LEU |
| 1 | P | 980 | TYR |
| 1 | P | 984 | ASP |
| 1 | P | 987 | LYS |
| 1 | P | 999 | LEU |
| 1 | P | 1001 | GLN |
| 1 | P | 1003 | ASP |
| 1 | P | 1015 | HIS |
| 1 | P | 1017 | HIS |
| 1 | P | 1018 | ILE |
| 1 | P | 1034 | GLU |
| 1 | P | 1067 | TYR |
| 1 | P | 1068 | ASN |
| 1 | P | 1075 | GLU |
| 1 | P | 1078 | ARG |
| 1 | P | 1086 | LEU |
| 1 | P | 1089 | ASP |
| 1 | P | 1093 | ASP |
| 1 | P | 1105 | VAL |
| 1 | P | 1109 | LYS |
| 1 | P | 1118 | THR |
| 1 | P | 1122 | ASN |
| 1 | P | 1125 | SER |
| 1 | P | 1126 | ILE |
| 1 | P | 1131 | ARG |
| 1 | P | 1137 | LYS |
| 1 | P | 1140 | ASN |
| 1 | P | 1153 | LYS |
| 1 | P | 1156 | LEU |
| 1 | P | 1157 | VAL |
| 1 | P | 1160 | PHE |
| 1 | P | 1161 | ILE |
| 1 | P | 1168 | GLN |
| 1 | P | 1174 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P | 1182 | ASN |
| 1 | P | 1196 | ILE |
| 1 | P | 1200 | MET |
| 1 | P | 1210 | LYS |
| 1 | P | 1213 | VAL |
| 1 | P | 1221 | THR |
| 1 | P | 1225 | VAL |
| 1 | P | 1226 | THR |
| 1 | P | 1230 | LEU |
| 1 | P | 1247 | ARG |
| 1 | P | 1249 | TRP |
| 1 | P | 1250 | ILE |
| 1 | P | 1255 | SER |
| 1 | P | 1258 | ARG |
| 1 | P | 1260 | ARG |
| 1 | P | 1266 | PHE |
| 1 | P | 1286 | ARG |
| 1 | P | 1302 | SER |
| 1 | P | 1304 | ASP |
| 1 | P | 1310 | THR |
| 1 | P | 1313 | LEU |
| 1 | P | 1330 | VAL |
| 1 | P | 1331 | GLU |
| 1 | P | 1357 | ARG |
| 1 | P | 1394 | GLN |
| 1 | P | 1421 | VAL |
| 1 | P | 1427 | HIS |
| 1 | P | 1430 | ILE |
| 1 | P | 1439 | VAL |
| 1 | P | 1441 | SER |
| 1 | P | 1461 | VAL |
| 1 | P | 1484 | CYS |
| 1 | P | 1494 | ARG |
| 1 | P | 1516 | VAL |
| 1 | P | 1541 | GLU |
| 1 | P | 1543 | ILE |
| 1 | P | 1551 | ASP |
| 1 | P | 1559 | LEU |
| 1 | P | 1568 | VAL |
| 1 | P | 1581 | GLU |
| 1 | P | 1622 | GLN |
| 1 | P | 1643 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P | 1644 | ILE |
| 2 | Q | 2089 | ARG |
| 2 | Q | 2104 | ILE |
| 2 | Q | 2131 | LEU |
| 2 | Q | 2132 | CYS |
| 2 | Q | 2145 | LEU |
| 2 | Q | 2160 | VAL |
| 2 | Q | 2185 | THR |
| 2 | Q | 2187 | VAL |
| 2 | Q | 2191 | LEU |
| 2 | Q | 2205 | THR |
| 2 | Q | 2211 | HIS |
| 2 | Q | 2220 | GLU |
| 2 | Q | 2222 | MET |
| 2 | Q | 2227 | VAL |
| 2 | Q | 2234 | GLN |
| 2 | Q | 2241 | THR |
| 2 | Q | 2260 | GLU |
| 2 | Q | 2267 | HIS |
| 2 | Q | 2270 | ILE |
| 2 | Q | 2274 | LEU |
| 2 | Q | 2326 | ILE |
| 2 | Q | 2327 | GLU |
| 2 | Q | 2333 | LEU |
| 2 | Q | 2361 | LYS |
| 2 | Q | 2441 | ARG |
| 2 | Q | 2445 | MET |
| 2 | Q | 2448 | THR |
| 2 | Q | 2450 | ILE |
| 2 | Q | 2466 | THR |
| 2 | Q | 2474 | THR |
| 2 | Q | 2497 | GLU |
| 2 | Q | 2500 | ILE |
| 2 | Q | 2502 | LEU |
| 2 | Q | 2547 | MET |
| 2 | Q | 2548 | CYS |
| 2 | Q | 2555 | GLU |
| 2 | Q | 2556 | TYR |
| 2 | Q | 2561 | HIS |
| 2 | Q | 2571 | ARG |
| 2 | Q | 2572 | VAL |
| 2 | Q | 2575 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Q | 2579 | GLU |
| 2 | Q | 2581 | MET |
| 2 | Q | 2593 | TRP |
| 2 | Q | 2595 | TRP |
| 2 | Q | 2597 | MET |
| 2 | Q | 2600 | ASP |
| 2 | Q | 2630 | LYS |
| 2 | Q | 2631 | TYR |
| 2 | Q | 2643 | GLU |
| 2 | Q | 2651 | GLN |
| 2 | Q | 2662 | LEU |
| 2 | Q | 2699 | MET |
| 2 | Q | 2750 | ILE |
| 2 | Q | 2758 | THR |
| 2 | Q | 2768 | LEU |
| 2 | Q | 2769 | PHE |
| 2 | Q | 2772 | LYS |
| 2 | Q | 2781 | LEU |
| 2 | Q | 2788 | ILE |
| 2 | Q | 2802 | ASP |
| 2 | Q | 2814 | LYS |
| 2 | Q | 2816 | SER |
| 2 | Q | 2823 | ILE |
| 2 | Q | 2829 | CYS |
| 2 | Q | 2847 | HIS |
| 2 | Q | 2848 | PHE |
| 2 | Q | 2851 | ASN |
| 2 | Q | 2863 | ARG |
| 2 | Q | 2868 | GLU |
| 2 | Q | 2877 | ILE |
| 2 | Q | 2878 | ARG |
| 2 | Q | 2879 | LEU |
| 2 | Q | 2880 | GLU |
| 2 | Q | 2882 | GLU |
| 2 | Q | 2883 | ILE |
| 2 | Q | 2891 | LEU |
| 2 | Q | 2895 | SER |
| 2 | Q | 2898 | LYS |
| 2 | Q | 2900 | SER |
| 2 | Q | 2907 | LYS |
| 3 | R | 2929[A] | SER |
| 3 | R | 2929[B] | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | R | 2930[A] | LEU |
| 3 | R | 2930[B] | LEU |
| 3 | R | 2931[A] | THR |
| 3 | R | 2931[B] | THR |
| 3 | R | 2933[A] | SER |
| 3 | R | 2933[B] | SER |
| 3 | R | 2935[A] | ILE |
| 3 | R | 2935[B] | ILE |
| 3 | R | 2938[A] | LEU |
| 3 | R | 2938[B] | LEU |
| 3 | R | 2942[A] | LEU |
| 3 | R | 2942[B] | LEU |
| 3 | R | 2946[A] | GLN |
| 3 | R | 2946[B] | GLN |
| 3 | R | 2949[A] | LYS |
| 3 | R | 2949[B] | LYS |
| 3 | R | 2954[A] | TYR |
| 3 | R | 2954[B] | TYR |
| 3 | R | 2956[A] | LYS |
| 3 | R | 2956[B] | LYS |
| 3 | R | 2959[A] | SER |
| 3 | R | 2959[B] | SER |
| 3 | R | 2960[A] | PHE |
| 3 | R | 2960[B] | PHE |
| 3 | R | 2963[A] | MET |
| 3 | R | 2963[B] | MET |
| 3 | R | 2965[A] | LEU |
| 3 | R | 2965[B] | LEU |
| 3 | R | 2968[A] | GLN |
| 3 | R | 2968[B] | GLN |
| 3 | R | 2973[A] | THR |
| 3 | R | 2973[B] | THR |
| 3 | R | 2980[A] | HIS |
| 3 | R | 2980[B] | HIS |
| 3 | R | 2982[A] | MET |
| 3 | R | 2982[B] | MET |
| 3 | R | 2990[A] | ARG |
| 3 | R | 2990[B] | ARG |
| 3 | R | 2995[A] | GLN |
| 3 | R | 2995[B] | GLN |
| 3 | R | 2996[A] | MET |
| 3 | R | 2996[B] | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | R | 2997[A] | GLU |
| 3 | R | 2997[B] | GLU |
| 3 | R | 3000[A] | LEU |
| 3 | R | 3000[B] | LEU |
| 3 | R | 3001[A] | LYS |
| 3 | R | 3001[B] | LYS |
| 3 | R | 3019[A] | HIS |
| 3 | R | 3019[B] | HIS |
| 3 | R | 3021[A] | LEU |
| 3 | R | 3021[B] | LEU |
| 3 | R | 3023[A] | ILE |
| 3 | R | 3023[B] | ILE |
| 3 | R | 3024[A] | LEU |
| 3 | R | 3024[B] | LEU |
| 3 | R | 3026[A] | THR |
| 3 | R | 3026[B] | THR |
| 3 | R | 3029[A] | LYS |
| 3 | R | 3029[B] | LYS |
| 3 | R | 3040[A] | VAL |
| 3 | R | 3040[B] | VAL |
| 3 | R | 3042[A] | ASP |
| 3 | R | 3042[B] | ASP |
| 3 | R | 3044[A] | LYS |
| 3 | R | 3044[B] | LYS |
| 3 | R | 3048[A] | ASP |
| 3 | R | 3048[B] | ASP |
| 3 | R | 3050[A] | ARG |
| 3 | R | 3050[B] | ARG |
| 3 | R | 3063[A] | SER |
| 3 | R | 3063[B] | SER |
| 3 | R | 3067[A] | ARG |
| 3 | R | 3067[B] | ARG |
| 3 | R | 3077[A] | ASP |
| 3 | R | 3077[B] | ASP |
| 3 | R | 3081[A] | PHE |
| 3 | R | 3081[B] | PHE |
| 3 | R | 3096[A] | VAL |
| 3 | R | 3096[B] | VAL |
| 3 | R | 3105[A] | SER |
| 3 | R | 3105[B] | SER |
| 3 | R | 3107[A] | LEU |
| 3 | R | 3107[B] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | R | 3110[A] | THR |
| 3 | R | 3110[B] | THR |
| 3 | R | 3111[A] | SER |
| 3 | R | 3111[B] | SER |
| 3 | R | 3115[A] | LEU |
| 3 | R | 3115[B] | LEU |
| 3 | R | 3123[A] | THR |
| 3 | R | 3123[B] | THR |
| 3 | R | 3131[A] | GLN |
| 3 | R | 3131[B] | GLN |
| 3 | R | 3133[A] | LEU |
| 3 | R | 3133[B] | LEU |
| 3 | R | 3134[A] | GLN |
| 3 | R | 3134[B] | GLN |
| 3 | R | 3135[A] | LYS |
| 3 | R | 3135[B] | LYS |
| 3 | R | 3139[A] | LEU |
| 3 | R | 3139[B] | LEU |
| 3 | R | 3141[A] | TYR |
| 3 | R | 3141[B] | TYR |
| 3 | R | 3147[A] | GLU |
| 3 | R | 3147[B] | GLU |
| 3 | R | 3151[A] | LEU |
| 3 | R | 3151[B] | LEU |
| 3 | R | 3156[A] | MET |
| 3 | R | 3156[B] | MET |
| 3 | R | 3159[A] | SER |
| 3 | R | 3159[B] | SER |
| 3 | R | 3160[A] | SER |
| 3 | R | 3160[B] | SER |
| 3 | R | 3161[A] | GLU |
| 3 | R | 3161[B] | GLU |
| 3 | R | 3162[A] | ASP |
| 3 | R | 3162[B] | ASP |
| 3 | R | 3163[A] | ASN |
| 3 | R | 3163[B] | ASN |
| 3 | R | 3169[A] | LYS |
| 3 | R | 3169[B] | LYS |
| 3 | R | 3172[A] | SER |
| 3 | R | 3172[B] | SER |
| 3 | R | 3176[A] | LYS |
| 3 | R | 3176[B] | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | R | 3181[A] | GLN |
| 3 | R | 3181[B] | GLN |
| 3 | R | 3182[A] | GLN |
| 3 | R | 3182[B] | GLN |
| 3 | R | 3183[A] | LEU |
| 3 | R | 3183[B] | LEU |
| 3 | R | 3185[A] | TYR |
| 3 | R | 3185[B] | TYR |
| 3 | R | 3186[A] | GLU |
| 3 | R | 3186[B] | GLU |
| 3 | R | 3188[A] | ASP |
| 3 | R | 3188[B] | ASP |
| 3 | R | 3191[A] | ASN |
| 3 | R | 3191[B] | ASN |
| 3 | R | 3192[A] | PHE |
| 3 | R | 3192[B] | PHE |
| 3 | R | 3193[A] | HIS |
| 3 | R | 3193[B] | HIS |
| 3 | R | 3195[A] | MET |
| 3 | R | 3195[B] | MET |
| 3 | R | 3196[A] | THR |
| 3 | R | 3196[B] | THR |
| 3 | R | 3200[A] | LEU |
| 3 | R | 3200[B] | LEU |
| 3 | R | 3201[A] | GLU |
| 3 | R | 3201[B] | GLU |
| 3 | R | 3204[A] | LEU |
| 3 | R | 3204[B] | LEU |
| 3 | R | 3205[A] | LYS |
| 3 | R | 3205[B] | LYS |
| 3 | R | 3210[A] | LYS |
| 3 | R | 3210[B] | LYS |
| 3 | R | 3211[A] | ASP |
| 3 | R | 3211[B] | ASP |
| 3 | R | 3212[A] | ARG |
| 3 | R | 3212[B] | ARG |
| 3 | R | 3218[A] | LEU |
| 3 | R | 3218[B] | LEU |
| 3 | R | 3220[A] | ARG |
| 3 | R | 3220[B] | ARG |
| 3 | R | 3222[A] | ILE |
| 3 | R | 3222[B] | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | R | 3224[A] | GLN |
| 3 | R | 3224[B] | GLN |
| 3 | R | 3225[A] | SER |
| 3 | R | 3225[B] | SER |
| 3 | R | 3230[A] | PHE |
| 3 | R | 3230[B] | PHE |
| 3 | R | 3244[A] | THR |
| 3 | R | 3244[B] | THR |
| 3 | R | 3251[A] | ASP |
| 3 | R | 3251[B] | ASP |
| 3 | R | 3254[A] | MET |
| 3 | R | 3254[B] | MET |
| 3 | R | 3260[A] | ARG |
| 3 | R | 3260[B] | ARG |
| 3 | R | 3267[A] | SER |
| 3 | R | 3267[B] | SER |
| 3 | R | 3268[A] | LYS |
| 3 | R | 3268[B] | LYS |
| 3 | R | 3271[A] | VAL |
| 3 | R | 3271[B] | VAL |
| 3 | R | 3272[A] | HIS |
| 3 | R | 3272[B] | HIS |
| 3 | R | 3274[A] | ARG |
| 3 | R | 3274[B] | ARG |
| 3 | R | 3276[A] | ASP |
| 3 | R | 3276[B] | ASP |
| 3 | R | 3278[A] | HIS |
| 3 | R | 3278[B] | HIS |
| 3 | R | 3279[A] | ASP |
| 3 | R | 3279[B] | ASP |
| 3 | R | 3283[A] | ILE |
| 3 | R | 3283[B] | ILE |
| 3 | R | 3286[A] | THR |
| 3 | R | 3286[B] | THR |
| 3 | R | 3287[A] | ILE |
| 3 | R | 3287[B] | ILE |
| 3 | R | 3288[A] | MET |
| 3 | R | 3288[B] | MET |
| 3 | R | 3290[A] | ILE |
| 3 | R | 3290[B] | ILE |
| 3 | R | 3293[A] | LYS |
| 3 | R | 3293[B] | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | R | 3297[A] | PRO |
| 3 | R | 3297[B] | PRO |
| 3 | R | 3299[A] | LEU |
| 3 | R | 3299[B] | LEU |
| 3 | R | 3302[A] | SER |
| 3 | R | 3302[B] | SER |
| 3 | R | 3304[A] | THR |
| 3 | R | 3304[B] | THR |
| 3 | R | 3306[A] | LEU |
| 3 | R | 3306[B] | LEU |
| 3 | R | 3308[A] | LYS |
| 3 | R | 3308[B] | LYS |
| 1 | S | 2 | LEU |
| 1 | S | 37 | ILE |
| 1 | S | 62 | MET |
| 1 | S | 67 | MET |
| 1 | S | 70 | ARG |
| 1 | S | 83 | HIS |
| 1 | S | 89 | ILE |
| 1 | S | 111 | ILE |
| 1 | S | 116 | LYS |
| 1 | S | 117 | LYS |
| 1 | S | 119 | LYS |
| 1 | S | 148 | GLN |
| 1 | S | 149 | GLU |
| 1 | S | 152 | LYS |
| 1 | S | 179 | HIS |
| 1 | S | 185 | LEU |
| 1 | S | 205 | LEU |
| 1 | S | 214 | GLU |
| 1 | S | 226 | HIS |
| 1 | S | 227 | ARG |
| 1 | S | 238 | ASN |
| 1 | S | 239 | LEU |
| 1 | S | 249 | ARG |
| 1 | S | 266 | LEU |
| 1 | S | 281 | LEU |
| 1 | S | 289 | LEU |
| 1 | S | 296 | ARG |
| 1 | S | 308 | LEU |
| 1 | S | 326 | GLU |
| 1 | S | 327 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 329 | ARG |
| 1 | S | 331 | SER |
| 1 | S | 332 | ASP |
| 1 | S | 336 | ASN |
| 1 | S | 386 | ILE |
| 1 | S | 391 | MET |
| 1 | S | 393 | THR |
| 1 | S | 394 | GLN |
| 1 | S | 407 | GLN |
| 1 | S | 415 | VAL |
| 1 | S | 420 | SER |
| 1 | S | 424 | PHE |
| 1 | S | 450 | LYS |
| 1 | S | 456 | GLN |
| 1 | S | 472 | ASP |
| 1 | S | 474 | LEU |
| 1 | S | 486 | THR |
| 1 | S | 494 | VAL |
| 1 | S | 509 | ILE |
| 1 | S | 511 | VAL |
| 1 | S | 525 | SER |
| 1 | S | 527 | LEU |
| 1 | S | 547 | LYS |
| 1 | S | 559 | THR |
| 1 | S | 562 | GLN |
| 1 | S | 564 | ASP |
| 1 | S | 568 | PHE |
| 1 | S | 569 | LYS |
| 1 | S | 570 | GLN |
| 1 | S | 572 | SER |
| 1 | S | 573 | LYS |
| 1 | S | 576 | HIS |
| 1 | S | 579 | LEU |
| 1 | S | 589 | GLN |
| 1 | S | 597 | VAL |
| 1 | S | 603 | HIS |
| 1 | S | 609 | TRP |
| 1 | S | 613 | SER |
| 1 | S | 618 | MET |
| 1 | S | 624 | THR |
| 1 | S | 633 | HIS |
| 1 | S | 688 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 705 | THR |
| 1 | S | 720 | VAL |
| 1 | S | 729 | VAL |
| 1 | S | 738 | ILE |
| 1 | S | 741 | SER |
| 1 | S | 744 | VAL |
| 1 | S | 749 | VAL |
| 1 | S | 754 | GLU |
| 1 | S | 757 | VAL |
| 1 | S | 797 | THR |
| 1 | S | 803 | LYS |
| 1 | S | 806 | ASN |
| 1 | S | 810 | LEU |
| 1 | S | 813 | THR |
| 1 | S | 828 | ASP |
| 1 | S | 831 | VAL |
| 1 | S | 832 | LYS |
| 1 | S | 836 | GLN |
| 1 | S | 838 | ARG |
| 1 | S | 841 | LYS |
| 1 | S | 842 | ASN |
| 1 | S | 865 | LYS |
| 1 | S | 868 | THR |
| 1 | S | 873 | VAL |
| 1 | S | 877 | HIS |
| 1 | S | 880 | THR |
| 1 | S | 881 | GLN |
| 1 | S | 890 | GLN |
| 1 | S | 891 | LYS |
| 1 | S | 896 | HIS |
| 1 | S | 917 | LEU |
| 1 | S | 920 | ASN |
| 1 | S | 930 | ASP |
| 1 | S | 935 | ILE |
| 1 | S | 941 | LEU |
| 1 | S | 943 | LEU |
| 1 | S | 944 | GLU |
| 1 | S | 953 | GLU |
| 1 | S | 955 | LYS |
| 1 | S | 977 | GLU |
| 1 | S | 989 | THR |
| 1 | S | 999 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 1012 | GLU |
| 1 | S | 1015 | HIS |
| 1 | S | 1017 | HIS |
| 1 | S | 1025 | THR |
| 1 | S | 1059 | LEU |
| 1 | S | 1061 | LYS |
| 1 | S | 1075 | GLU |
| 1 | S | 1076 | ILE |
| 1 | S | 1077 | LEU |
| 1 | S | 1078 | ARG |
| 1 | S | 1088 | SER |
| 1 | S | 1089 | ASP |
| 1 | S | 1090 | ILE |
| 1 | S | 1097 | ARG |
| 1 | S | 1120 | GLU |
| 1 | S | 1121 | LEU |
| 1 | S | 1122 | ASN |
| 1 | S | 1126 | ILE |
| 1 | S | 1131 | ARG |
| 1 | S | 1137 | LYS |
| 1 | S | 1145 | THR |
| 1 | S | 1153 | LYS |
| 1 | S | 1155 | LEU |
| 1 | S | 1157 | VAL |
| 1 | S | 1160 | PHE |
| 1 | S | 1161 | ILE |
| 1 | S | 1164 | ASP |
| 1 | S | 1166 | THR |
| 1 | S | 1167 | ASP |
| 1 | S | 1174 | GLU |
| 1 | S | 1181 | GLU |
| 1 | S | 1190 | ARG |
| 1 | S | 1196 | ILE |
| 1 | S | 1200 | MET |
| 1 | S | 1213 | VAL |
| 1 | S | 1217 | ILE |
| 1 | S | 1219 | ASP |
| 1 | S | 1224 | GLU |
| 1 | S | 1225 | VAL |
| 1 | S | 1228 | LEU |
| 1 | S | 1230 | LEU |
| 1 | S | 1242 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 1258 | ARG |
| 1 | S | 1260 | ARG |
| 1 | S | 1284 | GLU |
| 1 | S | 1286 | ARG |
| 1 | S | 1313 | LEU |
| 1 | S | 1325 | LEU |
| 1 | S | 1341 | VAL |
| 1 | S | 1354 | GLU |
| 1 | S | 1370 | LEU |
| 1 | S | 1396 | GLU |
| 1 | S | 1398 | PHE |
| 1 | S | 1408 | LEU |
| 1 | S | 1427 | HIS |
| 1 | S | 1429 | THR |
| 1 | S | 1439 | VAL |
| 1 | S | 1441 | SER |
| 1 | S | 1465 | TRP |
| 1 | S | 1473 | ARG |
| 1 | S | 1484 | CYS |
| 1 | S | 1494 | ARG |
| 1 | S | 1500 | THR |
| 1 | S | 1541 | GLU |
| 1 | S | 1559 | LEU |
| 1 | S | 1568 | VAL |
| 1 | S | 1597 | THR |
| 1 | S | 1620 | LEU |
| 1 | S | 1622 | GLN |
| 1 | S | 1632 | LEU |
| 1 | S | 1641 | THR |
| 1 | S | 1643 | LYS |
| 1 | S | 1644 | ILE |
| 1 | S | 1651 | ILE |
| 2 | T | 2089 | ARG |
| 2 | T | 2117 | ASP |
| 2 | T | 2131 | LEU |
| 2 | T | 2132 | CYS |
| 2 | T | 2145 | LEU |
| 2 | T | 2160 | VAL |
| 2 | T | 2166 | LEU |
| 2 | T | 2168 | ARG |
| 2 | T | 2180 | TRP |
| 2 | T | 2185 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | T | 2186 | GLU |
| 2 | T | 2191 | LEU |
| 2 | T | 2215 | SER |
| 2 | T | 2222 | MET |
| 2 | T | 2237 | LEU |
| 2 | T | 2241 | THR |
| 2 | T | 2248 | ILE |
| 2 | T | 2260 | GLU |
| 2 | T | 2267 | HIS |
| 2 | T | 2309 | GLN |
| 2 | T | 2327 | GLU |
| 2 | T | 2333 | LEU |
| 2 | T | 2344 | LEU |
| 2 | T | 2349 | THR |
| 2 | T | 2359 | ASN |
| 2 | T | 2361 | LYS |
| 2 | T | 2370 | MET |
| 2 | T | 2424 | SER |
| 2 | T | 2425 | HIS |
| 2 | T | 2445 | MET |
| 2 | T | 2478 | GLU |
| 2 | T | 2505 | ILE |
| 2 | T | 2507 | ARG |
| 2 | T | 2548 | CYS |
| 2 | T | 2556 | TYR |
| 2 | T | 2558 | CYS |
| 2 | T | 2561 | HIS |
| 2 | T | 2572 | VAL |
| 2 | T | 2575 | LEU |
| 2 | T | 2579 | GLU |
| 2 | T | 2580 | SER |
| 2 | T | 2581 | MET |
| 2 | T | 2595 | TRP |
| 2 | T | 2601 | ASN |
| 2 | T | 2617 | ASP |
| 2 | T | 2625 | LEU |
| 2 | T | 2630 | LYS |
| 2 | T | 2643 | GLU |
| 2 | T | 2652 | LYS |
| 2 | T | 2662 | LEU |
| 2 | T | 2680 | HIS |
| 2 | T | 2739 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | T | 2750 | ILE |
| 2 | T | 2758 | THR |
| 2 | T | 2768 | LEU |
| 2 | T | 2769 | PHE |
| 2 | T | 2772 | LYS |
| 2 | T | 2809 | LEU |
| 2 | T | 2823 | ILE |
| 2 | T | 2825 | ILE |
| 2 | T | 2828 | ASP |
| 2 | T | 2830 | GLN |
| 2 | T | 2831 | GLU |
| 2 | T | 2838 | LEU |
| 2 | T | 2848 | PHE |
| 2 | T | 2851 | ASN |
| 2 | T | 2856 | ILE |
| 2 | T | 2865 | ILE |
| 2 | T | 2872 | GLU |
| 2 | T | 2873 | HIS |
| 2 | T | 2876 | LYS |
| 2 | T | 2878 | ARG |
| 2 | T | 2879 | LEU |
| 2 | T | 2882 | GLU |
| 2 | T | 2890 | VAL |
| 2 | T | 2891 | LEU |
| 2 | T | 2892 | ASP |
| 2 | T | 2901 | LEU |
| 3 | U | 2929[A] | SER |
| 3 | U | 2929[B] | SER |
| 3 | U | 2930[A] | LEU |
| 3 | U | 2930[B] | LEU |
| 3 | U | 2931[A] | THR |
| 3 | U | 2931[B] | THR |
| 3 | U | 2933[A] | SER |
| 3 | U | 2933[B] | SER |
| 3 | U | 2935[A] | ILE |
| 3 | U | 2935[B] | ILE |
| 3 | U | 2938[A] | LEU |
| 3 | U | 2938[B] | LEU |
| 3 | U | 2942[A] | LEU |
| 3 | U | 2942[B] | LEU |
| 3 | U | 2946[A] | GLN |
| 3 | U | 2946[B] | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | U | 2949[A] | LYS |
| 3 | U | 2949[B] | LYS |
| 3 | U | 2954[A] | TYR |
| 3 | U | 2954[B] | TYR |
| 3 | U | 2956[A] | LYS |
| 3 | U | 2956[B] | LYS |
| 3 | U | 2959[A] | SER |
| 3 | U | 2959[B] | SER |
| 3 | U | 2960[A] | PHE |
| 3 | U | 2960[B] | PHE |
| 3 | U | 2963[A] | MET |
| 3 | U | 2963[B] | MET |
| 3 | U | 2965[A] | LEU |
| 3 | U | 2965[B] | LEU |
| 3 | U | 2968[A] | GLN |
| 3 | U | 2968[B] | GLN |
| 3 | U | 2973[A] | THR |
| 3 | U | 2973[B] | THR |
| 3 | U | 2980[A] | HIS |
| 3 | U | 2980[B] | HIS |
| 3 | U | 2982[A] | MET |
| 3 | U | 2982[B] | MET |
| 3 | U | 2990[A] | ARG |
| 3 | U | 2990[B] | ARG |
| 3 | U | 2995[A] | GLN |
| 3 | U | 2995[B] | GLN |
| 3 | U | 2996[A] | MET |
| 3 | U | 2996[B] | MET |
| 3 | U | 2997[A] | GLU |
| 3 | U | 2997[B] | GLU |
| 3 | U | 3000[A] | LEU |
| 3 | U | 3000[B] | LEU |
| 3 | U | 3001[A] | LYS |
| 3 | U | 3001[B] | LYS |
| 3 | U | 3019[A] | HIS |
| 3 | U | 3019[B] | HIS |
| 3 | U | 3021[A] | LEU |
| 3 | U | 3021[B] | LEU |
| 3 | U | 3023[A] | ILE |
| 3 | U | 3023[B] | ILE |
| 3 | U | 3024[A] | LEU |
| 3 | U | 3024[B] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | U | 3026[A] | THR |
| 3 | U | 3026[B] | THR |
| 3 | U | 3029[A] | LYS |
| 3 | U | 3029[B] | LYS |
| 3 | U | 3040[A] | VAL |
| 3 | U | 3040[B] | VAL |
| 3 | U | 3042[A] | ASP |
| 3 | U | 3042[B] | ASP |
| 3 | U | 3044[A] | LYS |
| 3 | U | 3044[B] | LYS |
| 3 | U | 3048[A] | ASP |
| 3 | U | 3048[B] | ASP |
| 3 | U | 3050[A] | ARG |
| 3 | U | 3050[B] | ARG |
| 3 | U | 3063[A] | SER |
| 3 | U | 3063[B] | SER |
| 3 | U | 3067[A] | ARG |
| 3 | U | 3067[B] | ARG |
| 3 | U | 3077[A] | ASP |
| 3 | U | 3077[B] | ASP |
| 3 | U | 3081[A] | PHE |
| 3 | U | 3081[B] | PHE |
| 3 | U | 3096[A] | VAL |
| 3 | U | 3096[B] | VAL |
| 3 | U | 3105[A] | SER |
| 3 | U | 3105[B] | SER |
| 3 | U | 3107[A] | LEU |
| 3 | U | 3107[B] | LEU |
| 3 | U | 3110[A] | THR |
| 3 | U | 3110[B] | THR |
| 3 | U | 3111[A] | SER |
| 3 | U | 3111[B] | SER |
| 3 | U | 3115[A] | LEU |
| 3 | U | 3115[B] | LEU |
| 3 | U | 3123[A] | THR |
| 3 | U | 3123[B] | THR |
| 3 | U | 3131[A] | GLN |
| 3 | U | 3131[B] | GLN |
| 3 | U | 3133[A] | LEU |
| 3 | U | 3133[B] | LEU |
| 3 | U | 3134[A] | GLN |
| 3 | U | 3134[B] | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | U | 3135[A] | LYS |
| 3 | U | 3135[B] | LYS |
| 3 | U | 3139[A] | LEU |
| 3 | U | 3139[B] | LEU |
| 3 | U | 3141[A] | TYR |
| 3 | U | 3141[B] | TYR |
| 3 | U | 3147[A] | GLU |
| 3 | U | 3147[B] | GLU |
| 3 | U | 3151[A] | LEU |
| 3 | U | 3151[B] | LEU |
| 3 | U | 3156[A] | MET |
| 3 | U | 3156[B] | MET |
| 3 | U | 3159[A] | SER |
| 3 | U | 3159[B] | SER |
| 3 | U | 3160[A] | SER |
| 3 | U | 3160[B] | SER |
| 3 | U | 3161[A] | GLU |
| 3 | U | 3161[B] | GLU |
| 3 | U | 3162[A] | ASP |
| 3 | U | 3162[B] | ASP |
| 3 | U | 3163[A] | ASN |
| 3 | U | 3163[B] | ASN |
| 3 | U | 3169[A] | LYS |
| 3 | U | 3169[B] | LYS |
| 3 | U | 3172[A] | SER |
| 3 | U | 3172[B] | SER |
| 3 | U | 3176[A] | LYS |
| 3 | U | 3176[B] | LYS |
| 3 | U | 3181[A] | GLN |
| 3 | U | 3181[B] | GLN |
| 3 | U | 3182[A] | GLN |
| 3 | U | 3182[B] | GLN |
| 3 | U | 3183[A] | LEU |
| 3 | U | 3183[B] | LEU |
| 3 | U | 3185[A] | TYR |
| 3 | U | 3185[B] | TYR |
| 3 | U | 3186[A] | GLU |
| 3 | U | 3186[B] | GLU |
| 3 | U | 3188[A] | ASP |
| 3 | U | 3188[B] | ASP |
| 3 | U | 3191[A] | ASN |
| 3 | U | 3191[B] | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | U | 3192[A] | PHE |
| 3 | U | 3192[B] | PHE |
| 3 | U | 3193[A] | HIS |
| 3 | U | 3193[B] | HIS |
| 3 | U | 3195[A] | MET |
| 3 | U | 3195[B] | MET |
| 3 | U | 3196[A] | THR |
| 3 | U | 3196[B] | THR |
| 3 | U | 3200[A] | LEU |
| 3 | U | 3200[B] | LEU |
| 3 | U | 3201[A] | GLU |
| 3 | U | 3201[B] | GLU |
| 3 | U | 3204[A] | LEU |
| 3 | U | 3204[B] | LEU |
| 3 | U | 3205[A] | LYS |
| 3 | U | 3205[B] | LYS |
| 3 | U | 3210[A] | LYS |
| 3 | U | 3210[B] | LYS |
| 3 | U | 3211[A] | ASP |
| 3 | U | 3211[B] | ASP |
| 3 | U | 3212[A] | ARG |
| 3 | U | 3212[B] | ARG |
| 3 | U | 3218[A] | LEU |
| 3 | U | 3218[B] | LEU |
| 3 | U | 3220[A] | ARG |
| 3 | U | 3220[B] | ARG |
| 3 | U | 3222[A] | ILE |
| 3 | U | 3222[B] | ILE |
| 3 | U | 3224[A] | GLN |
| 3 | U | 3224[B] | GLN |
| 3 | U | 3225[A] | SER |
| 3 | U | 3225[B] | SER |
| 3 | U | 3230[A] | PHE |
| 3 | U | 3230[B] | PHE |
| 3 | U | 3244[A] | THR |
| 3 | U | 3244[B] | THR |
| 3 | U | 3251[A] | ASP |
| 3 | U | 3251[B] | ASP |
| 3 | U | 3254[A] | MET |
| 3 | U | 3254[B] | MET |
| 3 | U | 3260[A] | ARG |
| 3 | U | 3260[B] | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | U | 3267[A] | SER |
| 3 | U | 3267[B] | SER |
| 3 | U | 3268[A] | LYS |
| 3 | U | 3268[B] | LYS |
| 3 | U | 3271[A] | VAL |
| 3 | U | 3271[B] | VAL |
| 3 | U | 3272[A] | HIS |
| 3 | U | 3272[B] | HIS |
| 3 | U | 3274[A] | ARG |
| 3 | U | 3274[B] | ARG |
| 3 | U | 3276[A] | ASP |
| 3 | U | 3276[B] | ASP |
| 3 | U | 3278[A] | HIS |
| 3 | U | 3278[B] | HIS |
| 3 | U | 3279[A] | ASP |
| 3 | U | 3279[B] | ASP |
| 3 | U | 3283[A] | ILE |
| 3 | U | 3283[B] | ILE |
| 3 | U | 3286[A] | THR |
| 3 | U | 3286[B] | THR |
| 3 | U | 3287[A] | ILE |
| 3 | U | 3287[B] | ILE |
| 3 | U | 3288[A] | MET |
| 3 | U | 3288[B] | MET |
| 3 | U | 3290[A] | ILE |
| 3 | U | 3290[B] | ILE |
| 3 | U | 3293[A] | LYS |
| 3 | U | 3293[B] | LYS |
| 3 | U | 3297[A] | PRO |
| 3 | U | 3297[B] | PRO |
| 3 | U | 3299[A] | LEU |
| 3 | U | 3299[B] | LEU |
| 3 | U | 3302[A] | SER |
| 3 | U | 3302[B] | SER |
| 3 | U | 3304[A] | THR |
| 3 | U | 3304[B] | THR |
| 3 | U | 3306[A] | LEU |
| 3 | U | 3306[B] | LEU |
| 3 | U | 3308[A] | LYS |
| 3 | U | 3308[B] | LYS |
| 1 | V | 4 | ARG |
| 1 | V | 37 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | V | 51 | ASP |
| 1 | V | 64 | THR |
| 1 | V | 67 | MET |
| 1 | V | 70 | ARG |
| 1 | V | 89 | ILE |
| 1 | V | 109 | LEU |
| 1 | V | 111 | ILE |
| 1 | V | 120 | LYS |
| 1 | V | 121 | ASN |
| 1 | V | 132 | ASN |
| 1 | V | 133 | LYS |
| 1 | V | 134 | VAL |
| 1 | V | 149 | GLU |
| 1 | V | 151 | GLN |
| 1 | V | 160 | LEU |
| 1 | V | 163 | LEU |
| 1 | V | 174 | GLN |
| 1 | V | 179 | HIS |
| 1 | V | 185 | LEU |
| 1 | V | 193 | SER |
| 1 | V | 205 | LEU |
| 1 | V | 223 | LEU |
| 1 | V | 235 | CYS |
| 1 | V | 237 | LEU |
| 1 | V | 245 | GLU |
| 1 | V | 249 | ARG |
| 1 | V | 250 | ASP |
| 1 | V | 264 | SER |
| 1 | V | 266 | LEU |
| 1 | V | 282 | ASN |
| 1 | V | 289 | LEU |
| 1 | V | 290 | GLU |
| 1 | V | 293 | LEU |
| 1 | V | 308 | LEU |
| 1 | V | 326 | GLU |
| 1 | V | 336 | ASN |
| 1 | V | 337 | ASP |
| 1 | V | 354 | PHE |
| 1 | V | 365 | THR |
| 1 | V | 386 | ILE |
| 1 | V | 387 | ASN |
| 1 | V | 390 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | V | 391 | MET |
| 1 | V | 393 | THR |
| 1 | V | 395 | THR |
| 1 | V | 407 | GLN |
| 1 | V | 416 | ASN |
| 1 | V | 424 | PHE |
| 1 | V | 434 | GLU |
| 1 | V | 450 | LYS |
| 1 | V | 456 | GLN |
| 1 | V | 464 | LEU |
| 1 | V | 472 | ASP |
| 1 | V | 474 | LEU |
| 1 | V | 494 | VAL |
| 1 | V | 509 | ILE |
| 1 | V | 511 | VAL |
| 1 | V | 518 | LYS |
| 1 | V | 527 | LEU |
| 1 | V | 547 | LYS |
| 1 | V | 560 | SER |
| 1 | V | 564 | ASP |
| 1 | V | 567 | LEU |
| 1 | V | 568 | PHE |
| 1 | V | 570 | GLN |
| 1 | V | 589 | GLN |
| 1 | V | 603 | HIS |
| 1 | V | 625 | SER |
| 1 | V | 650 | GLN |
| 1 | V | 688 | VAL |
| 1 | V | 744 | VAL |
| 1 | V | 749 | VAL |
| 1 | V | 762 | VAL |
| 1 | V | 770 | THR |
| 1 | V | 775 | ARG |
| 1 | V | 776 | VAL |
| 1 | V | 781 | ILE |
| 1 | V | 797 | THR |
| 1 | V | 819 | ILE |
| 1 | V | 830 | ASN |
| 1 | V | 831 | VAL |
| 1 | V | 834 | ASP |
| 1 | V | 841 | LYS |
| 1 | V | 842 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | V | 858 | MET |
| 1 | V | 864 | ASP |
| 1 | V | 865 | LYS |
| 1 | V | 873 | VAL |
| 1 | V | 879 | SER |
| 1 | V | 907 | ARG |
| 1 | V | 909 | ILE |
| 1 | V | 917 | LEU |
| 1 | V | 935 | ILE |
| 1 | V | 941 | LEU |
| 1 | V | 943 | LEU |
| 1 | V | 949 | ASP |
| 1 | V | 951 | ASN |
| 1 | V | 953 | GLU |
| 1 | V | 961 | SER |
| 1 | V | 965 | ASP |
| 1 | V | 979 | LEU |
| 1 | V | 980 | TYR |
| 1 | V | 981 | GLU |
| 1 | V | 984 | ASP |
| 1 | V | 987 | LYS |
| 1 | V | 999 | LEU |
| 1 | V | 1001 | GLN |
| 1 | V | 1002 | GLU |
| 1 | V | 1013 | ILE |
| 1 | V | 1015 | HIS |
| 1 | V | 1017 | HIS |
| 1 | V | 1018 | ILE |
| 1 | V | 1033 | LEU |
| 1 | V | 1041 | ILE |
| 1 | V | 1075 | GLU |
| 1 | V | 1077 | LEU |
| 1 | V | 1078 | ARG |
| 1 | V | 1086 | LEU |
| 1 | V | 1088 | SER |
| 1 | V | 1090 | ILE |
| 1 | V | 1091 | ASN |
| 1 | V | 1118 | THR |
| 1 | V | 1122 | ASN |
| 1 | V | 1126 | ILE |
| 1 | V | 1140 | ASN |
| 1 | V | 1153 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | V | 1157 | VAL |
| 1 | V | 1160 | PHE |
| 1 | V | 1174 | GLU |
| 1 | V | 1181 | GLU |
| 1 | V | 1196 | ILE |
| 1 | V | 1200 | MET |
| 1 | V | 1205 | LEU |
| 1 | V | 1206 | HIS |
| 1 | V | 1207 | TYR |
| 1 | V | 1210 | LYS |
| 1 | V | 1214 | GLU |
| 1 | V | 1215 | LEU |
| 1 | V | 1221 | THR |
| 1 | V | 1226 | THR |
| 1 | V | 1229 | LYS |
| 1 | V | 1230 | LEU |
| 1 | V | 1247 | ARG |
| 1 | V | 1258 | ARG |
| 1 | V | 1260 | ARG |
| 1 | V | 1267 | GLU |
| 1 | V | 1304 | ASP |
| 1 | V | 1309 | HIS |
| 1 | V | 1313 | LEU |
| 1 | V | 1381 | LYS |
| 1 | V | 1394 | GLN |
| 1 | V | 1396 | GLU |
| 1 | V | 1408 | LEU |
| 1 | V | 1415 | ASP |
| 1 | V | 1427 | HIS |
| 1 | V | 1430 | ILE |
| 1 | V | 1433 | TRP |
| 1 | V | 1439 | VAL |
| 1 | V | 1441 | SER |
| 1 | V | 1456 | LEU |
| 1 | V | 1461 | VAL |
| 1 | V | 1484 | CYS |
| 1 | V | 1491 | GLN |
| 1 | V | 1493 | MET |
| 1 | V | 1494 | ARG |
| 1 | V | 1509 | THR |
| 1 | V | 1516 | VAL |
| 1 | V | 1530 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | V | 1541 | GLU |
| 1 | V | 1568 | VAL |
| 1 | V | 1580 | GLU |
| 1 | V | 1620 | LEU |
| 1 | V | 1622 | GLN |
| 1 | V | 1629 | GLU |
| 1 | V | 1632 | LEU |
| 1 | V | 1641 | THR |
| 1 | V | 1643 | LYS |
| 1 | V | 1649 | THR |
| 2 | W | 2089 | ARG |
| 2 | W | 2108 | LYS |
| 2 | W | 2138 | LYS |
| 2 | W | 2143 | CYS |
| 2 | W | 2145 | LEU |
| 2 | W | 2160 | VAL |
| 2 | W | 2184 | MET |
| 2 | W | 2185 | THR |
| 2 | W | 2187 | VAL |
| 2 | W | 2191 | LEU |
| 2 | W | 2205 | THR |
| 2 | W | 2215 | SER |
| 2 | W | 2222 | MET |
| 2 | W | 2237 | LEU |
| 2 | W | 2241 | THR |
| 2 | W | 2260 | GLU |
| 2 | W | 2267 | HIS |
| 2 | W | 2270 | ILE |
| 2 | W | 2274 | LEU |
| 2 | W | 2309 | GLN |
| 2 | W | 2327 | GLU |
| 2 | W | 2328 | LEU |
| 2 | W | 2333 | LEU |
| 2 | W | 2349 | THR |
| 2 | W | 2361 | LYS |
| 2 | W | 2394 | VAL |
| 2 | W | 2403 | PHE |
| 2 | W | 2417 | VAL |
| 2 | W | 2445 | MET |
| 2 | W | 2448 | THR |
| 2 | W | 2480 | LEU |
| 2 | W | 2500 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | W | 2507 | ARG |
| 2 | W | 2533 | ASP |
| 2 | W | 2556 | TYR |
| 2 | W | 2561 | HIS |
| 2 | W | 2572 | VAL |
| 2 | W | 2575 | LEU |
| 2 | W | 2579 | GLU |
| 2 | W | 2581 | MET |
| 2 | W | 2595 | TRP |
| 2 | W | 2597 | MET |
| 2 | W | 2602 | LEU |
| 2 | W | 2617 | ASP |
| 2 | W | 2620 | ILE |
| 2 | W | 2631 | TYR |
| 2 | W | 2644 | LEU |
| 2 | W | 2655 | THR |
| 2 | W | 2680 | HIS |
| 2 | W | 2742 | MET |
| 2 | W | 2746 | MET |
| 2 | W | 2758 | THR |
| 2 | W | 2768 | LEU |
| 2 | W | 2769 | PHE |
| 2 | W | 2772 | LYS |
| 2 | W | 2780 | HIS |
| 2 | W | 2794 | LEU |
| 2 | W | 2800 | LYS |
| 2 | W | 2816 | SER |
| 2 | W | 2825 | ILE |
| 2 | W | 2826 | GLU |
| 2 | W | 2828 | ASP |
| 2 | W | 2830 | GLN |
| 2 | W | 2838 | LEU |
| 2 | W | 2848 | PHE |
| 2 | W | 2851 | ASN |
| 2 | W | 2856 | ILE |
| 2 | W | 2861 | LYS |
| 2 | W | 2865 | ILE |
| 2 | W | 2868 | GLU |
| 2 | W | 2873 | HIS |
| 2 | W | 2876 | LYS |
| 2 | W | 2879 | LEU |
| 2 | W | 2891 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | W | 2895 | SER |
| 2 | W | 2898 | LYS |
| 3 | X | 2929[A] | SER |
| 3 | X | 2929[B] | SER |
| 3 | X | 2930[A] | LEU |
| 3 | X | 2930[B] | LEU |
| 3 | X | 2931[A] | THR |
| 3 | X | 2931[B] | THR |
| 3 | X | 2933[A] | SER |
| 3 | X | 2933[B] | SER |
| 3 | X | 2935[A] | ILE |
| 3 | X | 2935[B] | ILE |
| 3 | X | 2938[A] | LEU |
| 3 | X | 2938[B] | LEU |
| 3 | X | 2942[A] | LEU |
| 3 | X | 2942[B] | LEU |
| 3 | X | 2946[A] | GLN |
| 3 | X | 2946[B] | GLN |
| 3 | X | 2949[A] | LYS |
| 3 | X | 2949[B] | LYS |
| 3 | X | 2954[A] | TYR |
| 3 | X | 2954[B] | TYR |
| 3 | X | 2956[A] | LYS |
| 3 | X | 2956[B] | LYS |
| 3 | X | 2959[A] | SER |
| 3 | X | 2959[B] | SER |
| 3 | X | 2960[A] | PHE |
| 3 | X | 2960[B] | PHE |
| 3 | X | 2963[A] | MET |
| 3 | X | 2963[B] | MET |
| 3 | X | 2965[A] | LEU |
| 3 | X | 2965[B] | LEU |
| 3 | X | 2968[A] | GLN |
| 3 | X | 2968[B] | GLN |
| 3 | X | 2973[A] | THR |
| 3 | X | 2973[B] | THR |
| 3 | X | 2980[A] | HIS |
| 3 | X | 2980[B] | HIS |
| 3 | X | 2982[A] | MET |
| 3 | X | 2982[B] | MET |
| 3 | X | 2990[A] | ARG |
| 3 | X | 2990[B] | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | X | 2995[A] | GLN |
| 3 | X | 2995[B] | GLN |
| 3 | X | 2996[A] | MET |
| 3 | X | 2996[B] | MET |
| 3 | X | 2997[A] | GLU |
| 3 | X | 2997[B] | GLU |
| 3 | X | 3000[A] | LEU |
| 3 | X | 3000[B] | LEU |
| 3 | X | 3001[A] | LYS |
| 3 | X | 3001[B] | LYS |
| 3 | X | 3019[A] | HIS |
| 3 | X | 3019[B] | HIS |
| 3 | X | 3021[A] | LEU |
| 3 | X | 3021[B] | LEU |
| 3 | X | 3023[A] | ILE |
| 3 | X | 3023[B] | ILE |
| 3 | X | 3024[A] | LEU |
| 3 | X | 3024[B] | LEU |
| 3 | X | 3026[A] | THR |
| 3 | X | 3026[B] | THR |
| 3 | X | 3029[A] | LYS |
| 3 | X | 3029[B] | LYS |
| 3 | X | 3040[A] | VAL |
| 3 | X | 3040[B] | VAL |
| 3 | X | 3042[A] | ASP |
| 3 | X | 3042[B] | ASP |
| 3 | X | 3044[A] | LYS |
| 3 | X | 3044[B] | LYS |
| 3 | X | 3048[A] | ASP |
| 3 | X | 3048[B] | ASP |
| 3 | X | 3050[A] | ARG |
| 3 | X | 3050[B] | ARG |
| 3 | X | 3063[A] | SER |
| 3 | X | 3063[B] | SER |
| 3 | X | 3067[A] | ARG |
| 3 | X | 3067[B] | ARG |
| 3 | X | 3077[A] | ASP |
| 3 | X | 3077[B] | ASP |
| 3 | X | 3081[A] | PHE |
| 3 | X | 3081[B] | PHE |
| 3 | X | 3096[A] | VAL |
| 3 | X | 3096[B] | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | X | 3105[A] | SER |
| 3 | X | 3105[B] | SER |
| 3 | X | 3107[A] | LEU |
| 3 | X | 3107[B] | LEU |
| 3 | X | 3110[A] | THR |
| 3 | X | 3110[B] | THR |
| 3 | X | 3111[A] | SER |
| 3 | X | 3111[B] | SER |
| 3 | X | 3115[A] | LEU |
| 3 | X | 3115[B] | LEU |
| 3 | X | 3123[A] | THR |
| 3 | X | 3123[B] | THR |
| 3 | X | 3131[A] | GLN |
| 3 | X | 3131[B] | GLN |
| 3 | X | 3133[A] | LEU |
| 3 | X | 3133[B] | LEU |
| 3 | X | 3134[A] | GLN |
| 3 | X | 3134[B] | GLN |
| 3 | X | 3135[A] | LYS |
| 3 | X | 3135[B] | LYS |
| 3 | X | 3139[A] | LEU |
| 3 | X | 3139[B] | LEU |
| 3 | X | 3141[A] | TYR |
| 3 | X | 3141[B] | TYR |
| 3 | X | 3147[A] | GLU |
| 3 | X | 3147[B] | GLU |
| 3 | X | 3151[A] | LEU |
| 3 | X | 3151[B] | LEU |
| 3 | X | 3156[A] | MET |
| 3 | X | 3156[B] | MET |
| 3 | X | 3159[A] | SER |
| 3 | X | 3159[B] | SER |
| 3 | X | 3160[A] | SER |
| 3 | X | 3160[B] | SER |
| 3 | X | 3161[A] | GLU |
| 3 | X | 3161[B] | GLU |
| 3 | X | 3162[A] | ASP |
| 3 | X | 3162[B] | ASP |
| 3 | X | 3163[A] | ASN |
| 3 | X | 3163[B] | ASN |
| 3 | X | 3169[A] | LYS |
| 3 | X | 3169[B] | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | X | 3172[A] | SER |
| 3 | X | 3172[B] | SER |
| 3 | X | 3176[A] | LYS |
| 3 | X | 3176[B] | LYS |
| 3 | X | 3181[A] | GLN |
| 3 | X | 3181[B] | GLN |
| 3 | X | 3182[A] | GLN |
| 3 | X | 3182[B] | GLN |
| 3 | X | 3183[A] | LEU |
| 3 | X | 3183[B] | LEU |
| 3 | X | 3185[A] | TYR |
| 3 | X | 3185[B] | TYR |
| 3 | X | 3186[A] | GLU |
| 3 | X | 3186[B] | GLU |
| 3 | X | 3188[A] | ASP |
| 3 | X | 3188[B] | ASP |
| 3 | X | 3191[A] | ASN |
| 3 | X | 3191[B] | ASN |
| 3 | X | 3192[A] | PHE |
| 3 | X | 3192[B] | PHE |
| 3 | X | 3193[A] | HIS |
| 3 | X | 3193[B] | HIS |
| 3 | X | 3195[A] | MET |
| 3 | X | 3195[B] | MET |
| 3 | X | 3196[A] | THR |
| 3 | X | 3196[B] | THR |
| 3 | X | 3200[A] | LEU |
| 3 | X | 3200[B] | LEU |
| 3 | X | 3201[A] | GLU |
| 3 | X | 3201[B] | GLU |
| 3 | X | 3204[A] | LEU |
| 3 | X | 3204[B] | LEU |
| 3 | X | 3205[A] | LYS |
| 3 | X | 3205[B] | LYS |
| 3 | X | 3210[A] | LYS |
| 3 | X | 3210[B] | LYS |
| 3 | X | 3211[A] | ASP |
| 3 | X | 3211[B] | ASP |
| 3 | X | 3212[A] | ARG |
| 3 | X | 3212[B] | ARG |
| 3 | X | 3218[A] | LEU |
| 3 | X | 3218[B] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | X | 3220[A] | ARG |
| 3 | X | 3220[B] | ARG |
| 3 | X | 3222[A] | ILE |
| 3 | X | 3222[B] | ILE |
| 3 | X | 3224[A] | GLN |
| 3 | X | 3224[B] | GLN |
| 3 | X | 3225[A] | SER |
| 3 | X | 3225[B] | SER |
| 3 | X | 3230[A] | PHE |
| 3 | X | 3230[B] | PHE |
| 3 | X | 3244[A] | THR |
| 3 | X | 3244[B] | THR |
| 3 | X | 3251[A] | ASP |
| 3 | X | 3251[B] | ASP |
| 3 | X | 3254[A] | MET |
| 3 | X | 3254[B] | MET |
| 3 | X | 3260[A] | ARG |
| 3 | X | 3260[B] | ARG |
| 3 | X | 3267[A] | SER |
| 3 | X | 3267[B] | SER |
| 3 | X | 3268[A] | LYS |
| 3 | X | 3268[B] | LYS |
| 3 | X | 3271[A] | VAL |
| 3 | X | 3271[B] | VAL |
| 3 | X | 3272[A] | HIS |
| 3 | X | 3272[B] | HIS |
| 3 | X | 3274[A] | ARG |
| 3 | X | 3274[B] | ARG |
| 3 | X | 3276[A] | ASP |
| 3 | X | 3276[B] | ASP |
| 3 | X | 3278[A] | HIS |
| 3 | X | 3278[B] | HIS |
| 3 | X | 3279[A] | ASP |
| 3 | X | 3279[B] | ASP |
| 3 | X | 3283[A] | ILE |
| 3 | X | 3283[B] | ILE |
| 3 | X | 3286[A] | THR |
| 3 | X | 3286[B] | THR |
| 3 | X | 3287[A] | ILE |
| 3 | X | 3287[B] | ILE |
| 3 | X | 3288[A] | MET |
| 3 | X | 3288[B] | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | X | 3290[A] | ILE |
| 3 | X | 3290[B] | ILE |
| 3 | X | 3293[A] | LYS |
| 3 | X | 3293[B] | LYS |
| 3 | X | 3297[A] | PRO |
| 3 | X | 3297[B] | PRO |
| 3 | X | 3299[A] | LEU |
| 3 | X | 3299[B] | LEU |
| 3 | X | 3302[A] | SER |
| 3 | X | 3302[B] | SER |
| 3 | X | 3304[A] | THR |
| 3 | X | 3304[B] | THR |
| 3 | X | 3306[A] | LEU |
| 3 | X | 3306[B] | LEU |
| 3 | X | 3308[A] | LYS |
| 3 | X | 3308[B] | LYS |
| 1 | Y | 2 | LEU |
| 1 | Y | 4 | ARG |
| 1 | Y | 19 | GLN |
| 1 | Y | 57 | CYS |
| 1 | Y | 62 | MET |
| 1 | Y | 67 | MET |
| 1 | Y | 70 | ARG |
| 1 | Y | 86 | THR |
| 1 | Y | 104 | LEU |
| 1 | Y | 109 | LEU |
| 1 | Y | 116 | LYS |
| 1 | Y | 117 | LYS |
| 1 | Y | 119 | LYS |
| 1 | Y | 133 | LYS |
| 1 | Y | 140 | ASP |
| 1 | Y | 152 | LYS |
| 1 | Y | 163 | LEU |
| 1 | Y | 167 | ASP |
| 1 | Y | 179 | HIS |
| 1 | Y | 182 | ILE |
| 1 | Y | 185 | LEU |
| 1 | Y | 193 | SER |
| 1 | Y | 194 | MET |
| 1 | Y | 205 | LEU |
| 1 | Y | 214 | GLU |
| 1 | Y | 221 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 226 | HIS |
| 1 | Y | 235 | CYS |
| 1 | Y | 238 | ASN |
| 1 | Y | 239 | LEU |
| 1 | Y | 249 | ARG |
| 1 | Y | 264 | SER |
| 1 | Y | 265 | SER |
| 1 | Y | 266 | LEU |
| 1 | Y | 281 | LEU |
| 1 | Y | 285 | THR |
| 1 | Y | 289 | LEU |
| 1 | Y | 308 | LEU |
| 1 | Y | 325 | THR |
| 1 | Y | 329 | ARG |
| 1 | Y | 330 | GLN |
| 1 | Y | 336 | ASN |
| 1 | Y | 350 | MET |
| 1 | Y | 365 | THR |
| 1 | Y | 371 | LEU |
| 1 | Y | 386 | ILE |
| 1 | Y | 387 | ASN |
| 1 | Y | 391 | MET |
| 1 | Y | 407 | GLN |
| 1 | Y | 411 | ASP |
| 1 | Y | 413 | ASN |
| 1 | Y | 415 | VAL |
| 1 | Y | 418 | ASP |
| 1 | Y | 424 | PHE |
| 1 | Y | 444 | GLU |
| 1 | Y | 448 | SER |
| 1 | Y | 450 | LYS |
| 1 | Y | 467 | LYS |
| 1 | Y | 476 | ARG |
| 1 | Y | 499 | GLU |
| 1 | Y | 509 | ILE |
| 1 | Y | 515 | ASP |
| 1 | Y | 527 | LEU |
| 1 | Y | 557 | VAL |
| 1 | Y | 560 | SER |
| 1 | Y | 565 | GLU |
| 1 | Y | 567 | LEU |
| 1 | Y | 569 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 570 | GLN |
| 1 | Y | 575 | ASP |
| 1 | Y | 578 | PHE |
| 1 | Y | 597 | VAL |
| 1 | Y | 603 | HIS |
| 1 | Y | 609 | TRP |
| 1 | Y | 610 | THR |
| 1 | Y | 619 | SER |
| 1 | Y | 624 | THR |
| 1 | Y | 633 | HIS |
| 1 | Y | 692 | VAL |
| 1 | Y | 696 | GLN |
| 1 | Y | 714 | ARG |
| 1 | Y | 720 | VAL |
| 1 | Y | 722 | GLU |
| 1 | Y | 729 | VAL |
| 1 | Y | 736 | MET |
| 1 | Y | 738 | ILE |
| 1 | Y | 739 | GLN |
| 1 | Y | 744 | VAL |
| 1 | Y | 749 | VAL |
| 1 | Y | 788 | LEU |
| 1 | Y | 797 | THR |
| 1 | Y | 805 | VAL |
| 1 | Y | 806 | ASN |
| 1 | Y | 819 | ILE |
| 1 | Y | 826 | ILE |
| 1 | Y | 832 | LYS |
| 1 | Y | 836 | GLN |
| 1 | Y | 865 | LYS |
| 1 | Y | 866 | GLU |
| 1 | Y | 896 | HIS |
| 1 | Y | 901 | THR |
| 1 | Y | 909 | ILE |
| 1 | Y | 912 | ASN |
| 1 | Y | 917 | LEU |
| 1 | Y | 930 | ASP |
| 1 | Y | 935 | ILE |
| 1 | Y | 948 | THR |
| 1 | Y | 965 | ASP |
| 1 | Y | 967 | ILE |
| 1 | Y | 973 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 979 | LEU |
| 1 | Y | 981 | GLU |
| 1 | Y | 987 | LYS |
| 1 | Y | 989 | THR |
| 1 | Y | 991 | LEU |
| 1 | Y | 995 | ILE |
| 1 | Y | 999 | LEU |
| 1 | Y | 1001 | GLN |
| 1 | Y | 1015 | HIS |
| 1 | Y | 1017 | HIS |
| 1 | Y | 1025 | THR |
| 1 | Y | 1030 | MET |
| 1 | Y | 1033 | LEU |
| 1 | Y | 1041 | ILE |
| 1 | Y | 1075 | GLU |
| 1 | Y | 1077 | LEU |
| 1 | Y | 1086 | LEU |
| 1 | Y | 1090 | ILE |
| 1 | Y | 1093 | ASP |
| 1 | Y | 1097 | ARG |
| 1 | Y | 1105 | VAL |
| 1 | Y | 1118 | THR |
| 1 | Y | 1121 | LEU |
| 1 | Y | 1122 | ASN |
| 1 | Y | 1142 | VAL |
| 1 | Y | 1145 | THR |
| 1 | Y | 1154 | SER |
| 1 | Y | 1157 | VAL |
| 1 | Y | 1160 | PHE |
| 1 | Y | 1161 | ILE |
| 1 | Y | 1164 | ASP |
| 1 | Y | 1168 | GLN |
| 1 | Y | 1170 | MET |
| 1 | Y | 1200 | MET |
| 1 | Y | 1213 | VAL |
| 1 | Y | 1228 | LEU |
| 1 | Y | 1230 | LEU |
| 1 | Y | 1231 | VAL |
| 1 | Y | 1232 | THR |
| 1 | Y | 1245 | GLU |
| 1 | Y | 1247 | ARG |
| 1 | Y | 1258 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 1260 | ARG |
| 1 | Y | 1286 | ARG |
| 1 | Y | 1304 | ASP |
| 1 | Y | 1307 | MET |
| 1 | Y | 1331 | GLU |
| 1 | Y | 1341 | VAL |
| 1 | Y | 1354 | GLU |
| 1 | Y | 1369 | THR |
| 1 | Y | 1372 | ILE |
| 1 | Y | 1381 | LYS |
| 1 | Y | 1396 | GLU |
| 1 | Y | 1401 | ARG |
| 1 | Y | 1421 | VAL |
| 1 | Y | 1427 | HIS |
| 1 | Y | 1430 | ILE |
| 1 | Y | 1471 | LEU |
| 1 | Y | 1488 | LEU |
| 1 | Y | 1494 | ARG |
| 1 | Y | 1506 | LEU |
| 1 | Y | 1516 | VAL |
| 1 | Y | 1541 | GLU |
| 1 | Y | 1543 | ILE |
| 1 | Y | 1559 | LEU |
| 1 | Y | 1568 | VAL |
| 1 | Y | 1578 | ILE |
| 1 | Y | 1581 | GLU |
| 1 | Y | 1583 | CYS |
| 1 | Y | 1597 | THR |
| 1 | Y | 1621 | ASN |
| 1 | Y | 1622 | GLN |
| 1 | Y | 1629 | GLU |
| 1 | Y | 1632 | LEU |
| 1 | Y | 1642 | GLN |
| 1 | Y | 1656 | ASP |
| 2 | Z | 2089 | ARG |
| 2 | Z | 2104 | ILE |
| 2 | Z | 2108 | LYS |
| 2 | Z | 2117 | ASP |
| 2 | Z | 2131 | LEU |
| 2 | Z | 2132 | CYS |
| 2 | Z | 2134 | ASN |
| 2 | Z | 2143 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Z | 2145 | LEU |
| 2 | Z | 2160 | VAL |
| 2 | Z | 2168 | ARG |
| 2 | Z | 2180 | TRP |
| 2 | Z | 2184 | MET |
| 2 | Z | 2187 | VAL |
| 2 | Z | 2190 | LEU |
| 2 | Z | 2191 | LEU |
| 2 | Z | 2205 | THR |
| 2 | Z | 2221 | THR |
| 2 | Z | 2227 | VAL |
| 2 | Z | 2233 | GLU |
| 2 | Z | 2237 | LEU |
| 2 | Z | 2241 | THR |
| 2 | Z | 2249 | LEU |
| 2 | Z | 2260 | GLU |
| 2 | Z | 2267 | HIS |
| 2 | Z | 2270 | ILE |
| 2 | Z | 2282 | LEU |
| 2 | Z | 2309 | GLN |
| 2 | Z | 2327 | GLU |
| 2 | Z | 2333 | LEU |
| 2 | Z | 2345 | ASN |
| 2 | Z | 2359 | ASN |
| 2 | Z | 2361 | LYS |
| 2 | Z | 2373 | MET |
| 2 | Z | 2381 | LEU |
| 2 | Z | 2394 | VAL |
| 2 | Z | 2425 | HIS |
| 2 | Z | 2441 | ARG |
| 2 | Z | 2445 | MET |
| 2 | Z | 2457 | LYS |
| 2 | Z | 2460 | SER |
| 2 | Z | 2469 | VAL |
| 2 | Z | 2495 | ASN |
| 2 | Z | 2502 | LEU |
| 2 | Z | 2507 | ARG |
| 2 | Z | 2548 | CYS |
| 2 | Z | 2556 | TYR |
| 2 | Z | 2558 | CYS |
| 2 | Z | 2560 | LEU |
| 2 | Z | 2561 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Z | 2565 | THR |
| 2 | Z | 2572 | VAL |
| 2 | Z | 2579 | GLU |
| 2 | Z | 2595 | TRP |
| 2 | Z | 2600 | ASP |
| 2 | Z | 2608 | ASP |
| 2 | Z | 2620 | ILE |
| 2 | Z | 2630 | LYS |
| 2 | Z | 2637 | VAL |
| 2 | Z | 2643 | GLU |
| 2 | Z | 2647 | LEU |
| 2 | Z | 2653 | GLU |
| 2 | Z | 2662 | LEU |
| 2 | Z | 2674 | VAL |
| 2 | Z | 2680 | HIS |
| 2 | Z | 2758 | THR |
| 2 | Z | 2768 | LEU |
| 2 | Z | 2769 | PHE |
| 2 | Z | 2772 | LYS |
| 2 | Z | 2780 | HIS |
| 2 | Z | 2781 | LEU |
| 2 | Z | 2809 | LEU |
| 2 | Z | 2813 | ILE |
| 2 | Z | 2825 | ILE |
| 2 | Z | 2828 | ASP |
| 2 | Z | 2835 | ILE |
| 2 | Z | 2838 | LEU |
| 2 | Z | 2848 | PHE |
| 2 | Z | 2850 | ARG |
| 2 | Z | 2851 | ASN |
| 2 | Z | 2856 | ILE |
| 2 | Z | 2863 | ARG |
| 2 | Z | 2868 | GLU |
| 2 | Z | 2870 | LEU |
| 2 | Z | 2873 | HIS |
| 2 | Z | 2876 | LYS |
| 2 | Z | 2878 | ARG |
| 2 | Z | 2884 | LYS |
| 2 | Z | 2891 | LEU |
| 2 | Z | 2895 | SER |
| 2 | Z | 2898 | LYS |
| 2 | Z | 2900 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | a | 2929[A] | SER |
| 3 | a | 2929[B] | SER |
| 3 | a | 2930[A] | LEU |
| 3 | a | 2930[B] | LEU |
| 3 | a | 2931[A] | THR |
| 3 | a | 2931[B] | THR |
| 3 | a | 2933[A] | SER |
| 3 | a | 2933[B] | SER |
| 3 | a | 2935[A] | ILE |
| 3 | a | 2935[B] | ILE |
| 3 | a | 2938[A] | LEU |
| 3 | a | 2938[B] | LEU |
| 3 | a | 2942[A] | LEU |
| 3 | a | 2942[B] | LEU |
| 3 | a | 2946[A] | GLN |
| 3 | a | 2946[B] | GLN |
| 3 | a | 2949[A] | LYS |
| 3 | a | 2949[B] | LYS |
| 3 | a | 2954[A] | TYR |
| 3 | a | 2954[B] | TYR |
| 3 | a | 2956[A] | LYS |
| 3 | a | 2956[B] | LYS |
| 3 | a | 2959[A] | SER |
| 3 | a | 2959[B] | SER |
| 3 | a | 2960[A] | PHE |
| 3 | a | 2960[B] | PHE |
| 3 | a | 2963[A] | MET |
| 3 | a | 2963[B] | MET |
| 3 | a | 2965[A] | LEU |
| 3 | a | 2965[B] | LEU |
| 3 | a | 2968[A] | GLN |
| 3 | a | 2968[B] | GLN |
| 3 | a | 2973[A] | THR |
| 3 | a | 2973[B] | THR |
| 3 | a | 2980[A] | HIS |
| 3 | a | 2980[B] | HIS |
| 3 | a | 2982[A] | MET |
| 3 | a | 2982[B] | MET |
| 3 | a | 2990[A] | ARG |
| 3 | a | 2990[B] | ARG |
| 3 | a | 2995[A] | GLN |
| 3 | a | 2995[B] | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | a | 2996[A] | MET |
| 3 | a | 2996[B] | MET |
| 3 | a | 2997[A] | GLU |
| 3 | a | 2997[B] | GLU |
| 3 | a | 3000[A] | LEU |
| 3 | a | 3000[B] | LEU |
| 3 | a | 3001[A] | LYS |
| 3 | a | 3001[B] | LYS |
| 3 | a | 3019[A] | HIS |
| 3 | a | 3019[B] | HIS |
| 3 | a | 3021[A] | LEU |
| 3 | a | 3021[B] | LEU |
| 3 | a | 3023[A] | ILE |
| 3 | a | 3023[B] | ILE |
| 3 | a | 3024[A] | LEU |
| 3 | a | 3024[B] | LEU |
| 3 | a | 3026[A] | THR |
| 3 | a | 3026[B] | THR |
| 3 | a | 3029[A] | LYS |
| 3 | a | 3029[B] | LYS |
| 3 | a | 3040[A] | VAL |
| 3 | a | 3040[B] | VAL |
| 3 | a | 3042[A] | ASP |
| 3 | a | 3042[B] | ASP |
| 3 | a | 3044[A] | LYS |
| 3 | a | 3044[B] | LYS |
| 3 | a | 3048[A] | ASP |
| 3 | a | 3048[B] | ASP |
| 3 | a | 3050[A] | ARG |
| 3 | a | 3050[B] | ARG |
| 3 | a | 3063[A] | SER |
| 3 | a | 3063[B] | SER |
| 3 | a | 3067[A] | ARG |
| 3 | a | 3067[B] | ARG |
| 3 | a | 3077[A] | ASP |
| 3 | a | 3077[B] | ASP |
| 3 | a | 3081[A] | PHE |
| 3 | a | 3081[B] | PHE |
| 3 | a | 3096[A] | VAL |
| 3 | a | 3096[B] | VAL |
| 3 | a | 3105[A] | SER |
| 3 | a | 3105[B] | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | a | 3107[A] | LEU |
| 3 | a | 3107[B] | LEU |
| 3 | a | 3110[A] | THR |
| 3 | a | 3110[B] | THR |
| 3 | a | 3111[A] | SER |
| 3 | a | 3111[B] | SER |
| 3 | a | 3115[A] | LEU |
| 3 | a | 3115[B] | LEU |
| 3 | a | 3123[A] | THR |
| 3 | a | 3123[B] | THR |
| 3 | a | 3131[A] | GLN |
| 3 | a | 3131[B] | GLN |
| 3 | a | 3133[A] | LEU |
| 3 | a | 3133[B] | LEU |
| 3 | a | 3134[A] | GLN |
| 3 | a | 3134[B] | GLN |
| 3 | a | 3135[A] | LYS |
| 3 | a | 3135[B] | LYS |
| 3 | a | 3139[A] | LEU |
| 3 | a | 3139[B] | LEU |
| 3 | a | 3141[A] | TYR |
| 3 | a | 3141[B] | TYR |
| 3 | a | 3147[A] | GLU |
| 3 | a | 3147[B] | GLU |
| 3 | a | 3151[A] | LEU |
| 3 | a | 3151[B] | LEU |
| 3 | a | 3156[A] | MET |
| 3 | a | 3156[B] | MET |
| 3 | a | 3159[A] | SER |
| 3 | a | 3159[B] | SER |
| 3 | a | 3160[A] | SER |
| 3 | a | 3160[B] | SER |
| 3 | a | 3161[A] | GLU |
| 3 | a | 3161[B] | GLU |
| 3 | a | 3162[A] | ASP |
| 3 | a | 3162[B] | ASP |
| 3 | a | 3163[A] | ASN |
| 3 | a | 3163[B] | ASN |
| 3 | a | 3169[A] | LYS |
| 3 | a | 3169[B] | LYS |
| 3 | a | 3172[A] | SER |
| 3 | a | 3172[B] | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | a | 3176[A] | LYS |
| 3 | a | 3176[B] | LYS |
| 3 | a | 3181[A] | GLN |
| 3 | a | 3181[B] | GLN |
| 3 | a | 3182[A] | GLN |
| 3 | a | 3182[B] | GLN |
| 3 | a | 3183[A] | LEU |
| 3 | a | 3183[B] | LEU |
| 3 | a | 3185[A] | TYR |
| 3 | a | 3185[B] | TYR |
| 3 | a | 3186[A] | GLU |
| 3 | a | 3186[B] | GLU |
| 3 | a | 3188[A] | ASP |
| 3 | a | 3188[B] | ASP |
| 3 | a | 3191[A] | ASN |
| 3 | a | 3191[B] | ASN |
| 3 | a | 3192[A] | PHE |
| 3 | a | 3192[B] | PHE |
| 3 | a | 3193[A] | HIS |
| 3 | a | 3193[B] | HIS |
| 3 | a | 3195[A] | MET |
| 3 | a | 3195[B] | MET |
| 3 | a | 3196[A] | THR |
| 3 | a | 3196[B] | THR |
| 3 | a | 3200[A] | LEU |
| 3 | a | 3200[B] | LEU |
| 3 | a | 3201[A] | GLU |
| 3 | a | 3201[B] | GLU |
| 3 | a | 3204[A] | LEU |
| 3 | a | 3204[B] | LEU |
| 3 | a | 3205[A] | LYS |
| 3 | a | 3205[B] | LYS |
| 3 | a | 3210[A] | LYS |
| 3 | a | 3210[B] | LYS |
| 3 | a | 3211[A] | ASP |
| 3 | a | 3211[B] | ASP |
| 3 | a | 3212[A] | ARG |
| 3 | a | 3212[B] | ARG |
| 3 | a | 3218[A] | LEU |
| 3 | a | 3218[B] | LEU |
| 3 | a | 3220[A] | ARG |
| 3 | a | 3220[B] | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | a | 3222[A] | ILE |
| 3 | a | 3222[B] | ILE |
| 3 | a | 3224[A] | GLN |
| 3 | a | 3224[B] | GLN |
| 3 | a | 3225[A] | SER |
| 3 | a | 3225[B] | SER |
| 3 | a | 3230[A] | PHE |
| 3 | a | 3230[B] | PHE |
| 3 | a | 3244[A] | THR |
| 3 | a | 3244[B] | THR |
| 3 | a | 3251[A] | ASP |
| 3 | a | 3251[B] | ASP |
| 3 | a | 3254[A] | MET |
| 3 | a | 3254[B] | MET |
| 3 | a | 3260[A] | ARG |
| 3 | a | 3260[B] | ARG |
| 3 | a | 3267[A] | SER |
| 3 | a | 3267[B] | SER |
| 3 | a | 3268[A] | LYS |
| 3 | a | 3268[B] | LYS |
| 3 | a | 3271[A] | VAL |
| 3 | a | 3271[B] | VAL |
| 3 | a | 3272[A] | HIS |
| 3 | a | 3272[B] | HIS |
| 3 | a | 3274[A] | ARG |
| 3 | a | 3274[B] | ARG |
| 3 | a | 3276[A] | ASP |
| 3 | a | 3276[B] | ASP |
| 3 | a | 3278[A] | HIS |
| 3 | a | 3278[B] | HIS |
| 3 | a | 3279[A] | ASP |
| 3 | a | 3279[B] | ASP |
| 3 | a | 3283[A] | ILE |
| 3 | a | 3283[B] | ILE |
| 3 | a | 3286[A] | THR |
| 3 | a | 3286[B] | THR |
| 3 | a | 3287[A] | ILE |
| 3 | a | 3287[B] | ILE |
| 3 | a | 3288[A] | MET |
| 3 | a | 3288[B] | MET |
| 3 | a | 3290[A] | ILE |
| 3 | a | 3290[B] | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | a | 3293[A] | LYS |
| 3 | a | 3293[B] | LYS |
| 3 | a | 3297[A] | PRO |
| 3 | a | 3297[B] | PRO |
| 3 | a | 3299[A] | LEU |
| 3 | a | 3299[B] | LEU |
| 3 | a | 3302[A] | SER |
| 3 | a | 3302[B] | SER |
| 3 | a | 3304[A] | THR |
| 3 | a | 3304[B] | THR |
| 3 | a | 3306[A] | LEU |
| 3 | a | 3306[B] | LEU |
| 3 | a | 3308[A] | LYS |
| 3 | a | 3308[B] | LYS |
| 1 | b | 2 | LEU |
| 1 | b | 4 | ARG |
| 1 | b | 17 | ASN |
| 1 | b | 19 | GLN |
| 1 | b | 25 | MET |
| 1 | b | 26 | GLN |
| 1 | b | 35 | GLN |
| 1 | b | 53 | SER |
| 1 | b | 55 | ILE |
| 1 | b | 56 | VAL |
| 1 | b | 62 | MET |
| 1 | b | 67 | MET |
| 1 | b | 89 | ILE |
| 1 | b | 119 | LYS |
| 1 | b | 120 | LYS |
| 1 | b | 127 | GLU |
| 1 | b | 128 | ILE |
| 1 | b | 129 | LYS |
| 1 | b | 130 | PHE |
| 1 | b | 148 | GLN |
| 1 | b | 163 | LEU |
| 1 | b | 179 | HIS |
| 1 | b | 185 | LEU |
| 1 | b | 205 | LEU |
| 1 | b | 213 | VAL |
| 1 | b | 214 | GLU |
| 1 | b | 219 | LEU |
| 1 | b | 223 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | b | 235 | CYS |
| 1 | b | 237 | LEU |
| 1 | b | 238 | ASN |
| 1 | b | 239 | LEU |
| 1 | b | 244 | MET |
| 1 | b | 249 | ARG |
| 1 | b | 266 | LEU |
| 1 | b | 279 | LEU |
| 1 | b | 281 | LEU |
| 1 | b | 285 | THR |
| 1 | b | 289 | LEU |
| 1 | b | 308 | LEU |
| 1 | b | 329 | ARG |
| 1 | b | 371 | LEU |
| 1 | b | 376 | ASN |
| 1 | b | 384 | THR |
| 1 | b | 387 | ASN |
| 1 | b | 391 | MET |
| 1 | b | 407 | GLN |
| 1 | b | 411 | ASP |
| 1 | b | 420 | SER |
| 1 | b | 423 | ARG |
| 1 | b | 424 | PHE |
| 1 | b | 448 | SER |
| 1 | b | 456 | GLN |
| 1 | b | 474 | LEU |
| 1 | b | 476 | ARG |
| 1 | b | 494 | VAL |
| 1 | b | 509 | ILE |
| 1 | b | 516 | TRP |
| 1 | b | 520 | PHE |
| 1 | b | 527 | LEU |
| 1 | b | 557 | VAL |
| 1 | b | 560 | SER |
| 1 | b | 561 | ARG |
| 1 | b | 564 | ASP |
| 1 | b | 569 | LYS |
| 1 | b | 572 | SER |
| 1 | b | 573 | LYS |
| 1 | b | 579 | LEU |
| 1 | b | 603 | HIS |
| 1 | b | 677 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | b | 687 | SER |
| 1 | b | 688 | VAL |
| 1 | b | 692 | VAL |
| 1 | b | 695 | TYR |
| 1 | b | 722 | GLU |
| 1 | b | 739 | GLN |
| 1 | b | 744 | VAL |
| 1 | b | 749 | VAL |
| 1 | b | 753 | ASN |
| 1 | b | 762 | VAL |
| 1 | b | 797 | THR |
| 1 | b | 819 | ILE |
| 1 | b | 821 | ILE |
| 1 | b | 830 | ASN |
| 1 | b | 836 | GLN |
| 1 | b | 838 | ARG |
| 1 | b | 877 | HIS |
| 1 | b | 883 | CYS |
| 1 | b | 885 | SER |
| 1 | b | 896 | HIS |
| 1 | b | 901 | THR |
| 1 | b | 909 | ILE |
| 1 | b | 930 | ASP |
| 1 | b | 935 | ILE |
| 1 | b | 955 | LYS |
| 1 | b | 965 | ASP |
| 1 | b | 967 | ILE |
| 1 | b | 979 | LEU |
| 1 | b | 980 | TYR |
| 1 | b | 982 | LYS |
| 1 | b | 984 | ASP |
| 1 | b | 987 | LYS |
| 1 | b | 999 | LEU |
| 1 | b | 1001 | GLN |
| 1 | b | 1013 | ILE |
| 1 | b | 1015 | HIS |
| 1 | b | 1017 | HIS |
| 1 | b | 1033 | LEU |
| 1 | b | 1041 | ILE |
| 1 | b | 1053 | TRP |
| 1 | b | 1067 | TYR |
| 1 | b | 1068 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | b | 1075 | GLU |
| 1 | b | 1077 | LEU |
| 1 | b | 1109 | LYS |
| 1 | b | 1118 | THR |
| 1 | b | 1153 | LYS |
| 1 | b | 1157 | VAL |
| 1 | b | 1160 | PHE |
| 1 | b | 1161 | ILE |
| 1 | b | 1167 | ASP |
| 1 | b | 1182 | ASN |
| 1 | b | 1183 | GLU |
| 1 | b | 1196 | ILE |
| 1 | b | 1200 | MET |
| 1 | b | 1209 | ASP |
| 1 | b | 1213 | VAL |
| 1 | b | 1221 | THR |
| 1 | b | 1224 | GLU |
| 1 | b | 1227 | ASP |
| 1 | b | 1230 | LEU |
| 1 | b | 1233 | SER |
| 1 | b | 1247 | ARG |
| 1 | b | 1258 | ARG |
| 1 | b | 1260 | ARG |
| 1 | b | 1284 | GLU |
| 1 | b | 1331 | GLU |
| 1 | b | 1368 | ARG |
| 1 | b | 1372 | ILE |
| 1 | b | 1381 | LYS |
| 1 | b | 1396 | GLU |
| 1 | b | 1401 | ARG |
| 1 | b | 1427 | HIS |
| 1 | b | 1430 | ILE |
| 1 | b | 1439 | VAL |
| 1 | b | 1441 | SER |
| 1 | b | 1494 | ARG |
| 1 | b | 1500 | THR |
| 1 | b | 1509 | THR |
| 1 | b | 1516 | VAL |
| 1 | b | 1541 | GLU |
| 1 | b | 1543 | ILE |
| 1 | b | 1568 | VAL |
| 1 | b | 1578 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | b | 1580 | GLU |
| 1 | b | 1581 | GLU |
| 1 | b | 1596 | GLU |
| 1 | b | 1598 | GLU |
| 1 | b | 1620 | LEU |
| 1 | b | 1622 | GLN |
| 1 | b | 1632 | LEU |
| 1 | b | 1640 | ILE |
| 1 | b | 1641 | THR |
| 1 | b | 1642 | GLN |
| 2 | c | 2089 | ARG |
| 2 | c | 2131 | LEU |
| 2 | c | 2132 | CYS |
| 2 | c | 2145 | LEU |
| 2 | c | 2160 | VAL |
| 2 | c | 2180 | TRP |
| 2 | c | 2185 | THR |
| 2 | c | 2187 | VAL |
| 2 | c | 2203 | ILE |
| 2 | c | 2221 | THR |
| 2 | c | 2226 | GLU |
| 2 | c | 2227 | VAL |
| 2 | c | 2234 | GLN |
| 2 | c | 2241 | THR |
| 2 | c | 2249 | LEU |
| 2 | c | 2252 | GLU |
| 2 | c | 2255 | ASP |
| 2 | c | 2267 | HIS |
| 2 | c | 2270 | ILE |
| 2 | c | 2277 | LYS |
| 2 | c | 2326 | ILE |
| 2 | c | 2327 | GLU |
| 2 | c | 2333 | LEU |
| 2 | c | 2344 | LEU |
| 2 | c | 2361 | LYS |
| 2 | c | 2373 | MET |
| 2 | c | 2394 | VAL |
| 2 | c | 2406 | SER |
| 2 | c | 2445 | MET |
| 2 | c | 2448 | THR |
| 2 | c | 2452 | GLN |
| 2 | c | 2480 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | c | 2495 | ASN |
| 2 | c | 2497 | GLU |
| 2 | c | 2498 | VAL |
| 2 | c | 2500 | ILE |
| 2 | c | 2507 | ARG |
| 2 | c | 2546 | LEU |
| 2 | c | 2548 | CYS |
| 2 | c | 2552 | GLU |
| 2 | c | 2556 | TYR |
| 2 | c | 2561 | HIS |
| 2 | c | 2563 | MET |
| 2 | c | 2565 | THR |
| 2 | c | 2572 | VAL |
| 2 | c | 2575 | LEU |
| 2 | c | 2579 | GLU |
| 2 | c | 2581 | MET |
| 2 | c | 2595 | TRP |
| 2 | c | 2597 | MET |
| 2 | c | 2602 | LEU |
| 2 | c | 2608 | ASP |
| 2 | c | 2616 | THR |
| 2 | c | 2620 | ILE |
| 2 | c | 2630 | LYS |
| 2 | c | 2631 | TYR |
| 2 | c | 2640 | ILE |
| 2 | c | 2649 | GLU |
| 2 | c | 2653 | GLU |
| 2 | c | 2662 | LEU |
| 2 | c | 2680 | HIS |
| 2 | c | 2683 | ILE |
| 2 | c | 2742 | MET |
| 2 | c | 2750 | ILE |
| 2 | c | 2758 | THR |
| 2 | c | 2763 | SER |
| 2 | c | 2769 | PHE |
| 2 | c | 2772 | LYS |
| 2 | c | 2782 | ASN |
| 2 | c | 2786 | MET |
| 2 | c | 2809 | LEU |
| 2 | c | 2823 | ILE |
| 2 | c | 2828 | ASP |
| 2 | c | 2830 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | c | 2848 | PHE |
| 2 | c | 2850 | ARG |
| 2 | c | 2851 | ASN |
| 2 | c | 2855 | ASP |
| 2 | c | 2856 | ILE |
| 2 | c | 2860 | LEU |
| 2 | c | 2865 | ILE |
| 2 | c | 2870 | LEU |
| 2 | c | 2874 | ASP |
| 2 | c | 2879 | LEU |
| 2 | c | 2882 | GLU |
| 2 | c | 2891 | LEU |
| 2 | c | 2892 | ASP |
| 2 | c | 2898 | LYS |
| 2 | c | 2900 | SER |
| 2 | c | 2901 | LEU |
| 3 | d | 2929[A] | SER |
| 3 | d | 2929[B] | SER |
| 3 | d | 2930[A] | LEU |
| 3 | d | 2930[B] | LEU |
| 3 | d | 2931[A] | THR |
| 3 | d | 2931[B] | THR |
| 3 | d | 2933[A] | SER |
| 3 | d | 2933[B] | SER |
| 3 | d | 2935[A] | ILE |
| 3 | d | 2935[B] | ILE |
| 3 | d | 2938[A] | LEU |
| 3 | d | 2938[B] | LEU |
| 3 | d | 2942[A] | LEU |
| 3 | d | 2942[B] | LEU |
| 3 | d | 2946[A] | GLN |
| 3 | d | 2946[B] | GLN |
| 3 | d | 2949[A] | LYS |
| 3 | d | 2949[B] | LYS |
| 3 | d | 2954[A] | TYR |
| 3 | d | 2954[B] | TYR |
| 3 | d | 2956[A] | LYS |
| 3 | d | 2956[B] | LYS |
| 3 | d | 2959[A] | SER |
| 3 | d | 2959[B] | SER |
| 3 | d | 2960[A] | PHE |
| 3 | d | 2960[B] | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | d | 2963[A] | MET |
| 3 | d | 2963[B] | MET |
| 3 | d | 2965[A] | LEU |
| 3 | d | 2965[B] | LEU |
| 3 | d | 2968[A] | GLN |
| 3 | d | 2968[B] | GLN |
| 3 | d | 2973[A] | THR |
| 3 | d | 2973[B] | THR |
| 3 | d | 2980[A] | HIS |
| 3 | d | 2980[B] | HIS |
| 3 | d | 2982[A] | MET |
| 3 | d | 2982[B] | MET |
| 3 | d | 2990[A] | ARG |
| 3 | d | 2990[B] | ARG |
| 3 | d | 2995[A] | GLN |
| 3 | d | 2995[B] | GLN |
| 3 | d | 2996[A] | MET |
| 3 | d | 2996[B] | MET |
| 3 | d | 2997[A] | GLU |
| 3 | d | 2997[B] | GLU |
| 3 | d | 3000[A] | LEU |
| 3 | d | 3000[B] | LEU |
| 3 | d | 3001[A] | LYS |
| 3 | d | 3001[B] | LYS |
| 3 | d | 3019[A] | HIS |
| 3 | d | 3019[B] | HIS |
| 3 | d | 3021[A] | LEU |
| 3 | d | 3021[B] | LEU |
| 3 | d | 3023[A] | ILE |
| 3 | d | 3023[B] | ILE |
| 3 | d | 3024[A] | LEU |
| 3 | d | 3024[B] | LEU |
| 3 | d | 3026[A] | THR |
| 3 | d | 3026[B] | THR |
| 3 | d | 3029[A] | LYS |
| 3 | d | 3029[B] | LYS |
| 3 | d | 3040[A] | VAL |
| 3 | d | 3040[B] | VAL |
| 3 | d | 3042[A] | ASP |
| 3 | d | 3042[B] | ASP |
| 3 | d | 3044[A] | LYS |
| 3 | d | 3044[B] | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | d | 3048[A] | ASP |
| 3 | d | 3048[B] | ASP |
| 3 | d | 3050[A] | ARG |
| 3 | d | 3050[B] | ARG |
| 3 | d | 3063[A] | SER |
| 3 | d | 3063[B] | SER |
| 3 | d | 3067[A] | ARG |
| 3 | d | 3067[B] | ARG |
| 3 | d | 3077[A] | ASP |
| 3 | d | 3077[B] | ASP |
| 3 | d | 3081[A] | PHE |
| 3 | d | 3081[B] | PHE |
| 3 | d | 3096[A] | VAL |
| 3 | d | 3096[B] | VAL |
| 3 | d | 3105[A] | SER |
| 3 | d | 3105[B] | SER |
| 3 | d | 3107[A] | LEU |
| 3 | d | 3107[B] | LEU |
| 3 | d | 3110[A] | THR |
| 3 | d | 3110[B] | THR |
| 3 | d | 3111[A] | SER |
| 3 | d | 3111[B] | SER |
| 3 | d | 3115[A] | LEU |
| 3 | d | 3115[B] | LEU |
| 3 | d | 3123[A] | THR |
| 3 | d | 3123[B] | THR |
| 3 | d | 3131[A] | GLN |
| 3 | d | 3131[B] | GLN |
| 3 | d | 3133[A] | LEU |
| 3 | d | 3133[B] | LEU |
| 3 | d | 3134[A] | GLN |
| 3 | d | 3134[B] | GLN |
| 3 | d | 3135[A] | LYS |
| 3 | d | 3135[B] | LYS |
| 3 | d | 3139[A] | LEU |
| 3 | d | 3139[B] | LEU |
| 3 | d | 3141[A] | TYR |
| 3 | d | 3141[B] | TYR |
| 3 | d | 3147[A] | GLU |
| 3 | d | 3147[B] | GLU |
| 3 | d | 3151[A] | LEU |
| 3 | d | 3151[B] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | d | 3156[A] | MET |
| 3 | d | 3156[B] | MET |
| 3 | d | 3159[A] | SER |
| 3 | d | 3159[B] | SER |
| 3 | d | 3160[A] | SER |
| 3 | d | 3160[B] | SER |
| 3 | d | 3161[A] | GLU |
| 3 | d | 3161[B] | GLU |
| 3 | d | 3162[A] | ASP |
| 3 | d | 3162[B] | ASP |
| 3 | d | 3163[A] | ASN |
| 3 | d | 3163[B] | ASN |
| 3 | d | 3169[A] | LYS |
| 3 | d | 3169[B] | LYS |
| 3 | d | 3172[A] | SER |
| 3 | d | 3172[B] | SER |
| 3 | d | 3176[A] | LYS |
| 3 | d | 3176[B] | LYS |
| 3 | d | 3181[A] | GLN |
| 3 | d | 3181[B] | GLN |
| 3 | d | 3182[A] | GLN |
| 3 | d | 3182[B] | GLN |
| 3 | d | 3183[A] | LEU |
| 3 | d | 3183[B] | LEU |
| 3 | d | 3185[A] | TYR |
| 3 | d | 3185[B] | TYR |
| 3 | d | 3186[A] | GLU |
| 3 | d | 3186[B] | GLU |
| 3 | d | 3188[A] | ASP |
| 3 | d | 3188[B] | ASP |
| 3 | d | 3191[A] | ASN |
| 3 | d | 3191[B] | ASN |
| 3 | d | 3192[A] | PHE |
| 3 | d | 3192[B] | PHE |
| 3 | d | 3193[A] | HIS |
| 3 | d | 3193[B] | HIS |
| 3 | d | 3195[A] | MET |
| 3 | d | 3195[B] | MET |
| 3 | d | 3196[A] | THR |
| 3 | d | 3196[B] | THR |
| 3 | d | 3200[A] | LEU |
| 3 | d | 3200[B] | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | d | 3201[A] | GLU |
| 3 | d | 3201[B] | GLU |
| 3 | d | 3204[A] | LEU |
| 3 | d | 3204[B] | LEU |
| 3 | d | 3205[A] | LYS |
| 3 | d | 3205[B] | LYS |
| 3 | d | 3210[A] | LYS |
| 3 | d | 3210[B] | LYS |
| 3 | d | 3211[A] | ASP |
| 3 | d | 3211[B] | ASP |
| 3 | d | 3212[A] | ARG |
| 3 | d | 3212[B] | ARG |
| 3 | d | 3218[A] | LEU |
| 3 | d | 3218[B] | LEU |
| 3 | d | 3220[A] | ARG |
| 3 | d | 3220[B] | ARG |
| 3 | d | 3222[A] | ILE |
| 3 | d | 3222[B] | ILE |
| 3 | d | 3224[A] | GLN |
| 3 | d | 3224[B] | GLN |
| 3 | d | 3225[A] | SER |
| 3 | d | 3225[B] | SER |
| 3 | d | 3230[A] | PHE |
| 3 | d | 3230[B] | PHE |
| 3 | d | 3244[A] | THR |
| 3 | d | 3244[B] | THR |
| 3 | d | 3251[A] | ASP |
| 3 | d | 3251[B] | ASP |
| 3 | d | 3254[A] | MET |
| 3 | d | 3254[B] | MET |
| 3 | d | 3260[A] | ARG |
| 3 | d | 3260[B] | ARG |
| 3 | d | 3267[A] | SER |
| 3 | d | 3267[B] | SER |
| 3 | d | 3268[A] | LYS |
| 3 | d | 3268[B] | LYS |
| 3 | d | 3271[A] | VAL |
| 3 | d | 3271[B] | VAL |
| 3 | d | 3272[A] | HIS |
| 3 | d | 3272[B] | HIS |
| 3 | d | 3274[A] | ARG |
| 3 | d | 3274[B] | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | d | 3276[A] | ASP |
| 3 | d | 3276[B] | ASP |
| 3 | d | 3278[A] | HIS |
| 3 | d | 3278[B] | HIS |
| 3 | d | 3279[A] | ASP |
| 3 | d | 3279[B] | ASP |
| 3 | d | 3283[A] | ILE |
| 3 | d | 3283[B] | ILE |
| 3 | d | 3286[A] | THR |
| 3 | d | 3286[B] | THR |
| 3 | d | 3287[A] | ILE |
| 3 | d | 3287[B] | ILE |
| 3 | d | 3288[A] | MET |
| 3 | d | 3288[B] | MET |
| 3 | d | 3290[A] | ILE |
| 3 | d | 3290[B] | ILE |
| 3 | d | 3293[A] | LYS |
| 3 | d | 3293[B] | LYS |
| 3 | d | 3297[A] | PRO |
| 3 | d | 3297[B] | PRO |
| 3 | d | 3299[A] | LEU |
| 3 | d | 3299[B] | LEU |
| 3 | d | 3302[A] | SER |
| 3 | d | 3302[B] | SER |
| 3 | d | 3304[A] | THR |
| 3 | d | 3304[B] | THR |
| 3 | d | 3306[A] | LEU |
| 3 | d | 3306[B] | LEU |
| 3 | d | 3308[A] | LYS |
| 3 | d | 3308[B] | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (420) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 19 | GLN |
| 1 | A | 100 | GLN |
| 1 | A | 106 | GLN |
| 1 | A | 121 | ASN |
| 1 | A | 151 | GLN |
| 1 | A | 165 | GLN |
| 1 | A | 180 | ASN |
| 1 | A | 183 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 238 | ASN |
| 1 | A | 376 | ASN |
| 1 | A | 416 | ASN |
| 1 | A | 497 | GLN |
| 1 | A | 636 | GLN |
| 1 | A | 648 | GLN |
| 1 | A | 696 | GLN |
| 1 | A | 779 | HIS |
| 1 | A | 836 | GLN |
| 1 | A | 871 | GLN |
| 1 | A | 877 | HIS |
| 1 | A | 897 | HIS |
| 1 | A | 912 | ASN |
| 1 | A | 1001 | GLN |
| 1 | A | 1045 | HIS |
| 1 | A | 1366 | ASN |
| 1 | A | 1400 | ASN |
| 1 | A | 1490 | ASN |
| 1 | A | 1524 | HIS |
| 1 | A | 1548 | GLN |
| 1 | A | 1622 | GLN |
| 2 | B | 2086 | ASN |
| 2 | B | 2161 | GLN |
| 2 | B | 2169 | HIS |
| 2 | B | 2240 | GLN |
| 2 | B | 2268 | ASN |
| 2 | B | 2297 | HIS |
| 2 | B | 2343 | ASN |
| 2 | B | 2345 | ASN |
| 2 | B | 2461 | HIS |
| 2 | B | 2780 | HIS |
| 2 | B | 2851 | ASN |
| 2 | B | 2894 | ASN |
| 1 | D | 100 | GLN |
| 1 | D | 106 | GLN |
| 1 | D | 151 | GLN |
| 1 | D | 153 | ASN |
| 1 | D | 192 | HIS |
| 1 | D | 340 | GLN |
| 1 | D | 353 | ASN |
| 1 | D | 482 | HIS |
| 1 | D | 500 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 570 | GLN |
| 1 | D | 636 | GLN |
| 1 | D | 645 | GLN |
| 1 | D | 648 | GLN |
| 1 | D | 650 | GLN |
| 1 | D | 679 | ASN |
| 1 | D | 696 | GLN |
| 1 | D | 753 | ASN |
| 1 | D | 904 | HIS |
| 1 | D | 1017 | HIS |
| 1 | D | 1057 | GLN |
| 1 | D | 1071 | ASN |
| 1 | D | 1107 | ASN |
| 1 | D | 1212 | HIS |
| 1 | D | 1242 | ASN |
| 1 | D | 1321 | HIS |
| 1 | D | 1366 | ASN |
| 1 | D | 1400 | ASN |
| 1 | D | 1520 | GLN |
| 1 | D | 1524 | HIS |
| 1 | D | 1531 | ASN |
| 1 | D | 1582 | ASN |
| 1 | D | 1647 | ASN |
| 2 | E | 2169 | HIS |
| 2 | E | 2210 | ASN |
| 2 | E | 2213 | HIS |
| 2 | E | 2230 | HIS |
| 2 | E | 2283 | ASN |
| 2 | E | 2297 | HIS |
| 2 | E | 2365 | HIS |
| 2 | E | 2412 | GLN |
| 2 | E | 2425 | HIS |
| 2 | E | 2471 | HIS |
| 2 | E | 2495 | ASN |
| 2 | E | 2568 | HIS |
| 2 | E | 2584 | HIS |
| 2 | E | 2651 | GLN |
| 2 | E | 2873 | HIS |
| 2 | E | 2894 | ASN |
| 1 | G | 161 | ASN |
| 1 | G | 180 | ASN |
| 1 | G | 224 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 558 | HIS |
| 1 | G | 679 | ASN |
| 1 | G | 877 | HIS |
| 1 | G | 881 | GLN |
| 1 | G | 897 | HIS |
| 1 | G | 957 | ASN |
| 1 | G | 1045 | HIS |
| 1 | G | 1140 | ASN |
| 1 | G | 1182 | ASN |
| 1 | G | 1242 | ASN |
| 1 | G | 1280 | GLN |
| 1 | G | 1321 | HIS |
| 1 | G | 1440 | HIS |
| 1 | G | 1457 | HIS |
| 1 | G | 1460 | ASN |
| 1 | G | 1524 | HIS |
| 1 | G | 1547 | ASN |
| 1 | G | 1642 | GLN |
| 2 | H | 2101 | ASN |
| 2 | H | 2141 | HIS |
| 2 | H | 2213 | HIS |
| 2 | H | 2230 | HIS |
| 2 | H | 2312 | GLN |
| 2 | H | 2390 | GLN |
| 2 | H | 2471 | HIS |
| 2 | H | 2675 | GLN |
| 2 | H | 2684 | HIS |
| 2 | H | 2782 | ASN |
| 2 | H | 2873 | HIS |
| 1 | J | 121 | ASN |
| 1 | J | 145 | GLN |
| 1 | J | 148 | GLN |
| 1 | J | 151 | GLN |
| 1 | J | 192 | HIS |
| 1 | J | 216 | HIS |
| 1 | J | 224 | GLN |
| 1 | J | 226 | HIS |
| 1 | J | 330 | GLN |
| 1 | J | 348 | ASN |
| 1 | J | 353 | ASN |
| 1 | J | 376 | ASN |
| 1 | J | 407 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 416 | ASN |
| 1 | J | 475 | ASN |
| 1 | J | 497 | GLN |
| 1 | J | 558 | HIS |
| 1 | J | 562 | GLN |
| 1 | J | 598 | GLN |
| 1 | J | 622 | HIS |
| 1 | J | 678 | ASN |
| 1 | J | 679 | ASN |
| 1 | J | 717 | GLN |
| 1 | J | 836 | GLN |
| 1 | J | 837 | HIS |
| 1 | J | 881 | GLN |
| 1 | J | 897 | HIS |
| 1 | J | 1010 | GLN |
| 1 | J | 1017 | HIS |
| 1 | J | 1122 | ASN |
| 1 | J | 1128 | GLN |
| 1 | J | 1168 | GLN |
| 1 | J | 1182 | ASN |
| 1 | J | 1242 | ASN |
| 1 | J | 1276 | ASN |
| 1 | J | 1280 | GLN |
| 1 | J | 1400 | ASN |
| 1 | J | 1440 | HIS |
| 1 | J | 1457 | HIS |
| 1 | J | 1502 | ASN |
| 1 | J | 1560 | HIS |
| 1 | J | 1585 | ASN |
| 1 | J | 1602 | GLN |
| 1 | J | 1621 | ASN |
| 1 | J | 1623 | ASN |
| 1 | J | 1625 | HIS |
| 2 | K | 2101 | ASN |
| 2 | K | 2111 | GLN |
| 2 | K | 2240 | GLN |
| 2 | K | 2283 | ASN |
| 2 | K | 2284 | HIS |
| 2 | K | 2312 | GLN |
| 2 | K | 2343 | ASN |
| 2 | K | 2345 | ASN |
| 2 | K | 2359 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | K | 2390 | GLN |
| 2 | K | 2584 | HIS |
| 2 | K | 2811 | HIS |
| 1 | M | 17 | ASN |
| 1 | M | 19 | GLN |
| 1 | M | 106 | GLN |
| 1 | M | 165 | GLN |
| 1 | M | 174 | GLN |
| 1 | M | 180 | ASN |
| 1 | M | 192 | HIS |
| 1 | M | 216 | HIS |
| 1 | M | 221 | GLN |
| 1 | M | 336 | ASN |
| 1 | M | 598 | GLN |
| 1 | M | 717 | GLN |
| 1 | M | 743 | ASN |
| 1 | M | 877 | HIS |
| 1 | M | 881 | GLN |
| 1 | M | 896 | HIS |
| 1 | M | 897 | HIS |
| 1 | M | 1001 | GLN |
| 1 | M | 1017 | HIS |
| 1 | M | 1068 | ASN |
| 1 | M | 1071 | ASN |
| 1 | M | 1128 | GLN |
| 1 | M | 1168 | GLN |
| 1 | M | 1206 | HIS |
| 1 | M | 1276 | ASN |
| 1 | M | 1280 | GLN |
| 1 | M | 1321 | HIS |
| 1 | M | 1406 | HIS |
| 1 | M | 1457 | HIS |
| 1 | M | 1480 | ASN |
| 1 | M | 1520 | GLN |
| 1 | M | 1524 | HIS |
| 2 | N | 2098 | GLN |
| 2 | N | 2161 | GLN |
| 2 | N | 2230 | HIS |
| 2 | N | 2246 | ASN |
| 2 | N | 2297 | HIS |
| 2 | N | 2374 | ASN |
| 2 | N | 2495 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | N | 2510 | ASN |
| 2 | N | 2568 | HIS |
| 2 | N | 2798 | GLN |
| 1 | P | 106 | GLN |
| 1 | P | 192 | HIS |
| 1 | P | 226 | HIS |
| 1 | P | 353 | ASN |
| 1 | P | 407 | GLN |
| 1 | P | 416 | ASN |
| 1 | P | 475 | ASN |
| 1 | P | 686 | HIS |
| 1 | P | 830 | ASN |
| 1 | P | 836 | GLN |
| 1 | P | 897 | HIS |
| 1 | P | 957 | ASN |
| 1 | P | 1017 | HIS |
| 1 | P | 1045 | HIS |
| 1 | P | 1128 | GLN |
| 1 | P | 1140 | ASN |
| 1 | P | 1276 | ASN |
| 1 | P | 1280 | GLN |
| 1 | P | 1321 | HIS |
| 1 | P | 1457 | HIS |
| 1 | P | 1520 | GLN |
| 1 | P | 1547 | ASN |
| 1 | P | 1621 | ASN |
| 2 | Q | 2111 | GLN |
| 2 | Q | 2297 | HIS |
| 2 | Q | 2374 | ASN |
| 2 | Q | 2387 | GLN |
| 2 | Q | 2503 | ASN |
| 2 | Q | 2537 | GLN |
| 2 | Q | 2568 | HIS |
| 2 | Q | 2732 | HIS |
| 2 | Q | 2873 | HIS |
| 2 | Q | 2894 | ASN |
| 1 | S | 165 | GLN |
| 1 | S | 241 | HIS |
| 1 | S | 340 | GLN |
| 1 | S | 348 | ASN |
| 1 | S | 353 | ASN |
| 1 | S | 394 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 562 | GLN |
| 1 | S | 696 | GLN |
| 1 | S | 830 | ASN |
| 1 | S | 871 | GLN |
| 1 | S | 897 | HIS |
| 1 | S | 904 | HIS |
| 1 | S | 912 | ASN |
| 1 | S | 957 | ASN |
| 1 | S | 1107 | ASN |
| 1 | S | 1128 | GLN |
| 1 | S | 1212 | HIS |
| 1 | S | 1276 | ASN |
| 1 | S | 1371 | GLN |
| 1 | S | 1520 | GLN |
| 1 | S | 1524 | HIS |
| 1 | S | 1585 | ASN |
| 1 | S | 1647 | ASN |
| 2 | T | 2211 | HIS |
| 2 | T | 2230 | HIS |
| 2 | T | 2240 | GLN |
| 2 | T | 2365 | HIS |
| 2 | T | 2387 | GLN |
| 2 | T | 2461 | HIS |
| 2 | T | 2537 | GLN |
| 2 | T | 2576 | HIS |
| 2 | T | 2584 | HIS |
| 2 | T | 2741 | GLN |
| 2 | T | 2756 | ASN |
| 2 | T | 2811 | HIS |
| 1 | V | 17 | ASN |
| 1 | V | 19 | GLN |
| 1 | V | 78 | GLN |
| 1 | V | 121 | ASN |
| 1 | V | 145 | GLN |
| 1 | V | 180 | ASN |
| 1 | V | 260 | ASN |
| 1 | V | 348 | ASN |
| 1 | V | 360 | HIS |
| 1 | V | 416 | ASN |
| 1 | V | 500 | ASN |
| 1 | V | 570 | GLN |
| 1 | V | 679 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | V | 837 | HIS |
| 1 | V | 871 | GLN |
| 1 | V | 890 | GLN |
| 1 | V | 897 | HIS |
| 1 | V | 912 | ASN |
| 1 | V | 1001 | GLN |
| 1 | V | 1068 | ASN |
| 1 | V | 1071 | ASN |
| 1 | V | 1140 | ASN |
| 1 | V | 1242 | ASN |
| 1 | V | 1309 | HIS |
| 1 | V | 1400 | ASN |
| 1 | V | 1428 | ASN |
| 1 | V | 1457 | HIS |
| 1 | V | 1460 | ASN |
| 1 | V | 1520 | GLN |
| 1 | V | 1524 | HIS |
| 1 | V | 1560 | HIS |
| 1 | V | 1582 | ASN |
| 2 | W | 2098 | GLN |
| 2 | W | 2240 | GLN |
| 2 | W | 2297 | HIS |
| 2 | W | 2380 | GLN |
| 2 | W | 2387 | GLN |
| 2 | W | 2425 | HIS |
| 2 | W | 2510 | ASN |
| 2 | W | 2741 | GLN |
| 2 | W | 2784 | HIS |
| 2 | W | 2830 | GLN |
| 2 | W | 2873 | HIS |
| 1 | Y | 35 | GLN |
| 1 | Y | 106 | GLN |
| 1 | Y | 153 | ASN |
| 1 | Y | 305 | ASN |
| 1 | Y | 353 | ASN |
| 1 | Y | 360 | HIS |
| 1 | Y | 413 | ASN |
| 1 | Y | 570 | GLN |
| 1 | Y | 679 | ASN |
| 1 | Y | 696 | GLN |
| 1 | Y | 871 | GLN |
| 1 | Y | 890 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 897 | HIS |
| 1 | Y | 912 | ASN |
| 1 | Y | 920 | ASN |
| 1 | Y | 951 | ASN |
| 1 | Y | 957 | ASN |
| 1 | Y | 1057 | GLN |
| 1 | Y | 1091 | ASN |
| 1 | Y | 1140 | ASN |
| 1 | Y | 1206 | HIS |
| 1 | Y | 1299 | GLN |
| 1 | Y | 1406 | HIS |
| 1 | Y | 1428 | ASN |
| 1 | Y | 1440 | HIS |
| 1 | Y | 1457 | HIS |
| 1 | Y | 1483 | ASN |
| 1 | Y | 1510 | ASN |
| 1 | Y | 1524 | HIS |
| 1 | Y | 1582 | ASN |
| 1 | Y | 1621 | ASN |
| 1 | Y | 1642 | GLN |
| 2 | Z | 2134 | ASN |
| 2 | Z | 2141 | HIS |
| 2 | Z | 2284 | HIS |
| 2 | Z | 2309 | GLN |
| 2 | Z | 2312 | GLN |
| 2 | Z | 2495 | ASN |
| 2 | Z | 2561 | HIS |
| 2 | Z | 2568 | HIS |
| 2 | Z | 2651 | GLN |
| 2 | Z | 2741 | GLN |
| 1 | b | 145 | GLN |
| 1 | b | 260 | ASN |
| 1 | b | 348 | ASN |
| 1 | b | 353 | ASN |
| 1 | b | 376 | ASN |
| 1 | b | 407 | GLN |
| 1 | b | 416 | ASN |
| 1 | b | 475 | ASN |
| 1 | b | 558 | HIS |
| 1 | b | 570 | GLN |
| 1 | b | 633 | HIS |
| 1 | b | 743 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | b | 779 | HIS |
| 1 | b | 881 | GLN |
| 1 | b | 897 | HIS |
| 1 | b | 912 | ASN |
| 1 | b | 951 | ASN |
| 1 | b | 1045 | HIS |
| 1 | b | 1122 | ASN |
| 1 | b | 1140 | ASN |
| 1 | b | 1182 | ASN |
| 1 | b | 1242 | ASN |
| 1 | b | 1276 | ASN |
| 1 | b | 1299 | GLN |
| 1 | b | 1321 | HIS |
| 1 | b | 1394 | GLN |
| 1 | b | 1400 | ASN |
| 1 | b | 1457 | HIS |
| 1 | b | 1510 | ASN |
| 1 | b | 1524 | HIS |
| 1 | b | 1621 | ASN |
| 2 | c | 2146 | HIS |
| 2 | c | 2211 | HIS |
| 2 | c | 2240 | GLN |
| 2 | c | 2297 | HIS |
| 2 | c | 2374 | ASN |
| 2 | c | 2390 | GLN |
| 2 | c | 2425 | HIS |
| 2 | c | 2495 | ASN |
| 2 | c | 2510 | ASN |
| 2 | c | 2576 | HIS |
| 2 | c | 2780 | HIS |
| 2 | c | 2798 | GLN |
| 2 | c | 2830 | GLN |
| 2 | c | 2847 | HIS |
| 2 | c | 2894 | 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)

130 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 | $\#\|Z\| > 2$ |
| 8 | NAG | 0 | 1 | 1,8 | 14,14,15 | 0.72 | 1 (7%) | 17,19,21 | 1.49 | 2 (11%) |
| 8 | NAG | 0 | 2 | 8 | 14,14,15 | 0.52 | 0 | 17,19,21 | 1.50 | 4 (23%) |
| 8 | BMA | 0 | 3 | 8 | 11,11,12 | 0.22 | 0 | 15,15,17 | 1.90 | 4 (26%) |
| 8 | MAN | 0 | 4 | 8 | 11,11,12 | 0.32 | 0 | 15,15,17 | 0.89 | 1 (6%) |
| 4 | NAG | 1 | 1 | 4,1 | 14,14,15 | 0.44 | 0 | 17,19,21 | 1.03 | 1 (5%) |
| 4 | NAG | 1 | 2 | 4 | 14,14,15 | 0.42 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 4 | NAG | 2 | 1 | 4,2 | 14,14,15 | 1.05 | 1 (7%) | 17,19,21 | 1.42 | 2 (11%) |
| 4 | NAG | 2 | 2 | 4 | 14,14,15 | 0.31 | 0 | 17,19,21 | 0.73 | 0 |
| 6 | NAG | 3 | 1 | 6,1 | 14,14,15 | 0.96 | 1 (7%) | 17,19,21 | 1.45 | 2 (11%) |
| 6 | NAG | 3 | 2 | 6 | 14,14,15 | 0.40 | 0 | 17,19,21 | 0.77 | 0 |
| 6 | BMA | 3 | 3 | 6 | 11,11,12 | 0.26 | 0 | 15,15,17 | 0.62 | 0 |
| 4 | NAG | 4 | 1 | 4,1 | 14,14,15 | 0.72 | 1 (7%) | 17,19,21 | 1.24 | 2 (11%) |
| 4 | NAG | 4 | 2 | 4 | 14,14,15 | 0.41 | 0 | 17,19,21 | 1.19 | 2 (11%) |
| 6 | NAG | 5 | 1 | 6,1 | 14,14,15 | 0.71 | 0 | 17,19,21 | 1.26 | 1 (5%) |
| 6 | NAG | 5 | 2 | 6 | 14,14,15 | 0.31 | 0 | 17,19,21 | 1.00 | 1 (5%) |
| 6 | BMA | 5 | 3 | 6 | 11,11,12 | 0.28 | 0 | 15,15,17 | 1.31 | 2 (13%) |
| 4 | NAG | 6 | 1 | 4,1 | 14,14,15 | 0.90 | 1 (7%) | 17,19,21 | 1.93 | 2 (11%) |
| 4 | NAG | 6 | 2 | 4 | 14,14,15 | 0.41 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 4 | NAG | 7 | 1 | 4,2 | 14,14,15 | 0.81 | 1 (7%) | 17,19,21 | 1.49 | 2 (11%) |
| 4 | NAG | 7 | 2 | 4 | 14,14,15 | 0.43 | 0 | 17,19,21 | 1.07 | 2 (11%) |
| 4 | NAG | 8 | 1 | 4,1 | 14,14,15 | 0.94 | 1 (7%) | 17,19,21 | 1.85 | 2 (11%) |
| 4 | NAG | 8 | 2 | 4 | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.69 | 1 (5%) |
| 4 | NAG | 9 | 1 | 4,1 | 14,14,15 | 0.89 | 1 (7%) | 17,19,21 | 1.51 | 3 (17%) |
| 4 | NAG | 9 | 2 | 4 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.78 | 1 (5%) |
| 5 | NAG | AA | 1 | 5,1 | 14,14,15 | 0.66 | 0 | 17,19,21 | 1.16 | 3 (17%) |
| 5 | NAG | AA | 2 | 5 | 14,14,15 | 0.42 | 0 | 17,19,21 | 0.88 | 1 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 5 | BMA | AA | 3 | 5 | 11,11,12 | 0.29 | 0 | 15,15,17 | 1.93 | 3 (20%) |
| 5 | MAN | AA | 4 | 5 | 11,11,12 | 0.24 | 0 | 15,15,17 | 0.53 | 0 |
| 4 | NAG | BA | 1 | 4,1 | 14,14,15 | 0.71 | 0 | 17,19,21 | 1.37 | 3 (17%) |
| 4 | NAG | BA | 2 | 4 | 14,14,15 | 0.57 | 0 | 17,19,21 | 1.10 | 1 (5%) |
| 6 | NAG | CA | 1 | 6,2 | 14,14,15 | 1.04 | 1 (7%) | 17,19,21 | 1.54 | 1 (5%) |
| 6 | NAG | CA | 2 | 6 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.94 | 1 (5%) |
| 6 | BMA | CA | 3 | 6 | 11,11,12 | 0.22 | 0 | 15,15,17 | 0.68 | 0 |
| 6 | NAG | DA | 1 | 6,1 | 14,14,15 | 0.76 | 1 (7%) | 17,19,21 | 1.17 | 1 (5%) |
| 6 | NAG | DA | 2 | 6 | 14,14,15 | 0.31 | 0 | 17,19,21 | 1.22 | 2 (11%) |
| 6 | BMA | DA | 3 | 6 | 11,11,12 | 0.25 | 0 | 15,15,17 | 1.01 | 1 (6%) |
| 6 | NAG | EA | 1 | 6,1 | 14,14,15 | 0.79 | 1 (7%) | 17,19,21 | 1.35 | 2 (11%) |
| 6 | NAG | EA | 2 | 6 | 14,14,15 | 0.37 | 0 | 17,19,21 | 2.26 | 4 (23%) |
| 6 | BMA | EA | 3 | 6 | 11,11,12 | 0.23 | 0 | 15,15,17 | 0.78 | 0 |
| 5 | NAG | FA | 1 | 5,1 | 14,14,15 | 0.78 | 1 (7%) | 17,19,21 | 1.36 | 2 (11%) |
| 5 | NAG | FA | 2 | 5 | 14,14,15 | 0.48 | 0 | 17,19,21 | 0.90 | 1 (5%) |
| 5 | BMA | FA | 3 | 5 | 11,11,12 | 0.61 | 0 | 15,15,17 | 1.41 | 2 (13%) |
| 5 | MAN | FA | 4 | 5 | 11,11,12 | 0.21 | 0 | 15,15,17 | 1.29 | 2 (13%) |
| 6 | NAG | GA | 1 | 6,1 | 14,14,15 | 0.71 | 0 | 17,19,21 | 1.32 | 1 (5%) |
| 6 | NAG | GA | 2 | 6 | 14,14,15 | 0.42 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 6 | BMA | GA | 3 | 6 | 11,11,12 | 0.31 | 0 | 15,15,17 | 1.09 | 2 (13%) |
| 4 | NAG | HA | 1 | 4,2 | 14,14,15 | 0.68 | 0 | 17,19,21 | 1.23 | 2 (11%) |
| 4 | NAG | HA | 2 | 4 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.61 | 0 |
| 4 | NAG | IA | 1 | 4,1 | 14,14,15 | 0.80 | 1 (7%) | 17,19,21 | 1.50 | 2 (11%) |
| 4 | NAG | IA | 2 | 4 | 14,14,15 | 0.54 | 0 | 17,19,21 | 0.92 | 1 (5%) |
| 4 | NAG | JA | 1 | 4,1 | 14,14,15 | 0.82 | 1 (7%) | 17,19,21 | 1.23 | 1 (5%) |
| 4 | NAG | JA | 2 | 4 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.75 | 0 |
| 5 | NAG | KA | 1 | 5,1 | 14,14,15 | 0.72 | 0 | 17,19,21 | 1.86 | 5 (29%) |
| 5 | NAG | KA | 2 | 5 | 14,14,15 | 0.37 | 0 | 17,19,21 | 1.30 | 2 (11%) |
| 5 | BMA | KA | 3 | 5 | 11,11,12 | 0.29 | 0 | 15,15,17 | 1.45 | 1 (6%) |
| 5 | MAN | KA | 4 | 5 | 11,11,12 | 0.42 | 0 | 15,15,17 | 1.92 | 3 (20%) |
| 6 | NAG | LA | 1 | 6,1 | 14,14,15 | 0.98 | 1 (7%) | 17,19,21 | 2.35 | 4 (23%) |
| 6 | NAG | LA | 2 | 6 | 14,14,15 | 0.46 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 6 | BMA | LA | 3 | 6 | 11,11,12 | 0.22 | 0 | 15,15,17 | 0.79 | 1 (6%) |
| 4 | NAG | MA | 1 | 4,2 | 14,14,15 | 0.99 | 1 (7%) | 17,19,21 | 2.38 | 3 (17%) |
| 4 | NAG | MA | 2 | 4 | 14,14,15 | 0.32 | 0 | 17,19,21 | 1.69 | 3 (17%) |
| 6 | NAG | NA | 1 | 6,1 | 14,14,15 | 0.72 | 1 (7%) | 17,19,21 | 1.02 | 1 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 6 | NAG | NA | 2 | 6 | 14,14,15 | 0.37 | 0 | 17,19,21 | 0.84 | 0 |
| 6 | BMA | NA | 3 | 6 | 11,11,12 | 0.25 | 0 | 15,15,17 | 0.95 | 1 (6%) |
| 4 | NAG | OA | 1 | 4,1 | 14,14,15 | 1.17 | 1 (7%) | 17,19,21 | 1.59 | 2 (11%) |
| 4 | NAG | OA | 2 | 4 | 14,14,15 | 0.55 | 0 | 17,19,21 | 0.98 | 1 (5%) |
| 5 | NAG | PA | 1 | 5,1 | 14,14,15 | 0.66 | 0 | 17,19,21 | 1.13 | 1 (5%) |
| 5 | NAG | PA | 2 | 5 | 14,14,15 | 0.37 | 0 | 17,19,21 | 0.98 | 1 (5%) |
| 5 | BMA | PA | 3 | 5 | 11,11,12 | 0.61 | 0 | 15,15,17 | 2.27 | 4 (26%) |
| 5 | MAN | PA | 4 | 5 | 11,11,12 | 0.27 | 0 | 15,15,17 | 0.90 | 1 (6%) |
| 4 | NAG | QA | 1 | 4,1 | 14,14,15 | 0.57 | 0 | 17,19,21 | 2.49 | 5 (29%) |
| 4 | NAG | QA | 2 | 4 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.69 | 0 |
| 4 | NAG | RA | 1 | 4,2 | 14,14,15 | 1.13 | 1 (7%) | 17,19,21 | 2.16 | 4 (23%) |
| 4 | NAG | RA | 2 | 4 | 14,14,15 | 0.45 | 0 | 17,19,21 | 0.72 | 0 |
| 4 | NAG | e | 1 | 4,1 | 14,14,15 | 0.60 | 0 | 17,19,21 | 1.67 | 4 (23%) |
| 4 | NAG | e | 2 | 4 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.52 | 0 |
| 4 | NAG | f | 1 | 4,1 | 14,14,15 | 0.90 | 1 (7%) | 17,19,21 | 1.42 | 2 (11%) |
| 4 | NAG | f | 2 | 4 | 14,14,15 | 0.24 | 0 | 17,19,21 | 1.01 | 1 (5%) |
| 5 | NAG | g | 1 | 5,1 | 14,14,15 | 0.60 | 0 | 17,19,21 | 1.51 | 2 (11%) |
| 5 | NAG | g | 2 | 5 | 14,14,15 | 0.50 | 0 | 17,19,21 | 1.05 | 0 |
| 5 | BMA | g | 3 | 5 | 11,11,12 | 0.49 | 0 | 15,15,17 | 2.19 | 4 (26%) |
| 5 | MAN | g | 4 | 5 | 11,11,12 | 0.24 | 0 | 15,15,17 | 0.73 | 0 |
| 6 | NAG | h | 1 | 6,1 | 14,14,15 | 0.62 | 0 | 17,19,21 | 1.14 | 2 (11%) |
| 6 | NAG | h | 2 | 6 | 14,14,15 | 0.57 | 0 | 17,19,21 | 1.09 | 1 (5%) |
| 6 | BMA | h | 3 | 6 | 11,11,12 | 0.26 | 0 | 15,15,17 | 1.15 | 2 (13%) |
| 4 | NAG | i | 1 | 4,2 | 14,14,15 | 1.06 | 1 (7%) | 17,19,21 | 1.23 | 2 (11%) |
| 4 | NAG | i | 2 | 4 | 14,14,15 | 0.42 | 0 | 17,19,21 | 0.86 | 0 |
| 4 | NAG | j | 1 | 4,1 | 14,14,15 | 1.00 | 1 (7%) | 17,19,21 | 1.65 | 2 (11%) |
| 4 | NAG | j | 2 | 4 | 14,14,15 | 0.49 | 0 | 17,19,21 | 1.36 | 3 (17%) |
| 6 | NAG | k | 1 | 6,1 | 14,14,15 | 0.78 | 1 (7%) | 17,19,21 | 1.10 | 1 (5%) |
| 6 | NAG | k | 2 | 6 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.66 | 1 (5%) |
| 6 | BMA | k | 3 | 6 | 11,11,12 | 0.25 | 0 | 15,15,17 | 0.53 | 0 |
| 5 | NAG | l | 1 | 5,1 | 14,14,15 | 0.69 | 0 | 17,19,21 | 1.21 | 1 (5%) |
| 5 | NAG | l | 2 | 5 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.61 | 0 |
| 5 | BMA | l | 3 | 5 | 11,11,12 | 0.27 | 0 | 15,15,17 | 0.83 | 0 |
| 5 | MAN | l | 4 | 5 | 11,11,12 | 0.27 | 0 | 15,15,17 | 0.99 | 1 (6%) |
| 4 | NAG | m | 1 | 4,1 | 14,14,15 | 0.40 | 0 | 17,19,21 | 0.97 | 1 (5%) |
| 4 | NAG | m | 2 | 4 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.91 | 1 (5%) |
| 4 | NAG | n | 1 | 4,2 | 14,14,15 | 0.53 | 0 | 17,19,21 | 1.57 | 3 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 4 | NAG | n | 2 | 4 | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.99 | 1 (5%) |
| 4 | NAG | o | 1 | 4,1 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.00 | 1 (5%) |
| 4 | NAG | o | 2 | 4 | 14,14,15 | 0.43 | 0 | 17,19,21 | 1.13 | 2 (11%) |
| 4 | NAG | p | 1 | 4 | 14,14,15 | 0.89 | 1 (7%) | 17,19,21 | 1.94 | 4 (23%) |
| 4 | NAG | p | 2 | 4 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.67 | 0 |
| 4 | NAG | q | 1 | 4,1 | 14,14,15 | 0.56 | 0 | 17,19,21 | 1.18 | 2 (11%) |
| 4 | NAG | q | 2 | 4 | 14,14,15 | 0.51 | 0 | 17,19,21 | 0.87 | 1 (5%) |
| 6 | NAG | r | 1 | 6,1 | 14,14,15 | 0.69 | 0 | 17,19,21 | 1.73 | 4 (23%) |
| 6 | NAG | r | 2 | 6 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.02 | 0 |
| 6 | BMA | r | 3 | 6 | 11,11,12 | 0.23 | 0 | 15,15,17 | 0.63 | 0 |
| 4 | NAG | s | 1 | 4,2 | 14,14,15 | 0.80 | 1 (7%) | 17,19,21 | 1.22 | 2 (11%) |
| 4 | NAG | s | 2 | 4 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.77 | 0 |
| 4 | NAG | t | 1 | 4,1 | 14,14,15 | 0.64 | 0 | 17,19,21 | 1.50 | 3 (17%) |
| 4 | NAG | t | 2 | 4 | 14,14,15 | 0.31 | 0 | 17,19,21 | 0.54 | 0 |
| 4 | NAG | u | 1 | 4,1 | 14,14,15 | 0.83 | 1 (7%) | 17,19,21 | 1.64 | 3 (17%) |
| 4 | NAG | u | 2 | 4 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.85 | 1 (5%) |
| 4 | NAG | v | 1 | 4,1 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.11 | 1 (5%) |
| 4 | NAG | v | 2 | 4 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.93 | 1 (5%) |
| 6 | NAG | w | 1 | 6,1 | 14,14,15 | 0.71 | 1 (7%) | 17,19,21 | 1.90 | 4 (23%) |
| 6 | NAG | w | 2 | 6 | 14,14,15 | 0.42 | 0 | 17,19,21 | 1.17 | 1 (5%) |
| 6 | BMA | w | 3 | 6 | 11,11,12 | 0.30 | 0 | 15,15,17 | 0.84 | 1 (6%) |
| 4 | NAG | x | 1 | 4,2 | 14,14,15 | 0.50 | 0 | 17,19,21 | 0.91 | 0 |
| 4 | NAG | x | 2 | 4 | 14,14,15 | 0.48 | 0 | 17,19,21 | 1.03 | 1 (5%) |
| 6 | NAG | y | 1 | 6,1 | 14,14,15 | 0.86 | 1 (7%) | 17,19,21 | 1.18 | 1 (5%) |
| 6 | NAG | y | 2 | 6 | 14,14,15 | 0.35 | 0 | 17,19,21 | 1.92 | 4 (23%) |
| 6 | BMA | y | 3 | 6 | 11,11,12 | 0.22 | 0 | 15,15,17 | 1.24 | 2 (13%) |
| 7 | NAG | z | 1 | 7,1 | 14,14,15 | 1.07 | 1 (7%) | 17,19,21 | 2.10 | 3 (17%) |
| 7 | NAG | z | 2 | 7 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.58 | 3 (17%) |
| 7 | BMA | z | 3 | 7 | 11,11,12 | 0.45 | 0 | 15,15,17 | 2.58 | 5 (33%) |
| 7 | MAN | z | 4 | 7 | 11,11,12 | 0.42 | 0 | 15,15,17 | 1.98 | 4 (26%) |
| 7 | MAN | z | 5 | 7 | 11,11,12 | 0.22 | 0 | 15,15,17 | 0.63 | 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 |
|---|---|---|---|---|---|---|---|
| 8 | NAG | 0 | 1 | 1,8 | - | 2/6/23/26 | 0/1/1/1 |
| 8 | NAG | 0 | 2 | 8 | - | 2/6/23/26 | 0/1/1/1 |
| 8 | BMA | 0 | 3 | 8 | - | 0/2/19/22 | 0/1/1/1 |
| 8 | MAN | 0 | 4 | 8 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | 1 | 1 | 4,1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | 1 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | 2 | 1 | 4,2 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | 2 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | 3 | 1 | 6,1 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | 3 | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | 3 | 3 | 6 | - | 2/2/19/22 | 0/1/1/1 |
| 4 | NAG | 4 | 1 | 4,1 | - | 5/6/23/26 | 0/1/1/1 |
| 4 | NAG | 4 | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | 5 | 1 | 6,1 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | 5 | 2 | 6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | BMA | 5 | 3 | 6 | - | 2/2/19/22 | 0/1/1/1 |
| 4 | NAG | 6 | 1 | 4,1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | 6 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | 7 | 1 | 4,2 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | 7 | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | 8 | 1 | 4,1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | 8 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | 9 | 1 | 4,1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | 9 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | AA | 1 | 5,1 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | AA | 2 | 5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | BMA | AA | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | AA | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | BA | 1 | 4,1 | - | 5/6/23/26 | 0/1/1/1 |
| 4 | NAG | BA | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | CA | 1 | 6,2 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | CA | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | CA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | DA | 1 | 6,1 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | DA | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | DA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | EA | 1 | 6,1 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | EA | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 6 | BMA | EA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | FA | 1 | 5,1 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | FA | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | FA | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | FA | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | GA | 1 | 6,1 | - | 5/6/23/26 | 0/1/1/1 |
| 6 | NAG | GA | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | GA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | HA | 1 | 4,2 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | NAG | HA | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | IA | 1 | 4,1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | IA | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | JA | 1 | 4,1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | JA | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | KA | 1 | 5,1 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | KA | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | KA | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | KA | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | LA | 1 | 6,1 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | LA | 2 | 6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | BMA | LA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | MA | 1 | 4,2 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | MA | 2 | 4 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | NAG | NA | 1 | 6,1 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | NA | 2 | 6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | BMA | NA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | OA | 1 | 4,1 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | NAG | OA | 2 | 4 | - | 3/6/23/26 | 0/1/1/1 |
| 5 | NAG | PA | 1 | 5,1 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | PA | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | PA | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | PA | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | QA | 1 | 4,1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | QA | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | RA | 1 | 4,2 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | RA | 2 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | e | 1 | 4,1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | e | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | NAG | f | 1 | 4,1 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | f | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | g | 1 | 5,1 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | g | 2 | 5 | - | 3/6/23/26 | 0/1/1/1 |
| 5 | BMA | g | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 5 | MAN | g | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | h | 1 | 6,1 | - | 3/6/23/26 | 0/1/1/1 |
| 6 | NAG | h | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | h | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | i | 1 | 4,2 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | NAG | i | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | j | 1 | 4,1 | - | 5/6/23/26 | 0/1/1/1 |
| 4 | NAG | j | 2 | 4 | - | 6/6/23/26 | 0/1/1/1 |
| 6 | NAG | k | 1 | 6,1 | - | 6/6/23/26 | 0/1/1/1 |
| 6 | NAG | k | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | k | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | l | 1 | 5,1 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | l | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | l | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | l | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | m | 1 | 4,1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | m | 2 | 4 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | NAG | n | 1 | 4,2 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | n | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | o | 1 | 4,1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | o | 2 | 4 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | p | 1 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | p | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | q | 1 | 4,1 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | q | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | r | 1 | 6,1 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | r | 2 | 6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | BMA | r | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | s | 1 | 4,2 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | s | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | t | 1 | 4,1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | t | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | NAG | u | 1 | 4,1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | u | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | v | 1 | 4,1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | v | 2 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | w | 1 | 6,1 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | w | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | w | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | x | 1 | 4,2 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | x | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | y | 1 | 6,1 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | y | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | y | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | NAG | z | 1 | 7,1 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | NAG | z | 2 | 7 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | BMA | z | 3 | 7 | - | 2/2/19/22 | 0/1/1/1 |
| 7 | MAN | z | 4 | 7 | - | 1/2/19/22 | 0/1/1/1 |
| 7 | MAN | z | 5 | 7 | - | 1/2/19/22 | 0/1/1/1 |

All (29) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | OA | 1 | NAG | C1-C2 | 4.08 | 1.58 | 1.52 |
| 4 | 2 | 1 | NAG | C1-C2 | 3.75 | 1.57 | 1.52 |
| 4 | i | 1 | NAG | C1-C2 | 3.72 | 1.57 | 1.52 |
| 4 | RA | 1 | NAG | C1-C2 | 3.70 | 1.57 | 1.52 |
| 7 | z | 1 | NAG | C1-C2 | 3.65 | 1.57 | 1.52 |
| 6 | CA | 1 | NAG | C1-C2 | 3.53 | 1.57 | 1.52 |
| 4 | j | 1 | NAG | C1-C2 | 3.44 | 1.57 | 1.52 |
| 6 | 3 | 1 | NAG | C1-C2 | 3.35 | 1.57 | 1.52 |
| 6 | LA | 1 | NAG | C1-C2 | 3.27 | 1.57 | 1.52 |
| 4 | MA | 1 | NAG | C1-C2 | 3.15 | 1.57 | 1.52 |
| 4 | f | 1 | NAG | C1-C2 | 3.12 | 1.57 | 1.52 |
| 4 | 9 | 1 | NAG | C1-C2 | 2.97 | 1.56 | 1.52 |
| 4 | 6 | 1 | NAG | C1-C2 | 2.95 | 1.56 | 1.52 |
| 4 | p | 1 | NAG | C1-C2 | 2.84 | 1.56 | 1.52 |
| 6 | k | 1 | NAG | C1-C2 | 2.75 | 1.56 | 1.52 |
| 4 | 8 | 1 | NAG | C1-C2 | 2.70 | 1.56 | 1.52 |
| 4 | u | 1 | NAG | C1-C2 | 2.66 | 1.56 | 1.52 |
| 4 | s | 1 | NAG | C1-C2 | 2.61 | 1.56 | 1.52 |
| 6 | y | 1 | NAG | C1-C2 | 2.58 | 1.56 | 1.52 |
| 6 | EA | 1 | NAG | C1-C2 | 2.39 | 1.55 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | 7 | 1 | NAG | C1-C2 | 2.33 | 1.55 | 1.52 |
| 4 | IA | 1 | NAG | C1-C2 | 2.25 | 1.55 | 1.52 |
| 5 | FA | 1 | NAG | C1-C2 | 2.25 | 1.55 | 1.52 |
| 6 | NA | 1 | NAG | C1-C2 | 2.15 | 1.55 | 1.52 |
| 4 | 4 | 1 | NAG | C1-C2 | 2.12 | 1.55 | 1.52 |
| 6 | w | 1 | NAG | C1-C2 | 2.11 | 1.55 | 1.52 |
| 6 | DA | 1 | NAG | C1-C2 | 2.06 | 1.55 | 1.52 |
| 8 | 0 | 1 | NAG | C1-C2 | 2.05 | 1.55 | 1.52 |
| 4 | JA | 1 | NAG | C1-C2 | 2.02 | 1.55 | 1.52 |

All (216) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | LA | 1 | NAG | C1-O5-C5 | 8.01 | 123.04 | 112.19 |
| 4 | MA | 1 | NAG | C1-O5-C5 | 7.93 | 122.94 | 112.19 |
| 4 | RA | 1 | NAG | C1-O5-C5 | 7.38 | 122.19 | 112.19 |
| 4 | QA | 1 | NAG | C2-N2-C7 | -7.33 | 112.46 | 122.90 |
| 7 | z | 1 | NAG | C1-O5-C5 | 7.09 | 121.79 | 112.19 |
| 7 | z | 3 | BMA | C1-O5-C5 | 6.82 | 121.43 | 112.19 |
| 4 | 6 | 1 | NAG | C1-O5-C5 | 6.33 | 120.76 | 112.19 |
| 6 | EA | 2 | NAG | C1-O5-C5 | 6.26 | 120.68 | 112.19 |
| 5 | g | 3 | BMA | C1-C2-C3 | 6.03 | 117.08 | 109.67 |
| 4 | 8 | 1 | NAG | C1-O5-C5 | 5.88 | 120.16 | 112.19 |
| 5 | PA | 3 | BMA | C1-C2-C3 | 5.85 | 116.85 | 109.67 |
| 4 | j | 1 | NAG | C1-O5-C5 | 5.52 | 119.67 | 112.19 |
| 5 | KA | 1 | NAG | C1-O5-C5 | 5.35 | 119.44 | 112.19 |
| 6 | CA | 1 | NAG | C1-O5-C5 | 5.25 | 119.31 | 112.19 |
| 7 | z | 3 | BMA | C2-C3-C4 | -5.25 | 101.81 | 110.89 |
| 5 | AA | 3 | BMA | C1-C2-C3 | 5.00 | 115.81 | 109.67 |
| 4 | MA | 2 | NAG | C2-N2-C7 | 4.89 | 129.87 | 122.90 |
| 6 | y | 2 | NAG | O4-C4-C3 | -4.85 | 99.14 | 110.35 |
| 4 | OA | 1 | NAG | C1-O5-C5 | 4.75 | 118.63 | 112.19 |
| 8 | 0 | 3 | BMA | C1-O5-C5 | 4.75 | 118.63 | 112.19 |
| 8 | 0 | 1 | NAG | C1-O5-C5 | 4.60 | 118.42 | 112.19 |
| 4 | p | 1 | NAG | C1-O5-C5 | 4.59 | 118.41 | 112.19 |
| 6 | EA | 2 | NAG | O4-C4-C3 | -4.57 | 99.78 | 110.35 |
| 4 | u | 1 | NAG | C1-O5-C5 | 4.52 | 118.32 | 112.19 |
| 5 | KA | 4 | MAN | C1-C2-C3 | 4.48 | 115.18 | 109.67 |
| 4 | QA | 1 | NAG | O5-C5-C6 | 4.45 | 114.18 | 107.20 |
| 7 | z | 4 | MAN | C1-O5-C5 | 4.41 | 118.17 | 112.19 |
| 6 | r | 1 | NAG | C1-O5-C5 | 4.34 | 118.08 | 112.19 |
| 5 | KA | 4 | MAN | C1-O5-C5 | 4.29 | 118.01 | 112.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | 7 | 1 | NAG | C1-O5-C5 | 4.25 | 117.95 | 112.19 |
| 6 | w | 1 | NAG | O4-C4-C3 | 4.23 | 120.13 | 110.35 |
| 4 | 9 | 1 | NAG | O5-C5-C6 | 4.23 | 113.83 | 107.20 |
| 6 | y | 2 | NAG | C1-O5-C5 | 4.21 | 117.89 | 112.19 |
| 5 | KA | 2 | NAG | C1-O5-C5 | 4.20 | 117.89 | 112.19 |
| 5 | AA | 3 | BMA | O3-C3-C2 | -4.11 | 102.13 | 109.99 |
| 4 | 2 | 1 | NAG | C1-O5-C5 | 4.08 | 117.72 | 112.19 |
| 7 | z | 2 | NAG | C1-O5-C5 | 4.05 | 117.68 | 112.19 |
| 5 | KA | 3 | BMA | C1-C2-C3 | 3.98 | 114.55 | 109.67 |
| 5 | g | 1 | NAG | C1-O5-C5 | 3.86 | 117.42 | 112.19 |
| 5 | g | 1 | NAG | O5-C1-C2 | -3.83 | 105.23 | 111.29 |
| 5 | FA | 1 | NAG | C1-O5-C5 | 3.83 | 117.38 | 112.19 |
| 6 | w | 1 | NAG | C1-O5-C5 | 3.81 | 117.35 | 112.19 |
| 5 | g | 3 | BMA | C1-O5-C5 | 3.78 | 117.31 | 112.19 |
| 4 | MA | 1 | NAG | C2-N2-C7 | -3.77 | 117.54 | 122.90 |
| 4 | f | 1 | NAG | C1-O5-C5 | 3.76 | 117.29 | 112.19 |
| 4 | t | 1 | NAG | C1-O5-C5 | 3.74 | 117.26 | 112.19 |
| 4 | IA | 1 | NAG | C1-O5-C5 | 3.73 | 117.24 | 112.19 |
| 6 | w | 1 | NAG | C3-C4-C5 | -3.67 | 103.69 | 110.24 |
| 6 | EA | 2 | NAG | O5-C5-C6 | -3.66 | 101.47 | 107.20 |
| 7 | z | 4 | MAN | C1-C2-C3 | 3.62 | 114.12 | 109.67 |
| 6 | 3 | 1 | NAG | O4-C4-C3 | -3.60 | 102.03 | 110.35 |
| 4 | QA | 1 | NAG | C6-C5-C4 | -3.58 | 104.63 | 113.00 |
| 6 | y | 2 | NAG | O4-C4-C5 | 3.57 | 118.16 | 109.30 |
| 6 | 5 | 3 | BMA | C1-O5-C5 | 3.51 | 116.95 | 112.19 |
| 6 | GA | 1 | NAG | C1-O5-C5 | 3.47 | 116.89 | 112.19 |
| 4 | s | 1 | NAG | C2-N2-C7 | -3.46 | 117.98 | 122.90 |
| 5 | FA | 3 | BMA | C1-C2-C3 | 3.43 | 113.89 | 109.67 |
| 4 | e | 1 | NAG | C2-N2-C7 | -3.43 | 118.02 | 122.90 |
| 6 | 5 | 1 | NAG | C1-O5-C5 | 3.40 | 116.80 | 112.19 |
| 4 | e | 1 | NAG | O4-C4-C3 | -3.40 | 102.50 | 110.35 |
| 4 | n | 1 | NAG | O4-C4-C3 | -3.32 | 102.67 | 110.35 |
| 6 | DA | 2 | NAG | O4-C4-C3 | -3.31 | 102.69 | 110.35 |
| 4 | j | 2 | NAG | C2-N2-C7 | -3.30 | 118.20 | 122.90 |
| 8 | 0 | 2 | NAG | O5-C1-C2 | -3.29 | 106.09 | 111.29 |
| 4 | p | 1 | NAG | C4-C3-C2 | 3.28 | 115.83 | 111.02 |
| 7 | z | 4 | MAN | C3-C4-C5 | 3.25 | 116.05 | 110.24 |
| 6 | h | 1 | NAG | C1-O5-C5 | 3.24 | 116.59 | 112.19 |
| 4 | p | 1 | NAG | O5-C1-C2 | -3.22 | 106.20 | 111.29 |
| 4 | n | 1 | NAG | C2-N2-C7 | -3.21 | 118.33 | 122.90 |
| 4 | 6 | 1 | NAG | C3-C4-C5 | -3.20 | 104.53 | 110.24 |
| 6 | 3 | 1 | NAG | C1-O5-C5 | 3.19 | 116.51 | 112.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | HA | 1 | NAG | C2-N2-C7 | -3.18 | 118.38 | 122.90 |
| 5 | PA | 3 | BMA | C1-O5-C5 | 3.17 | 116.48 | 112.19 |
| 4 | u | 1 | NAG | C2-N2-C7 | -3.14 | 118.43 | 122.90 |
| 7 | z | 2 | NAG | C4-C3-C2 | -3.13 | 106.43 | 111.02 |
| 6 | DA | 2 | NAG | C1-O5-C5 | 3.12 | 116.42 | 112.19 |
| 4 | IA | 1 | NAG | C2-N2-C7 | -3.11 | 118.47 | 122.90 |
| 4 | v | 1 | NAG | C1-O5-C5 | 3.11 | 116.41 | 112.19 |
| 6 | r | 1 | NAG | C4-C3-C2 | -3.11 | 106.46 | 111.02 |
| 4 | t | 1 | NAG | C2-N2-C7 | -3.11 | 118.47 | 122.90 |
| 7 | z | 1 | NAG | C3-C4-C5 | -3.09 | 104.73 | 110.24 |
| 8 | 0 | 3 | BMA | C1-C2-C3 | -3.09 | 105.87 | 109.67 |
| 5 | PA | 3 | BMA | C2-C3-C4 | 3.07 | 116.22 | 110.89 |
| 6 | EA | 1 | NAG | C1-O5-C5 | 3.04 | 116.32 | 112.19 |
| 7 | z | 3 | BMA | C1-C2-C3 | 3.04 | 113.40 | 109.67 |
| 4 | q | 1 | NAG | O5-C1-C2 | -3.02 | 106.53 | 111.29 |
| 5 | KA | 4 | MAN | O5-C1-C2 | 3.01 | 115.42 | 110.77 |
| 6 | CA | 2 | NAG | C1-O5-C5 | 3.01 | 116.27 | 112.19 |
| 4 | f | 2 | NAG | C1-O5-C5 | 2.99 | 116.25 | 112.19 |
| 6 | r | 1 | NAG | C2-N2-C7 | -2.99 | 118.65 | 122.90 |
| 5 | FA | 4 | MAN | O5-C1-C2 | -2.98 | 106.16 | 110.77 |
| 6 | h | 2 | NAG | O5-C1-C2 | -2.98 | 106.59 | 111.29 |
| 5 | PA | 3 | BMA | C3-C4-C5 | 2.97 | 115.53 | 110.24 |
| 6 | LA | 1 | NAG | C3-C4-C5 | -2.96 | 104.96 | 110.24 |
| 4 | JA | 1 | NAG | C4-C3-C2 | 2.95 | 115.35 | 111.02 |
| 6 | y | 3 | BMA | C1-C2-C3 | 2.94 | 113.28 | 109.67 |
| 7 | z | 2 | NAG | O4-C4-C5 | 2.93 | 116.58 | 109.30 |
| 8 | 0 | 2 | NAG | C1-O5-C5 | 2.93 | 116.16 | 112.19 |
| 6 | 5 | 2 | NAG | O5-C1-C2 | -2.89 | 106.73 | 111.29 |
| 4 | i | 1 | NAG | C1-O5-C5 | 2.88 | 116.10 | 112.19 |
| 4 | 8 | 1 | NAG | C2-N2-C7 | -2.84 | 118.85 | 122.90 |
| 4 | RA | 1 | NAG | C2-N2-C7 | -2.84 | 118.85 | 122.90 |
| 5 | KA | 1 | NAG | C2-N2-C7 | -2.82 | 118.88 | 122.90 |
| 6 | EA | 2 | NAG | O4-C4-C5 | 2.81 | 116.27 | 109.30 |
| 5 | FA | 2 | NAG | C1-O5-C5 | 2.80 | 115.98 | 112.19 |
| 4 | o | 2 | NAG | C1-O5-C5 | -2.78 | 108.42 | 112.19 |
| 8 | 0 | 3 | BMA | O5-C1-C2 | -2.78 | 106.48 | 110.77 |
| 5 | PA | 2 | NAG | O4-C4-C5 | -2.75 | 102.46 | 109.30 |
| 5 | l | 1 | NAG | O5-C1-C2 | -2.75 | 106.94 | 111.29 |
| 4 | x | 2 | NAG | C1-O5-C5 | 2.75 | 115.91 | 112.19 |
| 7 | z | 3 | BMA | C6-C5-C4 | -2.74 | 106.59 | 113.00 |
| 4 | e | 1 | NAG | C1-O5-C5 | 2.71 | 115.86 | 112.19 |
| 4 | n | 1 | NAG | O5-C1-C2 | -2.69 | 107.04 | 111.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | y | 1 | NAG | C1-O5-C5 | 2.67 | 115.80 | 112.19 |
| 5 | KA | 1 | NAG | O5-C1-C2 | -2.66 | 107.09 | 111.29 |
| 6 | LA | 1 | NAG | C4-C3-C2 | 2.65 | 114.91 | 111.02 |
| 5 | AA | 1 | NAG | C1-O5-C5 | 2.64 | 115.76 | 112.19 |
| 5 | FA | 1 | NAG | O5-C1-C2 | -2.63 | 107.13 | 111.29 |
| 4 | OA | 2 | NAG | O5-C1-C2 | -2.63 | 107.14 | 111.29 |
| 6 | y | 3 | BMA | C1-O5-C5 | 2.61 | 115.73 | 112.19 |
| 7 | z | 3 | BMA | O5-C5-C4 | 2.61 | 117.17 | 110.83 |
| 7 | z | 4 | MAN | C6-C5-C4 | -2.61 | 106.90 | 113.00 |
| 4 | 4 | 1 | NAG | O4-C4-C3 | -2.59 | 104.37 | 110.35 |
| 8 | 0 | 2 | NAG | C2-N2-C7 | -2.56 | 119.26 | 122.90 |
| 8 | 0 | 4 | MAN | C1-O5-C5 | -2.55 | 108.73 | 112.19 |
| 4 | BA | 1 | NAG | C4-C3-C2 | 2.55 | 114.75 | 111.02 |
| 5 | l | 4 | MAN | C1-C2-C3 | 2.54 | 112.79 | 109.67 |
| 6 | GA | 3 | BMA | O5-C1-C2 | -2.54 | 106.85 | 110.77 |
| 8 | 0 | 3 | BMA | C6-C5-C4 | -2.53 | 107.08 | 113.00 |
| 5 | g | 3 | BMA | O3-C3-C2 | -2.52 | 105.16 | 109.99 |
| 6 | DA | 3 | BMA | C1-C2-C3 | 2.47 | 112.70 | 109.67 |
| 6 | EA | 1 | NAG | O5-C1-C2 | -2.46 | 107.41 | 111.29 |
| 4 | MA | 2 | NAG | O7-C7-N2 | 2.45 | 126.45 | 121.95 |
| 6 | DA | 1 | NAG | O4-C4-C3 | -2.45 | 104.69 | 110.35 |
| 6 | h | 3 | BMA | C1-C2-C3 | 2.44 | 112.67 | 109.67 |
| 6 | 5 | 3 | BMA | C1-C2-C3 | 2.44 | 112.66 | 109.67 |
| 4 | e | 1 | NAG | C4-C3-C2 | 2.43 | 114.59 | 111.02 |
| 5 | KA | 2 | NAG | O4-C4-C3 | -2.43 | 104.72 | 110.35 |
| 6 | h | 3 | BMA | C1-O5-C5 | 2.43 | 115.48 | 112.19 |
| 6 | LA | 3 | BMA | O5-C5-C6 | 2.43 | 111.01 | 107.20 |
| 4 | MA | 1 | NAG | C3-C4-C5 | -2.42 | 105.93 | 110.24 |
| 4 | t | 1 | NAG | O4-C4-C3 | -2.42 | 104.76 | 110.35 |
| 4 | o | 2 | NAG | O5-C5-C6 | 2.40 | 110.97 | 107.20 |
| 5 | AA | 2 | NAG | O5-C1-C2 | -2.40 | 107.50 | 111.29 |
| 6 | GA | 3 | BMA | O5-C5-C6 | 2.39 | 110.95 | 107.20 |
| 4 | 9 | 2 | NAG | C1-O5-C5 | 2.35 | 115.38 | 112.19 |
| 4 | p | 1 | NAG | O5-C5-C6 | -2.35 | 103.52 | 107.20 |
| 4 | 2 | 1 | NAG | C3-C4-C5 | -2.35 | 106.05 | 110.24 |
| 4 | j | 1 | NAG | C3-C4-C5 | -2.34 | 106.06 | 110.24 |
| 4 | 7 | 2 | NAG | C2-N2-C7 | -2.34 | 119.57 | 122.90 |
| 6 | w | 2 | NAG | C8-C7-N2 | 2.34 | 120.05 | 116.10 |
| 6 | w | 3 | BMA | O5-C5-C6 | 2.33 | 110.86 | 107.20 |
| 4 | i | 1 | NAG | C4-C3-C2 | -2.32 | 107.62 | 111.02 |
| 5 | AA | 1 | NAG | O5-C1-C2 | -2.31 | 107.64 | 111.29 |
| 4 | OA | 1 | NAG | O5-C1-C2 | -2.30 | 107.65 | 111.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | 1 | 2 | NAG | C8-C7-N2 | 2.30 | 119.99 | 116.10 |
| 4 | 6 | 2 | NAG | C8-C7-N2 | 2.30 | 119.99 | 116.10 |
| 6 | NA | 3 | BMA | C1-O5-C5 | -2.30 | 109.08 | 112.19 |
| 4 | q | 1 | NAG | C2-N2-C7 | -2.29 | 119.64 | 122.90 |
| 5 | PA | 4 | MAN | O5-C5-C6 | 2.29 | 110.80 | 107.20 |
| 4 | 4 | 2 | NAG | C1-C2-N2 | -2.29 | 106.57 | 110.49 |
| 5 | FA | 3 | BMA | C3-C4-C5 | 2.28 | 114.31 | 110.24 |
| 5 | g | 3 | BMA | O3-C3-C4 | 2.28 | 115.62 | 110.35 |
| 6 | LA | 2 | NAG | O4-C4-C3 | -2.27 | 105.10 | 110.35 |
| 4 | 7 | 1 | NAG | C3-C4-C5 | -2.27 | 106.19 | 110.24 |
| 4 | m | 2 | NAG | C1-O5-C5 | 2.26 | 115.26 | 112.19 |
| 6 | GA | 2 | NAG | C8-C7-N2 | 2.26 | 119.92 | 116.10 |
| 4 | 1 | 1 | NAG | C1-O5-C5 | 2.24 | 115.23 | 112.19 |
| 8 | 0 | 1 | NAG | C3-C4-C5 | -2.24 | 106.24 | 110.24 |
| 4 | 4 | 1 | NAG | O5-C1-C2 | -2.24 | 107.75 | 111.29 |
| 7 | z | 1 | NAG | C4-C3-C2 | 2.23 | 114.28 | 111.02 |
| 8 | 0 | 2 | NAG | C3-C4-C5 | -2.23 | 106.27 | 110.24 |
| 4 | MA | 2 | NAG | C1-C2-N2 | -2.22 | 106.70 | 110.49 |
| 6 | LA | 1 | NAG | C2-N2-C7 | -2.21 | 119.75 | 122.90 |
| 5 | PA | 1 | NAG | O5-C1-C2 | -2.21 | 107.80 | 111.29 |
| 4 | v | 2 | NAG | C2-N2-C7 | -2.20 | 119.77 | 122.90 |
| 5 | AA | 3 | BMA | C1-O5-C5 | 2.20 | 115.17 | 112.19 |
| 4 | n | 2 | NAG | C1-O5-C5 | -2.19 | 109.23 | 112.19 |
| 6 | y | 2 | NAG | O5-C5-C6 | -2.18 | 103.78 | 107.20 |
| 4 | u | 1 | NAG | C3-C4-C5 | -2.18 | 106.35 | 110.24 |
| 5 | AA | 1 | NAG | C2-N2-C7 | -2.18 | 119.81 | 122.90 |
| 5 | KA | 1 | NAG | C3-C4-C5 | -2.17 | 106.36 | 110.24 |
| 4 | 7 | 2 | NAG | C1-O5-C5 | 2.16 | 115.12 | 112.19 |
| 4 | 4 | 2 | NAG | O5-C5-C4 | -2.16 | 105.58 | 110.83 |
| 4 | j | 2 | NAG | C4-C3-C2 | -2.15 | 107.87 | 111.02 |
| 4 | q | 2 | NAG | C1-C2-N2 | -2.15 | 106.82 | 110.49 |
| 4 | BA | 1 | NAG | O5-C1-C2 | -2.14 | 107.91 | 111.29 |
| 4 | BA | 2 | NAG | C1-C2-N2 | -2.12 | 106.86 | 110.49 |
| 6 | LA | 2 | NAG | C2-N2-C7 | -2.12 | 119.88 | 122.90 |
| 4 | QA | 1 | NAG | O5-C5-C4 | 2.11 | 115.97 | 110.83 |
| 4 | 9 | 1 | NAG | C1-O5-C5 | 2.10 | 115.04 | 112.19 |
| 4 | HA | 1 | NAG | O5-C5-C6 | 2.10 | 110.50 | 107.20 |
| 4 | 9 | 1 | NAG | C3-C4-C5 | -2.10 | 106.50 | 110.24 |
| 6 | k | 2 | NAG | C1-O5-C5 | 2.09 | 115.02 | 112.19 |
| 4 | f | 1 | NAG | C3-C4-C5 | -2.08 | 106.53 | 110.24 |
| 4 | o | 1 | NAG | C2-N2-C7 | -2.08 | 119.94 | 122.90 |
| 4 | QA | 1 | NAG | O4-C4-C3 | -2.08 | 105.55 | 110.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | FA | 4 | MAN | C2-C3-C4 | -2.08 | 107.30 | 110.89 |
| 6 | GA | 2 | NAG | C2-N2-C7 | -2.07 | 119.96 | 122.90 |
| 4 | 6 | 2 | NAG | C2-N2-C7 | -2.06 | 119.97 | 122.90 |
| 4 | u | 2 | NAG | O5-C5-C6 | 2.06 | 110.43 | 107.20 |
| 4 | IA | 2 | NAG | C2-N2-C7 | -2.05 | 119.98 | 122.90 |
| 4 | BA | 1 | NAG | O4-C4-C3 | 2.05 | 115.08 | 110.35 |
| 5 | KA | 1 | NAG | O4-C4-C3 | -2.04 | 105.62 | 110.35 |
| 6 | w | 1 | NAG | C2-N2-C7 | -2.04 | 120.00 | 122.90 |
| 6 | k | 1 | NAG | C1-O5-C5 | 2.04 | 114.95 | 112.19 |
| 6 | h | 1 | NAG | O5-C5-C4 | 2.03 | 115.77 | 110.83 |
| 4 | 8 | 2 | NAG | C1-O5-C5 | 2.03 | 114.94 | 112.19 |
| 6 | NA | 1 | NAG | C4-C3-C2 | 2.03 | 113.99 | 111.02 |
| 4 | j | 2 | NAG | C1-O5-C5 | 2.02 | 114.93 | 112.19 |
| 4 | m | 1 | NAG | O5-C1-C2 | -2.02 | 108.10 | 111.29 |
| 4 | RA | 1 | NAG | C6-C5-C4 | -2.02 | 108.28 | 113.00 |
| 6 | r | 1 | NAG | C3-C4-C5 | -2.02 | 106.64 | 110.24 |
| 4 | RA | 1 | NAG | C3-C4-C5 | -2.01 | 106.64 | 110.24 |
| 4 | 1 | 2 | NAG | C2-N2-C7 | -2.01 | 120.05 | 122.90 |
| 4 | s | 1 | NAG | C4-C3-C2 | -2.00 | 108.08 | 111.02 |

There are no chirality outliers.

All (240) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | e | 1 | NAG | C8-C7-N2-C2 |
| 4 | e | 1 | NAG | O7-C7-N2-C2 |
| 4 | j | 1 | NAG | C3-C2-N2-C7 |
| 4 | j | 1 | NAG | C8-C7-N2-C2 |
| 4 | j | 1 | NAG | O7-C7-N2-C2 |
| 4 | m | 2 | NAG | C1-C2-N2-C7 |
| 4 | n | 1 | NAG | C8-C7-N2-C2 |
| 4 | n | 1 | NAG | O7-C7-N2-C2 |
| 4 | o | 1 | NAG | O7-C7-N2-C2 |
| 4 | q | 2 | NAG | C3-C2-N2-C7 |
| 4 | q | 2 | NAG | C8-C7-N2-C2 |
| 4 | q | 2 | NAG | O7-C7-N2-C2 |
| 4 | t | 1 | NAG | C8-C7-N2-C2 |
| 4 | t | 1 | NAG | O7-C7-N2-C2 |
| 4 | u | 1 | NAG | C8-C7-N2-C2 |
| 4 | u | 1 | NAG | O7-C7-N2-C2 |
| 4 | 2 | 1 | NAG | C3-C2-N2-C7 |
| 4 | 4 | 2 | NAG | C8-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | 4 | 2 | NAG | O7-C7-N2-C2 |
| 4 | 7 | 1 | NAG | O7-C7-N2-C2 |
| 4 | BA | 1 | NAG | C3-C2-N2-C7 |
| 4 | BA | 1 | NAG | C8-C7-N2-C2 |
| 4 | BA | 1 | NAG | O7-C7-N2-C2 |
| 4 | IA | 1 | NAG | C8-C7-N2-C2 |
| 4 | IA | 1 | NAG | O7-C7-N2-C2 |
| 4 | JA | 2 | NAG | C3-C2-N2-C7 |
| 4 | MA | 1 | NAG | C8-C7-N2-C2 |
| 4 | MA | 1 | NAG | O7-C7-N2-C2 |
| 4 | MA | 2 | NAG | C3-C2-N2-C7 |
| 4 | OA | 1 | NAG | C3-C2-N2-C7 |
| 4 | OA | 1 | NAG | O7-C7-N2-C2 |
| 4 | OA | 2 | NAG | C3-C2-N2-C7 |
| 6 | k | 1 | NAG | C8-C7-N2-C2 |
| 6 | k | 1 | NAG | O7-C7-N2-C2 |
| 6 | w | 1 | NAG | C8-C7-N2-C2 |
| 6 | w | 1 | NAG | O7-C7-N2-C2 |
| 6 | LA | 2 | NAG | C3-C2-N2-C7 |
| 6 | NA | 1 | NAG | C3-C2-N2-C7 |
| 6 | NA | 1 | NAG | C8-C7-N2-C2 |
| 6 | NA | 1 | NAG | O7-C7-N2-C2 |
| 6 | NA | 2 | NAG | C8-C7-N2-C2 |
| 6 | NA | 2 | NAG | O7-C7-N2-C2 |
| 4 | j | 2 | NAG | C8-C7-N2-C2 |
| 4 | o | 1 | NAG | C8-C7-N2-C2 |
| 4 | 7 | 1 | NAG | C8-C7-N2-C2 |
| 4 | 7 | 2 | NAG | C8-C7-N2-C2 |
| 4 | 7 | 2 | NAG | O7-C7-N2-C2 |
| 4 | OA | 1 | NAG | C8-C7-N2-C2 |
| 5 | AA | 1 | NAG | C8-C7-N2-C2 |
| 5 | AA | 1 | NAG | O7-C7-N2-C2 |
| 6 | r | 1 | NAG | C8-C7-N2-C2 |
| 6 | r | 1 | NAG | O7-C7-N2-C2 |
| 6 | r | 2 | NAG | C8-C7-N2-C2 |
| 6 | r | 2 | NAG | O7-C7-N2-C2 |
| 4 | i | 1 | NAG | O5-C5-C6-O6 |
| 4 | x | 1 | NAG | O5-C5-C6-O6 |
| 4 | u | 1 | NAG | O5-C5-C6-O6 |
| 4 | 8 | 1 | NAG | O5-C5-C6-O6 |
| 4 | HA | 1 | NAG | O5-C5-C6-O6 |
| 6 | k | 1 | NAG | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 6 | y | 1 | NAG | O5-C5-C6-O6 |
| 6 | 5 | 3 | BMA | O5-C5-C6-O6 |
| 5 | g | 3 | BMA | C4-C5-C6-O6 |
| 4 | j | 1 | NAG | O5-C5-C6-O6 |
| 4 | j | 2 | NAG | O5-C5-C6-O6 |
| 4 | s | 2 | NAG | O5-C5-C6-O6 |
| 4 | BA | 2 | NAG | O5-C5-C6-O6 |
| 4 | JA | 1 | NAG | O5-C5-C6-O6 |
| 4 | MA | 1 | NAG | O5-C5-C6-O6 |
| 4 | OA | 1 | NAG | O5-C5-C6-O6 |
| 4 | RA | 1 | NAG | O5-C5-C6-O6 |
| 6 | 3 | 1 | NAG | O5-C5-C6-O6 |
| 6 | 5 | 1 | NAG | O5-C5-C6-O6 |
| 6 | EA | 1 | NAG | O5-C5-C6-O6 |
| 8 | 0 | 1 | NAG | O5-C5-C6-O6 |
| 4 | j | 2 | NAG | O7-C7-N2-C2 |
| 4 | m | 2 | NAG | C8-C7-N2-C2 |
| 5 | KA | 1 | NAG | C8-C7-N2-C2 |
| 5 | KA | 1 | NAG | O7-C7-N2-C2 |
| 6 | DA | 1 | NAG | C8-C7-N2-C2 |
| 6 | LA | 1 | NAG | C8-C7-N2-C2 |
| 8 | 0 | 2 | NAG | C8-C7-N2-C2 |
| 4 | o | 1 | NAG | O5-C5-C6-O6 |
| 4 | p | 1 | NAG | O5-C5-C6-O6 |
| 4 | 7 | 1 | NAG | O5-C5-C6-O6 |
| 4 | IA | 1 | NAG | O5-C5-C6-O6 |
| 5 | l | 1 | NAG | O5-C5-C6-O6 |
| 6 | LA | 1 | NAG | O5-C5-C6-O6 |
| 4 | u | 1 | NAG | C4-C5-C6-O6 |
| 4 | BA | 2 | NAG | C4-C5-C6-O6 |
| 4 | JA | 1 | NAG | C4-C5-C6-O6 |
| 4 | n | 1 | NAG | O5-C5-C6-O6 |
| 4 | 4 | 1 | NAG | O5-C5-C6-O6 |
| 5 | FA | 1 | NAG | O5-C5-C6-O6 |
| 4 | x | 1 | NAG | C4-C5-C6-O6 |
| 4 | OA | 1 | NAG | C4-C5-C6-O6 |
| 6 | y | 1 | NAG | C4-C5-C6-O6 |
| 8 | 0 | 1 | NAG | C4-C5-C6-O6 |
| 4 | f | 1 | NAG | O5-C5-C6-O6 |
| 4 | v | 2 | NAG | O5-C5-C6-O6 |
| 4 | p | 1 | NAG | C4-C5-C6-O6 |
| 4 | 7 | 1 | NAG | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | HA | 1 | NAG | C4-C5-C6-O6 |
| 6 | k | 1 | NAG | C4-C5-C6-O6 |
| 6 | 5 | 1 | NAG | C4-C5-C6-O6 |
| 4 | 4 | 2 | NAG | O5-C5-C6-O6 |
| 6 | GA | 1 | NAG | O5-C5-C6-O6 |
| 4 | i | 1 | NAG | C4-C5-C6-O6 |
| 4 | m | 2 | NAG | O7-C7-N2-C2 |
| 4 | HA | 1 | NAG | C8-C7-N2-C2 |
| 6 | DA | 1 | NAG | O7-C7-N2-C2 |
| 6 | LA | 1 | NAG | O7-C7-N2-C2 |
| 8 | 0 | 2 | NAG | O7-C7-N2-C2 |
| 4 | JA | 2 | NAG | O5-C5-C6-O6 |
| 5 | KA | 1 | NAG | O5-C5-C6-O6 |
| 6 | r | 1 | NAG | O5-C5-C6-O6 |
| 4 | j | 2 | NAG | C4-C5-C6-O6 |
| 4 | IA | 1 | NAG | C4-C5-C6-O6 |
| 6 | LA | 1 | NAG | C4-C5-C6-O6 |
| 4 | f | 1 | NAG | C1-C2-N2-C7 |
| 6 | h | 1 | NAG | C1-C2-N2-C7 |
| 6 | NA | 2 | NAG | C1-C2-N2-C7 |
| 5 | g | 3 | BMA | O5-C5-C6-O6 |
| 7 | z | 3 | BMA | C4-C5-C6-O6 |
| 4 | f | 1 | NAG | C4-C5-C6-O6 |
| 4 | o | 1 | NAG | C4-C5-C6-O6 |
| 4 | s | 1 | NAG | C4-C5-C6-O6 |
| 4 | m | 2 | NAG | O5-C5-C6-O6 |
| 5 | PA | 1 | NAG | C4-C5-C6-O6 |
| 4 | IA | 2 | NAG | O5-C5-C6-O6 |
| 5 | PA | 1 | NAG | O5-C5-C6-O6 |
| 4 | v | 2 | NAG | C4-C5-C6-O6 |
| 4 | 4 | 1 | NAG | C4-C5-C6-O6 |
| 4 | 4 | 2 | NAG | C4-C5-C6-O6 |
| 5 | FA | 1 | NAG | C4-C5-C6-O6 |
| 6 | 5 | 3 | BMA | C4-C5-C6-O6 |
| 6 | r | 2 | NAG | O5-C5-C6-O6 |
| 4 | 8 | 1 | NAG | C4-C5-C6-O6 |
| 4 | RA | 1 | NAG | C4-C5-C6-O6 |
| 5 | l | 1 | NAG | C4-C5-C6-O6 |
| 5 | KA | 1 | NAG | C4-C5-C6-O6 |
| 4 | s | 1 | NAG | C8-C7-N2-C2 |
| 4 | BA | 2 | NAG | C8-C7-N2-C2 |
| 4 | HA | 1 | NAG | O7-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 6 | GA | 1 | NAG | C8-C7-N2-C2 |
| 4 | j | 1 | NAG | C4-C5-C6-O6 |
| 4 | MA | 1 | NAG | C4-C5-C6-O6 |
| 6 | EA | 1 | NAG | C4-C5-C6-O6 |
| 4 | RA | 2 | NAG | O5-C5-C6-O6 |
| 4 | n | 1 | NAG | C4-C5-C6-O6 |
| 4 | q | 1 | NAG | O5-C5-C6-O6 |
| 4 | m | 2 | NAG | C4-C5-C6-O6 |
| 4 | IA | 2 | NAG | C4-C5-C6-O6 |
| 4 | JA | 2 | NAG | C4-C5-C6-O6 |
| 6 | r | 2 | NAG | C4-C5-C6-O6 |
| 6 | 3 | 1 | NAG | C4-C5-C6-O6 |
| 5 | AA | 2 | NAG | O5-C5-C6-O6 |
| 4 | s | 2 | NAG | C4-C5-C6-O6 |
| 6 | GA | 1 | NAG | C4-C5-C6-O6 |
| 6 | 3 | 1 | NAG | C1-C2-N2-C7 |
| 6 | GA | 1 | NAG | C1-C2-N2-C7 |
| 4 | 1 | 1 | NAG | C4-C5-C6-O6 |
| 6 | GA | 1 | NAG | O7-C7-N2-C2 |
| 6 | 5 | 2 | NAG | O5-C5-C6-O6 |
| 6 | 5 | 2 | NAG | C4-C5-C6-O6 |
| 4 | v | 1 | NAG | O5-C5-C6-O6 |
| 4 | s | 1 | NAG | O5-C5-C6-O6 |
| 4 | s | 1 | NAG | O7-C7-N2-C2 |
| 4 | 4 | 1 | NAG | C8-C7-N2-C2 |
| 4 | 8 | 1 | NAG | C8-C7-N2-C2 |
| 4 | BA | 2 | NAG | O7-C7-N2-C2 |
| 4 | BA | 1 | NAG | C4-C5-C6-O6 |
| 5 | g | 2 | NAG | C4-C5-C6-O6 |
| 4 | m | 1 | NAG | O5-C5-C6-O6 |
| 6 | k | 1 | NAG | C1-C2-N2-C7 |
| 4 | i | 1 | NAG | C8-C7-N2-C2 |
| 6 | 3 | 3 | BMA | O5-C5-C6-O6 |
| 4 | 1 | 1 | NAG | O5-C5-C6-O6 |
| 7 | z | 3 | BMA | O5-C5-C6-O6 |
| 5 | g | 2 | NAG | O5-C5-C6-O6 |
| 4 | j | 2 | NAG | C1-C2-N2-C7 |
| 4 | s | 2 | NAG | C1-C2-N2-C7 |
| 4 | q | 1 | NAG | C4-C5-C6-O6 |
| 5 | g | 1 | NAG | O5-C5-C6-O6 |
| 4 | 4 | 1 | NAG | O7-C7-N2-C2 |
| 5 | AA | 1 | NAG | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | i | 1 | NAG | C1-C2-N2-C7 |
| 4 | OA | 1 | NAG | C1-C2-N2-C7 |
| 4 | 8 | 1 | NAG | O7-C7-N2-C2 |
| 4 | OA | 2 | NAG | O5-C5-C6-O6 |
| 4 | q | 2 | NAG | O5-C5-C6-O6 |
| 5 | AA | 2 | NAG | C4-C5-C6-O6 |
| 4 | OA | 2 | NAG | C4-C5-C6-O6 |
| 7 | z | 5 | MAN | O5-C5-C6-O6 |
| 6 | w | 1 | NAG | O5-C5-C6-O6 |
| 4 | 2 | 1 | NAG | C1-C2-N2-C7 |
| 4 | i | 1 | NAG | C3-C2-N2-C7 |
| 4 | s | 2 | NAG | C3-C2-N2-C7 |
| 4 | x | 1 | NAG | C3-C2-N2-C7 |
| 6 | NA | 2 | NAG | C3-C2-N2-C7 |
| 5 | g | 1 | NAG | C4-C5-C6-O6 |
| 4 | i | 1 | NAG | O7-C7-N2-C2 |
| 4 | HA | 1 | NAG | C1-C2-N2-C7 |
| 5 | AA | 2 | NAG | C8-C7-N2-C2 |
| 4 | 9 | 1 | NAG | C4-C5-C6-O6 |
| 4 | v | 1 | NAG | C4-C5-C6-O6 |
| 4 | JA | 2 | NAG | C1-C2-N2-C7 |
| 5 | AA | 1 | NAG | C4-C5-C6-O6 |
| 4 | 7 | 2 | NAG | C4-C5-C6-O6 |
| 6 | h | 1 | NAG | C4-C5-C6-O6 |
| 5 | AA | 2 | NAG | O7-C7-N2-C2 |
| 7 | z | 4 | MAN | O5-C5-C6-O6 |
| 4 | BA | 1 | NAG | O5-C5-C6-O6 |
| 4 | j | 2 | NAG | C3-C2-N2-C7 |
| 4 | m | 2 | NAG | C3-C2-N2-C7 |
| 4 | 4 | 1 | NAG | C3-C2-N2-C7 |
| 4 | HA | 1 | NAG | C3-C2-N2-C7 |
| 5 | g | 2 | NAG | C3-C2-N2-C7 |
| 6 | h | 1 | NAG | C3-C2-N2-C7 |
| 6 | k | 1 | NAG | C3-C2-N2-C7 |
| 4 | RA | 2 | NAG | C4-C5-C6-O6 |
| 4 | m | 1 | NAG | C4-C5-C6-O6 |
| 6 | w | 1 | NAG | C4-C5-C6-O6 |
| 4 | 6 | 1 | NAG | O5-C5-C6-O6 |
| 6 | LA | 2 | NAG | C1-C2-N2-C7 |
| 4 | m | 1 | NAG | C8-C7-N2-C2 |
| 4 | RA | 1 | NAG | C8-C7-N2-C2 |
| 6 | NA | 1 | NAG | C1-C2-N2-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 6 | r | 1 | NAG | C4-C5-C6-O6 |
| 4 | q | 1 | NAG | C8-C7-N2-C2 |
| 4 | IA | 2 | NAG | C8-C7-N2-C2 |
| 4 | 9 | 1 | NAG | O5-C5-C6-O6 |
| 6 | 3 | 3 | BMA | C4-C5-C6-O6 |
| 4 | 6 | 1 | NAG | C4-C5-C6-O6 |
| 4 | 7 | 2 | NAG | O5-C5-C6-O6 |
| 4 | m | 1 | NAG | O7-C7-N2-C2 |
| 4 | RA | 1 | NAG | O7-C7-N2-C2 |
| 6 | 3 | 1 | NAG | C3-C2-N2-C7 |
| 4 | IA | 2 | NAG | O7-C7-N2-C2 |
| 4 | o | 2 | NAG | C8-C7-N2-C2 |

There are no ring outliers.

78 monomers are involved in 141 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 6 | NA | 1 | NAG | 3 | 0 |
| 5 | PA | 2 | NAG | 1 | 0 |
| 5 | FA | 2 | NAG | 1 | 0 |
| 4 | 6 | 1 | NAG | 2 | 0 |
| 4 | j | 1 | NAG | 4 | 0 |
| 4 | f | 1 | NAG | 2 | 0 |
| 5 | l | 1 | NAG | 1 | 0 |
| 5 | FA | 4 | MAN | 1 | 0 |
| 6 | LA | 1 | NAG | 3 | 0 |
| 4 | n | 1 | NAG | 1 | 0 |
| 4 | JA | 1 | NAG | 2 | 0 |
| 4 | 1 | 1 | NAG | 1 | 0 |
| 4 | n | 2 | NAG | 1 | 0 |
| 4 | u | 1 | NAG | 6 | 0 |
| 4 | JA | 2 | NAG | 1 | 0 |
| 6 | r | 1 | NAG | 8 | 0 |
| 4 | BA | 2 | NAG | 3 | 0 |
| 4 | q | 1 | NAG | 3 | 0 |
| 4 | m | 2 | NAG | 4 | 0 |
| 8 | 0 | 1 | NAG | 6 | 0 |
| 5 | AA | 1 | NAG | 1 | 0 |
| 6 | 3 | 2 | NAG | 1 | 0 |
| 4 | HA | 1 | NAG | 4 | 0 |
| 4 | v | 1 | NAG | 1 | 0 |
| 6 | 5 | 3 | BMA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | QA | 1 | NAG | 4 | 0 |
| 6 | GA | 2 | NAG | 9 | 0 |
| 8 | 0 | 3 | BMA | 1 | 0 |
| 4 | RA | 2 | NAG | 1 | 0 |
| 6 | CA | 2 | NAG | 3 | 0 |
| 4 | s | 1 | NAG | 2 | 0 |
| 6 | EA | 1 | NAG | 1 | 0 |
| 6 | k | 1 | NAG | 4 | 0 |
| 6 | h | 2 | NAG | 1 | 0 |
| 4 | m | 1 | NAG | 9 | 0 |
| 4 | 9 | 2 | NAG | 1 | 0 |
| 6 | 5 | 1 | NAG | 1 | 0 |
| 5 | PA | 1 | NAG | 1 | 0 |
| 4 | j | 2 | NAG | 3 | 0 |
| 4 | o | 1 | NAG | 3 | 0 |
| 8 | 0 | 2 | NAG | 8 | 0 |
| 7 | z | 4 | MAN | 2 | 0 |
| 6 | r | 2 | NAG | 3 | 0 |
| 6 | DA | 1 | NAG | 2 | 0 |
| 5 | l | 3 | BMA | 1 | 0 |
| 4 | RA | 1 | NAG | 1 | 0 |
| 5 | l | 4 | MAN | 1 | 0 |
| 4 | q | 2 | NAG | 7 | 0 |
| 4 | i | 2 | NAG | 1 | 0 |
| 4 | OA | 2 | NAG | 1 | 0 |
| 6 | GA | 3 | BMA | 2 | 0 |
| 4 | HA | 2 | NAG | 2 | 0 |
| 5 | FA | 1 | NAG | 1 | 0 |
| 6 | DA | 2 | NAG | 2 | 0 |
| 6 | w | 1 | NAG | 2 | 0 |
| 6 | LA | 3 | BMA | 1 | 0 |
| 4 | BA | 1 | NAG | 3 | 0 |
| 6 | 5 | 2 | NAG | 2 | 0 |
| 6 | k | 2 | NAG | 1 | 0 |
| 4 | OA | 1 | NAG | 2 | 0 |
| 6 | LA | 2 | NAG | 5 | 0 |
| 6 | CA | 1 | NAG | 2 | 0 |
| 6 | GA | 1 | NAG | 7 | 0 |
| 4 | v | 2 | NAG | 2 | 0 |
| 4 | 7 | 1 | NAG | 6 | 0 |
| 4 | 7 | 2 | NAG | 6 | 0 |
| 7 | z | 3 | BMA | 2 | 0 |

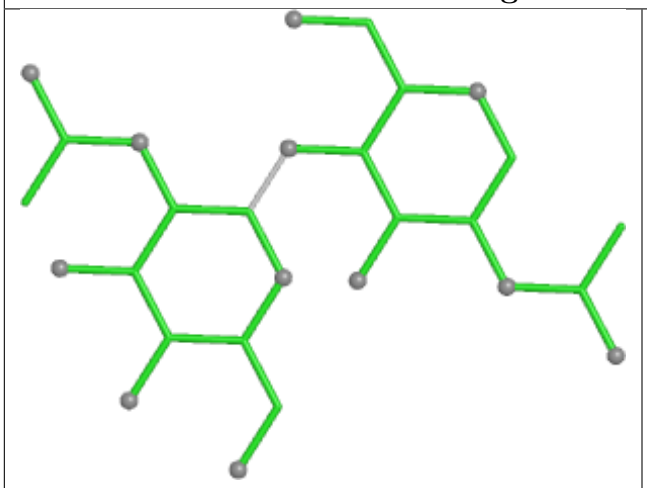
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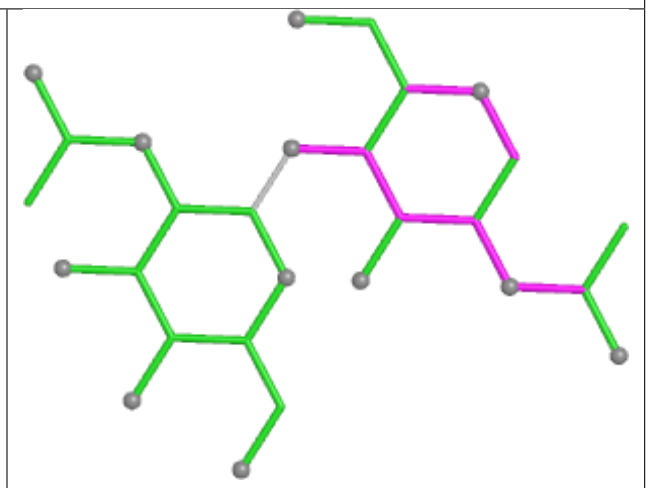
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | MA | 2 | NAG | 5 | 0 |
| 4 | 9 | 1 | NAG | 2 | 0 |
| 4 | 2 | 1 | NAG | 1 | 0 |
| 5 | l | 2 | NAG | 1 | 0 |
| 5 | KA | 1 | NAG | 1 | 0 |
| 6 | 3 | 1 | NAG | 3 | 0 |
| 6 | NA | 2 | NAG | 2 | 0 |
| 5 | FA | 3 | BMA | 1 | 0 |
| 4 | t | 1 | NAG | 1 | 0 |
| 4 | i | 1 | NAG | 3 | 0 |
| 4 | MA | 1 | NAG | 7 | 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.

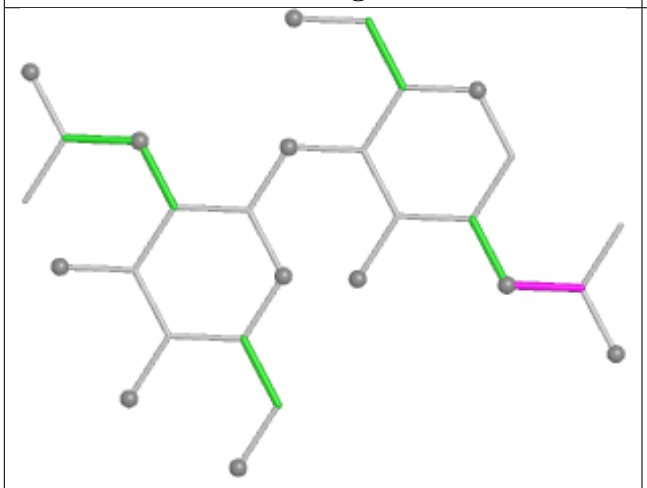
**Oligosaccharide Chain e**



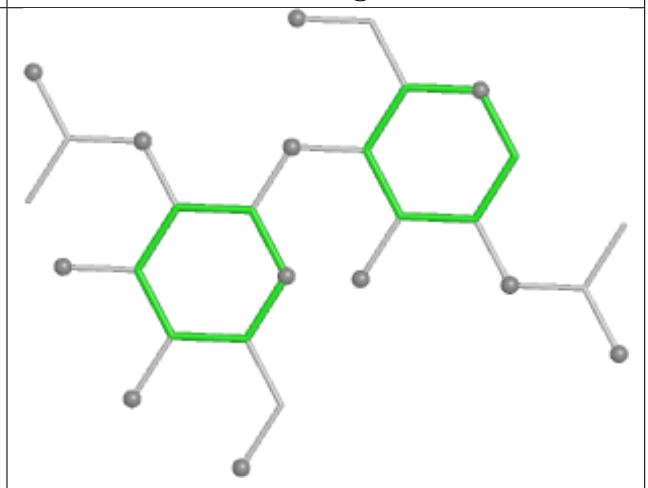
**Bond lengths**



**Bond angles**

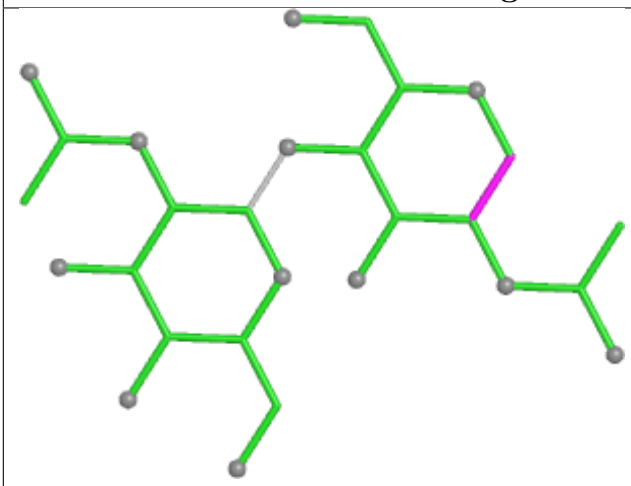


**Torsions**

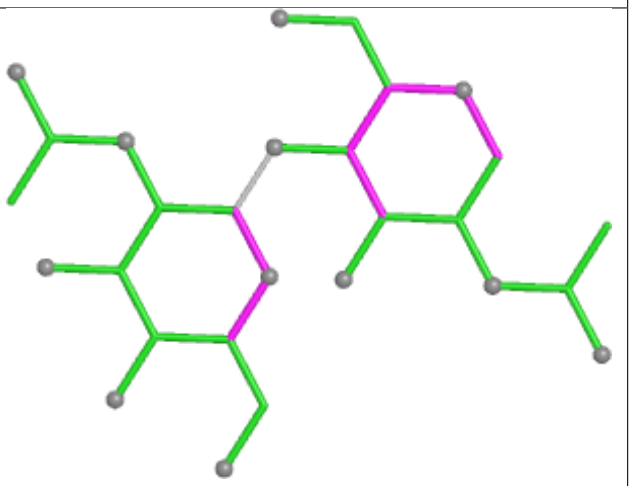


**Rings**

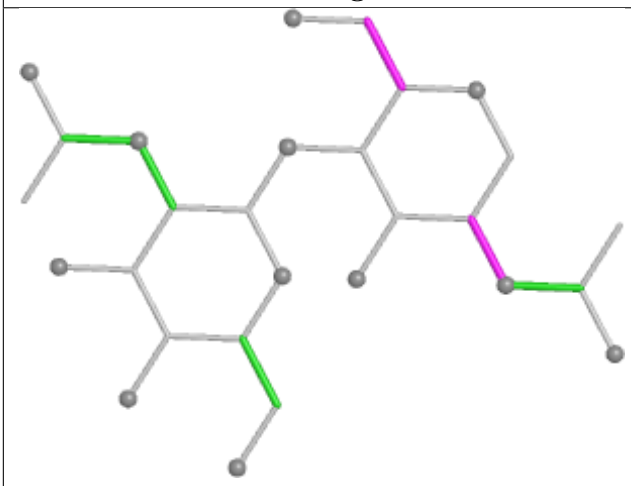
**Oligosaccharide Chain f**



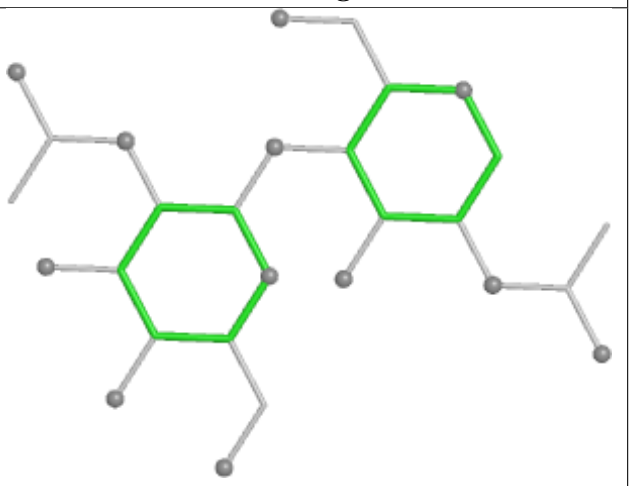
**Bond lengths**



**Bond angles**

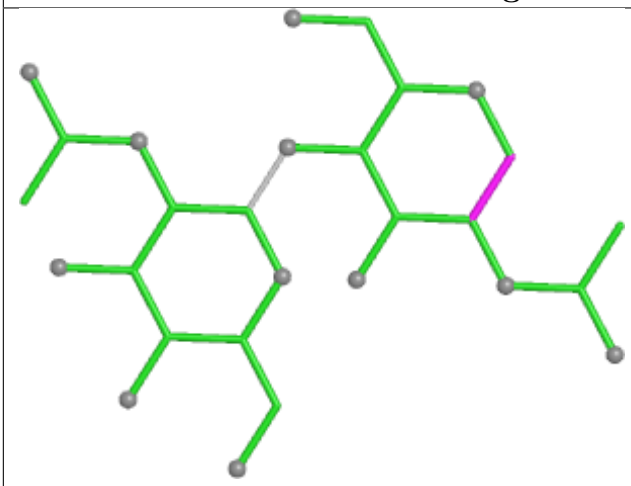


**Torsions**

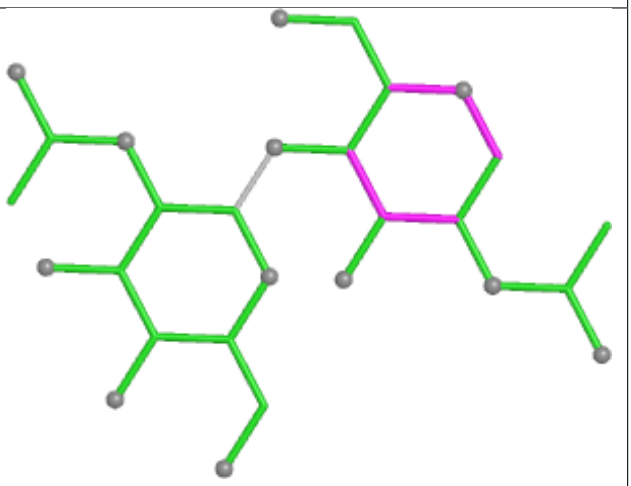


**Rings**

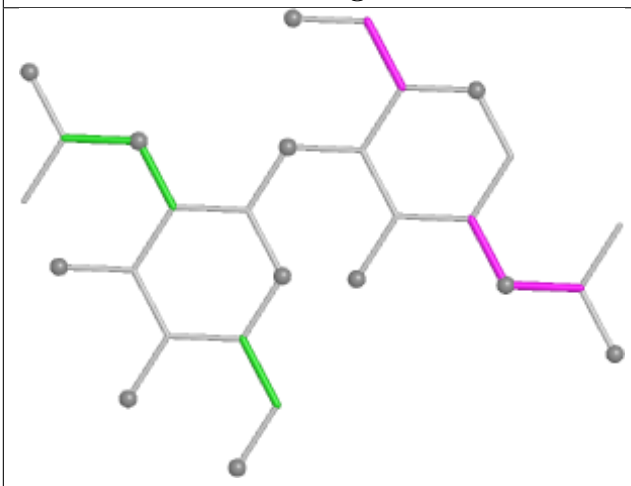
**Oligosaccharide Chain i**



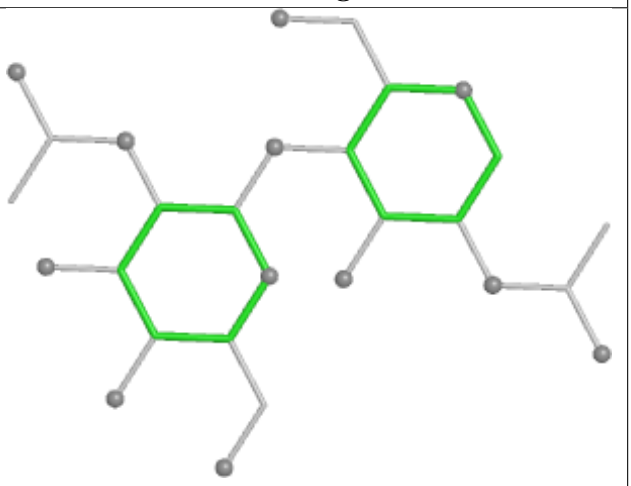
**Bond lengths**



**Bond angles**

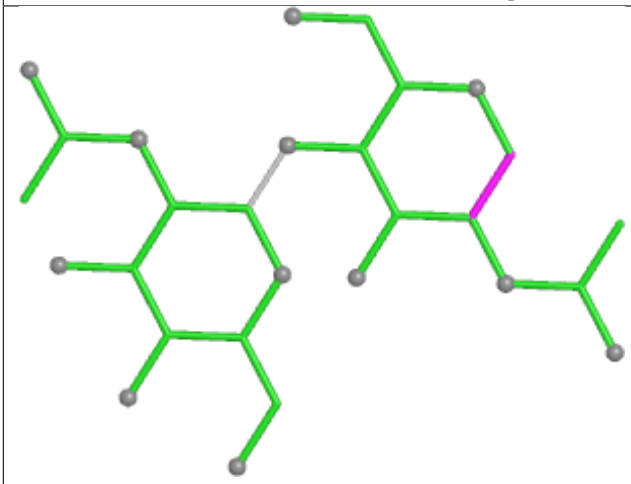


**Torsions**

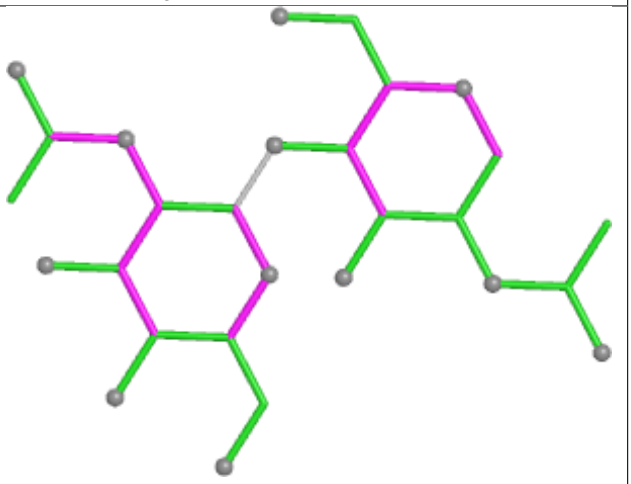


**Rings**

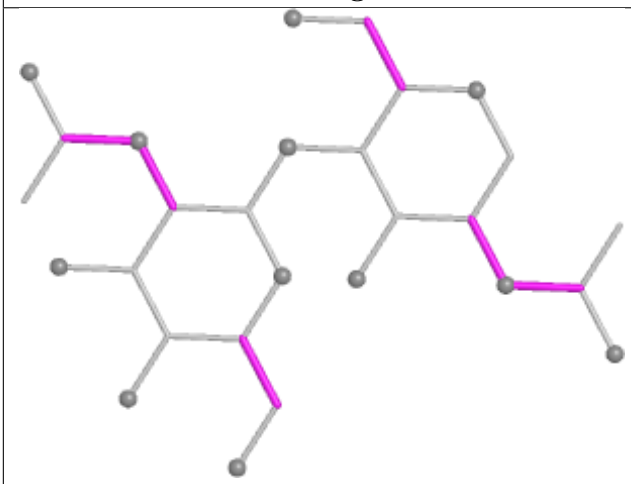
**Oligosaccharide Chain j**



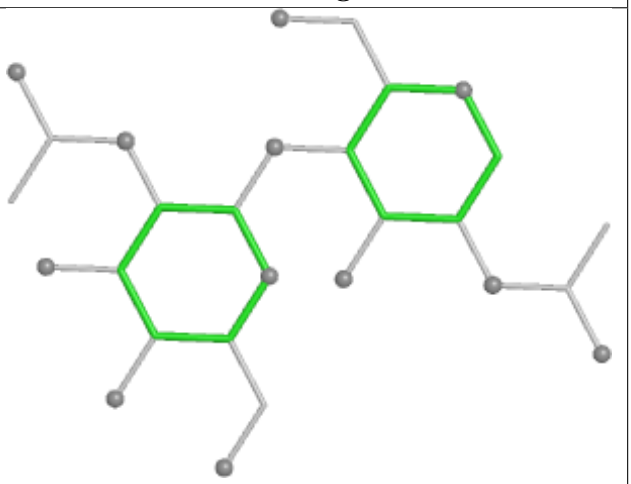
**Bond lengths**



**Bond angles**

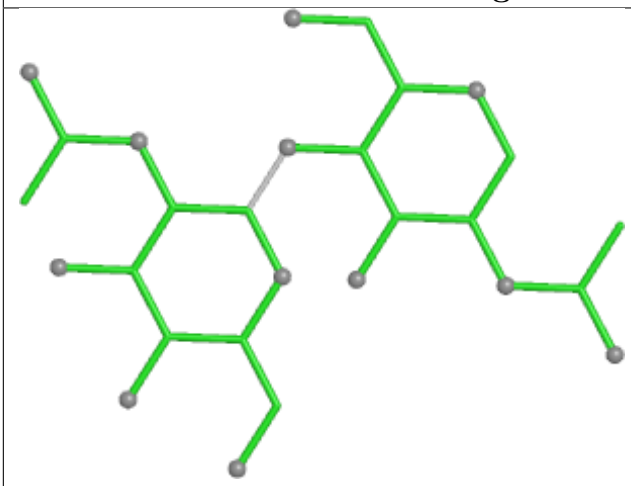


**Torsions**

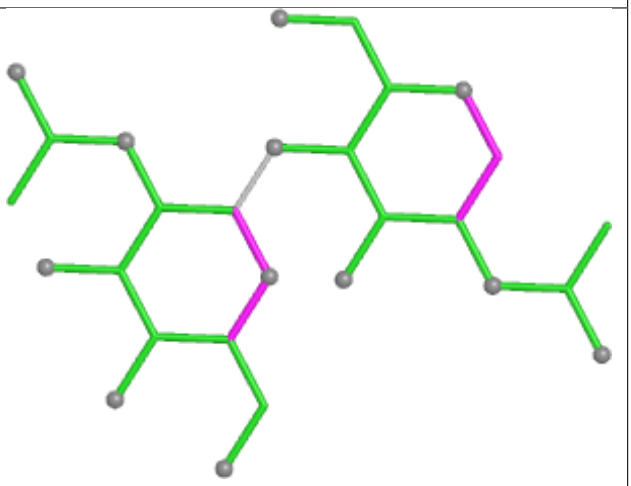


**Rings**

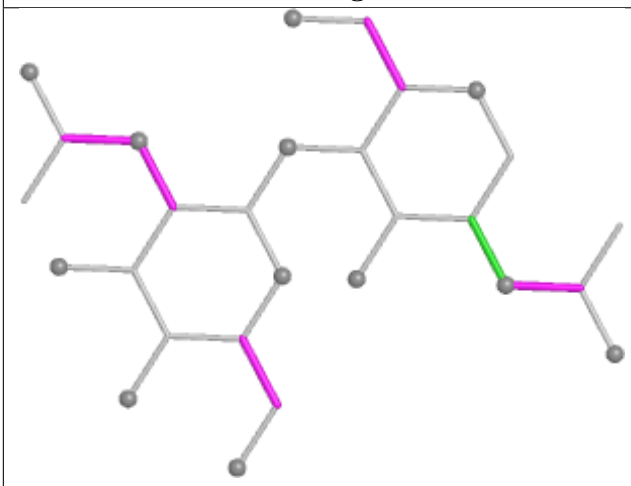
**Oligosaccharide Chain m**



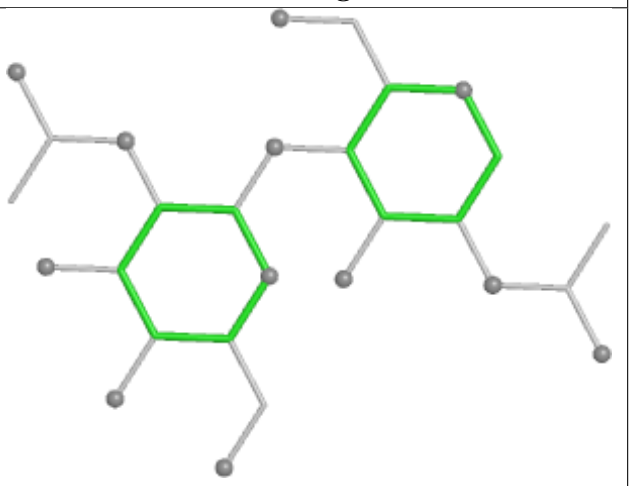
**Bond lengths**



**Bond angles**

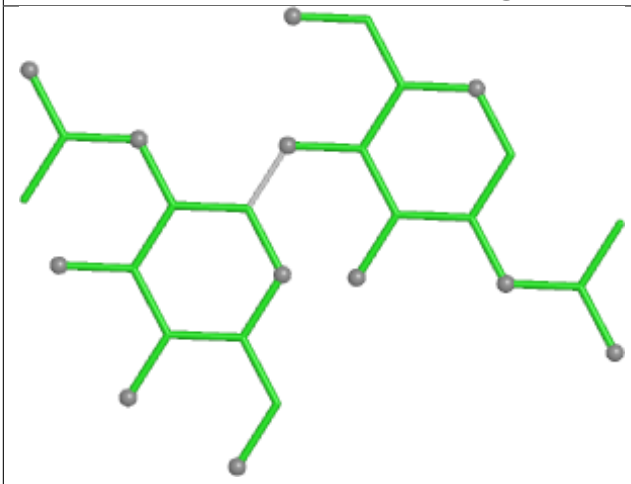


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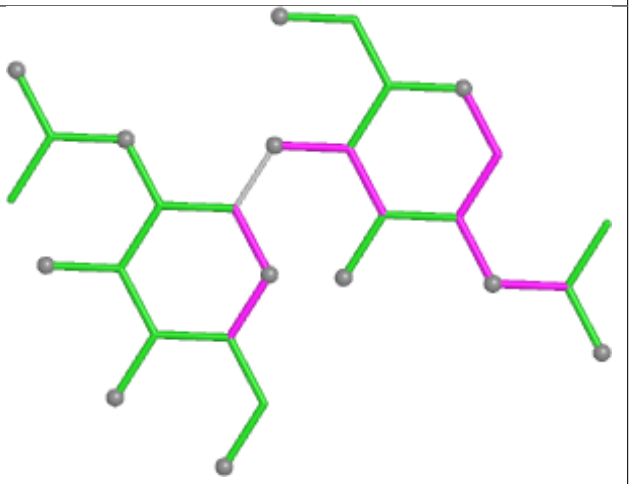


**Rings**

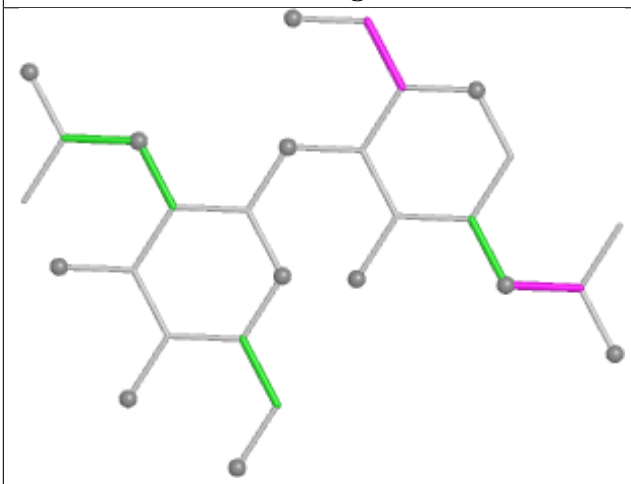
**Oligosaccharide Chain n**



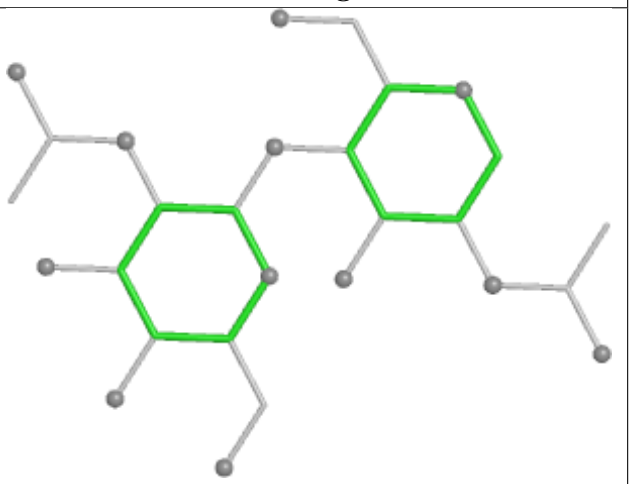
**Bond lengths**



**Bond angles**

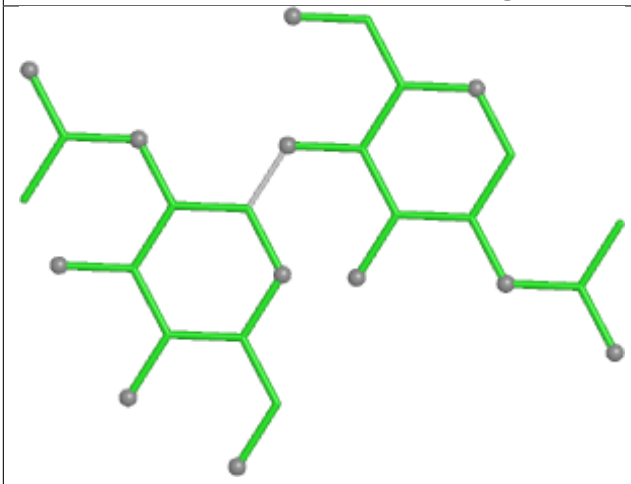


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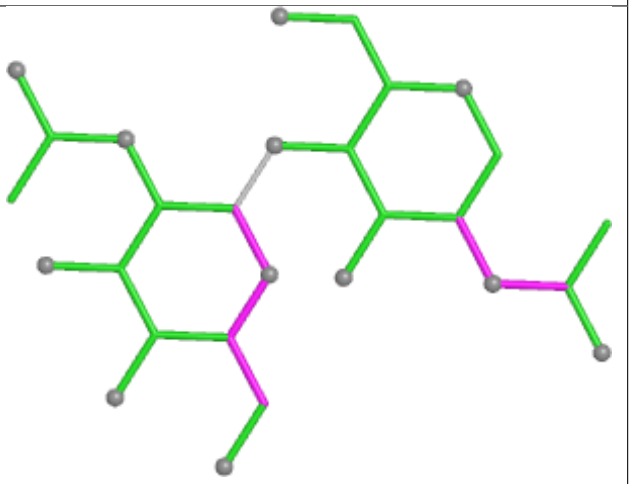


**Rings**

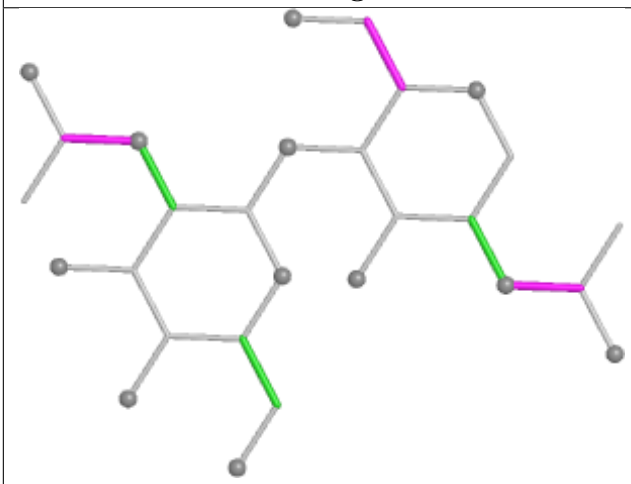
**Oligosaccharide Chain o**



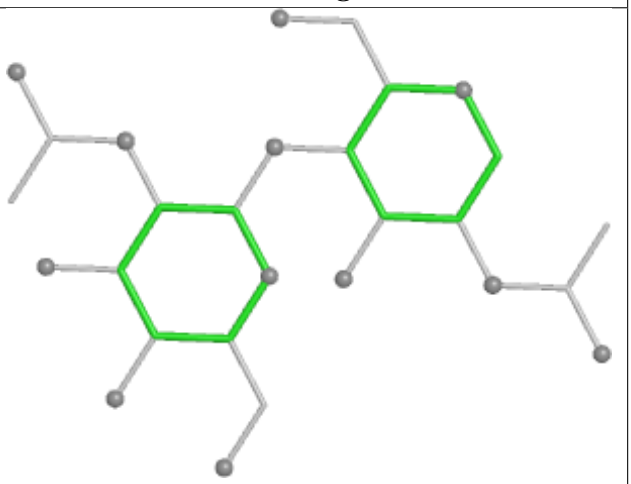
**Bond lengths**



**Bond angles**

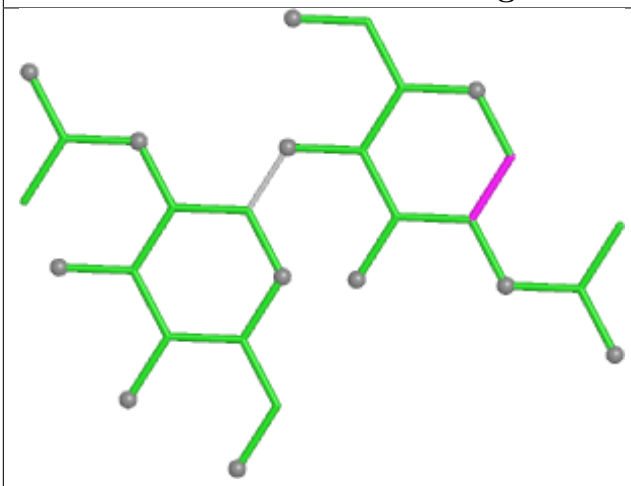


**Torsions**

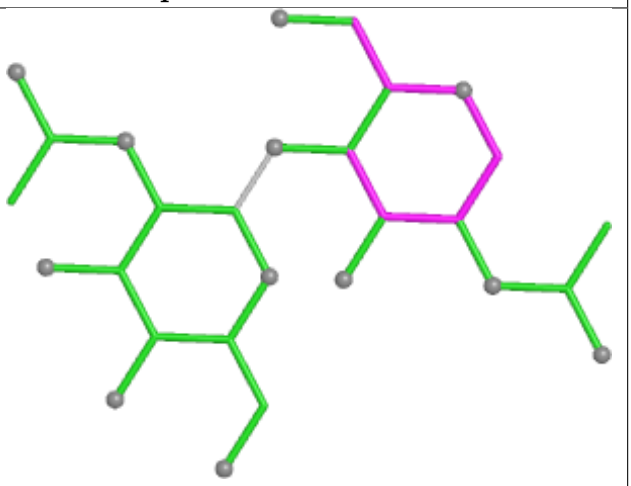


**Rings**

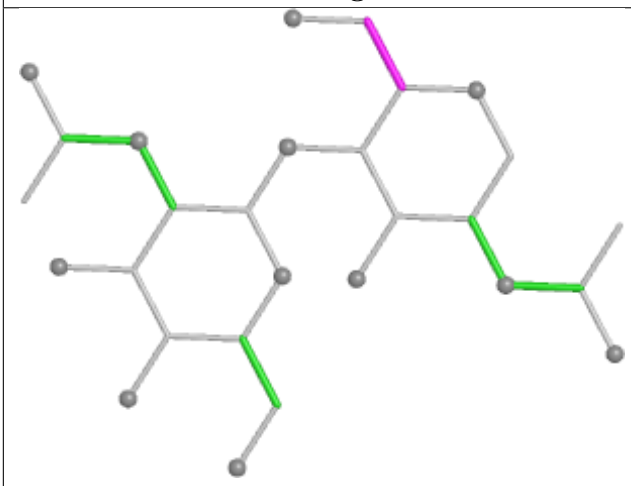
**Oligosaccharide Chain p**



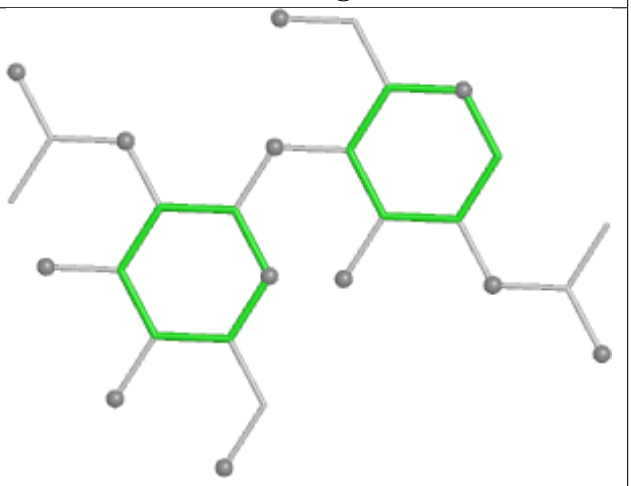
**Bond lengths**



**Bond angles**

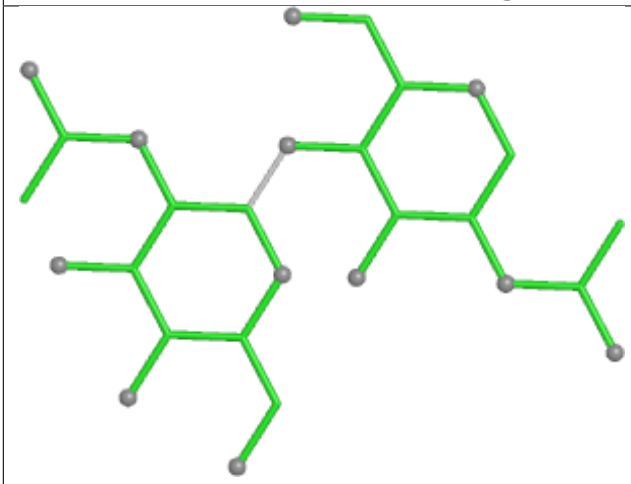


**Torsions**

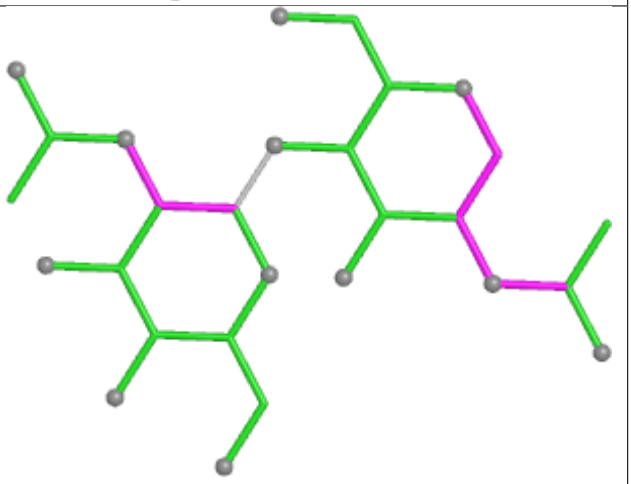


**Rings**

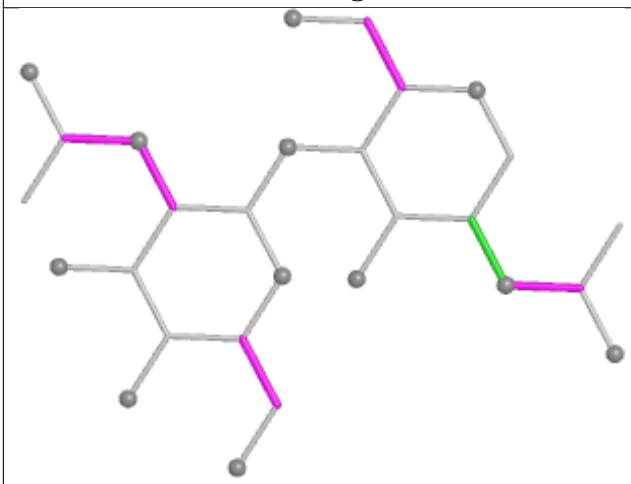
**Oligosaccharide Chain q**



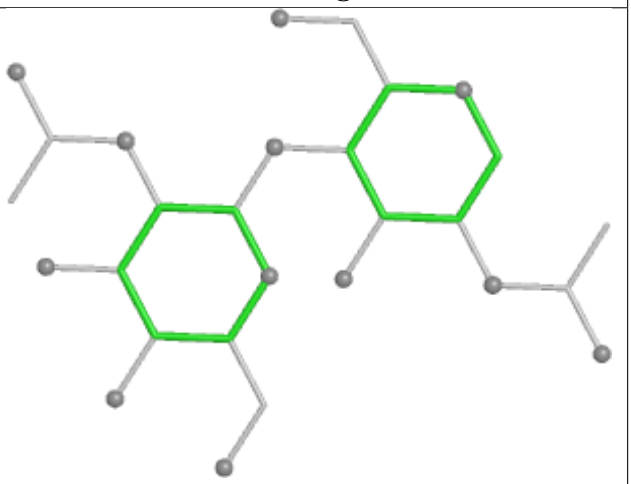
**Bond lengths**



**Bond angles**

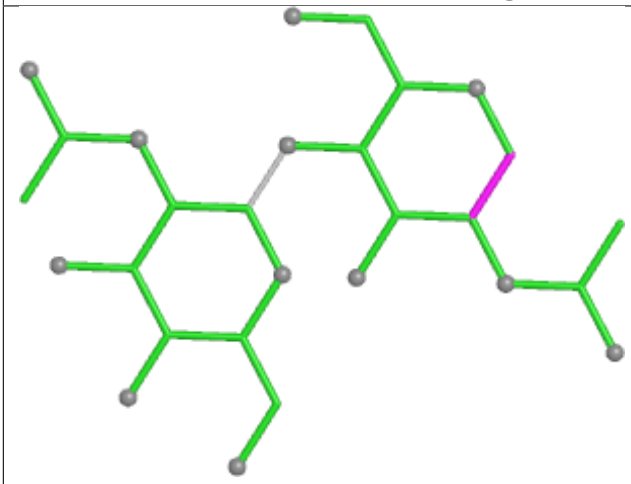


**Torsions**

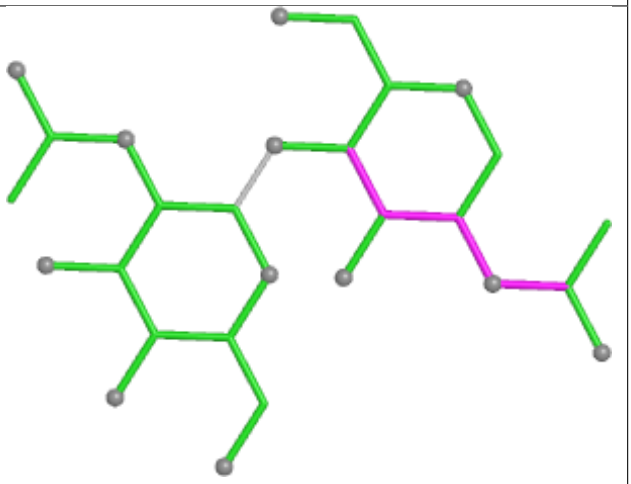


**Rings**

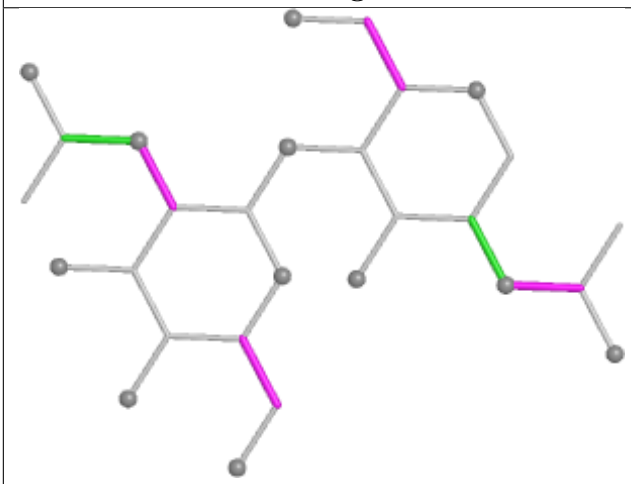
**Oligosaccharide Chain s**



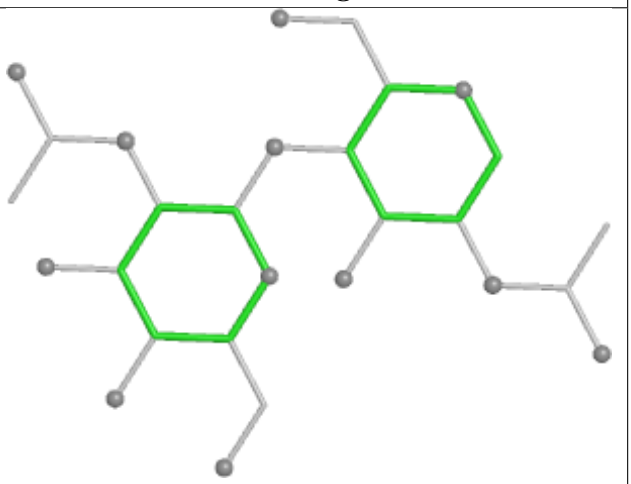
**Bond lengths**



**Bond angles**

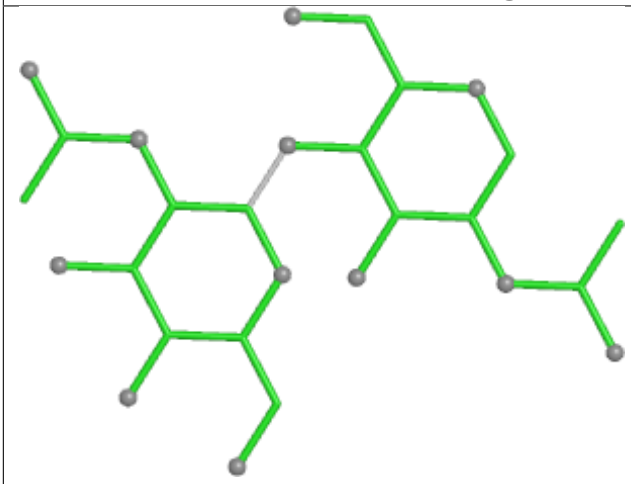


**Torsions**

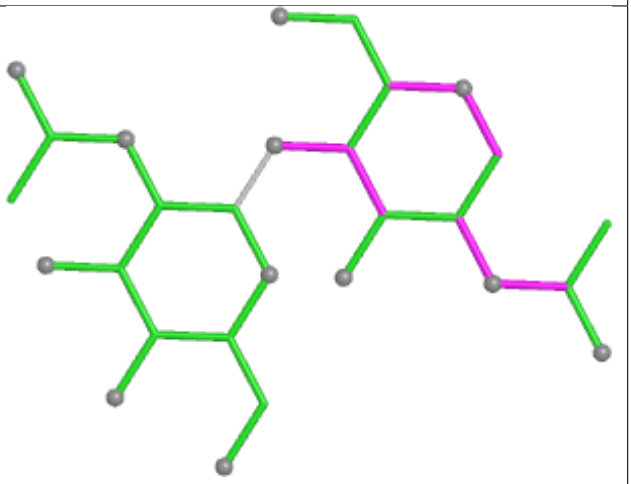


**Rings**

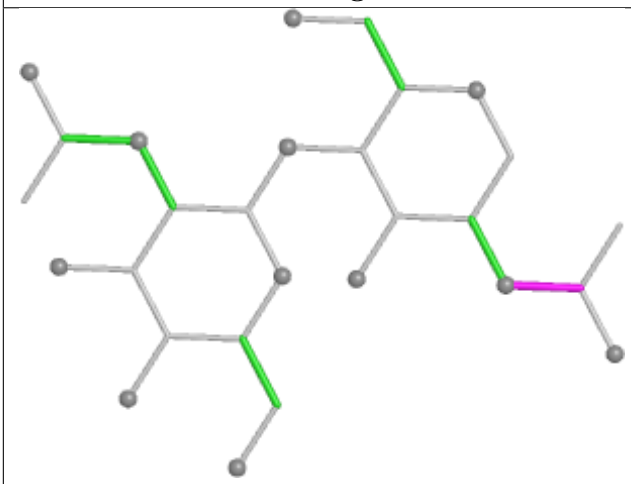
**Oligosaccharide Chain t**



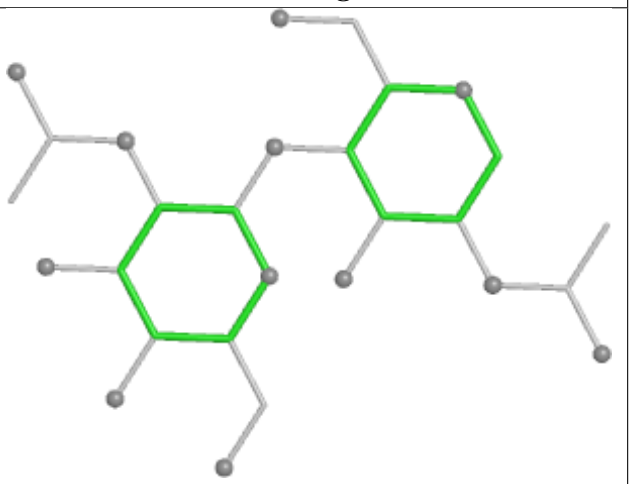
**Bond lengths**



**Bond angles**

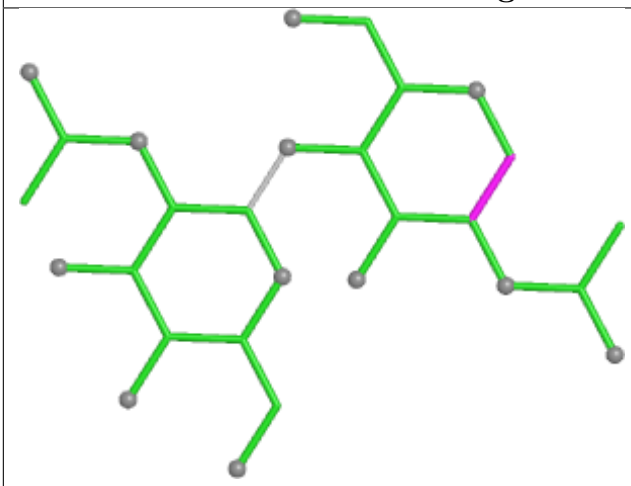


**Torsions**

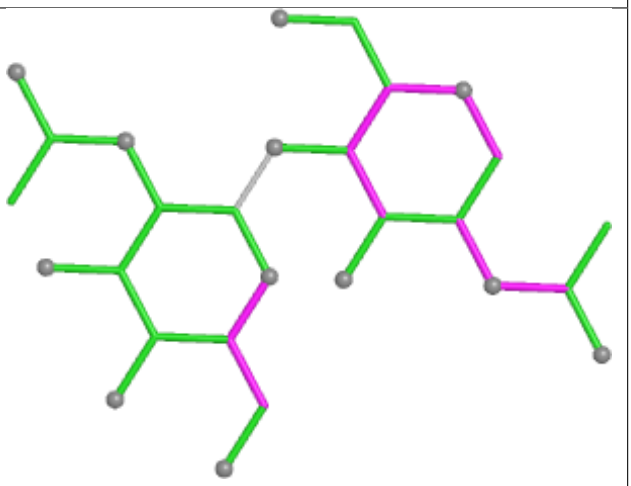


**Rings**

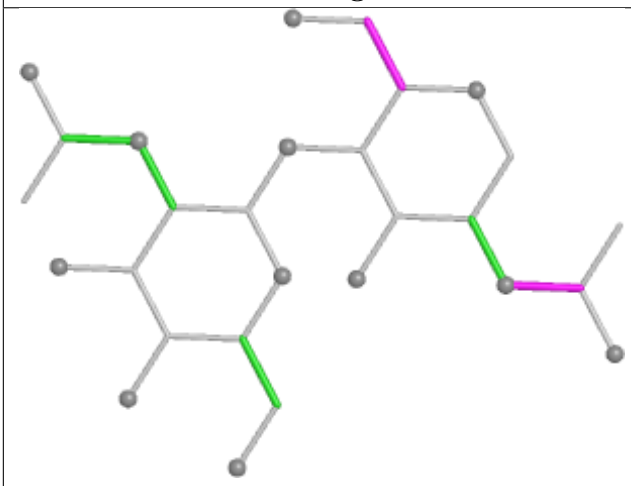
**Oligosaccharide Chain u**



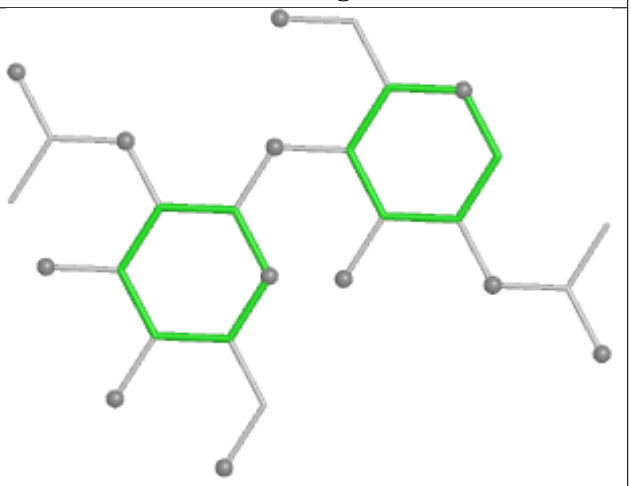
**Bond lengths**



**Bond angles**

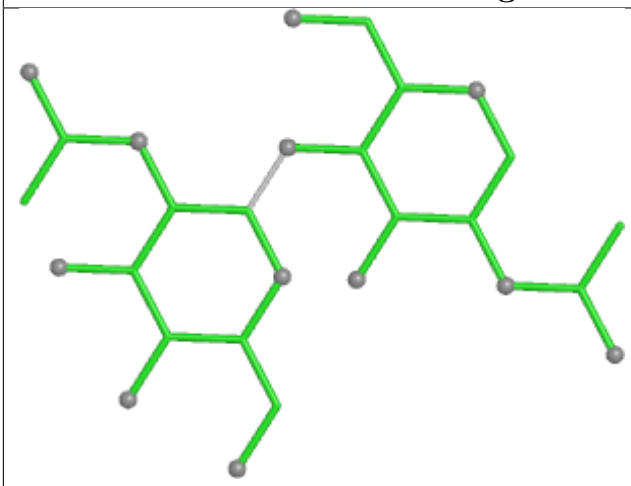


**Torsions**

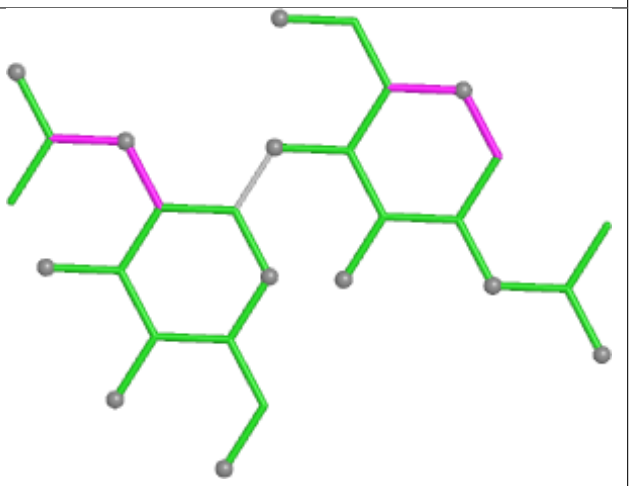


**Rings**

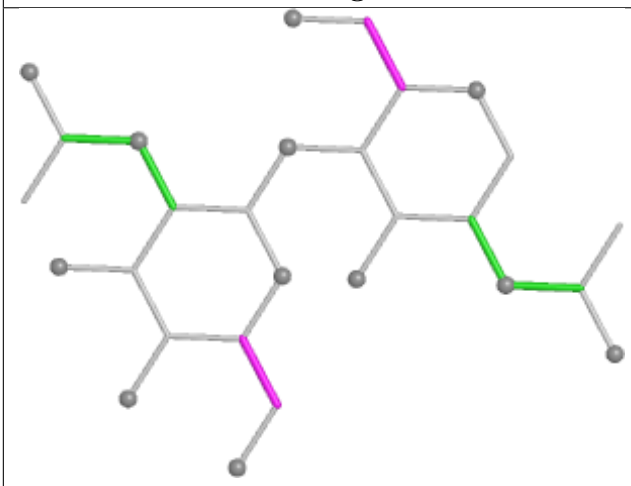
**Oligosaccharide Chain v**



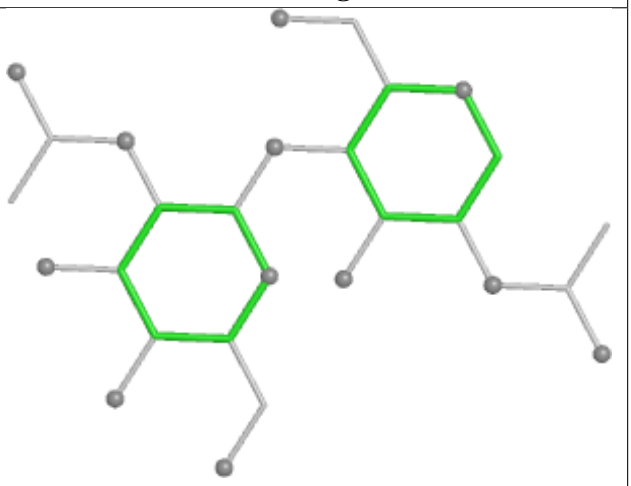
**Bond lengths**



**Bond angles**

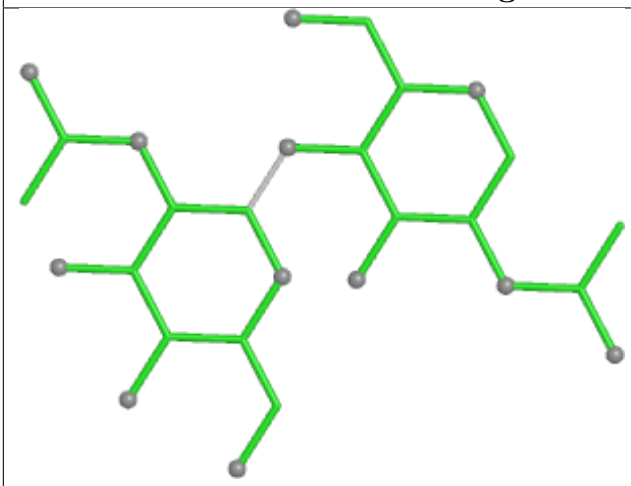


**Torsions**

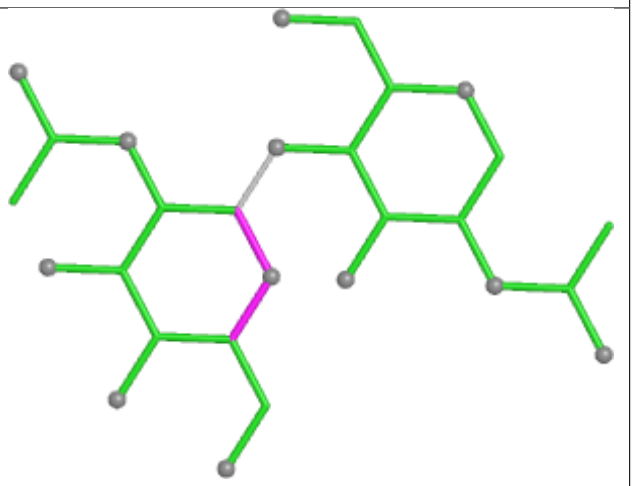


**Rings**

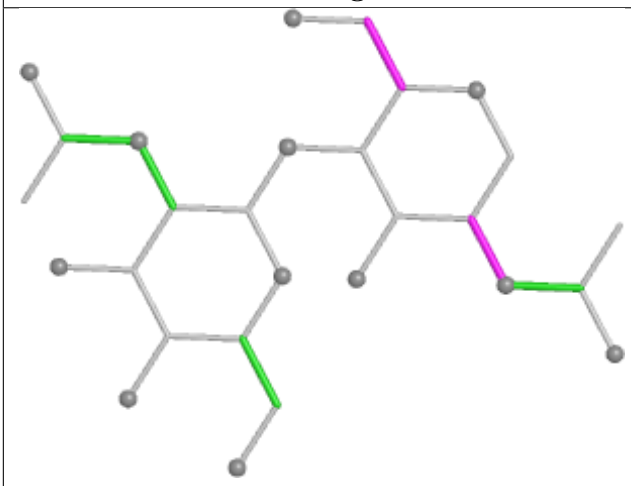
**Oligosaccharide Chain x**



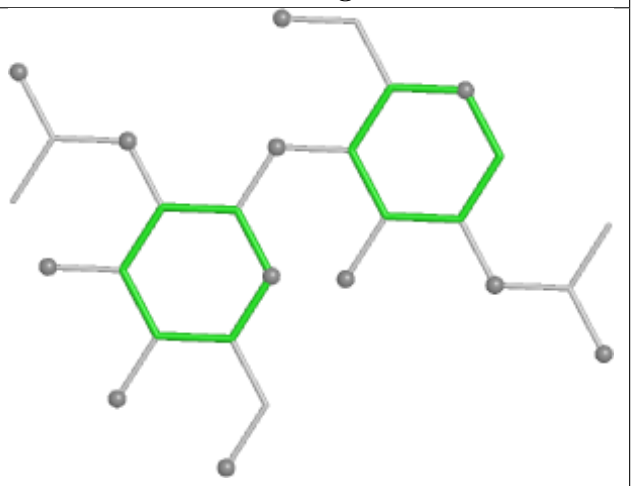
**Bond lengths**



**Bond angles**

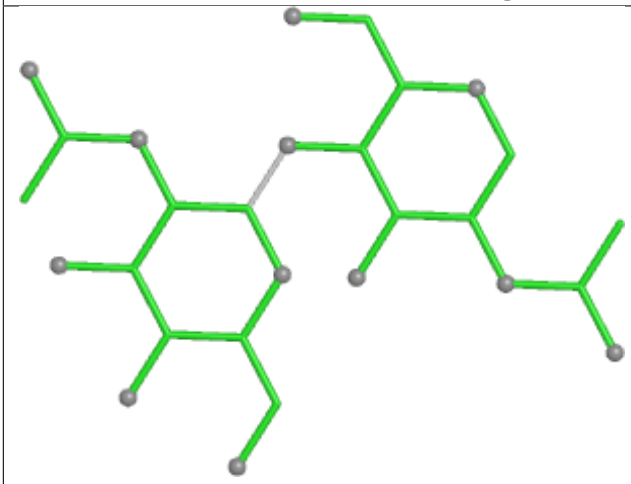


**Torsions**

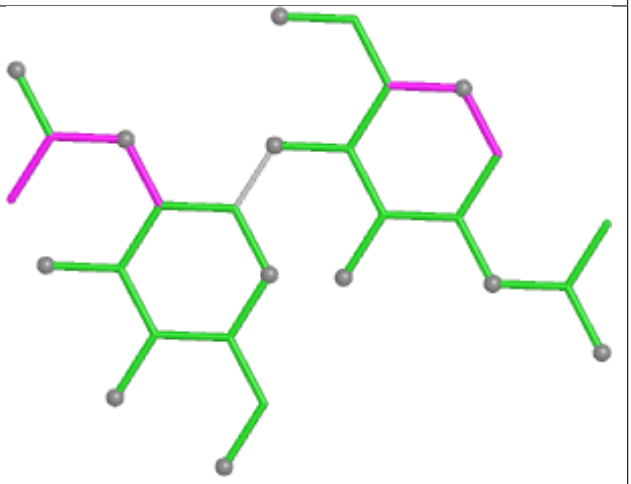


**Rings**

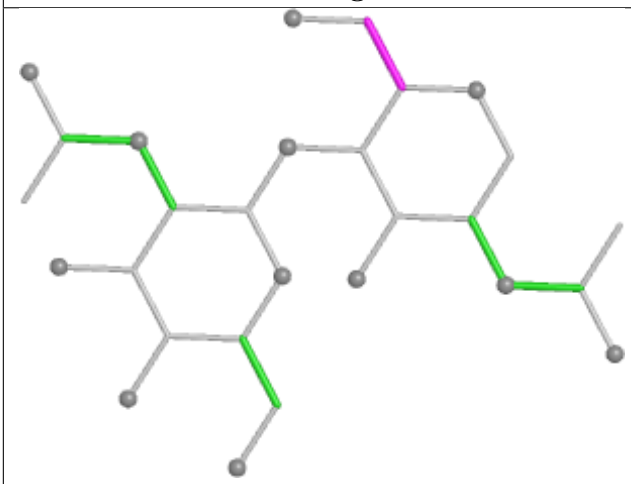
**Oligosaccharide Chain 1**



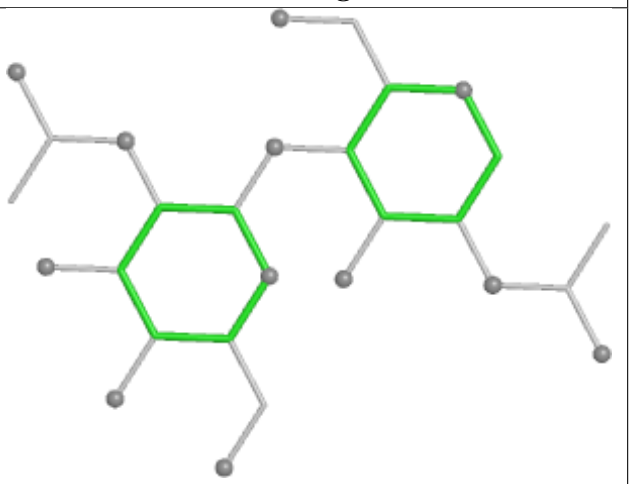
**Bond lengths**



**Bond angles**

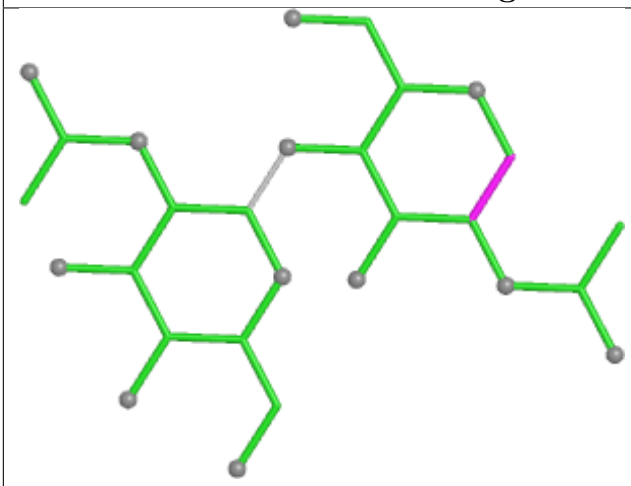


**Torsions**

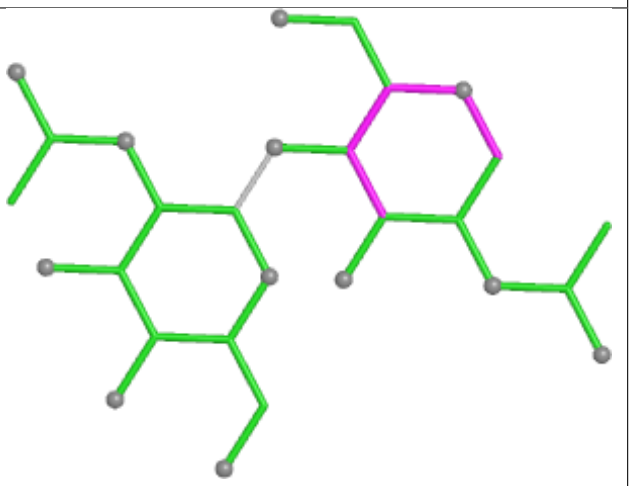


**Rings**

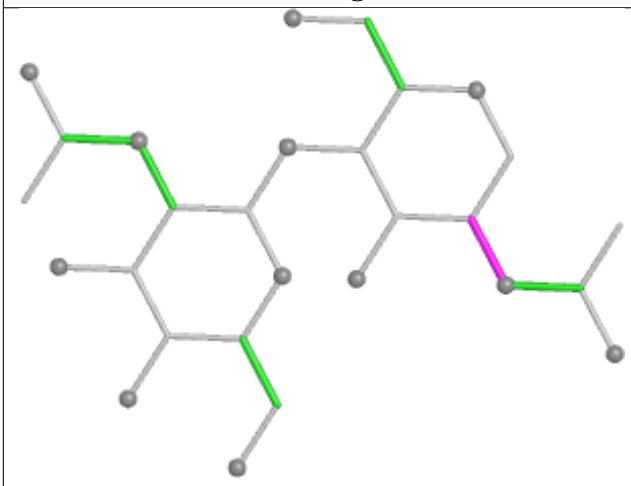
**Oligosaccharide Chain 2**



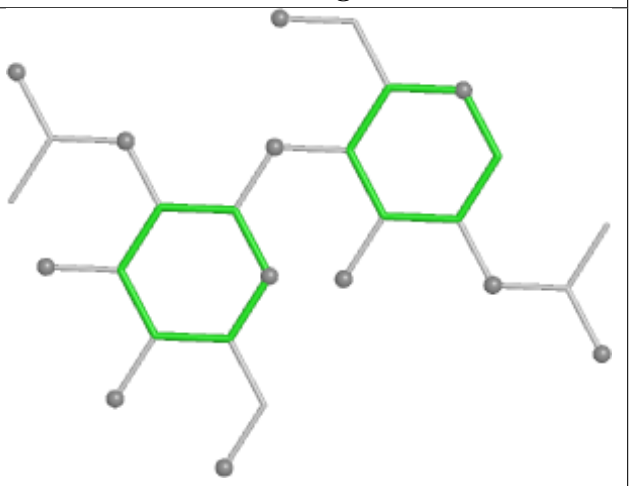
**Bond lengths**



**Bond angles**

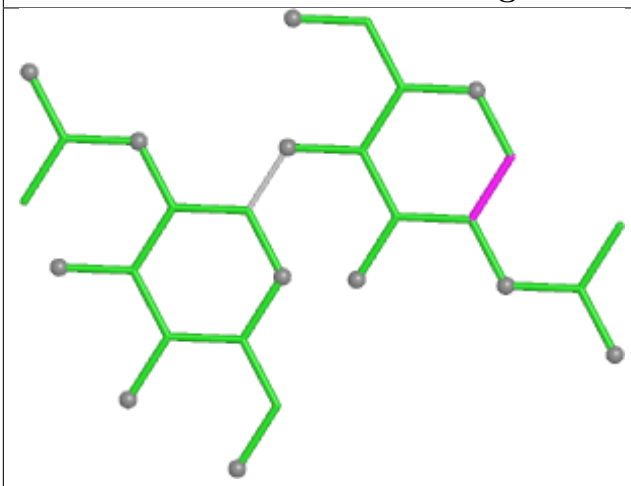


**Torsions**

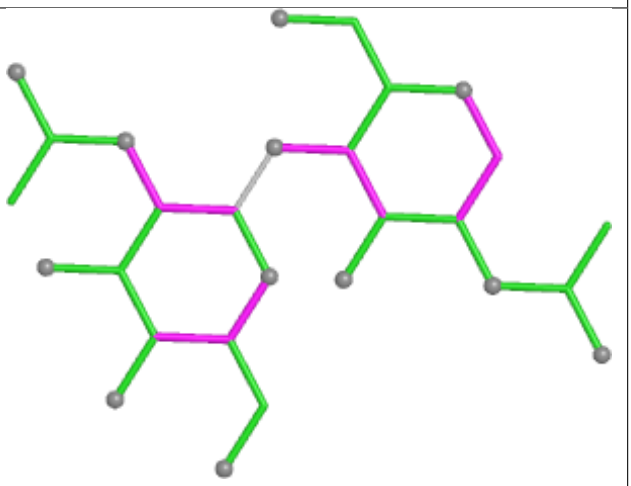


**Rings**

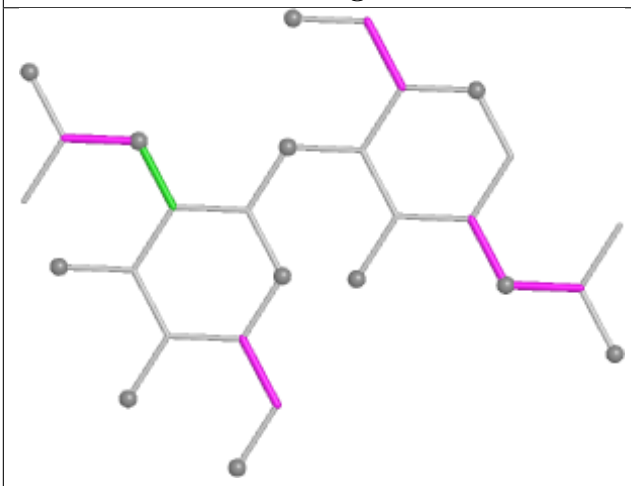
**Oligosaccharide Chain 4**



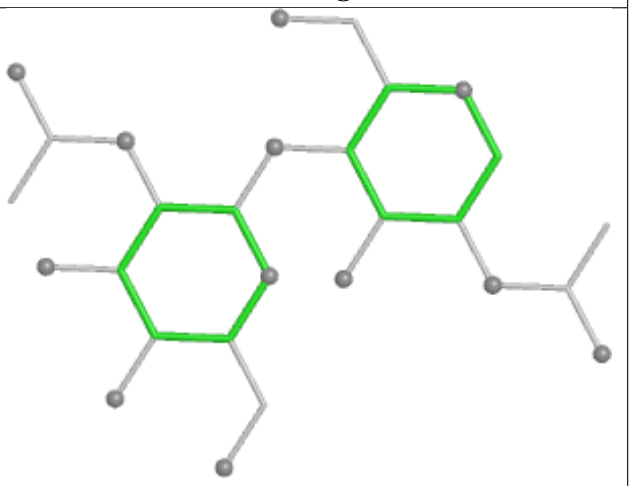
**Bond lengths**



**Bond angles**

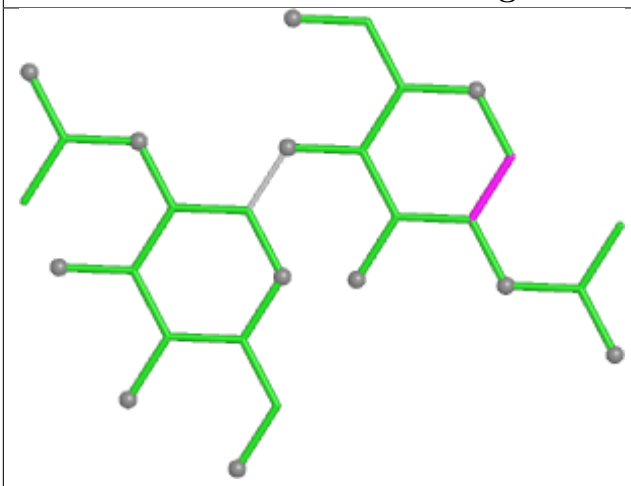


**Torsions**

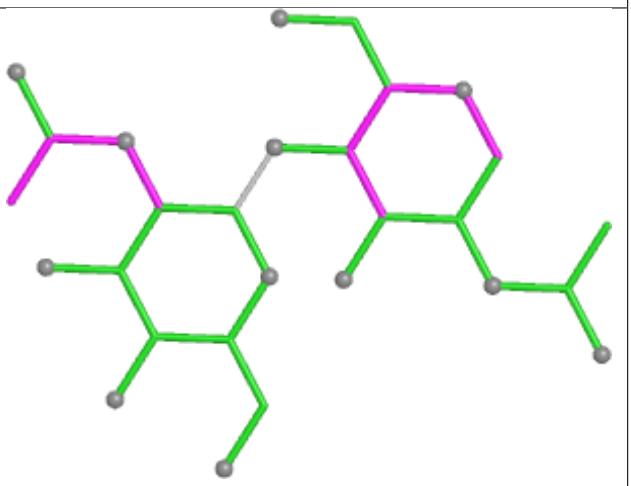


**Rings**

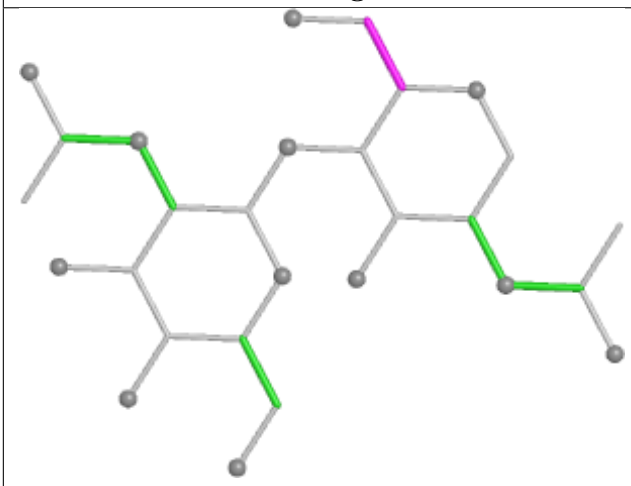
**Oligosaccharide Chain 6**



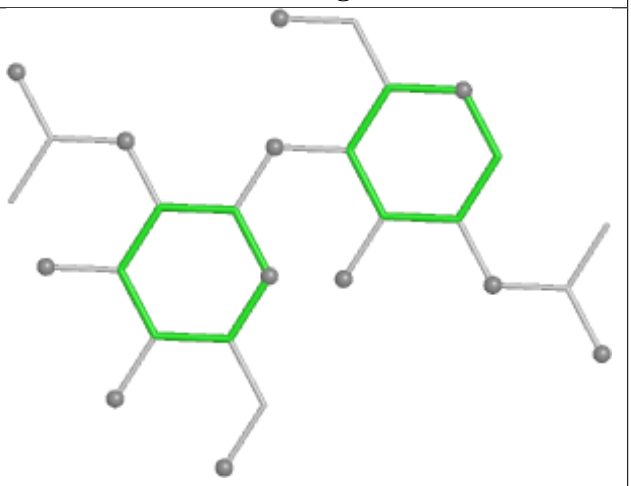
**Bond lengths**



**Bond angles**

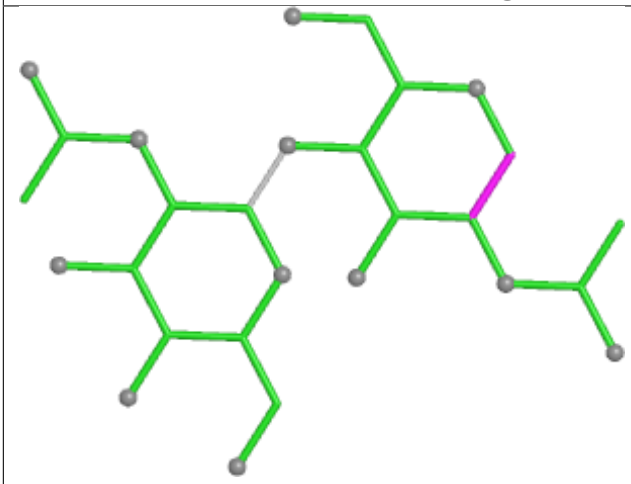


**Torsions**

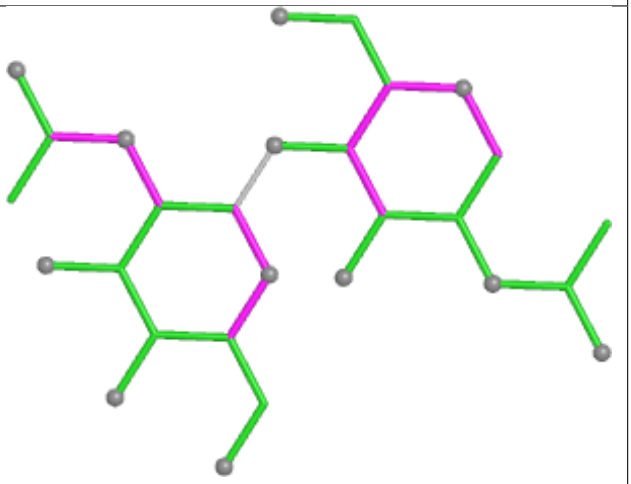


**Rings**

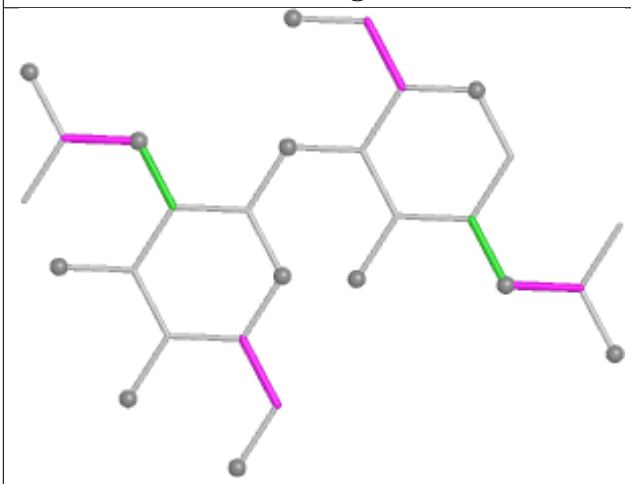
**Oligosaccharide Chain 7**



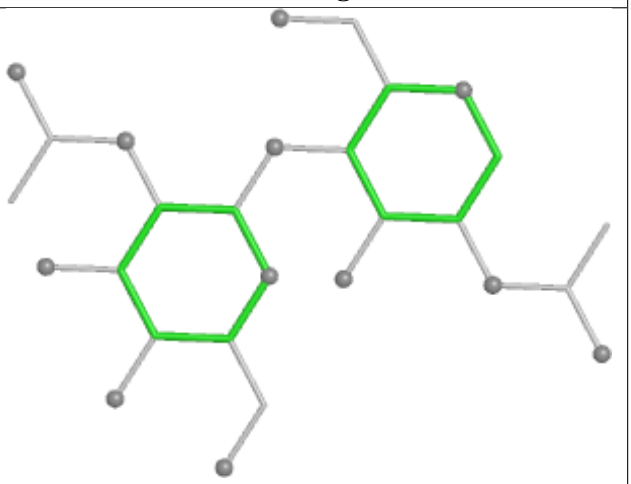
**Bond lengths**



**Bond angles**

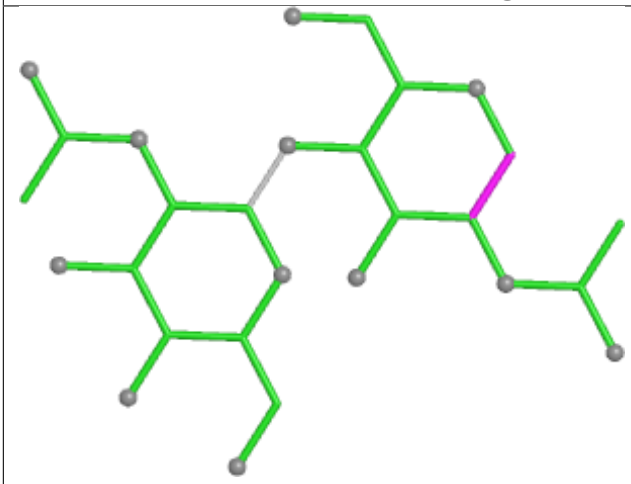


**Torsions**

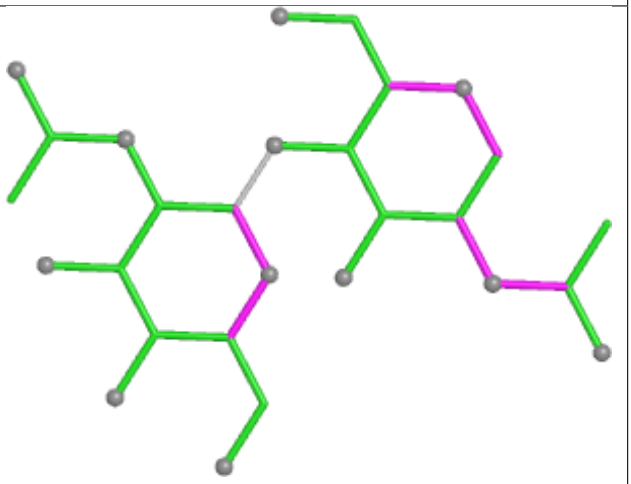


**Rings**

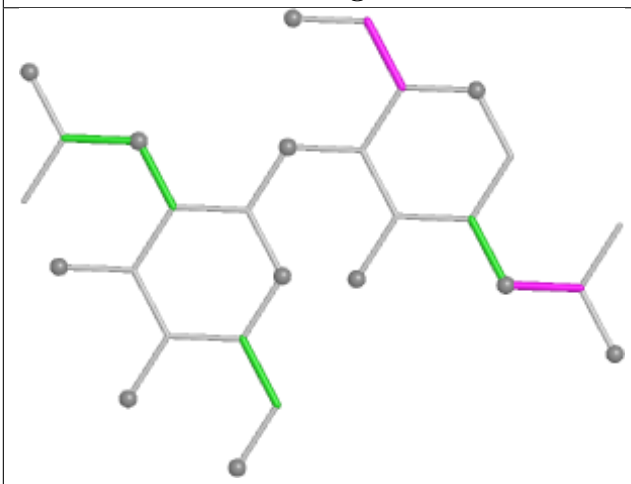
**Oligosaccharide Chain 8**



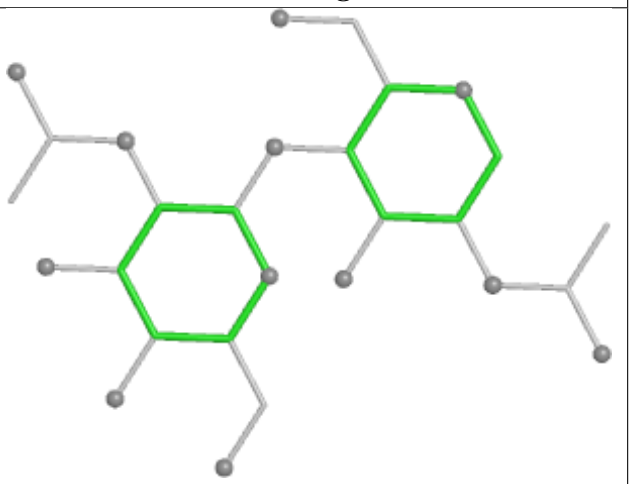
**Bond lengths**



**Bond angles**

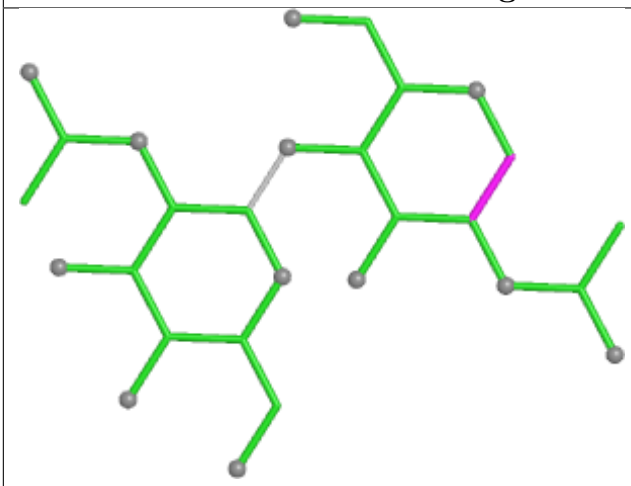


**Torsions**

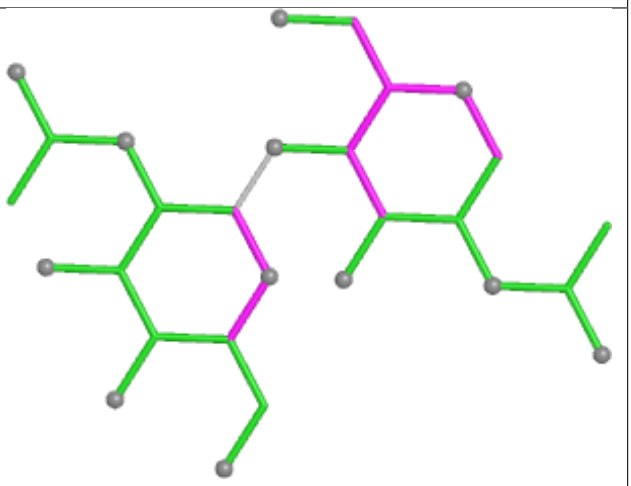


**Rings**

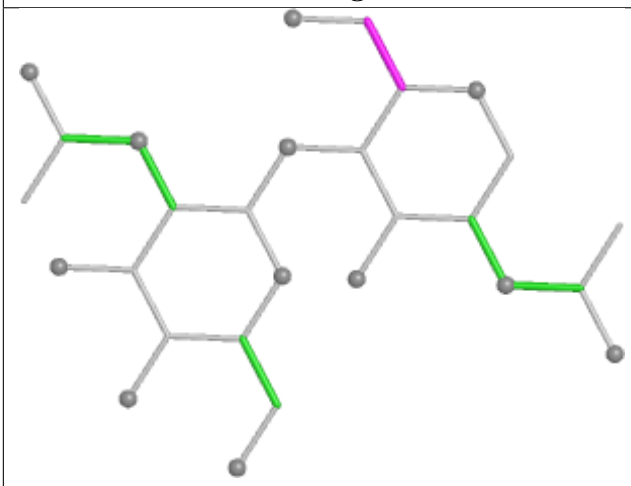
**Oligosaccharide Chain 9**



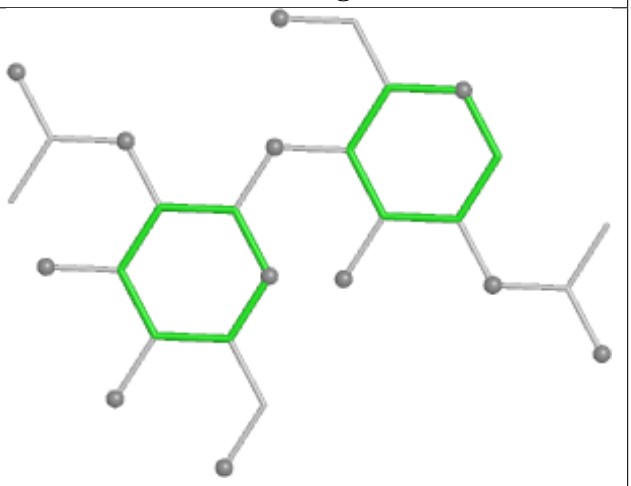
**Bond lengths**



**Bond angles**

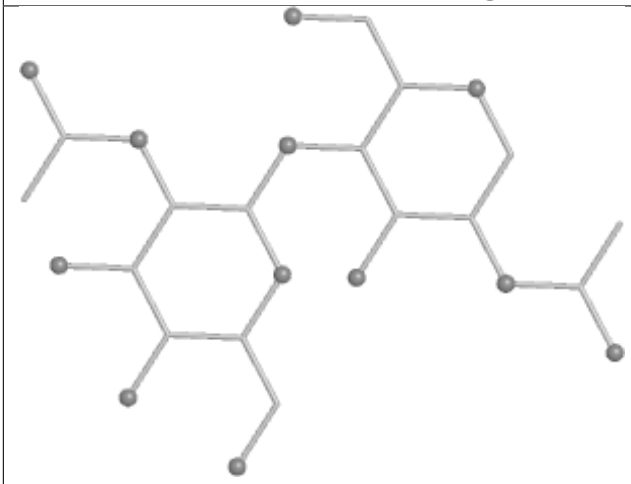


**Torsions**

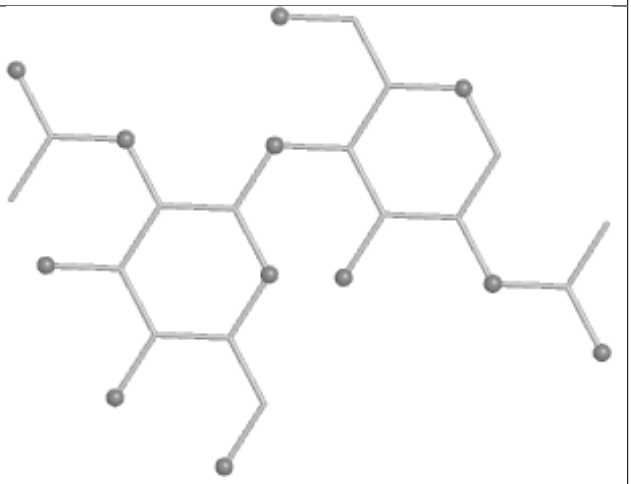


**Rings**

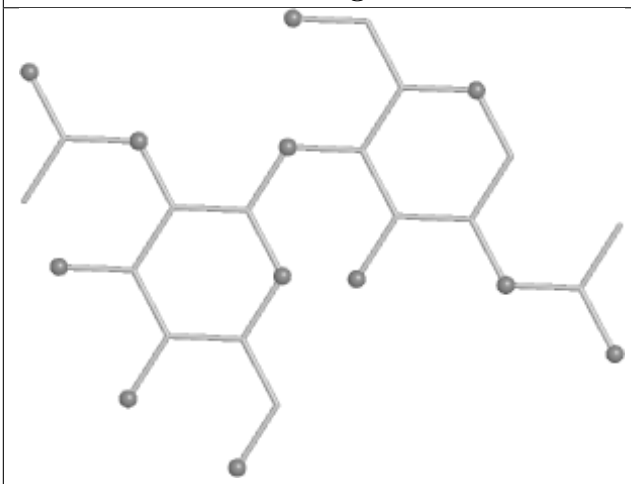
**Oligosaccharide Chain BA**



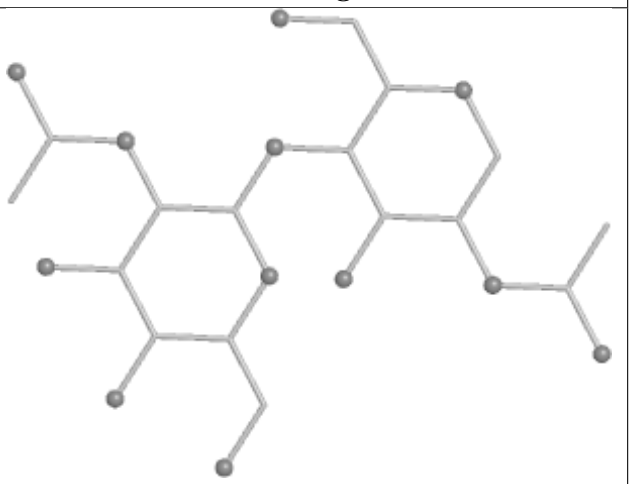
**Bond lengths**



**Bond angles**

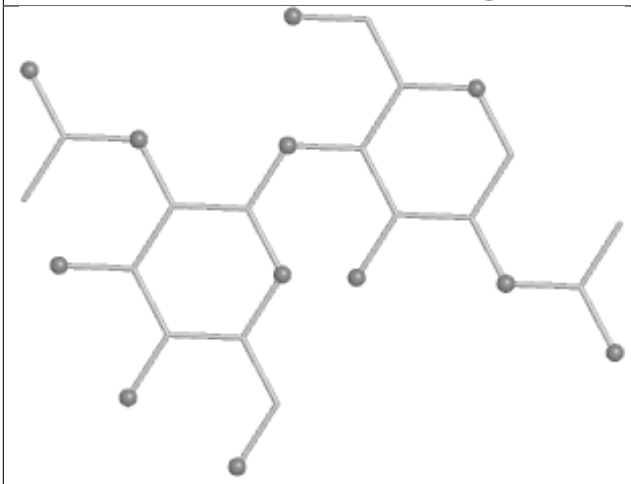


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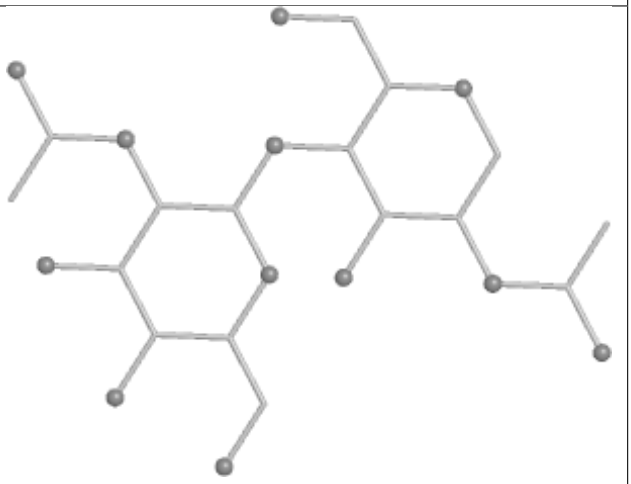


**Rings**

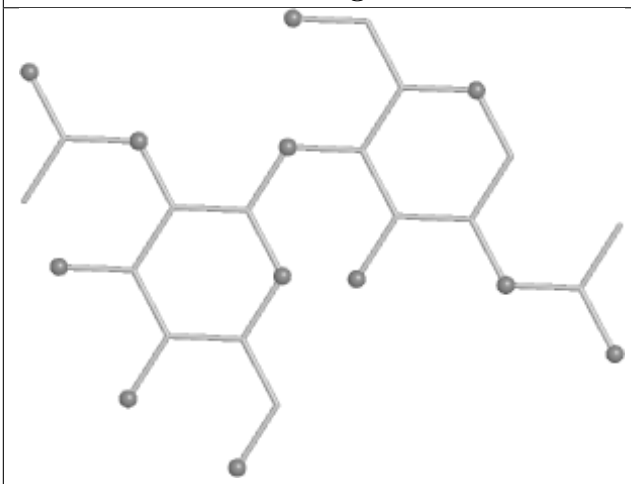
**Oligosaccharide Chain HA**



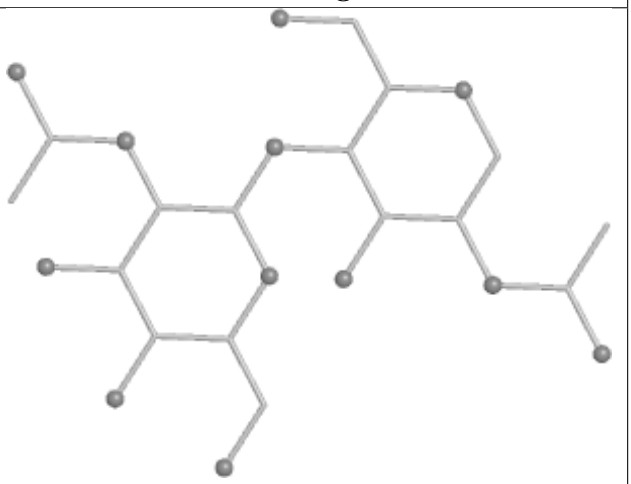
**Bond lengths**



**Bond angles**

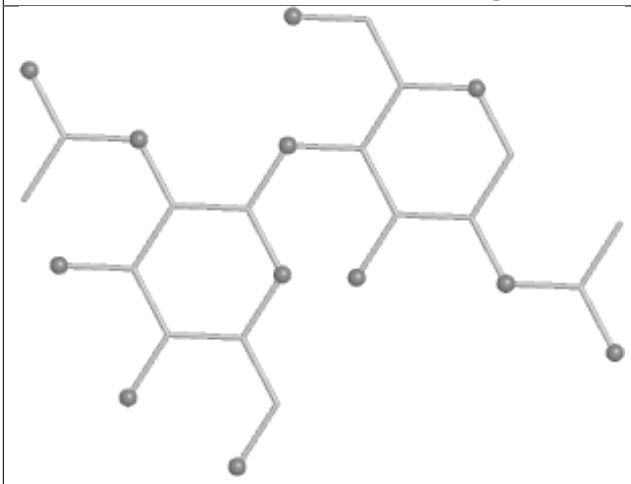


**Torsions**

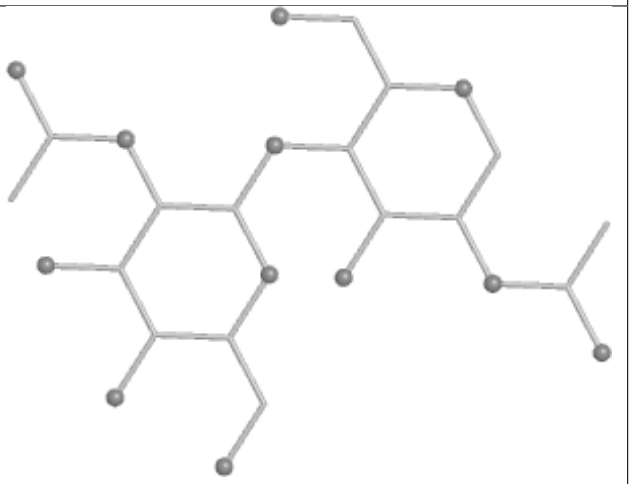


**Rings**

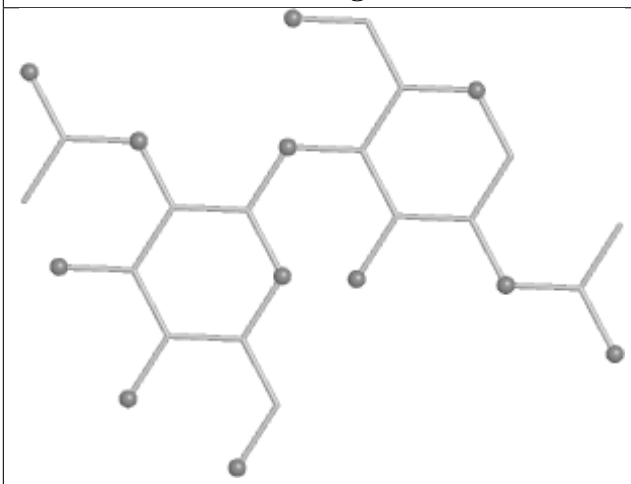
**Oligosaccharide Chain IA**



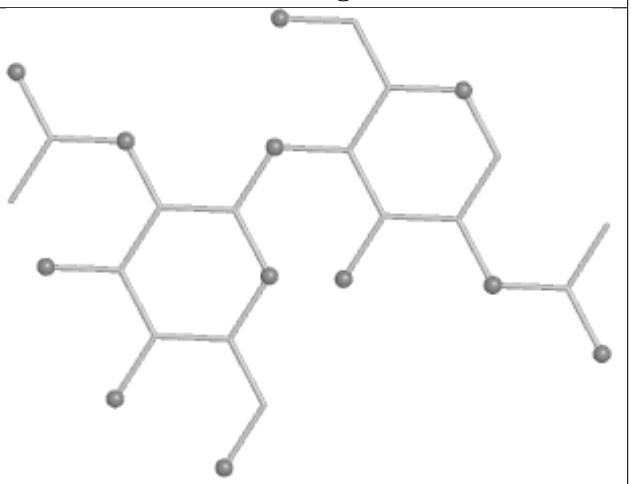
**Bond lengths**



**Bond angles**

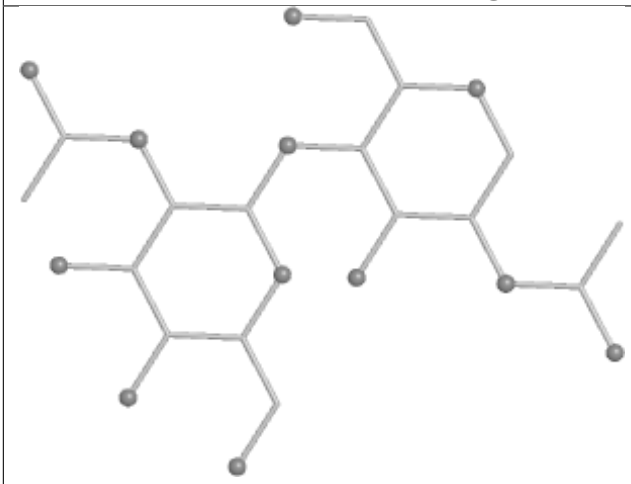


**Torsions**

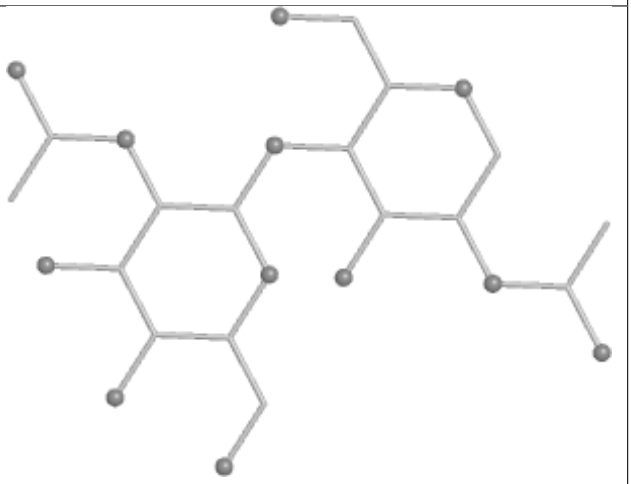


**Rings**

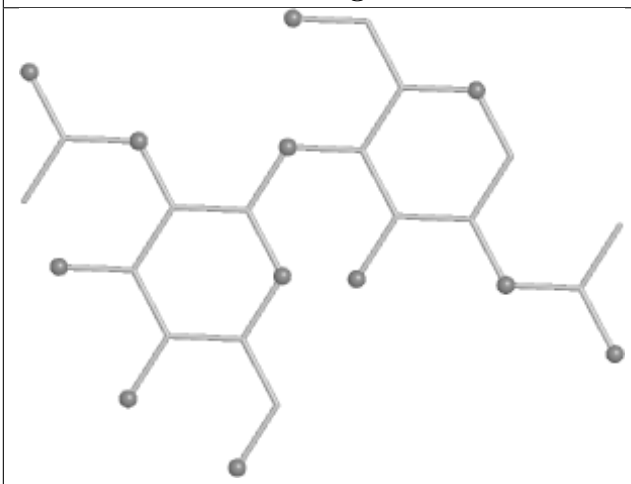
**Oligosaccharide Chain JA**



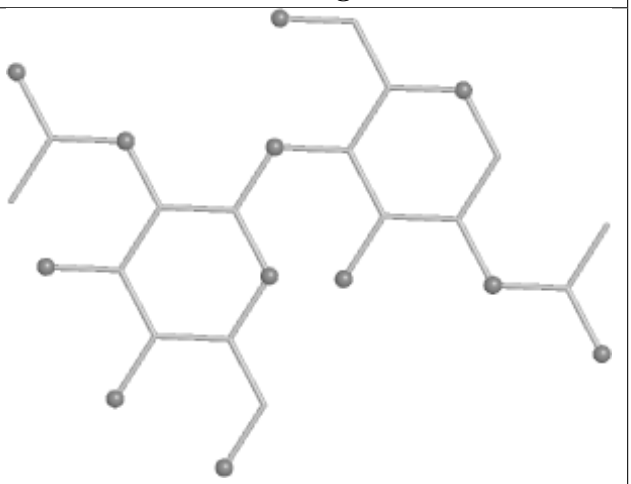
**Bond lengths**



**Bond angles**

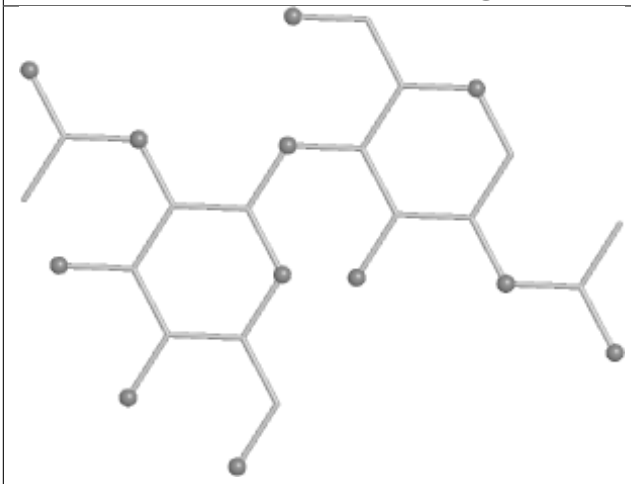


**Torsions**

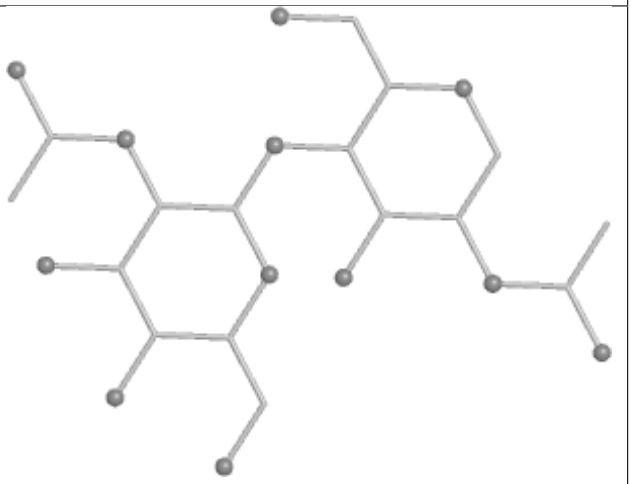


**Rings**

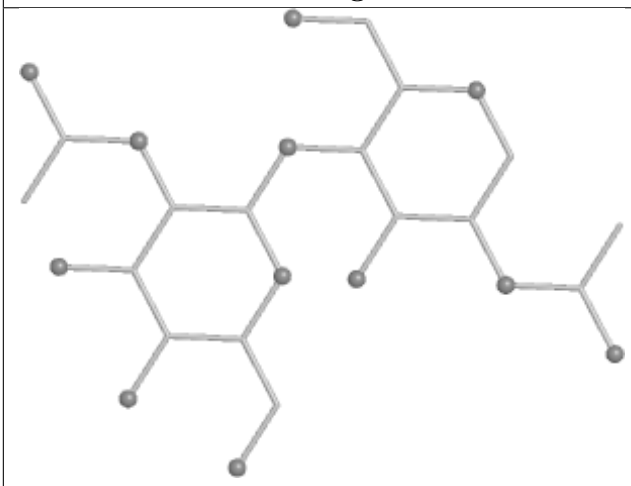
**Oligosaccharide Chain MA**



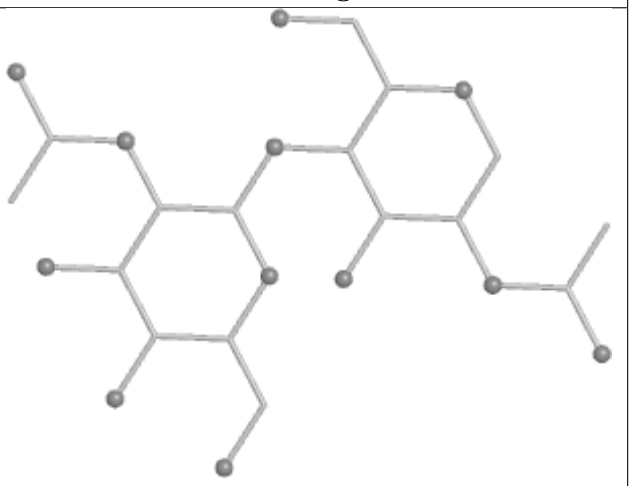
**Bond lengths**



**Bond angles**

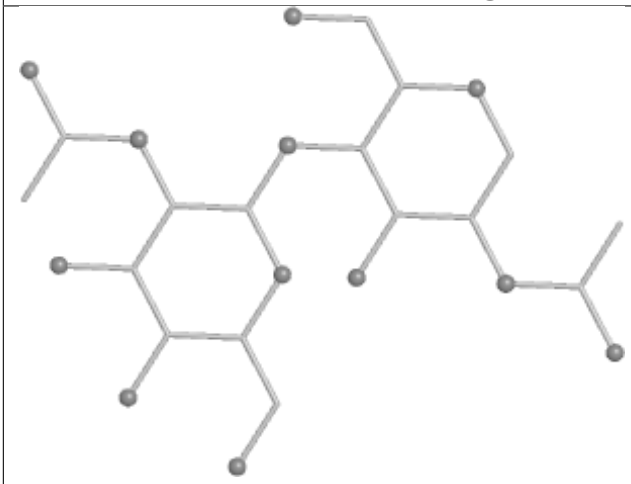


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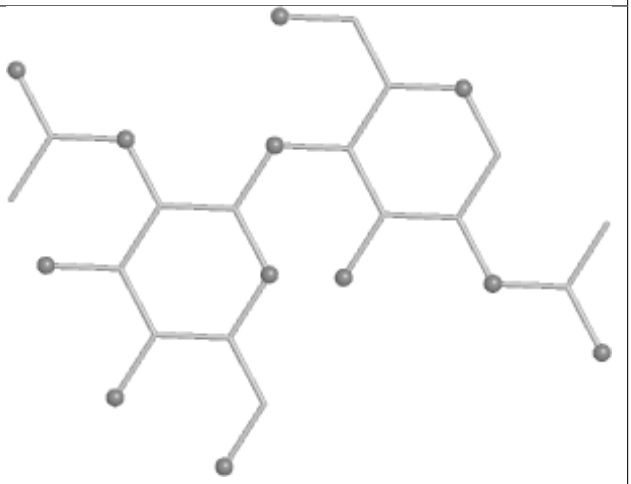


**Rings**

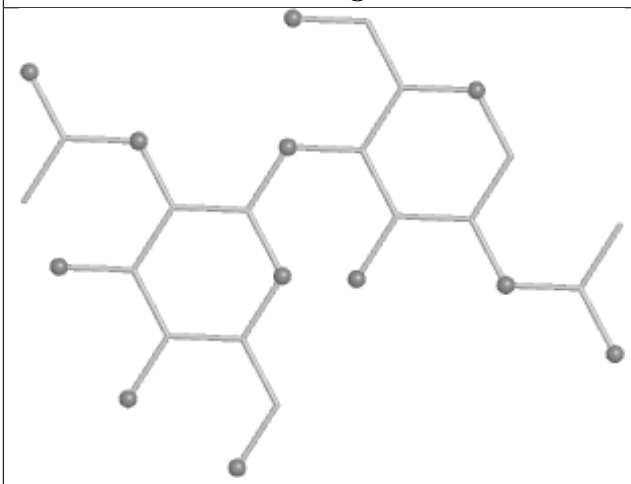
**Oligosaccharide Chain OA**



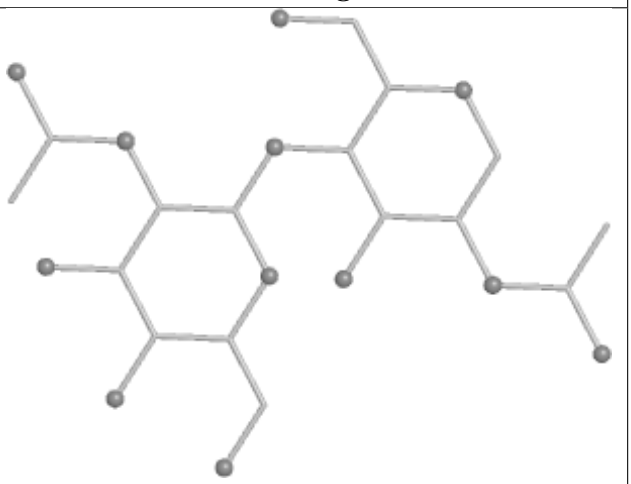
**Bond lengths**



**Bond angles**

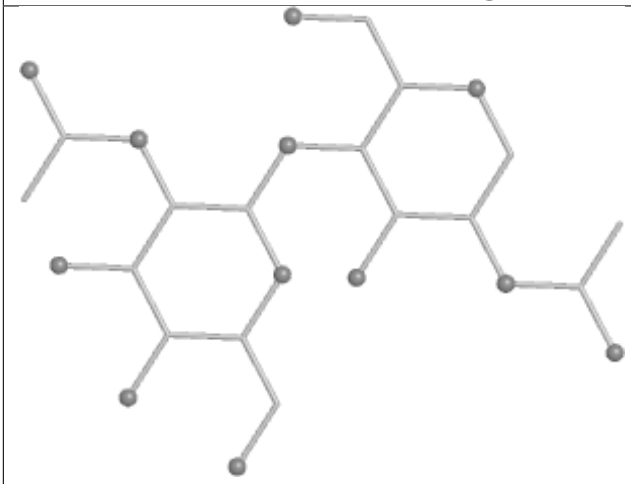


**Torsions**

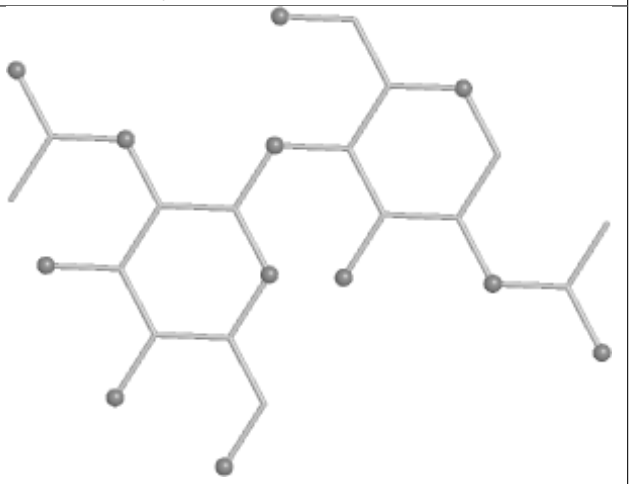


**Rings**

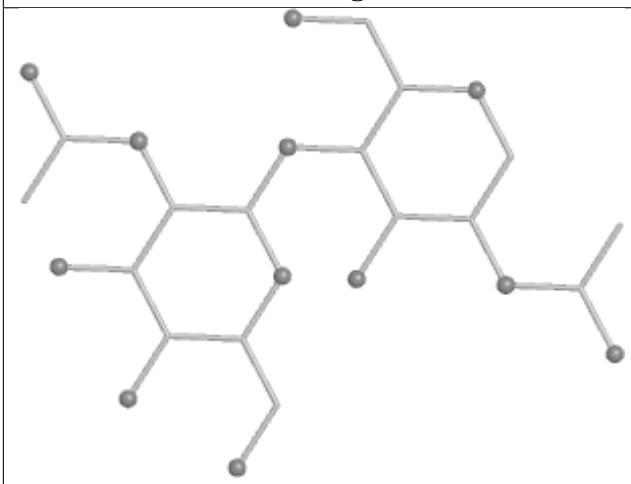
**Oligosaccharide Chain QA**



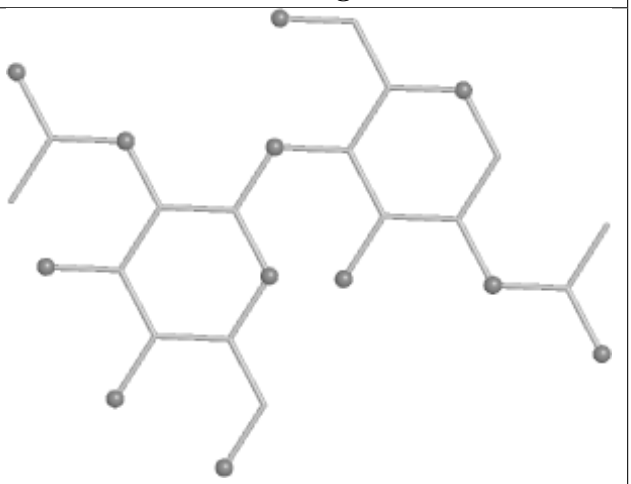
**Bond lengths**



**Bond angles**

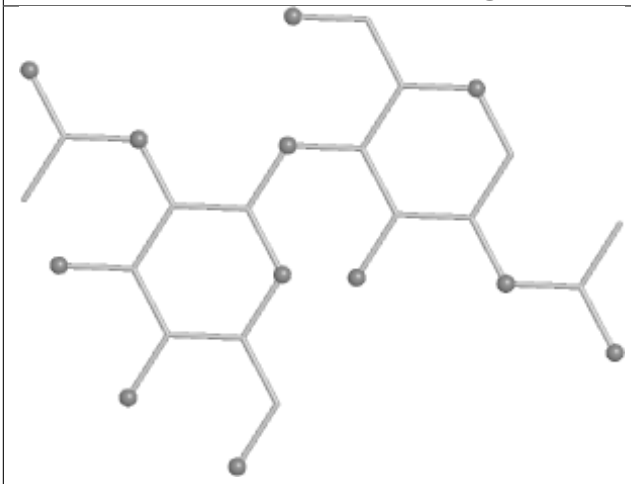


**Torsions**

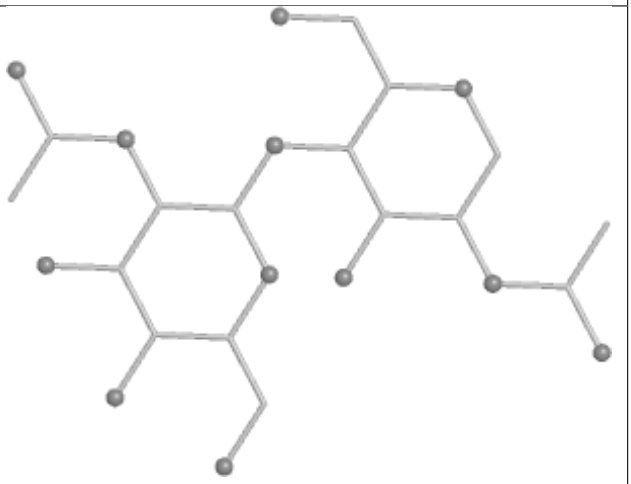


**Rings**

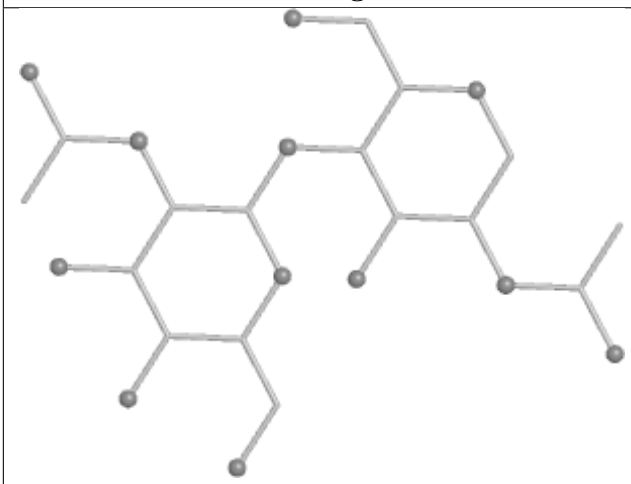
**Oligosaccharide Chain RA**



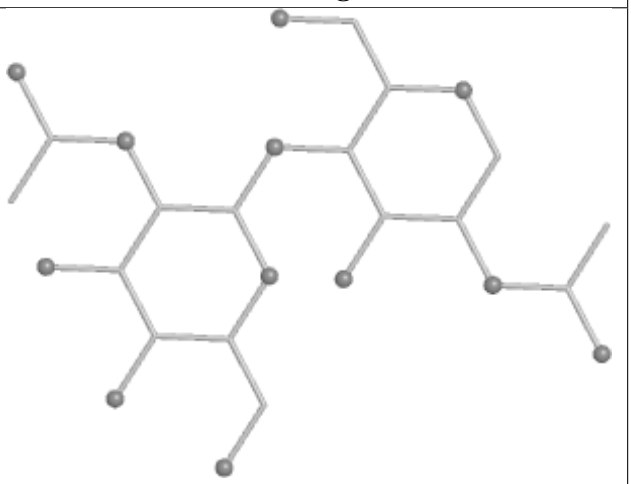
**Bond lengths**



**Bond angles**

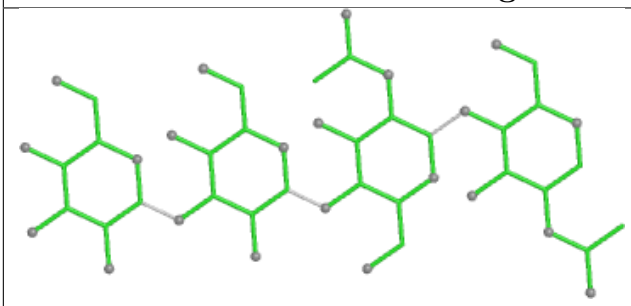


**Torsions**

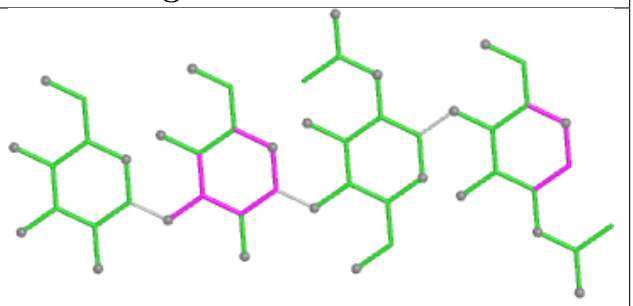


**Rings**

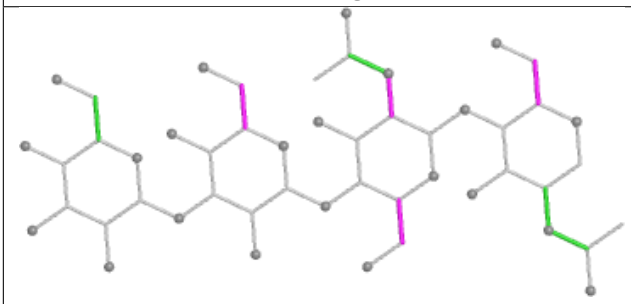
### Oligosaccharide Chain g



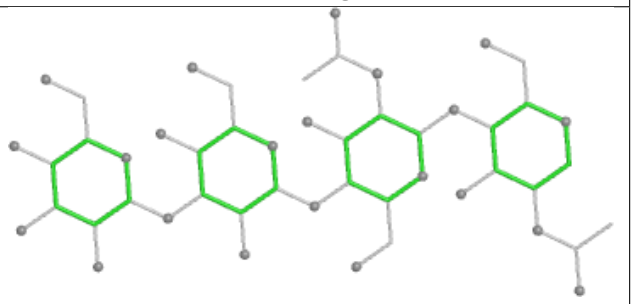
Bond lengths



Bond angles

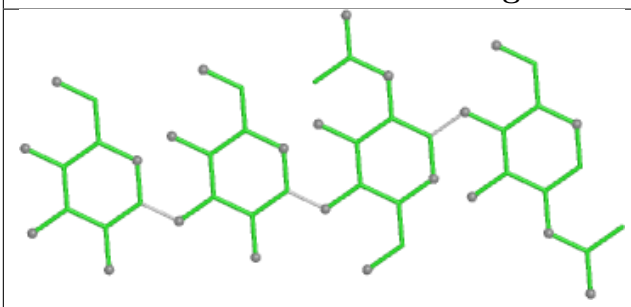


Torsions

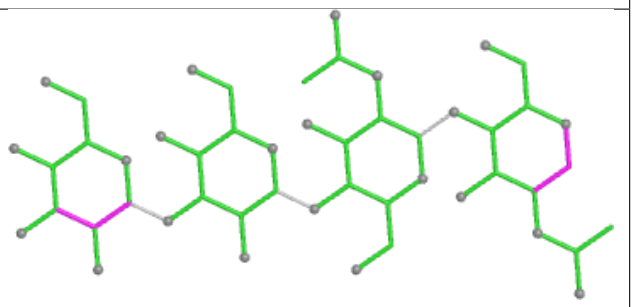


Rings

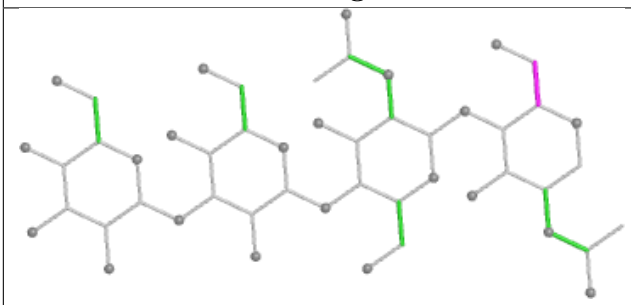
### Oligosaccharide Chain l



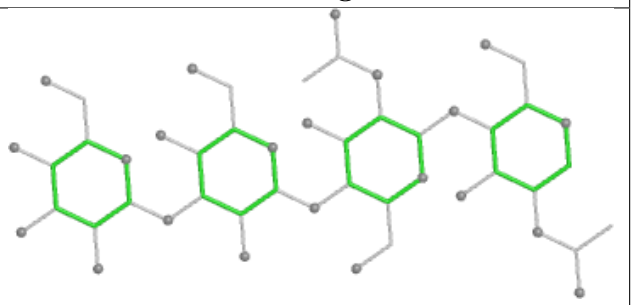
Bond lengths



Bond angles

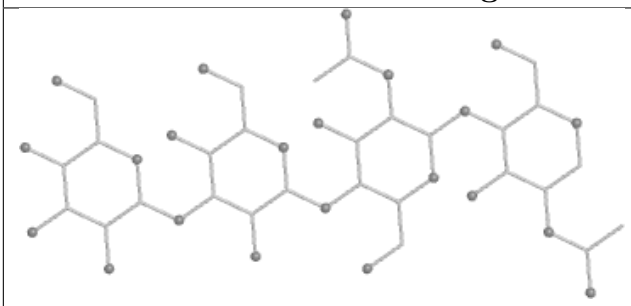


Torsions

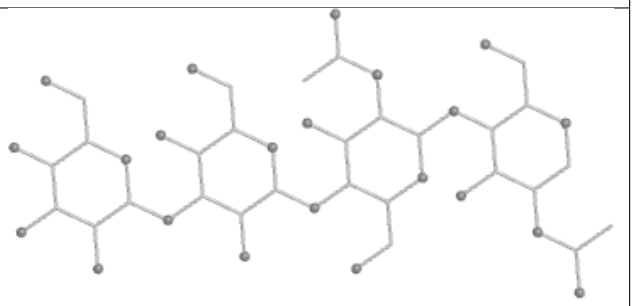


Rings

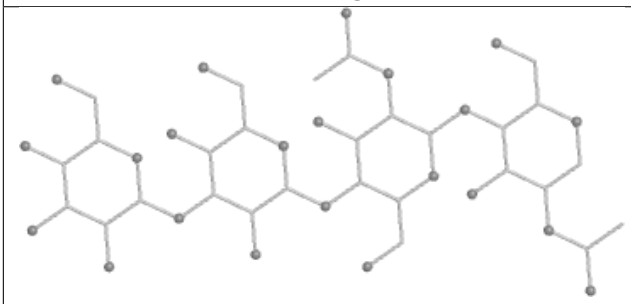
## Oligosaccharide Chain AA



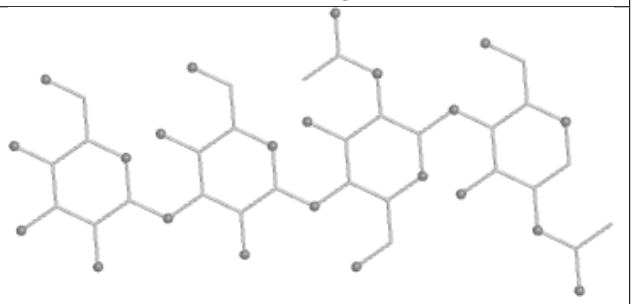
Bond lengths



Bond angles

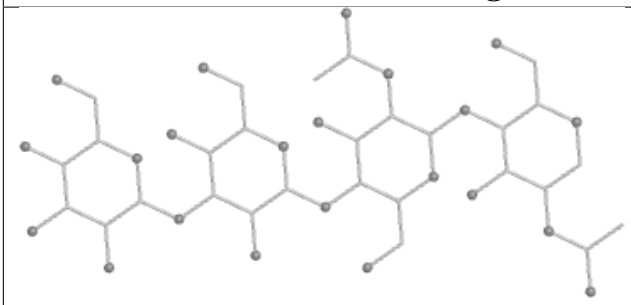


Torsions

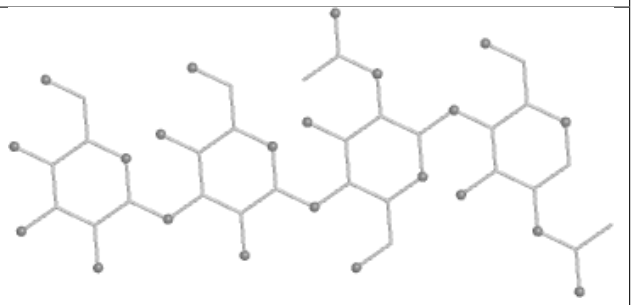


Rings

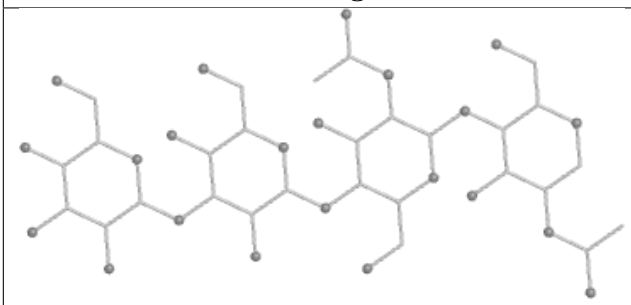
## Oligosaccharide Chain FA



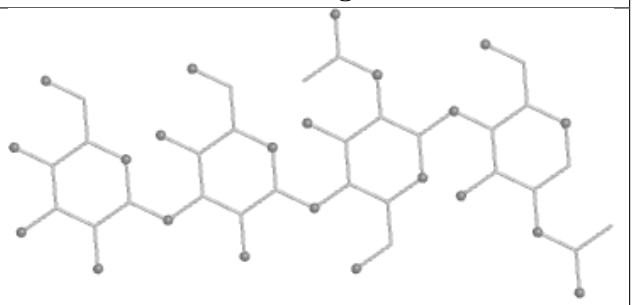
Bond lengths



Bond angles

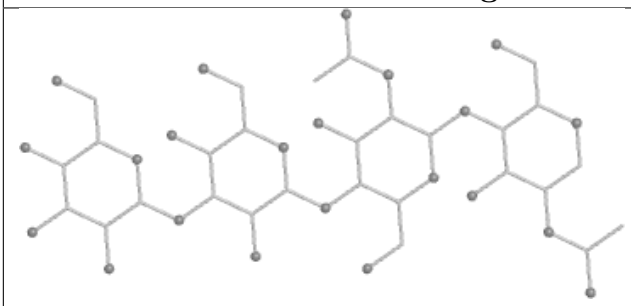


Torsions

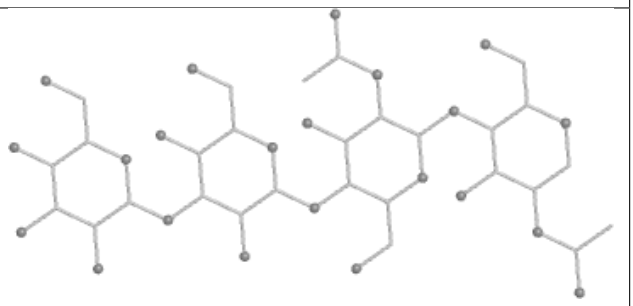


Rings

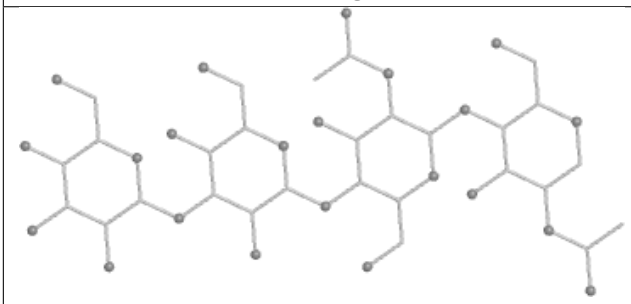
## Oligosaccharide Chain KA



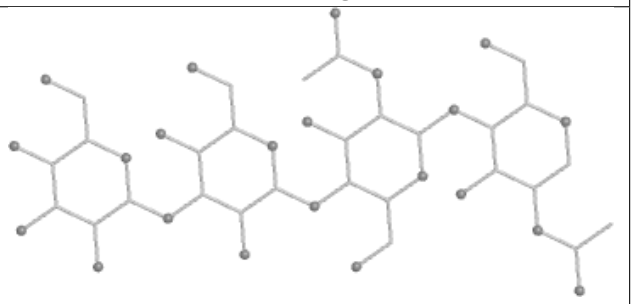
Bond lengths



Bond angles

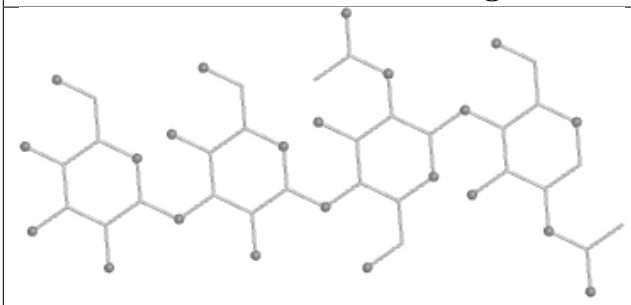


Torsions

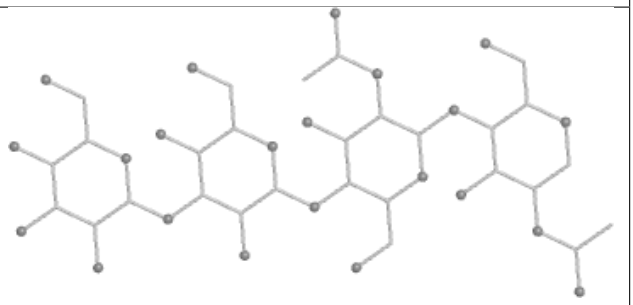


Rings

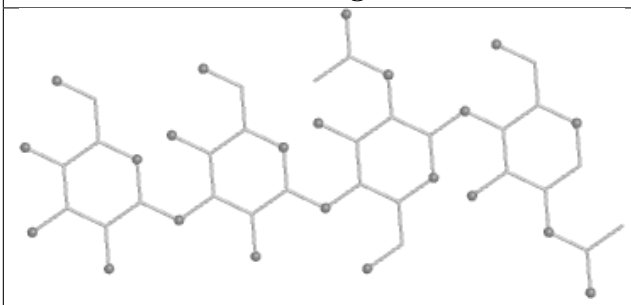
## Oligosaccharide Chain PA



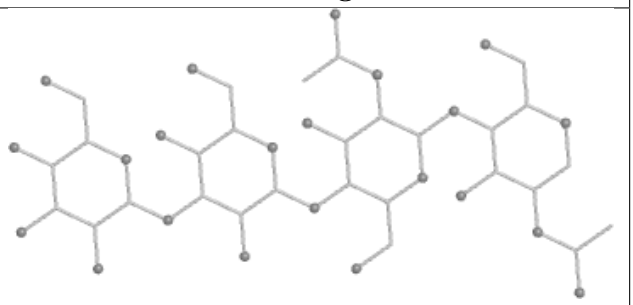
Bond lengths



Bond angles

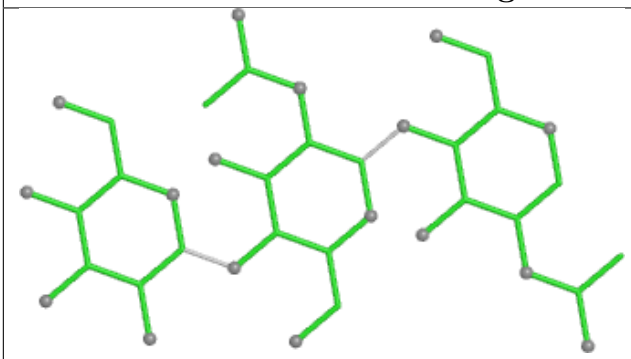


Torsions

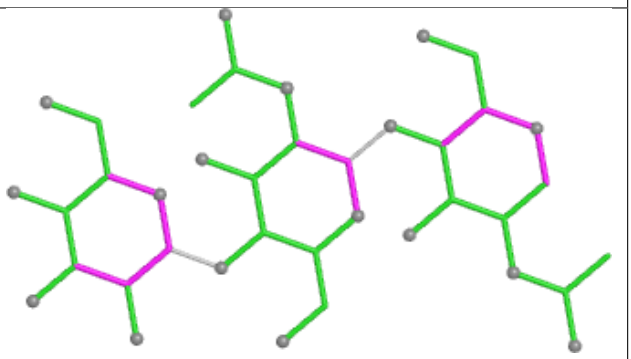


Rings

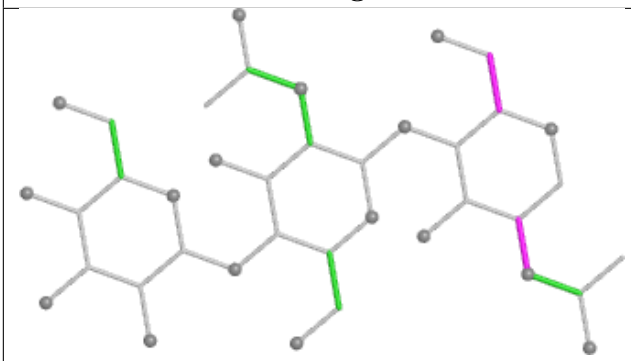
### Oligosaccharide Chain h



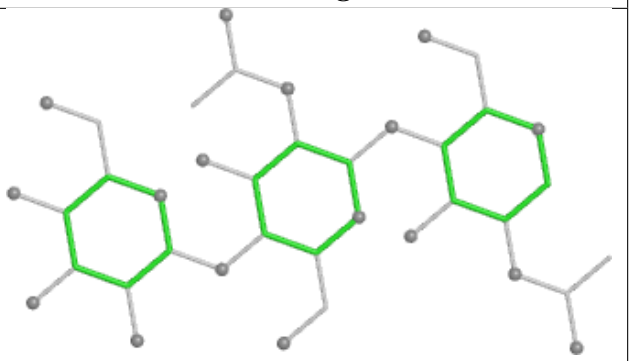
Bond lengths



Bond angles

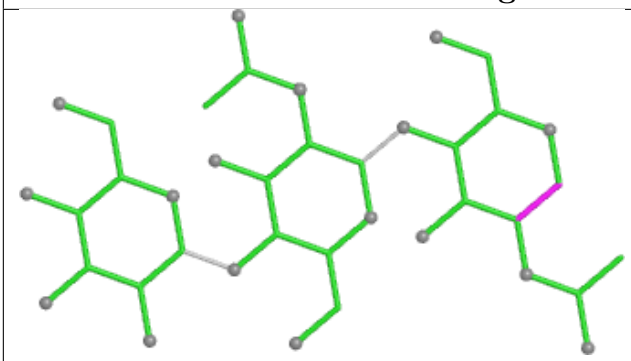


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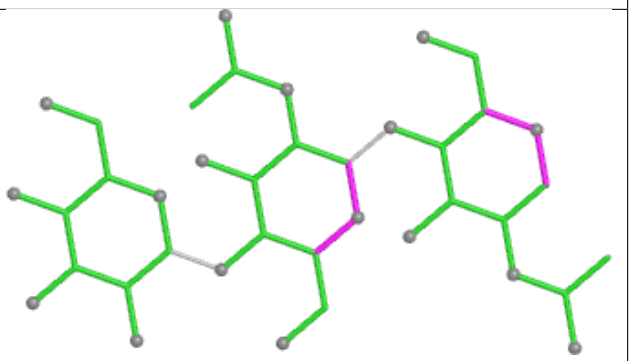


Rings

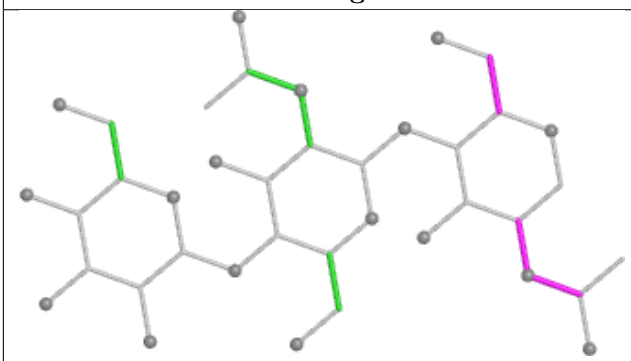
### Oligosaccharide Chain k



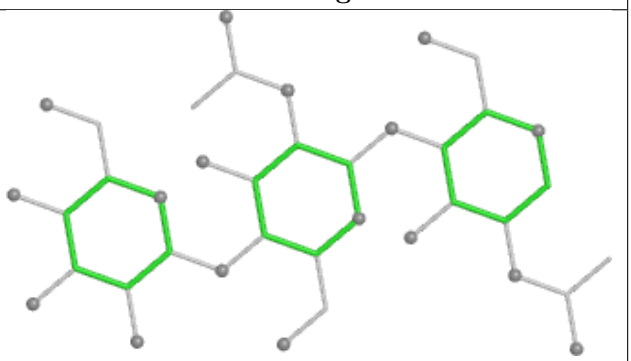
Bond lengths



Bond angles

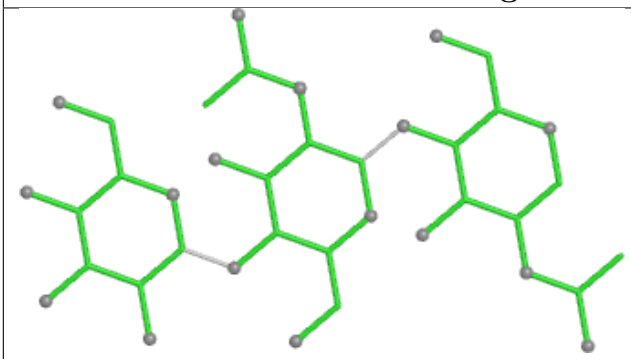


Torsions

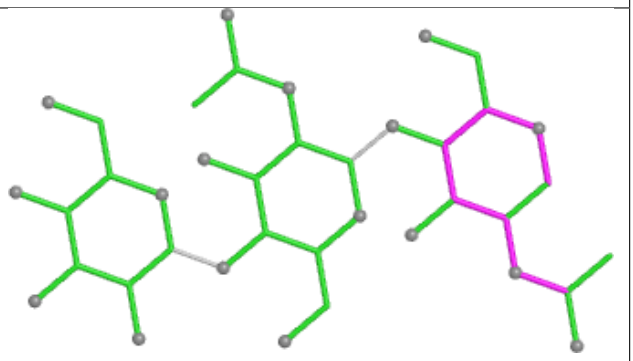


Rings

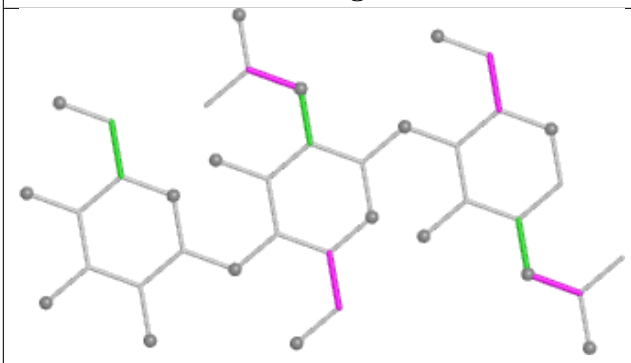
### Oligosaccharide Chain r



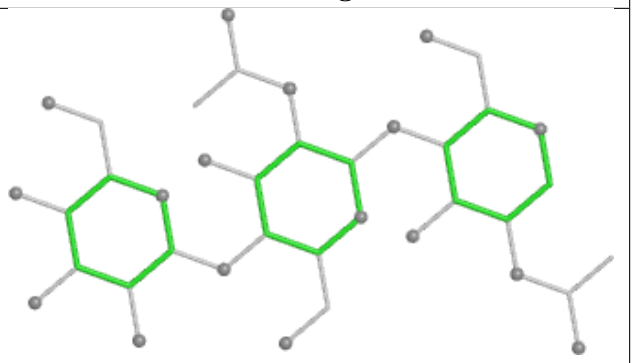
Bond lengths



Bond angles

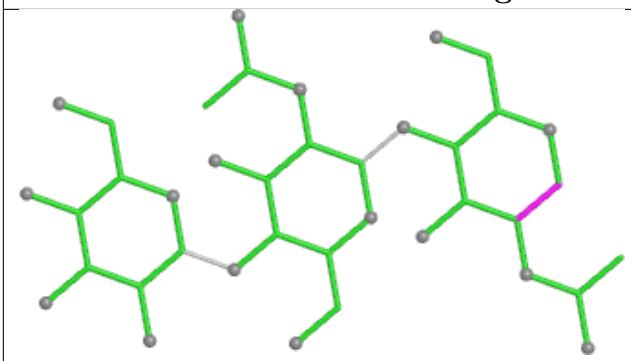


Torsions

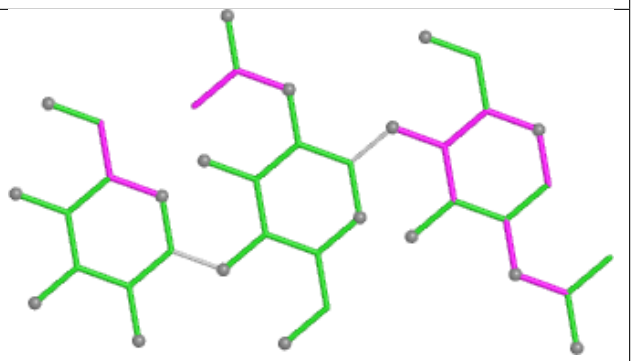


Rings

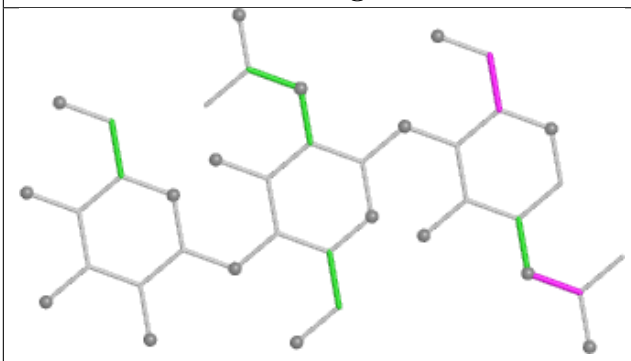
### Oligosaccharide Chain w



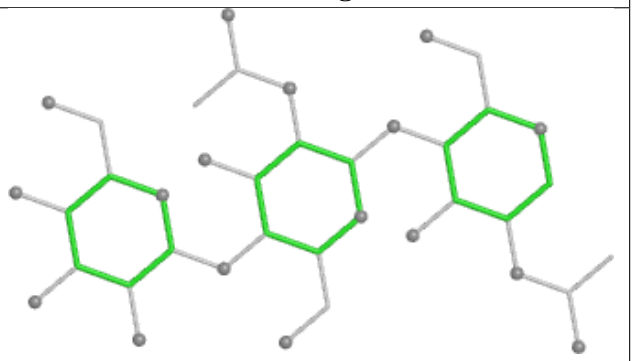
Bond lengths



Bond angles

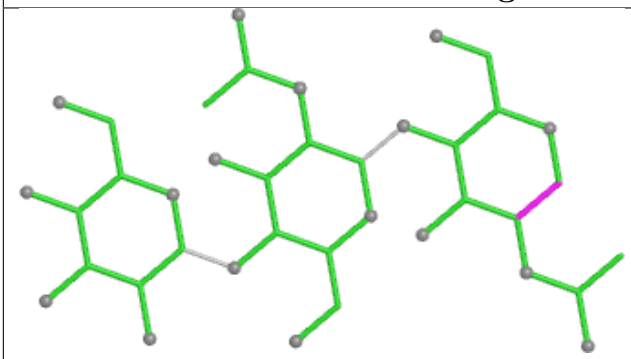


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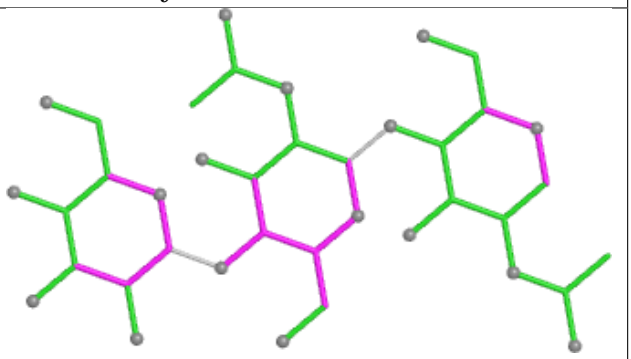


Rings

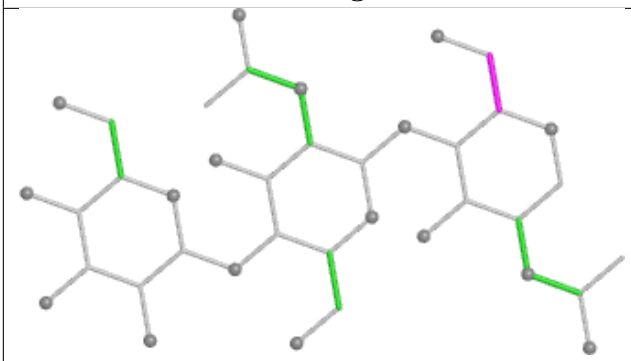
### Oligosaccharide Chain y



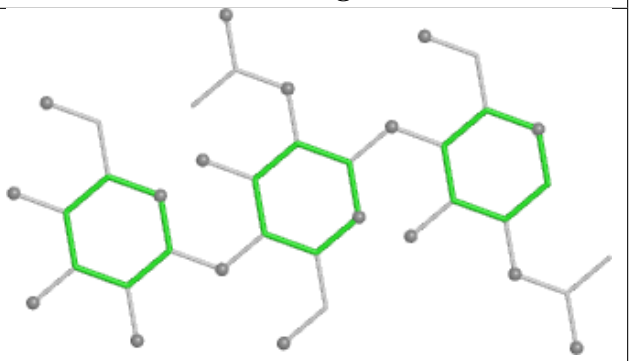
Bond lengths



Bond angles

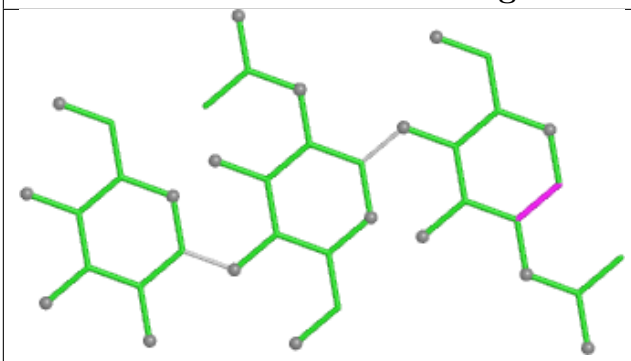


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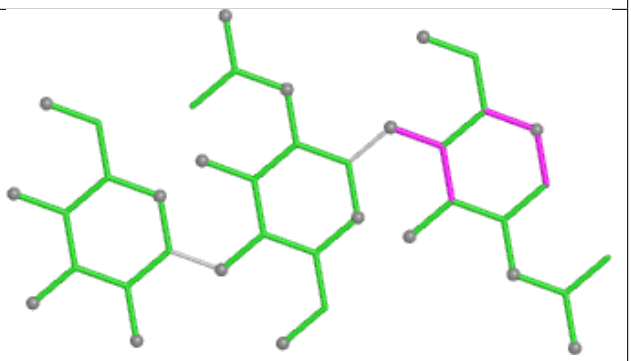


Rings

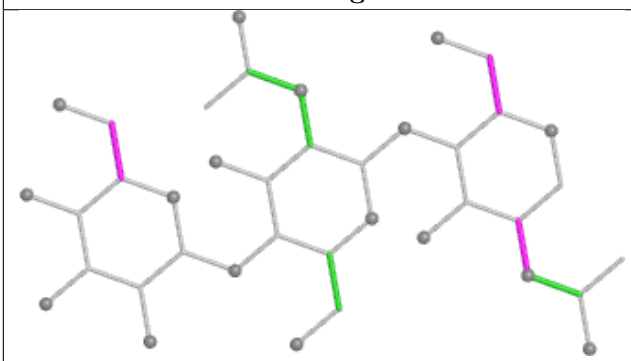
### Oligosaccharide Chain 3



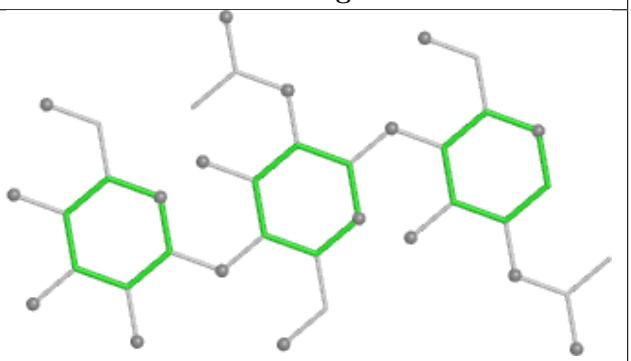
Bond lengths



Bond angles

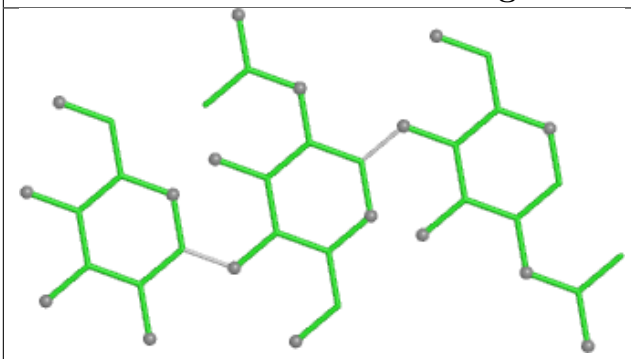


Torsions

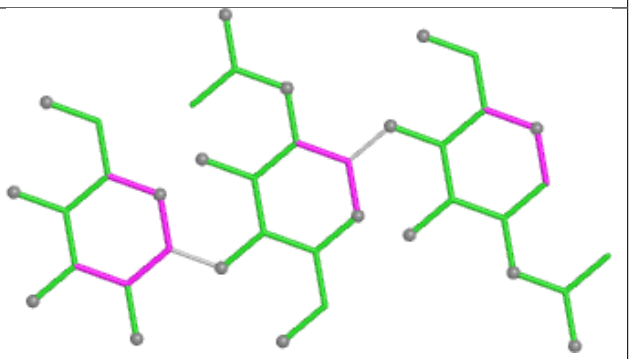


Rings

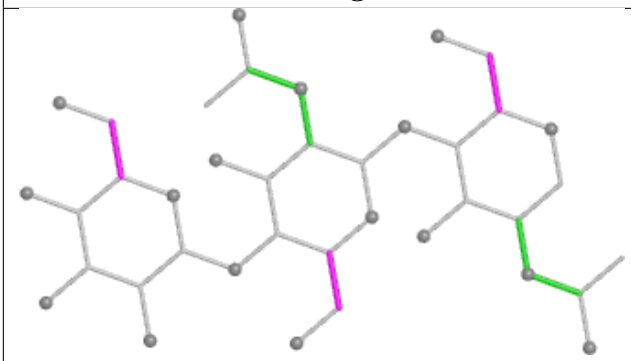
### Oligosaccharide Chain 5



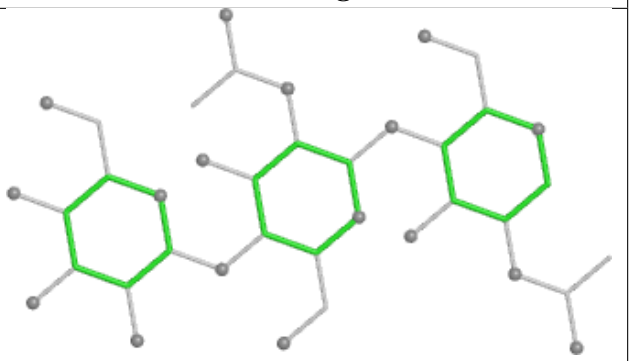
Bond lengths



Bond angles

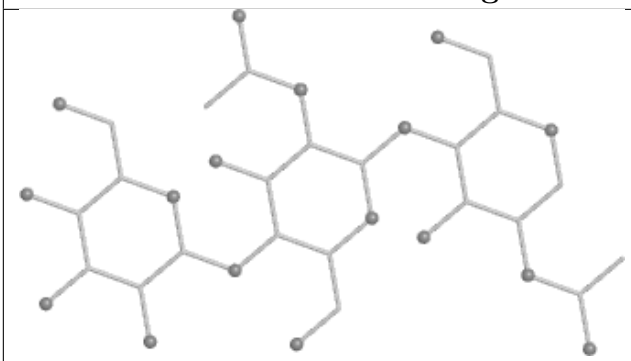


Torsions

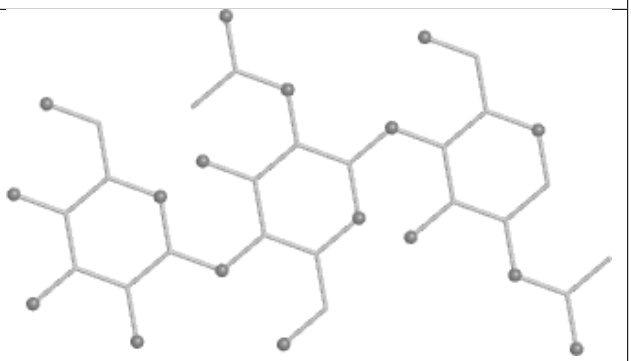


Rings

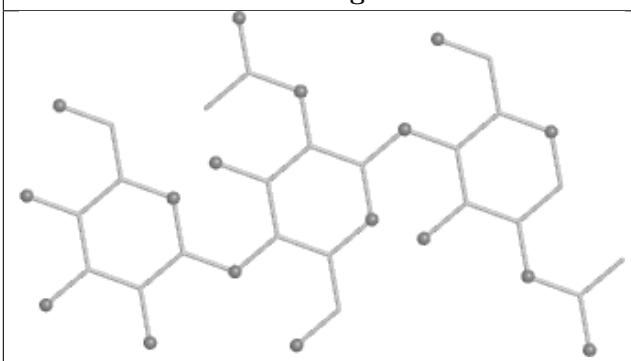
### Oligosaccharide Chain CA



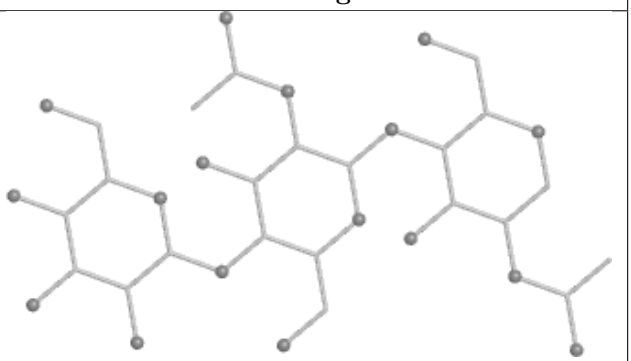
Bond lengths



Bond angles

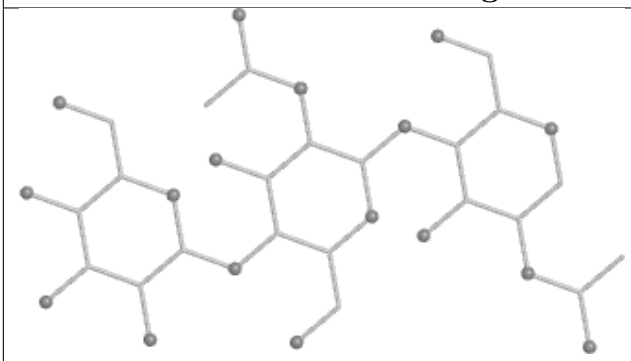


Torsions

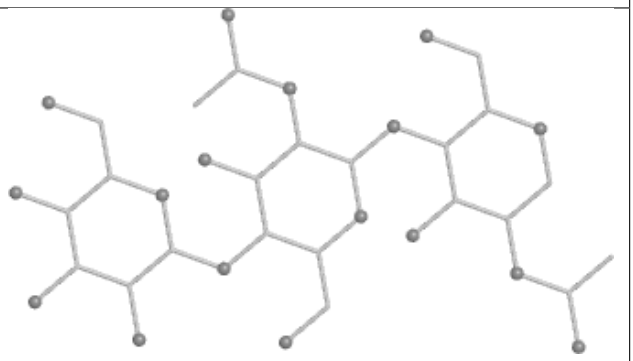


Rings

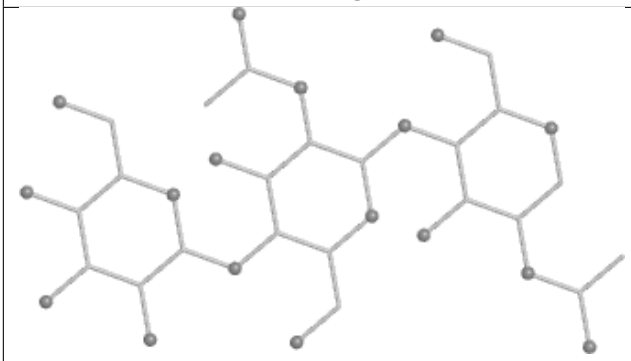
## Oligosaccharide Chain DA



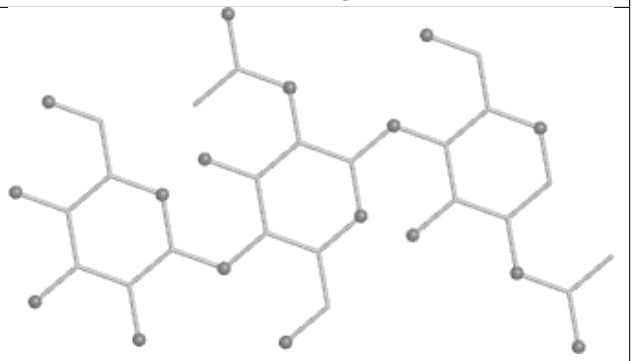
Bond lengths



Bond angles

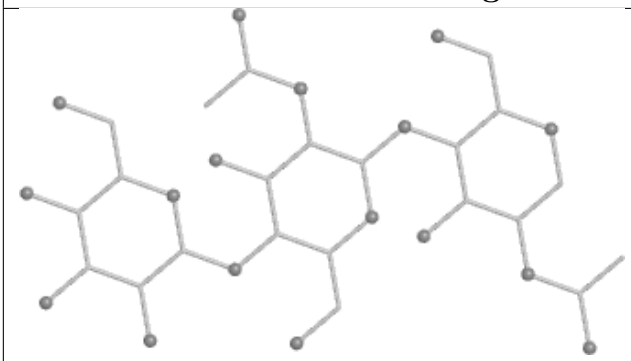


Torsions

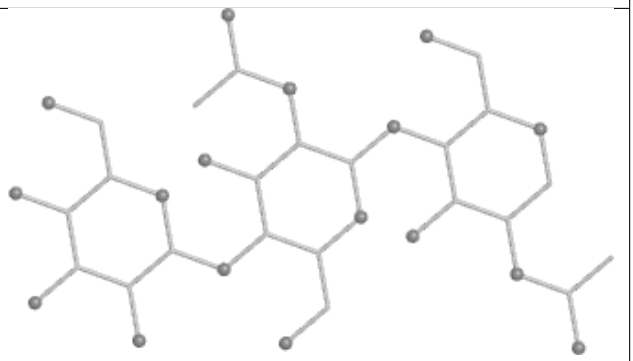


Rings

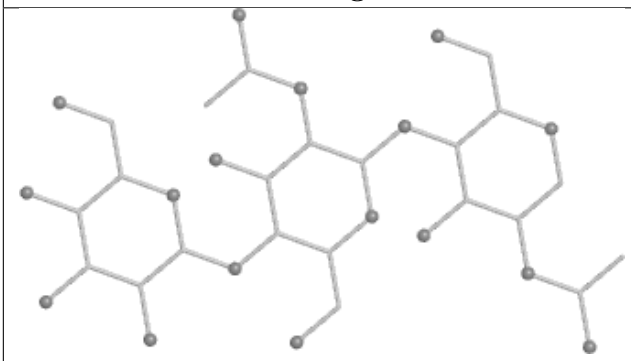
## Oligosaccharide Chain EA



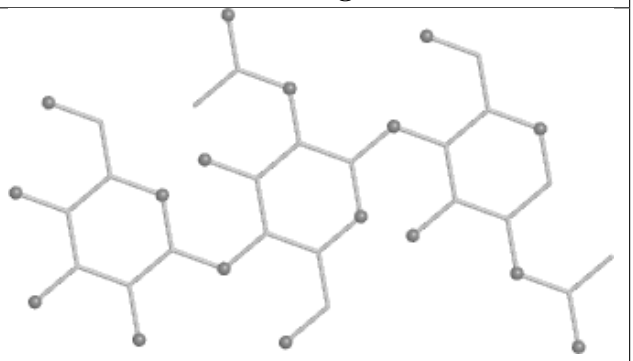
Bond lengths



Bond angles

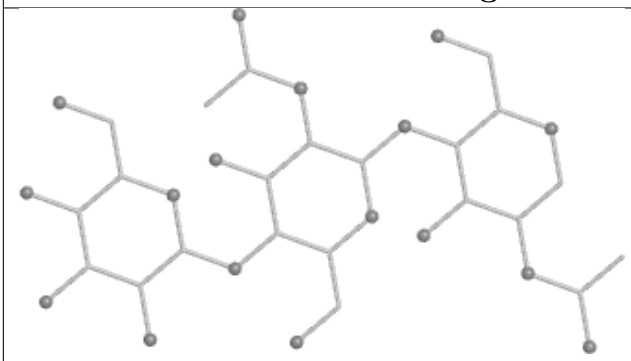


Torsions

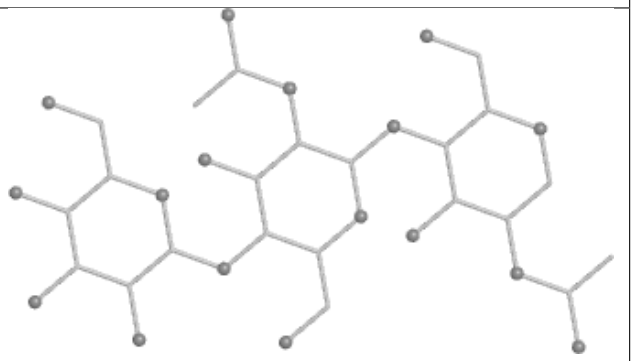


Rings

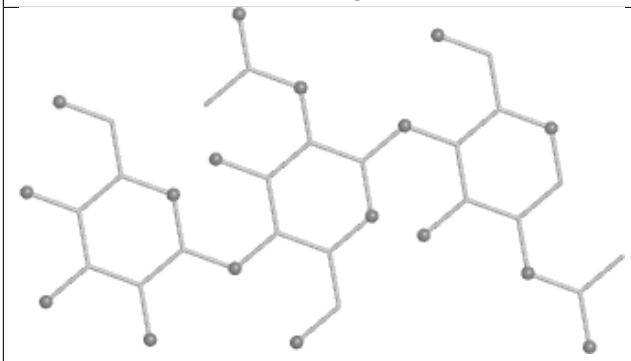
## Oligosaccharide Chain GA



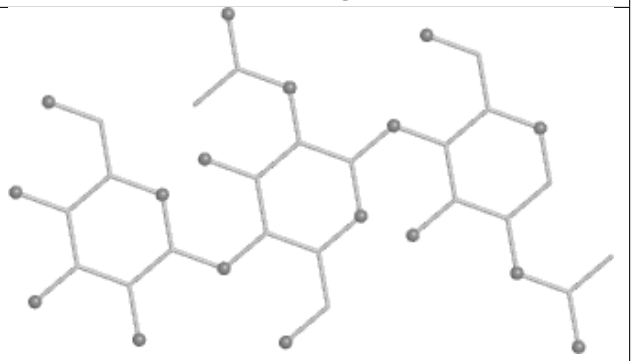
Bond lengths



Bond angles

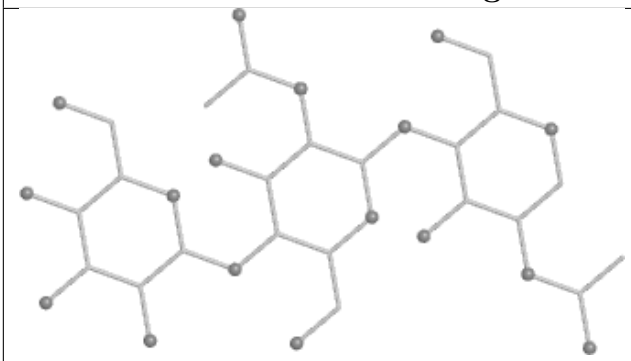


Torsions

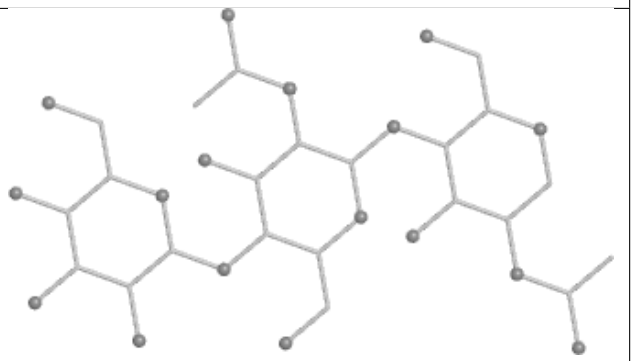


Rings

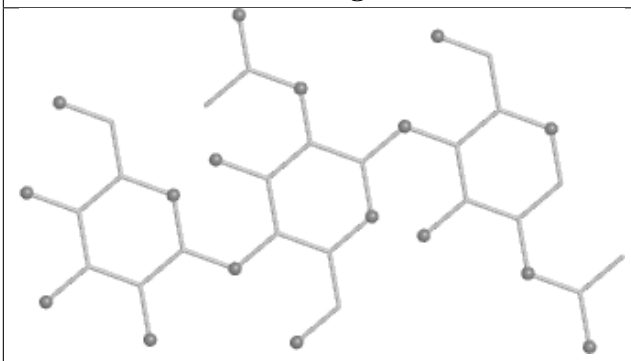
## Oligosaccharide Chain LA



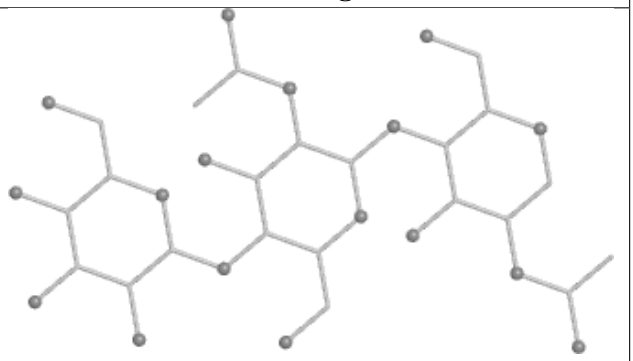
Bond lengths



Bond angles

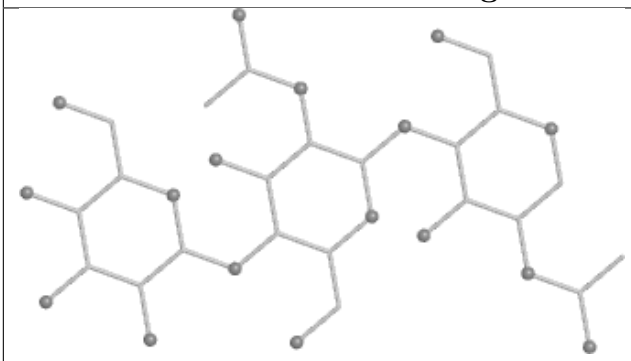


Torsions

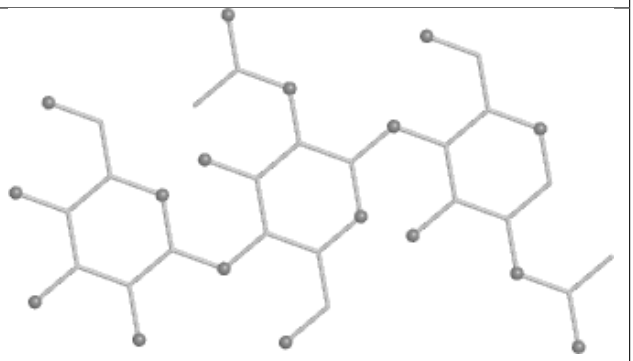


Rings

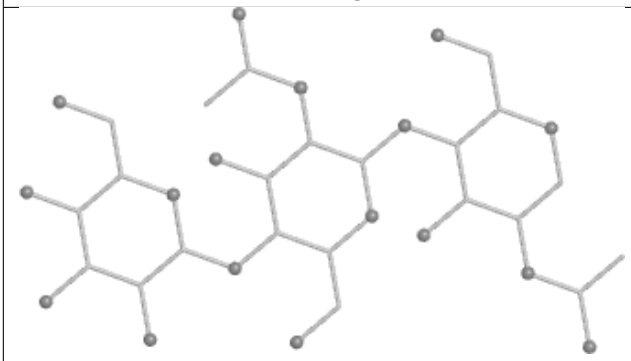
## Oligosaccharide Chain NA



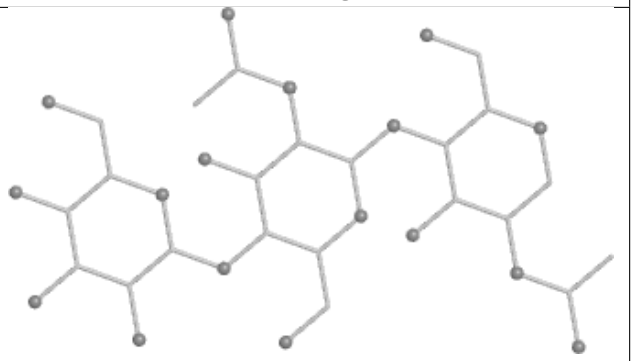
Bond lengths



Bond angles

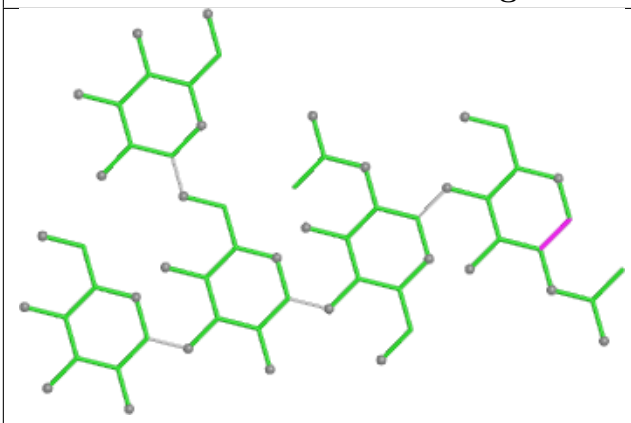


Torsions

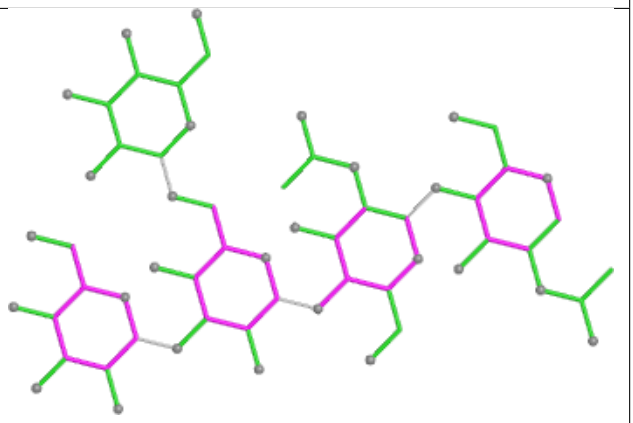


Rings

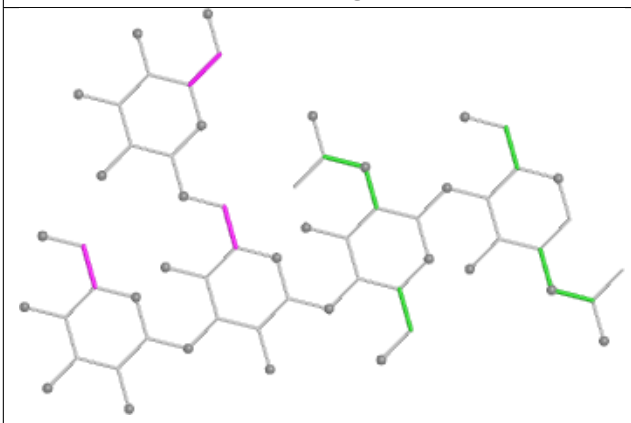
## Oligosaccharide Chain z



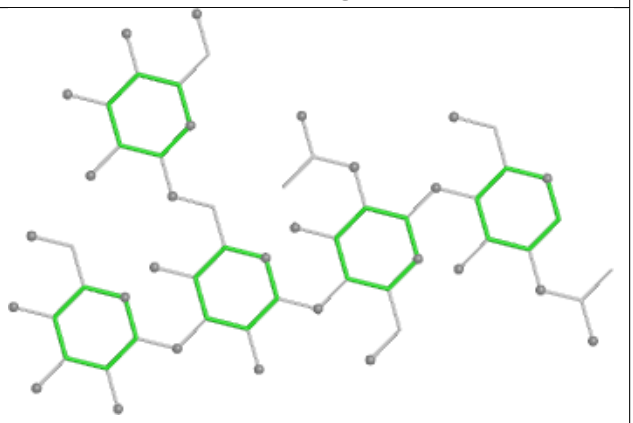
Bond lengths



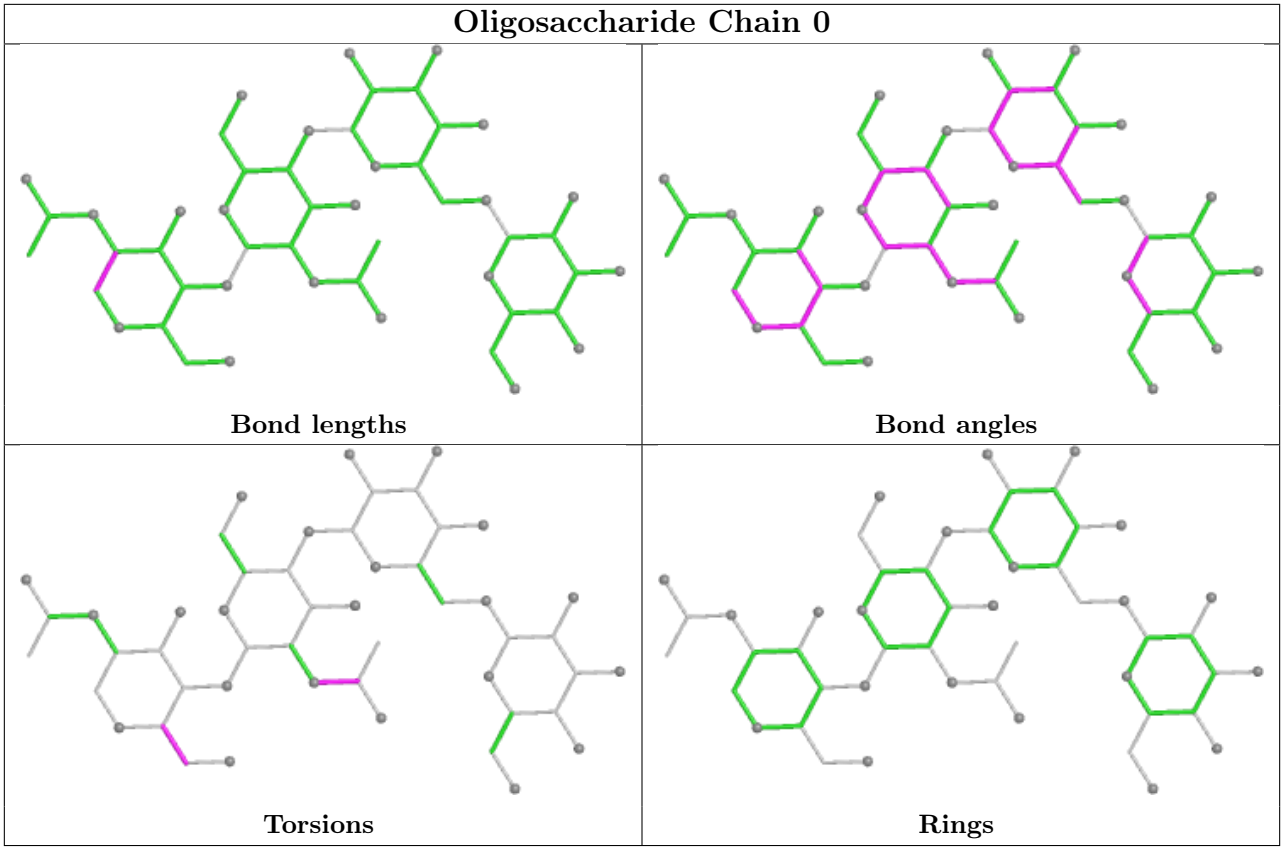
Bond angles



Torsions



Rings




## 5.6 Ligand geometry (i)

100 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 | $\#\|Z\| > 2$ |
| 9 | CUO | G | 2105 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | I | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | A | 5004 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | H | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | R | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | Y | 2105 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | S | 2103 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | K | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | G | 2104 | 1 | 0,5,5 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 9 | CUO | b | 2101[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | S | 2101[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | c | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | Z | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | P | 5004 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | W | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | M | 2101[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | B | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | T | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | S | 2102 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | Q | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | J | 5003 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | O | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | b | 2104 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | Y | 2102 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | Y | 2103 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | V | 5004 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | J | 5005[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | T | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | b | 2102 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | X | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | P | 5003 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | M | 2104 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | V | 5005[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | d | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | L | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | P | 5005[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | D | 5001 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | G | 2101[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | A | 5001 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | E | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | a | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | P | 5002 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | M | 2101[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | Y | 2101[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | H | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | S | 2105 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | D | 5002 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | X | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | U | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | F | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | Y | 2104 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | D | 5005[D] | - | 0,5,5 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 9 | CUO | J | 5002 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | L | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | d | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | c | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | Z | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | E | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | V | 5005[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | M | 2105 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | b | 2101[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | S | 2101[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | I | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | S | 2104 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | A | 5005[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | R | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | J | 5001 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | W | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | M | 2103 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | V | 5003 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | M | 2102 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | a | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | b | 2105 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | P | 5001 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | C | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | J | 5005[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | V | 5002 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | U | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | F | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | b | 2103 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | P | 5005[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | V | 5001 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | G | 2101[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | A | 5002 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | O | 3401[A] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | Y | 2101[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | A | 5005[D] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | A | 5003 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | D | 5004 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | K | 3001 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | C | 3401[B] | 3 | 0,5,5 | - | - | - | | |
| 9 | CUO | J | 5004 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | Q | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | G | 2102 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | G | 2103 | 1 | 0,5,5 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 9 | CUO | D | 5003 | 1 | 0,5,5 | - | - | - | | |
| 9 | CUO | B | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | N | 3002 | 2 | 0,5,5 | - | - | - | | |
| 9 | CUO | D | 5005[C] | - | 0,5,5 | - | - | - | | |
| 9 | CUO | N | 3001 | 2 | 0,5,5 | - | - | - | | |

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 |
|---|---|---|---|---|---|---|---|
| 9 | CUO | G | 2105 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | I | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | A | 5004 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | H | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | R | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | Y | 2105 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | S | 2103 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | K | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | G | 2104 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | b | 2101[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | S | 2101[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | c | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | Z | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | P | 5004 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | W | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | M | 2101[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | B | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | T | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | S | 2102 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | Q | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | J | 5003 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | O | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | b | 2104 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | Y | 2102 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | Y | 2103 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | V | 5004 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | J | 5005[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | T | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | b | 2102 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | X | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | P | 5003 | 1 | - | - | 0/2/2/2 |

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*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 9 | CUO | M | 2104 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | V | 5005[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | d | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | L | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | P | 5005[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | D | 5001 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | G | 2101[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | A | 5001 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | E | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | a | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | P | 5002 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | M | 2101[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | Y | 2101[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | H | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | S | 2105 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | D | 5002 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | X | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | U | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | F | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | Y | 2104 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | D | 5005[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | J | 5002 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | L | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | d | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | c | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | Z | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | E | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | V | 5005[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | M | 2105 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | b | 2101[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | S | 2101[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | I | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | S | 2104 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | A | 5005[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | R | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | J | 5001 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | W | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | M | 2103 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | V | 5003 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | M | 2102 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | a | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | b | 2105 | 1 | - | - | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 9 | CUO | P | 5001 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | C | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | J | 5005[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | V | 5002 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | U | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | F | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | b | 2103 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | P | 5005[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | V | 5001 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | G | 2101[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | A | 5002 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | O | 3401[A] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | Y | 2101[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | A | 5005[D] | - | - | - | 0/2/2/2 |
| 9 | CUO | A | 5003 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | D | 5004 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | K | 3001 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | C | 3401[B] | 3 | - | - | 0/2/2/2 |
| 9 | CUO | J | 5004 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | Q | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | G | 2102 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | G | 2103 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | D | 5003 | 1 | - | - | 0/2/2/2 |
| 9 | CUO | B | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | N | 3002 | 2 | - | - | 0/2/2/2 |
| 9 | CUO | D | 5005[C] | - | - | - | 0/2/2/2 |
| 9 | CUO | N | 3001 | 2 | - | - | 0/2/2/2 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 101 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 9 | I | 3401[B] | CUO | 1 | 0 |
| 9 | R | 3401[B] | CUO | 1 | 0 |
| 9 | Y | 2105 | CUO | 1 | 0 |
| 9 | G | 2104 | CUO | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 9 | T | 3002 | CUO | 1 | 0 |
| 9 | S | 2102 | CUO | 1 | 0 |
| 9 | O | 3401[B] | CUO | 5 | 0 |
| 9 | Y | 2102 | CUO | 1 | 0 |
| 9 | V | 5004 | CUO | 1 | 0 |
| 9 | X | 3401[A] | CUO | 5 | 0 |
| 9 | M | 2104 | CUO | 1 | 0 |
| 9 | d | 3401[A] | CUO | 5 | 0 |
| 9 | L | 3401[A] | CUO | 5 | 0 |
| 9 | D | 5001 | CUO | 1 | 0 |
| 9 | A | 5001 | CUO | 2 | 0 |
| 9 | a | 3401[A] | CUO | 5 | 0 |
| 9 | X | 3401[B] | CUO | 5 | 0 |
| 9 | U | 3401[A] | CUO | 5 | 0 |
| 9 | F | 3401[A] | CUO | 5 | 0 |
| 9 | Y | 2104 | CUO | 1 | 0 |
| 9 | J | 5002 | CUO | 1 | 0 |
| 9 | L | 3401[B] | CUO | 2 | 0 |
| 9 | d | 3401[B] | CUO | 5 | 0 |
| 9 | M | 2105 | CUO | 2 | 0 |
| 9 | I | 3401[A] | CUO | 5 | 0 |
| 9 | S | 2104 | CUO | 2 | 0 |
| 9 | R | 3401[A] | CUO | 5 | 0 |
| 9 | J | 5001 | CUO | 1 | 0 |
| 9 | W | 3002 | CUO | 1 | 0 |
| 9 | V | 5003 | CUO | 1 | 0 |
| 9 | a | 3401[B] | CUO | 2 | 0 |
| 9 | b | 2105 | CUO | 1 | 0 |
| 9 | C | 3401[A] | CUO | 5 | 0 |
| 9 | U | 3401[B] | CUO | 5 | 0 |
| 9 | F | 3401[B] | CUO | 2 | 0 |
| 9 | O | 3401[A] | CUO | 5 | 0 |
| 9 | D | 5004 | CUO | 1 | 0 |
| 9 | C | 3401[B] | CUO | 2 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 1656/2000 (82%) | -1.16 | 0 100 100 | 36, 70, 118, 164 | 0 |
| 1 | D | 1656/2000 (82%) | -1.17 | 0 100 100 | 37, 67, 114, 176 | 0 |
| 1 | G | 1656/2000 (82%) | -1.20 | 0 100 100 | 31, 68, 109, 152 | 0 |
| 1 | J | 1656/2000 (82%) | -1.16 | 0 100 100 | 30, 64, 119, 162 | 0 |
| 1 | M | 1656/2000 (82%) | -1.23 | 0 100 100 | 29, 56, 109, 157 | 0 |
| 1 | P | 1656/2000 (82%) | -1.27 | 0 100 100 | 27, 53, 97, 176 | 0 |
| 1 | S | 1656/2000 (82%) | -1.22 | 0 100 100 | 31, 60, 108, 164 | 0 |
| 1 | V | 1656/2000 (82%) | -1.26 | 1 (0%) 92 86 | 26, 55, 105, 154 | 0 |
| 1 | Y | 1656/2000 (82%) | -1.18 | 0 100 100 | 31, 66, 112, 160 | 0 |
| 1 | b | 1656/2000 (82%) | -1.21 | 0 100 100 | 30, 60, 105, 161 | 0 |
| 2 | B | 825/920 (89%) | -1.27 | 0 100 100 | 32, 57, 101, 140 | 0 |
| 2 | E | 825/920 (89%) | -1.26 | 0 100 100 | 30, 59, 106, 137 | 0 |
| 2 | H | 825/920 (89%) | -1.22 | 0 100 100 | 31, 63, 112, 147 | 0 |
| 2 | K | 825/920 (89%) | -1.24 | 0 100 100 | 34, 60, 101, 158 | 0 |
| 2 | N | 825/920 (89%) | -1.33 | 0 100 100 | 21, 46, 92, 135 | 0 |
| 2 | Q | 825/920 (89%) | -1.33 | 0 100 100 | 26, 49, 100, 134 | 0 |
| 2 | T | 825/920 (89%) | -1.28 | 0 100 100 | 30, 53, 93, 137 | 0 |
| 2 | W | 825/920 (89%) | -1.31 | 0 100 100 | 25, 53, 99, 129 | 0 |
| 2 | Z | 825/920 (89%) | -1.31 | 0 100 100 | 25, 52, 95, 130 | 0 |
| 2 | c | 825/920 (89%) | -1.27 | 0 100 100 | 26, 55, 103, 135 | 0 |
| 3 | C | 366/394 (92%) | -0.24 | 4 (1%) 78 57 | 34, 45, 49, 55 | 366 (100%) |
| 3 | F | 366/394 (92%) | -0.35 | 7 (1%) 66 43 | 28, 39, 44, 54 | 366 (100%) |
| 3 | I | 366/394 (92%) | -0.40 | 5 (1%) 73 51 | 29, 39, 46, 56 | 366 (100%) |
| 3 | L | 366/394 (92%) | -0.28 | 7 (1%) 66 43 | 32, 44, 49, 53 | 366 (100%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | O | 366/394 (92%) | -0.44 | 4 (1%) | 78 | 57 | 26, 37, 47, 53 | 366 (100%) |
| 3 | R | 366/394 (92%) | -0.56 | 1 (0%) | 90 | 79 | 29, 39, 45, 55 | 366 (100%) |
| 3 | U | 366/394 (92%) | -0.40 | 2 (0%) | 87 | 72 | 26, 37, 47, 51 | 366 (100%) |
| 3 | X | 366/394 (92%) | -0.08 | 10 (2%) | 56 | 33 | 39, 51, 56, 58 | 366 (100%) |
| 3 | a | 366/394 (92%) | -0.40 | 3 (0%) | 82 | 64 | 27, 38, 44, 48 | 366 (100%) |
| 3 | d | 366/394 (92%) | -0.28 | 5 (1%) | 73 | 51 | 41, 49, 53, 56 | 366 (100%) |
| All | All | 28470/33140 (85%) | -1.12 | 49 (0%) | 91 | 83 | 21, 56, 106, 176 | 3660 (12%) |

All (49) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | F | 3216[A] | GLY | 5.3 |
| 3 | F | 3282[A] | ASP | 4.9 |
| 3 | a | 3302[A] | SER | 4.8 |
| 3 | C | 2929[A] | SER | 4.8 |
| 3 | X | 3088[A] | GLY | 4.5 |
| 3 | d | 3221[A] | ALA | 4.3 |
| 3 | X | 3040[A] | VAL | 4.2 |
| 3 | F | 3283[A] | ILE | 4.1 |
| 3 | L | 2986[A] | PRO | 3.8 |
| 3 | L | 3303[A] | PRO | 3.8 |
| 3 | R | 3292[A] | GLY | 3.7 |
| 3 | O | 3220[A] | ARG | 3.4 |
| 3 | I | 3289[A] | GLY | 3.3 |
| 3 | I | 3179[A] | ASP | 3.3 |
| 3 | a | 3301[A] | PRO | 3.3 |
| 3 | X | 3108[A] | HIS | 3.1 |
| 3 | I | 3002[A] | ALA | 2.9 |
| 3 | F | 3215[A] | ALA | 2.9 |
| 3 | I | 2929[A] | SER | 2.8 |
| 3 | L | 2951[A] | ASP | 2.8 |
| 3 | C | 3282[A] | ASP | 2.8 |
| 3 | C | 3218[A] | LEU | 2.8 |
| 3 | X | 3158[A] | PHE | 2.7 |
| 3 | U | 3079[A] | CYS | 2.7 |
| 3 | F | 3002[A] | ALA | 2.6 |
| 3 | C | 3088[A] | GLY | 2.5 |
| 3 | O | 3146[A] | CYS | 2.4 |
| 3 | L | 3166[A] | GLU | 2.4 |
| 3 | L | 3079[A] | CYS | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | U | 3216[A] | GLY | 2.4 |
| 3 | X | 3138[A] | GLY | 2.3 |
| 3 | L | 3302[A] | SER | 2.3 |
| 3 | X | 3282[A] | ASP | 2.3 |
| 3 | X | 2929[A] | SER | 2.3 |
| 3 | L | 3085[A] | PHE | 2.3 |
| 3 | F | 3303[A] | PRO | 2.3 |
| 3 | O | 3101[A] | PRO | 2.3 |
| 3 | X | 3143[A] | SER | 2.2 |
| 3 | d | 3101[A] | PRO | 2.2 |
| 3 | d | 3247[A] | VAL | 2.2 |
| 3 | a | 3243[A] | GLY | 2.2 |
| 3 | d | 3282[A] | ASP | 2.2 |
| 1 | V | 886 | PRO | 2.1 |
| 3 | X | 2931[A] | THR | 2.1 |
| 3 | X | 3247[A] | VAL | 2.1 |
| 3 | d | 3220[A] | ARG | 2.1 |
| 3 | F | 3106[A] | THR | 2.1 |
| 3 | O | 3274[A] | ARG | 2.0 |
| 3 | I | 3288[A] | MET | 2.0 |

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

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

## 6.3 Carbohydrates (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 4 | NAG | e | 1 | 14/15 | - | - | 62,79,86,94 | 0 |
| 4 | NAG | e | 2 | 14/15 | - | - | 69,83,96,102 | 0 |
| 4 | NAG | f | 1 | 14/15 | - | - | 88,95,105,109 | 0 |
| 4 | NAG | f | 2 | 14/15 | - | - | 106,116,123,129 | 0 |
| 4 | NAG | i | 1 | 14/15 | - | - | 59,68,91,95 | 0 |
| 4 | NAG | i | 2 | 14/15 | - | - | 84,92,107,111 | 0 |
| 4 | NAG | j | 1 | 14/15 | - | - | 59,67,76,76 | 0 |
| 4 | NAG | j | 2 | 14/15 | - | - | 49,57,73,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 4 | NAG | m | 1 | 14/15 | - | - | 77,91,99,104 | 0 |
| 4 | NAG | m | 2 | 14/15 | - | - | 80,95,108,108 | 0 |
| 4 | NAG | n | 1 | 14/15 | - | - | 67,77,90,98 | 0 |
| 4 | NAG | n | 2 | 14/15 | - | - | 72,91,105,110 | 0 |
| 4 | NAG | o | 1 | 14/15 | - | - | 61,73,85,88 | 0 |
| 4 | NAG | o | 2 | 14/15 | - | - | 43,67,86,87 | 0 |
| 4 | NAG | p | 1 | 14/15 | - | - | 47,61,75,75 | 0 |
| 4 | NAG | p | 2 | 14/15 | - | - | 54,72,84,88 | 0 |
| 4 | NAG | q | 1 | 14/15 | - | - | 56,67,78,80 | 0 |
| 4 | NAG | q | 2 | 14/15 | - | - | 80,88,92,93 | 0 |
| 4 | NAG | s | 1 | 14/15 | - | - | 71,77,85,90 | 0 |
| 4 | NAG | s | 2 | 14/15 | - | - | 89,102,108,116 | 0 |
| 4 | NAG | t | 1 | 14/15 | - | - | 53,69,82,85 | 0 |
| 4 | NAG | t | 2 | 14/15 | - | - | 50,90,102,103 | 0 |
| 4 | NAG | u | 1 | 14/15 | - | - | 73,78,87,92 | 0 |
| 4 | NAG | u | 2 | 14/15 | - | - | 86,100,114,132 | 0 |
| 4 | NAG | v | 1 | 14/15 | - | - | 64,80,91,91 | 0 |
| 4 | NAG | v | 2 | 14/15 | - | - | 82,97,104,106 | 0 |
| 4 | NAG | x | 1 | 14/15 | - | - | 80,94,105,105 | 0 |
| 4 | NAG | x | 2 | 14/15 | - | - | 104,115,125,125 | 0 |
| 4 | NAG | 1 | 1 | 14/15 | - | - | 88,96,102,103 | 0 |
| 4 | NAG | 1 | 2 | 14/15 | - | - | 91,104,121,126 | 0 |
| 4 | NAG | 2 | 1 | 14/15 | - | - | 41,56,75,80 | 0 |
| 4 | NAG | 2 | 2 | 14/15 | - | - | 53,71,87,100 | 0 |
| 4 | NAG | 4 | 1 | 14/15 | - | - | 57,70,74,80 | 0 |
| 4 | NAG | 4 | 2 | 14/15 | - | - | 78,96,107,116 | 0 |
| 4 | NAG | 6 | 1 | 14/15 | - | - | 74,81,89,91 | 0 |
| 4 | NAG | 6 | 2 | 14/15 | - | - | 49,73,85,91 | 0 |
| 4 | NAG | 7 | 1 | 14/15 | - | - | 57,70,83,84 | 0 |
| 4 | NAG | 7 | 2 | 14/15 | - | - | 69,83,101,104 | 0 |
| 4 | NAG | 8 | 1 | 14/15 | - | - | 57,62,72,81 | 0 |
| 4 | NAG | 8 | 2 | 14/15 | - | - | 64,84,98,101 | 0 |
| 4 | NAG | 9 | 1 | 14/15 | - | - | 87,95,100,108 | 0 |
| 4 | NAG | 9 | 2 | 14/15 | - | - | 73,97,113,113 | 0 |
| 4 | NAG | BA | 1 | 14/15 | - | - | 80,84,96,97 | 0 |
| 4 | NAG | BA | 2 | 14/15 | - | - | 62,82,95,101 | 0 |
| 4 | NAG | MA | 2 | 14/15 | 0.95 | 0.07 | 84,93,116,127 | 0 |
| 5 | BMA | KA | 3 | 11/12 | 0.95 | 0.05 | 79,99,114,127 | 0 |
| 6 | NAG | GA | 2 | 14/15 | 0.96 | 0.07 | 88,108,127,131 | 0 |
| 4 | NAG | QA | 2 | 14/15 | 0.97 | 0.07 | 97,115,121,125 | 0 |
| 5 | NAG | FA | 2 | 14/15 | 0.97 | 0.07 | 74,88,101,105 | 0 |
| 4 | NAG | MA | 1 | 14/15 | 0.97 | 0.07 | 69,77,85,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | NAG | EA | 2 | 14/15 | 0.97 | 0.06 | 70,82,98,108 | 0 |
| 4 | NAG | IA | 2 | 14/15 | 0.97 | 0.07 | 75,89,96,100 | 0 |
| 6 | BMA | GA | 3 | 11/12 | 0.97 | 0.05 | 130,136,142,143 | 0 |
| 5 | NAG | FA | 1 | 14/15 | 0.98 | 0.04 | 49,68,77,78 | 0 |
| 4 | NAG | HA | 2 | 14/15 | 0.98 | 0.05 | 71,82,95,107 | 0 |
| 5 | NAG | KA | 1 | 14/15 | 0.98 | 0.04 | 60,66,76,78 | 0 |
| 5 | NAG | KA | 2 | 14/15 | 0.98 | 0.05 | 67,81,92,93 | 0 |
| 4 | NAG | HA | 1 | 14/15 | 0.98 | 0.04 | 56,63,83,93 | 0 |
| 5 | NAG | g | 1 | 14/15 | - | - | 57,79,95,97 | 0 |
| 5 | NAG | g | 2 | 14/15 | - | - | 99,105,109,109 | 0 |
| 5 | BMA | g | 3 | 11/12 | - | - | 110,124,133,139 | 0 |
| 5 | MAN | g | 4 | 11/12 | - | - | 103,117,133,133 | 0 |
| 5 | NAG | l | 1 | 14/15 | - | - | 52,57,72,76 | 0 |
| 5 | NAG | l | 2 | 14/15 | - | - | 69,84,96,97 | 0 |
| 5 | BMA | l | 3 | 11/12 | - | - | 98,113,119,128 | 0 |
| 5 | MAN | l | 4 | 11/12 | - | - | 114,118,122,128 | 0 |
| 5 | NAG | AA | 1 | 14/15 | - | - | 61,71,75,75 | 0 |
| 5 | NAG | AA | 2 | 14/15 | - | - | 87,92,98,104 | 0 |
| 5 | BMA | AA | 3 | 11/12 | - | - | 112,120,124,127 | 0 |
| 5 | MAN | AA | 4 | 11/12 | - | - | 114,125,132,145 | 0 |
| 5 | NAG | PA | 2 | 14/15 | 0.98 | 0.04 | 72,80,89,91 | 0 |
| 6 | NAG | EA | 1 | 14/15 | 0.98 | 0.05 | 46,58,71,75 | 0 |
| 5 | BMA | FA | 3 | 11/12 | - | - | 85,101,110,113 | 0 |
| 5 | MAN | FA | 4 | 11/12 | - | - | 94,107,126,132 | 0 |
| 4 | NAG | OA | 2 | 14/15 | 0.98 | 0.04 | 55,73,85,91 | 0 |
| 6 | NAG | GA | 1 | 14/15 | 0.98 | 0.06 | 79,97,106,109 | 0 |
| 4 | NAG | JA | 2 | 14/15 | 0.98 | 0.03 | 82,92,100,100 | 0 |
| 5 | MAN | KA | 4 | 11/12 | - | - | 87,103,122,135 | 0 |
| 4 | NAG | RA | 1 | 14/15 | 0.98 | 0.07 | 75,83,99,108 | 0 |
| 6 | BMA | LA | 3 | 11/12 | 0.98 | 0.05 | 101,110,119,119 | 0 |
| 5 | BMA | PA | 3 | 11/12 | - | - | 96,97,104,125 | 0 |
| 5 | MAN | PA | 4 | 11/12 | - | - | 107,112,125,133 | 0 |
| 6 | NAG | h | 1 | 14/15 | - | - | 85,93,112,115 | 0 |
| 6 | NAG | h | 2 | 14/15 | - | - | 84,94,107,114 | 0 |
| 6 | BMA | h | 3 | 11/12 | - | - | 108,114,120,126 | 0 |
| 6 | NAG | k | 1 | 14/15 | - | - | 71,83,92,99 | 0 |
| 6 | NAG | k | 2 | 14/15 | - | - | 88,104,119,123 | 0 |
| 6 | BMA | k | 3 | 11/12 | - | - | 110,119,126,133 | 0 |
| 6 | NAG | r | 1 | 14/15 | - | - | 79,88,107,112 | 0 |
| 6 | NAG | r | 2 | 14/15 | - | - | 84,91,98,102 | 0 |
| 6 | BMA | r | 3 | 11/12 | - | - | 111,120,128,129 | 0 |
| 6 | NAG | w | 1 | 14/15 | - | - | 78,100,106,118 | 0 |

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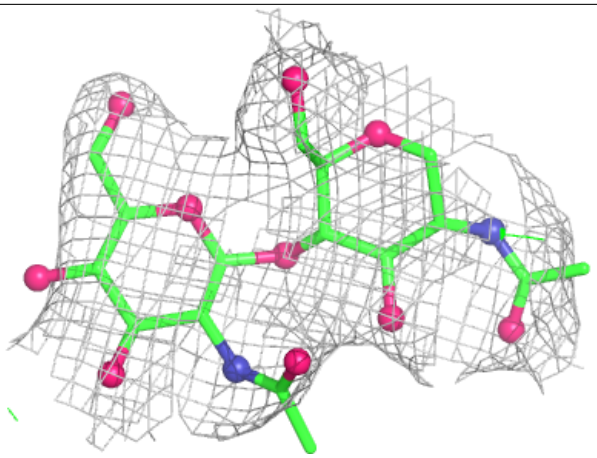
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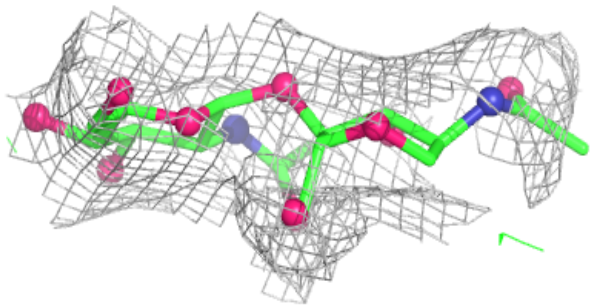
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | NAG | w | 2 | 14/15 | - | - | 88,104,108,111 | 0 |
| 6 | BMA | w | 3 | 11/12 | - | - | 107,110,117,128 | 0 |
| 6 | NAG | y | 1 | 14/15 | - | - | 52,67,74,75 | 0 |
| 6 | NAG | y | 2 | 14/15 | - | - | 65,83,94,109 | 0 |
| 6 | BMA | y | 3 | 11/12 | - | - | 102,116,123,123 | 0 |
| 6 | NAG | 3 | 1 | 14/15 | - | - | 46,67,81,90 | 0 |
| 6 | NAG | 3 | 2 | 14/15 | - | - | 61,82,96,102 | 0 |
| 6 | BMA | 3 | 3 | 11/12 | - | - | 114,119,149,149 | 0 |
| 6 | NAG | 5 | 1 | 14/15 | - | - | 52,60,70,76 | 0 |
| 6 | NAG | 5 | 2 | 14/15 | - | - | 61,77,95,103 | 0 |
| 6 | BMA | 5 | 3 | 11/12 | - | - | 98,114,124,127 | 0 |
| 6 | NAG | CA | 1 | 14/15 | - | - | 59,71,83,91 | 0 |
| 6 | NAG | CA | 2 | 14/15 | - | - | 88,97,115,124 | 0 |
| 6 | BMA | CA | 3 | 11/12 | - | - | 96,123,130,130 | 0 |
| 6 | NAG | DA | 1 | 14/15 | - | - | 50,66,77,82 | 0 |
| 6 | NAG | DA | 2 | 14/15 | - | - | 78,91,95,98 | 0 |
| 6 | BMA | DA | 3 | 11/12 | - | - | 82,103,108,108 | 0 |
| 6 | NAG | NA | 2 | 14/15 | 0.98 | 0.06 | 61,80,101,112 | 0 |
| 4 | NAG | IA | 1 | 14/15 | 0.99 | 0.04 | 51,66,83,92 | 0 |
| 6 | BMA | EA | 3 | 11/12 | - | - | 104,115,132,134 | 0 |
| 4 | NAG | OA | 1 | 14/15 | 0.99 | 0.05 | 57,70,80,85 | 0 |
| 4 | NAG | RA | 2 | 14/15 | 0.99 | 0.04 | 83,92,102,114 | 0 |
| 5 | NAG | PA | 1 | 14/15 | 0.99 | 0.03 | 62,72,77,78 | 0 |
| 6 | NAG | LA | 2 | 14/15 | 0.99 | 0.05 | 76,89,100,104 | 0 |
| 4 | NAG | JA | 1 | 14/15 | 0.99 | 0.03 | 70,80,88,90 | 0 |
| 6 | NAG | NA | 1 | 14/15 | 0.99 | 0.03 | 56,62,71,72 | 0 |
| 4 | NAG | QA | 1 | 14/15 | 0.99 | 0.04 | 97,107,114,118 | 0 |
| 6 | NAG | LA | 1 | 14/15 | 1.00 | 0.03 | 78,87,93,98 | 0 |
| 6 | BMA | NA | 3 | 11/12 | - | - | 102,117,134,138 | 0 |
| 7 | NAG | z | 1 | 14/15 | - | - | 79,85,93,96 | 0 |
| 7 | NAG | z | 2 | 14/15 | - | - | 92,105,121,128 | 0 |
| 7 | BMA | z | 3 | 11/12 | - | - | 124,134,140,150 | 0 |
| 7 | MAN | z | 4 | 11/12 | - | - | 135,140,150,154 | 0 |
| 7 | MAN | z | 5 | 11/12 | - | - | 121,135,151,154 | 0 |
| 8 | NAG | 0 | 1 | 14/15 | - | - | 60,67,72,81 | 0 |
| 8 | NAG | 0 | 2 | 14/15 | - | - | 58,78,82,90 | 0 |
| 8 | BMA | 0 | 3 | 11/12 | - | - | 97,112,128,130 | 0 |
| 8 | MAN | 0 | 4 | 11/12 | - | - | 94,114,123,126 | 0 |

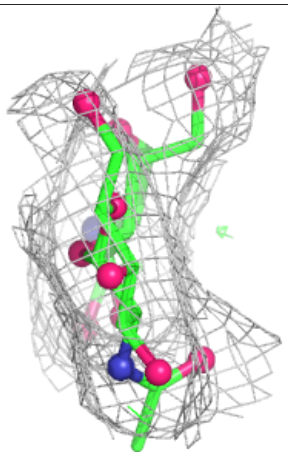
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain e:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

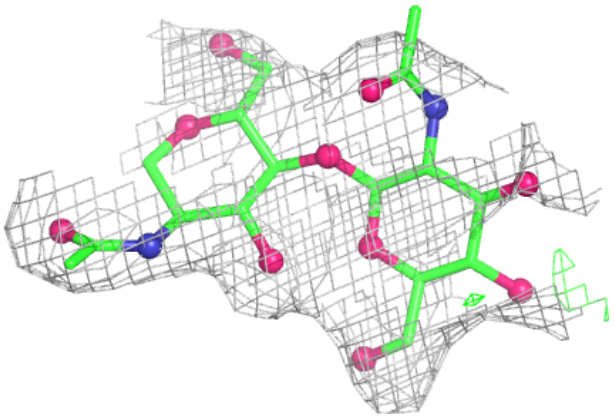


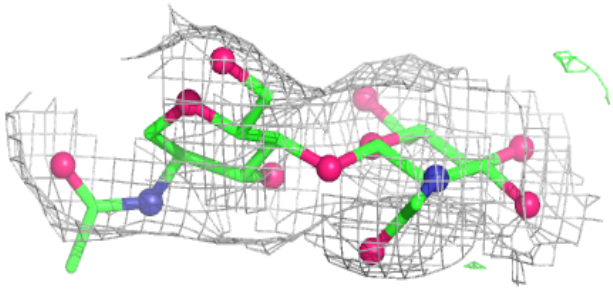


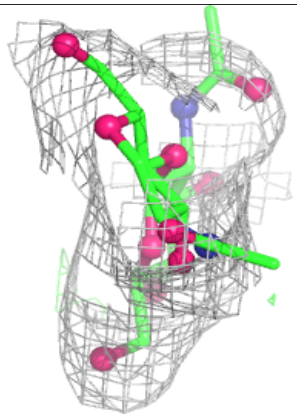


**Electron density around Chain f:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

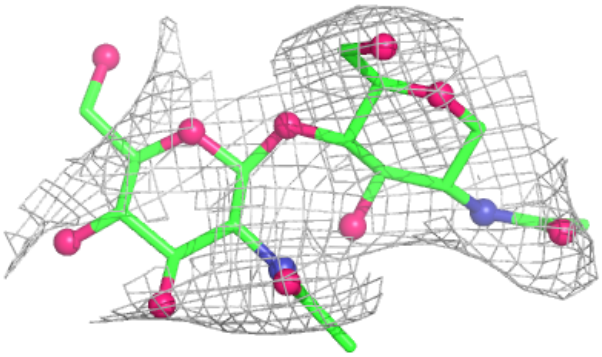


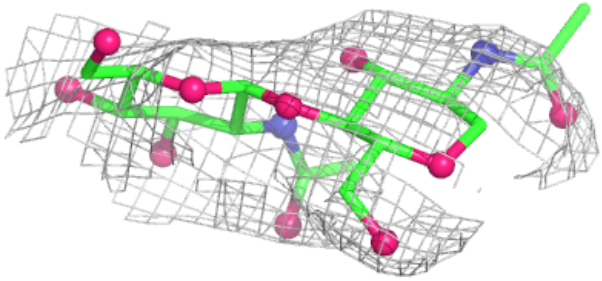




**Electron density around Chain i:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

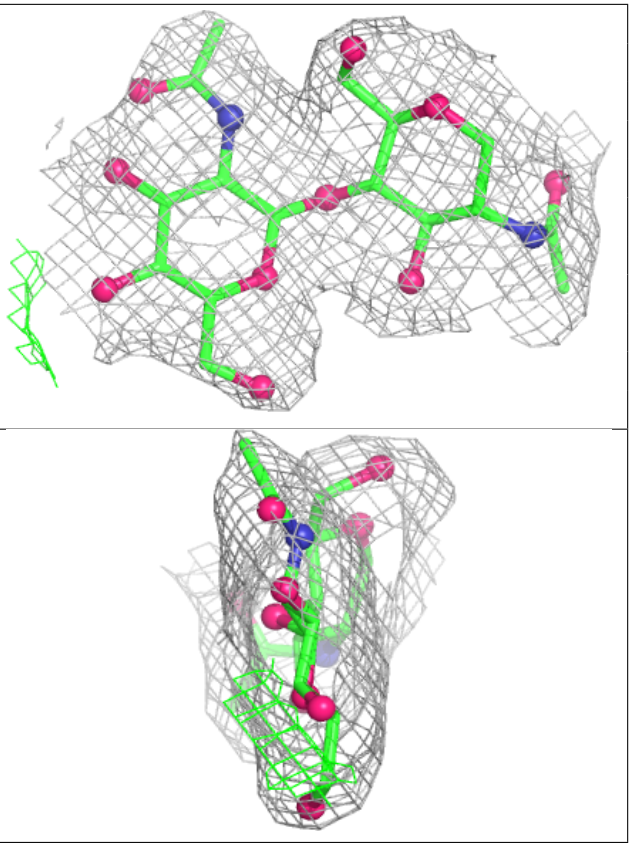






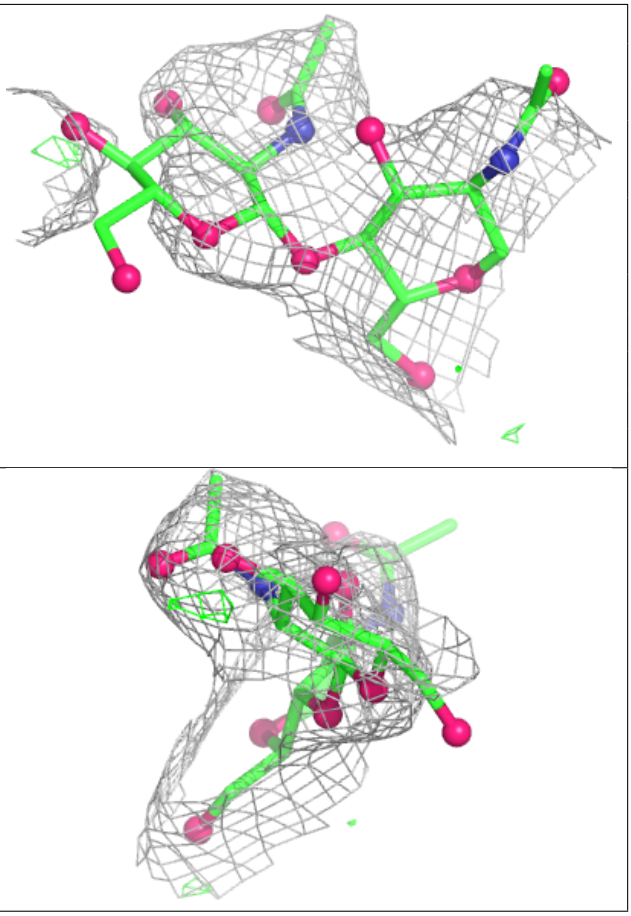
**Electron density around Chain j:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



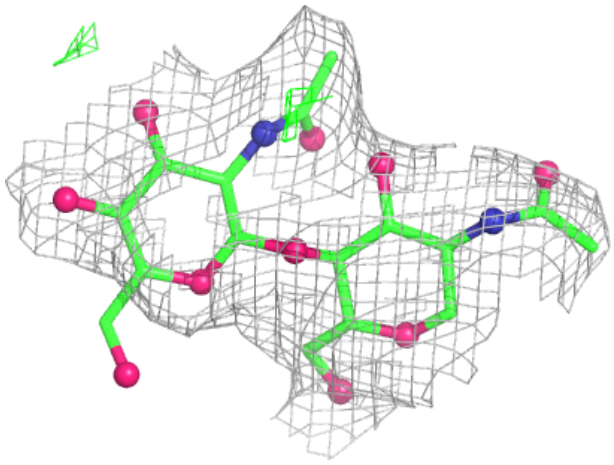
**Electron density around Chain m:**

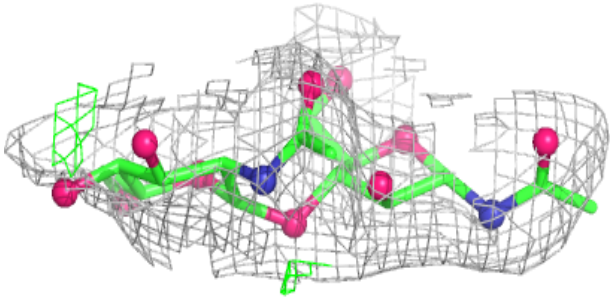
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

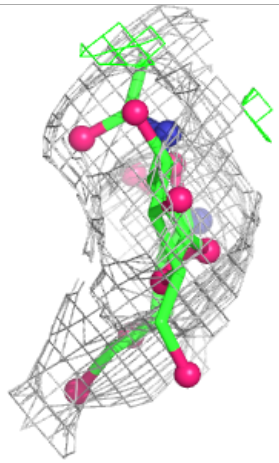


**Electron density around Chain n:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

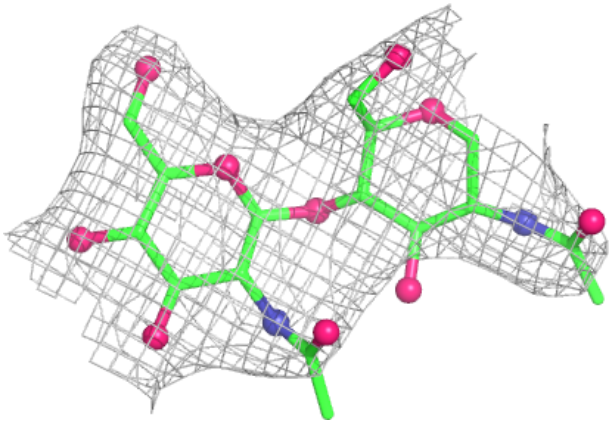


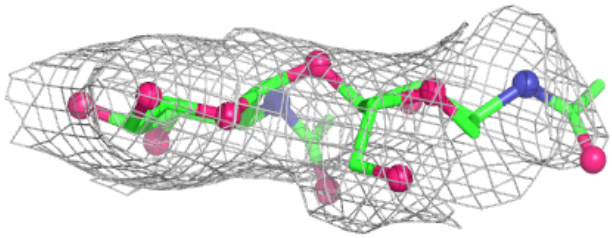


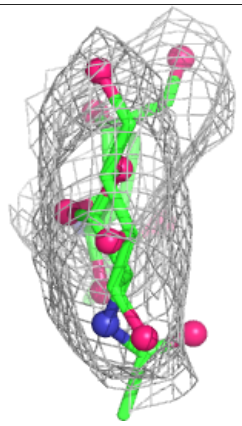


**Electron density around Chain o:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

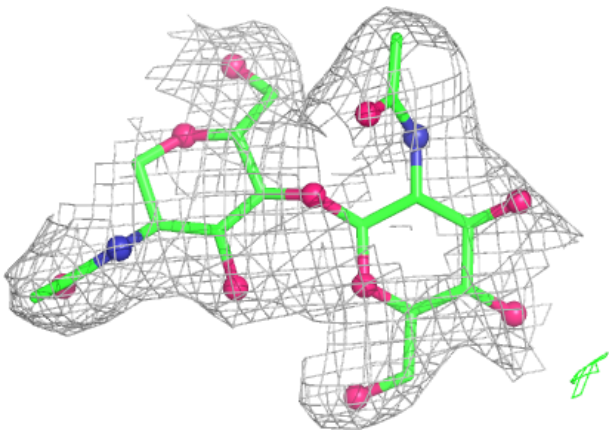


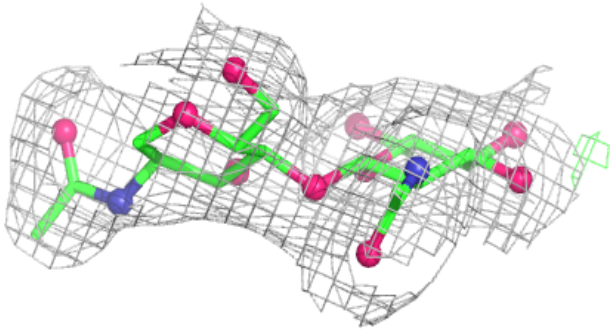


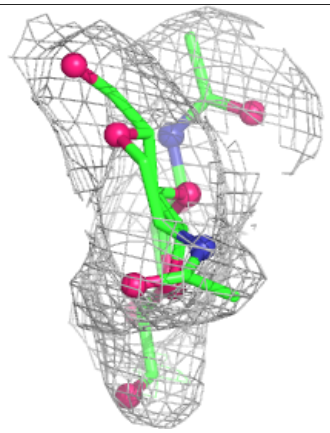


**Electron density around Chain p:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

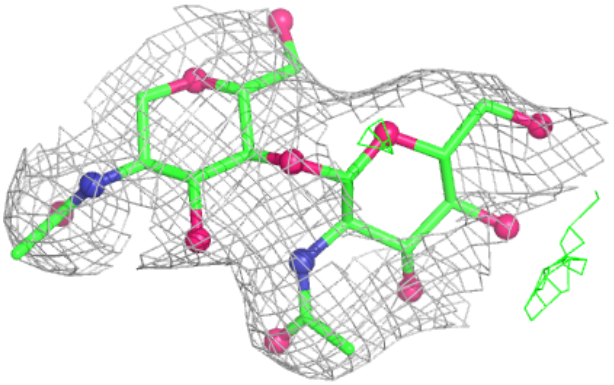


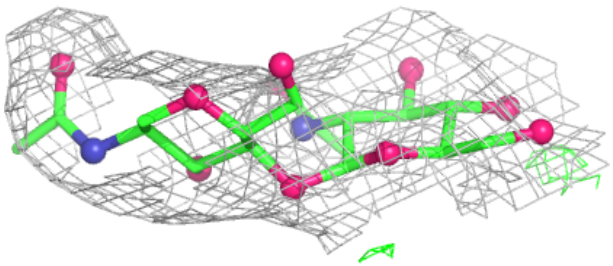


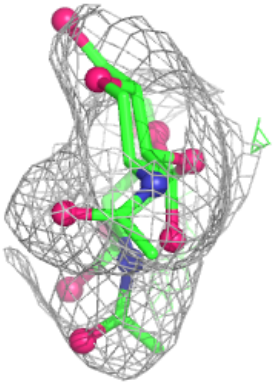


**Electron density around Chain q:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

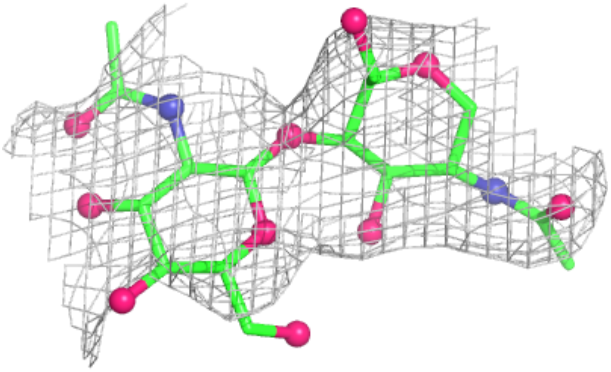


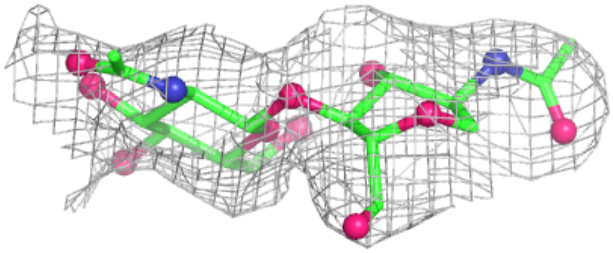


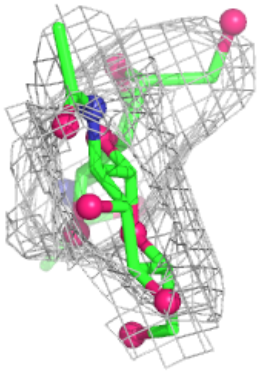


**Electron density around Chain s:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

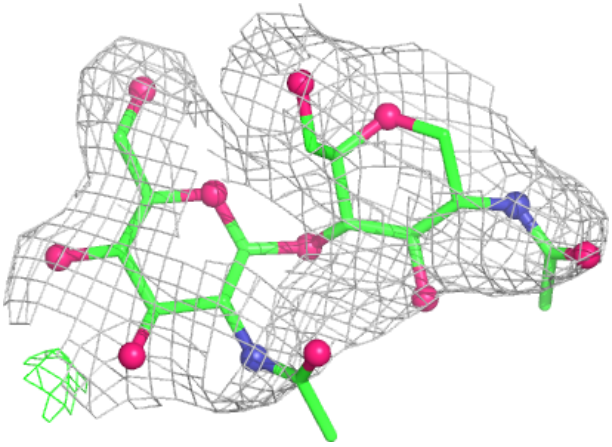


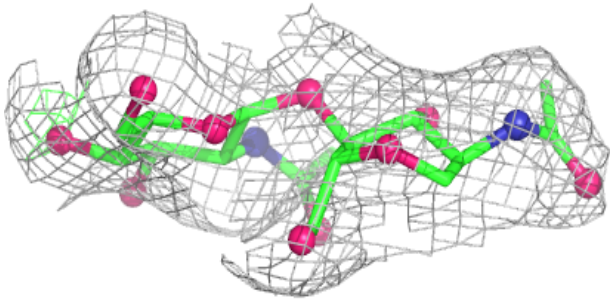


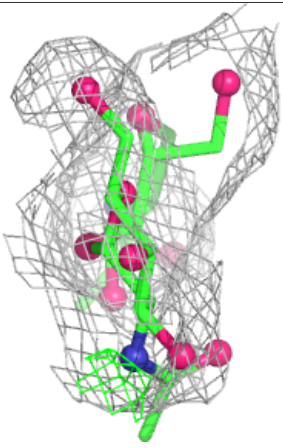


**Electron density around Chain t:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

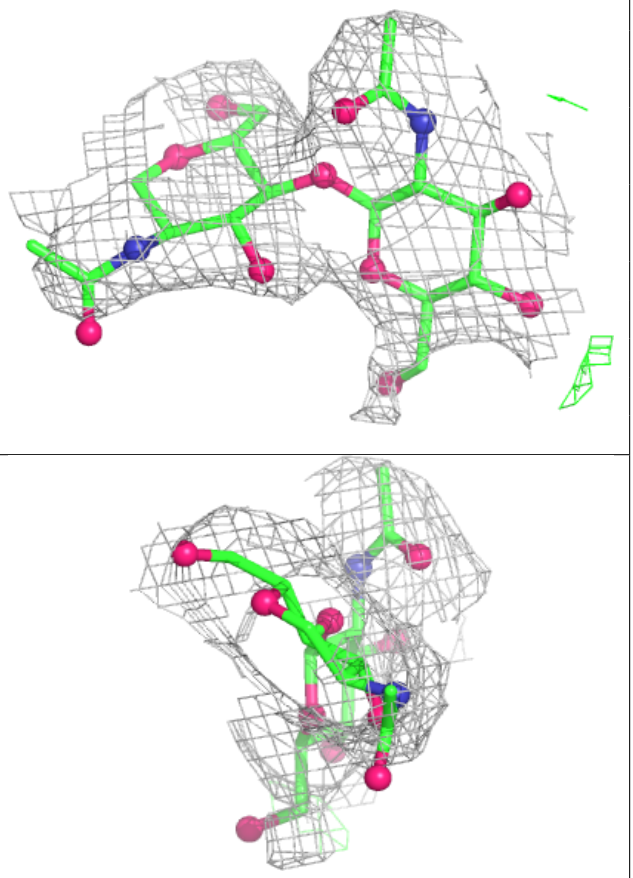






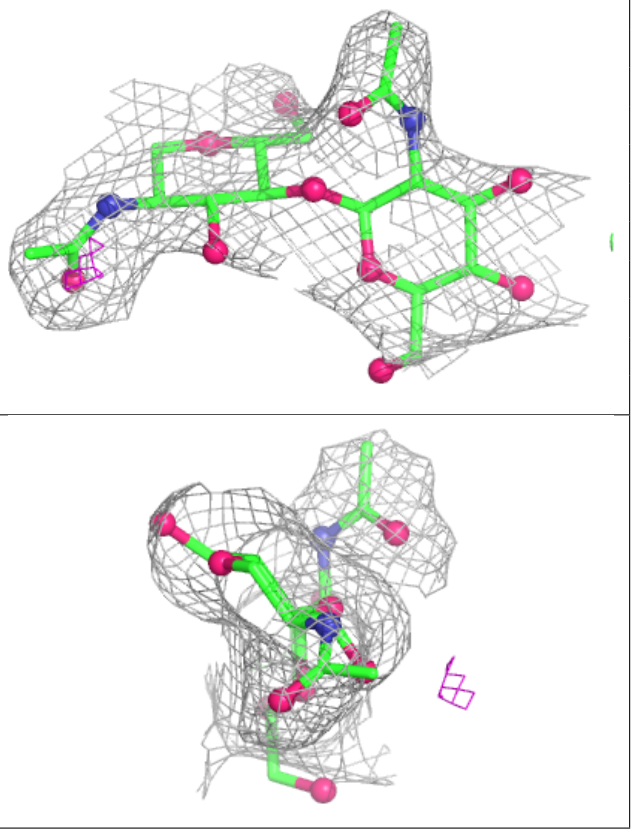
**Electron density around Chain u:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



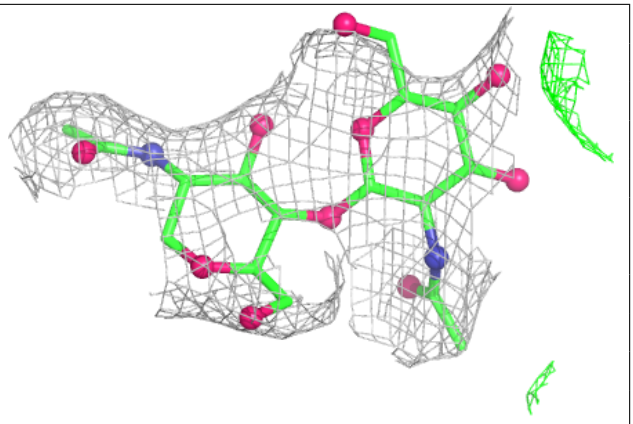
**Electron density around Chain v:**

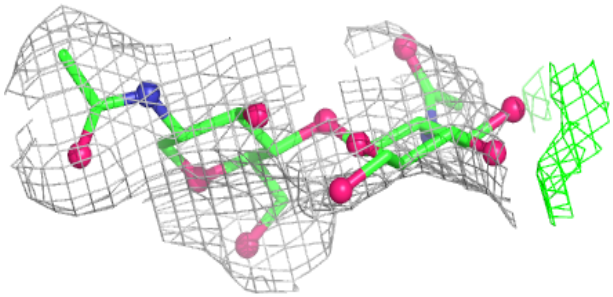
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

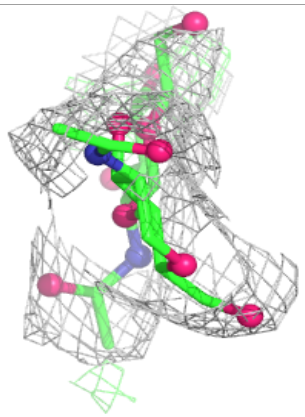


**Electron density around Chain x:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

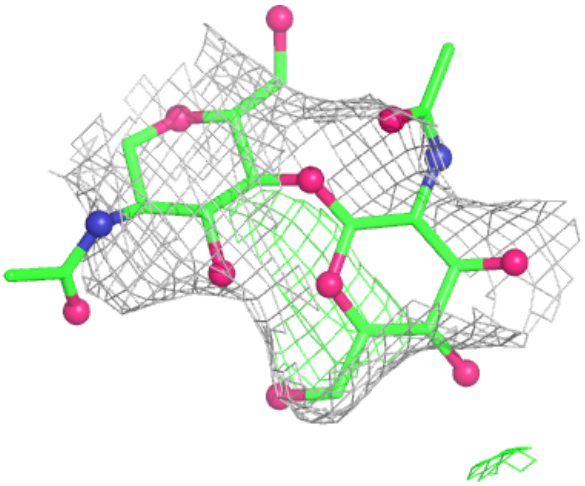


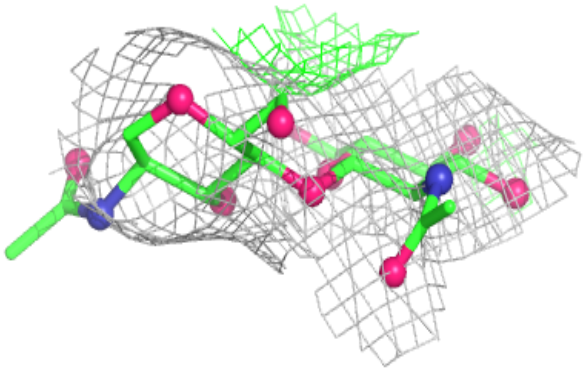


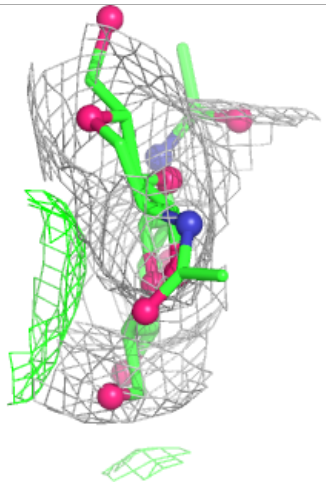


**Electron density around Chain 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

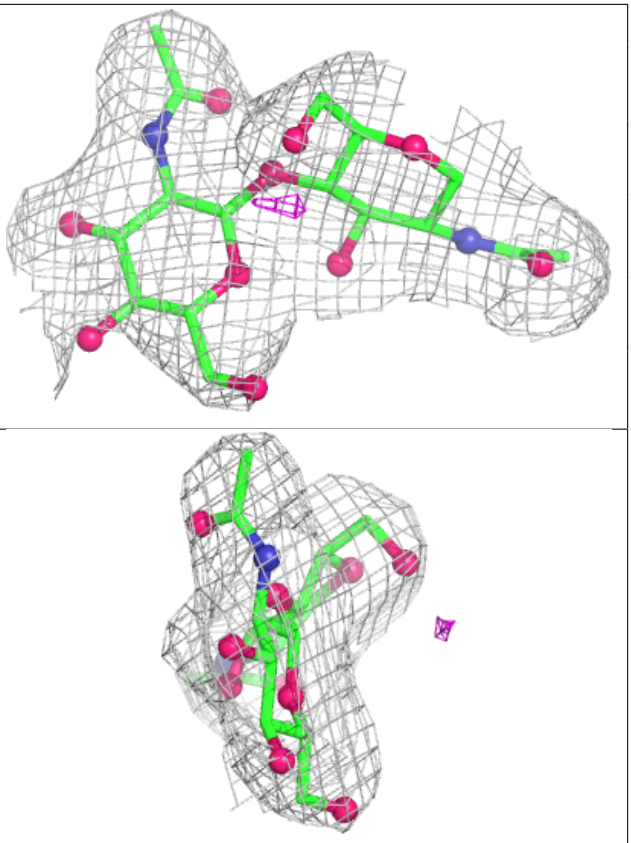






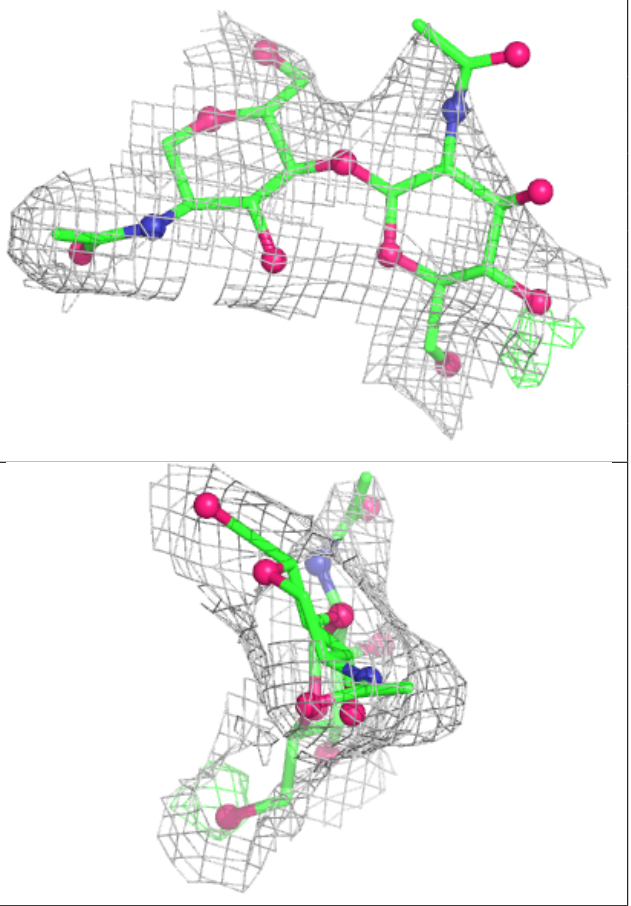
**Electron density around Chain 2:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



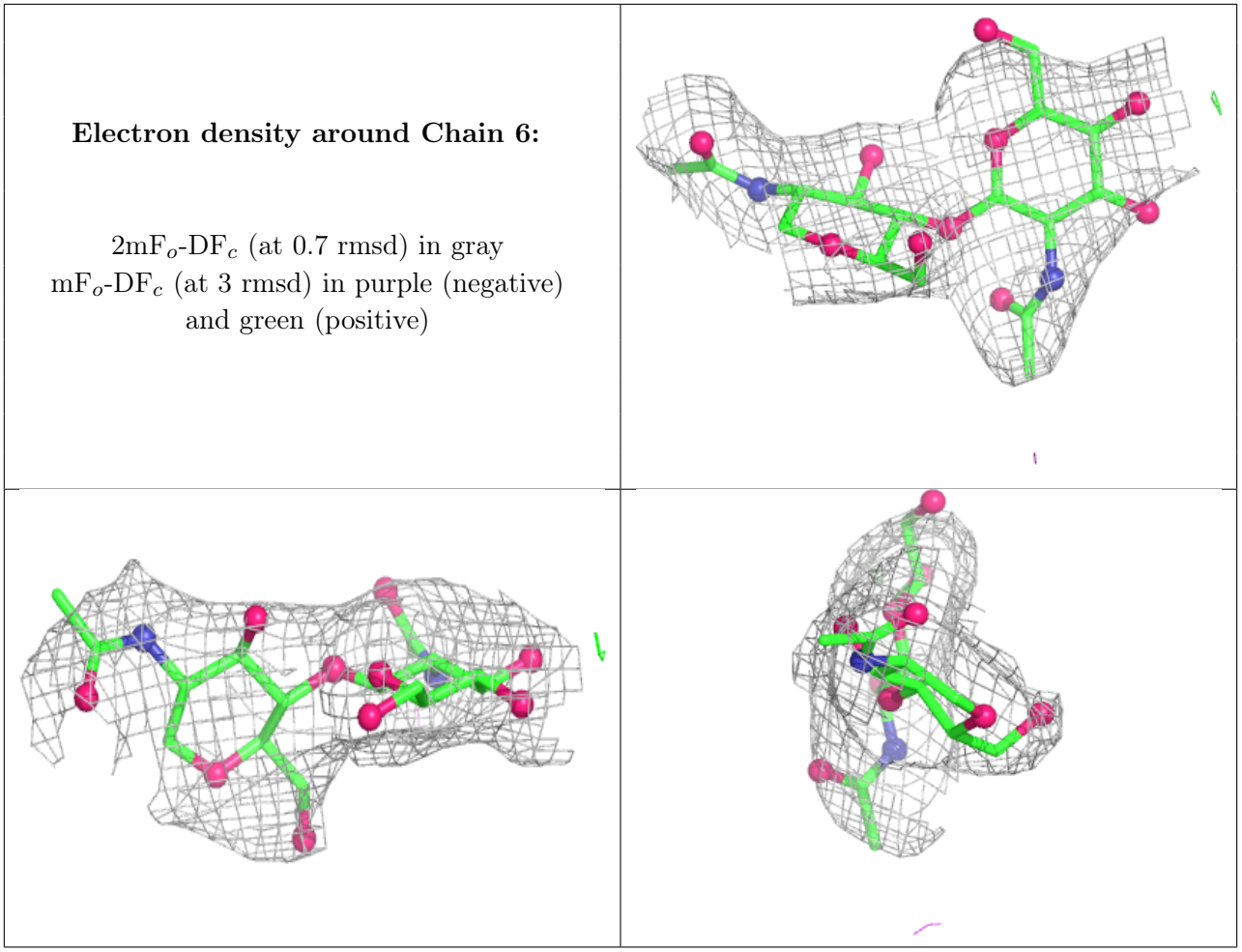
**Electron density around Chain 4:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



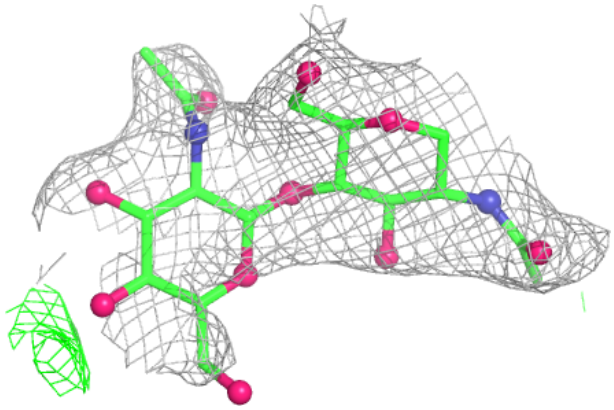
**Electron density around Chain 6:**

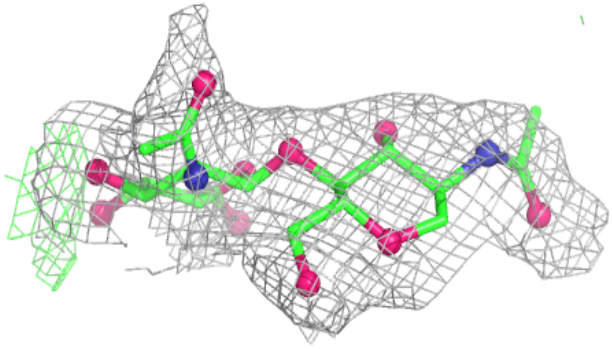
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

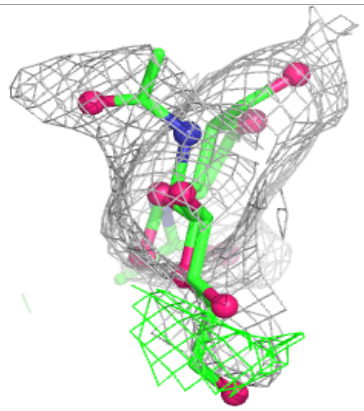


**Electron density around Chain 7:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

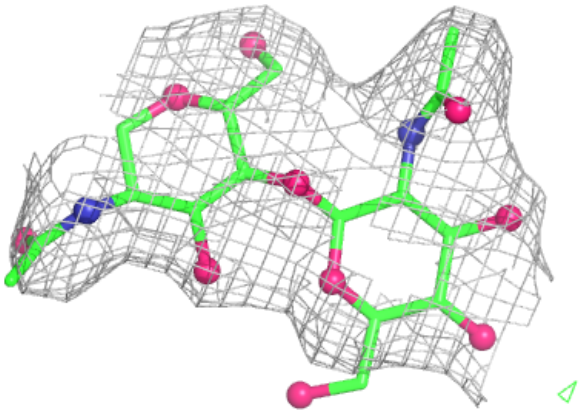


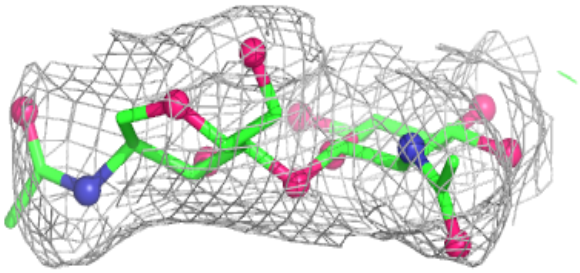


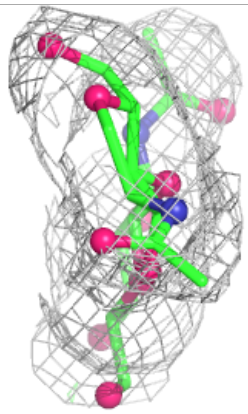


**Electron density around Chain 8:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

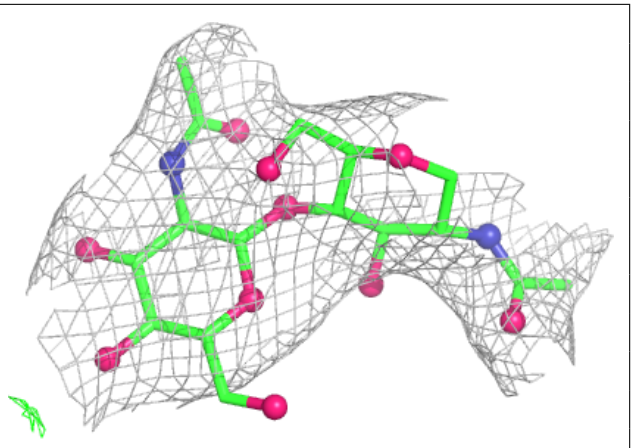


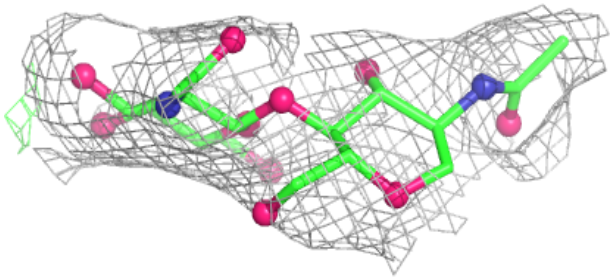


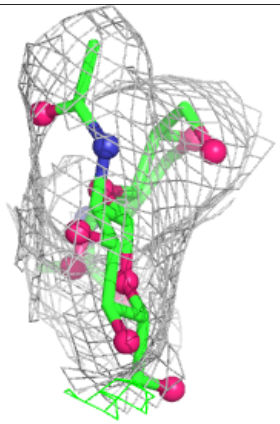


**Electron density around Chain 9:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

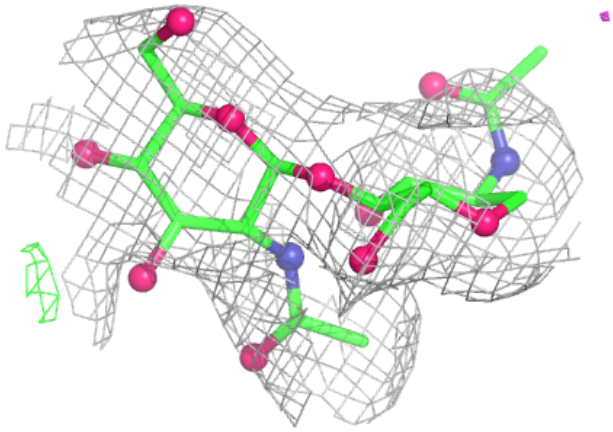


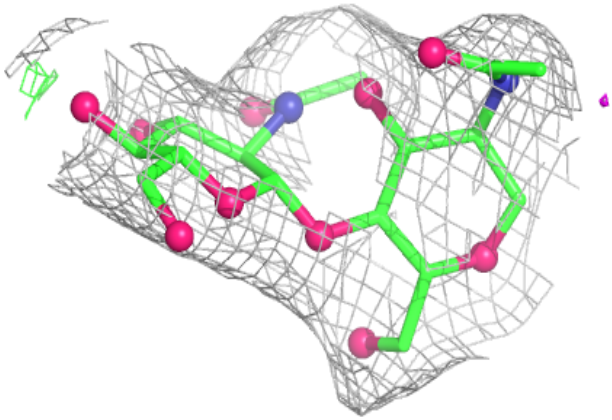


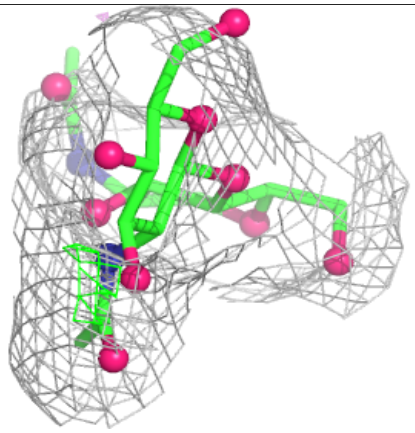


**Electron density around Chain BA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

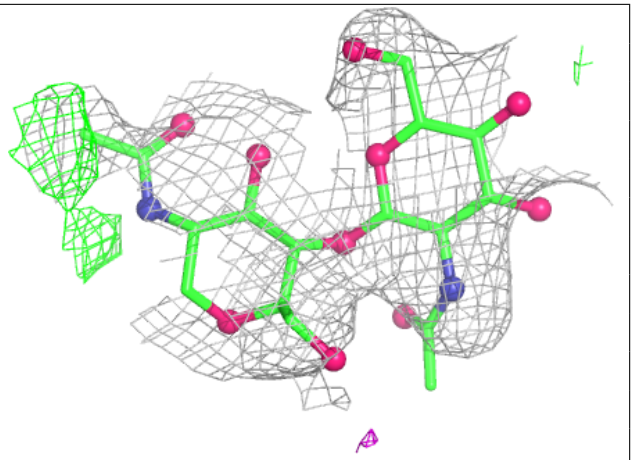


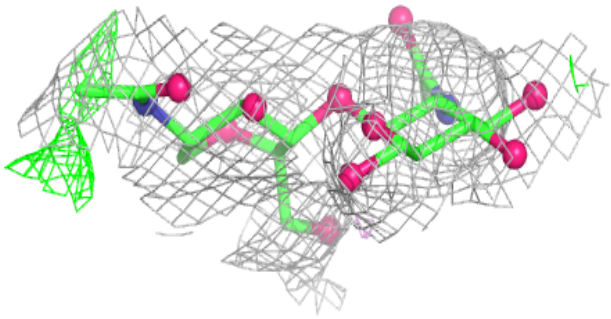


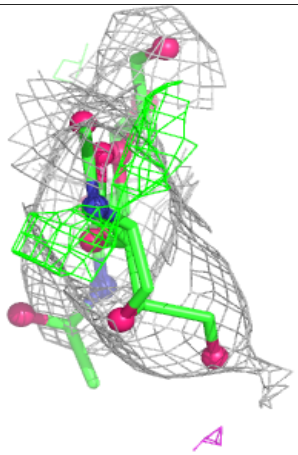


**Electron density around Chain HA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

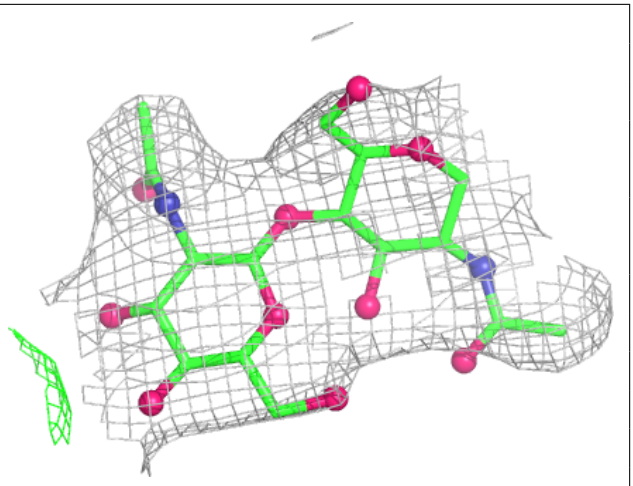


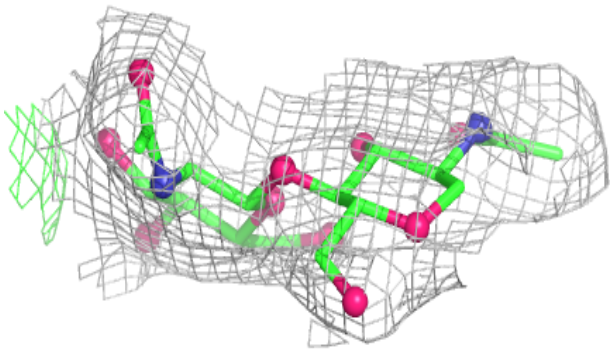


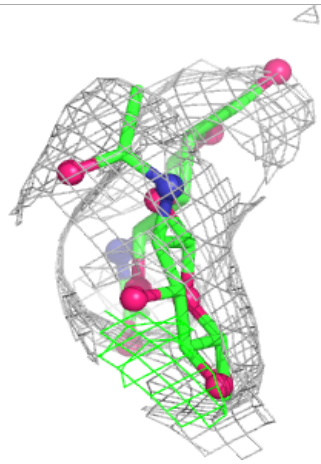


**Electron density around Chain IA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

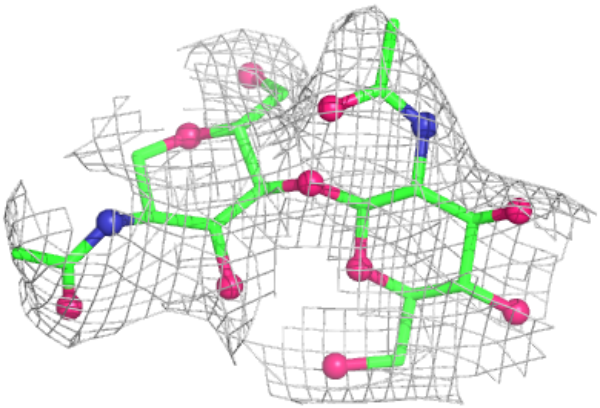


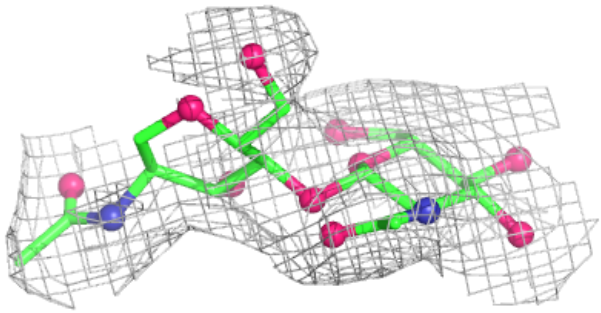


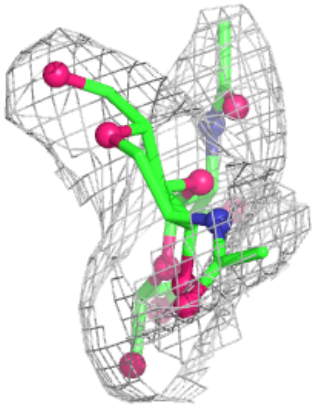


**Electron density around Chain JA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

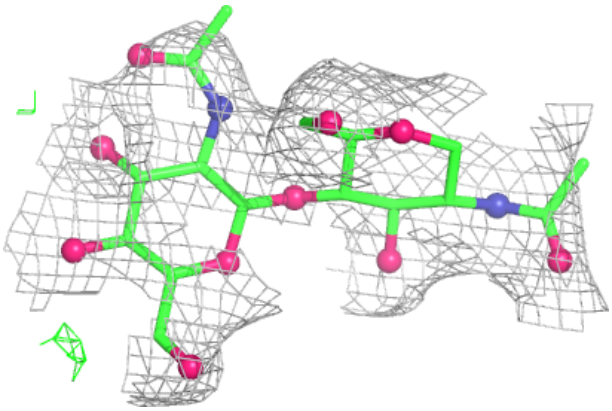


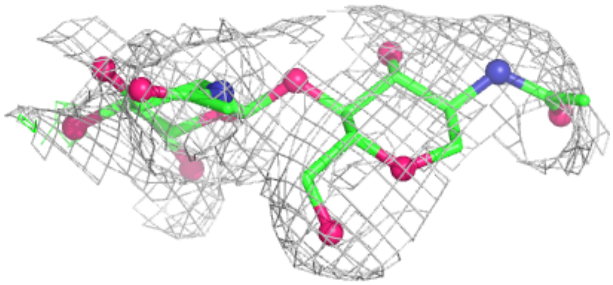


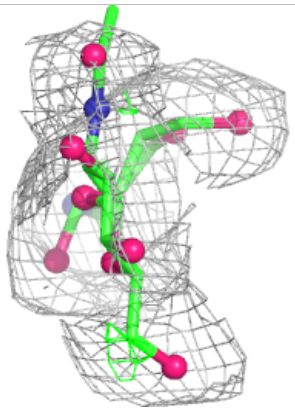


**Electron density around Chain MA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

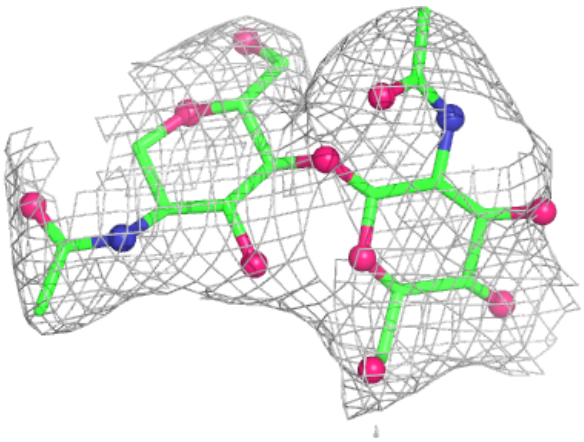


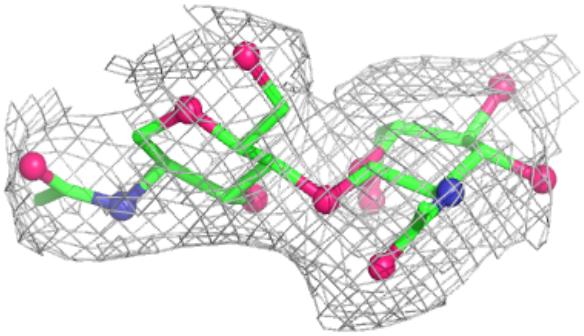


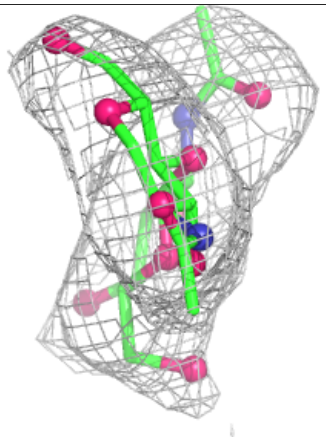


**Electron density around Chain OA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

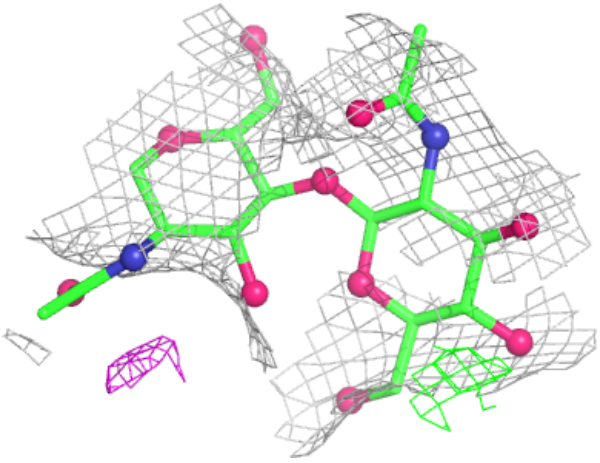


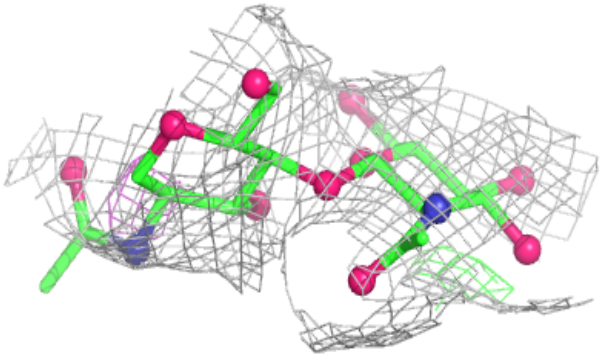


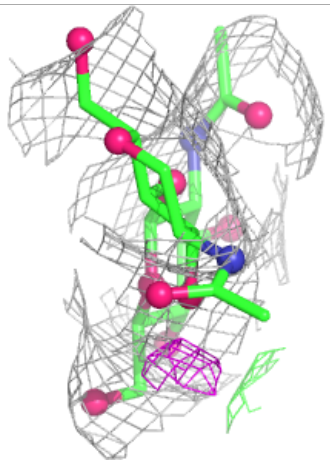


**Electron density around Chain QA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

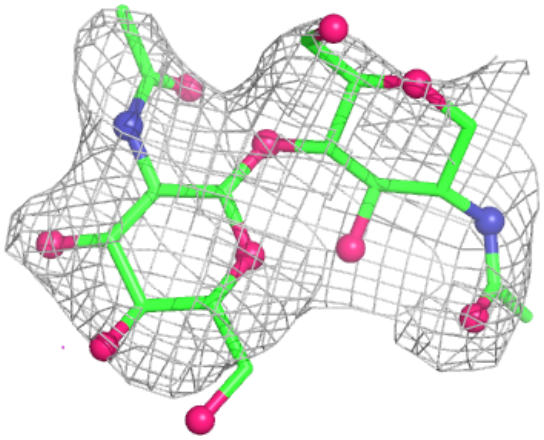


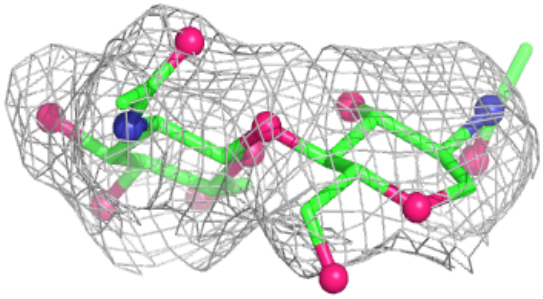


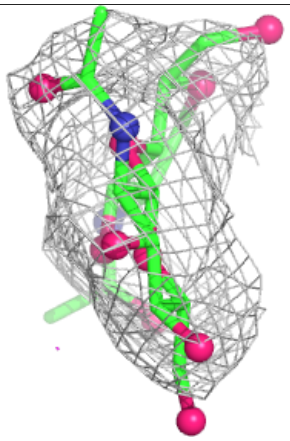


**Electron density around Chain RA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

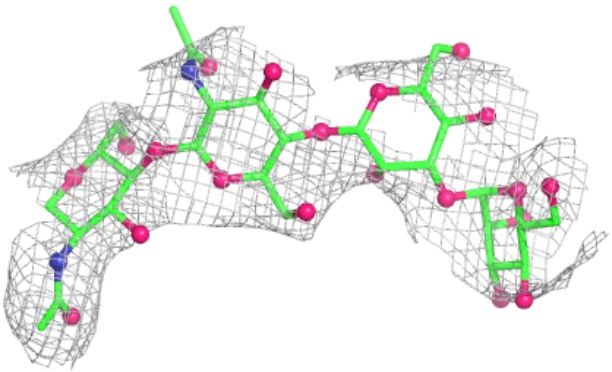


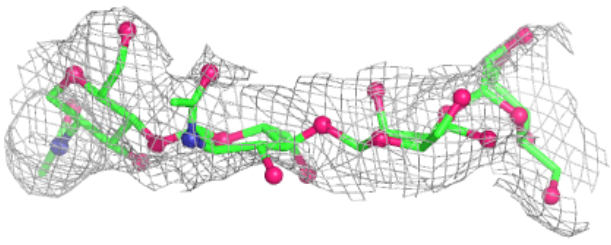


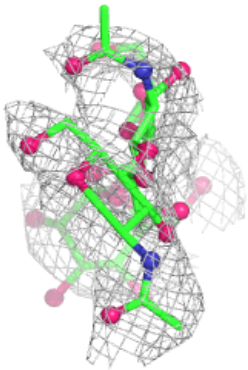


**Electron density around Chain g:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

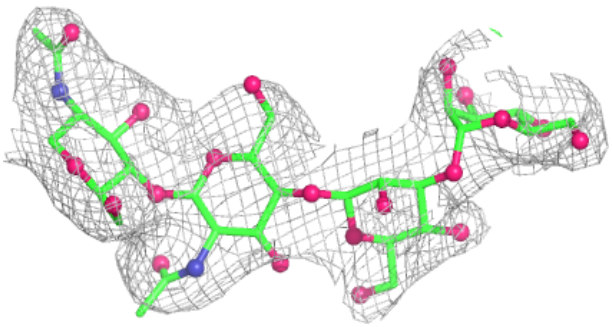


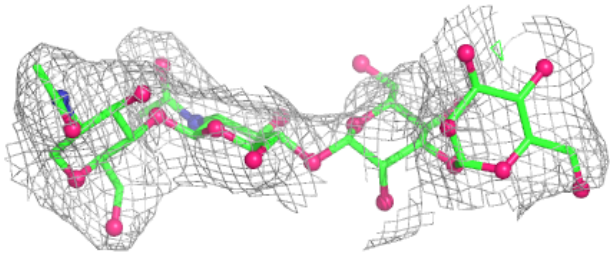


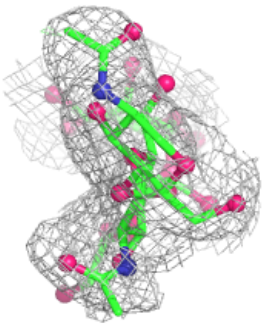


**Electron density around Chain l:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

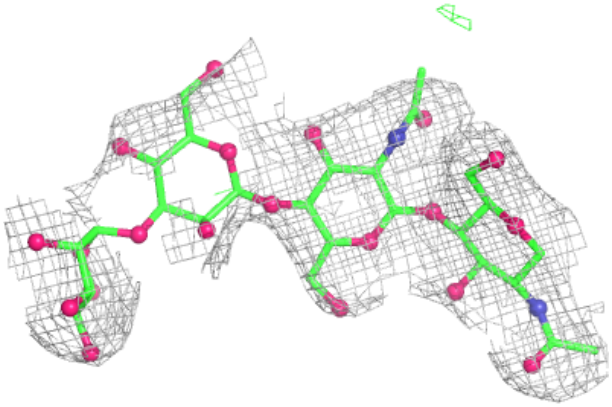


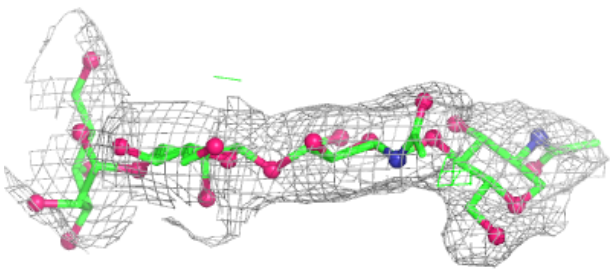


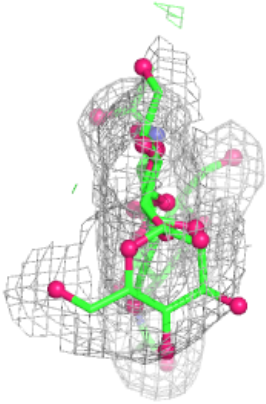


**Electron density around Chain AA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

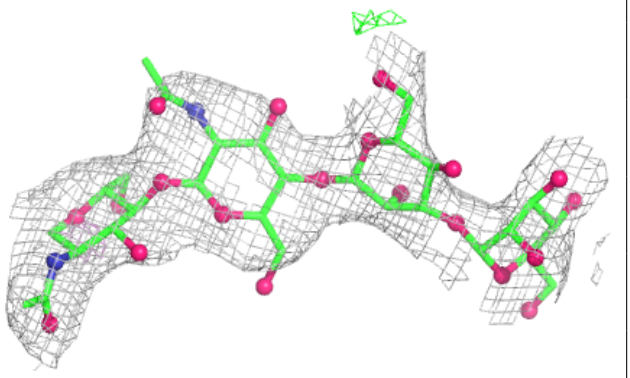


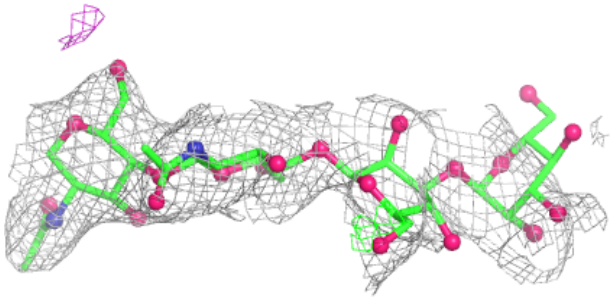


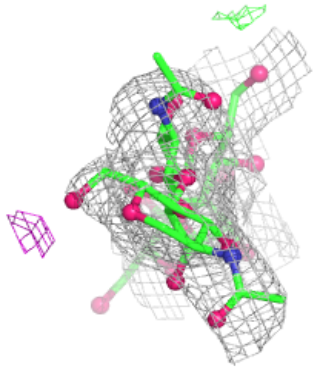


**Electron density around Chain FA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

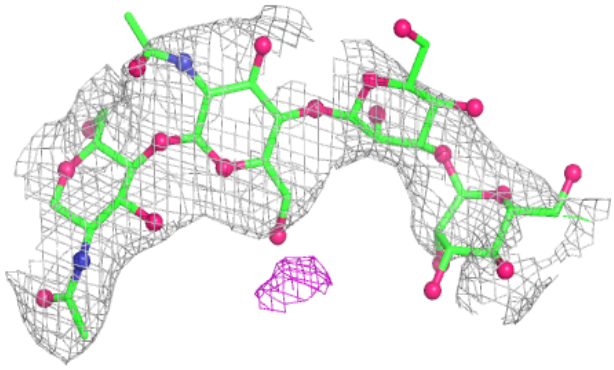


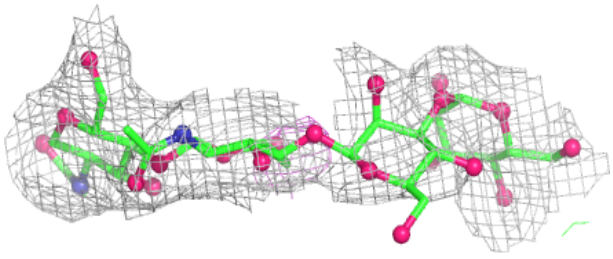


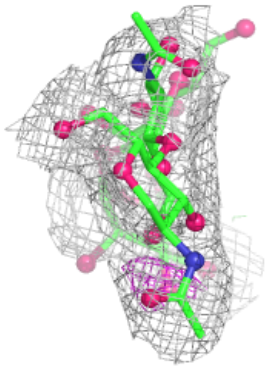


**Electron density around Chain KA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

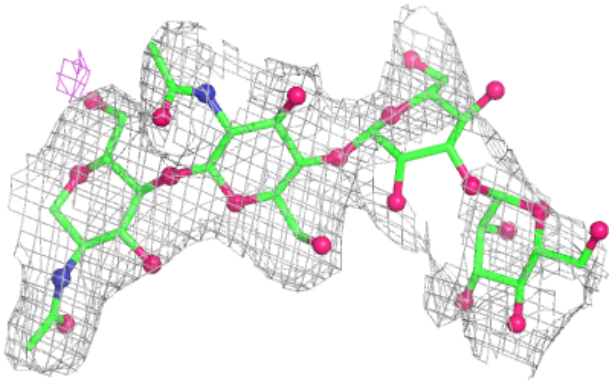


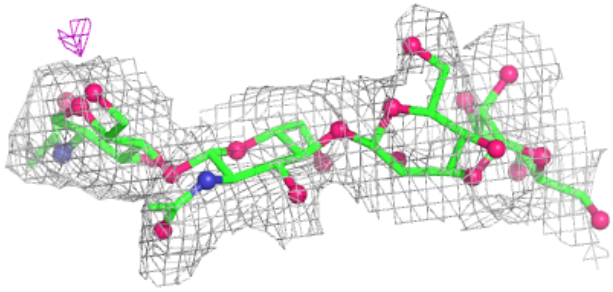


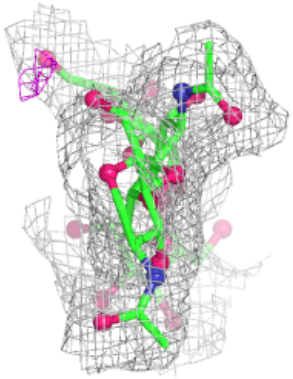


**Electron density around Chain PA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

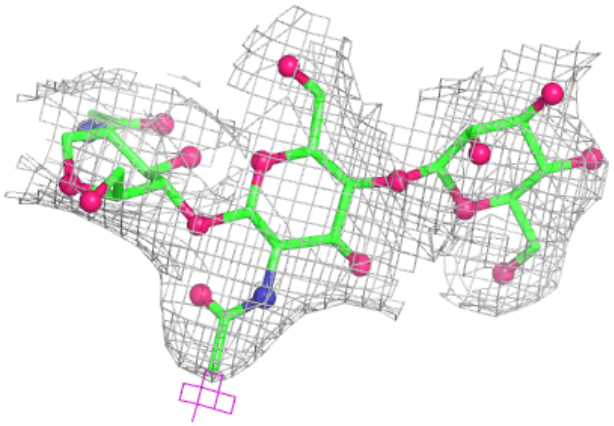


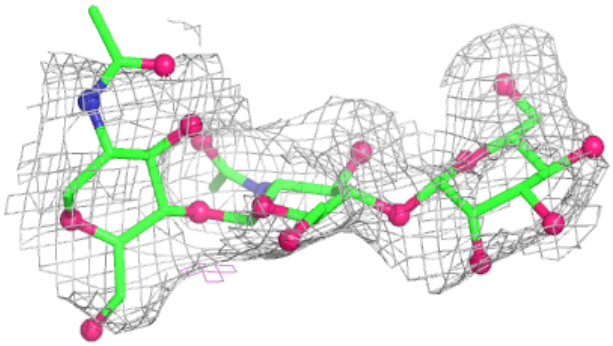


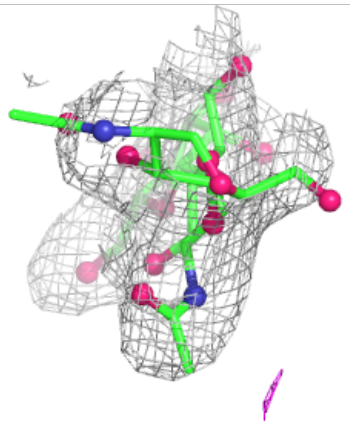


**Electron density around Chain h:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

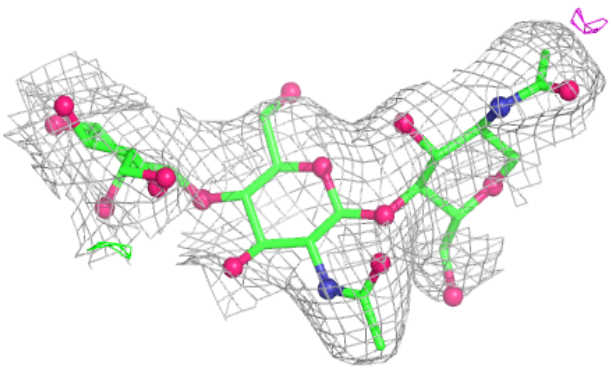


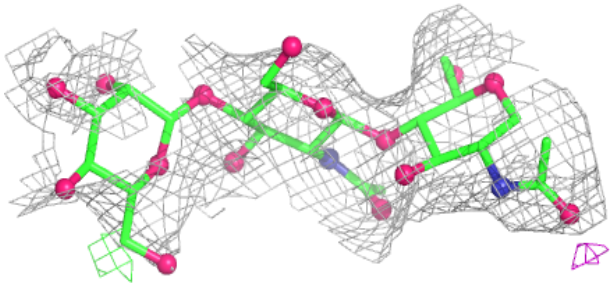


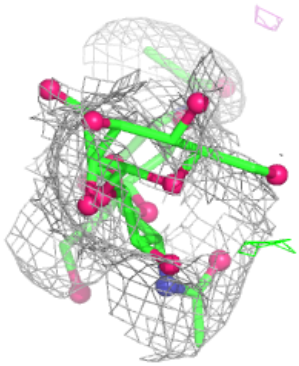


**Electron density around Chain k:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

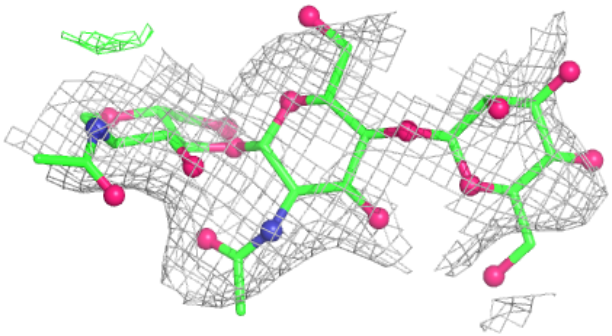


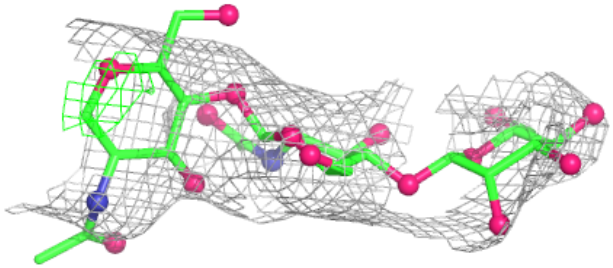


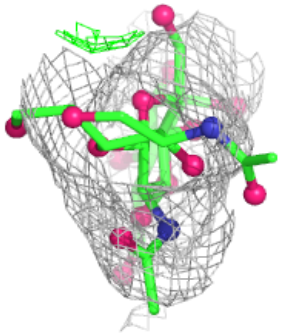


**Electron density around Chain r:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

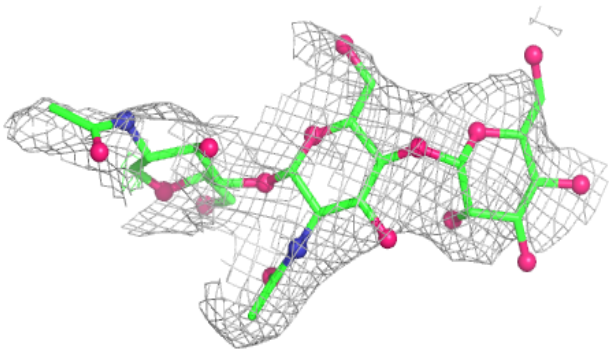


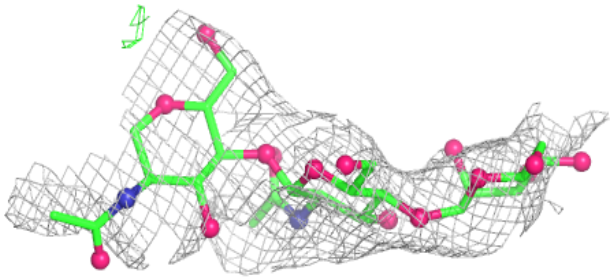


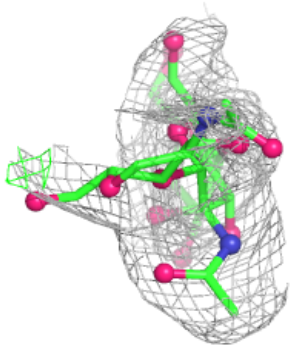


**Electron density around Chain w:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

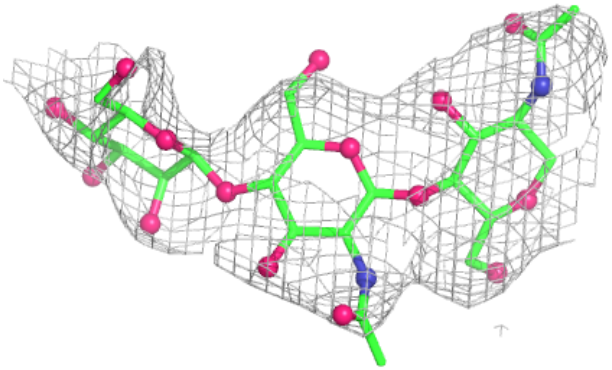


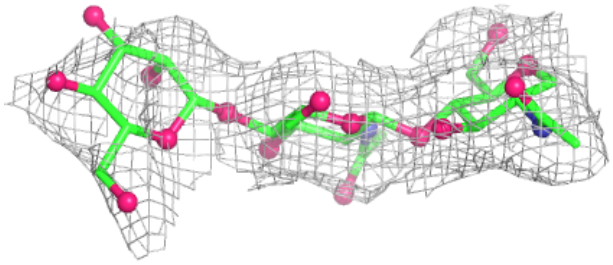


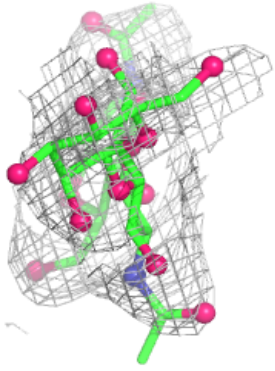


**Electron density around Chain y:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

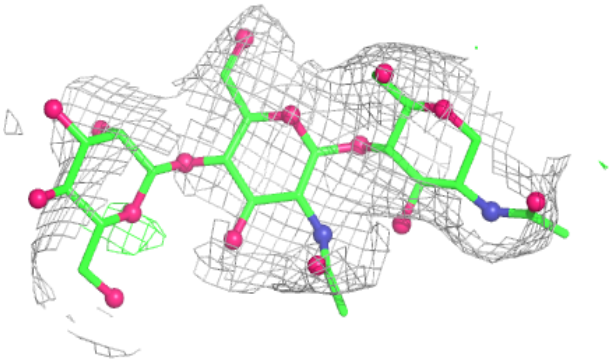


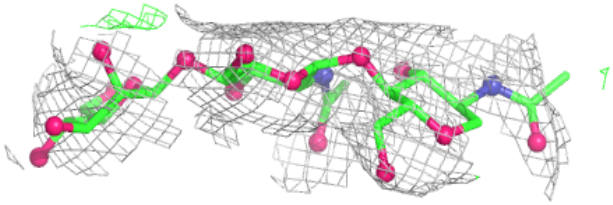


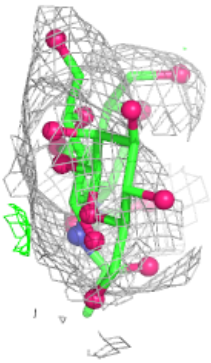


**Electron density around Chain 3:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

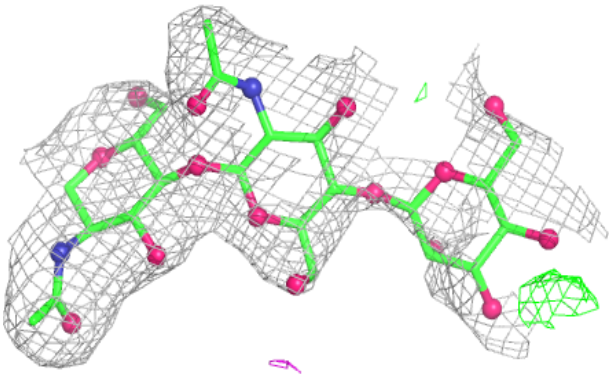


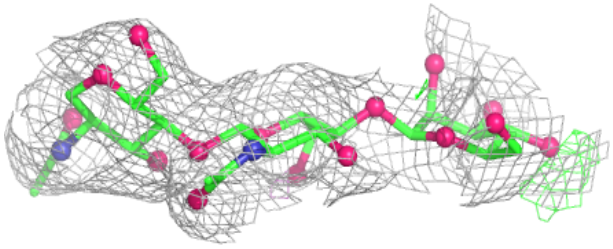


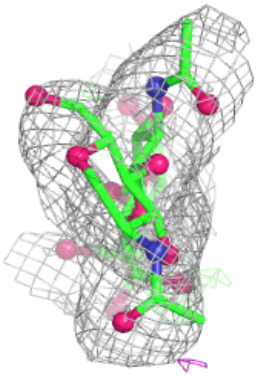


**Electron density around Chain 5:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

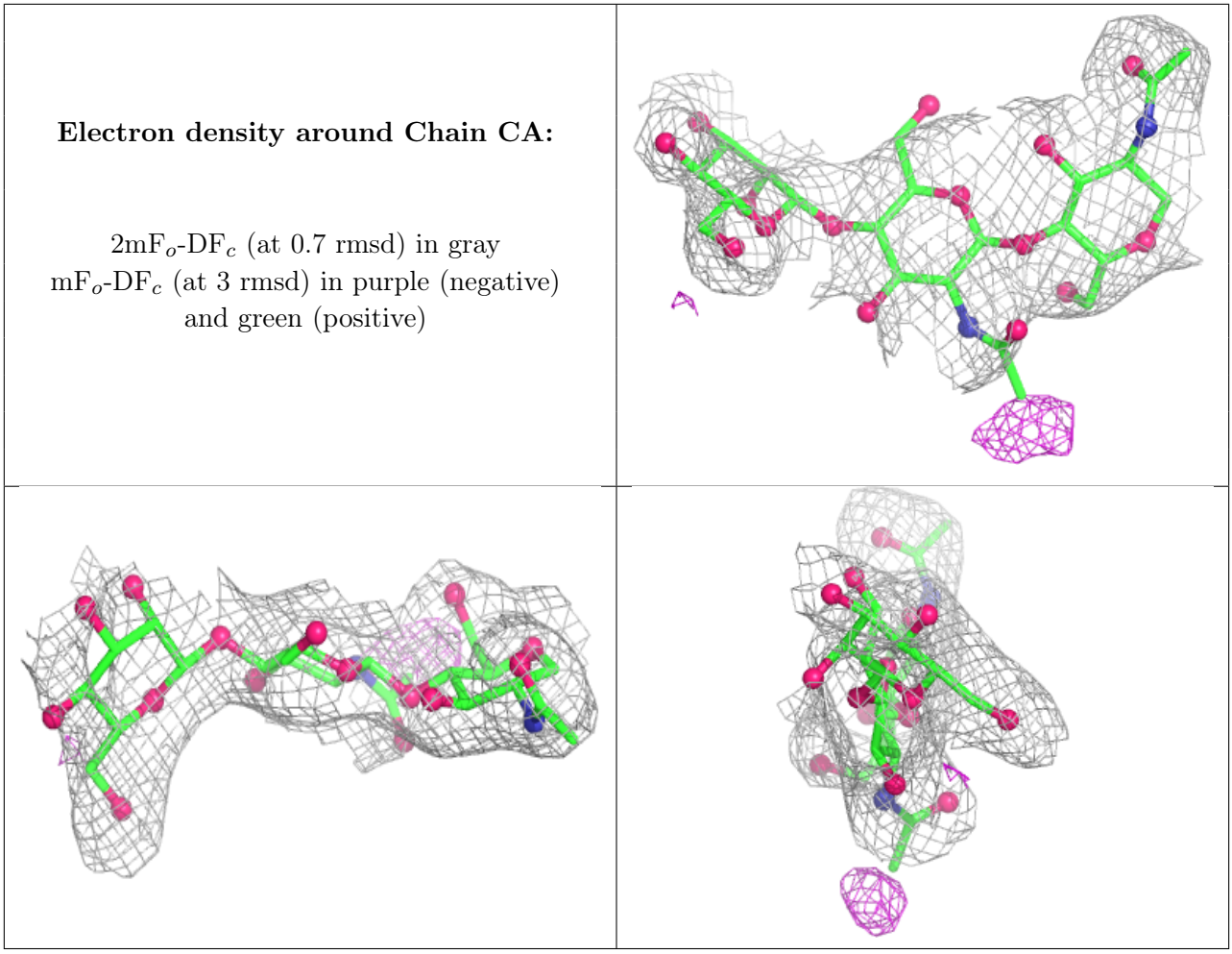






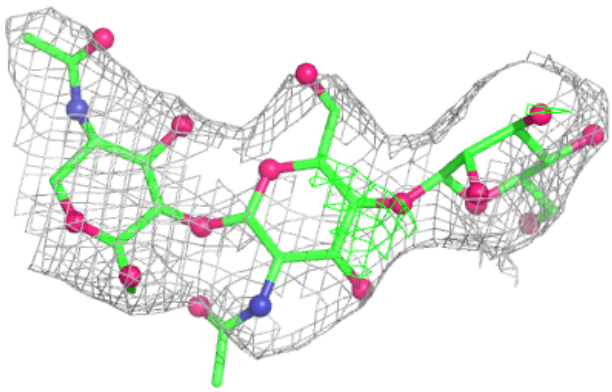
**Electron density around Chain CA:**

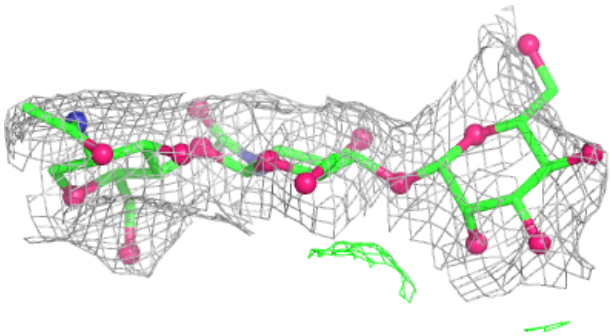
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

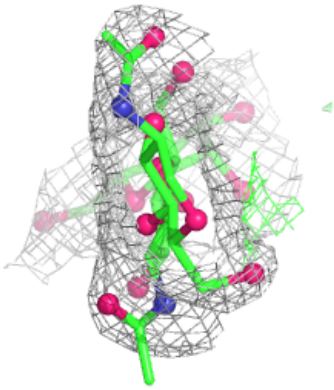


**Electron density around Chain DA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

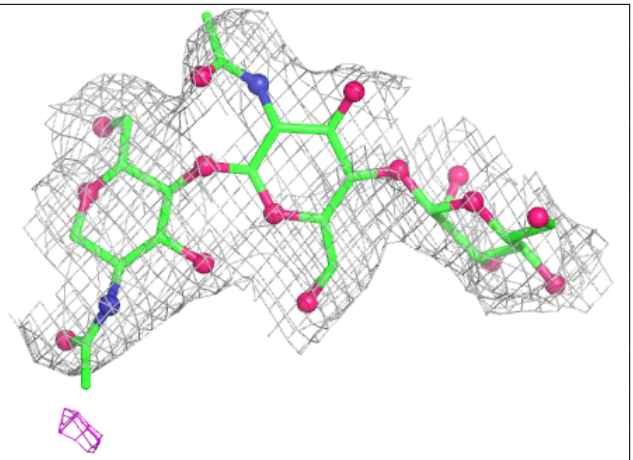


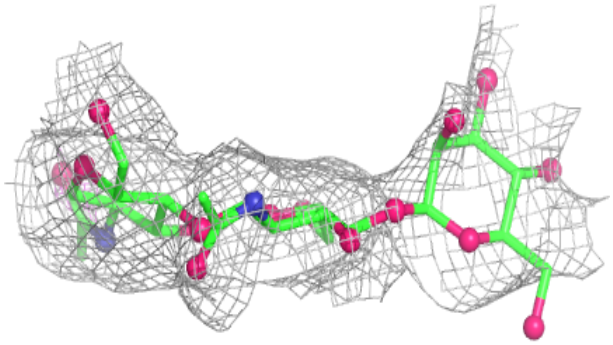


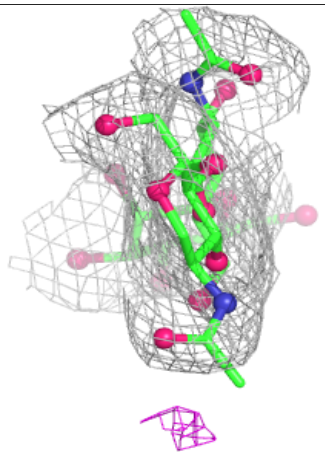


**Electron density around Chain EA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

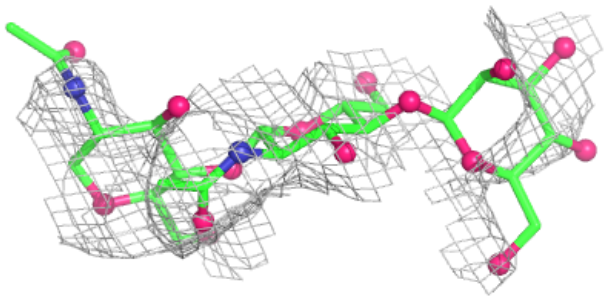


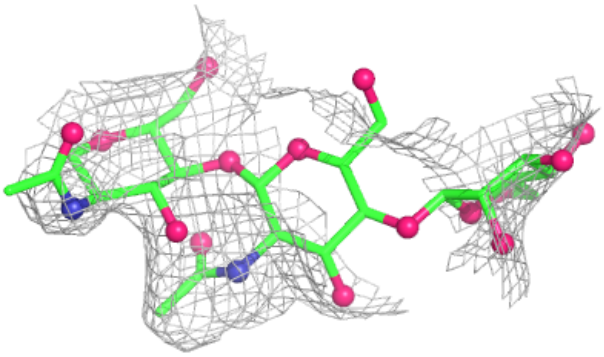


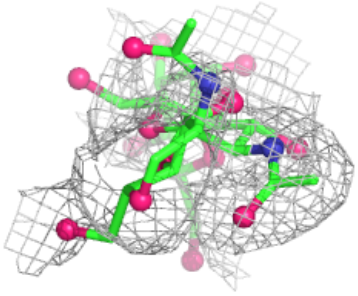


**Electron density around Chain GA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

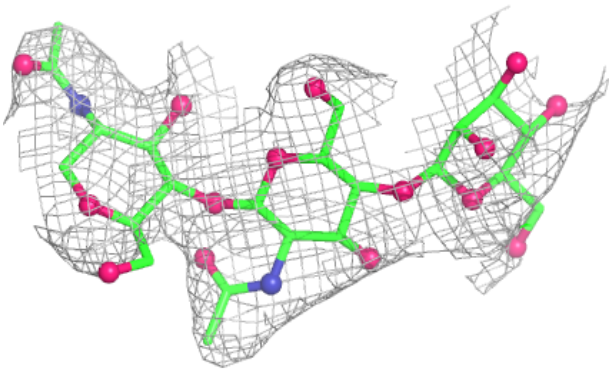


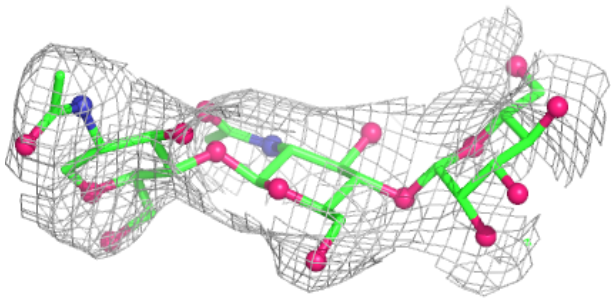


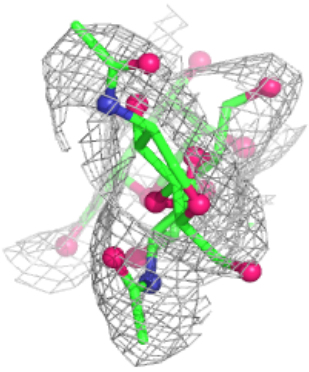


**Electron density around Chain LA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

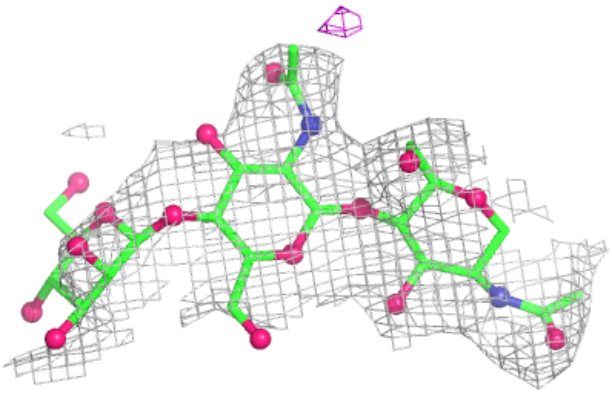


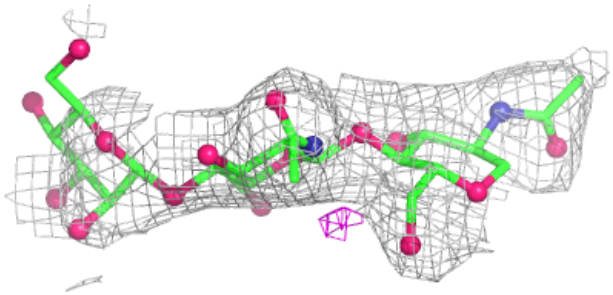


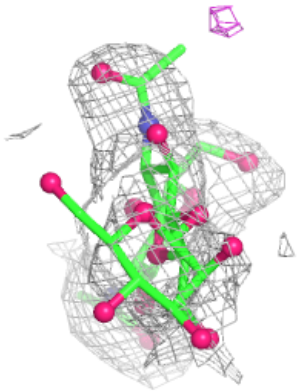


**Electron density around Chain NA:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

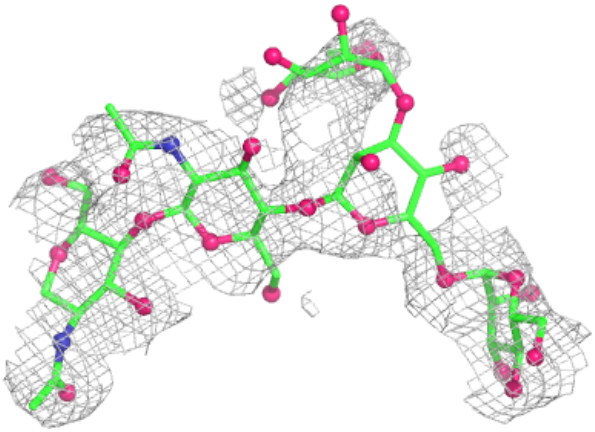


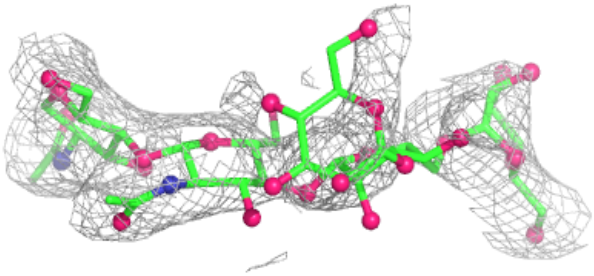


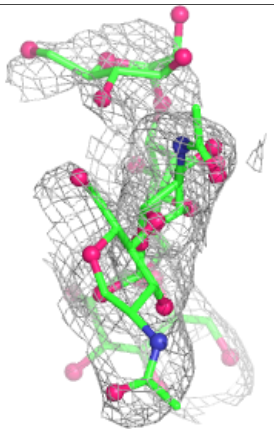


**Electron density around Chain z:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

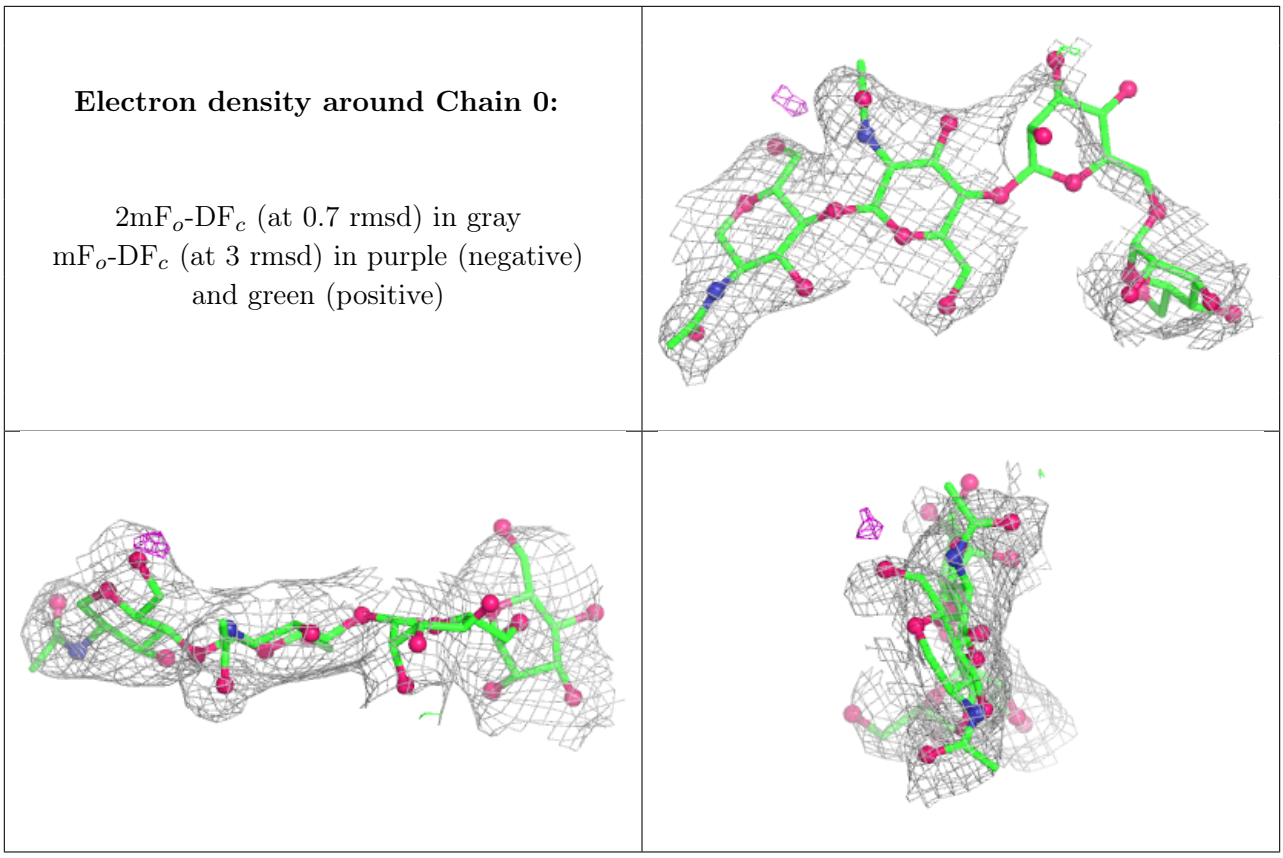






**Electron density around Chain 0:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 6.4 Ligands

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 9 | CUO | A | 5005[C] | 4/4 | 0.98 | 0.06 | 95,95,95,95 | 4 |
| 9 | CUO | A | 5005[D] | 4/4 | 0.98 | 0.06 | 95,95,95,95 | 4 |
| 9 | CUO | D | 5005[C] | 4/4 | 0.98 | 0.06 | 109,109,109,109 | 4 |
| 9 | CUO | D | 5005[D] | 4/4 | 0.98 | 0.06 | 109,109,109,109 | 4 |
| 9 | CUO | G | 2101[C] | 4/4 | 0.98 | 0.07 | 104,104,104,104 | 4 |
| 9 | CUO | G | 2101[D] | 4/4 | 0.98 | 0.07 | 104,104,104,104 | 4 |
| 9 | CUO | P | 5005[C] | 4/4 | 0.98 | 0.10 | 114,114,114,114 | 4 |
| 9 | CUO | P | 5005[D] | 4/4 | 0.98 | 0.10 | 114,114,114,114 | 4 |
| 9 | CUO | M | 2101[C] | 4/4 | 0.99 | 0.04 | 103,103,103,103 | 4 |
| 9 | CUO | M | 2101[D] | 4/4 | 0.99 | 0.04 | 103,103,103,103 | 4 |
| 9 | CUO | J | 5005[C] | 4/4 | 0.99 | 0.05 | 98,98,98,98 | 4 |
| 9 | CUO | J | 5005[D] | 4/4 | 0.99 | 0.05 | 98,98,98,98 | 4 |
| 9 | CUO | S | 2101[C] | 4/4 | 0.99 | 0.06 | 94,94,94,94 | 4 |
| 9 | CUO | S | 2101[D] | 4/4 | 0.99 | 0.06 | 94,94,94,94 | 4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 9 | CUO | U | 3401[A] | 4/4 | 0.99 | 0.08 | 81,81,81,81 | 4 |
| 9 | CUO | U | 3401[B] | 4/4 | 0.99 | 0.08 | 81,81,81,81 | 4 |
| 9 | CUO | V | 5005[C] | 4/4 | 0.99 | 0.07 | 113,113,113,113 | 4 |
| 9 | CUO | V | 5005[D] | 4/4 | 0.99 | 0.07 | 113,113,113,113 | 4 |
| 9 | CUO | Y | 2101[C] | 4/4 | 0.99 | 0.04 | 99,99,99,99 | 4 |
| 9 | CUO | Y | 2101[D] | 4/4 | 0.99 | 0.04 | 99,99,99,99 | 4 |
| 9 | CUO | a | 3401[A] | 4/4 | 0.99 | 0.04 | 85,85,85,85 | 4 |
| 9 | CUO | a | 3401[B] | 4/4 | 0.99 | 0.04 | 85,85,85,85 | 4 |
| 9 | CUO | b | 2101[C] | 4/4 | 0.99 | 0.05 | 106,106,106,106 | 4 |
| 9 | CUO | b | 2101[D] | 4/4 | 0.99 | 0.05 | 106,106,106,106 | 4 |
| 9 | CUO | G | 2104 | 4/4 | 1.00 | 0.03 | 58,85,92,97 | 0 |
| 9 | CUO | G | 2105 | 4/4 | 1.00 | 0.01 | 58,60,66,69 | 0 |
| 9 | CUO | H | 3001 | 4/4 | 1.00 | 0.02 | 58,60,72,78 | 0 |
| 9 | CUO | H | 3002 | 4/4 | 1.00 | 0.02 | 67,79,83,84 | 0 |
| 9 | CUO | I | 3401[A] | 4/4 | 1.00 | 0.04 | 84,84,84,84 | 4 |
| 9 | CUO | I | 3401[B] | 4/4 | 1.00 | 0.04 | 84,84,84,84 | 4 |
| 9 | CUO | J | 5001 | 4/4 | 1.00 | 0.03 | 49,52,60,69 | 0 |
| 9 | CUO | J | 5002 | 4/4 | 1.00 | 0.03 | 53,56,80,83 | 0 |
| 9 | CUO | J | 5003 | 4/4 | 1.00 | 0.03 | 89,96,96,103 | 0 |
| 9 | CUO | J | 5004 | 4/4 | 1.00 | 0.03 | 49,58,62,63 | 0 |
| 9 | CUO | B | 3001 | 4/4 | 1.00 | 0.03 | 49,55,75,88 | 0 |
| 9 | CUO | B | 3002 | 4/4 | 1.00 | 0.02 | 57,58,80,91 | 0 |
| 9 | CUO | K | 3001 | 4/4 | 1.00 | 0.01 | 57,73,73,80 | 0 |
| 9 | CUO | K | 3002 | 4/4 | 1.00 | 0.02 | 52,69,75,79 | 0 |
| 9 | CUO | L | 3401[A] | 4/4 | 1.00 | 0.02 | 100,100,100,100 | 4 |
| 9 | CUO | L | 3401[B] | 4/4 | 1.00 | 0.02 | 100,100,100,100 | 4 |
| 9 | CUO | C | 3401[A] | 4/4 | 1.00 | 0.03 | 99,99,99,99 | 4 |
| 9 | CUO | C | 3401[B] | 4/4 | 1.00 | 0.03 | 99,99,99,99 | 4 |
| 9 | CUO | M | 2102 | 4/4 | 1.00 | 0.03 | 41,52,59,63 | 0 |
| 9 | CUO | M | 2103 | 4/4 | 1.00 | 0.03 | 50,59,66,68 | 0 |
| 9 | CUO | M | 2104 | 4/4 | 1.00 | 0.06 | 58,70,74,76 | 0 |
| 9 | CUO | M | 2105 | 4/4 | 1.00 | 0.04 | 48,60,61,62 | 0 |
| 9 | CUO | N | 3001 | 4/4 | 1.00 | 0.02 | 36,39,74,80 | 0 |
| 9 | CUO | N | 3002 | 4/4 | 1.00 | 0.02 | 48,51,70,74 | 0 |
| 9 | CUO | O | 3401[A] | 4/4 | 1.00 | 0.03 | 85,85,85,85 | 4 |
| 9 | CUO | O | 3401[B] | 4/4 | 1.00 | 0.03 | 85,85,85,85 | 4 |
| 9 | CUO | P | 5001 | 4/4 | 1.00 | 0.03 | 36,38,56,71 | 0 |
| 9 | CUO | P | 5002 | 4/4 | 1.00 | 0.03 | 56,59,75,82 | 0 |
| 9 | CUO | P | 5003 | 4/4 | 1.00 | 0.03 | 45,54,76,83 | 0 |
| 9 | CUO | P | 5004 | 4/4 | 1.00 | 0.02 | 40,48,67,68 | 0 |
| 9 | CUO | D | 5001 | 4/4 | 1.00 | 0.03 | 64,68,95,98 | 0 |
| 9 | CUO | D | 5002 | 4/4 | 1.00 | 0.03 | 51,60,82,85 | 0 |

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*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 9 | CUO | Q | 3001 | 4/4 | 1.00 | 0.04 | 37,43,64,70 | 0 |
| 9 | CUO | Q | 3002 | 4/4 | 1.00 | 0.01 | 53,62,64,73 | 0 |
| 9 | CUO | R | 3401[A] | 4/4 | 1.00 | 0.02 | 84,84,84,84 | 4 |
| 9 | CUO | R | 3401[B] | 4/4 | 1.00 | 0.02 | 84,84,84,84 | 4 |
| 9 | CUO | D | 5003 | 4/4 | 1.00 | 0.02 | 60,62,67,79 | 0 |
| 9 | CUO | D | 5004 | 4/4 | 1.00 | 0.03 | 52,54,59,62 | 0 |
| 9 | CUO | S | 2102 | 4/4 | 1.00 | 0.03 | 54,65,85,90 | 0 |
| 9 | CUO | S | 2103 | 4/4 | 1.00 | 0.04 | 49,52,72,80 | 0 |
| 9 | CUO | S | 2104 | 4/4 | 1.00 | 0.05 | 74,79,82,87 | 0 |
| 9 | CUO | S | 2105 | 4/4 | 1.00 | 0.02 | 45,45,62,71 | 0 |
| 9 | CUO | T | 3001 | 4/4 | 1.00 | 0.02 | 44,59,84,85 | 0 |
| 9 | CUO | T | 3002 | 4/4 | 1.00 | 0.03 | 52,69,74,84 | 0 |
| 9 | CUO | A | 5003 | 4/4 | 1.00 | 0.02 | 79,87,89,89 | 0 |
| 9 | CUO | A | 5004 | 4/4 | 1.00 | 0.03 | 51,60,67,70 | 0 |
| 9 | CUO | V | 5001 | 4/4 | 1.00 | 0.05 | 39,39,64,66 | 0 |
| 9 | CUO | V | 5002 | 4/4 | 1.00 | 0.03 | 50,61,67,72 | 0 |
| 9 | CUO | V | 5003 | 4/4 | 1.00 | 0.05 | 66,79,89,90 | 0 |
| 9 | CUO | V | 5004 | 4/4 | 1.00 | 0.03 | 44,50,62,65 | 0 |
| 9 | CUO | E | 3001 | 4/4 | 1.00 | 0.01 | 55,55,80,85 | 0 |
| 9 | CUO | E | 3002 | 4/4 | 1.00 | 0.03 | 57,61,67,68 | 0 |
| 9 | CUO | W | 3001 | 4/4 | 1.00 | 0.05 | 37,41,72,78 | 0 |
| 9 | CUO | W | 3002 | 4/4 | 1.00 | 0.03 | 58,62,70,77 | 0 |
| 9 | CUO | X | 3401[A] | 4/4 | 1.00 | 0.04 | 121,121,121,121 | 4 |
| 9 | CUO | X | 3401[B] | 4/4 | 1.00 | 0.04 | 121,121,121,121 | 4 |
| 9 | CUO | F | 3401[A] | 4/4 | 1.00 | 0.03 | 86,86,86,86 | 4 |
| 9 | CUO | F | 3401[B] | 4/4 | 1.00 | 0.03 | 86,86,86,86 | 4 |
| 9 | CUO | Y | 2102 | 4/4 | 1.00 | 0.04 | 59,67,69,83 | 0 |
| 9 | CUO | Y | 2103 | 4/4 | 1.00 | 0.06 | 58,65,82,85 | 0 |
| 9 | CUO | Y | 2104 | 4/4 | 1.00 | 0.02 | 69,75,80,100 | 0 |
| 9 | CUO | Y | 2105 | 4/4 | 1.00 | 0.02 | 47,59,61,62 | 0 |
| 9 | CUO | Z | 3001 | 4/4 | 1.00 | 0.04 | 46,54,67,69 | 0 |
| 9 | CUO | Z | 3002 | 4/4 | 1.00 | 0.04 | 48,68,69,72 | 0 |
| 9 | CUO | A | 5001 | 4/4 | 1.00 | 0.03 | 70,73,87,92 | 0 |
| 9 | CUO | A | 5002 | 4/4 | 1.00 | 0.05 | 55,75,89,91 | 0 |
| 9 | CUO | G | 2102 | 4/4 | 1.00 | 0.02 | 57,62,65,70 | 0 |
| 9 | CUO | G | 2103 | 4/4 | 1.00 | 0.03 | 49,58,62,73 | 0 |
| 9 | CUO | b | 2102 | 4/4 | 1.00 | 0.02 | 60,63,73,78 | 0 |
| 9 | CUO | b | 2103 | 4/4 | 1.00 | 0.01 | 55,59,71,73 | 0 |
| 9 | CUO | b | 2104 | 4/4 | 1.00 | 0.04 | 60,75,83,94 | 0 |
| 9 | CUO | b | 2105 | 4/4 | 1.00 | 0.02 | 54,57,68,74 | 0 |
| 9 | CUO | c | 3001 | 4/4 | 1.00 | 0.03 | 48,56,77,80 | 0 |
| 9 | CUO | c | 3002 | 4/4 | 1.00 | 0.03 | 70,71,79,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 9 | CUO | d | 3401[A] | 4/4 | 1.00 | 0.03 | 111,111,111,111 | 4 |
| 9 | CUO | d | 3401[B] | 4/4 | 1.00 | 0.03 | 111,111,111,111 | 4 |

## 6.5 Other polymers (i)

There are no such residues in this entry.