# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 2Q6N / pdb_00002q6n |
| Title | : | Structure of Cytochrome P450 2B4 with Bound 1-(4-cholorophenyl)imidazole |
| Authors | : | Zhao, Y.; Sun, L.; Muralidhara, B.K.; Kumar, S.; White, M.A.; Stout, C.D.; Halpert, J.R. |
| Deposited on | : | 2007-06-05 |
| Resolution | : | 3.20 Å(reported) |

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

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

The 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 ⓘ) were used in the production of this report:

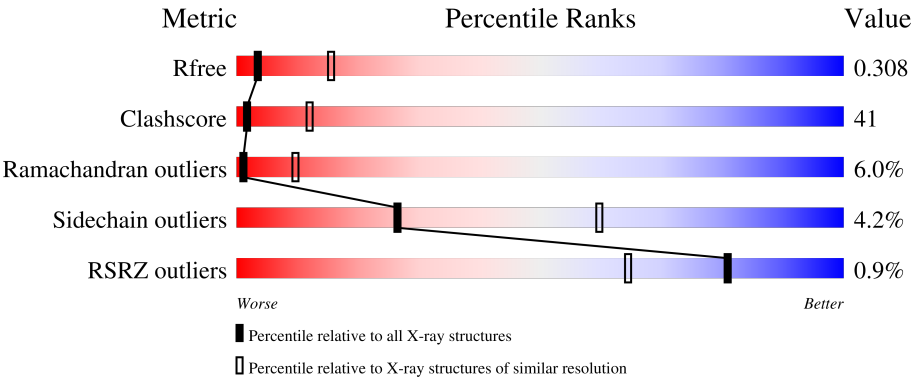
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4 | : | 9.0.010 (Gargrove) |
| Density-Fitness | : | 1.0.12 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 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 3.20 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 | 1466 (3.20-3.20) |
| Clashscore | 190562 | 1573 (3.20-3.20) |
| Ramachandran outliers | 187476 | 1548 (3.20-3.20) |
| Sidechain outliers | 187428 | 1547 (3.20-3.20) |
| RSRZ outliers | 180081 | 1466 (3.20-3.20) |

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 | 478 | 42% 48% 7% |
| 1 | B | 478 | % 40% 50% 7% |
| 1 | C | 478 | % 31% 57% 9% |
| 1 | D | 478 | % 36% 53% 9% |
| 1 | E | 478 | % 33% 56% 8% |

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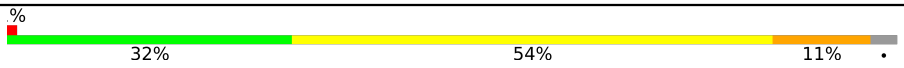
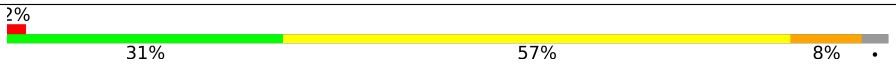
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 478 |   |
| 1 | G | 478 |   |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 3 | 1CI | G | 501 | - | - | X | - |

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26523 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 Cytochrome P450 2B4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3734 | 2405 | 649 | 669 | 11 | | | |
| 1 | B | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3734 | 2405 | 649 | 669 | 11 | | | |
| 1 | C | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3734 | 2405 | 649 | 669 | 11 | | | |
| 1 | D | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3734 | 2405 | 649 | 669 | 11 | | | |
| 1 | E | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3734 | 2405 | 649 | 669 | 11 | | | |
| 1 | F | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3734 | 2405 | 649 | 669 | 11 | | | |
| 1 | G | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3734 | 2405 | 649 | 669 | 11 | | | |

There are 245 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 21 | ALA | GLU | engineered mutation | UNP P00178 |
| A | ? | - | PHE | deletion | UNP P00178 |
| A | ? | - | SER | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | ALA | deletion | UNP P00178 |
| A | ? | - | PHE | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | ALA | deletion | UNP P00178 |
| A | ? | - | GLY | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | LEU | deletion | UNP P00178 |
| A | ? | - | PHE | deletion | UNP P00178 |
| A | ? | - | ARG | deletion | UNP P00178 |
| A | 22 | LYS | GLY | engineered mutation | UNP P00178 |
| A | 23 | LYS | HIS | engineered mutation | UNP P00178 |
| A | 24 | THR | PRO | engineered mutation | UNP P00178 |
| A | 25 | SER | LYS | engineered mutation | UNP P00178 |
| A | 26 | SER | ALA | engineered mutation | UNP P00178 |
| A | 27 | LYS | HIS | engineered mutation | UNP P00178 |
| A | 29 | LYS | ARG | engineered mutation | UNP P00178 |
| A | 221 | SER | PRO | engineered mutation | UNP P00178 |
| A | 226 | TYR | HIS | engineered mutation | UNP P00178 |
| A | 492 | HIS | - | expression tag | UNP P00178 |
| A | 493 | HIS | - | expression tag | UNP P00178 |
| A | 494 | HIS | - | expression tag | UNP P00178 |
| A | 495 | HIS | - | expression tag | UNP P00178 |
| A | 496 | HIS | - | expression tag | UNP P00178 |
| A | 497 | HIS | - | expression tag | UNP P00178 |
| B | 21 | ALA | GLU | engineered mutation | UNP P00178 |
| B | ? | - | PHE | deletion | UNP P00178 |
| B | ? | - | SER | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | ALA | deletion | UNP P00178 |
| B | ? | - | PHE | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | ALA | deletion | UNP P00178 |
| B | ? | - | GLY | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | LEU | deletion | UNP P00178 |
| B | ? | - | PHE | deletion | UNP P00178 |
| B | ? | - | ARG | deletion | UNP P00178 |
| B | 22 | LYS | GLY | engineered mutation | UNP P00178 |
| B | 23 | LYS | HIS | engineered mutation | UNP P00178 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 24 | THR | PRO | engineered mutation | UNP P00178 |
| B | 25 | SER | LYS | engineered mutation | UNP P00178 |
| B | 26 | SER | ALA | engineered mutation | UNP P00178 |
| B | 27 | LYS | HIS | engineered mutation | UNP P00178 |
| B | 29 | LYS | ARG | engineered mutation | UNP P00178 |
| B | 221 | SER | PRO | engineered mutation | UNP P00178 |
| B | 226 | TYR | HIS | engineered mutation | UNP P00178 |
| B | 492 | HIS | - | expression tag | UNP P00178 |
| B | 493 | HIS | - | expression tag | UNP P00178 |
| B | 494 | HIS | - | expression tag | UNP P00178 |
| B | 495 | HIS | - | expression tag | UNP P00178 |
| B | 496 | HIS | - | expression tag | UNP P00178 |
| B | 497 | HIS | - | expression tag | UNP P00178 |
| C | 21 | ALA | GLU | engineered mutation | UNP P00178 |
| C | ? | - | PHE | deletion | UNP P00178 |
| C | ? | - | SER | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | ALA | deletion | UNP P00178 |
| C | ? | - | PHE | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | ALA | deletion | UNP P00178 |
| C | ? | - | GLY | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | LEU | deletion | UNP P00178 |
| C | ? | - | PHE | deletion | UNP P00178 |
| C | ? | - | ARG | deletion | UNP P00178 |
| C | 22 | LYS | GLY | engineered mutation | UNP P00178 |
| C | 23 | LYS | HIS | engineered mutation | UNP P00178 |
| C | 24 | THR | PRO | engineered mutation | UNP P00178 |
| C | 25 | SER | LYS | engineered mutation | UNP P00178 |
| C | 26 | SER | ALA | engineered mutation | UNP P00178 |
| C | 27 | LYS | HIS | engineered mutation | UNP P00178 |
| C | 29 | LYS | ARG | engineered mutation | UNP P00178 |
| C | 221 | SER | PRO | engineered mutation | UNP P00178 |
| C | 226 | TYR | HIS | engineered mutation | UNP P00178 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 492 | HIS | - | expression tag | UNP P00178 |
| C | 493 | HIS | - | expression tag | UNP P00178 |
| C | 494 | HIS | - | expression tag | UNP P00178 |
| C | 495 | HIS | - | expression tag | UNP P00178 |
| C | 496 | HIS | - | expression tag | UNP P00178 |
| C | 497 | HIS | - | expression tag | UNP P00178 |
| D | 21 | ALA | GLU | engineered mutation | UNP P00178 |
| D | ? | - | PHE | deletion | UNP P00178 |
| D | ? | - | SER | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | ALA | deletion | UNP P00178 |
| D | ? | - | PHE | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | ALA | deletion | UNP P00178 |
| D | ? | - | GLY | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | LEU | deletion | UNP P00178 |
| D | ? | - | PHE | deletion | UNP P00178 |
| D | ? | - | ARG | deletion | UNP P00178 |
| D | 22 | LYS | GLY | engineered mutation | UNP P00178 |
| D | 23 | LYS | HIS | engineered mutation | UNP P00178 |
| D | 24 | THR | PRO | engineered mutation | UNP P00178 |
| D | 25 | SER | LYS | engineered mutation | UNP P00178 |
| D | 26 | SER | ALA | engineered mutation | UNP P00178 |
| D | 27 | LYS | HIS | engineered mutation | UNP P00178 |
| D | 29 | LYS | ARG | engineered mutation | UNP P00178 |
| D | 221 | SER | PRO | engineered mutation | UNP P00178 |
| D | 226 | TYR | HIS | engineered mutation | UNP P00178 |
| D | 492 | HIS | - | expression tag | UNP P00178 |
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| D | 494 | HIS | - | expression tag | UNP P00178 |
| D | 495 | HIS | - | expression tag | UNP P00178 |
| D | 496 | HIS | - | expression tag | UNP P00178 |
| D | 497 | HIS | - | expression tag | UNP P00178 |
| E | 21 | ALA | GLU | engineered mutation | UNP P00178 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
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| E | ? | - | PHE | deletion | UNP P00178 |
| E | ? | - | SER | deletion | UNP P00178 |
| E | ? | - | LEU | deletion | UNP P00178 |
| E | ? | - | LEU | deletion | UNP P00178 |
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| E | ? | - | ALA | deletion | UNP P00178 |
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| E | ? | - | LEU | deletion | UNP P00178 |
| E | ? | - | LEU | deletion | UNP P00178 |
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| E | 22 | LYS | GLY | engineered mutation | UNP P00178 |
| E | 23 | LYS | HIS | engineered mutation | UNP P00178 |
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| E | 25 | SER | LYS | engineered mutation | UNP P00178 |
| E | 26 | SER | ALA | engineered mutation | UNP P00178 |
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| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | ? | - | ALA | deletion | UNP P00178 |
| F | ? | - | PHE | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | ALA | deletion | UNP P00178 |
| F | ? | - | GLY | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | LEU | deletion | UNP P00178 |
| F | ? | - | PHE | deletion | UNP P00178 |
| F | ? | - | ARG | deletion | UNP P00178 |
| F | 22 | LYS | GLY | engineered mutation | UNP P00178 |
| F | 23 | LYS | HIS | engineered mutation | UNP P00178 |
| F | 24 | THR | PRO | engineered mutation | UNP P00178 |
| F | 25 | SER | LYS | engineered mutation | UNP P00178 |
| F | 26 | SER | ALA | engineered mutation | UNP P00178 |
| F | 27 | LYS | HIS | engineered mutation | UNP P00178 |
| F | 29 | LYS | ARG | engineered mutation | UNP P00178 |
| F | 221 | SER | PRO | engineered mutation | UNP P00178 |
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| F | 493 | HIS | - | expression tag | UNP P00178 |
| F | 494 | HIS | - | expression tag | UNP P00178 |
| F | 495 | HIS | - | expression tag | UNP P00178 |
| F | 496 | HIS | - | expression tag | UNP P00178 |
| F | 497 | HIS | - | expression tag | UNP P00178 |
| G | 21 | ALA | GLU | engineered mutation | UNP P00178 |
| G | ? | - | PHE | deletion | UNP P00178 |
| G | ? | - | SER | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | ALA | deletion | UNP P00178 |
| G | ? | - | PHE | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | ALA | deletion | UNP P00178 |
| G | ? | - | GLY | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |

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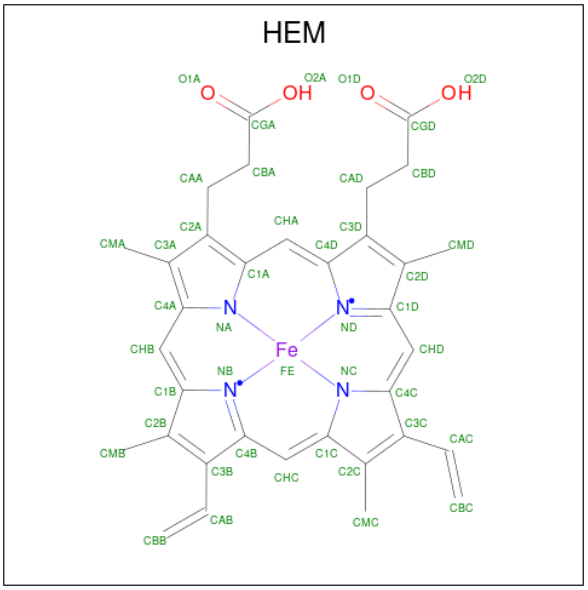
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | LEU | deletion | UNP P00178 |
| G | ? | - | PHE | deletion | UNP P00178 |
| G | ? | - | ARG | deletion | UNP P00178 |
| G | 22 | LYS | GLY | engineered mutation | UNP P00178 |
| G | 23 | LYS | HIS | engineered mutation | UNP P00178 |
| G | 24 | THR | PRO | engineered mutation | UNP P00178 |
| G | 25 | SER | LYS | engineered mutation | UNP P00178 |
| G | 26 | SER | ALA | engineered mutation | UNP P00178 |
| G | 27 | LYS | HIS | engineered mutation | UNP P00178 |
| G | 29 | LYS | ARG | engineered mutation | UNP P00178 |
| G | 221 | SER | PRO | engineered mutation | UNP P00178 |
| G | 226 | TYR | HIS | engineered mutation | UNP P00178 |
| G | 492 | HIS | - | expression tag | UNP P00178 |
| G | 493 | HIS | - | expression tag | UNP P00178 |
| G | 494 | HIS | - | expression tag | UNP P00178 |
| G | 495 | HIS | - | expression tag | UNP P00178 |
| G | 496 | HIS | - | expression tag | UNP P00178 |
| G | 497 | HIS | - | expression tag | UNP P00178 |

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

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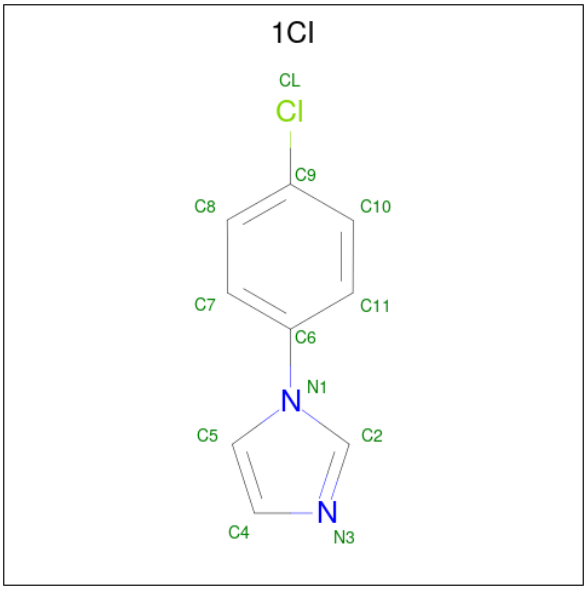
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | C | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | D | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | E | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | F | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | G | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

- Molecule 3 is 1-(4-CHLOROPHENYL)-1H-IMIDAZOLE (CCD ID: 1CI) (formula: $C_9H_7ClN_2$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 3 | A | 1 | Total | C | Cl | N | 0 | 0 |
| | | | 12 | 9 | 1 | 2 | | |
| 3 | B | 1 | Total | C | Cl | N | 0 | 0 |
| | | | 12 | 9 | 1 | 2 | | |
| 3 | C | 1 | Total | C | Cl | N | 0 | 0 |
| | | | 12 | 9 | 1 | 2 | | |
| 3 | D | 1 | Total | C | Cl | N | 0 | 0 |
| | | | 12 | 9 | 1 | 2 | | |
| 3 | E | 1 | Total | C | Cl | N | 0 | 0 |
| | | | 12 | 9 | 1 | 2 | | |

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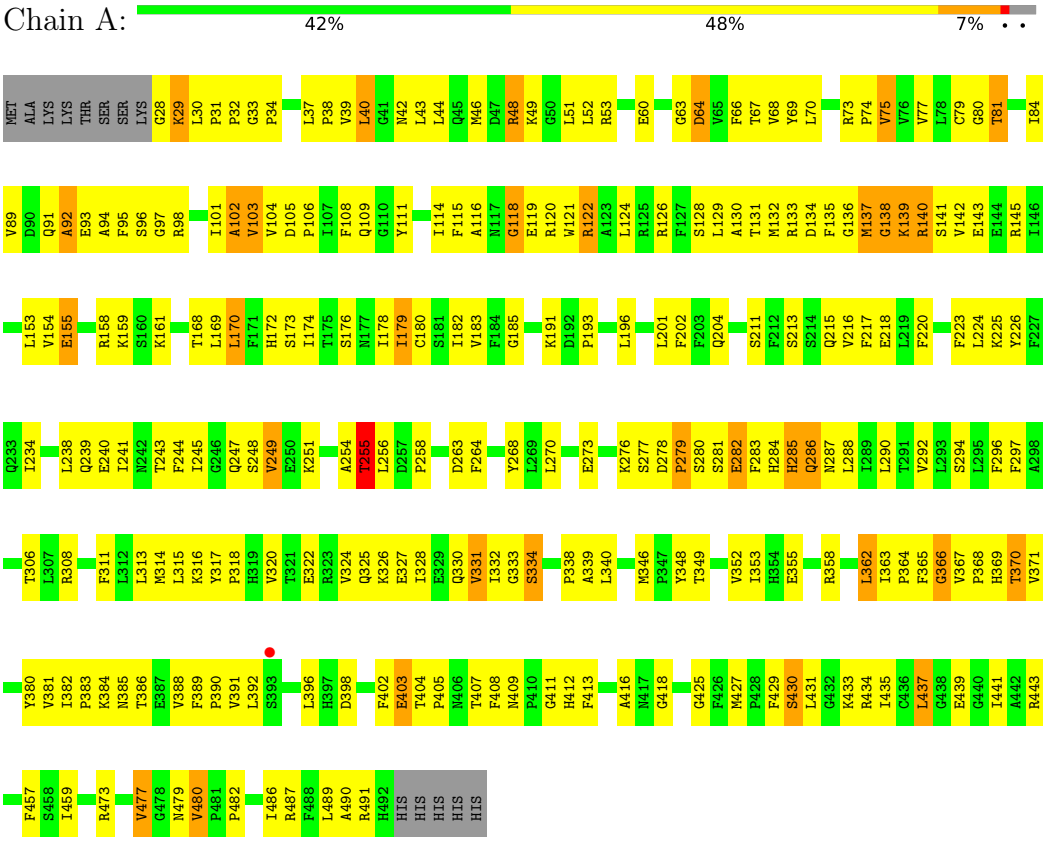
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 3 | F | 1 | Total | C | Cl | N | 0 | 0 |
| | | | 12 | 9 | 1 | 2 | | |
| 3 | G | 1 | Total | C | Cl | N | 0 | 0 |
| | | | 12 | 9 | 1 | 2 | | |

# 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.

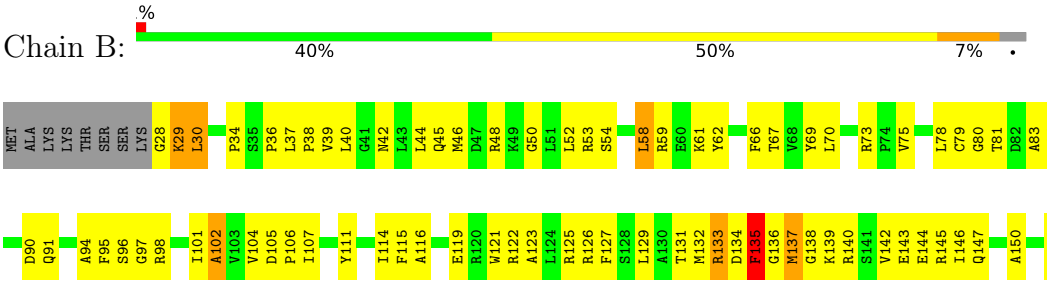
• Molecule 1: Cytochrome P450 2B4

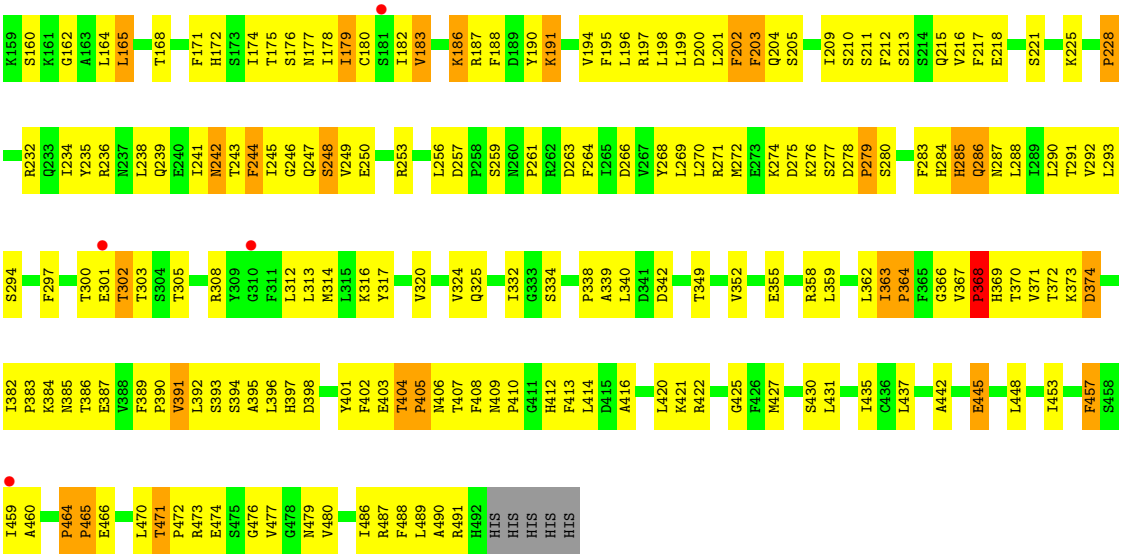
Chain A:




• Molecule 1: Cytochrome P450 2B4

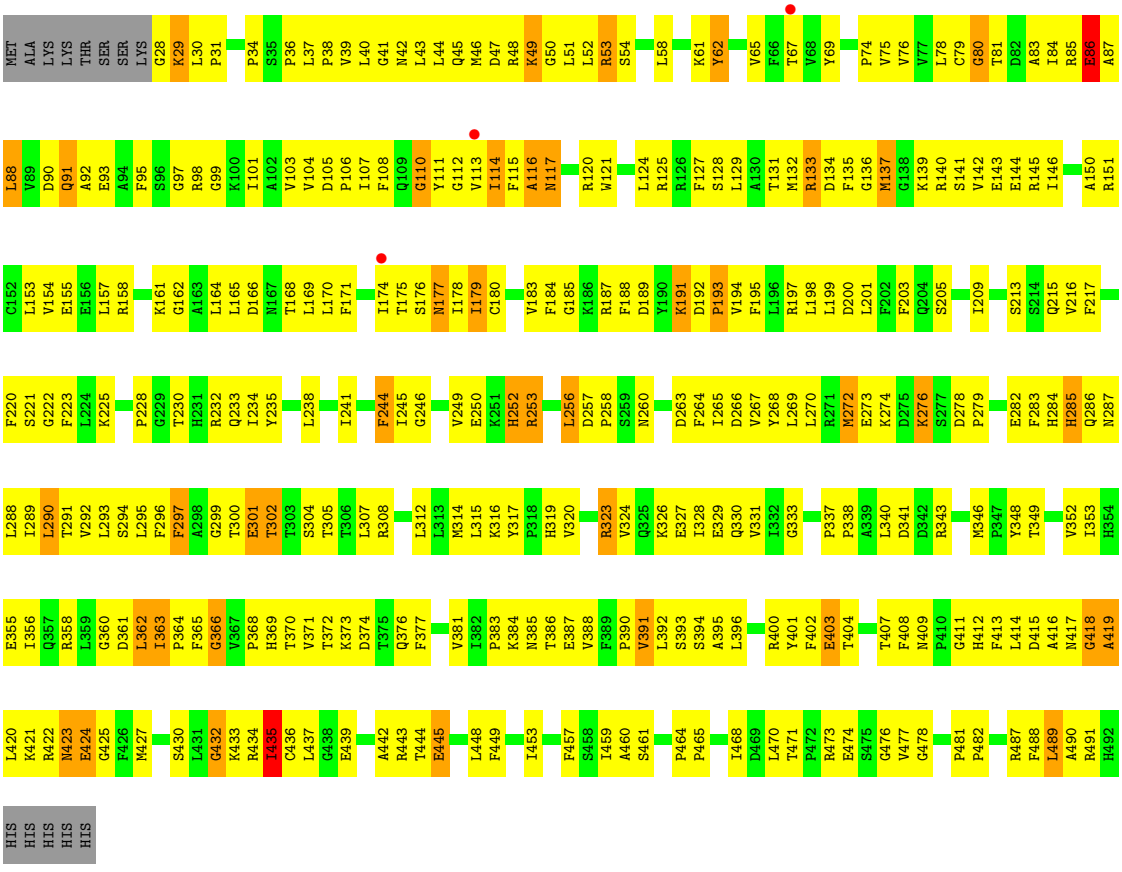
Chain B:





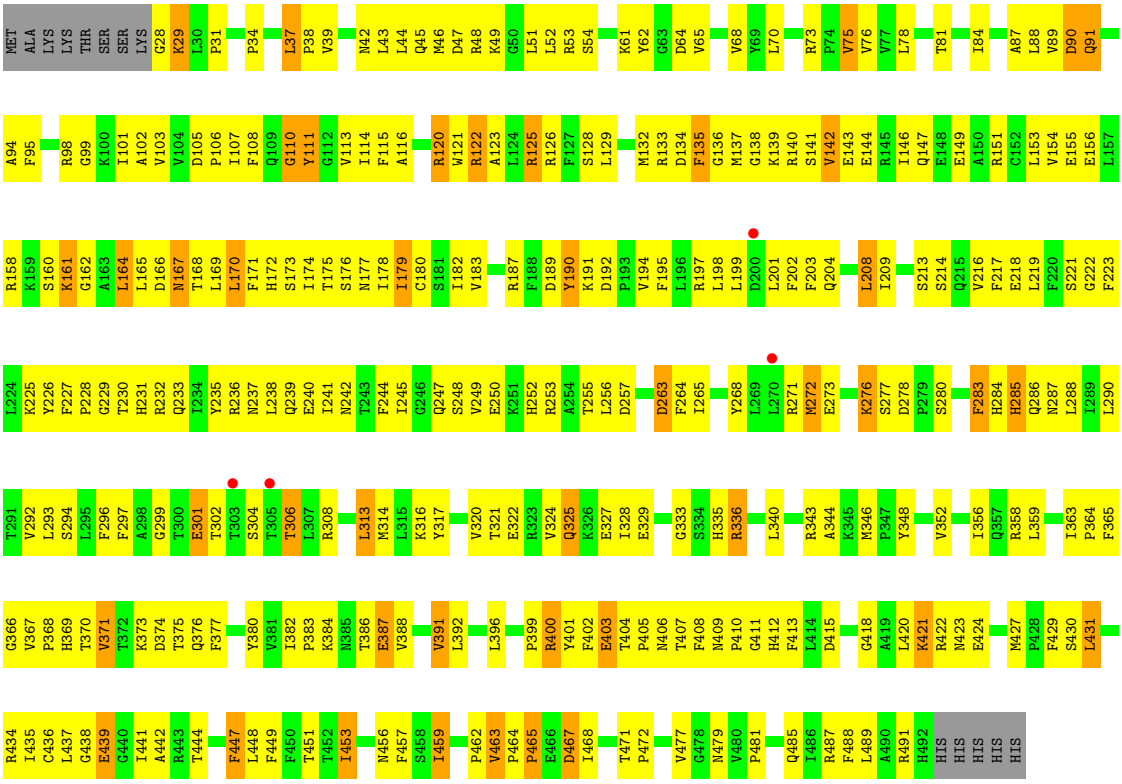

• Molecule 1: Cytochrome P450 2B4

Chain C:



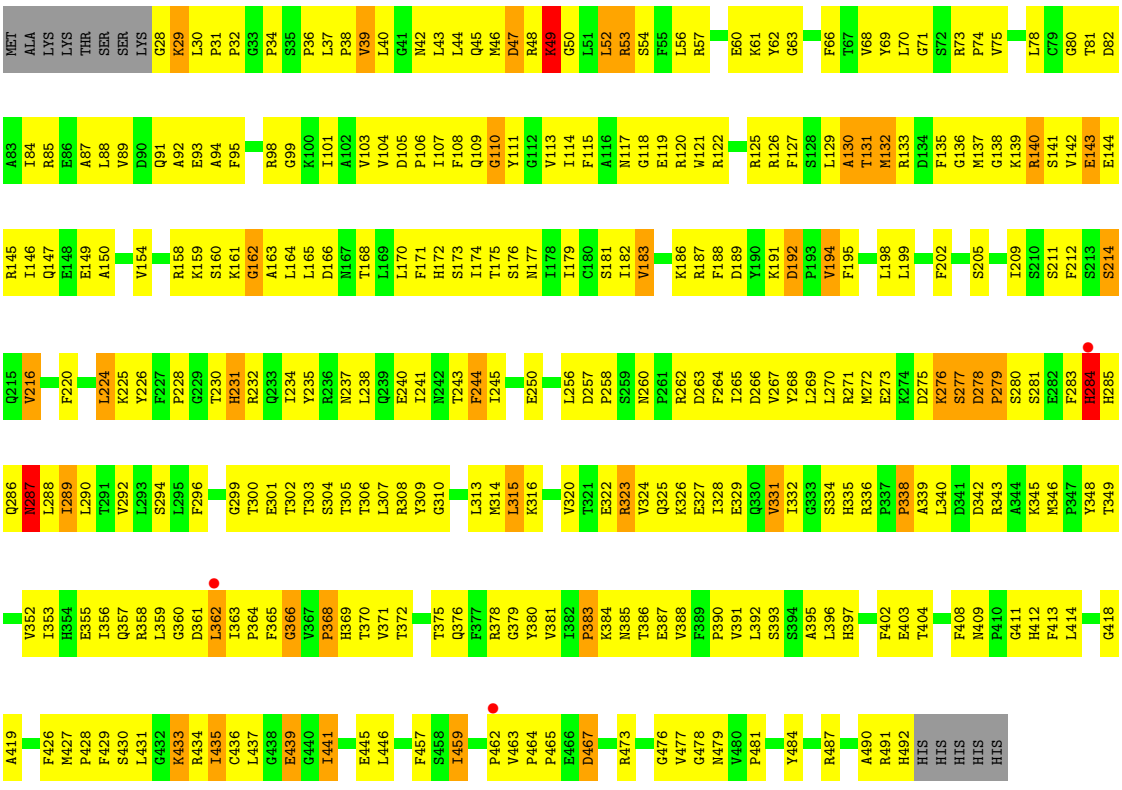

• Molecule 1: Cytochrome P450 2B4

Chain D:



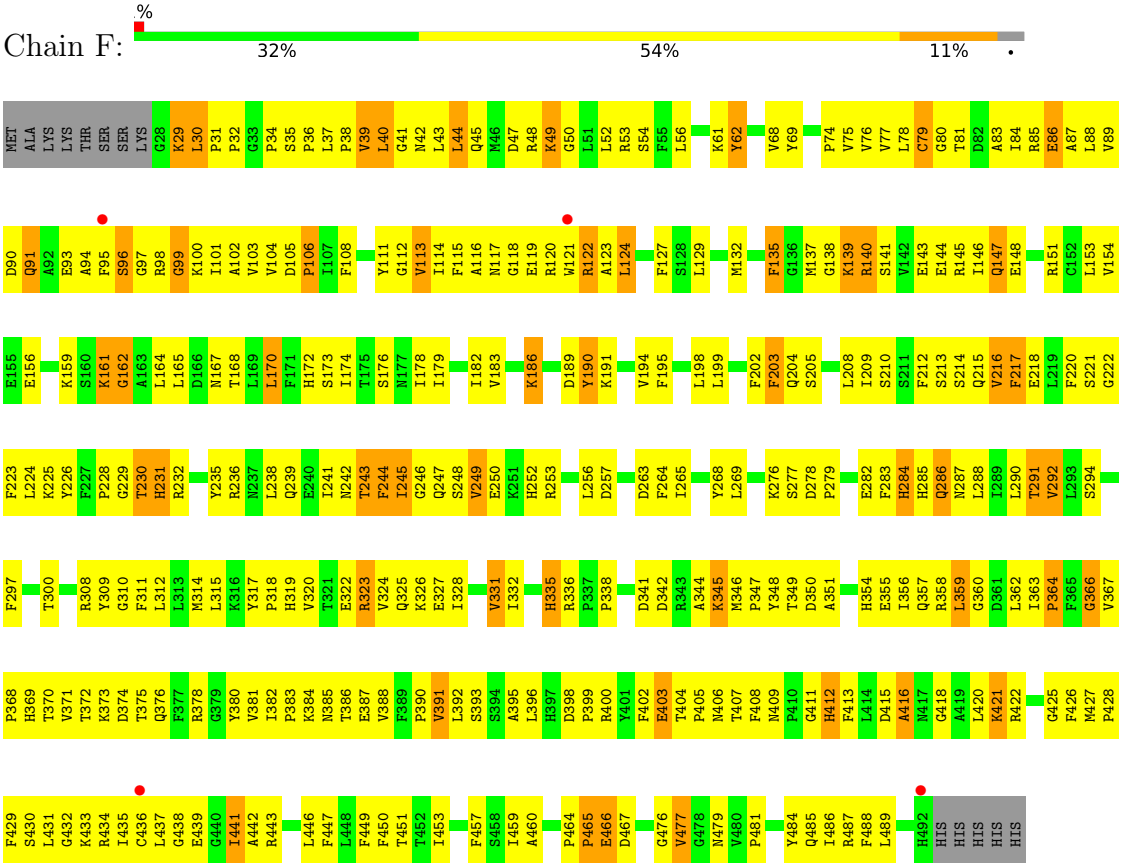
• Molecule 1: Cytochrome P450 2B4

Chain E:



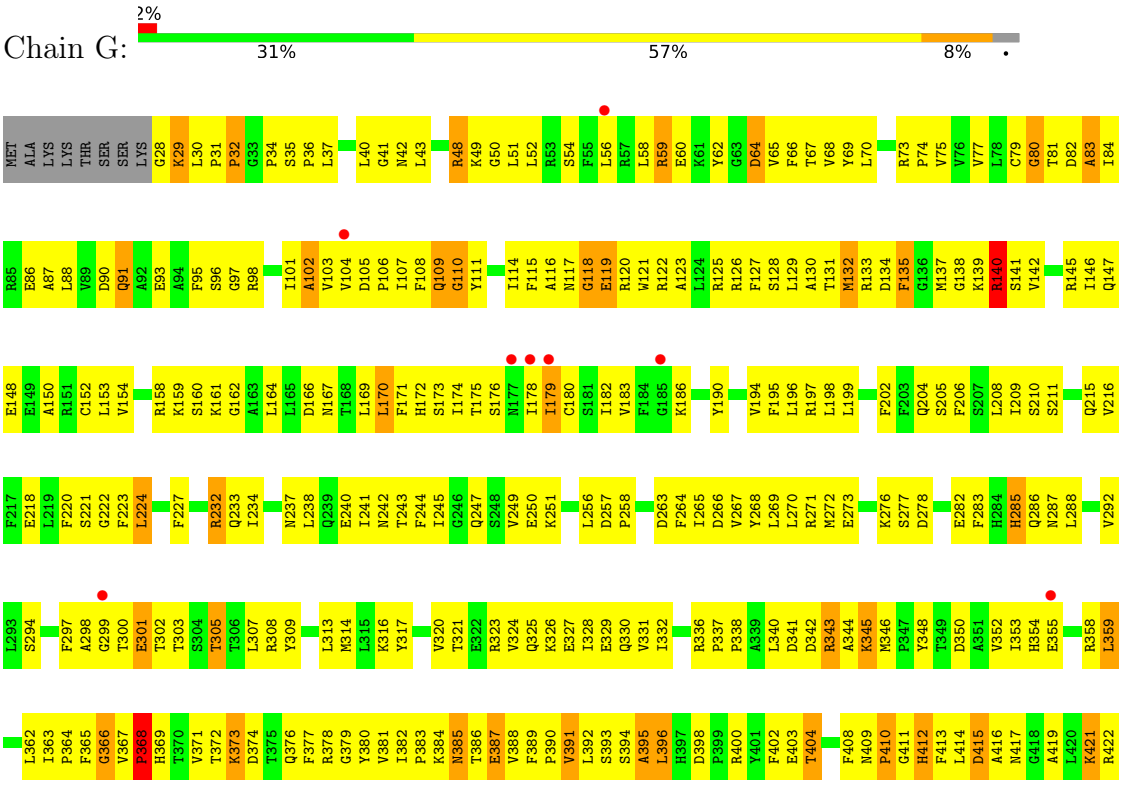
• Molecule 1: Cytochrome P450 2B4

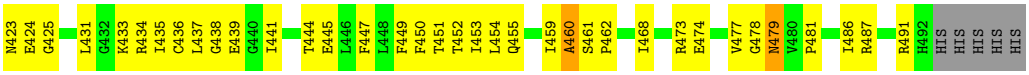
Chain F:




• Molecule 1: Cytochrome P450 2B4

Chain G:




N423
E424
G425
L431
G432
K433
R434
I435
C436
L437
G438
E439
G440
I441
T444
E445
L446
F447
L448
F449
F450
T451
T452
I453
L454
Q455
I459
A460
S461
P462
I468
R473
E474
V477
G478
N479
V480
P481
I486
R487
R491
H492
HIS
HIS
HIS
HIS
HIS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 140.00Å 147.31Å 238.49Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 3.20<br>30.00 – 3.20 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.8 (30.00-3.20)<br>99.0 (30.00-3.20) | Depositor<br>EDS |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | 0.11 | Depositor |
| $< I/\sigma(I) >$ [1] | 0.27 (at 3.19Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.233 , 0.311<br>0.233 , 0.308 | Depositor<br>DCC |
| $R_{free}$ test set | 4077 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 82.5 | Xtriage |
| Anisotropy | 0.131 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 67.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.45$, $< L^2 > = 0.27$ | Xtriage |
| Estimated twinning fraction | 0.026 for k,h,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 26523 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 111.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: HEM, 1CI

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 | 0.41 | 0/3828 | 0.97 | 16/5181 (0.3%) |
| 1 | B | 0.37 | 0/3828 | 0.93 | 18/5181 (0.3%) |
| 1 | C | 0.35 | 0/3828 | 0.90 | 19/5181 (0.4%) |
| 1 | D | 0.37 | 0/3828 | 0.96 | 21/5181 (0.4%) |
| 1 | E | 0.35 | 0/3828 | 0.94 | 12/5181 (0.2%) |
| 1 | F | 0.35 | 0/3828 | 0.91 | 13/5181 (0.3%) |
| 1 | G | 0.35 | 0/3828 | 0.94 | 15/5181 (0.3%) |
| All | All | 0.37 | 0/26796 | 0.94 | 114/36267 (0.3%) |

There are no bond length outliers.

All (114) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 202 | PHE | N-CA-C | -9.69 | 98.17 | 110.19 |
| 1 | G | 51 | LEU | N-CA-C | -8.81 | 102.66 | 113.41 |
| 1 | F | 96 | SER | N-CA-C | -8.03 | 103.98 | 113.21 |
| 1 | A | 302 | THR | N-CA-C | 8.02 | 119.71 | 110.97 |
| 1 | E | 183 | VAL | N-CA-C | 7.94 | 118.83 | 111.45 |
| 1 | D | 313 | LEU | N-CA-C | -7.92 | 103.22 | 113.12 |
| 1 | B | 302 | THR | N-CA-C | 7.89 | 120.58 | 111.11 |
| 1 | G | 59 | ARG | N-CA-C | -7.88 | 103.81 | 113.50 |
| 1 | G | 272 | MET | N-CA-C | -7.85 | 104.19 | 114.31 |
| 1 | A | 224 | LEU | N-CA-C | 7.84 | 119.91 | 111.36 |
| 1 | A | 403 | GLU | N-CA-C | -7.70 | 99.64 | 110.50 |
| 1 | C | 331 | VAL | N-CA-C | 7.51 | 117.59 | 110.53 |
| 1 | F | 249 | VAL | N-CA-C | -7.42 | 102.47 | 113.39 |
| 1 | A | 398 | ASP | CA-C-N | 7.24 | 126.94 | 119.56 |
| 1 | A | 398 | ASP | C-N-CA | 7.24 | 126.94 | 119.56 |
| 1 | F | 243 | THR | N-CA-C | -7.19 | 104.94 | 113.21 |
| 1 | F | 291 | THR | N-CA-C | -7.16 | 104.70 | 113.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 58 | LEU | N-CA-C | -7.14 | 105.09 | 113.88 |
| 1 | D | 217 | PHE | N-CA-C | -7.13 | 104.21 | 113.12 |
| 1 | G | 396 | LEU | N-CA-C | -6.95 | 105.34 | 114.31 |
| 1 | F | 44 | LEU | N-CA-C | 6.89 | 119.63 | 111.71 |
| 1 | D | 301 | GLU | N-CA-C | 6.82 | 119.34 | 111.02 |
| 1 | C | 144 | GLU | N-CA-C | -6.79 | 103.95 | 111.36 |
| 1 | D | 403 | GLU | N-CA-C | -6.76 | 99.56 | 110.32 |
| 1 | G | 273 | GLU | N-CA-C | -6.64 | 105.18 | 113.28 |
| 1 | D | 272 | MET | N-CA-C | -6.62 | 104.84 | 113.12 |
| 1 | B | 248 | SER | N-CA-C | -6.58 | 104.17 | 112.93 |
| 1 | D | 302 | THR | N-CA-C | 6.58 | 118.14 | 110.97 |
| 1 | B | 457 | PHE | N-CA-C | 6.55 | 117.77 | 108.74 |
| 1 | C | 403 | GLU | N-CA-C | -6.31 | 99.35 | 109.96 |
| 1 | G | 133 | ARG | N-CA-C | -6.30 | 104.51 | 111.82 |
| 1 | G | 404 | THR | CA-C-N | 6.28 | 127.69 | 119.84 |
| 1 | G | 404 | THR | C-N-CA | 6.28 | 127.69 | 119.84 |
| 1 | E | 225 | LYS | N-CA-C | -6.27 | 105.57 | 113.72 |
| 1 | F | 403 | GLU | N-CA-C | -6.20 | 102.35 | 110.53 |
| 1 | B | 183 | VAL | N-CA-C | 6.19 | 116.88 | 111.56 |
| 1 | B | 471 | THR | CA-C-N | 6.10 | 126.12 | 119.89 |
| 1 | B | 471 | THR | C-N-CA | 6.10 | 126.12 | 119.89 |
| 1 | F | 245 | ILE | N-CA-C | -6.09 | 105.37 | 112.98 |
| 1 | B | 473 | ARG | N-CA-C | -6.04 | 105.95 | 113.38 |
| 1 | E | 306 | THR | N-CA-C | -6.01 | 105.44 | 112.89 |
| 1 | C | 252 | HIS | N-CA-C | -5.99 | 106.52 | 113.88 |
| 1 | A | 103 | VAL | N-CA-C | 5.98 | 120.50 | 111.89 |
| 1 | B | 135 | PHE | N-CA-C | -5.96 | 103.92 | 113.28 |
| 1 | B | 363 | ILE | CA-C-N | 5.95 | 127.28 | 119.84 |
| 1 | B | 363 | ILE | C-N-CA | 5.95 | 127.28 | 119.84 |
| 1 | C | 317 | TYR | CA-C-N | 5.95 | 125.33 | 118.85 |
| 1 | C | 317 | TYR | C-N-CA | 5.95 | 125.33 | 118.85 |
| 1 | D | 142 | VAL | N-CA-C | -5.93 | 105.28 | 113.00 |
| 1 | D | 263 | ASP | N-CA-C | 5.93 | 116.11 | 108.34 |
| 1 | C | 312 | LEU | N-CA-C | -5.88 | 104.88 | 111.28 |
| 1 | A | 346 | MET | CA-C-N | 5.86 | 125.53 | 119.56 |
| 1 | A | 346 | MET | C-N-CA | 5.86 | 125.53 | 119.56 |
| 1 | F | 217 | PHE | N-CA-C | -5.83 | 105.01 | 111.71 |
| 1 | G | 166 | ASP | N-CA-C | -5.82 | 100.51 | 109.76 |
| 1 | D | 363 | ILE | CA-C-N | 5.78 | 127.07 | 119.84 |
| 1 | D | 363 | ILE | C-N-CA | 5.78 | 127.07 | 119.84 |
| 1 | E | 433 | LYS | N-CA-C | -5.78 | 106.19 | 113.18 |
| 1 | C | 363 | ILE | CA-C-N | 5.76 | 127.05 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 363 | ILE | C-N-CA | 5.76 | 127.05 | 119.84 |
| 1 | C | 445 | GLU | N-CA-C | -5.75 | 105.01 | 111.28 |
| 1 | A | 480 | VAL | N-CA-C | 5.72 | 113.53 | 107.76 |
| 1 | C | 272 | MET | N-CA-C | -5.71 | 106.45 | 113.41 |
| 1 | E | 473 | ARG | N-CA-C | -5.70 | 106.18 | 113.01 |
| 1 | A | 40 | LEU | N-CA-C | 5.67 | 118.40 | 111.82 |
| 1 | D | 367 | VAL | CA-C-N | 5.67 | 126.92 | 119.84 |
| 1 | D | 367 | VAL | C-N-CA | 5.67 | 126.92 | 119.84 |
| 1 | B | 445 | GLU | N-CA-C | -5.64 | 105.21 | 111.36 |
| 1 | E | 276 | LYS | N-CA-C | -5.62 | 105.53 | 112.38 |
| 1 | E | 459 | ILE | N-CA-C | 5.58 | 117.93 | 109.12 |
| 1 | A | 477 | VAL | N-CA-C | -5.53 | 105.81 | 113.00 |
| 1 | G | 147 | GLN | N-CA-C | -5.51 | 104.66 | 111.33 |
| 1 | C | 274 | LYS | N-CA-C | -5.50 | 104.69 | 111.40 |
| 1 | G | 395 | ALA | N-CA-C | -5.47 | 106.45 | 114.39 |
| 1 | C | 62 | TYR | N-CA-C | 5.45 | 119.23 | 112.59 |
| 1 | D | 120 | ARG | N-CA-C | -5.44 | 105.04 | 110.97 |
| 1 | D | 459 | ILE | N-CA-C | 5.43 | 117.47 | 108.99 |
| 1 | D | 421 | LYS | N-CA-C | 5.42 | 113.23 | 108.78 |
| 1 | C | 302 | THR | N-CA-C | 5.41 | 119.38 | 112.34 |
| 1 | C | 88 | LEU | N-CA-C | 5.33 | 119.85 | 113.23 |
| 1 | B | 464 | PRO | CA-C-N | 5.28 | 126.44 | 119.84 |
| 1 | B | 464 | PRO | C-N-CA | 5.28 | 126.44 | 119.84 |
| 1 | C | 253 | ARG | N-CA-C | -5.27 | 106.82 | 113.20 |
| 1 | E | 315 | LEU | N-CA-C | -5.27 | 106.98 | 113.41 |
| 1 | B | 158 | ARG | N-CA-C | -5.26 | 105.54 | 111.28 |
| 1 | E | 192 | ASP | CA-C-N | 5.26 | 124.71 | 119.24 |
| 1 | E | 192 | ASP | C-N-CA | 5.26 | 124.71 | 119.24 |
| 1 | F | 231 | HIS | N-CA-C | -5.26 | 107.52 | 114.31 |
| 1 | D | 64 | ASP | N-CA-C | -5.23 | 106.74 | 113.02 |
| 1 | C | 290 | LEU | N-CA-C | 5.22 | 116.66 | 111.07 |
| 1 | F | 244 | PHE | N-CA-C | -5.22 | 106.24 | 113.18 |
| 1 | A | 396 | LEU | N-CA-C | -5.22 | 106.76 | 113.23 |
| 1 | G | 342 | ASP | N-CA-C | -5.21 | 106.98 | 113.19 |
| 1 | B | 242 | ASN | N-CA-C | -5.21 | 106.92 | 113.28 |
| 1 | D | 306 | THR | N-CA-C | -5.18 | 105.25 | 112.45 |
| 1 | A | 249 | VAL | N-CA-C | -5.18 | 105.36 | 111.00 |
| 1 | E | 287 | ASN | N-CA-C | -5.16 | 107.12 | 113.41 |
| 1 | C | 114 | ILE | CB-CA-C | -5.16 | 107.33 | 111.71 |
| 1 | F | 292 | VAL | N-CA-C | -5.14 | 105.40 | 111.00 |
| 1 | E | 244 | PHE | N-CA-C | -5.13 | 105.58 | 111.07 |
| 1 | D | 374 | ASP | N-CA-C | -5.11 | 100.75 | 108.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 216 | VAL | N-CA-C | -5.11 | 105.41 | 110.62 |
| 1 | D | 37 | LEU | N-CA-C | -5.10 | 103.04 | 110.08 |
| 1 | A | 301 | GLU | N-CA-C | 5.09 | 121.65 | 110.80 |
| 1 | A | 158 | ARG | N-CA-C | -5.08 | 105.83 | 111.36 |
| 1 | D | 182 | ILE | N-CA-C | -5.08 | 106.98 | 113.22 |
| 1 | F | 174 | ILE | N-CA-C | 5.08 | 115.29 | 110.42 |
| 1 | G | 251 | LYS | N-CA-C | -5.07 | 105.83 | 111.36 |
| 1 | D | 421 | LYS | CA-C-O | 5.07 | 120.88 | 117.94 |
| 1 | A | 315 | LEU | N-CA-C | -5.06 | 107.24 | 113.41 |
| 1 | G | 473 | ARG | N-CA-C | -5.05 | 106.54 | 113.30 |
| 1 | B | 244 | PHE | N-CA-C | -5.04 | 104.78 | 112.04 |
| 1 | F | 147 | GLN | N-CA-C | -5.01 | 105.29 | 111.40 |
| 1 | C | 58 | LEU | N-CA-C | -5.01 | 106.34 | 112.90 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 3734 | 0 | 3744 | 259 | 0 |
| 1 | B | 3734 | 0 | 3744 | 278 | 0 |
| 1 | C | 3734 | 0 | 3744 | 334 | 0 |
| 1 | D | 3734 | 0 | 3744 | 293 | 0 |
| 1 | E | 3734 | 0 | 3745 | 347 | 0 |
| 1 | F | 3734 | 0 | 3744 | 345 | 0 |
| 1 | G | 3734 | 0 | 3744 | 325 | 0 |
| 2 | A | 43 | 0 | 30 | 2 | 0 |
| 2 | B | 43 | 0 | 30 | 3 | 0 |
| 2 | C | 43 | 0 | 30 | 4 | 0 |
| 2 | D | 43 | 0 | 30 | 6 | 0 |
| 2 | E | 43 | 0 | 30 | 8 | 0 |
| 2 | F | 43 | 0 | 30 | 7 | 0 |
| 2 | G | 43 | 0 | 30 | 4 | 0 |
| 3 | A | 12 | 0 | 7 | 1 | 0 |
| 3 | B | 12 | 0 | 7 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | C | 12 | 0 | 7 | 3 | 0 |
| 3 | D | 12 | 0 | 7 | 2 | 0 |
| 3 | E | 12 | 0 | 7 | 1 | 0 |
| 3 | F | 12 | 0 | 7 | 3 | 0 |
| 3 | G | 12 | 0 | 7 | 4 | 0 |
| All | All | 26523 | 0 | 26468 | 2149 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (2149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:114:ILE:HD13 | 1:D:294:SER:HB3 | 1.38 | 1.05 |
| 1:E:111:TYR:HB2 | 1:E:290:LEU:HD12 | 1.35 | 1.03 |
| 1:E:75:VAL:HG12 | 1:E:387:GLU:HB2 | 1.44 | 1.00 |
| 1:E:98:ARG:HG2 | 1:E:115:PHE:HA | 1.47 | 0.97 |
| 1:D:216:VAL:HG11 | 1:F:228:PRO:HD3 | 1.48 | 0.96 |
| 1:A:111:TYR:HB2 | 1:A:290:LEU:HD12 | 1.47 | 0.95 |
| 1:B:209:ILE:HD13 | 1:B:234:ILE:HD13 | 1.48 | 0.94 |
| 1:A:213:SER:HA | 1:A:216:VAL:HG12 | 1.47 | 0.94 |
| 1:G:232:ARG:NH1 | 1:G:232:ARG:HA | 1.84 | 0.92 |
| 1:D:373:LYS:HA | 1:D:384:LYS:HG3 | 1.51 | 0.92 |
| 1:C:132:MET:HG3 | 1:C:137:MET:HE2 | 1.50 | 0.92 |
| 1:G:140:ARG:NH1 | 1:G:140:ARG:HB2 | 1.86 | 0.91 |
| 1:E:362:LEU:H | 1:E:362:LEU:HD22 | 1.35 | 0.91 |
| 1:C:253:ARG:HH22 | 1:C:272:MET:HE1 | 1.34 | 0.90 |
| 1:B:232:ARG:HB3 | 1:B:232:ARG:HH11 | 1.33 | 0.90 |
| 1:F:135:PHE:HE1 | 1:F:145:ARG:HH12 | 1.21 | 0.89 |
| 1:E:284:HIS:H | 1:E:284:HIS:CD2 | 1.83 | 0.89 |
| 1:E:52:LEU:HD13 | 1:E:364:PRO:HB3 | 1.56 | 0.88 |
| 1:B:373:LYS:HA | 1:B:384:LYS:HG3 | 1.56 | 0.87 |
| 1:F:141:SER:HB3 | 1:F:144:GLU:HG3 | 1.56 | 0.87 |
| 1:E:177:ASN:HD21 | 1:E:187:ARG:HB2 | 1.39 | 0.87 |
| 1:E:376:GLN:HE22 | 1:E:379:GLY:H | 1.23 | 0.86 |
| 1:A:256:LEU:HD21 | 1:A:270:LEU:HD23 | 1.53 | 0.86 |
| 1:A:34:PRO:HG2 | 1:A:42:ASN:ND2 | 1.90 | 0.86 |
| 1:B:253:ARG:HH22 | 1:B:272:MET:HE1 | 1.38 | 0.86 |
| 1:E:176:SER:HB2 | 1:E:300:THR:HG23 | 1.56 | 0.86 |
| 1:C:107:ILE:HG13 | 1:C:238:LEU:HD12 | 1.58 | 0.86 |
| 1:D:325:GLN:HA | 1:D:325:GLN:HE21 | 1.39 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:37:LEU:H | 1:F:37:LEU:HD12 | 1.38 | 0.86 |
| 1:E:332:ILE:HG21 | 1:E:338:PRO:HG3 | 1.56 | 0.85 |
| 1:A:368:PRO:HG3 | 1:A:389:PHE:HE2 | 1.41 | 0.85 |
| 1:A:94:ALA:O | 1:A:371:VAL:HA | 1.75 | 0.85 |
| 1:C:49:LYS:HE3 | 1:C:53:ARG:NH1 | 1.91 | 0.85 |
| 1:D:228:PRO:HD3 | 1:E:216:VAL:HG11 | 1.58 | 0.84 |
| 1:F:53:ARG:HA | 1:F:53:ARG:HH11 | 1.42 | 0.84 |
| 1:D:276:LYS:HD2 | 1:D:277:SER:H | 1.43 | 0.84 |
| 1:A:124:LEU:HD21 | 1:A:287:ASN:HD22 | 1.40 | 0.84 |
| 1:E:268:TYR:O | 1:E:272:MET:HG2 | 1.77 | 0.84 |
| 1:G:232:ARG:HA | 1:G:232:ARG:HH11 | 1.37 | 0.84 |
| 1:E:107:ILE:HG13 | 1:E:238:LEU:HD12 | 1.59 | 0.83 |
| 1:F:320:VAL:HG21 | 1:F:408:PHE:HE2 | 1.41 | 0.83 |
| 1:C:395:ALA:HB1 | 1:C:427:MET:HE3 | 1.58 | 0.83 |
| 1:A:102:ALA:HB2 | 1:A:218:GLU:HA | 1.59 | 0.82 |
| 1:G:328:ILE:HG23 | 1:G:332:ILE:HD12 | 1.59 | 0.82 |
| 1:B:409:ASN:HB3 | 1:B:412:HIS:CE1 | 2.15 | 0.82 |
| 1:D:53:ARG:HH11 | 1:D:53:ARG:HA | 1.43 | 0.82 |
| 1:A:153:LEU:HD22 | 1:A:174:ILE:HD13 | 1.60 | 0.82 |
| 1:B:409:ASN:HB3 | 1:B:412:HIS:HE1 | 1.44 | 0.82 |
| 1:A:69:TYR:CE2 | 1:A:74:PRO:HB3 | 2.14 | 0.82 |
| 1:A:273:GLU:HA | 1:A:276:LYS:HE3 | 1.61 | 0.81 |
| 1:G:140:ARG:HB2 | 1:G:140:ARG:HH11 | 1.44 | 0.81 |
| 1:C:52:LEU:HD22 | 1:C:364:PRO:HB3 | 1.60 | 0.81 |
| 1:D:232:ARG:HB3 | 1:D:232:ARG:HH11 | 1.45 | 0.81 |
| 1:G:422:ARG:HG2 | 1:G:423:ASN:H | 1.45 | 0.81 |
| 1:A:52:LEU:HD22 | 1:A:364:PRO:HB3 | 1.63 | 0.81 |
| 1:E:194:VAL:O | 1:E:198:LEU:HD23 | 1.81 | 0.81 |
| 1:G:164:LEU:HG | 1:G:487:ARG:HH21 | 1.45 | 0.81 |
| 1:E:177:ASN:ND2 | 1:E:187:ARG:HB2 | 1.96 | 0.80 |
| 1:E:358:ARG:HG3 | 1:E:396:LEU:HD22 | 1.61 | 0.80 |
| 1:A:362:LEU:HD22 | 1:A:362:LEU:H | 1.45 | 0.80 |
| 1:B:164:LEU:HD23 | 1:B:487:ARG:HB3 | 1.62 | 0.80 |
| 1:F:320:VAL:HA | 1:F:323:ARG:HB2 | 1.62 | 0.80 |
| 1:D:164:LEU:HD22 | 1:D:485:GLN:HB3 | 1.63 | 0.80 |
| 1:G:362:LEU:HD22 | 1:G:362:LEU:H | 1.46 | 0.80 |
| 1:G:138:GLY:HA3 | 1:G:145:ARG:HH21 | 1.46 | 0.80 |
| 1:G:303:THR:HG21 | 1:G:445:GLU:OE1 | 1.82 | 0.80 |
| 1:C:417:ASN:OD1 | 1:G:271:ARG:HB2 | 1.81 | 0.80 |
| 1:B:364:PRO:HG3 | 1:B:479:ASN:ND2 | 1.97 | 0.79 |
| 1:F:49:LYS:HE2 | 1:F:53:ARG:HG2 | 1.63 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:102:ALA:HB1 | 1:A:217:PHE:HD2 | 1.48 | 0.79 |
| 1:E:99:GLY:HA3 | 1:E:368:PRO:HB2 | 1.64 | 0.79 |
| 1:G:138:GLY:HA3 | 1:G:145:ARG:NH2 | 1.98 | 0.79 |
| 1:E:328:ILE:HG23 | 1:E:332:ILE:HD12 | 1.66 | 0.78 |
| 1:C:98:ARG:HG2 | 1:C:115:PHE:HA | 1.63 | 0.78 |
| 1:D:222:GLY:HA2 | 1:D:225:LYS:HE3 | 1.64 | 0.78 |
| 1:G:224:LEU:HD23 | 1:G:227:PHE:HB2 | 1.64 | 0.78 |
| 1:D:352:VAL:HG13 | 1:D:408:PHE:HZ | 1.48 | 0.78 |
| 1:G:245:ILE:O | 1:G:249:VAL:HG23 | 1.84 | 0.78 |
| 1:E:122:ARG:HB3 | 1:E:126:ARG:HH11 | 1.48 | 0.78 |
| 1:C:125:ARG:HH12 | 1:C:437:LEU:HB2 | 1.49 | 0.78 |
| 1:B:101:ILE:HD11 | 1:B:368:PRO:HD2 | 1.66 | 0.77 |
| 1:B:232:ARG:HB3 | 1:B:232:ARG:NH1 | 1.98 | 0.77 |
| 1:F:140:ARG:HH22 | 1:F:148:GLU:HG2 | 1.48 | 0.77 |
| 1:D:245:ILE:O | 1:D:249:VAL:HG23 | 1.84 | 0.77 |
| 1:C:179:ILE:O | 1:C:179:ILE:HD13 | 1.83 | 0.77 |
| 1:G:123:ALA:HA | 1:G:126:ARG:HG2 | 1.66 | 0.77 |
| 1:E:53:ARG:HA | 1:E:53:ARG:HH11 | 1.49 | 0.77 |
| 1:F:194:VAL:O | 1:F:198:LEU:HD23 | 1.84 | 0.77 |
| 1:C:38:PRO:O | 1:C:40:LEU:HD23 | 1.85 | 0.77 |
| 1:C:232:ARG:NH1 | 1:C:232:ARG:HB3 | 2.00 | 0.76 |
| 1:D:52:LEU:HD22 | 1:D:364:PRO:HB3 | 1.68 | 0.76 |
| 1:E:328:ILE:HG12 | 1:E:346:MET:HE1 | 1.66 | 0.76 |
| 1:E:147:GLN:HE22 | 1:E:339:ALA:HA | 1.49 | 0.76 |
| 1:A:138:GLY:O | 1:A:139:LYS:HD2 | 1.85 | 0.76 |
| 1:B:305:THR:HG22 | 1:B:308:ARG:HH21 | 1.51 | 0.76 |
| 1:E:125:ARG:HH12 | 1:E:437:LEU:HB2 | 1.50 | 0.76 |
| 1:G:79:CYS:O | 1:G:83:ALA:HB3 | 1.86 | 0.76 |
| 1:G:130:ALA:O | 1:G:134:ASP:HB2 | 1.86 | 0.76 |
| 1:G:101:ILE:HB | 1:G:104:VAL:HG22 | 1.68 | 0.76 |
| 1:C:297:PHE:CD2 | 3:C:501:1CI:H8 | 2.20 | 0.76 |
| 1:E:258:PRO:HG3 | 1:E:270:LEU:HD21 | 1.68 | 0.75 |
| 1:B:34:PRO:HG2 | 1:B:42:ASN:ND2 | 2.02 | 0.75 |
| 1:A:129:LEU:HD21 | 1:A:133:ARG:NH2 | 2.01 | 0.75 |
| 1:D:70:LEU:HD22 | 1:D:219:LEU:HD11 | 1.67 | 0.75 |
| 1:D:409:ASN:HB3 | 1:D:412:HIS:CE1 | 2.21 | 0.75 |
| 1:E:147:GLN:NE2 | 1:E:339:ALA:HA | 2.01 | 0.75 |
| 1:E:370:THR:HA | 1:E:386:THR:O | 1.87 | 0.75 |
| 1:G:285:HIS:O | 1:G:287:ASN:N | 2.20 | 0.75 |
| 1:F:320:VAL:HG21 | 1:F:408:PHE:CE2 | 2.21 | 0.75 |
| 1:C:75:VAL:HG12 | 1:C:387:GLU:HB2 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:101:ILE:HB | 1:F:104:VAL:HG22 | 1.68 | 0.74 |
| 1:F:132:MET:HE1 | 1:F:441:ILE:HD11 | 1.69 | 0.74 |
| 1:A:95:PHE:O | 1:A:369:HIS:HD2 | 1.70 | 0.74 |
| 1:B:217:PHE:O | 1:B:221:SER:HB3 | 1.87 | 0.74 |
| 1:D:44:LEU:H | 1:D:44:LEU:HD12 | 1.49 | 0.74 |
| 1:D:276:LYS:HD2 | 1:D:277:SER:N | 2.01 | 0.74 |
| 1:C:409:ASN:HB3 | 1:C:412:HIS:ND1 | 2.02 | 0.74 |
| 1:G:98:ARG:HG2 | 1:G:115:PHE:HA | 1.68 | 0.74 |
| 1:E:75:VAL:HG12 | 1:E:387:GLU:CB | 2.16 | 0.74 |
| 1:E:98:ARG:HD3 | 1:E:99:GLY:H | 1.51 | 0.74 |
| 1:F:95:PHE:CE1 | 1:F:371:VAL:HG12 | 2.22 | 0.74 |
| 1:G:73:ARG:HH21 | 1:G:387:GLU:HB2 | 1.51 | 0.74 |
| 1:G:415:ASP:CG | 1:G:416:ALA:H | 1.96 | 0.74 |
| 1:G:29:LYS:HE3 | 1:G:379:GLY:O | 1.86 | 0.74 |
| 1:B:133:ARG:NH2 | 1:B:139:LYS:HE2 | 2.03 | 0.74 |
| 1:B:53:ARG:HH11 | 1:B:53:ARG:HA | 1.53 | 0.74 |
| 1:B:136:GLY:O | 1:B:142:VAL:HG13 | 1.87 | 0.74 |
| 1:C:205:SER:O | 1:C:209:ILE:HG13 | 1.87 | 0.74 |
| 1:E:125:ARG:NH1 | 1:E:437:LEU:HB2 | 2.03 | 0.74 |
| 1:F:249:VAL:HG21 | 1:F:288:LEU:HD21 | 1.69 | 0.74 |
| 1:F:446:LEU:O | 1:F:450:PHE:HB2 | 1.88 | 0.74 |
| 1:E:256:LEU:HD11 | 1:E:270:LEU:HG | 1.69 | 0.73 |
| 1:B:383:PRO:HG2 | 1:B:386:THR:OG1 | 1.89 | 0.73 |
| 1:D:101:ILE:HD11 | 1:D:368:PRO:HD2 | 1.70 | 0.73 |
| 1:D:411:GLY:O | 1:D:413:PHE:N | 2.20 | 0.73 |
| 1:G:209:ILE:HG22 | 1:G:477:VAL:HG11 | 1.70 | 0.73 |
| 1:C:245:ILE:O | 1:C:249:VAL:HG23 | 1.88 | 0.73 |
| 1:D:158:ARG:HG2 | 1:D:457:PHE:HZ | 1.53 | 0.73 |
| 1:G:409:ASN:HB3 | 1:G:412:HIS:CE1 | 2.23 | 0.73 |
| 1:B:297:PHE:CE2 | 3:B:501:1CI:H8 | 2.24 | 0.73 |
| 1:B:364:PRO:HG3 | 1:B:479:ASN:HD21 | 1.54 | 0.73 |
| 1:F:443:ARG:NH1 | 1:F:443:ARG:HB3 | 2.03 | 0.73 |
| 1:G:371:VAL:HG11 | 1:G:382:ILE:HG21 | 1.71 | 0.73 |
| 1:G:398:ASP:OD2 | 1:G:400:ARG:HB2 | 1.88 | 0.73 |
| 1:G:139:LYS:C | 1:G:140:ARG:HG3 | 2.13 | 0.73 |
| 1:E:140:ARG:HB2 | 1:E:144:GLU:HG2 | 1.71 | 0.72 |
| 1:B:153:LEU:HD22 | 1:B:174:ILE:HD13 | 1.70 | 0.72 |
| 1:C:402:PHE:CD1 | 1:C:412:HIS:HD2 | 2.06 | 0.72 |
| 1:G:364:PRO:HG3 | 1:G:479:ASN:ND2 | 2.05 | 0.72 |
| 1:D:98:ARG:HB2 | 1:D:434:ARG:HH12 | 1.53 | 0.72 |
| 1:E:441:ILE:HD11 | 2:E:500:HEM:HBC2 | 1.70 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:276:LYS:HD2 | 1:F:276:LYS:C | 2.15 | 0.72 |
| 1:D:76:VAL:HB | 1:D:388:VAL:HG22 | 1.71 | 0.72 |
| 1:F:358:ARG:HG3 | 1:F:396:LEU:HD22 | 1.71 | 0.72 |
| 1:E:113:VAL:HG13 | 1:E:114:ILE:CD1 | 2.19 | 0.72 |
| 1:E:413:PHE:O | 1:E:414:LEU:HD23 | 1.89 | 0.72 |
| 1:F:137:MET:HG3 | 1:F:138:GLY:H | 1.54 | 0.72 |
| 1:G:461:SER:HB2 | 1:G:462:PRO:HD2 | 1.69 | 0.72 |
| 1:F:114:ILE:HG12 | 2:F:500:HEM:HAD1 | 1.69 | 0.72 |
| 1:A:256:LEU:O | 1:A:258:PRO:HD3 | 1.88 | 0.72 |
| 1:C:257:ASP:OD2 | 1:C:260:ASN:HB3 | 1.90 | 0.72 |
| 1:D:168:THR:HG22 | 1:D:169:LEU:HD12 | 1.71 | 0.72 |
| 1:A:368:PRO:HG3 | 1:A:389:PHE:CE2 | 2.24 | 0.72 |
| 1:C:340:LEU:HD11 | 1:C:343:ARG:NH2 | 2.05 | 0.72 |
| 1:G:305:THR:CG2 | 1:G:481:PRO:HD2 | 2.20 | 0.72 |
| 1:C:114:ILE:HG12 | 2:C:500:HEM:HAD1 | 1.73 | 0.71 |
| 1:E:284:HIS:H | 1:E:284:HIS:HD2 | 1.36 | 0.71 |
| 1:D:335:HIS:O | 1:D:336:ARG:HB3 | 1.89 | 0.71 |
| 1:F:388:VAL:O | 1:F:390:PRO:HD3 | 1.90 | 0.71 |
| 1:E:272:MET:HE1 | 1:E:283:PHE:HD2 | 1.56 | 0.71 |
| 1:B:44:LEU:HB2 | 1:B:45:GLN:NE2 | 2.05 | 0.71 |
| 1:C:411:GLY:HA2 | 1:C:414:LEU:HD12 | 1.73 | 0.71 |
| 1:A:137:MET:O | 1:A:138:GLY:C | 2.33 | 0.71 |
| 1:F:143:GLU:O | 1:F:147:GLN:HG3 | 1.91 | 0.71 |
| 1:A:132:MET:HE2 | 1:A:137:MET:HE3 | 1.72 | 0.70 |
| 1:G:409:ASN:HB3 | 1:G:412:HIS:HE1 | 1.56 | 0.70 |
| 1:C:50:GLY:O | 1:C:54:SER:HB2 | 1.89 | 0.70 |
| 1:D:273:GLU:O | 1:D:276:LYS:HG3 | 1.90 | 0.70 |
| 1:D:132:MET:C | 1:D:134:ASP:H | 1.99 | 0.70 |
| 1:B:168:THR:HA | 1:B:308:ARG:HD3 | 1.72 | 0.70 |
| 1:C:90:ASP:O | 1:C:91:GLN:HG3 | 1.90 | 0.70 |
| 1:C:358:ARG:HA | 1:C:396:LEU:HD22 | 1.72 | 0.70 |
| 1:D:174:ILE:HG13 | 1:D:175:THR:H | 1.56 | 0.70 |
| 1:F:217:PHE:HA | 1:F:224:LEU:HD12 | 1.74 | 0.70 |
| 1:F:241:ILE:O | 1:F:245:ILE:HG13 | 1.91 | 0.70 |
| 1:B:97:GLY:HA3 | 1:B:370:THR:O | 1.90 | 0.70 |
| 1:D:241:ILE:O | 1:D:245:ILE:HG13 | 1.92 | 0.70 |
| 1:F:332:ILE:HG21 | 1:F:338:PRO:HG3 | 1.72 | 0.70 |
| 1:C:232:ARG:HB3 | 1:C:232:ARG:HH11 | 1.56 | 0.70 |
| 1:D:321:THR:O | 1:D:325:GLN:HG2 | 1.92 | 0.70 |
| 1:E:258:PRO:HA | 1:E:270:LEU:HD11 | 1.73 | 0.69 |
| 1:B:422:ARG:NH1 | 1:B:422:ARG:HB2 | 2.07 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:220:PHE:HB3 | 1:A:223:PHE:HB3 | 1.74 | 0.69 |
| 1:E:32:PRO:HB2 | 1:E:62:TYR:HD1 | 1.57 | 0.69 |
| 1:G:305:THR:HG22 | 1:G:481:PRO:HD2 | 1.74 | 0.69 |
| 1:C:171:PHE:HB3 | 1:C:304:SER:OG | 1.92 | 0.69 |
| 1:C:489:LEU:HD12 | 1:C:489:LEU:H | 1.57 | 0.69 |
| 1:F:95:PHE:C | 1:F:97:GLY:H | 1.99 | 0.69 |
| 1:C:128:SER:O | 1:C:132:MET:HG2 | 1.90 | 0.69 |
| 1:G:139:LYS:O | 1:G:140:ARG:HG3 | 1.91 | 0.69 |
| 1:A:32:PRO:O | 1:A:66:PHE:HB2 | 1.93 | 0.69 |
| 1:E:273:GLU:O | 1:E:276:LYS:HE2 | 1.92 | 0.69 |
| 1:F:99:GLY:HA3 | 1:F:368:PRO:HB2 | 1.75 | 0.69 |
| 1:C:121:TRP:HE1 | 1:C:125:ARG:HD2 | 1.58 | 0.69 |
| 1:D:167:ASN:HD22 | 1:D:171:PHE:HE2 | 1.41 | 0.69 |
| 1:A:128:SER:O | 1:A:132:MET:HG2 | 1.92 | 0.69 |
| 1:A:28:GLY:O | 1:A:29:LYS:HG2 | 1.92 | 0.69 |
| 1:A:216:VAL:HG11 | 1:B:228:PRO:HD3 | 1.73 | 0.69 |
| 1:C:155:GLU:O | 1:C:158:ARG:HB2 | 1.92 | 0.69 |
| 1:C:161:LYS:NZ | 1:F:485:GLN:HE22 | 1.91 | 0.68 |
| 1:E:114:ILE:HD13 | 1:E:294:SER:HB3 | 1.76 | 0.68 |
| 1:A:284:HIS:O | 1:A:286:GLN:N | 2.27 | 0.68 |
| 1:C:253:ARG:HH22 | 1:C:272:MET:CE | 2.03 | 0.68 |
| 1:F:323:ARG:HB3 | 1:F:348:TYR:CE2 | 2.28 | 0.68 |
| 1:D:412:HIS:O | 1:D:421:LYS:HE2 | 1.93 | 0.68 |
| 1:B:79:CYS:O | 1:B:83:ALA:HB3 | 1.93 | 0.68 |
| 1:C:323:ARG:HB3 | 1:C:348:TYR:CE2 | 2.29 | 0.68 |
| 1:C:421:LYS:HG2 | 1:C:422:ARG:H | 1.58 | 0.68 |
| 1:F:364:PRO:HG3 | 1:F:479:ASN:ND2 | 2.08 | 0.68 |
| 1:F:53:ARG:NH1 | 1:F:56:LEU:HD12 | 2.08 | 0.68 |
| 1:G:164:LEU:HG | 1:G:487:ARG:NH2 | 2.09 | 0.68 |
| 1:D:114:ILE:HD13 | 1:D:294:SER:CB | 2.20 | 0.68 |
| 1:E:113:VAL:HG13 | 1:E:114:ILE:HD12 | 1.75 | 0.68 |
| 1:F:77:VAL:HG12 | 1:F:78:LEU:N | 2.09 | 0.68 |
| 1:F:369:HIS:O | 1:F:387:GLU:HA | 1.93 | 0.68 |
| 1:G:68:VAL:O | 1:G:74:PRO:HA | 1.93 | 0.68 |
| 1:B:410:PRO:O | 1:B:414:LEU:HD12 | 1.94 | 0.68 |
| 1:D:441:ILE:HD12 | 1:D:441:ILE:H | 1.58 | 0.68 |
| 1:A:126:ARG:HE | 1:A:130:ALA:HB2 | 1.58 | 0.68 |
| 1:B:284:HIS:O | 1:B:285:HIS:C | 2.37 | 0.67 |
| 1:D:90:ASP:O | 1:D:91:GLN:HG3 | 1.93 | 0.67 |
| 1:D:392:LEU:HD11 | 1:D:430:SER:HB2 | 1.76 | 0.67 |
| 1:E:176:SER:HB2 | 1:E:300:THR:CG2 | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:395:ALA:CB | 1:C:427:MET:HE3 | 2.25 | 0.67 |
| 1:A:98:ARG:NH1 | 1:A:367:VAL:HB | 2.10 | 0.67 |
| 1:F:282:GLU:HB3 | 1:F:287:ASN:ND2 | 2.10 | 0.67 |
| 1:D:232:ARG:HB3 | 1:D:232:ARG:NH1 | 2.09 | 0.67 |
| 1:G:325:GLN:HE21 | 1:G:491:ARG:HH11 | 1.42 | 0.67 |
| 1:D:116:ALA:HB1 | 1:D:120:ARG:HG2 | 1.77 | 0.67 |
| 1:D:129:LEU:HB2 | 1:D:437:LEU:HD11 | 1.76 | 0.67 |
| 1:F:278:ASP:OD1 | 1:F:279:PRO:HD2 | 1.95 | 0.67 |
| 1:F:357:GLN:HE22 | 2:F:500:HEM:HBB2 | 1.60 | 0.67 |
| 1:D:430:SER:O | 1:D:435:ILE:HG13 | 1.95 | 0.67 |
| 1:A:489:LEU:HD21 | 1:D:489:LEU:CD1 | 2.26 | 0.66 |
| 1:C:129:LEU:O | 1:C:133:ARG:HB2 | 1.94 | 0.66 |
| 1:E:114:ILE:HD13 | 1:E:294:SER:CB | 2.25 | 0.66 |
| 1:G:40:LEU:O | 1:G:43:LEU:HB2 | 1.95 | 0.66 |
| 1:D:87:ALA:HB2 | 1:D:377:PHE:CZ | 2.30 | 0.66 |
| 1:A:114:ILE:HG12 | 2:A:500:HEM:HAD1 | 1.78 | 0.66 |
| 1:E:302:THR:OG1 | 3:E:501:1CI:H4 | 1.93 | 0.66 |
| 1:G:32:PRO:HB2 | 1:G:62:TYR:HB3 | 1.76 | 0.66 |
| 1:F:186:LYS:HD2 | 1:F:186:LYS:H | 1.60 | 0.66 |
| 1:A:129:LEU:C | 1:A:129:LEU:HD23 | 2.21 | 0.66 |
| 1:B:81:THR:HG21 | 1:B:425:GLY:HA2 | 1.77 | 0.66 |
| 1:D:364:PRO:HG3 | 1:D:479:ASN:ND2 | 2.11 | 0.66 |
| 1:A:98:ARG:HG2 | 1:A:115:PHE:HA | 1.78 | 0.66 |
| 1:F:137:MET:HG3 | 1:F:138:GLY:N | 2.11 | 0.66 |
| 1:F:320:VAL:O | 1:F:324:VAL:HG23 | 1.96 | 0.66 |
| 1:C:409:ASN:HB3 | 1:C:412:HIS:CE1 | 2.31 | 0.66 |
| 1:B:391:VAL:HG12 | 1:B:394:SER:H | 1.61 | 0.66 |
| 1:E:114:ILE:HD11 | 2:E:500:HEM:HMD3 | 1.77 | 0.66 |
| 1:F:205:SER:O | 1:F:209:ILE:HG13 | 1.96 | 0.66 |
| 1:B:107:ILE:HG13 | 1:B:238:LEU:HD12 | 1.77 | 0.66 |
| 1:D:308:ARG:HG2 | 1:D:308:ARG:HH11 | 1.61 | 0.65 |
| 1:E:50:GLY:O | 1:E:54:SER:HB2 | 1.96 | 0.65 |
| 1:E:94:ALA:O | 1:E:371:VAL:HA | 1.96 | 0.65 |
| 1:B:98:ARG:HG2 | 1:B:115:PHE:HA | 1.79 | 0.65 |
| 1:C:272:MET:O | 1:C:276:LYS:HB3 | 1.95 | 0.65 |
| 1:E:139:LYS:HE2 | 1:E:145:ARG:HD3 | 1.77 | 0.65 |
| 1:E:183:VAL:HG11 | 1:E:292:VAL:HG13 | 1.78 | 0.65 |
| 1:E:314:MET:HE3 | 1:E:356:ILE:HD11 | 1.78 | 0.65 |
| 1:A:119:GLU:HA | 1:A:122:ARG:HD3 | 1.77 | 0.65 |
| 1:D:42:ASN:O | 1:D:46:MET:HG2 | 1.96 | 0.65 |
| 1:G:107:ILE:HG13 | 1:G:238:LEU:HD12 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:231:HIS:CE1 | 1:F:232:ARG:HG2 | 2.30 | 0.65 |
| 1:F:232:ARG:NH1 | 1:F:232:ARG:HB3 | 2.12 | 0.65 |
| 1:A:111:TYR:HB2 | 1:A:290:LEU:CD1 | 2.25 | 0.65 |
| 1:C:103:VAL:HG11 | 1:C:234:ILE:HD12 | 1.79 | 0.65 |
| 1:G:167:ASN:HB2 | 1:G:171:PHE:CE1 | 2.31 | 0.65 |
| 1:G:374:ASP:HA | 1:G:382:ILE:O | 1.96 | 0.65 |
| 1:D:105:ASP:HB3 | 1:D:106:PRO:HD3 | 1.79 | 0.65 |
| 1:D:348:TYR:O | 1:D:352:VAL:HG23 | 1.97 | 0.65 |
| 1:C:352:VAL:HG13 | 1:C:408:PHE:HZ | 1.62 | 0.65 |
| 1:D:316:LYS:HG3 | 1:D:465:PRO:O | 1.97 | 0.65 |
| 1:E:258:PRO:HA | 1:E:270:LEU:CD1 | 2.27 | 0.65 |
| 1:F:357:GLN:HG2 | 1:F:428:PRO:HG3 | 1.78 | 0.65 |
| 1:A:133:ARG:HA | 1:A:137:MET:HB3 | 1.78 | 0.65 |
| 1:D:73:ARG:HH21 | 1:D:387:GLU:CD | 2.05 | 0.65 |
| 1:D:174:ILE:HG13 | 1:D:175:THR:N | 2.12 | 0.65 |
| 1:G:363:ILE:HG13 | 2:G:500:HEM:HMA3 | 1.77 | 0.65 |
| 1:G:73:ARG:HB2 | 1:G:73:ARG:CZ | 2.27 | 0.64 |
| 1:G:153:LEU:CD1 | 1:G:170:LEU:HD22 | 2.27 | 0.64 |
| 1:A:383:PRO:HG2 | 1:A:386:THR:OG1 | 1.97 | 0.64 |
| 1:B:200:ASP:O | 1:B:204:GLN:HB2 | 1.96 | 0.64 |
| 1:C:105:ASP:HB3 | 1:C:106:PRO:HD3 | 1.78 | 0.64 |
| 1:E:305:THR:HG22 | 1:E:308:ARG:HE | 1.62 | 0.64 |
| 1:F:430:SER:HB2 | 2:F:500:HEM:HBA1 | 1.79 | 0.64 |
| 1:G:422:ARG:HG2 | 1:G:423:ASN:N | 2.11 | 0.64 |
| 1:D:164:LEU:HG | 1:D:487:ARG:HG3 | 1.79 | 0.64 |
| 1:G:52:LEU:HD13 | 1:G:364:PRO:HB3 | 1.79 | 0.64 |
| 1:G:344:ALA:C | 1:G:346:MET:H | 2.05 | 0.64 |
| 1:C:139:LYS:HE2 | 1:C:340:LEU:HB3 | 1.78 | 0.64 |
| 1:E:352:VAL:HG13 | 1:E:408:PHE:HZ | 1.63 | 0.64 |
| 1:C:141:SER:O | 1:C:145:ARG:HG2 | 1.98 | 0.64 |
| 1:B:178:ILE:O | 1:B:182:ILE:HD13 | 1.97 | 0.64 |
| 1:C:93:GLU:OE1 | 1:C:433:LYS:HE3 | 1.97 | 0.64 |
| 1:C:374:ASP:OD2 | 1:C:384:LYS:HB2 | 1.98 | 0.64 |
| 1:G:308:ARG:HG2 | 1:G:308:ARG:HH11 | 1.63 | 0.64 |
| 1:E:80:GLY:O | 1:E:84:ILE:HG12 | 1.97 | 0.64 |
| 1:F:390:PRO:O | 1:F:392:LEU:N | 2.30 | 0.64 |
| 1:C:44:LEU:HB2 | 1:C:45:GLN:NE2 | 2.13 | 0.64 |
| 1:G:40:LEU:HD22 | 1:G:43:LEU:HD23 | 1.80 | 0.64 |
| 1:A:147:GLN:NE2 | 1:A:339:ALA:HA | 2.13 | 0.64 |
| 1:B:136:GLY:HA2 | 1:B:145:ARG:HH12 | 1.62 | 0.64 |
| 1:C:85:ARG:NE | 1:C:424:GLU:HG3 | 2.13 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:153:LEU:HD22 | 1:D:174:ILE:HD13 | 1.80 | 0.64 |
| 1:F:135:PHE:HE1 | 1:F:145:ARG:NH1 | 1.92 | 0.64 |
| 1:G:95:PHE:C | 1:G:97:GLY:H | 2.06 | 0.64 |
| 1:G:137:MET:HG3 | 1:G:138:GLY:H | 1.63 | 0.64 |
| 1:G:479:ASN:O | 1:G:481:PRO:HD3 | 1.98 | 0.64 |
| 1:C:352:VAL:O | 1:C:356:ILE:HG13 | 1.99 | 0.63 |
| 1:E:29:LYS:C | 1:E:30:LEU:HD12 | 2.22 | 0.63 |
| 1:D:114:ILE:CD1 | 1:D:294:SER:HB3 | 2.23 | 0.63 |
| 1:A:308:ARG:HG2 | 1:A:308:ARG:HH11 | 1.64 | 0.63 |
| 1:C:443:ARG:HG2 | 1:C:443:ARG:HH11 | 1.62 | 0.63 |
| 1:B:253:ARG:HH12 | 1:B:272:MET:HE3 | 1.64 | 0.63 |
| 1:B:442:ALA:HB1 | 2:B:500:HEM:HAB | 1.81 | 0.63 |
| 1:B:474:GLU:HB3 | 1:B:480:VAL:HG12 | 1.80 | 0.63 |
| 1:E:93:GLU:OE1 | 1:E:433:LYS:HE3 | 1.98 | 0.63 |
| 1:A:213:SER:HA | 1:A:216:VAL:CG1 | 2.25 | 0.63 |
| 1:E:205:SER:O | 1:E:209:ILE:HG13 | 1.98 | 0.63 |
| 1:F:376:GLN:HE21 | 1:F:381:VAL:HG22 | 1.64 | 0.63 |
| 1:C:349:THR:O | 1:C:353:ILE:HG13 | 1.99 | 0.63 |
| 1:E:174:ILE:HG13 | 1:E:175:THR:H | 1.64 | 0.63 |
| 1:E:224:LEU:H | 1:E:224:LEU:HD23 | 1.64 | 0.63 |
| 1:A:404:THR:HG21 | 1:A:409:ASN:HD22 | 1.64 | 0.63 |
| 1:B:202:PHE:CE1 | 1:B:241:ILE:HD13 | 2.34 | 0.63 |
| 1:D:37:LEU:H | 1:D:37:LEU:HD12 | 1.63 | 0.63 |
| 1:G:336:ARG:HB2 | 1:G:337:PRO:HD2 | 1.81 | 0.63 |
| 1:E:114:ILE:CD1 | 1:E:294:SER:HB3 | 2.29 | 0.63 |
| 1:E:158:ARG:HH11 | 1:E:158:ARG:HG3 | 1.64 | 0.63 |
| 1:E:105:ASP:HB3 | 1:E:106:PRO:HD3 | 1.80 | 0.62 |
| 1:F:202:PHE:CE1 | 1:F:241:ILE:HD13 | 2.34 | 0.62 |
| 1:C:81:THR:HG23 | 1:C:425:GLY:HA2 | 1.81 | 0.62 |
| 1:E:272:MET:HE1 | 1:E:283:PHE:CD2 | 2.34 | 0.62 |
| 1:F:425:GLY:O | 1:F:427:MET:HG2 | 1.99 | 0.62 |
| 1:A:120:ARG:HA | 1:A:282:GLU:HG3 | 1.81 | 0.62 |
| 1:C:139:LYS:HD3 | 1:C:140:ARG:CZ | 2.29 | 0.62 |
| 1:C:174:ILE:HD12 | 1:C:449:PHE:CD1 | 2.34 | 0.62 |
| 1:F:371:VAL:HG22 | 1:F:386:THR:H | 1.64 | 0.62 |
| 1:B:70:LEU:O | 1:B:73:ARG:HG2 | 1.98 | 0.62 |
| 1:B:129:LEU:O | 1:B:129:LEU:HD23 | 1.99 | 0.62 |
| 1:C:340:LEU:HD11 | 1:C:343:ARG:CZ | 2.28 | 0.62 |
| 1:F:105:ASP:HB3 | 1:F:106:PRO:HD3 | 1.81 | 0.62 |
| 1:F:364:PRO:O | 1:F:393:SER:HB2 | 1.98 | 0.62 |
| 1:G:299:GLY:HA2 | 2:G:500:HEM:HMC3 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:52:LEU:O | 1:E:56:LEU:HG | 2.00 | 0.62 |
| 1:A:268:TYR:CD1 | 1:A:288:LEU:HD13 | 2.34 | 0.62 |
| 1:A:363:ILE:CG2 | 1:A:366:GLY:HA2 | 2.30 | 0.62 |
| 1:F:118:GLY:O | 1:F:122:ARG:HD3 | 1.99 | 0.62 |
| 1:A:429:PHE:HE2 | 1:A:443:ARG:HD3 | 1.63 | 0.62 |
| 1:D:179:ILE:HD13 | 1:D:179:ILE:C | 2.24 | 0.62 |
| 1:E:409:ASN:HB3 | 1:E:412:HIS:CE1 | 2.34 | 0.62 |
| 1:F:162:GLY:O | 1:F:487:ARG:HB2 | 2.00 | 0.62 |
| 1:B:78:LEU:HB2 | 1:B:84:ILE:HD13 | 1.81 | 0.62 |
| 1:C:198:LEU:O | 1:C:201:LEU:HB2 | 1.99 | 0.62 |
| 1:D:113:VAL:HG13 | 1:D:114:ILE:HD12 | 1.80 | 0.62 |
| 1:E:362:LEU:H | 1:E:362:LEU:CD2 | 2.12 | 0.62 |
| 1:F:49:LYS:CE | 1:F:53:ARG:HG2 | 2.30 | 0.62 |
| 1:A:349:THR:O | 1:A:353:ILE:HG13 | 2.00 | 0.62 |
| 1:B:101:ILE:HB | 1:B:104:VAL:CG2 | 2.30 | 0.62 |
| 1:G:95:PHE:O | 1:G:369:HIS:HD2 | 1.83 | 0.62 |
| 1:B:98:ARG:NH1 | 1:B:367:VAL:HB | 2.15 | 0.62 |
| 1:E:258:PRO:HG3 | 1:E:270:LEU:CD2 | 2.29 | 0.62 |
| 1:C:170:LEU:O | 1:C:170:LEU:HD23 | 2.00 | 0.61 |
| 1:F:288:LEU:O | 1:F:292:VAL:HG23 | 2.00 | 0.61 |
| 1:F:323:ARG:HB3 | 1:F:348:TYR:HE2 | 1.65 | 0.61 |
| 1:A:320:VAL:O | 1:A:324:VAL:HG23 | 2.00 | 0.61 |
| 1:C:209:ILE:HG22 | 1:C:477:VAL:HG11 | 1.82 | 0.61 |
| 1:D:98:ARG:HB2 | 1:D:434:ARG:NH1 | 2.14 | 0.61 |
| 1:G:324:VAL:O | 1:G:328:ILE:HG13 | 1.99 | 0.61 |
| 1:A:124:LEU:HD11 | 1:A:287:ASN:ND2 | 2.16 | 0.61 |
| 1:B:81:THR:CG2 | 1:B:425:GLY:HA2 | 2.30 | 0.61 |
| 1:B:297:PHE:CD2 | 3:B:501:1CI:H8 | 2.35 | 0.61 |
| 1:F:132:MET:CE | 1:F:441:ILE:HD11 | 2.30 | 0.61 |
| 1:F:138:GLY:O | 1:F:139:LYS:HG2 | 1.99 | 0.61 |
| 1:F:146:ILE:HG12 | 1:F:178:ILE:HD12 | 1.82 | 0.61 |
| 1:F:238:LEU:HD23 | 1:F:241:ILE:HD12 | 1.83 | 0.61 |
| 1:A:369:HIS:O | 1:A:370:THR:HG23 | 1.99 | 0.61 |
| 1:C:125:ARG:NH1 | 1:C:437:LEU:HB2 | 2.14 | 0.61 |
| 1:D:31:PRO:HB3 | 1:D:65:VAL:HG12 | 1.80 | 0.61 |
| 1:D:324:VAL:O | 1:D:328:ILE:HG13 | 2.00 | 0.61 |
| 1:E:168:THR:HA | 1:E:308:ARG:CD | 2.30 | 0.61 |
| 1:G:82:ASP:C | 1:G:84:ILE:H | 2.06 | 0.61 |
| 1:B:422:ARG:HB2 | 1:B:422:ARG:HH11 | 1.65 | 0.61 |
| 1:C:363:ILE:HG22 | 1:C:366:GLY:H | 1.65 | 0.61 |
| 1:E:163:ALA:HA | 1:E:487:ARG:HH12 | 1.64 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:328:ILE:HG12 | 1:G:346:MET:HE1 | 1.82 | 0.61 |
| 1:C:121:TRP:NE1 | 1:C:125:ARG:HD2 | 2.14 | 0.61 |
| 1:C:154:VAL:HG12 | 1:C:158:ARG:NH1 | 2.16 | 0.61 |
| 1:D:204:GLN:O | 1:D:208:LEU:HD23 | 2.00 | 0.61 |
| 1:A:245:ILE:O | 1:A:249:VAL:HG23 | 2.00 | 0.61 |
| 1:B:253:ARG:HH12 | 1:B:272:MET:CE | 2.14 | 0.61 |
| 1:E:237:ASN:O | 1:E:241:ILE:HG13 | 2.01 | 0.61 |
| 1:F:99:GLY:HA3 | 1:F:368:PRO:CB | 2.31 | 0.61 |
| 1:C:136:GLY:O | 1:C:142:VAL:HB | 2.01 | 0.60 |
| 1:C:308:ARG:HG2 | 1:C:308:ARG:HH11 | 1.66 | 0.60 |
| 1:F:242:ASN:C | 1:F:244:PHE:H | 2.09 | 0.60 |
| 1:A:137:MET:O | 1:A:139:LYS:N | 2.34 | 0.60 |
| 1:B:143:GLU:O | 1:B:147:GLN:HG3 | 2.01 | 0.60 |
| 1:C:84:ILE:HG21 | 1:C:427:MET:SD | 2.41 | 0.60 |
| 1:D:299:GLY:HA2 | 2:D:500:HEM:HMC3 | 1.83 | 0.60 |
| 1:E:168:THR:HA | 1:E:308:ARG:HD2 | 1.82 | 0.60 |
| 1:B:183:VAL:HG11 | 1:B:292:VAL:HG13 | 1.83 | 0.60 |
| 1:D:284:HIS:O | 1:D:286:GLN:N | 2.34 | 0.60 |
| 1:D:370:THR:HA | 1:D:386:THR:O | 2.00 | 0.60 |
| 1:F:250:GLU:C | 1:F:252:HIS:H | 2.08 | 0.60 |
| 1:G:328:ILE:O | 1:G:332:ILE:HB | 2.01 | 0.60 |
| 1:F:249:VAL:CG2 | 1:F:288:LEU:HD21 | 2.31 | 0.60 |
| 1:G:423:ASN:C | 1:G:425:GLY:H | 2.10 | 0.60 |
| 1:B:134:ASP:O | 1:B:135:PHE:HB3 | 2.00 | 0.60 |
| 1:D:125:ARG:HH11 | 1:D:125:ARG:HG3 | 1.65 | 0.60 |
| 1:B:127:PHE:O | 1:B:131:THR:HG22 | 2.01 | 0.60 |
| 1:C:81:THR:CG2 | 1:C:425:GLY:HA2 | 2.31 | 0.60 |
| 1:C:376:GLN:HG2 | 1:C:381:VAL:HG22 | 1.83 | 0.60 |
| 1:E:136:GLY:O | 1:E:141:SER:HA | 2.01 | 0.60 |
| 1:E:145:ARG:HD2 | 1:E:181:SER:HB3 | 1.82 | 0.60 |
| 1:E:154:VAL:O | 1:E:158:ARG:HG2 | 2.01 | 0.60 |
| 1:B:102:ALA:HB2 | 1:B:218:GLU:HA | 1.84 | 0.60 |
| 1:G:316:LYS:HB2 | 1:G:468:ILE:HG21 | 1.84 | 0.60 |
| 1:B:369:HIS:HE1 | 2:B:500:HEM:O2A | 1.85 | 0.60 |
| 1:C:244:PHE:CD1 | 1:C:244:PHE:C | 2.80 | 0.60 |
| 1:D:340:LEU:HD11 | 1:D:343:ARG:NH2 | 2.17 | 0.60 |
| 1:B:245:ILE:O | 1:B:249:VAL:HG23 | 2.02 | 0.60 |
| 1:B:285:HIS:O | 1:B:286:GLN:C | 2.44 | 0.60 |
| 1:C:78:LEU:O | 1:C:84:ILE:HD11 | 2.01 | 0.60 |
| 1:C:404:THR:HG23 | 1:C:412:HIS:HE1 | 1.67 | 0.60 |
| 1:F:327:GLU:OE2 | 1:F:347:PRO:HD2 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:265:ILE:O | 1:G:269:LEU:HG | 2.02 | 0.60 |
| 1:G:383:PRO:O | 1:G:386:THR:HG22 | 2.02 | 0.60 |
| 1:D:442:ALA:HB2 | 2:D:500:HEM:HMC2 | 1.83 | 0.59 |
| 1:F:245:ILE:O | 1:F:249:VAL:HB | 2.02 | 0.59 |
| 1:G:421:LYS:HG2 | 1:G:422:ARG:H | 1.67 | 0.59 |
| 1:A:179:ILE:HD13 | 1:A:179:ILE:O | 2.02 | 0.59 |
| 1:A:404:THR:OG1 | 1:A:407:THR:HB | 2.01 | 0.59 |
| 1:C:288:LEU:O | 1:C:292:VAL:HG23 | 2.01 | 0.59 |
| 1:C:363:ILE:HG21 | 1:C:366:GLY:HA2 | 1.83 | 0.59 |
| 1:A:69:TYR:CZ | 1:A:74:PRO:HB3 | 2.37 | 0.59 |
| 1:A:365:PHE:O | 1:A:366:GLY:O | 2.20 | 0.59 |
| 1:C:256:LEU:HD12 | 1:C:257:ASP:H | 1.67 | 0.59 |
| 1:D:404:THR:HB | 1:D:407:THR:HB | 1.83 | 0.59 |
| 1:G:56:LEU:C | 1:G:58:LEU:H | 2.10 | 0.59 |
| 1:G:90:ASP:O | 1:G:91:GLN:HB2 | 2.03 | 0.59 |
| 1:G:105:ASP:N | 1:G:106:PRO:CD | 2.65 | 0.59 |
| 1:D:427:MET:HE2 | 1:D:431:LEU:HD21 | 1.83 | 0.59 |
| 1:F:167:ASN:ND2 | 1:F:486:ILE:HG21 | 2.17 | 0.59 |
| 1:C:390:PRO:O | 1:C:392:LEU:N | 2.35 | 0.59 |
| 1:C:457:PHE:CD1 | 1:C:490:ALA:HA | 2.37 | 0.59 |
| 1:E:53:ARG:HH11 | 1:E:53:ARG:CA | 2.15 | 0.59 |
| 1:A:473:ARG:HB2 | 1:A:482:PRO:HA | 1.84 | 0.59 |
| 1:D:133:ARG:HD2 | 1:D:142:VAL:CG2 | 2.33 | 0.59 |
| 1:F:464:PRO:HB2 | 1:F:467:ASP:CB | 2.33 | 0.59 |
| 1:G:54:SER:O | 1:G:58:LEU:HB2 | 2.03 | 0.59 |
| 1:F:132:MET:HB2 | 1:F:182:ILE:HG21 | 1.85 | 0.59 |
| 1:B:91:GLN:HB3 | 1:B:94:ALA:HB3 | 1.84 | 0.59 |
| 1:E:303:THR:HG21 | 1:E:445:GLU:OE1 | 2.02 | 0.59 |
| 1:B:205:SER:O | 1:B:209:ILE:HG12 | 2.03 | 0.59 |
| 1:C:191:LYS:HE3 | 1:C:191:LYS:HA | 1.85 | 0.59 |
| 1:C:316:LYS:O | 1:C:465:PRO:HB3 | 2.02 | 0.59 |
| 1:G:50:GLY:HA2 | 1:G:215:GLN:OE1 | 2.03 | 0.59 |
| 1:G:384:LYS:O | 1:G:385:ASN:HB2 | 2.03 | 0.59 |
| 1:B:236:ARG:O | 1:B:239:GLN:HB2 | 2.03 | 0.59 |
| 1:C:402:PHE:HD1 | 1:C:412:HIS:HD2 | 1.47 | 0.59 |
| 1:E:220:PHE:HB2 | 1:E:224:LEU:HD21 | 1.84 | 0.59 |
| 1:G:348:TYR:O | 1:G:352:VAL:HG23 | 2.02 | 0.59 |
| 1:A:226:TYR:CD2 | 1:C:43:LEU:HG | 2.37 | 0.58 |
| 1:A:313:LEU:O | 1:A:313:LEU:HD23 | 2.02 | 0.58 |
| 1:D:101:ILE:HD11 | 1:D:368:PRO:CD | 2.32 | 0.58 |
| 1:E:34:PRO:HG2 | 1:E:42:ASN:OD1 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:116:ALA:O | 1:G:121:TRP:HB2 | 2.03 | 0.58 |
| 1:D:43:LEU:HD11 | 1:F:226:TYR:HD2 | 1.68 | 0.58 |
| 1:E:99:GLY:HA3 | 1:E:368:PRO:CB | 2.30 | 0.58 |
| 1:G:73:ARG:HB2 | 1:G:73:ARG:NH1 | 2.19 | 0.58 |
| 1:G:256:LEU:HD22 | 1:G:269:LEU:HD12 | 1.86 | 0.58 |
| 1:G:358:ARG:HA | 1:G:396:LEU:HD13 | 1.86 | 0.58 |
| 1:A:364:PRO:HG3 | 1:A:479:ASN:ND2 | 2.18 | 0.58 |
| 1:B:52:LEU:HD22 | 1:B:364:PRO:HB3 | 1.84 | 0.58 |
| 1:B:203:PHE:HA | 1:B:301:GLU:OE1 | 2.02 | 0.58 |
| 1:D:325:GLN:HA | 1:D:325:GLN:NE2 | 2.14 | 0.58 |
| 1:F:398:ASP:OD2 | 1:F:400:ARG:HB2 | 2.04 | 0.58 |
| 1:G:376:GLN:CD | 1:G:376:GLN:H | 2.11 | 0.58 |
| 1:A:37:LEU:HD11 | 1:A:44:LEU:HD12 | 1.85 | 0.58 |
| 1:B:279:PRO:HG2 | 1:B:280:SER:H | 1.67 | 0.58 |
| 1:B:320:VAL:HG21 | 1:B:408:PHE:CE2 | 2.38 | 0.58 |
| 1:D:108:PHE:O | 1:D:110:GLY:N | 2.32 | 0.58 |
| 1:D:202:PHE:CD1 | 1:D:297:PHE:HD1 | 2.21 | 0.58 |
| 1:D:322:GLU:HA | 1:D:325:GLN:HB2 | 1.85 | 0.58 |
| 1:D:405:PRO:HG2 | 1:D:406:ASN:OD1 | 2.02 | 0.58 |
| 1:E:94:ALA:HB1 | 1:E:375:THR:OG1 | 2.03 | 0.58 |
| 1:A:70:LEU:HD12 | 1:A:75:VAL:HG11 | 1.85 | 0.58 |
| 1:E:111:TYR:HB2 | 1:E:290:LEU:CD1 | 2.23 | 0.58 |
| 1:E:173:SER:O | 1:E:177:ASN:HB2 | 2.03 | 0.58 |
| 1:F:362:LEU:H | 1:F:362:LEU:HD22 | 1.69 | 0.58 |
| 1:F:363:ILE:HG22 | 1:F:366:GLY:H | 1.69 | 0.58 |
| 1:B:190:TYR:O | 1:B:196:LEU:HD21 | 2.03 | 0.58 |
| 1:C:449:PHE:O | 1:C:453:ILE:HG13 | 2.04 | 0.58 |
| 1:C:489:LEU:HD12 | 1:C:489:LEU:N | 2.18 | 0.58 |
| 1:D:314:MET:HE2 | 1:D:314:MET:HA | 1.85 | 0.58 |
| 1:E:47:ASP:HB3 | 1:E:54:SER:HA | 1.86 | 0.58 |
| 1:E:108:PHE:HA | 1:E:290:LEU:HD13 | 1.85 | 0.58 |
| 1:E:305:THR:HG22 | 1:E:308:ARG:HH21 | 1.69 | 0.58 |
| 1:F:61:LYS:HD3 | 1:F:62:TYR:HE2 | 1.69 | 0.58 |
| 1:F:253:ARG:NH2 | 1:F:269:LEU:HD22 | 2.19 | 0.58 |
| 1:G:70:LEU:HB2 | 1:G:73:ARG:HG3 | 1.85 | 0.58 |
| 1:G:142:VAL:O | 1:G:146:ILE:HG13 | 2.04 | 0.58 |
| 1:A:324:VAL:HG13 | 1:A:349:THR:OG1 | 2.04 | 0.58 |
| 1:C:319:HIS:CE1 | 1:C:320:VAL:HG23 | 2.39 | 0.58 |
| 1:C:327:GLU:OE1 | 1:C:346:MET:HB3 | 2.03 | 0.58 |
| 1:D:225:LYS:C | 1:D:227:PHE:H | 2.10 | 0.58 |
| 1:D:236:ARG:O | 1:D:239:GLN:HB2 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:320:VAL:O | 1:D:324:VAL:HG23 | 2.04 | 0.58 |
| 1:E:228:PRO:HG3 | 1:F:213:SER:OG | 2.04 | 0.58 |
| 1:E:308:ARG:HH11 | 1:E:308:ARG:HB3 | 1.69 | 0.58 |
| 1:A:174:ILE:O | 1:A:178:ILE:HG12 | 2.04 | 0.58 |
| 1:G:332:ILE:HD13 | 1:G:338:PRO:HG3 | 1.84 | 0.58 |
| 1:G:362:LEU:HD22 | 1:G:362:LEU:N | 2.18 | 0.58 |
| 1:D:70:LEU:HD12 | 1:D:75:VAL:HG11 | 1.84 | 0.57 |
| 1:E:164:LEU:HD21 | 1:E:462:PRO:HD3 | 1.86 | 0.57 |
| 1:F:222:GLY:HA2 | 1:F:225:LYS:HE3 | 1.86 | 0.57 |
| 1:G:276:LYS:HD2 | 1:G:277:SER:N | 2.19 | 0.57 |
| 1:A:138:GLY:C | 1:A:139:LYS:HD2 | 2.28 | 0.57 |
| 1:B:75:VAL:HG12 | 1:B:387:GLU:HB2 | 1.84 | 0.57 |
| 1:E:372:THR:O | 1:E:384:LYS:HE3 | 2.03 | 0.57 |
| 1:B:371:VAL:HG21 | 1:B:382:ILE:HG22 | 1.85 | 0.57 |
| 1:D:44:LEU:HD12 | 1:D:44:LEU:N | 2.19 | 0.57 |
| 1:G:28:GLY:O | 1:G:380:TYR:HD1 | 1.87 | 0.57 |
| 1:B:158:ARG:HH11 | 1:B:158:ARG:HG3 | 1.67 | 0.57 |
| 1:B:248:SER:C | 1:B:250:GLU:H | 2.12 | 0.57 |
| 1:C:51:LEU:O | 1:C:54:SER:HB3 | 2.04 | 0.57 |
| 1:C:272:MET:HG3 | 1:C:283:PHE:O | 2.03 | 0.57 |
| 1:F:48:ARG:HG3 | 1:F:48:ARG:HH11 | 1.69 | 0.57 |
| 1:F:404:THR:OG1 | 1:F:407:THR:HB | 2.05 | 0.57 |
| 1:G:137:MET:HG3 | 1:G:138:GLY:N | 2.19 | 0.57 |
| 1:G:202:PHE:CE1 | 1:G:241:ILE:HD13 | 2.39 | 0.57 |
| 1:C:413:PHE:O | 1:C:420:LEU:HD12 | 2.04 | 0.57 |
| 1:E:174:ILE:HG13 | 1:E:175:THR:N | 2.19 | 0.57 |
| 1:E:404:THR:O | 1:E:404:THR:HG23 | 2.04 | 0.57 |
| 1:F:98:ARG:N | 1:F:117:ASN:OD1 | 2.36 | 0.57 |
| 1:A:132:MET:HB2 | 1:A:182:ILE:HG21 | 1.86 | 0.57 |
| 1:B:362:LEU:H | 1:B:362:LEU:HD22 | 1.69 | 0.57 |
| 1:F:229:GLY:C | 1:F:231:HIS:H | 2.12 | 0.57 |
| 1:G:150:ALA:O | 1:G:154:VAL:HG23 | 2.05 | 0.57 |
| 1:G:460:ALA:O | 1:G:487:ARG:HG2 | 2.04 | 0.57 |
| 1:A:324:VAL:O | 1:A:328:ILE:HG13 | 2.05 | 0.57 |
| 1:B:253:ARG:NH2 | 1:B:272:MET:HE1 | 2.15 | 0.57 |
| 1:C:284:HIS:O | 1:C:286:GLN:N | 2.37 | 0.57 |
| 1:D:158:ARG:HG2 | 1:D:457:PHE:CZ | 2.37 | 0.57 |
| 1:E:414:LEU:HA | 1:E:419:ALA:O | 2.05 | 0.57 |
| 1:C:111:TYR:HB2 | 1:C:290:LEU:HD12 | 1.86 | 0.57 |
| 1:E:37:LEU:HD12 | 1:E:37:LEU:N | 2.20 | 0.57 |
| 1:C:34:PRO:HD2 | 1:C:67:THR:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:145:ARG:HD2 | 1:E:181:SER:CB | 2.35 | 0.57 |
| 1:F:315:LEU:HG | 1:F:459:ILE:HD12 | 1.86 | 0.57 |
| 1:C:79:CYS:O | 1:C:83:ALA:HB3 | 2.05 | 0.56 |
| 1:D:103:VAL:HG21 | 1:D:209:ILE:HG23 | 1.87 | 0.56 |
| 1:E:140:ARG:HB2 | 1:E:144:GLU:CB | 2.35 | 0.56 |
| 1:C:108:PHE:O | 1:C:110:GLY:N | 2.34 | 0.56 |
| 1:C:372:THR:O | 1:C:384:LYS:HE3 | 2.05 | 0.56 |
| 1:E:358:ARG:HG3 | 1:E:396:LEU:HB3 | 1.88 | 0.56 |
| 1:A:268:TYR:CE1 | 1:A:288:LEU:HB2 | 2.41 | 0.56 |
| 1:C:174:ILE:O | 1:C:178:ILE:HG12 | 2.05 | 0.56 |
| 1:C:457:PHE:HA | 1:C:491:ARG:HG3 | 1.88 | 0.56 |
| 1:D:133:ARG:HD2 | 1:D:142:VAL:HG21 | 1.87 | 0.56 |
| 1:D:268:TYR:O | 1:D:272:MET:HB2 | 2.06 | 0.56 |
| 1:E:161:LYS:O | 1:E:162:GLY:C | 2.49 | 0.56 |
| 1:E:171:PHE:CD2 | 1:E:307:LEU:HB3 | 2.40 | 0.56 |
| 1:E:271:ARG:C | 1:E:272:MET:HE2 | 2.31 | 0.56 |
| 1:E:358:ARG:HD2 | 1:E:396:LEU:O | 2.06 | 0.56 |
| 1:F:183:VAL:O | 1:F:265:ILE:HG13 | 2.06 | 0.56 |
| 1:F:232:ARG:HB3 | 1:F:232:ARG:HH11 | 1.71 | 0.56 |
| 1:F:243:THR:O | 1:F:243:THR:HG22 | 2.05 | 0.56 |
| 1:G:41:GLY:C | 1:G:43:LEU:H | 2.13 | 0.56 |
| 1:G:145:ARG:O | 1:G:148:GLU:HB3 | 2.06 | 0.56 |
| 1:G:298:ALA:HB1 | 3:G:501:1CI:H4 | 1.87 | 0.56 |
| 1:G:341:ASP:C | 1:G:343:ARG:H | 2.10 | 0.56 |
| 1:A:85:ARG:HA | 1:A:89:VAL:HG23 | 1.87 | 0.56 |
| 1:E:358:ARG:HG3 | 1:E:396:LEU:CD2 | 2.32 | 0.56 |
| 1:F:140:ARG:NH2 | 1:F:148:GLU:HG2 | 2.19 | 0.56 |
| 1:G:372:THR:O | 1:G:373:LYS:HB3 | 2.05 | 0.56 |
| 1:C:112:GLY:O | 1:C:116:ALA:HB2 | 2.05 | 0.56 |
| 1:G:210:SER:O | 1:G:474:GLU:HG3 | 2.06 | 0.56 |
| 1:D:94:ALA:O | 1:D:371:VAL:HA | 2.05 | 0.56 |
| 1:D:238:LEU:HD22 | 1:D:293:LEU:HD21 | 1.86 | 0.56 |
| 1:F:285:HIS:O | 1:F:287:ASN:N | 2.38 | 0.56 |
| 1:A:81:THR:CG2 | 1:A:425:GLY:HA2 | 2.36 | 0.56 |
| 1:A:362:LEU:HD22 | 1:A:362:LEU:N | 2.18 | 0.56 |
| 1:C:158:ARG:HH11 | 1:C:158:ARG:HG3 | 1.70 | 0.56 |
| 1:C:391:VAL:HG12 | 1:C:394:SER:H | 1.69 | 0.56 |
| 1:A:137:MET:HA | 1:A:142:VAL:HG21 | 1.88 | 0.56 |
| 1:B:48:ARG:HH11 | 1:B:48:ARG:HG3 | 1.70 | 0.56 |
| 1:B:268:TYR:CD1 | 1:B:288:LEU:HD13 | 2.40 | 0.56 |
| 1:B:352:VAL:HG13 | 1:B:408:PHE:HZ | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:279:PRO:HG2 | 1:E:280:SER:H | 1.70 | 0.56 |
| 1:F:435:ILE:HG12 | 1:F:436:CYS:N | 2.20 | 0.56 |
| 1:D:141:SER:HB2 | 1:D:144:GLU:HG2 | 1.88 | 0.56 |
| 1:E:332:ILE:HD13 | 1:E:338:PRO:HB3 | 1.87 | 0.56 |
| 1:C:421:LYS:CG | 1:C:422:ARG:H | 2.17 | 0.56 |
| 1:C:437:LEU:C | 1:C:437:LEU:HD23 | 2.31 | 0.56 |
| 1:D:98:ARG:HG3 | 1:D:99:GLY:O | 2.06 | 0.56 |
| 1:E:69:TYR:CZ | 1:E:74:PRO:HB3 | 2.40 | 0.56 |
| 1:F:176:SER:HB2 | 1:F:300:THR:HG23 | 1.88 | 0.56 |
| 1:F:215:GLN:O | 1:F:218:GLU:HB3 | 2.06 | 0.56 |
| 1:G:358:ARG:HG3 | 1:G:396:LEU:HB3 | 1.86 | 0.56 |
| 1:C:34:PRO:HG2 | 1:C:42:ASN:OD1 | 2.06 | 0.55 |
| 1:E:98:ARG:HD3 | 1:E:99:GLY:N | 2.20 | 0.55 |
| 1:E:132:MET:SD | 1:E:133:ARG:N | 2.79 | 0.55 |
| 1:G:320:VAL:HG21 | 1:G:408:PHE:HE2 | 1.70 | 0.55 |
| 1:C:183:VAL:O | 1:C:265:ILE:HG13 | 2.06 | 0.55 |
| 1:C:198:LEU:H | 1:C:198:LEU:HD22 | 1.71 | 0.55 |
| 1:F:167:ASN:HD22 | 1:F:486:ILE:HG21 | 1.71 | 0.55 |
| 1:C:400:ARG:HG2 | 1:C:400:ARG:HH11 | 1.70 | 0.55 |
| 1:D:308:ARG:NH2 | 1:D:481:PRO:O | 2.39 | 0.55 |
| 1:E:273:GLU:OE2 | 1:E:276:LYS:HD3 | 2.06 | 0.55 |
| 1:F:93:GLU:HB2 | 1:F:433:LYS:HE3 | 1.88 | 0.55 |
| 1:F:415:ASP:CG | 1:F:416:ALA:N | 2.64 | 0.55 |
| 1:E:29:LYS:HE3 | 1:E:380:TYR:CD1 | 2.41 | 0.55 |
| 1:E:111:TYR:CB | 1:E:290:LEU:HD12 | 2.25 | 0.55 |
| 1:F:88:LEU:HD11 | 1:F:369:HIS:NE2 | 2.22 | 0.55 |
| 1:A:94:ALA:HB2 | 1:A:373:LYS:HE2 | 1.89 | 0.55 |
| 1:A:459:ILE:HB | 1:A:486:ILE:HD11 | 1.89 | 0.55 |
| 1:E:70:LEU:O | 1:E:73:ARG:HG2 | 2.06 | 0.55 |
| 1:E:127:PHE:CD2 | 1:E:283:PHE:HE2 | 2.25 | 0.55 |
| 1:F:443:ARG:HB3 | 1:F:443:ARG:HH11 | 1.69 | 0.55 |
| 1:A:231:HIS:CE1 | 1:A:232:ARG:HG2 | 2.41 | 0.55 |
| 1:B:105:ASP:N | 1:B:106:PRO:CD | 2.70 | 0.55 |
| 1:G:363:ILE:HD13 | 1:G:478:GLY:HA2 | 1.88 | 0.55 |
| 1:A:33:GLY:HA3 | 1:A:67:THR:O | 2.05 | 0.55 |
| 1:A:102:ALA:HB1 | 1:A:217:PHE:CD2 | 2.36 | 0.55 |
| 1:A:308:ARG:HG2 | 1:A:308:ARG:NH1 | 2.22 | 0.55 |
| 1:E:140:ARG:HB2 | 1:E:144:GLU:CG | 2.36 | 0.55 |
| 1:F:246:GLY:C | 1:F:248:SER:H | 2.14 | 0.55 |
| 1:B:73:ARG:NH2 | 1:B:387:GLU:OE1 | 2.39 | 0.55 |
| 1:F:48:ARG:HG3 | 1:F:48:ARG:NH1 | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:145:ARG:HG2 | 1:G:145:ARG:HH11 | 1.72 | 0.55 |
| 1:A:390:PRO:O | 1:A:392:LEU:N | 2.40 | 0.55 |
| 1:B:134:ASP:C | 1:B:136:GLY:H | 2.14 | 0.55 |
| 1:B:162:GLY:HA3 | 1:B:489:LEU:HD23 | 1.89 | 0.55 |
| 1:B:202:PHE:O | 1:B:203:PHE:HB3 | 2.07 | 0.55 |
| 1:B:302:THR:HG21 | 3:B:501:1CI:H4 | 1.88 | 0.55 |
| 1:C:88:LEU:HD22 | 1:C:432:GLY:HA3 | 1.89 | 0.55 |
| 1:D:70:LEU:HD22 | 1:D:219:LEU:CD1 | 2.36 | 0.55 |
| 1:D:98:ARG:HG2 | 1:D:115:PHE:HA | 1.87 | 0.55 |
| 1:E:133:ARG:CZ | 1:E:141:SER:HB2 | 2.36 | 0.55 |
| 1:F:276:LYS:HD2 | 1:F:277:SER:N | 2.22 | 0.55 |
| 1:G:128:SER:O | 1:G:131:THR:HB | 2.07 | 0.55 |
| 1:G:362:LEU:H | 1:G:362:LEU:CD2 | 2.19 | 0.55 |
| 1:G:380:TYR:OH | 1:G:383:PRO:HD3 | 2.07 | 0.55 |
| 1:A:52:LEU:CD2 | 1:A:364:PRO:HB3 | 2.36 | 0.55 |
| 1:A:129:LEU:HD23 | 1:A:129:LEU:O | 2.07 | 0.55 |
| 1:C:183:VAL:HG11 | 1:C:292:VAL:HG13 | 1.88 | 0.55 |
| 1:G:31:PRO:HD3 | 1:G:380:TYR:CB | 2.36 | 0.55 |
| 1:E:146:ILE:HD13 | 1:E:445:GLU:HG2 | 1.89 | 0.54 |
| 1:E:376:GLN:NE2 | 1:E:379:GLY:H | 1.99 | 0.54 |
| 1:G:101:ILE:HD11 | 1:G:368:PRO:HD2 | 1.89 | 0.54 |
| 1:G:331:VAL:HG21 | 1:G:345:LYS:O | 2.06 | 0.54 |
| 1:A:60:GLU:OE2 | 1:A:60:GLU:HA | 2.06 | 0.54 |
| 1:A:362:LEU:C | 1:A:363:ILE:HD12 | 2.32 | 0.54 |
| 1:C:49:LYS:HG2 | 1:C:53:ARG:HB2 | 1.88 | 0.54 |
| 1:C:340:LEU:O | 1:C:340:LEU:HD12 | 2.07 | 0.54 |
| 1:D:167:ASN:HB2 | 1:D:171:PHE:CE2 | 2.42 | 0.54 |
| 1:E:316:LYS:O | 1:E:465:PRO:HB3 | 2.07 | 0.54 |
| 1:G:362:LEU:O | 1:G:363:ILE:HD13 | 2.07 | 0.54 |
| 1:A:39:VAL:HG12 | 1:A:40:LEU:HD23 | 1.89 | 0.54 |
| 1:A:355:GLU:OE2 | 1:A:358:ARG:NH2 | 2.39 | 0.54 |
| 1:C:241:ILE:O | 1:C:245:ILE:HG13 | 2.07 | 0.54 |
| 1:D:132:MET:C | 1:D:134:ASP:N | 2.66 | 0.54 |
| 1:D:297:PHE:CD2 | 3:D:501:1CI:H10 | 2.42 | 0.54 |
| 1:F:62:TYR:HD2 | 1:F:62:TYR:N | 2.05 | 0.54 |
| 1:B:59:ARG:O | 1:B:59:ARG:HG2 | 2.06 | 0.54 |
| 1:B:172:HIS:CE1 | 1:B:203:PHE:HB2 | 2.42 | 0.54 |
| 1:E:355:GLU:HG2 | 1:E:409:ASN:H | 1.73 | 0.54 |
| 1:G:128:SER:O | 1:G:132:MET:HG2 | 2.07 | 0.54 |
| 1:G:422:ARG:CG | 1:G:423:ASN:H | 2.20 | 0.54 |
| 1:C:168:THR:HA | 1:C:308:ARG:HD2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:222:GLY:HA2 | 1:C:225:LYS:HE3 | 1.89 | 0.54 |
| 1:C:223:PHE:C | 1:C:223:PHE:CD2 | 2.85 | 0.54 |
| 1:F:29:LYS:C | 1:F:30:LEU:HD23 | 2.32 | 0.54 |
| 1:G:400:ARG:HG2 | 1:G:400:ARG:HH11 | 1.71 | 0.54 |
| 1:B:142:VAL:C | 1:B:144:GLU:N | 2.64 | 0.54 |
| 1:C:308:ARG:NH2 | 1:C:481:PRO:HB2 | 2.23 | 0.54 |
| 1:D:369:HIS:HE1 | 2:D:500:HEM:O2A | 1.90 | 0.54 |
| 1:E:32:PRO:HB2 | 1:E:62:TYR:CD1 | 2.41 | 0.54 |
| 1:F:403:GLU:O | 1:F:404:THR:C | 2.51 | 0.54 |
| 1:A:80:GLY:O | 1:A:84:ILE:HG12 | 2.07 | 0.54 |
| 1:C:268:TYR:CD1 | 1:C:288:LEU:HD13 | 2.42 | 0.54 |
| 1:D:198:LEU:O | 1:D:201:LEU:HB2 | 2.08 | 0.54 |
| 1:F:357:GLN:CG | 1:F:428:PRO:HG3 | 2.37 | 0.54 |
| 1:G:65:VAL:HG21 | 1:G:377:PHE:HE2 | 1.71 | 0.54 |
| 1:A:131:THR:O | 1:A:135:PHE:HB2 | 2.08 | 0.54 |
| 1:C:75:VAL:HG12 | 1:C:387:GLU:CB | 2.37 | 0.54 |
| 1:C:97:GLY:O | 1:C:370:THR:N | 2.41 | 0.54 |
| 1:C:150:ALA:O | 1:C:154:VAL:HG23 | 2.07 | 0.54 |
| 1:C:437:LEU:HD23 | 1:C:437:LEU:O | 2.07 | 0.54 |
| 1:A:429:PHE:O | 1:A:430:SER:HB3 | 2.08 | 0.54 |
| 1:B:101:ILE:HB | 1:B:104:VAL:HG22 | 1.89 | 0.54 |
| 1:B:179:ILE:HG22 | 1:B:180:CYS:N | 2.22 | 0.54 |
| 1:D:29:LYS:HE3 | 1:D:380:TYR:HE1 | 1.72 | 0.54 |
| 1:E:34:PRO:HG2 | 1:E:42:ASN:CG | 2.33 | 0.54 |
| 1:E:129:LEU:HG | 1:E:437:LEU:HD11 | 1.89 | 0.54 |
| 1:A:136:GLY:C | 1:A:142:VAL:HG23 | 2.33 | 0.54 |
| 1:B:272:MET:HG3 | 1:B:283:PHE:O | 2.07 | 0.54 |
| 1:C:388:VAL:O | 1:C:390:PRO:HD3 | 2.07 | 0.54 |
| 1:D:202:PHE:HD1 | 1:D:297:PHE:HD1 | 1.56 | 0.54 |
| 1:E:163:ALA:HA | 1:E:487:ARG:NH1 | 2.23 | 0.54 |
| 1:F:223:PHE:C | 1:F:223:PHE:CD2 | 2.85 | 0.54 |
| 1:A:114:ILE:HG13 | 1:A:294:SER:HB3 | 1.91 | 0.53 |
| 1:A:183:VAL:HA | 1:A:264:PHE:HB3 | 1.90 | 0.53 |
| 1:A:369:HIS:HE1 | 2:A:500:HEM:O2A | 1.90 | 0.53 |
| 1:C:161:LYS:HZ3 | 1:F:485:GLN:HE22 | 1.56 | 0.53 |
| 1:D:249:VAL:HG11 | 1:D:288:LEU:HD21 | 1.91 | 0.53 |
| 1:D:438:GLY:O | 1:D:439:GLU:C | 2.51 | 0.53 |
| 1:E:164:LEU:HG | 1:E:487:ARG:NH2 | 2.24 | 0.53 |
| 1:E:284:HIS:CD2 | 1:E:284:HIS:N | 2.62 | 0.53 |
| 1:F:98:ARG:NH1 | 1:F:367:VAL:HB | 2.23 | 0.53 |
| 1:F:464:PRO:HB2 | 1:F:467:ASP:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:172:HIS:CE1 | 1:G:301:GLU:HA | 2.43 | 0.53 |
| 1:G:172:HIS:HE1 | 1:G:301:GLU:HA | 1.73 | 0.53 |
| 1:G:403:GLU:O | 1:G:404:THR:C | 2.51 | 0.53 |
| 1:A:402:PHE:O | 1:A:405:PRO:HD3 | 2.08 | 0.53 |
| 1:B:242:ASN:HD21 | 1:B:290:LEU:HD23 | 1.73 | 0.53 |
| 1:C:88:LEU:O | 1:C:432:GLY:HA2 | 2.07 | 0.53 |
| 1:C:103:VAL:CG1 | 1:C:234:ILE:HD12 | 2.38 | 0.53 |
| 1:C:170:LEU:HD23 | 1:C:170:LEU:C | 2.33 | 0.53 |
| 1:C:442:ALA:HB1 | 2:C:500:HEM:CBB | 2.39 | 0.53 |
| 1:D:108:PHE:C | 1:D:110:GLY:H | 2.14 | 0.53 |
| 1:D:409:ASN:C | 1:D:411:GLY:H | 2.16 | 0.53 |
| 1:E:42:ASN:HB3 | 1:E:45:GLN:HB2 | 1.90 | 0.53 |
| 1:E:436:CYS:SG | 1:E:439:GLU:N | 2.81 | 0.53 |
| 1:F:62:TYR:N | 1:F:62:TYR:CD2 | 2.76 | 0.53 |
| 1:C:61:LYS:HG2 | 1:C:62:TYR:CE2 | 2.43 | 0.53 |
| 1:D:228:PRO:CD | 1:E:216:VAL:HG11 | 2.36 | 0.53 |
| 1:D:429:PHE:CD2 | 1:D:439:GLU:HG3 | 2.42 | 0.53 |
| 1:E:257:ASP:OD2 | 1:E:260:ASN:HB3 | 2.09 | 0.53 |
| 1:E:305:THR:HG22 | 1:E:308:ARG:NE | 2.23 | 0.53 |
| 1:F:297:PHE:CD2 | 3:F:501:1CI:H10 | 2.42 | 0.53 |
| 1:A:43:LEU:HD22 | 1:A:220:PHE:CZ | 2.44 | 0.53 |
| 1:A:278:ASP:C | 1:A:280:SER:H | 2.16 | 0.53 |
| 1:C:153:LEU:HD13 | 1:C:170:LEU:HD21 | 1.89 | 0.53 |
| 1:C:370:THR:HA | 1:C:386:THR:O | 2.08 | 0.53 |
| 1:C:403:GLU:O | 1:C:412:HIS:NE2 | 2.41 | 0.53 |
| 1:D:139:LYS:HD2 | 1:D:144:GLU:OE1 | 2.09 | 0.53 |
| 1:E:272:MET:SD | 1:E:283:PHE:O | 2.67 | 0.53 |
| 1:G:174:ILE:HD12 | 1:G:449:PHE:CD2 | 2.44 | 0.53 |
| 1:A:49:LYS:HE2 | 1:A:53:ARG:HG2 | 1.90 | 0.53 |
| 1:G:101:ILE:HB | 1:G:104:VAL:CG2 | 2.37 | 0.53 |
| 1:A:64:ASP:HA | 1:A:79:CYS:HB2 | 1.91 | 0.53 |
| 1:A:213:SER:C | 1:A:215:GLN:H | 2.16 | 0.53 |
| 1:B:183:VAL:HA | 1:B:264:PHE:HB3 | 1.90 | 0.53 |
| 1:E:114:ILE:HD12 | 1:E:114:ILE:N | 2.23 | 0.53 |
| 1:F:415:ASP:CG | 1:F:416:ALA:H | 2.16 | 0.53 |
| 1:G:88:LEU:HD13 | 1:G:431:LEU:O | 2.08 | 0.53 |
| 1:G:195:PHE:O | 1:G:199:LEU:HG | 2.09 | 0.53 |
| 1:G:404:THR:HG23 | 1:G:404:THR:O | 2.09 | 0.53 |
| 1:B:409:ASN:O | 1:B:412:HIS:ND1 | 2.40 | 0.53 |
| 1:C:187:ARG:O | 1:C:187:ARG:HG3 | 2.07 | 0.53 |
| 1:F:409:ASN:HB3 | 1:F:412:HIS:HE1 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:172:HIS:ND1 | 1:G:300:THR:HG22 | 2.23 | 0.53 |
| 1:G:415:ASP:CG | 1:G:416:ALA:N | 2.66 | 0.53 |
| 1:A:487:ARG:CD | 1:A:489:LEU:HD11 | 2.39 | 0.53 |
| 1:D:105:ASP:N | 1:D:106:PRO:CD | 2.71 | 0.53 |
| 1:D:142:VAL:O | 1:D:146:ILE:HG13 | 2.08 | 0.53 |
| 1:D:383:PRO:HG2 | 1:D:386:THR:OG1 | 2.08 | 0.53 |
| 1:F:449:PHE:O | 1:F:453:ILE:HG13 | 2.09 | 0.53 |
| 1:G:73:ARG:NH2 | 1:G:387:GLU:HB2 | 2.21 | 0.53 |
| 1:D:129:LEU:C | 1:D:129:LEU:HD23 | 2.33 | 0.53 |
| 1:D:297:PHE:CE2 | 3:D:501:1CI:H10 | 2.44 | 0.53 |
| 1:E:85:ARG:HG2 | 1:E:85:ARG:NH1 | 2.23 | 0.53 |
| 1:E:195:PHE:CE2 | 1:E:199:LEU:HD11 | 2.44 | 0.53 |
| 1:G:31:PRO:HD3 | 1:G:380:TYR:CG | 2.43 | 0.53 |
| 1:B:140:ARG:O | 1:B:144:GLU:HG3 | 2.09 | 0.53 |
| 1:C:176:SER:O | 1:C:180:CYS:HB2 | 2.08 | 0.53 |
| 1:E:393:SER:O | 1:E:397:HIS:HB2 | 2.09 | 0.53 |
| 1:G:244:PHE:CD1 | 1:G:244:PHE:C | 2.86 | 0.53 |
| 1:G:326:LYS:O | 1:G:329:GLU:HB3 | 2.09 | 0.53 |
| 1:E:464:PRO:HB2 | 1:E:467:ASP:HB2 | 1.92 | 0.52 |
| 1:F:324:VAL:HG13 | 1:F:349:THR:OG1 | 2.08 | 0.52 |
| 1:G:234:ILE:O | 1:G:238:LEU:HG | 2.09 | 0.52 |
| 1:G:320:VAL:O | 1:G:324:VAL:HG23 | 2.08 | 0.52 |
| 1:G:421:LYS:HG2 | 1:G:422:ARG:N | 2.23 | 0.52 |
| 1:B:177:ASN:OD1 | 1:B:187:ARG:HB2 | 2.09 | 0.52 |
| 1:C:49:LYS:HG2 | 1:C:53:ARG:CB | 2.39 | 0.52 |
| 1:C:363:ILE:CG2 | 1:C:366:GLY:HA2 | 2.39 | 0.52 |
| 1:D:87:ALA:HB1 | 1:D:95:PHE:CE2 | 2.44 | 0.52 |
| 1:E:101:ILE:CG2 | 1:E:104:VAL:HG22 | 2.39 | 0.52 |
| 1:E:171:PHE:CE2 | 1:E:307:LEU:HB3 | 2.44 | 0.52 |
| 1:E:171:PHE:HB3 | 1:E:304:SER:OG | 2.10 | 0.52 |
| 1:E:340:LEU:HD11 | 1:E:343:ARG:NH2 | 2.24 | 0.52 |
| 1:E:388:VAL:O | 1:E:390:PRO:HD3 | 2.08 | 0.52 |
| 1:E:430:SER:O | 1:E:431:LEU:HD23 | 2.08 | 0.52 |
| 1:F:168:THR:HA | 1:F:308:ARG:HD2 | 1.90 | 0.52 |
| 1:F:213:SER:HA | 1:F:216:VAL:CG1 | 2.38 | 0.52 |
| 1:A:129:LEU:HD21 | 1:A:133:ARG:CZ | 2.39 | 0.52 |
| 1:A:223:PHE:C | 1:A:223:PHE:CD2 | 2.88 | 0.52 |
| 1:D:135:PHE:HE1 | 1:D:263:ASP:HA | 1.75 | 0.52 |
| 1:E:129:LEU:O | 1:E:132:MET:HG3 | 2.10 | 0.52 |
| 1:F:103:VAL:HG11 | 1:F:214:SER:HA | 1.91 | 0.52 |
| 1:F:250:GLU:C | 1:F:252:HIS:N | 2.66 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:31:PRO:HB2 | 1:G:66:PHE:HA | 1.91 | 0.52 |
| 1:G:73:ARG:HH21 | 1:G:387:GLU:CB | 2.21 | 0.52 |
| 1:A:248:SER:HA | 1:A:251:LYS:HD2 | 1.90 | 0.52 |
| 1:A:489:LEU:HD21 | 1:D:489:LEU:HD11 | 1.90 | 0.52 |
| 1:A:352:VAL:HG13 | 1:A:408:PHE:HZ | 1.74 | 0.52 |
| 1:B:62:TYR:HB3 | 1:B:66:PHE:HB3 | 1.92 | 0.52 |
| 1:C:43:LEU:HD22 | 1:C:220:PHE:HZ | 1.74 | 0.52 |
| 1:C:120:ARG:HB2 | 1:C:282:GLU:OE2 | 2.08 | 0.52 |
| 1:D:34:PRO:HG2 | 1:D:42:ASN:OD1 | 2.09 | 0.52 |
| 1:A:153:LEU:HD21 | 1:A:453:ILE:HD11 | 1.91 | 0.52 |
| 1:A:369:HIS:HB2 | 1:A:388:VAL:O | 2.10 | 0.52 |
| 1:C:373:LYS:O | 1:C:374:ASP:C | 2.52 | 0.52 |
| 1:D:195:PHE:CE2 | 1:D:199:LEU:HD11 | 2.44 | 0.52 |
| 1:E:111:TYR:HD2 | 1:E:287:ASN:HD22 | 1.58 | 0.52 |
| 1:G:108:PHE:O | 1:G:110:GLY:N | 2.43 | 0.52 |
| 1:A:88:LEU:O | 1:A:92:ALA:HB2 | 2.10 | 0.52 |
| 1:A:105:ASP:N | 1:A:106:PRO:CD | 2.73 | 0.52 |
| 1:A:137:MET:HE2 | 1:A:441:ILE:CD1 | 2.39 | 0.52 |
| 1:A:297:PHE:O | 1:A:301:GLU:HB2 | 2.10 | 0.52 |
| 1:B:119:GLU:OE2 | 1:B:123:ALA:HB2 | 2.10 | 0.52 |
| 1:B:132:MET:O | 1:B:133:ARG:C | 2.53 | 0.52 |
| 1:B:212:PHE:CD1 | 1:B:212:PHE:C | 2.87 | 0.52 |
| 1:B:257:ASP:C | 1:B:259:SER:H | 2.18 | 0.52 |
| 1:B:373:LYS:O | 1:B:374:ASP:C | 2.52 | 0.52 |
| 1:B:404:THR:HG23 | 1:B:412:HIS:CE1 | 2.43 | 0.52 |
| 1:C:85:ARG:HE | 1:C:424:GLU:HG3 | 1.73 | 0.52 |
| 1:C:189:ASP:OD2 | 1:E:159:LYS:HE2 | 2.10 | 0.52 |
| 1:D:78:LEU:HB2 | 1:D:84:ILE:HD13 | 1.92 | 0.52 |
| 1:F:327:GLU:OE2 | 1:F:346:MET:HA | 2.10 | 0.52 |
| 1:F:430:SER:CB | 2:F:500:HEM:HBA1 | 2.38 | 0.52 |
| 1:G:180:CYS:C | 1:G:182:ILE:H | 2.17 | 0.52 |
| 1:G:206:PHE:CZ | 1:G:478:GLY:HA3 | 2.45 | 0.52 |
| 1:A:94:ALA:HB1 | 1:A:375:THR:OG1 | 2.10 | 0.52 |
| 1:B:153:LEU:HD22 | 1:B:174:ILE:HG21 | 1.91 | 0.52 |
| 1:C:176:SER:O | 1:C:180:CYS:N | 2.40 | 0.52 |
| 1:D:285:HIS:O | 1:D:286:GLN:C | 2.52 | 0.52 |
| 1:D:308:ARG:HH11 | 1:D:308:ARG:CG | 2.22 | 0.52 |
| 1:F:31:PRO:HA | 1:F:380:TYR:CE1 | 2.45 | 0.52 |
| 1:F:182:ILE:HD12 | 1:F:182:ILE:N | 2.25 | 0.52 |
| 1:F:265:ILE:O | 1:F:269:LEU:HG | 2.10 | 0.52 |
| 1:B:98:ARG:HH12 | 1:B:367:VAL:HB | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:89:VAL:C | 1:D:91:GLN:H | 2.18 | 0.52 |
| 1:E:78:LEU:O | 1:E:84:ILE:HD11 | 2.09 | 0.52 |
| 1:E:324:VAL:O | 1:E:328:ILE:HG13 | 2.10 | 0.52 |
| 1:A:34:PRO:HG2 | 1:A:42:ASN:CG | 2.35 | 0.52 |
| 1:B:457:PHE:CD1 | 1:B:490:ALA:HA | 2.45 | 0.52 |
| 1:D:189:ASP:C | 1:D:191:LYS:H | 2.17 | 0.52 |
| 1:D:268:TYR:CE1 | 1:D:288:LEU:HB2 | 2.45 | 0.52 |
| 1:E:375:THR:HG22 | 1:E:376:GLN:N | 2.25 | 0.52 |
| 1:F:165:LEU:C | 1:F:165:LEU:HD12 | 2.35 | 0.52 |
| 1:G:32:PRO:HB2 | 1:G:62:TYR:CD1 | 2.45 | 0.52 |
| 1:G:171:PHE:CE2 | 1:G:307:LEU:HB3 | 2.45 | 0.52 |
| 1:A:202:PHE:CE1 | 1:A:241:ILE:HD13 | 2.45 | 0.51 |
| 1:B:271:ARG:HA | 1:B:274:LYS:HB3 | 1.92 | 0.51 |
| 1:D:42:ASN:HA | 1:D:45:GLN:OE1 | 2.10 | 0.51 |
| 1:F:285:HIS:O | 1:F:286:GLN:C | 2.53 | 0.51 |
| 1:G:380:TYR:CG | 1:G:381:VAL:N | 2.78 | 0.51 |
| 1:A:42:ASN:O | 1:A:46:MET:HG2 | 2.10 | 0.51 |
| 1:B:202:PHE:O | 1:B:204:GLN:N | 2.43 | 0.51 |
| 1:C:372:THR:O | 1:C:384:LYS:HG3 | 2.09 | 0.51 |
| 1:F:34:PRO:O | 1:F:36:PRO:HD3 | 2.10 | 0.51 |
| 1:F:362:LEU:HD22 | 1:F:362:LEU:N | 2.25 | 0.51 |
| 1:A:176:SER:O | 1:A:179:ILE:HG22 | 2.10 | 0.51 |
| 1:B:303:THR:HG21 | 1:B:445:GLU:OE1 | 2.10 | 0.51 |
| 1:B:384:LYS:O | 1:B:385:ASN:HB2 | 2.11 | 0.51 |
| 1:D:136:GLY:CA | 1:D:140:ARG:HB3 | 2.40 | 0.51 |
| 1:E:403:GLU:O | 1:E:412:HIS:NE2 | 2.43 | 0.51 |
| 1:F:178:ILE:O | 1:F:182:ILE:HD13 | 2.10 | 0.51 |
| 1:F:223:PHE:C | 1:F:223:PHE:HD2 | 2.18 | 0.51 |
| 1:G:80:GLY:O | 1:G:84:ILE:HG12 | 2.10 | 0.51 |
| 1:B:242:ASN:OD1 | 1:B:293:LEU:HD22 | 2.10 | 0.51 |
| 1:C:140:ARG:H | 1:C:143:GLU:HB3 | 1.76 | 0.51 |
| 1:C:299:GLY:HA2 | 2:C:500:HEM:HMC3 | 1.91 | 0.51 |
| 1:D:164:LEU:HB2 | 1:D:487:ARG:CZ | 2.40 | 0.51 |
| 1:E:87:ALA:O | 1:E:95:PHE:HD2 | 1.94 | 0.51 |
| 1:E:299:GLY:HA2 | 2:E:500:HEM:HMC3 | 1.91 | 0.51 |
| 1:G:327:GLU:OE2 | 1:G:346:MET:HA | 2.11 | 0.51 |
| 1:A:430:SER:O | 1:A:431:LEU:HD23 | 2.10 | 0.51 |
| 1:B:70:LEU:HB2 | 1:B:73:ARG:CG | 2.40 | 0.51 |
| 1:C:103:VAL:HG22 | 1:C:217:PHE:HD2 | 1.76 | 0.51 |
| 1:C:460:ALA:HB3 | 1:C:489:LEU:HD11 | 1.92 | 0.51 |
| 1:D:111:TYR:HB2 | 1:D:290:LEU:HD12 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:114:ILE:HD11 | 2:D:500:HEM:HMD3 | 1.93 | 0.51 |
| 1:D:192:ASP:HB3 | 1:D:195:PHE:HB3 | 1.92 | 0.51 |
| 1:D:209:ILE:HG22 | 1:D:477:VAL:HG11 | 1.93 | 0.51 |
| 1:D:256:LEU:HD12 | 1:D:257:ASP:N | 2.26 | 0.51 |
| 1:E:78:LEU:HB3 | 1:E:84:ILE:HD13 | 1.91 | 0.51 |
| 1:E:127:PHE:CZ | 1:E:267:VAL:HG12 | 2.45 | 0.51 |
| 1:A:340:LEU:HD13 | 1:A:444:THR:HG23 | 1.92 | 0.51 |
| 1:B:127:PHE:C | 1:B:127:PHE:CD1 | 2.89 | 0.51 |
| 1:B:384:LYS:HG2 | 1:B:385:ASN:ND2 | 2.25 | 0.51 |
| 1:C:142:VAL:O | 1:C:145:ARG:HB2 | 2.10 | 0.51 |
| 1:E:113:VAL:HG22 | 1:E:113:VAL:O | 2.10 | 0.51 |
| 1:E:138:GLY:C | 1:E:139:LYS:HD3 | 2.35 | 0.51 |
| 1:E:435:ILE:O | 1:E:436:CYS:C | 2.53 | 0.51 |
| 1:F:52:LEU:C | 1:F:54:SER:H | 2.17 | 0.51 |
| 1:G:341:ASP:C | 1:G:343:ARG:N | 2.69 | 0.51 |
| 1:A:49:LYS:CE | 1:A:53:ARG:HE | 2.24 | 0.51 |
| 1:B:248:SER:C | 1:B:250:GLU:N | 2.65 | 0.51 |
| 1:D:198:LEU:HD11 | 1:D:244:PHE:CD2 | 2.45 | 0.51 |
| 1:E:390:PRO:O | 1:E:392:LEU:N | 2.44 | 0.51 |
| 1:F:31:PRO:HB3 | 1:F:32:PRO:HD2 | 1.92 | 0.51 |
| 1:F:439:GLU:O | 1:F:443:ARG:HG2 | 2.10 | 0.51 |
| 1:G:326:LYS:O | 1:G:330:GLN:HG3 | 2.11 | 0.51 |
| 1:G:332:ILE:HA | 1:G:336:ARG:NH2 | 2.26 | 0.51 |
| 1:C:107:ILE:HG22 | 1:C:108:PHE:N | 2.26 | 0.51 |
| 1:D:149:GLU:CD | 1:D:187:ARG:HH21 | 2.19 | 0.51 |
| 1:E:430:SER:CB | 2:E:500:HEM:HBA1 | 2.41 | 0.51 |
| 1:F:37:LEU:H | 1:F:37:LEU:CD1 | 2.17 | 0.51 |
| 1:F:95:PHE:HE1 | 1:F:371:VAL:HG12 | 1.72 | 0.51 |
| 1:G:35:SER:O | 1:G:37:LEU:HD12 | 2.10 | 0.51 |
| 1:G:95:PHE:O | 1:G:97:GLY:N | 2.43 | 0.51 |
| 1:G:403:GLU:O | 1:G:412:HIS:NE2 | 2.44 | 0.51 |
| 1:A:43:LEU:HD22 | 1:A:220:PHE:HZ | 1.75 | 0.51 |
| 1:B:73:ARG:NH2 | 1:B:387:GLU:CD | 2.69 | 0.51 |
| 1:D:316:LYS:O | 1:D:465:PRO:HB3 | 2.10 | 0.51 |
| 1:D:409:ASN:C | 1:D:411:GLY:N | 2.69 | 0.51 |
| 1:E:170:LEU:HD23 | 1:E:170:LEU:O | 2.11 | 0.51 |
| 1:F:50:GLY:O | 1:F:54:SER:HB2 | 2.10 | 0.51 |
| 1:F:61:LYS:CD | 1:F:62:TYR:HE2 | 2.23 | 0.51 |
| 1:F:77:VAL:HG13 | 1:F:391:VAL:CG2 | 2.41 | 0.51 |
| 1:A:285:HIS:O | 1:A:286:GLN:C | 2.52 | 0.51 |
| 1:A:487:ARG:HD2 | 1:A:489:LEU:HD11 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:136:GLY:C | 1:C:142:VAL:HB | 2.36 | 0.51 |
| 1:C:302:THR:OG1 | 3:C:501:1CI:H4 | 2.11 | 0.51 |
| 1:E:48:ARG:HH11 | 1:E:48:ARG:HG3 | 1.76 | 0.51 |
| 1:E:53:ARG:NH1 | 1:E:53:ARG:HB2 | 2.26 | 0.51 |
| 1:F:84:ILE:HG13 | 1:F:395:ALA:HB2 | 1.93 | 0.51 |
| 1:F:235:TYR:O | 1:F:236:ARG:C | 2.54 | 0.51 |
| 1:F:246:GLY:O | 1:F:249:VAL:HG12 | 2.11 | 0.51 |
| 1:G:459:ILE:O | 1:G:460:ALA:HB2 | 2.10 | 0.51 |
| 1:A:213:SER:C | 1:A:215:GLN:N | 2.68 | 0.50 |
| 1:B:80:GLY:O | 1:B:84:ILE:HG12 | 2.11 | 0.50 |
| 1:C:404:THR:HG23 | 1:C:412:HIS:CE1 | 2.45 | 0.50 |
| 1:E:304:SER:O | 1:E:307:LEU:HB2 | 2.10 | 0.50 |
| 1:F:77:VAL:CG1 | 1:F:78:LEU:N | 2.72 | 0.50 |
| 1:G:309:TYR:HB2 | 1:G:481:PRO:HG2 | 1.93 | 0.50 |
| 1:B:460:ALA:HB3 | 1:B:487:ARG:HG3 | 1.94 | 0.50 |
| 1:E:477:VAL:O | 1:E:477:VAL:HG22 | 2.11 | 0.50 |
| 1:F:140:ARG:HH12 | 1:F:148:GLU:CG | 2.25 | 0.50 |
| 1:F:364:PRO:HD2 | 1:F:477:VAL:O | 2.12 | 0.50 |
| 1:F:402:PHE:O | 1:F:405:PRO:HD3 | 2.11 | 0.50 |
| 1:G:441:ILE:O | 1:G:445:GLU:HG3 | 2.11 | 0.50 |
| 1:A:256:LEU:HD21 | 1:A:270:LEU:CD2 | 2.32 | 0.50 |
| 1:A:363:ILE:HG22 | 1:A:363:ILE:O | 2.11 | 0.50 |
| 1:B:174:ILE:O | 1:B:178:ILE:HG12 | 2.12 | 0.50 |
| 1:C:76:VAL:HB | 1:C:388:VAL:HG22 | 1.93 | 0.50 |
| 1:C:151:ARG:HG2 | 1:C:151:ARG:HH11 | 1.76 | 0.50 |
| 1:C:195:PHE:HA | 1:C:198:LEU:HD23 | 1.92 | 0.50 |
| 1:E:129:LEU:O | 1:E:130:ALA:C | 2.55 | 0.50 |
| 1:F:435:ILE:HG12 | 1:F:436:CYS:H | 1.75 | 0.50 |
| 1:G:43:LEU:HD13 | 1:G:220:PHE:HZ | 1.76 | 0.50 |
| 1:A:382:ILE:HG22 | 1:A:386:THR:HB | 1.93 | 0.50 |
| 1:E:127:PHE:C | 1:E:127:PHE:CD1 | 2.89 | 0.50 |
| 1:E:272:MET:SD | 1:E:283:PHE:HB3 | 2.52 | 0.50 |
| 1:F:40:LEU:HD22 | 1:F:40:LEU:H | 1.76 | 0.50 |
| 1:F:44:LEU:HB2 | 1:F:45:GLN:NE2 | 2.26 | 0.50 |
| 1:F:140:ARG:HH12 | 1:F:148:GLU:HG2 | 1.76 | 0.50 |
| 1:F:268:TYR:CD1 | 1:F:288:LEU:HD13 | 2.46 | 0.50 |
| 1:G:69:TYR:CD1 | 1:G:74:PRO:HB3 | 2.46 | 0.50 |
| 1:B:34:PRO:HB3 | 1:B:62:TYR:OH | 2.11 | 0.50 |
| 1:C:326:LYS:O | 1:C:329:GLU:HB3 | 2.12 | 0.50 |
| 1:D:160:SER:O | 1:D:161:LYS:C | 2.54 | 0.50 |
| 1:F:47:ASP:HB3 | 1:F:54:SER:HA | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:120:ARG:HA | 1:F:282:GLU:HG3 | 1.93 | 0.50 |
| 1:F:328:ILE:HG12 | 1:F:346:MET:HE1 | 1.94 | 0.50 |
| 1:F:359:LEU:O | 1:F:359:LEU:HD13 | 2.11 | 0.50 |
| 1:A:135:PHE:CE1 | 1:A:263:ASP:HA | 2.46 | 0.50 |
| 1:C:99:GLY:HA3 | 1:C:368:PRO:HB2 | 1.94 | 0.50 |
| 1:D:201:LEU:HD11 | 1:D:240:GLU:CD | 2.37 | 0.50 |
| 1:E:195:PHE:CZ | 1:E:199:LEU:HD11 | 2.47 | 0.50 |
| 1:E:395:ALA:HB1 | 1:E:427:MET:HE3 | 1.94 | 0.50 |
| 1:G:238:LEU:O | 1:G:242:ASN:ND2 | 2.44 | 0.50 |
| 1:G:386:THR:HG23 | 1:G:386:THR:O | 2.11 | 0.50 |
| 1:A:48:ARG:HG3 | 1:A:48:ARG:HH11 | 1.76 | 0.50 |
| 1:B:216:VAL:HG11 | 1:C:228:PRO:HD3 | 1.93 | 0.50 |
| 1:B:268:TYR:OH | 1:B:283:PHE:HA | 2.11 | 0.50 |
| 1:B:395:ALA:HB1 | 1:B:427:MET:HE3 | 1.94 | 0.50 |
| 1:C:28:GLY:O | 1:C:29:LYS:HG2 | 2.11 | 0.50 |
| 1:C:38:PRO:C | 1:C:40:LEU:H | 2.18 | 0.50 |
| 1:C:362:LEU:O | 1:C:362:LEU:HD13 | 2.12 | 0.50 |
| 1:E:73:ARG:HG3 | 1:E:73:ARG:O | 2.12 | 0.50 |
| 1:E:85:ARG:HG2 | 1:E:85:ARG:HH11 | 1.76 | 0.50 |
| 1:E:476:GLY:C | 1:E:478:GLY:H | 2.20 | 0.50 |
| 1:F:39:VAL:O | 1:F:41:GLY:N | 2.44 | 0.50 |
| 1:F:402:PHE:CE2 | 1:F:425:GLY:HA3 | 2.47 | 0.50 |
| 1:G:36:PRO:HA | 1:G:42:ASN:ND2 | 2.26 | 0.50 |
| 1:C:363:ILE:HG22 | 1:C:366:GLY:N | 2.27 | 0.50 |
| 1:C:369:HIS:HB2 | 1:C:388:VAL:O | 2.12 | 0.50 |
| 1:D:402:PHE:CD1 | 1:D:412:HIS:HD2 | 2.30 | 0.50 |
| 1:D:415:ASP:OD1 | 1:D:418:GLY:N | 2.39 | 0.50 |
| 1:E:121:TRP:HE1 | 1:E:125:ARG:HD2 | 1.75 | 0.50 |
| 1:E:220:PHE:HB2 | 1:E:224:LEU:CD2 | 2.42 | 0.50 |
| 1:G:75:VAL:HG23 | 1:G:77:VAL:HG23 | 1.94 | 0.50 |
| 1:A:170:LEU:O | 1:A:173:SER:HB2 | 2.12 | 0.50 |
| 1:C:328:ILE:HG12 | 1:C:346:MET:HE1 | 1.92 | 0.50 |
| 1:C:477:VAL:O | 1:C:477:VAL:HG22 | 2.12 | 0.50 |
| 1:A:247:GLN:O | 1:A:251:LYS:HE3 | 2.12 | 0.49 |
| 1:A:429:PHE:CE2 | 1:A:443:ARG:HD3 | 2.44 | 0.49 |
| 1:B:153:LEU:HD21 | 1:B:453:ILE:HD11 | 1.95 | 0.49 |
| 1:B:186:LYS:H | 1:B:186:LYS:HD3 | 1.77 | 0.49 |
| 1:B:358:ARG:HG2 | 1:B:358:ARG:HH11 | 1.77 | 0.49 |
| 1:F:75:VAL:HG12 | 1:F:387:GLU:HB2 | 1.93 | 0.49 |
| 1:A:362:LEU:H | 1:A:362:LEU:CD2 | 2.19 | 0.49 |
| 1:B:165:LEU:HD12 | 1:B:486:ILE:O | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:244:PHE:C | 1:B:246:GLY:N | 2.70 | 0.49 |
| 1:C:30:LEU:HD21 | 1:C:383:PRO:HD2 | 1.94 | 0.49 |
| 1:D:322:GLU:O | 1:D:325:GLN:HB2 | 2.13 | 0.49 |
| 1:E:305:THR:HG22 | 1:E:308:ARG:NH2 | 2.27 | 0.49 |
| 1:E:403:GLU:O | 1:E:404:THR:HG22 | 2.11 | 0.49 |
| 1:F:409:ASN:HB3 | 1:F:412:HIS:CE1 | 2.47 | 0.49 |
| 1:G:167:ASN:HB2 | 1:G:171:PHE:CD1 | 2.46 | 0.49 |
| 1:B:382:ILE:CG2 | 1:B:386:THR:HB | 2.42 | 0.49 |
| 1:D:268:TYR:CD1 | 1:D:288:LEU:HD13 | 2.48 | 0.49 |
| 1:F:77:VAL:HG12 | 1:F:78:LEU:H | 1.77 | 0.49 |
| 1:F:77:VAL:HG13 | 1:F:391:VAL:HG21 | 1.94 | 0.49 |
| 1:D:202:PHE:CE1 | 1:D:241:ILE:HD13 | 2.47 | 0.49 |
| 1:E:73:ARG:NH2 | 1:E:387:GLU:OE1 | 2.45 | 0.49 |
| 1:F:390:PRO:O | 1:F:391:VAL:C | 2.55 | 0.49 |
| 1:C:38:PRO:O | 1:C:40:LEU:N | 2.39 | 0.49 |
| 1:C:174:ILE:HG13 | 1:C:175:THR:N | 2.28 | 0.49 |
| 1:D:122:ARG:HG2 | 1:D:122:ARG:HH11 | 1.78 | 0.49 |
| 1:E:230:THR:O | 1:E:234:ILE:HG13 | 2.13 | 0.49 |
| 1:E:329:GLU:OE2 | 1:E:334:SER:HB3 | 2.11 | 0.49 |
| 1:E:457:PHE:CD1 | 1:E:490:ALA:HA | 2.48 | 0.49 |
| 1:F:409:ASN:O | 1:F:412:HIS:ND1 | 2.46 | 0.49 |
| 1:F:415:ASP:HA | 1:F:421:LYS:HD3 | 1.95 | 0.49 |
| 1:F:443:ARG:HH11 | 1:F:443:ARG:CB | 2.25 | 0.49 |
| 1:G:123:ALA:CA | 1:G:126:ARG:HG2 | 2.40 | 0.49 |
| 1:G:205:SER:O | 1:G:209:ILE:HG13 | 2.13 | 0.49 |
| 1:B:188:PHE:HB2 | 1:B:195:PHE:CG | 2.47 | 0.49 |
| 1:B:213:SER:O | 1:B:216:VAL:HG12 | 2.13 | 0.49 |
| 1:C:203:PHE:HA | 1:C:301:GLU:OE1 | 2.13 | 0.49 |
| 1:C:329:GLU:O | 1:C:333:GLY:N | 2.46 | 0.49 |
| 1:F:108:PHE:HA | 1:F:290:LEU:HD13 | 1.93 | 0.49 |
| 1:F:405:PRO:C | 1:F:407:THR:H | 2.20 | 0.49 |
| 1:G:209:ILE:HG22 | 1:G:477:VAL:CG1 | 2.42 | 0.49 |
| 1:B:362:LEU:HD22 | 1:B:362:LEU:N | 2.27 | 0.49 |
| 1:C:128:SER:HA | 1:C:264:PHE:HE2 | 1.77 | 0.49 |
| 1:C:194:VAL:O | 1:C:197:ARG:HB3 | 2.12 | 0.49 |
| 1:C:328:ILE:HA | 1:C:346:MET:HE3 | 1.95 | 0.49 |
| 1:C:352:VAL:HG13 | 1:C:408:PHE:CZ | 2.46 | 0.49 |
| 1:C:392:LEU:HD21 | 1:C:430:SER:HA | 1.95 | 0.49 |
| 1:D:43:LEU:HD21 | 1:F:226:TYR:CD2 | 2.47 | 0.49 |
| 1:D:44:LEU:HB2 | 1:D:45:GLN:HE22 | 1.78 | 0.49 |
| 1:E:263:ASP:OD1 | 1:E:265:ILE:HB | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:88:LEU:HD21 | 1:F:369:HIS:NE2 | 2.27 | 0.49 |
| 1:F:189:ASP:C | 1:F:191:LYS:H | 2.21 | 0.49 |
| 1:G:114:ILE:HG12 | 2:G:500:HEM:HAD1 | 1.93 | 0.49 |
| 1:A:122:ARG:CD | 1:A:122:ARG:H | 2.26 | 0.49 |
| 1:A:427:MET:HE2 | 1:A:431:LEU:HD11 | 1.95 | 0.49 |
| 1:B:111:TYR:CD2 | 1:B:286:GLN:HB3 | 2.48 | 0.49 |
| 1:B:253:ARG:HA | 1:B:269:LEU:HD13 | 1.94 | 0.49 |
| 1:E:362:LEU:HD22 | 1:E:362:LEU:N | 2.16 | 0.49 |
| 1:F:90:ASP:O | 1:F:91:GLN:CG | 2.61 | 0.49 |
| 1:B:234:ILE:O | 1:B:238:LEU:HG | 2.13 | 0.49 |
| 1:C:263:ASP:OD1 | 1:C:265:ILE:HB | 2.13 | 0.49 |
| 1:C:434:ARG:O | 1:C:435:ILE:C | 2.55 | 0.49 |
| 1:D:229:GLY:C | 1:D:231:HIS:H | 2.20 | 0.49 |
| 1:D:413:PHE:O | 1:D:420:LEU:HD12 | 2.13 | 0.49 |
| 1:E:42:ASN:ND2 | 1:E:69:TYR:HB2 | 2.28 | 0.49 |
| 1:E:277:SER:O | 1:E:278:ASP:C | 2.56 | 0.49 |
| 1:F:99:GLY:H | 1:F:368:PRO:C | 2.20 | 0.49 |
| 1:G:65:VAL:HG21 | 1:G:377:PHE:CE2 | 2.47 | 0.49 |
| 1:G:355:GLU:CD | 1:G:358:ARG:HH21 | 2.21 | 0.49 |
| 1:A:284:HIS:O | 1:A:285:HIS:C | 2.55 | 0.49 |
| 1:B:316:LYS:HD3 | 1:B:317:TYR:HE1 | 1.76 | 0.49 |
| 1:B:340:LEU:C | 1:B:342:ASP:H | 2.20 | 0.49 |
| 1:C:49:LYS:HE3 | 1:C:53:ARG:HH12 | 1.74 | 0.49 |
| 1:D:137:MET:HE3 | 1:D:138:GLY:N | 2.27 | 0.49 |
| 1:D:139:LYS:HG3 | 1:D:139:LYS:O | 2.12 | 0.49 |
| 1:D:146:ILE:HG21 | 1:D:448:LEU:HD12 | 1.95 | 0.49 |
| 1:D:155:GLU:HA | 1:D:158:ARG:HG3 | 1.93 | 0.49 |
| 1:E:121:TRP:CZ2 | 1:E:434:ARG:HD3 | 2.47 | 0.49 |
| 1:E:131:THR:OG1 | 1:E:135:PHE:HD1 | 1.95 | 0.49 |
| 1:F:137:MET:CG | 1:F:138:GLY:H | 2.25 | 0.49 |
| 1:A:302:THR:OG1 | 3:A:501:1CI:H4 | 2.13 | 0.48 |
| 1:B:325:GLN:NE2 | 1:B:491:ARG:HH11 | 2.11 | 0.48 |
| 1:D:136:GLY:HA3 | 1:D:140:ARG:HB3 | 1.93 | 0.48 |
| 1:D:154:VAL:O | 1:D:158:ARG:HG3 | 2.12 | 0.48 |
| 1:D:176:SER:O | 1:D:180:CYS:HB2 | 2.13 | 0.48 |
| 1:D:411:GLY:C | 1:D:413:PHE:H | 2.17 | 0.48 |
| 1:F:118:GLY:O | 1:F:122:ARG:HB2 | 2.13 | 0.48 |
| 1:F:122:ARG:HB2 | 1:F:122:ARG:HH11 | 1.78 | 0.48 |
| 1:F:355:GLU:HG2 | 1:F:408:PHE:CD1 | 2.46 | 0.48 |
| 1:B:194:VAL:O | 1:B:198:LEU:HD23 | 2.13 | 0.48 |
| 1:D:202:PHE:HD1 | 1:D:297:PHE:CD1 | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:344:ALA:C | 1:D:346:MET:H | 2.20 | 0.48 |
| 1:D:449:PHE:O | 1:D:453:ILE:HG13 | 2.14 | 0.48 |
| 1:E:137:MET:HA | 1:E:137:MET:HE3 | 1.95 | 0.48 |
| 1:E:232:ARG:HG2 | 1:E:232:ARG:HH11 | 1.78 | 0.48 |
| 1:E:331:VAL:HG21 | 1:E:345:LYS:O | 2.14 | 0.48 |
| 1:F:464:PRO:HB2 | 1:F:467:ASP:HB3 | 1.94 | 0.48 |
| 1:G:305:THR:HG21 | 1:G:481:PRO:HD2 | 1.92 | 0.48 |
| 1:G:371:VAL:HG11 | 1:G:382:ILE:CG2 | 2.40 | 0.48 |
| 1:A:314:MET:HE2 | 1:A:314:MET:HA | 1.95 | 0.48 |
| 1:B:171:PHE:O | 1:B:174:ILE:HG12 | 2.14 | 0.48 |
| 1:E:81:THR:O | 1:E:85:ARG:HG3 | 2.13 | 0.48 |
| 1:E:172:HIS:HB3 | 1:E:199:LEU:HD22 | 1.95 | 0.48 |
| 1:E:188:PHE:CD2 | 1:E:195:PHE:HB2 | 2.48 | 0.48 |
| 1:F:268:TYR:CE1 | 1:F:288:LEU:HB2 | 2.48 | 0.48 |
| 1:F:373:LYS:C | 1:F:375:THR:H | 2.21 | 0.48 |
| 1:G:325:GLN:NE2 | 1:G:491:ARG:HH11 | 2.09 | 0.48 |
| 1:A:28:GLY:C | 1:A:29:LYS:HG2 | 2.38 | 0.48 |
| 1:C:360:GLY:O | 1:C:361:ASP:C | 2.56 | 0.48 |
| 2:C:500:HEM:NA | 3:C:501:1CI:N3 | 2.61 | 0.48 |
| 1:D:324:VAL:HG12 | 1:D:328:ILE:HD11 | 1.95 | 0.48 |
| 1:D:399:PRO:O | 1:D:401:TYR:N | 2.47 | 0.48 |
| 1:E:31:PRO:HB3 | 1:E:32:PRO:HD2 | 1.95 | 0.48 |
| 1:E:42:ASN:HD22 | 1:E:42:ASN:N | 2.12 | 0.48 |
| 1:E:85:ARG:HA | 1:E:89:VAL:HG23 | 1.94 | 0.48 |
| 1:F:97:GLY:HA2 | 1:F:117:ASN:OD1 | 2.13 | 0.48 |
| 1:F:327:GLU:CD | 1:F:346:MET:HA | 2.39 | 0.48 |
| 1:G:364:PRO:HG3 | 1:G:479:ASN:HD22 | 1.77 | 0.48 |
| 1:A:119:GLU:OE1 | 1:A:122:ARG:NH1 | 2.46 | 0.48 |
| 1:A:168:THR:HA | 1:A:308:ARG:HD3 | 1.95 | 0.48 |
| 1:A:317:TYR:HB3 | 1:A:320:VAL:HG23 | 1.95 | 0.48 |
| 1:A:384:LYS:O | 1:A:385:ASN:HB2 | 2.12 | 0.48 |
| 1:A:409:ASN:C | 1:A:411:GLY:H | 2.21 | 0.48 |
| 1:C:52:LEU:CD2 | 1:C:364:PRO:HB3 | 2.36 | 0.48 |
| 1:C:124:LEU:HD11 | 1:C:287:ASN:OD1 | 2.14 | 0.48 |
| 1:C:476:GLY:C | 1:C:478:GLY:H | 2.21 | 0.48 |
| 1:D:37:LEU:HD13 | 1:D:44:LEU:HD13 | 1.95 | 0.48 |
| 1:E:108:PHE:C | 1:E:110:GLY:H | 2.21 | 0.48 |
| 1:F:61:LYS:HD3 | 1:F:62:TYR:CE2 | 2.48 | 0.48 |
| 1:G:197:ARG:HH21 | 1:G:240:GLU:CD | 2.20 | 0.48 |
| 1:A:136:GLY:HA3 | 1:A:145:ARG:HH12 | 1.79 | 0.48 |
| 1:B:211:SER:HA | 1:B:474:GLU:CD | 2.39 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:241:ILE:O | 1:B:245:ILE:HG13 | 2.13 | 0.48 |
| 1:B:486:ILE:O | 1:B:486:ILE:HG23 | 2.12 | 0.48 |
| 1:C:146:ILE:HD13 | 1:C:445:GLU:HG2 | 1.96 | 0.48 |
| 1:C:323:ARG:HB3 | 1:C:348:TYR:HE2 | 1.77 | 0.48 |
| 1:C:365:PHE:O | 1:C:366:GLY:O | 2.31 | 0.48 |
| 1:D:400:ARG:HG2 | 1:D:400:ARG:HH11 | 1.78 | 0.48 |
| 1:E:173:SER:HA | 1:E:199:LEU:HD11 | 1.94 | 0.48 |
| 1:F:96:SER:HB2 | 1:F:121:TRP:CZ3 | 2.49 | 0.48 |
| 1:F:114:ILE:CD1 | 1:F:294:SER:HB3 | 2.43 | 0.48 |
| 1:F:122:ARG:HB2 | 1:F:122:ARG:NH1 | 2.29 | 0.48 |
| 1:G:373:LYS:HA | 1:G:384:LYS:HD2 | 1.94 | 0.48 |
| 1:A:37:LEU:H | 1:A:37:LEU:HD12 | 1.78 | 0.48 |
| 1:A:49:LYS:HE3 | 1:A:53:ARG:HE | 1.78 | 0.48 |
| 1:A:128:SER:HA | 1:A:264:PHE:HE2 | 1.79 | 0.48 |
| 1:C:457:PHE:CA | 1:C:491:ARG:HG3 | 2.44 | 0.48 |
| 1:C:489:LEU:HD23 | 1:F:487:ARG:HD2 | 1.96 | 0.48 |
| 1:D:102:ALA:CB | 1:D:218:GLU:HA | 2.44 | 0.48 |
| 1:E:140:ARG:O | 1:E:144:GLU:HB3 | 2.14 | 0.48 |
| 1:E:327:GLU:O | 1:E:346:MET:HE3 | 2.13 | 0.48 |
| 1:F:39:VAL:C | 1:F:41:GLY:H | 2.22 | 0.48 |
| 1:F:411:GLY:C | 1:F:413:PHE:N | 2.72 | 0.48 |
| 1:F:465:PRO:C | 1:F:467:ASP:H | 2.20 | 0.48 |
| 1:G:194:VAL:O | 1:G:198:LEU:HD13 | 2.14 | 0.48 |
| 1:G:344:ALA:O | 1:G:346:MET:N | 2.47 | 0.48 |
| 1:G:368:PRO:HG3 | 1:G:389:PHE:CZ | 2.49 | 0.48 |
| 1:G:411:GLY:O | 1:G:413:PHE:N | 2.46 | 0.48 |
| 1:A:191:LYS:O | 1:A:193:PRO:HD3 | 2.13 | 0.48 |
| 1:C:129:LEU:O | 1:C:133:ARG:HD3 | 2.13 | 0.48 |
| 1:C:157:LEU:HD22 | 1:C:488:PHE:CD2 | 2.48 | 0.48 |
| 1:D:487:ARG:HG2 | 1:D:487:ARG:HH11 | 1.78 | 0.48 |
| 1:E:139:LYS:O | 1:E:140:ARG:C | 2.57 | 0.48 |
| 1:F:53:ARG:HH11 | 1:F:53:ARG:CA | 2.20 | 0.48 |
| 1:F:80:GLY:O | 1:F:84:ILE:HG12 | 2.12 | 0.48 |
| 1:G:30:LEU:HD22 | 1:G:67:THR:OG1 | 2.14 | 0.48 |
| 1:G:79:CYS:O | 1:G:80:GLY:O | 2.31 | 0.48 |
| 1:G:152:CYS:HB3 | 1:G:190:TYR:HE2 | 1.78 | 0.48 |
| 1:A:155:GLU:O | 1:A:159:LYS:HG3 | 2.14 | 0.48 |
| 1:B:316:LYS:HG3 | 1:B:465:PRO:O | 2.14 | 0.48 |
| 1:C:174:ILE:HD12 | 1:C:449:PHE:CG | 2.49 | 0.48 |
| 1:D:225:LYS:C | 1:D:227:PHE:N | 2.71 | 0.48 |
| 1:D:247:GLN:O | 1:D:250:GLU:HB2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:284:HIS:HB2 | 1:E:285:HIS:H | 1.56 | 0.48 |
| 1:F:40:LEU:H | 1:F:40:LEU:CD2 | 2.27 | 0.48 |
| 1:F:88:LEU:HD11 | 1:F:369:HIS:CE1 | 2.49 | 0.48 |
| 1:F:223:PHE:HD2 | 1:F:223:PHE:O | 1.97 | 0.48 |
| 1:G:87:ALA:HB1 | 1:G:95:PHE:CE2 | 2.49 | 0.48 |
| 1:A:320:VAL:HG21 | 1:A:408:PHE:HE2 | 1.79 | 0.48 |
| 1:A:407:THR:O | 1:A:408:PHE:C | 2.55 | 0.48 |
| 1:B:142:VAL:C | 1:B:144:GLU:H | 2.20 | 0.48 |
| 1:C:52:LEU:C | 1:C:54:SER:H | 2.21 | 0.48 |
| 1:C:188:PHE:HB2 | 1:C:195:PHE:CG | 2.48 | 0.48 |
| 1:D:358:ARG:HG3 | 1:D:396:LEU:HB3 | 1.94 | 0.48 |
| 1:G:174:ILE:HG13 | 1:G:175:THR:N | 2.28 | 0.48 |
| 1:B:136:GLY:HA2 | 1:B:145:ARG:NH1 | 2.29 | 0.47 |
| 1:B:139:LYS:HD2 | 1:B:139:LYS:N | 2.29 | 0.47 |
| 1:B:186:LYS:H | 1:B:186:LYS:CD | 2.27 | 0.47 |
| 1:B:243:THR:O | 1:B:247:GLN:HG2 | 2.14 | 0.47 |
| 1:B:288:LEU:O | 1:B:292:VAL:HG23 | 2.13 | 0.47 |
| 1:B:370:THR:HG22 | 1:B:387:GLU:HG2 | 1.95 | 0.47 |
| 1:B:480:VAL:O | 1:B:480:VAL:HG13 | 2.13 | 0.47 |
| 1:C:107:ILE:HG21 | 1:C:238:LEU:HD13 | 1.96 | 0.47 |
| 1:C:113:VAL:HG22 | 1:C:113:VAL:O | 2.13 | 0.47 |
| 1:D:121:TRP:CZ2 | 1:D:434:ARG:HD3 | 2.49 | 0.47 |
| 1:E:52:LEU:HD23 | 1:E:53:ARG:HH12 | 1.78 | 0.47 |
| 1:E:244:PHE:CD1 | 1:E:244:PHE:C | 2.91 | 0.47 |
| 1:F:162:GLY:HA2 | 1:F:488:PHE:O | 2.14 | 0.47 |
| 1:G:477:VAL:HG13 | 1:G:478:GLY:N | 2.29 | 0.47 |
| 1:C:108:PHE:CD1 | 1:C:290:LEU:HD22 | 2.49 | 0.47 |
| 1:C:161:LYS:HZ1 | 1:F:485:GLN:HE22 | 1.61 | 0.47 |
| 1:C:285:HIS:O | 1:C:288:LEU:N | 2.47 | 0.47 |
| 1:E:122:ARG:C | 1:E:126:ARG:HD3 | 2.39 | 0.47 |
| 1:E:125:ARG:HG3 | 1:E:437:LEU:CD1 | 2.43 | 0.47 |
| 1:E:129:LEU:O | 1:E:132:MET:CG | 2.62 | 0.47 |
| 1:E:240:GLU:O | 1:E:243:THR:HB | 2.14 | 0.47 |
| 1:F:90:ASP:O | 1:F:91:GLN:CB | 2.61 | 0.47 |
| 1:F:312:LEU:HD13 | 1:F:484:TYR:CD2 | 2.48 | 0.47 |
| 1:A:140:ARG:O | 1:A:141:SER:C | 2.57 | 0.47 |
| 1:A:153:LEU:HB2 | 1:A:174:ILE:HG21 | 1.96 | 0.47 |
| 1:A:404:THR:HG21 | 1:A:409:ASN:ND2 | 2.27 | 0.47 |
| 1:B:73:ARG:HG3 | 1:B:73:ARG:O | 2.14 | 0.47 |
| 1:D:153:LEU:HD22 | 1:D:174:ILE:HG21 | 1.95 | 0.47 |
| 1:E:139:LYS:HD3 | 1:E:139:LYS:N | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:143:GLU:OE1 | 1:E:340:LEU:HB3 | 2.15 | 0.47 |
| 1:E:269:LEU:O | 1:E:272:MET:HB2 | 2.13 | 0.47 |
| 1:E:358:ARG:CG | 1:E:396:LEU:HB3 | 2.44 | 0.47 |
| 1:E:376:GLN:CD | 1:E:376:GLN:C | 2.82 | 0.47 |
| 1:F:101:ILE:CB | 1:F:104:VAL:HG22 | 2.42 | 0.47 |
| 1:F:129:LEU:O | 1:F:129:LEU:HD23 | 2.13 | 0.47 |
| 1:G:277:SER:O | 1:G:278:ASP:C | 2.57 | 0.47 |
| 1:G:320:VAL:HG21 | 1:G:408:PHE:CE2 | 2.50 | 0.47 |
| 1:G:410:PRO:O | 1:G:414:LEU:HD12 | 2.14 | 0.47 |
| 1:A:326:LYS:O | 1:A:330:GLN:HG3 | 2.14 | 0.47 |
| 1:B:48:ARG:HG3 | 1:B:48:ARG:NH1 | 2.29 | 0.47 |
| 1:D:249:VAL:HG22 | 1:D:265:ILE:HD13 | 1.94 | 0.47 |
| 1:D:456:ASN:O | 1:D:491:ARG:HB2 | 2.14 | 0.47 |
| 1:F:203:PHE:C | 1:F:205:SER:H | 2.23 | 0.47 |
| 1:F:384:LYS:O | 1:F:385:ASN:HB2 | 2.13 | 0.47 |
| 1:G:82:ASP:C | 1:G:84:ILE:N | 2.72 | 0.47 |
| 1:B:54:SER:O | 1:B:58:LEU:HG | 2.15 | 0.47 |
| 1:E:198:LEU:HD21 | 1:E:244:PHE:HD2 | 1.80 | 0.47 |
| 1:F:90:ASP:O | 1:F:91:GLN:HG3 | 2.14 | 0.47 |
| 1:G:183:VAL:HG11 | 1:G:292:VAL:HG13 | 1.96 | 0.47 |
| 1:G:233:GLN:HG3 | 1:G:237:ASN:ND2 | 2.30 | 0.47 |
| 1:A:150:ALA:O | 1:A:154:VAL:HG23 | 2.14 | 0.47 |
| 1:B:275:ASP:O | 1:B:276:LYS:C | 2.57 | 0.47 |
| 1:B:407:THR:O | 1:B:408:PHE:C | 2.58 | 0.47 |
| 1:C:270:LEU:C | 1:C:272:MET:H | 2.23 | 0.47 |
| 1:D:141:SER:C | 1:D:143:GLU:N | 2.70 | 0.47 |
| 1:D:288:LEU:O | 1:D:292:VAL:HG23 | 2.15 | 0.47 |
| 1:D:327:GLU:OE1 | 1:D:348:TYR:HB3 | 2.14 | 0.47 |
| 1:D:463:VAL:HB | 1:D:468:ILE:HD11 | 1.96 | 0.47 |
| 1:E:336:ARG:NH2 | 1:E:342:ASP:OD1 | 2.47 | 0.47 |
| 1:E:484:TYR:N | 1:E:484:TYR:CD1 | 2.82 | 0.47 |
| 1:F:102:ALA:HB3 | 1:F:218:GLU:HA | 1.96 | 0.47 |
| 1:F:438:GLY:HA3 | 2:F:500:HEM:HBC2 | 1.96 | 0.47 |
| 1:G:256:LEU:HD12 | 1:G:257:ASP:N | 2.30 | 0.47 |
| 1:A:223:PHE:C | 1:A:223:PHE:HD2 | 2.23 | 0.47 |
| 1:A:241:ILE:O | 1:A:245:ILE:HG13 | 2.14 | 0.47 |
| 1:A:254:ALA:O | 1:A:255:THR:HG23 | 2.15 | 0.47 |
| 1:B:172:HIS:HB3 | 1:B:199:LEU:HD22 | 1.97 | 0.47 |
| 1:B:314:MET:HB3 | 1:B:459:ILE:HD13 | 1.97 | 0.47 |
| 1:B:324:VAL:HG13 | 1:B:349:THR:OG1 | 2.14 | 0.47 |
| 1:C:48:ARG:HH11 | 1:C:48:ARG:HG3 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:116:ALA:O | 1:C:117:ASN:HB2 | 2.15 | 0.47 |
| 1:C:135:PHE:CE2 | 1:C:263:ASP:HA | 2.50 | 0.47 |
| 1:C:176:SER:HB2 | 1:C:300:THR:HG23 | 1.97 | 0.47 |
| 1:C:370:THR:CG2 | 1:C:385:ASN:HA | 2.45 | 0.47 |
| 1:C:489:LEU:CD2 | 1:F:489:LEU:HD11 | 2.45 | 0.47 |
| 1:D:125:ARG:NH1 | 2:D:500:HEM:O1D | 2.48 | 0.47 |
| 1:D:244:PHE:C | 1:D:244:PHE:CD1 | 2.93 | 0.47 |
| 1:D:371:VAL:C | 1:D:373:LYS:H | 2.22 | 0.47 |
| 1:E:129:LEU:HG | 1:E:437:LEU:CD1 | 2.45 | 0.47 |
| 1:E:275:ASP:C | 1:E:277:SER:N | 2.71 | 0.47 |
| 1:E:310:GLY:O | 1:E:314:MET:HG2 | 2.15 | 0.47 |
| 1:F:85:ARG:O | 1:F:86:GLU:C | 2.57 | 0.47 |
| 1:G:118:GLY:O | 1:G:119:GLU:C | 2.58 | 0.47 |
| 1:G:146:ILE:HG12 | 1:G:178:ILE:HD12 | 1.97 | 0.47 |
| 1:A:403:GLU:O | 1:A:412:HIS:NE2 | 2.47 | 0.47 |
| 1:B:157:LEU:HD13 | 1:B:488:PHE:CG | 2.50 | 0.47 |
| 1:B:312:LEU:HG | 1:B:470:LEU:HD23 | 1.97 | 0.47 |
| 1:B:464:PRO:HG3 | 1:E:492:HIS:CE1 | 2.50 | 0.47 |
| 1:C:415:ASP:OD1 | 1:C:418:GLY:N | 2.45 | 0.47 |
| 1:D:95:PHE:O | 1:D:369:HIS:HD2 | 1.98 | 0.47 |
| 1:D:108:PHE:C | 1:D:110:GLY:N | 2.71 | 0.47 |
| 1:D:179:ILE:HG21 | 1:D:299:GLY:HA3 | 1.96 | 0.47 |
| 1:D:194:VAL:O | 1:D:197:ARG:HB3 | 2.15 | 0.47 |
| 1:D:316:LYS:HD3 | 1:D:317:TYR:HE1 | 1.78 | 0.47 |
| 1:E:42:ASN:O | 1:E:46:MET:HG2 | 2.15 | 0.47 |
| 1:E:114:ILE:HG13 | 2:E:500:HEM:HAD1 | 1.96 | 0.47 |
| 1:F:415:ASP:O | 1:F:416:ALA:HB2 | 2.14 | 0.47 |
| 1:G:36:PRO:HA | 1:G:42:ASN:HD22 | 1.80 | 0.47 |
| 1:G:43:LEU:HD13 | 1:G:220:PHE:CZ | 2.49 | 0.47 |
| 1:G:107:ILE:HG13 | 1:G:238:LEU:CD1 | 2.42 | 0.47 |
| 1:G:241:ILE:O | 1:G:245:ILE:HG13 | 2.14 | 0.47 |
| 1:B:162:GLY:O | 1:B:487:ARG:NH1 | 2.47 | 0.47 |
| 1:B:202:PHE:CD1 | 1:B:297:PHE:CD1 | 3.03 | 0.47 |
| 1:C:291:THR:O | 1:C:295:LEU:HG | 2.14 | 0.47 |
| 1:D:248:SER:O | 1:D:252:HIS:ND1 | 2.47 | 0.47 |
| 1:D:287:ASN:O | 1:D:288:LEU:C | 2.56 | 0.47 |
| 1:A:176:SER:HB2 | 1:A:300:THR:HG23 | 1.97 | 0.47 |
| 1:A:247:GLN:O | 1:A:251:LYS:HG3 | 2.14 | 0.47 |
| 1:B:174:ILE:HG13 | 1:B:175:THR:N | 2.30 | 0.47 |
| 1:C:323:ARG:HD3 | 1:C:348:TYR:CD2 | 2.50 | 0.47 |
| 1:D:44:LEU:H | 1:D:44:LEU:CD1 | 2.22 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:286:GLN:OE1 | 1:E:286:GLN:HA | 2.14 | 0.47 |
| 1:F:101:ILE:HB | 1:F:104:VAL:CG2 | 2.40 | 0.47 |
| 1:F:350:ASP:OD1 | 1:F:420:LEU:HD21 | 2.15 | 0.47 |
| 1:G:60:GLU:HA | 1:G:60:GLU:OE2 | 2.15 | 0.47 |
| 1:G:95:PHE:C | 1:G:97:GLY:N | 2.72 | 0.47 |
| 1:G:101:ILE:O | 1:G:103:VAL:N | 2.47 | 0.47 |
| 1:G:305:THR:HA | 1:G:308:ARG:HD3 | 1.96 | 0.47 |
| 1:C:241:ILE:HG22 | 1:C:245:ILE:HD11 | 1.97 | 0.46 |
| 1:C:301:GLU:OE2 | 1:C:305:THR:HG21 | 2.15 | 0.46 |
| 1:D:38:PRO:O | 1:D:39:VAL:HB | 2.15 | 0.46 |
| 1:D:371:VAL:HG23 | 1:D:386:THR:H | 1.80 | 0.46 |
| 1:E:104:VAL:O | 1:E:105:ASP:C | 2.58 | 0.46 |
| 1:F:85:ARG:O | 1:F:89:VAL:HG23 | 2.15 | 0.46 |
| 1:F:253:ARG:HG3 | 1:F:253:ARG:HH11 | 1.80 | 0.46 |
| 1:F:286:GLN:O | 1:F:287:ASN:C | 2.58 | 0.46 |
| 1:G:233:GLN:HE21 | 1:G:237:ASN:ND2 | 2.12 | 0.46 |
| 1:A:278:ASP:O | 1:A:280:SER:N | 2.43 | 0.46 |
| 1:B:114:ILE:CD1 | 1:B:294:SER:HB3 | 2.45 | 0.46 |
| 1:B:285:HIS:HB3 | 1:B:286:GLN:H | 1.57 | 0.46 |
| 1:E:182:ILE:HD12 | 1:E:182:ILE:N | 2.30 | 0.46 |
| 1:F:30:LEU:HD22 | 1:F:383:PRO:HD2 | 1.97 | 0.46 |
| 1:F:121:TRP:O | 1:F:124:LEU:N | 2.48 | 0.46 |
| 1:A:30:LEU:HD21 | 1:A:383:PRO:HD2 | 1.98 | 0.46 |
| 1:A:268:TYR:OH | 1:A:287:ASN:HB2 | 2.16 | 0.46 |
| 1:C:315:LEU:HD13 | 1:C:461:SER:HB3 | 1.97 | 0.46 |
| 1:E:38:PRO:O | 1:E:39:VAL:HB | 2.15 | 0.46 |
| 1:E:158:ARG:C | 1:E:160:SER:H | 2.23 | 0.46 |
| 1:E:250:GLU:OE2 | 1:E:250:GLU:HA | 2.15 | 0.46 |
| 1:G:102:ALA:CB | 1:G:218:GLU:HA | 2.46 | 0.46 |
| 1:G:182:ILE:O | 1:G:263:ASP:HB2 | 2.14 | 0.46 |
| 1:G:316:LYS:HD3 | 1:G:317:TYR:CE1 | 2.50 | 0.46 |
| 1:B:287:ASN:O | 1:B:291:THR:HB | 2.15 | 0.46 |
| 1:B:362:LEU:C | 1:B:363:ILE:HG13 | 2.40 | 0.46 |
| 1:D:141:SER:C | 1:D:143:GLU:H | 2.24 | 0.46 |
| 1:E:98:ARG:HB2 | 1:E:434:ARG:NH2 | 2.30 | 0.46 |
| 1:E:325:GLN:NE2 | 1:E:491:ARG:NH1 | 2.63 | 0.46 |
| 1:F:208:LEU:HD22 | 1:F:230:THR:HB | 1.98 | 0.46 |
| 1:F:336:ARG:NH2 | 1:F:342:ASP:OD1 | 2.48 | 0.46 |
| 1:G:90:ASP:O | 1:G:91:GLN:CB | 2.62 | 0.46 |
| 1:G:146:ILE:HD12 | 1:G:444:THR:HG22 | 1.97 | 0.46 |
| 1:A:70:LEU:CD1 | 1:A:75:VAL:HG11 | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:409:ASN:C | 1:A:411:GLY:N | 2.73 | 0.46 |
| 1:B:466:GLU:OE1 | 1:B:466:GLU:N | 2.37 | 0.46 |
| 1:C:46:MET:HE3 | 1:C:54:SER:OG | 2.15 | 0.46 |
| 1:C:253:ARG:NH2 | 1:C:272:MET:HE1 | 2.15 | 0.46 |
| 1:E:68:VAL:O | 1:E:75:VAL:HG22 | 2.16 | 0.46 |
| 1:E:403:GLU:O | 1:E:404:THR:CG2 | 2.64 | 0.46 |
| 1:F:36:PRO:HB3 | 1:F:69:TYR:CD1 | 2.50 | 0.46 |
| 1:F:364:PRO:HD2 | 1:F:477:VAL:C | 2.41 | 0.46 |
| 1:G:116:ALA:HB1 | 1:G:120:ARG:HD2 | 1.97 | 0.46 |
| 1:G:134:ASP:O | 1:G:135:PHE:C | 2.58 | 0.46 |
| 1:G:316:LYS:HB2 | 1:G:468:ILE:CG2 | 2.46 | 0.46 |
| 1:G:435:ILE:HG12 | 1:G:436:CYS:N | 2.31 | 0.46 |
| 1:G:444:THR:HG22 | 1:G:444:THR:O | 2.15 | 0.46 |
| 1:A:31:PRO:HA | 1:A:380:TYR:CD1 | 2.50 | 0.46 |
| 1:A:215:GLN:C | 1:A:217:PHE:N | 2.72 | 0.46 |
| 1:A:281:SER:C | 1:A:283:PHE:H | 2.23 | 0.46 |
| 1:B:143:GLU:OE2 | 1:B:340:LEU:HB3 | 2.16 | 0.46 |
| 1:B:211:SER:HA | 1:B:474:GLU:OE2 | 2.16 | 0.46 |
| 1:C:44:LEU:HB2 | 1:C:45:GLN:HE21 | 1.80 | 0.46 |
| 1:D:399:PRO:C | 1:D:401:TYR:N | 2.74 | 0.46 |
| 1:D:409:ASN:O | 1:D:411:GLY:N | 2.48 | 0.46 |
| 1:E:371:VAL:HG21 | 1:E:383:PRO:O | 2.16 | 0.46 |
| 1:F:119:GLU:C | 1:F:121:TRP:N | 2.73 | 0.46 |
| 1:G:298:ALA:C | 1:G:300:THR:N | 2.72 | 0.46 |
| 1:G:422:ARG:CG | 1:G:423:ASN:N | 2.79 | 0.46 |
| 1:C:43:LEU:HD22 | 1:C:220:PHE:CZ | 2.50 | 0.46 |
| 1:C:139:LYS:HZ2 | 1:C:140:ARG:HD3 | 1.81 | 0.46 |
| 1:C:192:ASP:HB3 | 1:C:195:PHE:HB3 | 1.97 | 0.46 |
| 1:C:443:ARG:CZ | 1:C:443:ARG:HB3 | 2.46 | 0.46 |
| 1:C:457:PHE:CE1 | 1:C:490:ALA:HA | 2.51 | 0.46 |
| 1:E:212:PHE:CD1 | 1:E:212:PHE:C | 2.93 | 0.46 |
| 1:E:325:GLN:O | 1:E:329:GLU:HB2 | 2.16 | 0.46 |
| 1:F:78:LEU:HD11 | 1:F:388:VAL:HG11 | 1.97 | 0.46 |
| 1:F:202:PHE:CD1 | 1:F:297:PHE:HD1 | 2.34 | 0.46 |
| 1:G:98:ARG:N | 1:G:117:ASN:OD1 | 2.47 | 0.46 |
| 1:G:325:GLN:NE2 | 1:G:491:ARG:NH1 | 2.64 | 0.46 |
| 1:A:284:HIS:O | 1:A:284:HIS:CG | 2.68 | 0.46 |
| 1:B:34:PRO:HD2 | 1:B:67:THR:O | 2.15 | 0.46 |
| 1:B:37:LEU:HD12 | 1:B:37:LEU:N | 2.31 | 0.46 |
| 1:B:122:ARG:O | 1:B:126:ARG:HB2 | 2.16 | 0.46 |
| 1:C:370:THR:HG23 | 1:C:386:THR:N | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:441:ILE:H | 1:D:441:ILE:CD1 | 2.28 | 0.46 |
| 1:E:133:ARG:NH2 | 1:E:141:SER:CB | 2.78 | 0.46 |
| 1:E:355:GLU:CD | 1:E:358:ARG:HH21 | 2.23 | 0.46 |
| 1:F:52:LEU:C | 1:F:54:SER:N | 2.72 | 0.46 |
| 1:F:153:LEU:HD21 | 1:F:453:ILE:HD11 | 1.97 | 0.46 |
| 1:F:202:PHE:HE1 | 1:F:241:ILE:HD13 | 1.78 | 0.46 |
| 1:G:179:ILE:HG13 | 1:G:299:GLY:HA3 | 1.98 | 0.46 |
| 1:G:380:TYR:CE2 | 1:G:382:ILE:HA | 2.51 | 0.46 |
| 1:A:240:GLU:O | 1:A:243:THR:HB | 2.16 | 0.46 |
| 1:A:244:PHE:C | 1:A:244:PHE:CD1 | 2.93 | 0.46 |
| 1:B:101:ILE:O | 1:B:102:ALA:C | 2.58 | 0.46 |
| 1:B:121:TRP:C | 1:B:123:ALA:N | 2.73 | 0.46 |
| 1:D:189:ASP:C | 1:D:191:LYS:N | 2.74 | 0.46 |
| 1:E:93:GLU:O | 1:E:94:ALA:C | 2.58 | 0.46 |
| 1:E:457:PHE:HD1 | 1:E:490:ALA:HA | 1.79 | 0.46 |
| 1:F:245:ILE:O | 1:F:245:ILE:HG22 | 2.15 | 0.46 |
| 1:F:432:GLY:C | 1:F:434:ARG:H | 2.24 | 0.46 |
| 1:G:164:LEU:CG | 1:G:487:ARG:HH21 | 2.24 | 0.46 |
| 1:G:282:GLU:O | 1:G:287:ASN:ND2 | 2.45 | 0.46 |
| 1:G:308:ARG:HG2 | 1:G:308:ARG:NH1 | 2.31 | 0.46 |
| 1:G:340:LEU:HD22 | 1:G:444:THR:HG23 | 1.98 | 0.46 |
| 1:B:474:GLU:HB3 | 1:B:480:VAL:CG1 | 2.44 | 0.46 |
| 1:D:29:LYS:HE3 | 1:D:380:TYR:CE1 | 2.50 | 0.46 |
| 1:D:151:ARG:O | 1:D:154:VAL:HB | 2.16 | 0.46 |
| 1:D:171:PHE:HA | 1:D:174:ILE:HG12 | 1.97 | 0.46 |
| 1:D:213:SER:HA | 1:D:216:VAL:HG12 | 1.98 | 0.46 |
| 1:E:166:ASP:OD1 | 1:E:168:THR:HB | 2.15 | 0.46 |
| 1:E:231:HIS:ND1 | 1:E:231:HIS:C | 2.73 | 0.46 |
| 1:E:355:GLU:OE1 | 1:E:355:GLU:HA | 2.16 | 0.46 |
| 1:F:85:ARG:HG3 | 1:F:89:VAL:HG21 | 1.96 | 0.46 |
| 1:F:354:HIS:HB3 | 1:F:413:PHE:CD2 | 2.51 | 0.46 |
| 1:G:114:ILE:HG22 | 1:G:115:PHE:CD2 | 2.51 | 0.46 |
| 1:G:268:TYR:CE1 | 1:G:288:LEU:HB2 | 2.50 | 0.46 |
| 1:A:234:ILE:O | 1:A:238:LEU:HG | 2.16 | 0.45 |
| 1:A:285:HIS:O | 1:A:288:LEU:N | 2.49 | 0.45 |
| 1:B:38:PRO:C | 1:B:40:LEU:H | 2.24 | 0.45 |
| 1:C:85:ARG:HG2 | 1:C:85:ARG:NH1 | 2.31 | 0.45 |
| 1:C:177:ASN:HA | 1:C:180:CYS:HB3 | 1.98 | 0.45 |
| 1:D:47:ASP:OD1 | 1:D:53:ARG:HG3 | 2.16 | 0.45 |
| 1:E:111:TYR:N | 1:E:111:TYR:CD1 | 2.85 | 0.45 |
| 1:E:324:VAL:C | 1:E:326:LYS:H | 2.24 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:186:LYS:H | 1:F:186:LYS:CD | 2.29 | 0.45 |
| 1:G:321:THR:HG23 | 1:G:454:LEU:HD13 | 1.98 | 0.45 |
| 1:A:69:TYR:CD2 | 1:A:74:PRO:HB3 | 2.49 | 0.45 |
| 1:B:125:ARG:HH12 | 1:B:437:LEU:HB2 | 1.80 | 0.45 |
| 1:B:382:ILE:HG22 | 1:B:386:THR:HB | 1.98 | 0.45 |
| 1:C:65:VAL:HG22 | 1:C:78:LEU:CD2 | 2.45 | 0.45 |
| 1:C:111:TYR:CD1 | 1:C:111:TYR:N | 2.83 | 0.45 |
| 1:D:98:ARG:NE | 1:D:434:ARG:HH12 | 2.14 | 0.45 |
| 1:D:256:LEU:HD12 | 1:D:257:ASP:H | 1.79 | 0.45 |
| 1:E:119:GLU:HA | 1:E:122:ARG:NH1 | 2.31 | 0.45 |
| 1:E:429:PHE:O | 1:E:430:SER:HB3 | 2.16 | 0.45 |
| 1:F:113:VAL:CG1 | 1:F:291:THR:HG23 | 2.45 | 0.45 |
| 1:F:310:GLY:O | 1:F:314:MET:HG2 | 2.16 | 0.45 |
| 1:G:411:GLY:O | 1:G:414:LEU:N | 2.45 | 0.45 |
| 1:G:435:ILE:HG12 | 1:G:436:CYS:H | 1.81 | 0.45 |
| 1:A:48:ARG:NH2 | 1:B:235:TYR:CD2 | 2.84 | 0.45 |
| 1:C:139:LYS:HD3 | 1:C:140:ARG:NH1 | 2.31 | 0.45 |
| 1:D:373:LYS:CA | 1:D:384:LYS:HG3 | 2.33 | 0.45 |
| 1:D:429:PHE:HB3 | 1:D:436:CYS:HB3 | 1.98 | 0.45 |
| 1:D:447:PHE:O | 1:D:448:LEU:C | 2.59 | 0.45 |
| 1:E:150:ALA:O | 1:E:154:VAL:HG23 | 2.17 | 0.45 |
| 1:E:235:TYR:CG | 1:F:48:ARG:NH2 | 2.83 | 0.45 |
| 1:E:241:ILE:C | 1:E:243:THR:N | 2.73 | 0.45 |
| 1:F:210:SER:HB3 | 1:F:476:GLY:H | 1.80 | 0.45 |
| 1:G:32:PRO:CB | 1:G:62:TYR:HB3 | 2.46 | 0.45 |
| 1:G:131:THR:O | 1:G:134:ASP:HB3 | 2.16 | 0.45 |
| 1:A:161:LYS:HE3 | 1:D:462:PRO:HG3 | 1.97 | 0.45 |
| 1:A:489:LEU:N | 1:A:489:LEU:HD12 | 2.31 | 0.45 |
| 1:B:373:LYS:O | 1:B:373:LYS:HD2 | 2.16 | 0.45 |
| 1:D:253:ARG:HH11 | 1:D:253:ARG:HG3 | 1.80 | 0.45 |
| 1:E:142:VAL:O | 1:E:146:ILE:HG13 | 2.16 | 0.45 |
| 1:F:77:VAL:CG1 | 1:F:78:LEU:H | 2.30 | 0.45 |
| 1:F:77:VAL:O | 1:F:78:LEU:HD23 | 2.16 | 0.45 |
| 1:F:195:PHE:O | 1:F:199:LEU:HG | 2.15 | 0.45 |
| 1:G:40:LEU:HB3 | 1:G:43:LEU:HB3 | 1.98 | 0.45 |
| 1:C:140:ARG:N | 1:C:143:GLU:HB3 | 2.31 | 0.45 |
| 1:D:107:ILE:HD11 | 1:D:235:TYR:CD1 | 2.52 | 0.45 |
| 1:D:123:ALA:O | 1:D:126:ARG:HB3 | 2.16 | 0.45 |
| 1:D:371:VAL:HG21 | 1:D:382:ILE:HG22 | 1.98 | 0.45 |
| 1:E:108:PHE:O | 1:E:110:GLY:N | 2.40 | 0.45 |
| 1:E:127:PHE:HZ | 1:E:267:VAL:HG12 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:139:LYS:CE | 1:E:145:ARG:HD3 | 2.45 | 0.45 |
| 1:F:284:HIS:O | 1:F:285:HIS:C | 2.60 | 0.45 |
| 1:F:404:THR:HG1 | 1:F:407:THR:HB | 1.80 | 0.45 |
| 1:G:355:GLU:O | 1:G:359:LEU:HB2 | 2.16 | 0.45 |
| 1:A:28:GLY:HA2 | 1:A:381:VAL:HG23 | 1.97 | 0.45 |
| 1:A:121:TRP:HH2 | 1:A:433:LYS:HB3 | 1.80 | 0.45 |
| 1:B:157:LEU:O | 1:B:160:SER:OG | 2.29 | 0.45 |
| 1:C:164:LEU:HD23 | 1:C:487:ARG:HB3 | 1.98 | 0.45 |
| 1:D:43:LEU:C | 1:D:45:GLN:H | 2.25 | 0.45 |
| 1:D:340:LEU:HD13 | 1:D:444:THR:HG23 | 1.98 | 0.45 |
| 1:E:29:LYS:HE3 | 1:E:380:TYR:HD1 | 1.82 | 0.45 |
| 1:E:262:ARG:HH21 | 1:E:266:ASP:CG | 2.24 | 0.45 |
| 1:E:320:VAL:O | 1:E:324:VAL:HG23 | 2.17 | 0.45 |
| 1:F:111:TYR:HB2 | 1:F:290:LEU:HD12 | 1.99 | 0.45 |
| 1:F:137:MET:CG | 1:F:138:GLY:N | 2.80 | 0.45 |
| 1:G:129:LEU:HG | 1:G:437:LEU:HD11 | 1.99 | 0.45 |
| 1:G:138:GLY:HA3 | 1:G:145:ARG:CZ | 2.47 | 0.45 |
| 1:A:81:THR:HG23 | 1:A:425:GLY:HA2 | 1.97 | 0.45 |
| 1:A:318:PRO:O | 1:A:322:GLU:HG2 | 2.16 | 0.45 |
| 1:B:221:SER:O | 1:B:225:LYS:HD3 | 2.15 | 0.45 |
| 1:C:52:LEU:C | 1:C:54:SER:N | 2.72 | 0.45 |
| 1:C:85:ARG:HG2 | 1:C:85:ARG:HH11 | 1.82 | 0.45 |
| 1:C:256:LEU:HG | 1:C:258:PRO:HD3 | 1.99 | 0.45 |
| 1:C:308:ARG:NH2 | 1:C:481:PRO:O | 2.49 | 0.45 |
| 1:D:81:THR:HG23 | 1:D:424:GLU:O | 2.17 | 0.45 |
| 1:D:271:ARG:O | 1:D:271:ARG:HG2 | 2.17 | 0.45 |
| 1:D:313:LEU:HD12 | 1:D:356:ILE:HG12 | 1.99 | 0.45 |
| 1:D:464:PRO:O | 1:D:467:ASP:HB2 | 2.17 | 0.45 |
| 1:E:149:GLU:OE1 | 1:E:177:ASN:ND2 | 2.37 | 0.45 |
| 1:E:202:PHE:HZ | 1:E:296:PHE:CD2 | 2.35 | 0.45 |
| 1:E:363:ILE:CG2 | 1:E:366:GLY:HA2 | 2.46 | 0.45 |
| 1:F:229:GLY:O | 1:F:231:HIS:N | 2.44 | 0.45 |
| 1:F:297:PHE:HD2 | 3:F:501:1CI:H10 | 1.81 | 0.45 |
| 1:G:314:MET:SD | 1:G:450:PHE:HZ | 2.39 | 0.45 |
| 1:G:423:ASN:O | 1:G:425:GLY:N | 2.50 | 0.45 |
| 1:A:228:PRO:HD3 | 1:C:216:VAL:HG11 | 1.99 | 0.45 |
| 1:A:281:SER:O | 1:A:283:PHE:N | 2.50 | 0.45 |
| 1:A:331:VAL:HG12 | 1:A:332:ILE:N | 2.31 | 0.45 |
| 1:B:134:ASP:C | 1:B:136:GLY:N | 2.75 | 0.45 |
| 1:B:313:LEU:HD23 | 1:B:470:LEU:HD11 | 1.99 | 0.45 |
| 1:B:430:SER:O | 1:B:431:LEU:HD23 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:90:ASP:O | 1:C:91:GLN:CB | 2.64 | 0.45 |
| 1:D:335:HIS:O | 1:D:336:ARG:CB | 2.62 | 0.45 |
| 1:F:283:PHE:N | 1:F:283:PHE:CD1 | 2.85 | 0.45 |
| 1:A:429:PHE:O | 1:A:430:SER:CB | 2.64 | 0.45 |
| 1:C:176:SER:O | 1:C:180:CYS:CB | 2.65 | 0.45 |
| 1:C:285:HIS:O | 1:C:286:GLN:C | 2.60 | 0.45 |
| 1:E:127:PHE:HE2 | 1:E:271:ARG:HG2 | 1.82 | 0.45 |
| 1:E:308:ARG:NH1 | 1:E:308:ARG:CB | 2.80 | 0.45 |
| 1:F:145:ARG:HH11 | 1:F:182:ILE:CD1 | 2.30 | 0.45 |
| 1:F:268:TYR:OH | 1:F:283:PHE:HA | 2.16 | 0.45 |
| 1:F:464:PRO:HA | 1:F:465:PRO:HD3 | 1.88 | 0.45 |
| 1:G:209:ILE:CG2 | 1:G:477:VAL:HG11 | 2.43 | 0.45 |
| 1:B:135:PHE:C | 1:B:135:PHE:CD1 | 2.94 | 0.45 |
| 1:B:200:ASP:O | 1:B:204:GLN:CB | 2.65 | 0.45 |
| 1:C:221:SER:O | 1:C:225:LYS:HG2 | 2.17 | 0.45 |
| 1:D:329:GLU:CD | 1:D:333:GLY:HA2 | 2.42 | 0.45 |
| 1:E:34:PRO:HG3 | 1:E:45:GLN:HG2 | 1.99 | 0.45 |
| 1:E:309:TYR:CE2 | 1:E:313:LEU:HD12 | 2.52 | 0.45 |
| 1:F:146:ILE:HA | 1:F:178:ILE:HD11 | 1.98 | 0.45 |
| 1:F:363:ILE:HG22 | 1:F:366:GLY:N | 2.32 | 0.45 |
| 1:F:447:PHE:O | 1:F:451:THR:HG23 | 2.17 | 0.45 |
| 1:A:333:GLY:O | 1:A:334:SER:HB3 | 2.17 | 0.44 |
| 1:A:352:VAL:HG13 | 1:A:408:PHE:CZ | 2.52 | 0.44 |
| 1:B:244:PHE:C | 1:B:246:GLY:H | 2.24 | 0.44 |
| 1:B:285:HIS:O | 1:B:287:ASN:N | 2.51 | 0.44 |
| 1:B:398:ASP:OD2 | 1:B:401:TYR:HD1 | 2.00 | 0.44 |
| 1:C:80:GLY:O | 1:C:84:ILE:HG12 | 2.17 | 0.44 |
| 1:C:125:ARG:NH2 | 1:C:435:ILE:O | 2.50 | 0.44 |
| 1:C:435:ILE:HG12 | 1:C:436:CYS:N | 2.31 | 0.44 |
| 1:C:464:PRO:O | 1:C:468:ILE:HG12 | 2.17 | 0.44 |
| 1:D:125:ARG:HG3 | 1:D:125:ARG:NH1 | 2.30 | 0.44 |
| 1:D:172:HIS:CE1 | 1:D:301:GLU:HA | 2.52 | 0.44 |
| 1:D:375:THR:HG22 | 1:D:376:GLN:N | 2.32 | 0.44 |
| 1:D:411:GLY:C | 1:D:413:PHE:N | 2.73 | 0.44 |
| 1:E:278:ASP:HB3 | 1:E:281:SER:HB2 | 1.99 | 0.44 |
| 1:E:357:GLN:NE2 | 1:E:446:LEU:HD11 | 2.32 | 0.44 |
| 1:G:211:SER:HA | 1:G:474:GLU:CG | 2.46 | 0.44 |
| 1:A:98:ARG:HB2 | 1:A:434:ARG:CZ | 2.47 | 0.44 |
| 1:C:36:PRO:HA | 1:C:42:ASN:ND2 | 2.32 | 0.44 |
| 1:C:256:LEU:CD1 | 1:C:257:ASP:H | 2.30 | 0.44 |
| 1:C:403:GLU:O | 1:C:404:THR:CG2 | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:170:LEU:O | 1:D:173:SER:HB2 | 2.17 | 0.44 |
| 1:D:232:ARG:CZ | 1:E:212:PHE:CE2 | 3.01 | 0.44 |
| 1:E:103:VAL:CG1 | 1:E:234:ILE:HD12 | 2.47 | 0.44 |
| 1:F:40:LEU:HD22 | 1:F:40:LEU:N | 2.32 | 0.44 |
| 1:G:73:ARG:HG3 | 1:G:73:ARG:O | 2.17 | 0.44 |
| 1:G:129:LEU:C | 1:G:131:THR:N | 2.74 | 0.44 |
| 1:A:327:GLU:CD | 1:A:348:TYR:HB3 | 2.42 | 0.44 |
| 1:A:403:GLU:HG3 | 1:A:404:THR:HG22 | 1.99 | 0.44 |
| 1:B:97:GLY:CA | 1:B:370:THR:O | 2.63 | 0.44 |
| 1:C:146:ILE:CD1 | 1:C:445:GLU:HG2 | 2.47 | 0.44 |
| 1:D:70:LEU:CD2 | 1:D:219:LEU:HD11 | 2.44 | 0.44 |
| 1:D:401:TYR:O | 1:D:423:ASN:ND2 | 2.44 | 0.44 |
| 1:D:435:ILE:O | 1:D:436:CYS:C | 2.59 | 0.44 |
| 1:F:276:LYS:NZ | 1:F:277:SER:HB2 | 2.33 | 0.44 |
| 1:G:325:GLN:HE21 | 1:G:491:ARG:NH1 | 2.13 | 0.44 |
| 1:A:137:MET:HE2 | 1:A:441:ILE:HD11 | 2.00 | 0.44 |
| 1:C:223:PHE:C | 1:C:223:PHE:HD2 | 2.25 | 0.44 |
| 1:D:154:VAL:HA | 1:D:457:PHE:HE2 | 1.83 | 0.44 |
| 1:E:36:PRO:HB3 | 1:E:69:TYR:HB2 | 1.99 | 0.44 |
| 1:E:183:VAL:HA | 1:E:264:PHE:HB3 | 1.99 | 0.44 |
| 1:F:102:ALA:CB | 1:F:218:GLU:HA | 2.47 | 0.44 |
| 1:F:256:LEU:HG | 1:F:257:ASP:N | 2.32 | 0.44 |
| 1:G:41:GLY:C | 1:G:43:LEU:N | 2.76 | 0.44 |
| 1:G:86:GLU:HA | 1:G:90:ASP:OD2 | 2.18 | 0.44 |
| 1:G:298:ALA:HB2 | 3:G:501:1CI:H5 | 1.99 | 0.44 |
| 1:A:37:LEU:HD12 | 1:A:37:LEU:N | 2.32 | 0.44 |
| 1:B:34:PRO:HG2 | 1:B:42:ASN:HD21 | 1.79 | 0.44 |
| 1:C:143:GLU:OE1 | 1:C:340:LEU:HB3 | 2.18 | 0.44 |
| 1:C:400:ARG:HG2 | 1:C:400:ARG:NH1 | 2.32 | 0.44 |
| 1:D:53:ARG:HA | 1:D:53:ARG:NH1 | 2.21 | 0.44 |
| 1:D:221:SER:C | 1:D:223:PHE:N | 2.75 | 0.44 |
| 1:D:429:PHE:CE2 | 1:D:439:GLU:HG3 | 2.53 | 0.44 |
| 1:D:487:ARG:HG2 | 1:D:487:ARG:NH1 | 2.31 | 0.44 |
| 1:E:363:ILE:HG21 | 1:E:366:GLY:HA2 | 1.99 | 0.44 |
| 1:F:98:ARG:HG2 | 1:F:115:PHE:HA | 2.00 | 0.44 |
| 1:F:116:ALA:C | 1:F:121:TRP:HB2 | 2.43 | 0.44 |
| 1:A:281:SER:C | 1:A:283:PHE:N | 2.76 | 0.44 |
| 1:C:31:PRO:HD2 | 1:C:67:THR:OG1 | 2.18 | 0.44 |
| 1:C:418:GLY:O | 1:C:419:ALA:O | 2.36 | 0.44 |
| 1:D:61:LYS:HD3 | 1:D:62:TYR:CE2 | 2.53 | 0.44 |
| 1:E:479:ASN:O | 1:E:481:PRO:HD3 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:242:ASN:C | 1:F:244:PHE:N | 2.75 | 0.44 |
| 1:F:411:GLY:C | 1:F:413:PHE:H | 2.25 | 0.44 |
| 1:G:34:PRO:HG2 | 1:G:42:ASN:OD1 | 2.17 | 0.44 |
| 1:G:98:ARG:NH2 | 1:G:434:ARG:HD2 | 2.32 | 0.44 |
| 1:A:68:VAL:HG12 | 1:A:75:VAL:HG22 | 2.00 | 0.44 |
| 1:A:136:GLY:HA3 | 1:A:145:ARG:NH1 | 2.33 | 0.44 |
| 1:B:339:ALA:O | 1:B:342:ASP:HB2 | 2.18 | 0.44 |
| 1:B:410:PRO:C | 1:B:414:LEU:HD12 | 2.42 | 0.44 |
| 1:C:176:SER:OG | 1:C:296:PHE:HE1 | 2.00 | 0.44 |
| 1:D:325:GLN:NE2 | 1:D:491:ARG:NH1 | 2.66 | 0.44 |
| 1:F:93:GLU:HA | 1:F:433:LYS:HD2 | 2.00 | 0.44 |
| 1:F:121:TRP:O | 1:F:123:ALA:N | 2.51 | 0.44 |
| 1:F:244:PHE:CD1 | 1:F:244:PHE:C | 2.94 | 0.44 |
| 1:F:351:ALA:O | 1:F:354:HIS:HB2 | 2.18 | 0.44 |
| 1:G:140:ARG:HB2 | 1:G:140:ARG:CZ | 2.45 | 0.44 |
| 1:G:363:ILE:HG22 | 1:G:366:GLY:N | 2.32 | 0.44 |
| 1:G:417:ASN:C | 1:G:419:ALA:H | 2.26 | 0.44 |
| 1:G:451:THR:O | 1:G:455:GLN:N | 2.46 | 0.44 |
| 1:B:202:PHE:CD1 | 1:B:297:PHE:HD1 | 2.36 | 0.44 |
| 1:B:249:VAL:HG11 | 1:B:288:LEU:HD21 | 1.98 | 0.44 |
| 1:C:364:PRO:HA | 1:C:393:SER:HB2 | 1.98 | 0.44 |
| 1:C:369:HIS:O | 1:C:388:VAL:N | 2.49 | 0.44 |
| 1:C:418:GLY:O | 1:C:419:ALA:C | 2.60 | 0.44 |
| 1:D:111:TYR:N | 1:D:111:TYR:CD1 | 2.86 | 0.44 |
| 1:D:223:PHE:C | 1:D:223:PHE:CD2 | 2.95 | 0.44 |
| 1:D:239:GLN:OE1 | 1:D:239:GLN:HA | 2.18 | 0.44 |
| 1:E:324:VAL:C | 1:E:326:LYS:N | 2.76 | 0.44 |
| 1:E:365:PHE:O | 1:E:366:GLY:O | 2.36 | 0.44 |
| 2:F:500:HEM:NA | 3:F:501:1CI:N3 | 2.65 | 0.44 |
| 1:G:158:ARG:C | 1:G:160:SER:H | 2.25 | 0.44 |
| 1:G:378:ARG:HG3 | 1:G:378:ARG:O | 2.17 | 0.44 |
| 1:A:81:THR:HG21 | 1:A:425:GLY:HA2 | 1.99 | 0.44 |
| 1:A:362:LEU:O | 1:A:364:PRO:HD3 | 2.18 | 0.44 |
| 1:B:390:PRO:O | 1:B:392:LEU:N | 2.47 | 0.44 |
| 1:B:403:GLU:O | 1:B:404:THR:HB | 2.18 | 0.44 |
| 1:B:413:PHE:O | 1:B:420:LEU:HA | 2.17 | 0.44 |
| 1:C:86:GLU:HB3 | 1:C:377:PHE:CE1 | 2.53 | 0.44 |
| 1:C:135:PHE:CG | 1:C:135:PHE:O | 2.70 | 0.44 |
| 1:C:326:LYS:HG2 | 1:C:330:GLN:HE21 | 1.82 | 0.44 |
| 1:E:42:ASN:ND2 | 1:E:42:ASN:N | 2.66 | 0.44 |
| 1:E:164:LEU:HG | 1:E:487:ARG:CZ | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:271:ARG:HG3 | 1:E:272:MET:HE2 | 2.00 | 0.44 |
| 1:E:308:ARG:HB3 | 1:E:308:ARG:NH1 | 2.31 | 0.44 |
| 1:F:141:SER:HB3 | 1:F:144:GLU:CG | 2.36 | 0.44 |
| 1:F:183:VAL:HA | 1:F:264:PHE:HB3 | 2.00 | 0.44 |
| 1:F:370:THR:HA | 1:F:386:THR:O | 2.18 | 0.44 |
| 1:F:402:PHE:HZ | 1:F:426:PHE:N | 2.15 | 0.44 |
| 1:G:111:TYR:HB3 | 1:G:287:ASN:OD1 | 2.18 | 0.44 |
| 1:G:459:ILE:CG2 | 1:G:486:ILE:HD11 | 2.48 | 0.44 |
| 1:A:172:HIS:O | 1:A:176:SER:HB2 | 2.17 | 0.43 |
| 1:A:332:ILE:HD13 | 1:A:338:PRO:HB3 | 2.00 | 0.43 |
| 1:B:30:LEU:HD22 | 1:B:383:PRO:HD3 | 2.00 | 0.43 |
| 1:B:201:LEU:C | 1:B:202:PHE:O | 2.58 | 0.43 |
| 1:B:209:ILE:CD1 | 1:B:234:ILE:HD13 | 2.35 | 0.43 |
| 1:B:427:MET:HG3 | 1:B:427:MET:O | 2.18 | 0.43 |
| 1:C:104:VAL:HG11 | 1:C:209:ILE:HD13 | 2.00 | 0.43 |
| 1:C:154:VAL:HG12 | 1:C:158:ARG:HH12 | 1.83 | 0.43 |
| 1:C:171:PHE:CE2 | 1:C:307:LEU:HB3 | 2.52 | 0.43 |
| 1:D:231:HIS:CE1 | 1:D:232:ARG:HG2 | 2.52 | 0.43 |
| 1:F:79:CYS:O | 1:F:83:ALA:HB3 | 2.17 | 0.43 |
| 1:F:98:ARG:H | 1:F:117:ASN:CG | 2.26 | 0.43 |
| 1:F:116:ALA:O | 1:F:434:ARG:NH2 | 2.37 | 0.43 |
| 1:F:320:VAL:HG22 | 1:F:348:TYR:OH | 2.17 | 0.43 |
| 1:G:414:LEU:HD23 | 1:G:419:ALA:O | 2.18 | 0.43 |
| 1:B:36:PRO:HG3 | 1:B:69:TYR:CD1 | 2.53 | 0.43 |
| 1:B:116:ALA:O | 1:B:121:TRP:HB2 | 2.18 | 0.43 |
| 1:B:213:SER:HA | 1:C:228:PRO:HB3 | 2.00 | 0.43 |
| 1:B:244:PHE:C | 1:B:244:PHE:CD1 | 2.96 | 0.43 |
| 1:B:367:VAL:O | 1:B:368:PRO:C | 2.60 | 0.43 |
| 1:B:487:ARG:HB3 | 1:B:487:ARG:NH1 | 2.33 | 0.43 |
| 1:C:269:LEU:O | 1:C:272:MET:HB3 | 2.18 | 0.43 |
| 1:C:293:LEU:O | 1:C:297:PHE:HB2 | 2.18 | 0.43 |
| 1:F:32:PRO:HD3 | 1:F:380:TYR:OH | 2.18 | 0.43 |
| 1:G:364:PRO:CG | 1:G:479:ASN:ND2 | 2.80 | 0.43 |
| 1:B:137:MET:C | 1:B:139:LYS:H | 2.27 | 0.43 |
| 1:B:249:VAL:HG11 | 1:B:288:LEU:CD2 | 2.48 | 0.43 |
| 1:B:257:ASP:C | 1:B:259:SER:N | 2.76 | 0.43 |
| 1:B:373:LYS:HD2 | 1:B:373:LYS:C | 2.42 | 0.43 |
| 1:C:30:LEU:HB3 | 1:C:31:PRO:CD | 2.48 | 0.43 |
| 1:C:213:SER:O | 1:C:216:VAL:HG12 | 2.18 | 0.43 |
| 1:F:140:ARG:HH22 | 1:F:148:GLU:CG | 2.24 | 0.43 |
| 1:F:457:PHE:HA | 1:F:489:LEU:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:479:ASN:O | 1:F:481:PRO:HD3 | 2.18 | 0.43 |
| 1:B:285:HIS:O | 1:B:288:LEU:N | 2.22 | 0.43 |
| 1:B:368:PRO:HG3 | 1:B:389:PHE:CZ | 2.53 | 0.43 |
| 1:C:46:MET:HE2 | 1:C:51:LEU:HD23 | 2.00 | 0.43 |
| 1:C:90:ASP:O | 1:C:91:GLN:CG | 2.61 | 0.43 |
| 1:C:139:LYS:HZ3 | 1:C:143:GLU:CD | 2.26 | 0.43 |
| 1:C:166:ASP:C | 1:C:168:THR:H | 2.26 | 0.43 |
| 1:D:87:ALA:HB2 | 1:D:377:PHE:CE1 | 2.53 | 0.43 |
| 1:D:143:GLU:O | 1:D:147:GLN:HG3 | 2.19 | 0.43 |
| 1:D:441:ILE:HD12 | 1:D:441:ILE:N | 2.30 | 0.43 |
| 1:E:113:VAL:O | 1:E:113:VAL:CG2 | 2.66 | 0.43 |
| 1:E:409:ASN:C | 1:E:411:GLY:H | 2.25 | 0.43 |
| 1:E:409:ASN:C | 1:E:411:GLY:N | 2.75 | 0.43 |
| 1:B:50:GLY:O | 1:B:54:SER:HB2 | 2.19 | 0.43 |
| 1:B:153:LEU:CD2 | 1:B:174:ILE:HD13 | 2.45 | 0.43 |
| 1:C:188:PHE:HB3 | 1:C:195:PHE:HB2 | 2.00 | 0.43 |
| 1:C:270:LEU:C | 1:C:272:MET:N | 2.75 | 0.43 |
| 1:C:444:THR:HG22 | 1:C:448:LEU:HD12 | 2.00 | 0.43 |
| 1:D:308:ARG:CG | 1:D:308:ARG:NH1 | 2.81 | 0.43 |
| 1:E:99:GLY:HA3 | 1:E:368:PRO:C | 2.44 | 0.43 |
| 1:F:77:VAL:HG12 | 1:F:79:CYS:H | 1.82 | 0.43 |
| 1:F:153:LEU:HD13 | 1:F:170:LEU:HD22 | 1.99 | 0.43 |
| 1:F:203:PHE:C | 1:F:205:SER:N | 2.74 | 0.43 |
| 1:F:371:VAL:HG23 | 1:F:385:ASN:H | 1.84 | 0.43 |
| 1:G:202:PHE:CD1 | 1:G:297:PHE:HD1 | 2.37 | 0.43 |
| 1:G:438:GLY:O | 1:G:439:GLU:C | 2.61 | 0.43 |
| 1:A:191:LYS:HA | 1:A:196:LEU:HD11 | 1.99 | 0.43 |
| 1:A:316:LYS:HD3 | 1:A:317:TYR:CE1 | 2.54 | 0.43 |
| 1:B:53:ARG:HH11 | 1:B:53:ARG:CA | 2.26 | 0.43 |
| 1:C:127:PHE:CZ | 1:C:267:VAL:HG12 | 2.54 | 0.43 |
| 1:C:401:TYR:CE2 | 1:C:424:GLU:HB2 | 2.54 | 0.43 |
| 1:D:371:VAL:C | 1:D:373:LYS:N | 2.76 | 0.43 |
| 1:D:427:MET:CE | 1:D:431:LEU:HD21 | 2.48 | 0.43 |
| 1:E:49:LYS:HG2 | 1:E:49:LYS:O | 2.18 | 0.43 |
| 1:E:114:ILE:CD1 | 1:E:114:ILE:N | 2.81 | 0.43 |
| 1:E:441:ILE:O | 1:E:445:GLU:HG3 | 2.17 | 0.43 |
| 1:F:68:VAL:O | 1:F:75:VAL:HG22 | 2.19 | 0.43 |
| 1:F:331:VAL:HG11 | 1:F:345:LYS:HB2 | 2.01 | 0.43 |
| 1:G:344:ALA:C | 1:G:346:MET:N | 2.71 | 0.43 |
| 1:G:455:GLN:O | 1:G:455:GLN:HG2 | 2.19 | 0.43 |
| 1:A:338:PRO:HD2 | 1:A:452:THR:OG1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:183:VAL:HA | 1:C:264:PHE:HB3 | 2.01 | 0.43 |
| 1:C:184:PHE:CD1 | 1:C:265:ILE:HD11 | 2.54 | 0.43 |
| 1:C:348:TYR:O | 1:C:352:VAL:HG23 | 2.18 | 0.43 |
| 1:D:98:ARG:HD3 | 1:D:368:PRO:O | 2.18 | 0.43 |
| 1:D:226:TYR:O | 1:E:216:VAL:HG21 | 2.18 | 0.43 |
| 1:E:135:PHE:C | 1:E:135:PHE:CD2 | 2.94 | 0.43 |
| 1:E:284:HIS:NE2 | 1:E:287:ASN:ND2 | 2.66 | 0.43 |
| 1:F:38:PRO:O | 1:F:39:VAL:HB | 2.19 | 0.43 |
| 1:F:170:LEU:O | 1:F:173:SER:N | 2.51 | 0.43 |
| 1:F:189:ASP:O | 1:F:191:LYS:N | 2.51 | 0.43 |
| 1:F:344:ALA:C | 1:F:346:MET:H | 2.26 | 0.43 |
| 1:G:373:LYS:HA | 1:G:384:LYS:HB2 | 2.00 | 0.43 |
| 1:A:108:PHE:HA | 1:A:290:LEU:HD13 | 2.01 | 0.43 |
| 1:B:253:ARG:HH22 | 1:B:272:MET:CE | 2.21 | 0.43 |
| 1:B:312:LEU:CD2 | 1:B:470:LEU:HD23 | 2.48 | 0.43 |
| 1:B:487:ARG:CB | 1:B:487:ARG:HH11 | 2.32 | 0.43 |
| 1:C:131:THR:HG23 | 1:C:267:VAL:HG11 | 2.01 | 0.43 |
| 1:D:78:LEU:O | 1:D:84:ILE:HD11 | 2.19 | 0.43 |
| 1:E:172:HIS:O | 1:E:176:SER:HB3 | 2.19 | 0.43 |
| 1:E:268:TYR:CG | 1:E:288:LEU:HD13 | 2.54 | 0.43 |
| 1:G:98:ARG:NH1 | 1:G:367:VAL:HB | 2.34 | 0.43 |
| 1:G:169:LEU:HD11 | 1:G:196:LEU:CD2 | 2.49 | 0.43 |
| 1:G:268:TYR:CZ | 1:G:288:LEU:HB2 | 2.54 | 0.43 |
| 1:A:320:VAL:HG21 | 1:A:408:PHE:CE2 | 2.54 | 0.43 |
| 1:B:134:ASP:O | 1:B:135:PHE:CB | 2.66 | 0.43 |
| 1:B:135:PHE:HZ | 1:B:263:ASP:C | 2.27 | 0.43 |
| 1:B:158:ARG:HG3 | 1:B:158:ARG:NH1 | 2.31 | 0.43 |
| 1:B:290:LEU:O | 1:B:293:LEU:HB3 | 2.19 | 0.43 |
| 1:B:402:PHE:O | 1:B:405:PRO:HD3 | 2.19 | 0.43 |
| 1:C:363:ILE:HG22 | 1:C:363:ILE:O | 2.18 | 0.43 |
| 1:D:42:ASN:OD1 | 1:D:68:VAL:HA | 2.19 | 0.43 |
| 1:D:111:TYR:HB2 | 1:D:290:LEU:CD1 | 2.48 | 0.43 |
| 1:D:365:PHE:HA | 1:D:391:VAL:HA | 2.00 | 0.43 |
| 1:E:34:PRO:CG | 1:E:45:GLN:HG2 | 2.49 | 0.43 |
| 1:E:101:ILE:HG22 | 1:E:104:VAL:HG22 | 2.01 | 0.43 |
| 1:E:117:ASN:O | 1:E:120:ARG:HB3 | 2.19 | 0.43 |
| 1:E:402:PHE:HZ | 1:E:426:PHE:N | 2.17 | 0.43 |
| 1:E:430:SER:HB3 | 2:E:500:HEM:HBA1 | 2.00 | 0.43 |
| 1:G:305:THR:HA | 1:G:308:ARG:HB2 | 2.01 | 0.43 |
| 1:A:66:PHE:CE1 | 1:A:77:VAL:HB | 2.54 | 0.43 |
| 1:A:101:ILE:O | 1:A:102:ALA:C | 2.61 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:116:ALA:HB1 | 1:A:120:ARG:HG2 | 2.00 | 0.43 |
| 1:A:126:ARG:HH21 | 1:A:126:ARG:HG2 | 1.84 | 0.43 |
| 1:A:178:ILE:O | 1:A:182:ILE:HD13 | 2.19 | 0.43 |
| 1:B:85:ARG:O | 1:B:86:GLU:C | 2.61 | 0.43 |
| 1:B:249:VAL:O | 1:B:249:VAL:HG12 | 2.17 | 0.43 |
| 1:B:370:THR:HA | 1:B:386:THR:O | 2.19 | 0.43 |
| 1:D:156:GLU:HG2 | 1:D:190:TYR:HD2 | 1.83 | 0.43 |
| 1:E:158:ARG:HG3 | 1:E:158:ARG:NH1 | 2.31 | 0.43 |
| 1:E:349:THR:O | 1:E:353:ILE:HG13 | 2.17 | 0.43 |
| 1:F:39:VAL:C | 1:F:41:GLY:N | 2.76 | 0.43 |
| 1:F:311:PHE:CD1 | 1:F:459:ILE:HG21 | 2.53 | 0.43 |
| 1:G:31:PRO:HB3 | 1:G:32:PRO:HD2 | 2.01 | 0.43 |
| 1:G:34:PRO:HD3 | 1:G:62:TYR:CE2 | 2.54 | 0.43 |
| 1:G:93:GLU:OE1 | 1:G:433:LYS:HE3 | 2.19 | 0.43 |
| 1:G:174:ILE:HD12 | 1:G:449:PHE:CE2 | 2.54 | 0.43 |
| 1:G:250:GLU:HA | 1:G:250:GLU:OE2 | 2.18 | 0.43 |
| 1:G:390:PRO:O | 1:G:392:LEU:N | 2.51 | 0.43 |
| 1:A:142:VAL:O | 1:A:145:ARG:HB2 | 2.19 | 0.42 |
| 1:B:53:ARG:NH1 | 1:B:53:ARG:HB2 | 2.33 | 0.42 |
| 1:B:147:GLN:O | 1:B:150:ALA:HB3 | 2.19 | 0.42 |
| 1:B:176:SER:HB2 | 1:B:300:THR:HG23 | 2.00 | 0.42 |
| 1:C:166:ASP:C | 1:C:168:THR:N | 2.75 | 0.42 |
| 1:C:188:PHE:CZ | 1:C:244:PHE:HZ | 2.37 | 0.42 |
| 1:C:217:PHE:CE1 | 1:C:221:SER:HA | 2.54 | 0.42 |
| 1:C:320:VAL:HG11 | 1:C:408:PHE:HE2 | 1.84 | 0.42 |
| 1:C:489:LEU:O | 1:C:490:ALA:C | 2.62 | 0.42 |
| 1:D:43:LEU:HG | 1:F:226:TYR:CE2 | 2.54 | 0.42 |
| 1:D:235:TYR:CD2 | 1:E:48:ARG:NH2 | 2.86 | 0.42 |
| 1:E:91:GLN:O | 1:E:93:GLU:N | 2.52 | 0.42 |
| 1:E:241:ILE:C | 1:E:243:THR:H | 2.26 | 0.42 |
| 1:E:309:TYR:HE2 | 1:E:313:LEU:HD12 | 1.84 | 0.42 |
| 1:F:369:HIS:HE1 | 2:F:500:HEM:O2A | 2.02 | 0.42 |
| 1:A:287:ASN:O | 1:A:288:LEU:C | 2.61 | 0.42 |
| 1:B:34:PRO:O | 1:B:36:PRO:HD3 | 2.19 | 0.42 |
| 1:B:102:ALA:CB | 1:B:218:GLU:HA | 2.47 | 0.42 |
| 1:B:215:GLN:NE2 | 1:B:476:GLY:HA3 | 2.34 | 0.42 |
| 1:B:391:VAL:HG12 | 1:B:391:VAL:O | 2.18 | 0.42 |
| 1:C:151:ARG:HG2 | 1:C:151:ARG:NH1 | 2.34 | 0.42 |
| 1:D:48:ARG:NH2 | 1:F:235:TYR:CG | 2.87 | 0.42 |
| 1:D:471:THR:HA | 1:D:472:PRO:HD3 | 1.92 | 0.42 |
| 1:E:119:GLU:HA | 1:E:122:ARG:HD3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:271:ARG:HG3 | 1:E:272:MET:CE | 2.49 | 0.42 |
| 1:F:119:GLU:C | 1:F:121:TRP:H | 2.27 | 0.42 |
| 1:F:121:TRP:O | 1:F:122:ARG:C | 2.62 | 0.42 |
| 1:F:127:PHE:C | 1:F:129:LEU:H | 2.26 | 0.42 |
| 1:F:139:LYS:O | 1:F:140:ARG:C | 2.61 | 0.42 |
| 1:F:399:PRO:HA | 1:F:402:PHE:O | 2.20 | 0.42 |
| 1:G:137:MET:CG | 1:G:138:GLY:H | 2.25 | 0.42 |
| 1:G:409:ASN:C | 1:G:411:GLY:H | 2.27 | 0.42 |
| 1:A:95:PHE:C | 1:A:97:GLY:H | 2.27 | 0.42 |
| 1:A:213:SER:O | 1:A:215:GLN:N | 2.51 | 0.42 |
| 1:A:325:GLN:NE2 | 1:A:491:ARG:NH1 | 2.67 | 0.42 |
| 1:C:103:VAL:HG22 | 1:C:217:PHE:CD2 | 2.54 | 0.42 |
| 1:C:215:GLN:NE2 | 1:C:476:GLY:CA | 2.82 | 0.42 |
| 1:D:411:GLY:O | 1:D:412:HIS:HB2 | 2.19 | 0.42 |
| 1:D:459:ILE:HG22 | 1:D:488:PHE:CE1 | 2.54 | 0.42 |
| 1:E:111:TYR:CD2 | 1:E:287:ASN:ND2 | 2.87 | 0.42 |
| 1:E:119:GLU:HA | 1:E:122:ARG:HH11 | 1.84 | 0.42 |
| 1:F:164:LEU:HG | 1:F:487:ARG:NH2 | 2.34 | 0.42 |
| 1:F:382:ILE:HG22 | 1:F:386:THR:HB | 2.02 | 0.42 |
| 1:G:176:SER:O | 1:G:179:ILE:HG22 | 2.19 | 0.42 |
| 1:A:38:PRO:O | 1:A:40:LEU:N | 2.46 | 0.42 |
| 1:A:111:TYR:CB | 1:A:290:LEU:HD12 | 2.32 | 0.42 |
| 1:B:96:SER:HB3 | 1:B:372:THR:CG2 | 2.49 | 0.42 |
| 1:C:176:SER:C | 1:C:178:ILE:H | 2.27 | 0.42 |
| 1:C:471:THR:O | 1:C:482:PRO:HD3 | 2.20 | 0.42 |
| 1:D:132:MET:O | 1:D:134:ASP:N | 2.38 | 0.42 |
| 1:D:168:THR:HG22 | 1:D:169:LEU:N | 2.33 | 0.42 |
| 1:F:30:LEU:HD23 | 1:F:30:LEU:N | 2.35 | 0.42 |
| 1:F:203:PHE:O | 1:F:205:SER:N | 2.52 | 0.42 |
| 1:F:309:TYR:CZ | 1:F:360:GLY:HA2 | 2.54 | 0.42 |
| 1:G:69:TYR:HA | 1:G:74:PRO:HA | 2.00 | 0.42 |
| 1:G:127:PHE:O | 1:G:128:SER:C | 2.62 | 0.42 |
| 1:G:423:ASN:C | 1:G:425:GLY:N | 2.74 | 0.42 |
| 1:A:103:VAL:HG23 | 1:A:104:VAL:HG13 | 2.00 | 0.42 |
| 1:B:266:ASP:O | 1:B:270:LEU:HG | 2.19 | 0.42 |
| 1:C:30:LEU:HD21 | 1:C:383:PRO:CD | 2.49 | 0.42 |
| 1:C:203:PHE:CZ | 1:C:473:ARG:NH2 | 2.87 | 0.42 |
| 1:C:404:THR:HG23 | 1:C:404:THR:O | 2.19 | 0.42 |
| 1:D:114:ILE:HG22 | 1:D:115:PHE:CG | 2.54 | 0.42 |
| 1:D:176:SER:O | 1:D:180:CYS:CB | 2.67 | 0.42 |
| 1:D:179:ILE:HD13 | 1:D:179:ILE:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:233:GLN:NE2 | 1:D:237:ASN:OD1 | 2.52 | 0.42 |
| 1:F:198:LEU:CD2 | 1:F:198:LEU:N | 2.82 | 0.42 |
| 1:F:310:GLY:HA3 | 1:F:356:ILE:HD13 | 2.02 | 0.42 |
| 1:G:43:LEU:HD22 | 1:G:220:PHE:CZ | 2.54 | 0.42 |
| 1:G:264:PHE:CD1 | 1:G:264:PHE:C | 2.97 | 0.42 |
| 1:G:323:ARG:HB2 | 1:G:348:TYR:CE2 | 2.54 | 0.42 |
| 1:A:134:ASP:OD1 | 1:A:134:ASP:O | 2.37 | 0.42 |
| 1:B:355:GLU:OE2 | 1:B:358:ARG:NE | 2.53 | 0.42 |
| 1:B:398:ASP:OD2 | 1:B:401:TYR:CD1 | 2.72 | 0.42 |
| 1:B:471:THR:HA | 1:B:472:PRO:HD3 | 1.89 | 0.42 |
| 1:C:87:ALA:O | 1:C:95:PHE:HB2 | 2.20 | 0.42 |
| 1:C:443:ARG:HH11 | 1:C:443:ARG:CG | 2.26 | 0.42 |
| 1:E:28:GLY:HA3 | 1:E:381:VAL:CG2 | 2.49 | 0.42 |
| 1:E:88:LEU:HD21 | 1:E:369:HIS:CE1 | 2.54 | 0.42 |
| 1:E:121:TRP:NE1 | 1:E:125:ARG:HD2 | 2.34 | 0.42 |
| 1:E:198:LEU:HD21 | 1:E:244:PHE:CD2 | 2.54 | 0.42 |
| 1:F:283:PHE:H | 1:F:283:PHE:HD1 | 1.67 | 0.42 |
| 1:F:373:LYS:HG3 | 1:F:375:THR:OG1 | 2.20 | 0.42 |
| 1:G:365:PHE:CE1 | 1:G:477:VAL:HA | 2.54 | 0.42 |
| 1:G:388:VAL:HG12 | 1:G:389:PHE:N | 2.35 | 0.42 |
| 1:A:137:MET:CE | 1:A:441:ILE:HD11 | 2.50 | 0.42 |
| 1:A:153:LEU:HD22 | 1:A:174:ILE:CD1 | 2.41 | 0.42 |
| 1:A:215:GLN:C | 1:A:217:PHE:H | 2.25 | 0.42 |
| 1:B:268:TYR:CG | 1:B:288:LEU:HD13 | 2.55 | 0.42 |
| 1:C:36:PRO:C | 1:C:37:LEU:HD12 | 2.45 | 0.42 |
| 1:C:246:GLY:HA2 | 1:C:289:ILE:HD11 | 2.01 | 0.42 |
| 1:C:314:MET:HB3 | 1:C:459:ILE:HD11 | 2.01 | 0.42 |
| 1:C:392:LEU:O | 1:C:395:ALA:HB3 | 2.19 | 0.42 |
| 1:C:401:TYR:HB3 | 1:C:423:ASN:OD1 | 2.20 | 0.42 |
| 1:C:470:LEU:O | 1:C:471:THR:C | 2.63 | 0.42 |
| 1:D:238:LEU:O | 1:D:242:ASN:ND2 | 2.53 | 0.42 |
| 1:D:369:HIS:O | 1:D:387:GLU:HA | 2.19 | 0.42 |
| 1:E:348:TYR:O | 1:E:352:VAL:HG23 | 2.18 | 0.42 |
| 1:F:53:ARG:HG3 | 1:F:53:ARG:O | 2.20 | 0.42 |
| 1:F:159:LYS:C | 1:F:161:LYS:H | 2.28 | 0.42 |
| 1:F:189:ASP:C | 1:F:191:LYS:N | 2.76 | 0.42 |
| 1:G:153:LEU:HD13 | 1:G:170:LEU:HD22 | 2.02 | 0.42 |
| 1:G:256:LEU:HD12 | 1:G:256:LEU:C | 2.44 | 0.42 |
| 1:G:313:LEU:O | 1:G:316:LYS:N | 2.53 | 0.42 |
| 2:G:500:HEM:NC | 3:G:501:1CI:H4 | 2.34 | 0.42 |
| 1:A:38:PRO:O | 1:A:39:VAL:HB | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:139:LYS:O | 1:A:140:ARG:HB2 | 2.20 | 0.42 |
| 1:A:437:LEU:O | 1:A:437:LEU:HD23 | 2.20 | 0.42 |
| 1:B:284:HIS:O | 1:B:284:HIS:ND1 | 2.52 | 0.42 |
| 1:C:407:THR:HG22 | 1:C:408:PHE:N | 2.35 | 0.42 |
| 1:C:416:ALA:HB3 | 1:G:267:VAL:HG11 | 2.01 | 0.42 |
| 1:D:403:GLU:O | 1:D:404:THR:C | 2.61 | 0.42 |
| 1:E:268:TYR:CE1 | 1:E:272:MET:SD | 3.13 | 0.42 |
| 1:G:402:PHE:CD1 | 1:G:412:HIS:HD2 | 2.38 | 0.42 |
| 1:G:454:LEU:HA | 1:G:454:LEU:HD23 | 1.85 | 0.42 |
| 1:A:183:VAL:HA | 1:A:264:PHE:CB | 2.50 | 0.42 |
| 1:A:489:LEU:HD12 | 1:A:489:LEU:H | 1.84 | 0.42 |
| 1:B:42:ASN:O | 1:B:46:MET:HG2 | 2.20 | 0.42 |
| 1:B:90:ASP:O | 1:B:91:GLN:HG3 | 2.20 | 0.42 |
| 1:C:69:TYR:CE2 | 1:C:74:PRO:HB3 | 2.55 | 0.42 |
| 1:C:199:LEU:O | 1:C:200:ASP:C | 2.63 | 0.42 |
| 1:C:319:HIS:ND1 | 1:C:320:VAL:HG23 | 2.34 | 0.42 |
| 1:C:371:VAL:HG23 | 1:C:371:VAL:O | 2.19 | 0.42 |
| 1:D:44:LEU:HB2 | 1:D:45:GLN:NE2 | 2.34 | 0.42 |
| 1:D:49:LYS:HE2 | 1:D:53:ARG:HG2 | 2.02 | 0.42 |
| 1:D:121:TRP:HZ2 | 1:D:125:ARG:HH11 | 1.68 | 0.42 |
| 1:D:139:LYS:C | 1:D:144:GLU:HG3 | 2.45 | 0.42 |
| 1:E:29:LYS:O | 1:E:30:LEU:HD12 | 2.19 | 0.42 |
| 1:E:82:ASP:O | 1:E:85:ARG:HB2 | 2.20 | 0.42 |
| 1:F:36:PRO:O | 1:F:37:LEU:C | 2.62 | 0.42 |
| 1:F:98:ARG:HD3 | 1:F:368:PRO:O | 2.20 | 0.42 |
| 1:F:322:GLU:O | 1:F:326:LYS:HB2 | 2.20 | 0.42 |
| 1:F:441:ILE:O | 1:F:442:ALA:C | 2.63 | 0.42 |
| 1:G:59:ARG:NH1 | 1:G:394:SER:HB2 | 2.35 | 0.42 |
| 1:G:204:GLN:O | 1:G:208:LEU:HG | 2.20 | 0.42 |
| 1:G:221:SER:C | 1:G:223:PHE:N | 2.78 | 0.42 |
| 1:G:353:ILE:CD1 | 1:G:447:PHE:HA | 2.50 | 0.42 |
| 1:A:63:GLY:O | 1:A:64:ASP:C | 2.63 | 0.42 |
| 1:A:143:GLU:O | 1:A:147:GLN:HG3 | 2.19 | 0.42 |
| 1:A:277:SER:C | 1:A:279:PRO:HD3 | 2.45 | 0.42 |
| 1:A:473:ARG:NH2 | 1:A:480:VAL:HG11 | 2.34 | 0.42 |
| 1:B:364:PRO:HA | 1:B:393:SER:HB2 | 2.02 | 0.42 |
| 1:D:272:MET:HG3 | 1:D:283:PHE:O | 2.20 | 0.42 |
| 1:E:34:PRO:CB | 1:E:45:GLN:HG2 | 2.50 | 0.42 |
| 1:E:168:THR:HA | 1:E:308:ARG:HD3 | 2.00 | 0.42 |
| 1:E:226:TYR:CD1 | 1:F:43:LEU:HD21 | 2.55 | 0.42 |
| 1:E:270:LEU:C | 1:E:272:MET:N | 2.78 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:434:ARG:O | 1:E:435:ILE:C | 2.63 | 0.42 |
| 1:F:239:GLN:HA | 1:F:239:GLN:OE1 | 2.19 | 0.42 |
| 1:F:466:GLU:OE1 | 1:F:466:GLU:N | 2.53 | 0.42 |
| 1:G:82:ASP:O | 1:G:84:ILE:N | 2.53 | 0.42 |
| 1:G:221:SER:O | 1:G:223:PHE:N | 2.53 | 0.42 |
| 1:A:91:GLN:C | 1:A:93:GLU:H | 2.27 | 0.41 |
| 1:A:487:ARG:HG3 | 1:A:489:LEU:CD1 | 2.49 | 0.41 |
| 1:C:265:ILE:O | 1:C:266:ASP:C | 2.62 | 0.41 |
| 1:C:403:GLU:O | 1:C:404:THR:HG22 | 2.20 | 0.41 |
| 1:D:164:LEU:CD2 | 1:D:485:GLN:HB3 | 2.41 | 0.41 |
| 1:D:166:ASP:O | 1:D:168:THR:N | 2.53 | 0.41 |
| 1:D:299:GLY:HA2 | 2:D:500:HEM:CMC | 2.49 | 0.41 |
| 1:D:325:GLN:NE2 | 1:D:491:ARG:HH12 | 2.18 | 0.41 |
| 1:E:37:LEU:HD12 | 1:E:37:LEU:H | 1.84 | 0.41 |
| 1:E:323:ARG:HB3 | 1:E:348:TYR:CE2 | 2.55 | 0.41 |
| 1:G:64:ASP:O | 1:G:66:PHE:HD1 | 2.03 | 0.41 |
| 1:G:211:SER:HA | 1:G:474:GLU:CD | 2.45 | 0.41 |
| 1:G:243:THR:O | 1:G:247:GLN:HG2 | 2.19 | 0.41 |
| 1:G:266:ASP:O | 1:G:270:LEU:HG | 2.19 | 0.41 |
| 1:G:390:PRO:O | 1:G:391:VAL:C | 2.61 | 0.41 |
| 1:A:434:ARG:O | 1:A:435:ILE:C | 2.64 | 0.41 |
| 1:B:61:LYS:C | 1:B:62:TYR:CD2 | 2.99 | 0.41 |
| 1:C:176:SER:C | 1:C:178:ILE:N | 2.78 | 0.41 |
| 1:C:403:GLU:O | 1:C:403:GLU:HG3 | 2.20 | 0.41 |
| 1:D:183:VAL:HA | 1:D:264:PHE:HB3 | 2.02 | 0.41 |
| 1:F:98:ARG:O | 1:F:99:GLY:O | 2.39 | 0.41 |
| 1:G:42:ASN:HD22 | 1:G:42:ASN:N | 2.18 | 0.41 |
| 1:A:28:GLY:O | 1:A:29:LYS:CG | 2.65 | 0.41 |
| 1:A:118:GLY:O | 1:A:122:ARG:HD2 | 2.20 | 0.41 |
| 1:A:136:GLY:O | 1:A:137:MET:C | 2.62 | 0.41 |
| 1:A:363:ILE:HD12 | 1:A:363:ILE:N | 2.35 | 0.41 |
| 1:B:125:ARG:HG3 | 1:B:125:ARG:HH11 | 1.85 | 0.41 |
| 1:B:305:THR:HG22 | 1:B:308:ARG:NH2 | 2.27 | 0.41 |
| 1:C:133:ARG:HB3 | 1:C:134:ASP:H | 1.74 | 0.41 |
| 1:D:51:LEU:O | 1:D:54:SER:HB2 | 2.20 | 0.41 |
| 1:E:43:LEU:C | 1:E:45:GLN:H | 2.27 | 0.41 |
| 1:E:63:GLY:O | 1:E:66:PHE:HD1 | 2.03 | 0.41 |
| 1:E:111:TYR:HD2 | 1:E:287:ASN:ND2 | 2.17 | 0.41 |
| 1:E:113:VAL:C | 1:E:114:ILE:HD12 | 2.45 | 0.41 |
| 1:E:273:GLU:C | 1:E:275:ASP:H | 2.28 | 0.41 |
| 1:E:464:PRO:HA | 1:E:465:PRO:HD3 | 1.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:362:LEU:H | 1:F:362:LEU:CD2 | 2.32 | 0.41 |
| 1:F:430:SER:O | 1:F:431:LEU:HD23 | 2.20 | 0.41 |
| 1:G:114:ILE:CD1 | 1:G:294:SER:HB3 | 2.50 | 0.41 |
| 1:G:138:GLY:CA | 1:G:145:ARG:HE | 2.32 | 0.41 |
| 1:G:169:LEU:HD11 | 1:G:196:LEU:HD23 | 2.02 | 0.41 |
| 1:G:367:VAL:O | 1:G:368:PRO:C | 2.64 | 0.41 |
| 1:A:31:PRO:HG3 | 1:A:380:TYR:CG | 2.55 | 0.41 |
| 1:A:457:PHE:HD1 | 1:A:490:ALA:HA | 1.84 | 0.41 |
| 1:B:62:TYR:CB | 1:B:66:PHE:HB3 | 2.50 | 0.41 |
| 1:B:146:ILE:CG2 | 1:B:448:LEU:HD12 | 2.50 | 0.41 |
| 1:B:194:VAL:O | 1:B:197:ARG:HB3 | 2.21 | 0.41 |
| 1:B:332:ILE:HD13 | 1:B:338:PRO:HG3 | 2.02 | 0.41 |
| 1:C:320:VAL:O | 1:C:320:VAL:HG12 | 2.20 | 0.41 |
| 1:E:85:ARG:C | 1:E:87:ALA:N | 2.77 | 0.41 |
| 1:E:428:PRO:HG2 | 1:E:429:PHE:CD2 | 2.54 | 0.41 |
| 1:F:87:ALA:O | 1:F:95:PHE:CD2 | 2.74 | 0.41 |
| 1:F:344:ALA:O | 1:F:346:MET:N | 2.54 | 0.41 |
| 1:G:198:LEU:HD21 | 1:G:244:PHE:CD2 | 2.54 | 0.41 |
| 1:G:449:PHE:O | 1:G:453:ILE:HG13 | 2.19 | 0.41 |
| 1:A:145:ARG:O | 1:A:148:GLU:HB3 | 2.21 | 0.41 |
| 1:C:52:LEU:HD22 | 1:C:364:PRO:CB | 2.42 | 0.41 |
| 1:E:108:PHE:O | 1:E:109:GLN:HB2 | 2.21 | 0.41 |
| 1:E:457:PHE:O | 1:E:491:ARG:HD2 | 2.20 | 0.41 |
| 1:F:78:LEU:HD11 | 1:F:388:VAL:CG1 | 2.51 | 0.41 |
| 1:F:429:PHE:HB3 | 1:F:436:CYS:CB | 2.50 | 0.41 |
| 1:G:171:PHE:HE2 | 1:G:307:LEU:HB3 | 1.84 | 0.41 |
| 1:B:28:GLY:O | 1:B:29:LYS:O | 2.38 | 0.41 |
| 1:C:403:GLU:C | 1:C:404:THR:HG22 | 2.45 | 0.41 |
| 1:F:42:ASN:O | 1:F:43:LEU:C | 2.63 | 0.41 |
| 1:G:102:ALA:HB2 | 1:G:218:GLU:HA | 2.02 | 0.41 |
| 1:G:409:ASN:O | 1:G:411:GLY:N | 2.53 | 0.41 |
| 1:A:122:ARG:H | 1:A:122:ARG:HD2 | 1.85 | 0.41 |
| 1:C:213:SER:HA | 1:C:216:VAL:HG12 | 2.02 | 0.41 |
| 1:C:223:PHE:HD2 | 1:C:223:PHE:O | 2.03 | 0.41 |
| 1:D:177:ASN:HA | 1:D:180:CYS:HB3 | 2.02 | 0.41 |
| 1:D:278:ASP:C | 1:D:280:SER:H | 2.28 | 0.41 |
| 1:E:40:LEU:C | 1:E:71:GLY:HA2 | 2.46 | 0.41 |
| 1:E:299:GLY:HA2 | 2:E:500:HEM:CMC | 2.50 | 0.41 |
| 1:E:302:THR:HB | 2:E:500:HEM:HAB | 2.02 | 0.41 |
| 1:F:154:VAL:HG13 | 1:F:457:PHE:CZ | 2.55 | 0.41 |
| 1:F:460:ALA:O | 1:F:487:ARG:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:73:ARG:NH1 | 1:G:73:ARG:CB | 2.83 | 0.41 |
| 1:G:81:THR:HG23 | 1:G:425:GLY:HA2 | 2.03 | 0.41 |
| 1:G:125:ARG:HH12 | 1:G:437:LEU:HB2 | 1.85 | 0.41 |
| 1:G:162:GLY:O | 1:G:487:ARG:HD3 | 2.21 | 0.41 |
| 1:G:336:ARG:HB2 | 1:G:337:PRO:CD | 2.50 | 0.41 |
| 1:G:461:SER:HB2 | 1:G:462:PRO:CD | 2.46 | 0.41 |
| 1:A:213:SER:O | 1:A:217:PHE:HB2 | 2.20 | 0.41 |
| 1:A:217:PHE:O | 1:A:218:GLU:C | 2.64 | 0.41 |
| 1:A:439:GLU:O | 1:A:443:ARG:HG3 | 2.21 | 0.41 |
| 1:B:320:VAL:O | 1:B:324:VAL:HG23 | 2.21 | 0.41 |
| 1:C:34:PRO:N | 1:C:62:TYR:HE1 | 2.19 | 0.41 |
| 1:C:101:ILE:CG2 | 1:C:104:VAL:HG22 | 2.50 | 0.41 |
| 1:C:278:ASP:OD1 | 1:C:279:PRO:HD2 | 2.20 | 0.41 |
| 1:C:443:ARG:CG | 1:C:443:ARG:NH1 | 2.82 | 0.41 |
| 1:D:162:GLY:O | 1:D:487:ARG:NH1 | 2.54 | 0.41 |
| 1:D:179:ILE:HD12 | 1:D:296:PHE:HA | 2.02 | 0.41 |
| 1:D:232:ARG:NE | 1:E:212:PHE:CE2 | 2.89 | 0.41 |
| 1:D:253:ARG:C | 1:D:255:THR:H | 2.29 | 0.41 |
| 1:E:69:TYR:CE1 | 1:E:74:PRO:HB3 | 2.56 | 0.41 |
| 1:E:103:VAL:HG21 | 1:E:214:SER:CB | 2.50 | 0.41 |
| 1:F:411:GLY:O | 1:F:413:PHE:N | 2.54 | 0.41 |
| 1:G:31:PRO:CB | 1:G:66:PHE:HA | 2.51 | 0.41 |
| 1:G:111:TYR:CD1 | 1:G:111:TYR:N | 2.89 | 0.41 |
| 1:A:51:LEU:O | 1:A:52:LEU:C | 2.62 | 0.41 |
| 1:A:75:VAL:HG21 | 1:A:389:PHE:HD1 | 1.85 | 0.41 |
| 1:A:180:CYS:O | 1:A:185:GLY:N | 2.54 | 0.41 |
| 1:A:202:PHE:CD1 | 1:A:297:PHE:CD1 | 3.09 | 0.41 |
| 1:A:404:THR:HG23 | 1:A:412:HIS:NE2 | 2.36 | 0.41 |
| 1:A:411:GLY:C | 1:A:413:PHE:N | 2.78 | 0.41 |
| 1:A:416:ALA:C | 1:A:418:GLY:H | 2.29 | 0.41 |
| 1:B:138:GLY:O | 1:B:139:LYS:HB2 | 2.20 | 0.41 |
| 1:B:355:GLU:OE2 | 1:B:358:ARG:NH2 | 2.53 | 0.41 |
| 1:B:358:ARG:HG2 | 1:B:358:ARG:NH1 | 2.34 | 0.41 |
| 1:B:358:ARG:HA | 1:B:396:LEU:HD22 | 2.02 | 0.41 |
| 1:B:397:HIS:HD2 | 1:B:405:PRO:O | 2.03 | 0.41 |
| 1:C:252:HIS:CD2 | 1:C:265:ILE:HD12 | 2.55 | 0.41 |
| 1:C:324:VAL:O | 1:C:328:ILE:HG13 | 2.20 | 0.41 |
| 1:D:121:TRP:HZ2 | 1:D:125:ARG:NH1 | 2.19 | 0.41 |
| 1:D:129:LEU:CB | 1:D:437:LEU:HD11 | 2.48 | 0.41 |
| 1:D:155:GLU:CA | 1:D:158:ARG:HG3 | 2.51 | 0.41 |
| 1:D:247:GLN:O | 1:D:250:GLU:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:47:ASP:HB2 | 1:E:57:ARG:HD3 | 2.03 | 0.41 |
| 1:E:48:ARG:HG3 | 1:E:48:ARG:NH1 | 2.36 | 0.41 |
| 1:E:61:LYS:O | 1:E:61:LYS:HG2 | 2.21 | 0.41 |
| 1:E:154:VAL:HG12 | 1:E:158:ARG:NH1 | 2.36 | 0.41 |
| 1:E:361:ASP:OD1 | 1:E:364:PRO:HA | 2.21 | 0.41 |
| 1:F:95:PHE:C | 1:F:97:GLY:N | 2.66 | 0.41 |
| 1:F:212:PHE:O | 1:F:216:VAL:HG12 | 2.20 | 0.41 |
| 1:F:220:PHE:O | 1:F:224:LEU:HG | 2.20 | 0.41 |
| 1:F:249:VAL:HG21 | 1:F:288:LEU:CD2 | 2.45 | 0.41 |
| 1:G:256:LEU:O | 1:G:258:PRO:HD3 | 2.21 | 0.41 |
| 1:G:314:MET:HE2 | 1:G:314:MET:N | 2.36 | 0.41 |
| 1:G:350:ASP:O | 1:G:354:HIS:ND1 | 2.53 | 0.41 |
| 1:G:393:SER:C | 1:G:395:ALA:H | 2.28 | 0.41 |
| 1:A:457:PHE:CD1 | 1:A:490:ALA:HA | 2.56 | 0.41 |
| 1:B:111:TYR:HD2 | 1:B:286:GLN:HB3 | 1.86 | 0.41 |
| 1:B:131:THR:HG23 | 1:B:132:MET:N | 2.35 | 0.41 |
| 1:B:256:LEU:HD21 | 1:B:270:LEU:HD23 | 2.03 | 0.41 |
| 1:B:404:THR:C | 1:B:406:ASN:H | 2.29 | 0.41 |
| 1:C:197:ARG:O | 1:C:198:LEU:C | 2.64 | 0.41 |
| 1:C:355:GLU:HA | 1:C:355:GLU:OE1 | 2.21 | 0.41 |
| 1:D:179:ILE:CD1 | 1:D:296:PHE:HA | 2.51 | 0.41 |
| 1:E:315:LEU:HD23 | 1:E:459:ILE:HD12 | 2.02 | 0.41 |
| 1:F:156:GLU:HG2 | 1:F:190:TYR:CD2 | 2.56 | 0.41 |
| 1:F:198:LEU:N | 1:F:198:LEU:HD22 | 2.36 | 0.41 |
| 1:F:308:ARG:HG2 | 1:F:308:ARG:HH11 | 1.86 | 0.41 |
| 1:F:477:VAL:O | 1:F:477:VAL:HG22 | 2.21 | 0.41 |
| 1:G:451:THR:O | 1:G:452:THR:C | 2.64 | 0.41 |
| 1:A:239:GLN:HA | 1:A:239:GLN:OE1 | 2.21 | 0.40 |
| 1:A:403:GLU:O | 1:A:404:THR:C | 2.65 | 0.40 |
| 1:B:114:ILE:HG13 | 1:B:294:SER:HB3 | 2.04 | 0.40 |
| 1:B:191:LYS:NZ | 1:B:191:LYS:CB | 2.85 | 0.40 |
| 1:B:487:ARG:NH2 | 1:E:162:GLY:O | 2.54 | 0.40 |
| 1:C:120:ARG:HD3 | 1:C:287:ASN:OD1 | 2.21 | 0.40 |
| 1:C:142:VAL:HA | 1:C:145:ARG:HG3 | 2.03 | 0.40 |
| 1:C:250:GLU:HA | 1:C:250:GLU:OE2 | 2.20 | 0.40 |
| 1:C:273:GLU:O | 1:C:276:LYS:HE3 | 2.22 | 0.40 |
| 1:F:69:TYR:HA | 1:F:74:PRO:HA | 2.02 | 0.40 |
| 1:F:94:ALA:HA | 1:F:372:THR:OG1 | 2.21 | 0.40 |
| 1:F:100:LYS:HE2 | 1:F:105:ASP:CG | 2.46 | 0.40 |
| 1:F:325:GLN:HA | 1:F:328:ILE:HD12 | 2.02 | 0.40 |
| 1:G:400:ARG:CZ | 1:G:400:ARG:HB3 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:85:ARG:C | 1:A:87:ALA:N | 2.79 | 0.40 |
| 1:A:311:PHE:HD1 | 1:A:459:ILE:HG21 | 1.86 | 0.40 |
| 1:B:210:SER:HA | 1:B:477:VAL:HG12 | 2.04 | 0.40 |
| 1:B:257:ASP:O | 1:B:259:SER:N | 2.55 | 0.40 |
| 1:B:284:HIS:CE1 | 1:B:287:ASN:ND2 | 2.89 | 0.40 |
| 1:B:430:SER:HB3 | 2:B:500:HEM:HBA1 | 2.03 | 0.40 |
| 1:C:125:ARG:HH11 | 1:C:125:ARG:HG3 | 1.86 | 0.40 |
| 1:C:230:THR:O | 1:C:233:GLN:N | 2.54 | 0.40 |
| 1:D:28:GLY:O | 1:D:29:LYS:O | 2.39 | 0.40 |
| 1:D:88:LEU:HD12 | 1:D:431:LEU:HD12 | 2.02 | 0.40 |
| 1:D:216:VAL:HG22 | 1:D:216:VAL:O | 2.21 | 0.40 |
| 1:D:276:LYS:C | 1:D:278:ASP:H | 2.30 | 0.40 |
| 1:D:316:LYS:HA | 1:D:465:PRO:HA | 2.03 | 0.40 |
| 1:E:323:ARG:O | 1:E:326:LYS:HB3 | 2.21 | 0.40 |
| 1:E:463:VAL:HA | 1:E:464:PRO:HD3 | 1.93 | 0.40 |
| 1:F:35:SER:O | 1:F:37:LEU:HD12 | 2.20 | 0.40 |
| 1:F:209:ILE:O | 1:F:209:ILE:HG22 | 2.20 | 0.40 |
| 1:F:216:VAL:HG22 | 1:F:224:LEU:CD1 | 2.52 | 0.40 |
| 1:F:317:TYR:N | 1:F:317:TYR:CD1 | 2.88 | 0.40 |
| 1:G:108:PHE:O | 1:G:109:GLN:HB2 | 2.21 | 0.40 |
| 1:G:170:LEU:O | 1:G:173:SER:HB2 | 2.22 | 0.40 |
| 1:G:411:GLY:C | 1:G:413:PHE:N | 2.78 | 0.40 |
| 1:A:283:PHE:N | 1:A:283:PHE:CD1 | 2.87 | 0.40 |
| 1:A:288:LEU:O | 1:A:292:VAL:HG23 | 2.20 | 0.40 |
| 1:B:81:THR:HG23 | 1:B:427:MET:HE3 | 2.03 | 0.40 |
| 1:B:186:LYS:CD | 1:B:186:LYS:N | 2.84 | 0.40 |
| 1:B:421:LYS:HE2 | 1:B:421:LYS:HB3 | 1.92 | 0.40 |
| 1:C:113:VAL:HB | 1:C:291:THR:HG23 | 2.03 | 0.40 |
| 1:C:114:ILE:HG13 | 1:C:294:SER:HB3 | 2.04 | 0.40 |
| 1:C:250:GLU:C | 1:C:252:HIS:H | 2.30 | 0.40 |
| 1:C:370:THR:HG23 | 1:C:386:THR:H | 1.87 | 0.40 |
| 1:C:393:SER:C | 1:C:395:ALA:N | 2.78 | 0.40 |
| 1:F:441:ILE:H | 1:F:441:ILE:HG13 | 1.69 | 0.40 |
| 1:G:48:ARG:HG2 | 1:G:49:LYS:N | 2.36 | 0.40 |
| 1:G:125:ARG:HG3 | 1:G:437:LEU:HD13 | 2.02 | 0.40 |
| 1:G:298:ALA:O | 1:G:300:THR:N | 2.55 | 0.40 |
| 1:G:372:THR:O | 1:G:373:LYS:CB | 2.69 | 0.40 |
| 1:B:48:ARG:NH2 | 1:C:235:TYR:CG | 2.90 | 0.40 |
| 1:B:201:LEU:HB3 | 1:B:241:ILE:HD11 | 2.03 | 0.40 |
| 1:B:277:SER:O | 1:B:278:ASP:C | 2.64 | 0.40 |
| 1:C:47:ASP:O | 1:C:48:ARG:C | 2.63 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:192:ASP:HA | 1:C:193:PRO:HD3 | 1.94 | 0.40 |
| 1:C:337:PRO:HA | 1:C:338:PRO:HD3 | 1.94 | 0.40 |
| 1:C:445:GLU:HB3 | 1:C:449:PHE:CE2 | 2.56 | 0.40 |
| 1:D:103:VAL:HG11 | 1:D:214:SER:HB3 | 2.03 | 0.40 |
| 1:D:304:SER:C | 1:D:306:THR:H | 2.30 | 0.40 |
| 1:E:133:ARG:NH2 | 1:E:141:SER:HB2 | 2.37 | 0.40 |
| 1:E:189:ASP:HB3 | 1:E:192:ASP:HB2 | 2.03 | 0.40 |
| 1:E:322:GLU:O | 1:E:323:ARG:C | 2.64 | 0.40 |
| 1:F:81:THR:HG23 | 1:F:425:GLY:HA2 | 2.03 | 0.40 |
| 1:F:96:SER:HB2 | 1:F:121:TRP:HZ3 | 1.85 | 0.40 |
| 1:F:215:GLN:NE2 | 1:F:476:GLY:HA2 | 2.37 | 0.40 |
| 1:G:298:ALA:HB1 | 3:G:501:1CI:C4 | 2.50 | 0.40 |
| 1:A:180:CYS:SG | 1:A:296:PHE:CE1 | 3.15 | 0.40 |
| 1:B:95:PHE:O | 1:B:369:HIS:HD2 | 2.04 | 0.40 |
| 1:B:203:PHE:O | 1:B:204:GLN:C | 2.65 | 0.40 |
| 1:B:403:GLU:O | 1:B:404:THR:CB | 2.70 | 0.40 |
| 1:C:140:ARG:H | 1:C:143:GLU:CB | 2.34 | 0.40 |
| 1:D:226:TYR:OH | 1:E:44:LEU:HD23 | 2.22 | 0.40 |
| 1:E:125:ARG:NH2 | 1:E:435:ILE:O | 2.55 | 0.40 |
| 1:E:245:ILE:HG22 | 1:E:289:ILE:CD1 | 2.51 | 0.40 |
| 1:E:359:LEU:O | 1:E:360:GLY:C | 2.65 | 0.40 |
| 1:F:97:GLY:HA3 | 1:F:370:THR:OG1 | 2.22 | 0.40 |
| 1:F:151:ARG:HG2 | 1:F:151:ARG:HH11 | 1.87 | 0.40 |
| 1:F:318:PRO:O | 1:F:319:HIS:C | 2.64 | 0.40 |
| 1:G:42:ASN:H | 1:G:69:TYR:HB2 | 1.87 | 0.40 |
| 1:G:87:ALA:HB1 | 1:G:95:PHE:CZ | 2.57 | 0.40 |
| 1:G:116:ALA:HB1 | 1:G:120:ARG:CD | 2.51 | 0.40 |
| 1:G:119:GLU:HA | 1:G:122:ARG:HH11 | 1.87 | 0.40 |
| 1:G:139:LYS:C | 1:G:141:SER:H | 2.30 | 0.40 |
| 1:G:221:SER:C | 1:G:223:PHE:H | 2.30 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 463/478 (97%) | 380 (82%) | 60 (13%) | 23 (5%) | 1 13 |
| 1 | B | 463/478 (97%) | 365 (79%) | 76 (16%) | 22 (5%) | 2 14 |
| 1 | C | 463/478 (97%) | 356 (77%) | 80 (17%) | 27 (6%) | 1 10 |
| 1 | D | 463/478 (97%) | 360 (78%) | 82 (18%) | 21 (4%) | 2 15 |
| 1 | E | 463/478 (97%) | 366 (79%) | 69 (15%) | 28 (6%) | 1 10 |
| 1 | F | 463/478 (97%) | 327 (71%) | 97 (21%) | 39 (8%) | 0 4 |
| 1 | G | 463/478 (97%) | 339 (73%) | 88 (19%) | 36 (8%) | 1 5 |
| All | All | 3241/3346 (97%) | 2493 (77%) | 552 (17%) | 196 (6%) | 1 10 |

All (196) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 29 | LYS |
| 1 | A | 102 | ALA |
| 1 | A | 137 | MET |
| 1 | A | 255 | THR |
| 1 | A | 285 | HIS |
| 1 | A | 334 | SER |
| 1 | A | 366 | GLY |
| 1 | A | 391 | VAL |
| 1 | B | 29 | LYS |
| 1 | B | 133 | ARG |
| 1 | B | 137 | MET |
| 1 | B | 285 | HIS |
| 1 | B | 286 | GLN |
| 1 | B | 334 | SER |
| 1 | B | 404 | THR |
| 1 | C | 29 | LYS |
| 1 | C | 91 | GLN |
| 1 | C | 285 | HIS |
| 1 | C | 301 | GLU |
| 1 | C | 391 | VAL |
| 1 | C | 419 | ALA |
| 1 | D | 29 | LYS |
| 1 | D | 167 | ASN |
| 1 | D | 285 | HIS |
| 1 | D | 336 | ARG |
| 1 | E | 301 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 391 | VAL |
| 1 | F | 79 | CYS |
| 1 | F | 86 | GLU |
| 1 | F | 91 | GLN |
| 1 | F | 140 | ARG |
| 1 | F | 286 | GLN |
| 1 | F | 391 | VAL |
| 1 | G | 48 | ARG |
| 1 | G | 64 | ASP |
| 1 | G | 102 | ALA |
| 1 | G | 286 | GLN |
| 1 | G | 373 | LYS |
| 1 | G | 391 | VAL |
| 1 | G | 415 | ASP |
| 1 | A | 64 | ASP |
| 1 | A | 92 | ALA |
| 1 | A | 118 | GLY |
| 1 | A | 138 | GLY |
| 1 | A | 331 | VAL |
| 1 | A | 430 | SER |
| 1 | B | 102 | ALA |
| 1 | B | 368 | PRO |
| 1 | C | 39 | VAL |
| 1 | C | 41 | GLY |
| 1 | C | 116 | ALA |
| 1 | C | 297 | PHE |
| 1 | C | 366 | GLY |
| 1 | C | 435 | ILE |
| 1 | D | 91 | GLN |
| 1 | D | 161 | LYS |
| 1 | D | 400 | ARG |
| 1 | D | 447 | PHE |
| 1 | E | 29 | LYS |
| 1 | E | 92 | ALA |
| 1 | E | 118 | GLY |
| 1 | E | 162 | GLY |
| 1 | E | 331 | VAL |
| 1 | E | 366 | GLY |
| 1 | E | 378 | ARG |
| 1 | F | 40 | LEU |
| 1 | F | 122 | ARG |
| 1 | F | 230 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 263 | ASP |
| 1 | F | 345 | LYS |
| 1 | F | 416 | ALA |
| 1 | G | 29 | LYS |
| 1 | G | 80 | GLY |
| 1 | G | 91 | GLN |
| 1 | G | 96 | SER |
| 1 | G | 118 | GLY |
| 1 | G | 119 | GLU |
| 1 | G | 140 | ARG |
| 1 | G | 159 | LYS |
| 1 | G | 283 | PHE |
| 1 | G | 285 | HIS |
| 1 | G | 343 | ARG |
| 1 | G | 345 | LYS |
| 1 | G | 366 | GLY |
| 1 | G | 368 | PRO |
| 1 | G | 387 | GLU |
| 1 | G | 412 | HIS |
| 1 | G | 424 | GLU |
| 1 | G | 460 | ALA |
| 1 | A | 96 | SER |
| 1 | A | 225 | LYS |
| 1 | A | 282 | GLU |
| 1 | A | 286 | GLN |
| 1 | C | 49 | LYS |
| 1 | C | 110 | GLY |
| 1 | C | 137 | MET |
| 1 | C | 432 | GLY |
| 1 | D | 128 | SER |
| 1 | D | 203 | PHE |
| 1 | E | 140 | ARG |
| 1 | E | 284 | HIS |
| 1 | E | 418 | GLY |
| 1 | F | 29 | LYS |
| 1 | F | 99 | GLY |
| 1 | F | 161 | LYS |
| 1 | F | 190 | TYR |
| 1 | F | 247 | GLN |
| 1 | F | 421 | LYS |
| 1 | G | 32 | PRO |
| 1 | G | 83 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 301 | GLU |
| 1 | A | 140 | ARG |
| 1 | A | 279 | PRO |
| 1 | B | 39 | VAL |
| 1 | B | 87 | ALA |
| 1 | B | 228 | PRO |
| 1 | B | 279 | PRO |
| 1 | B | 374 | ASP |
| 1 | C | 92 | ALA |
| 1 | C | 133 | ARG |
| 1 | C | 177 | ASN |
| 1 | C | 193 | PRO |
| 1 | D | 90 | ASP |
| 1 | D | 110 | GLY |
| 1 | D | 283 | PHE |
| 1 | D | 422 | ARG |
| 1 | D | 453 | ILE |
| 1 | E | 60 | GLU |
| 1 | E | 211 | SER |
| 1 | E | 277 | SER |
| 1 | E | 278 | ASP |
| 1 | E | 279 | PRO |
| 1 | F | 49 | LYS |
| 1 | F | 139 | LYS |
| 1 | F | 331 | VAL |
| 1 | F | 374 | ASP |
| 1 | F | 422 | ARG |
| 1 | G | 109 | GLN |
| 1 | G | 410 | PRO |
| 1 | G | 421 | LYS |
| 1 | A | 109 | GLN |
| 1 | A | 211 | SER |
| 1 | A | 301 | GLU |
| 1 | B | 366 | GLY |
| 1 | B | 405 | PRO |
| 1 | B | 416 | ALA |
| 1 | C | 117 | ASN |
| 1 | D | 190 | TYR |
| 1 | E | 110 | GLY |
| 1 | E | 130 | ALA |
| 1 | E | 368 | PRO |
| 1 | E | 385 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 439 | GLU |
| 1 | F | 203 | PHE |
| 1 | F | 335 | HIS |
| 1 | F | 378 | ARG |
| 1 | F | 406 | ASN |
| 1 | G | 135 | PHE |
| 1 | B | 203 | PHE |
| 1 | C | 80 | GLY |
| 1 | C | 86 | GLU |
| 1 | C | 256 | LEU |
| 1 | D | 178 | ILE |
| 1 | D | 439 | GLU |
| 1 | E | 39 | VAL |
| 1 | E | 49 | LYS |
| 1 | F | 221 | SER |
| 1 | F | 366 | GLY |
| 1 | F | 412 | HIS |
| 1 | F | 418 | GLY |
| 1 | F | 437 | LEU |
| 1 | G | 161 | LYS |
| 1 | G | 385 | ASN |
| 1 | B | 435 | ILE |
| 1 | C | 185 | GLY |
| 1 | D | 391 | VAL |
| 1 | D | 410 | PRO |
| 1 | E | 289 | ILE |
| 1 | E | 435 | ILE |
| 1 | F | 39 | VAL |
| 1 | F | 441 | ILE |
| 1 | B | 261 | PRO |
| 1 | B | 391 | VAL |
| 1 | F | 112 | GLY |
| 1 | G | 222 | GLY |
| 1 | C | 162 | GLY |
| 1 | G | 110 | GLY |
| 1 | B | 364 | PRO |
| 1 | C | 418 | GLY |
| 1 | D | 366 | GLY |
| 1 | E | 383 | PRO |
| 1 | F | 106 | PRO |
| 1 | F | 162 | GLY |
| 1 | F | 364 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 465 | PRO |
| 1 | E | 338 | 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 | 411/423 (97%) | 392 (95%) | 19 (5%) | 24 | 58 |
| 1 | B | 411/423 (97%) | 402 (98%) | 9 (2%) | 45 | 71 |
| 1 | C | 411/423 (97%) | 394 (96%) | 17 (4%) | 27 | 60 |
| 1 | D | 411/423 (97%) | 390 (95%) | 21 (5%) | 21 | 54 |
| 1 | E | 411/423 (97%) | 388 (94%) | 23 (6%) | 19 | 52 |
| 1 | F | 411/423 (97%) | 392 (95%) | 19 (5%) | 24 | 58 |
| 1 | G | 411/423 (97%) | 399 (97%) | 12 (3%) | 37 | 67 |
| All | All | 2877/2961 (97%) | 2757 (96%) | 120 (4%) | 26 | 60 |

All (120) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 48 | ARG |
| 1 | A | 73 | ARG |
| 1 | A | 75 | VAL |
| 1 | A | 81 | THR |
| 1 | A | 122 | ARG |
| 1 | A | 139 | LYS |
| 1 | A | 155 | GLU |
| 1 | A | 169 | LEU |
| 1 | A | 170 | LEU |
| 1 | A | 179 | ILE |
| 1 | A | 201 | LEU |
| 1 | A | 204 | GLN |
| 1 | A | 255 | THR |
| 1 | A | 302 | THR |
| 1 | A | 306 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 362 | LEU |
| 1 | A | 370 | THR |
| 1 | A | 437 | LEU |
| 1 | A | 477 | VAL |
| 1 | B | 30 | LEU |
| 1 | B | 135 | PHE |
| 1 | B | 165 | LEU |
| 1 | B | 179 | ILE |
| 1 | B | 186 | LYS |
| 1 | B | 191 | LYS |
| 1 | B | 359 | LEU |
| 1 | B | 368 | PRO |
| 1 | B | 465 | PRO |
| 1 | C | 53 | ARG |
| 1 | C | 86 | GLU |
| 1 | C | 165 | LEU |
| 1 | C | 169 | LEU |
| 1 | C | 179 | ILE |
| 1 | C | 191 | LYS |
| 1 | C | 244 | PHE |
| 1 | C | 276 | LYS |
| 1 | C | 323 | ARG |
| 1 | C | 341 | ASP |
| 1 | C | 362 | LEU |
| 1 | C | 423 | ASN |
| 1 | C | 424 | GLU |
| 1 | C | 435 | ILE |
| 1 | C | 439 | GLU |
| 1 | C | 474 | GLU |
| 1 | C | 489 | LEU |
| 1 | D | 75 | VAL |
| 1 | D | 111 | TYR |
| 1 | D | 122 | ARG |
| 1 | D | 125 | ARG |
| 1 | D | 135 | PHE |
| 1 | D | 164 | LEU |
| 1 | D | 165 | LEU |
| 1 | D | 170 | LEU |
| 1 | D | 179 | ILE |
| 1 | D | 208 | LEU |
| 1 | D | 230 | THR |
| 1 | D | 276 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 325 | GLN |
| 1 | D | 359 | LEU |
| 1 | D | 371 | VAL |
| 1 | D | 387 | GLU |
| 1 | D | 431 | LEU |
| 1 | D | 451 | THR |
| 1 | D | 463 | VAL |
| 1 | D | 465 | PRO |
| 1 | D | 467 | ASP |
| 1 | E | 47 | ASP |
| 1 | E | 49 | LYS |
| 1 | E | 52 | LEU |
| 1 | E | 53 | ARG |
| 1 | E | 131 | THR |
| 1 | E | 132 | MET |
| 1 | E | 143 | GLU |
| 1 | E | 165 | LEU |
| 1 | E | 179 | ILE |
| 1 | E | 186 | LYS |
| 1 | E | 191 | LYS |
| 1 | E | 194 | VAL |
| 1 | E | 214 | SER |
| 1 | E | 216 | VAL |
| 1 | E | 224 | LEU |
| 1 | E | 231 | HIS |
| 1 | E | 284 | HIS |
| 1 | E | 287 | ASN |
| 1 | E | 323 | ARG |
| 1 | E | 335 | HIS |
| 1 | E | 362 | LEU |
| 1 | E | 441 | ILE |
| 1 | E | 467 | ASP |
| 1 | F | 30 | LEU |
| 1 | F | 62 | TYR |
| 1 | F | 76 | VAL |
| 1 | F | 113 | VAL |
| 1 | F | 124 | LEU |
| 1 | F | 135 | PHE |
| 1 | F | 170 | LEU |
| 1 | F | 172 | HIS |
| 1 | F | 179 | ILE |
| 1 | F | 186 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 204 | GLN |
| 1 | F | 216 | VAL |
| 1 | F | 284 | HIS |
| 1 | F | 323 | ARG |
| 1 | F | 335 | HIS |
| 1 | F | 341 | ASP |
| 1 | F | 359 | LEU |
| 1 | F | 466 | GLU |
| 1 | F | 477 | VAL |
| 1 | G | 132 | MET |
| 1 | G | 140 | ARG |
| 1 | G | 170 | LEU |
| 1 | G | 179 | ILE |
| 1 | G | 186 | LYS |
| 1 | G | 224 | LEU |
| 1 | G | 232 | ARG |
| 1 | G | 302 | THR |
| 1 | G | 305 | THR |
| 1 | G | 359 | LEU |
| 1 | G | 368 | PRO |
| 1 | G | 479 | ASN |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 117 | ASN |
| 1 | A | 147 | GLN |
| 1 | A | 204 | GLN |
| 1 | A | 233 | GLN |
| 1 | A | 287 | ASN |
| 1 | A | 325 | GLN |
| 1 | A | 369 | HIS |
| 1 | A | 385 | ASN |
| 1 | A | 479 | ASN |
| 1 | B | 172 | HIS |
| 1 | B | 242 | ASN |
| 1 | B | 286 | GLN |
| 1 | B | 287 | ASN |
| 1 | B | 325 | GLN |
| 1 | B | 369 | HIS |
| 1 | B | 385 | ASN |
| 1 | B | 397 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 479 | ASN |
| 1 | B | 492 | HIS |
| 1 | C | 117 | ASN |
| 1 | C | 215 | GLN |
| 1 | C | 247 | GLN |
| 1 | C | 260 | ASN |
| 1 | C | 285 | HIS |
| 1 | C | 330 | GLN |
| 1 | C | 335 | HIS |
| 1 | C | 369 | HIS |
| 1 | C | 385 | ASN |
| 1 | C | 412 | HIS |
| 1 | C | 492 | HIS |
| 1 | D | 45 | GLN |
| 1 | D | 204 | GLN |
| 1 | D | 233 | GLN |
| 1 | D | 237 | ASN |
| 1 | D | 284 | HIS |
| 1 | D | 325 | GLN |
| 1 | D | 354 | HIS |
| 1 | D | 369 | HIS |
| 1 | D | 397 | HIS |
| 1 | D | 412 | HIS |
| 1 | E | 42 | ASN |
| 1 | E | 172 | HIS |
| 1 | E | 284 | HIS |
| 1 | E | 287 | ASN |
| 1 | E | 325 | GLN |
| 1 | E | 330 | GLN |
| 1 | E | 335 | HIS |
| 1 | E | 357 | GLN |
| 1 | E | 376 | GLN |
| 1 | E | 417 | ASN |
| 1 | F | 45 | GLN |
| 1 | F | 167 | ASN |
| 1 | F | 204 | GLN |
| 1 | F | 233 | GLN |
| 1 | F | 237 | ASN |
| 1 | F | 319 | HIS |
| 1 | F | 325 | GLN |
| 1 | F | 330 | GLN |
| 1 | F | 357 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 376 | GLN |
| 1 | F | 485 | GLN |
| 1 | G | 42 | ASN |
| 1 | G | 45 | GLN |
| 1 | G | 204 | GLN |
| 1 | G | 233 | GLN |
| 1 | G | 285 | HIS |
| 1 | G | 325 | GLN |
| 1 | G | 369 | HIS |
| 1 | G | 479 | ASN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | HEM | G | 500 | 3,1 | 50,50,50 | 2.41 | 23 (46%) | 67,82,82 | 1.48 | 14 (20%) |
| 2 | HEM | F | 500 | 3,1 | 50,50,50 | 2.39 | 22 (44%) | 67,82,82 | 1.40 | 13 (19%) |
| 3 | 1CI | C | 501 | 2 | 13,13,13 | 1.89 | 2 (15%) | 17,17,17 | 0.75 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | 1CI | G | 501 | 2 | 13,13,13 | 1.88 | 2 (15%) | 17,17,17 | 0.73 | 0 |
| 2 | HEM | C | 500 | 3,1 | 50,50,50 | 2.36 | 25 (50%) | 67,82,82 | 1.40 | 11 (16%) |
| 2 | HEM | A | 500 | 3,1 | 50,50,50 | 2.38 | 24 (48%) | 67,82,82 | 1.38 | 11 (16%) |
| 3 | 1CI | F | 501 | 2 | 13,13,13 | 1.91 | 2 (15%) | 17,17,17 | 0.74 | 0 |
| 3 | 1CI | B | 501 | - | 13,13,13 | 1.90 | 2 (15%) | 17,17,17 | 0.78 | 0 |
| 2 | HEM | D | 500 | 3,1 | 50,50,50 | 2.39 | 21 (42%) | 67,82,82 | 1.39 | 11 (16%) |
| 3 | 1CI | E | 501 | - | 13,13,13 | 1.89 | 2 (15%) | 17,17,17 | 0.74 | 0 |
| 3 | 1CI | A | 501 | 2 | 13,13,13 | 1.90 | 2 (15%) | 17,17,17 | 0.73 | 0 |
| 2 | HEM | E | 500 | - | 50,50,50 | 2.47 | 23 (46%) | 67,82,82 | 1.40 | 13 (19%) |
| 3 | 1CI | D | 501 | 2 | 13,13,13 | 1.90 | 2 (15%) | 17,17,17 | 0.75 | 0 |
| 2 | HEM | B | 500 | 1 | 50,50,50 | 2.41 | 23 (46%) | 67,82,82 | 1.42 | 14 (20%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | HEM | G | 500 | 3,1 | - | 8/14/54/54 | - |
| 2 | HEM | F | 500 | 3,1 | - | 8/14/54/54 | - |
| 3 | 1CI | C | 501 | 2 | - | 0/4/4/4 | 0/2/2/2 |
| 3 | 1CI | G | 501 | 2 | - | 0/4/4/4 | 0/2/2/2 |
| 2 | HEM | C | 500 | 3,1 | - | 6/14/54/54 | - |
| 2 | HEM | A | 500 | 3,1 | - | 5/14/54/54 | - |
| 3 | 1CI | F | 501 | 2 | - | 0/4/4/4 | 0/2/2/2 |
| 3 | 1CI | B | 501 | - | - | 0/4/4/4 | 0/2/2/2 |
| 2 | HEM | D | 500 | 3,1 | - | 4/14/54/54 | - |
| 3 | 1CI | E | 501 | - | - | 0/4/4/4 | 0/2/2/2 |
| 3 | 1CI | A | 501 | 2 | - | 0/4/4/4 | 0/2/2/2 |
| 2 | HEM | E | 500 | - | - | 8/14/54/54 | - |
| 3 | 1CI | D | 501 | 2 | - | 0/4/4/4 | 0/2/2/2 |
| 2 | HEM | B | 500 | 1 | - | 6/14/54/54 | - |

All (175) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | F | 501 | 1CI | C6-N1 | -5.96 | 1.33 | 1.43 |
| 3 | D | 501 | 1CI | C6-N1 | -5.94 | 1.33 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | B | 501 | 1CI | C6-N1 | -5.91 | 1.33 | 1.43 |
| 3 | E | 501 | 1CI | C6-N1 | -5.91 | 1.33 | 1.43 |
| 3 | A | 501 | 1CI | C6-N1 | -5.90 | 1.33 | 1.43 |
| 3 | C | 501 | 1CI | C6-N1 | -5.86 | 1.33 | 1.43 |
| 3 | G | 501 | 1CI | C6-N1 | -5.83 | 1.33 | 1.43 |
| 2 | E | 500 | HEM | C4A-NA | -4.73 | 1.30 | 1.39 |
| 2 | E | 500 | HEM | C1D-ND | -4.67 | 1.29 | 1.38 |
| 2 | A | 500 | HEM | C1B-NB | -4.57 | 1.32 | 1.40 |
| 2 | B | 500 | HEM | C4A-NA | -4.45 | 1.31 | 1.39 |
| 2 | F | 500 | HEM | C1D-ND | -4.45 | 1.30 | 1.38 |
| 2 | D | 500 | HEM | C1D-ND | -4.41 | 1.30 | 1.38 |
| 2 | G | 500 | HEM | C1D-ND | -4.41 | 1.30 | 1.38 |
| 2 | C | 500 | HEM | C1D-ND | -4.38 | 1.30 | 1.38 |
| 2 | A | 500 | HEM | C1D-ND | -4.35 | 1.30 | 1.38 |
| 2 | D | 500 | HEM | C1B-NB | -4.33 | 1.32 | 1.40 |
| 2 | E | 500 | HEM | C1B-NB | -4.26 | 1.32 | 1.40 |
| 2 | F | 500 | HEM | C1B-NB | -4.25 | 1.32 | 1.40 |
| 2 | G | 500 | HEM | C4D-ND | -4.21 | 1.33 | 1.40 |
| 2 | B | 500 | HEM | C1C-NC | -4.21 | 1.31 | 1.39 |
| 2 | B | 500 | HEM | C1D-ND | -4.17 | 1.30 | 1.38 |
| 2 | B | 500 | HEM | C1B-NB | -4.15 | 1.33 | 1.40 |
| 2 | A | 500 | HEM | C4A-NA | -4.13 | 1.31 | 1.39 |
| 2 | G | 500 | HEM | C4A-NA | -4.08 | 1.31 | 1.39 |
| 2 | F | 500 | HEM | C4A-NA | -4.07 | 1.32 | 1.39 |
| 2 | D | 500 | HEM | CAC-C3C | -4.06 | 1.36 | 1.47 |
| 2 | G | 500 | HEM | C1B-NB | -4.01 | 1.33 | 1.40 |
| 2 | D | 500 | HEM | C4A-NA | -4.00 | 1.32 | 1.39 |
| 2 | G | 500 | HEM | C1C-NC | -3.98 | 1.32 | 1.39 |
| 2 | G | 500 | HEM | FE-NB | 3.93 | 2.07 | 1.94 |
| 2 | E | 500 | HEM | C1C-NC | -3.92 | 1.32 | 1.39 |
| 2 | B | 500 | HEM | FE-ND | 3.91 | 2.06 | 1.94 |
| 2 | A | 500 | HEM | C1C-NC | -3.91 | 1.32 | 1.39 |
| 2 | D | 500 | HEM | FE-NB | 3.91 | 2.06 | 1.94 |
| 2 | C | 500 | HEM | FE-NB | 3.90 | 2.06 | 1.94 |
| 2 | C | 500 | HEM | C1C-NC | -3.89 | 1.32 | 1.39 |
| 2 | D | 500 | HEM | CBB-CAB | 3.85 | 1.48 | 1.30 |
| 2 | F | 500 | HEM | C1C-NC | -3.85 | 1.32 | 1.39 |
| 2 | E | 500 | HEM | C4D-ND | -3.84 | 1.33 | 1.40 |
| 2 | F | 500 | HEM | CAC-C3C | -3.83 | 1.37 | 1.47 |
| 2 | G | 500 | HEM | CBB-CAB | 3.80 | 1.48 | 1.30 |
| 2 | C | 500 | HEM | CBB-CAB | 3.79 | 1.48 | 1.30 |
| 2 | E | 500 | HEM | CAC-C3C | -3.79 | 1.37 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 500 | HEM | CAC-C3C | -3.78 | 1.37 | 1.47 |
| 2 | F | 500 | HEM | CBB-CAB | 3.77 | 1.48 | 1.30 |
| 2 | F | 500 | HEM | C4D-ND | -3.76 | 1.33 | 1.40 |
| 2 | C | 500 | HEM | C1B-NB | -3.75 | 1.33 | 1.40 |
| 2 | B | 500 | HEM | CBB-CAB | 3.75 | 1.48 | 1.30 |
| 2 | E | 500 | HEM | CMA-C3A | 3.75 | 1.58 | 1.50 |
| 2 | E | 500 | HEM | C1C-C2C | -3.75 | 1.37 | 1.45 |
| 2 | A | 500 | HEM | CMA-C3A | 3.75 | 1.58 | 1.50 |
| 2 | C | 500 | HEM | C4A-NA | -3.74 | 1.32 | 1.39 |
| 2 | A | 500 | HEM | FE-NB | 3.74 | 2.06 | 1.94 |
| 2 | A | 500 | HEM | CAC-C3C | -3.73 | 1.37 | 1.47 |
| 2 | E | 500 | HEM | FE-NB | 3.72 | 2.06 | 1.94 |
| 2 | F | 500 | HEM | FE-ND | 3.69 | 2.06 | 1.94 |
| 2 | A | 500 | HEM | CBB-CAB | 3.69 | 1.48 | 1.30 |
| 2 | C | 500 | HEM | C4D-ND | -3.68 | 1.33 | 1.40 |
| 2 | E | 500 | HEM | CBB-CAB | 3.68 | 1.48 | 1.30 |
| 2 | B | 500 | HEM | CAC-C3C | -3.68 | 1.37 | 1.47 |
| 2 | B | 500 | HEM | CMA-C3A | 3.66 | 1.58 | 1.50 |
| 2 | D | 500 | HEM | CMA-C3A | 3.65 | 1.58 | 1.50 |
| 2 | G | 500 | HEM | CMA-C3A | 3.64 | 1.58 | 1.50 |
| 2 | G | 500 | HEM | FE-ND | 3.62 | 2.06 | 1.94 |
| 2 | C | 500 | HEM | CAC-C3C | -3.62 | 1.37 | 1.47 |
| 2 | D | 500 | HEM | C1C-C2C | -3.62 | 1.38 | 1.45 |
| 2 | G | 500 | HEM | FE-NC | 3.62 | 2.07 | 1.95 |
| 2 | C | 500 | HEM | CMA-C3A | 3.60 | 1.58 | 1.50 |
| 2 | D | 500 | HEM | FE-NC | 3.59 | 2.07 | 1.95 |
| 2 | A | 500 | HEM | C4B-NB | -3.59 | 1.31 | 1.38 |
| 2 | D | 500 | HEM | FE-ND | 3.58 | 2.05 | 1.94 |
| 2 | F | 500 | HEM | CMA-C3A | 3.58 | 1.58 | 1.50 |
| 2 | A | 500 | HEM | FE-ND | 3.58 | 2.05 | 1.94 |
| 2 | A | 500 | HEM | C1C-C2C | -3.56 | 1.38 | 1.45 |
| 2 | E | 500 | HEM | FE-NC | 3.55 | 2.06 | 1.95 |
| 2 | F | 500 | HEM | FE-NB | 3.54 | 2.05 | 1.94 |
| 2 | D | 500 | HEM | C1C-NC | -3.53 | 1.33 | 1.39 |
| 2 | D | 500 | HEM | C4D-ND | -3.53 | 1.34 | 1.40 |
| 2 | C | 500 | HEM | FE-NA | 3.50 | 2.06 | 1.95 |
| 2 | C | 500 | HEM | FE-ND | 3.50 | 2.05 | 1.94 |
| 2 | F | 500 | HEM | C4B-NB | -3.50 | 1.32 | 1.38 |
| 2 | B | 500 | HEM | FE-NA | 3.50 | 2.06 | 1.95 |
| 2 | B | 500 | HEM | C1C-C2C | -3.49 | 1.38 | 1.45 |
| 2 | G | 500 | HEM | C4B-NB | -3.47 | 1.32 | 1.38 |
| 2 | F | 500 | HEM | FE-NC | 3.47 | 2.06 | 1.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | G | 500 | HEM | C1C-C2C | -3.45 | 1.38 | 1.45 |
| 2 | G | 500 | HEM | FE-NA | 3.45 | 2.06 | 1.95 |
| 2 | E | 500 | HEM | FE-ND | 3.44 | 2.05 | 1.94 |
| 2 | B | 500 | HEM | FE-NB | 3.42 | 2.05 | 1.94 |
| 2 | D | 500 | HEM | FE-NA | 3.40 | 2.06 | 1.95 |
| 2 | F | 500 | HEM | FE-NA | 3.40 | 2.06 | 1.95 |
| 2 | E | 500 | HEM | C4B-NB | -3.35 | 1.32 | 1.38 |
| 2 | B | 500 | HEM | C4B-NB | -3.35 | 1.32 | 1.38 |
| 2 | C | 500 | HEM | C1C-C2C | -3.34 | 1.38 | 1.45 |
| 2 | C | 500 | HEM | C4B-NB | -3.33 | 1.32 | 1.38 |
| 2 | A | 500 | HEM | C4D-ND | -3.33 | 1.34 | 1.40 |
| 2 | F | 500 | HEM | C1C-C2C | -3.32 | 1.38 | 1.45 |
| 2 | B | 500 | HEM | FE-NC | 3.31 | 2.06 | 1.95 |
| 2 | B | 500 | HEM | C4D-ND | -3.29 | 1.34 | 1.40 |
| 2 | A | 500 | HEM | FE-NC | 3.28 | 2.06 | 1.95 |
| 2 | C | 500 | HEM | FE-NC | 3.26 | 2.05 | 1.95 |
| 2 | D | 500 | HEM | C4B-NB | -3.24 | 1.32 | 1.38 |
| 2 | E | 500 | HEM | FE-NA | 3.11 | 2.05 | 1.95 |
| 2 | A | 500 | HEM | FE-NA | 3.09 | 2.05 | 1.95 |
| 2 | E | 500 | HEM | C4C-NC | -3.02 | 1.33 | 1.39 |
| 2 | F | 500 | HEM | CMC-C2C | 3.01 | 1.56 | 1.50 |
| 2 | B | 500 | HEM | CMC-C2C | 2.94 | 1.56 | 1.50 |
| 2 | A | 500 | HEM | CMC-C2C | 2.91 | 1.56 | 1.50 |
| 2 | G | 500 | HEM | CMC-C2C | 2.90 | 1.56 | 1.50 |
| 2 | B | 500 | HEM | C3B-C2B | 2.89 | 1.43 | 1.37 |
| 2 | D | 500 | HEM | CMC-C2C | 2.84 | 1.56 | 1.50 |
| 2 | C | 500 | HEM | CMC-C2C | 2.84 | 1.56 | 1.50 |
| 2 | E | 500 | HEM | CMC-C2C | 2.71 | 1.56 | 1.50 |
| 2 | F | 500 | HEM | O2A-CGA | -2.70 | 1.21 | 1.30 |
| 2 | B | 500 | HEM | C4C-NC | -2.69 | 1.34 | 1.39 |
| 2 | A | 500 | HEM | C4C-NC | -2.69 | 1.34 | 1.39 |
| 2 | C | 500 | HEM | O2A-CGA | -2.69 | 1.21 | 1.30 |
| 2 | C | 500 | HEM | C4C-NC | -2.65 | 1.34 | 1.39 |
| 2 | E | 500 | HEM | CBD-CGD | 2.64 | 1.56 | 1.50 |
| 2 | D | 500 | HEM | O2A-CGA | -2.62 | 1.22 | 1.30 |
| 2 | B | 500 | HEM | O2A-CGA | -2.62 | 1.22 | 1.30 |
| 2 | C | 500 | HEM | C3B-C2B | 2.61 | 1.42 | 1.37 |
| 2 | B | 500 | HEM | CBC-CAC | 2.61 | 1.42 | 1.30 |
| 2 | A | 500 | HEM | O2A-CGA | -2.60 | 1.22 | 1.30 |
| 2 | D | 500 | HEM | C4C-NC | -2.59 | 1.34 | 1.39 |
| 2 | D | 500 | HEM | C3B-C2B | 2.59 | 1.42 | 1.37 |
| 2 | F | 500 | HEM | CAD-C3D | 2.58 | 1.58 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 500 | HEM | CAD-C3D | 2.57 | 1.58 | 1.51 |
| 2 | E | 500 | HEM | CAD-C3D | 2.57 | 1.57 | 1.51 |
| 2 | G | 500 | HEM | C4C-NC | -2.54 | 1.34 | 1.39 |
| 2 | E | 500 | HEM | CBC-CAC | 2.53 | 1.42 | 1.30 |
| 3 | B | 501 | 1CI | C5-N1 | -2.51 | 1.33 | 1.38 |
| 3 | G | 501 | 1CI | C5-N1 | -2.51 | 1.33 | 1.38 |
| 2 | G | 500 | HEM | C3B-C2B | 2.51 | 1.42 | 1.37 |
| 3 | A | 501 | 1CI | C5-N1 | -2.49 | 1.33 | 1.38 |
| 2 | C | 500 | HEM | CBC-CAC | 2.48 | 1.42 | 1.30 |
| 2 | F | 500 | HEM | C4C-NC | -2.46 | 1.35 | 1.39 |
| 2 | E | 500 | HEM | C3B-C2B | 2.46 | 1.42 | 1.37 |
| 3 | D | 501 | 1CI | C5-N1 | -2.46 | 1.33 | 1.38 |
| 3 | C | 501 | 1CI | C5-N1 | -2.46 | 1.33 | 1.38 |
| 2 | A | 500 | HEM | CBC-CAC | 2.45 | 1.42 | 1.30 |
| 3 | F | 501 | 1CI | C5-N1 | -2.44 | 1.33 | 1.38 |
| 2 | G | 500 | HEM | CBC-CAC | 2.44 | 1.42 | 1.30 |
| 2 | E | 500 | HEM | C3C-C4C | -2.43 | 1.41 | 1.46 |
| 3 | E | 501 | 1CI | C5-N1 | -2.43 | 1.33 | 1.38 |
| 2 | F | 500 | HEM | CBC-CAC | 2.41 | 1.42 | 1.30 |
| 2 | G | 500 | HEM | CAD-C3D | 2.40 | 1.57 | 1.51 |
| 2 | G | 500 | HEM | C4D-C3D | -2.38 | 1.41 | 1.45 |
| 2 | F | 500 | HEM | C3B-C2B | 2.36 | 1.42 | 1.37 |
| 2 | D | 500 | HEM | CBC-CAC | 2.35 | 1.41 | 1.30 |
| 2 | B | 500 | HEM | C3C-C4C | -2.33 | 1.42 | 1.46 |
| 2 | G | 500 | HEM | O2A-CGA | -2.30 | 1.23 | 1.30 |
| 2 | A | 500 | HEM | C3B-C2B | 2.29 | 1.41 | 1.37 |
| 2 | C | 500 | HEM | C3C-C4C | -2.29 | 1.42 | 1.46 |
| 2 | D | 500 | HEM | C4D-C3D | -2.28 | 1.41 | 1.45 |
| 2 | C | 500 | HEM | CBD-CGD | 2.25 | 1.55 | 1.50 |
| 2 | D | 500 | HEM | CAD-C3D | 2.24 | 1.57 | 1.51 |
| 2 | C | 500 | HEM | CAD-C3D | 2.23 | 1.57 | 1.51 |
| 2 | E | 500 | HEM | C4D-C3D | -2.23 | 1.41 | 1.45 |
| 2 | F | 500 | HEM | CBD-CGD | 2.20 | 1.55 | 1.50 |
| 2 | A | 500 | HEM | C3C-C4C | -2.18 | 1.42 | 1.46 |
| 2 | B | 500 | HEM | CBD-CGD | 2.18 | 1.55 | 1.50 |
| 2 | B | 500 | HEM | C4D-C3D | -2.16 | 1.41 | 1.45 |
| 2 | A | 500 | HEM | C4D-C3D | -2.15 | 1.41 | 1.45 |
| 2 | C | 500 | HEM | CMD-C2D | 2.10 | 1.55 | 1.50 |
| 2 | G | 500 | HEM | CBD-CGD | 2.10 | 1.55 | 1.50 |
| 2 | G | 500 | HEM | O2D-CGD | -2.09 | 1.23 | 1.30 |
| 2 | E | 500 | HEM | C1D-C2D | -2.06 | 1.40 | 1.44 |
| 2 | C | 500 | HEM | C3C-C2C | 2.06 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 500 | HEM | CAB-C3B | -2.06 | 1.41 | 1.47 |
| 2 | A | 500 | HEM | C1D-C2D | -2.04 | 1.40 | 1.44 |
| 2 | A | 500 | HEM | CAB-C3B | -2.04 | 1.41 | 1.47 |
| 2 | F | 500 | HEM | C3C-C4C | -2.04 | 1.42 | 1.46 |
| 2 | A | 500 | HEM | C3C-C2C | 2.03 | 1.41 | 1.37 |

All (87) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 500 | HEM | CHD-C4C-NC | -4.58 | 119.47 | 124.45 |
| 2 | F | 500 | HEM | CHD-C4C-NC | -3.95 | 120.15 | 124.45 |
| 2 | G | 500 | HEM | CHD-C4C-NC | -3.82 | 120.29 | 124.45 |
| 2 | G | 500 | HEM | CHB-C1B-NB | -3.78 | 119.69 | 124.37 |
| 2 | B | 500 | HEM | CHD-C4C-NC | -3.56 | 120.57 | 124.45 |
| 2 | D | 500 | HEM | CHD-C4C-NC | -3.53 | 120.61 | 124.45 |
| 2 | E | 500 | HEM | CHD-C4C-NC | -3.43 | 120.72 | 124.45 |
| 2 | A | 500 | HEM | CHD-C4C-NC | -3.35 | 120.81 | 124.45 |
| 2 | E | 500 | HEM | CHB-C1B-NB | -3.07 | 120.57 | 124.37 |
| 2 | B | 500 | HEM | C1B-NB-C4B | 3.03 | 108.79 | 105.21 |
| 2 | F | 500 | HEM | CHB-C1B-NB | -2.98 | 120.68 | 124.37 |
| 2 | C | 500 | HEM | C1C-CHC-C4B | 2.93 | 132.24 | 126.02 |
| 2 | G | 500 | HEM | C1B-NB-C4B | 2.85 | 108.58 | 105.21 |
| 2 | E | 500 | HEM | C1B-NB-C4B | 2.82 | 108.54 | 105.21 |
| 2 | A | 500 | HEM | CHB-C1B-NB | -2.79 | 120.92 | 124.37 |
| 2 | D | 500 | HEM | C4B-C3B-C2B | -2.73 | 104.77 | 107.28 |
| 2 | G | 500 | HEM | C4C-C3C-C2C | -2.71 | 104.47 | 106.81 |
| 2 | F | 500 | HEM | C1B-NB-C4B | 2.71 | 108.41 | 105.21 |
| 2 | D | 500 | HEM | CHB-C1B-NB | -2.71 | 121.02 | 124.37 |
| 2 | B | 500 | HEM | C4B-C3B-C2B | -2.70 | 104.80 | 107.28 |
| 2 | A | 500 | HEM | C3B-C2B-C1B | -2.70 | 104.39 | 106.41 |
| 2 | B | 500 | HEM | C4C-C3C-C2C | -2.69 | 104.48 | 106.81 |
| 2 | A | 500 | HEM | C3B-C4B-NB | 2.67 | 111.39 | 109.47 |
| 2 | E | 500 | HEM | C4D-ND-C1D | 2.67 | 108.36 | 105.21 |
| 2 | B | 500 | HEM | CHC-C4B-NB | -2.63 | 121.59 | 124.42 |
| 2 | G | 500 | HEM | CAD-CBD-CGD | 2.62 | 120.60 | 113.67 |
| 2 | E | 500 | HEM | C1C-CHC-C4B | 2.61 | 131.57 | 126.02 |
| 2 | A | 500 | HEM | C4C-C3C-C2C | -2.61 | 104.56 | 106.81 |
| 2 | E | 500 | HEM | C4B-C3B-C2B | -2.60 | 104.89 | 107.28 |
| 2 | D | 500 | HEM | C4D-ND-C1D | 2.60 | 108.28 | 105.21 |
| 2 | G | 500 | HEM | C4B-C3B-C2B | -2.59 | 104.90 | 107.28 |
| 2 | F | 500 | HEM | C1C-CHC-C4B | 2.57 | 131.48 | 126.02 |
| 2 | A | 500 | HEM | C4B-C3B-C2B | -2.56 | 104.92 | 107.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | F | 500 | HEM | C4B-C3B-C2B | -2.56 | 104.92 | 107.28 |
| 2 | D | 500 | HEM | C1C-CHC-C4B | 2.56 | 131.46 | 126.02 |
| 2 | B | 500 | HEM | C1C-CHC-C4B | 2.52 | 131.38 | 126.02 |
| 2 | B | 500 | HEM | C4D-ND-C1D | 2.52 | 108.19 | 105.21 |
| 2 | C | 500 | HEM | C1B-NB-C4B | 2.51 | 108.18 | 105.21 |
| 2 | E | 500 | HEM | C4C-C3C-C2C | -2.49 | 104.66 | 106.81 |
| 2 | D | 500 | HEM | C3B-C4B-NB | 2.48 | 111.25 | 109.47 |
| 2 | D | 500 | HEM | C3B-C2B-C1B | -2.48 | 104.55 | 106.41 |
| 2 | A | 500 | HEM | C1C-CHC-C4B | 2.46 | 131.26 | 126.02 |
| 2 | C | 500 | HEM | C3B-C2B-C1B | -2.45 | 104.57 | 106.41 |
| 2 | B | 500 | HEM | C4A-CHB-C1B | 2.45 | 132.01 | 126.25 |
| 2 | A | 500 | HEM | C4D-ND-C1D | 2.42 | 108.07 | 105.21 |
| 2 | G | 500 | HEM | C4D-ND-C1D | 2.42 | 108.07 | 105.21 |
| 2 | C | 500 | HEM | C4C-C3C-C2C | -2.42 | 104.72 | 106.81 |
| 2 | G | 500 | HEM | CHD-C4C-C3C | 2.41 | 129.26 | 125.21 |
| 2 | F | 500 | HEM | C3B-C4B-NB | 2.40 | 111.19 | 109.47 |
| 2 | A | 500 | HEM | C1B-NB-C4B | 2.40 | 108.05 | 105.21 |
| 2 | C | 500 | HEM | CHB-C1B-NB | -2.40 | 121.40 | 124.37 |
| 2 | C | 500 | HEM | C4D-ND-C1D | 2.39 | 108.04 | 105.21 |
| 2 | B | 500 | HEM | CHB-C1B-NB | -2.37 | 121.44 | 124.37 |
| 2 | D | 500 | HEM | C4C-C3C-C2C | -2.37 | 104.76 | 106.81 |
| 2 | F | 500 | HEM | C3B-C2B-C1B | -2.36 | 104.64 | 106.41 |
| 2 | B | 500 | HEM | C3B-C2B-C1B | -2.36 | 104.64 | 106.41 |
| 2 | E | 500 | HEM | CAD-CBD-CGD | 2.35 | 119.91 | 113.67 |
| 2 | C | 500 | HEM | C4B-C3B-C2B | -2.34 | 105.13 | 107.28 |
| 2 | B | 500 | HEM | CHD-C4C-C3C | 2.34 | 129.16 | 125.21 |
| 2 | F | 500 | HEM | C4C-CHD-C1D | 2.34 | 130.99 | 126.02 |
| 2 | D | 500 | HEM | C1B-NB-C4B | 2.30 | 107.93 | 105.21 |
| 2 | F | 500 | HEM | CHC-C1C-NC | -2.30 | 121.95 | 124.45 |
| 2 | G | 500 | HEM | C3B-C4B-NB | 2.28 | 111.10 | 109.47 |
| 2 | G | 500 | HEM | C1C-CHC-C4B | 2.27 | 130.83 | 126.02 |
| 2 | F | 500 | HEM | C4A-CHB-C1B | 2.26 | 131.57 | 126.25 |
| 2 | G | 500 | HEM | O2A-CGA-CBA | 2.26 | 121.14 | 114.00 |
| 2 | G | 500 | HEM | CHC-C4B-NB | -2.23 | 122.02 | 124.42 |
| 2 | A | 500 | HEM | CAD-C3D-C4D | 2.23 | 128.58 | 124.70 |
| 2 | E | 500 | HEM | CHD-C4C-C3C | 2.22 | 128.96 | 125.21 |
| 2 | B | 500 | HEM | CAD-CBD-CGD | 2.22 | 119.55 | 113.67 |
| 2 | E | 500 | HEM | O2A-CGA-CBA | 2.21 | 120.99 | 114.00 |
| 2 | A | 500 | HEM | CHC-C1C-NC | -2.21 | 122.05 | 124.45 |
| 2 | G | 500 | HEM | CHC-C1C-NC | -2.20 | 122.06 | 124.45 |
| 2 | F | 500 | HEM | O2A-CGA-CBA | 2.18 | 120.89 | 114.00 |
| 2 | D | 500 | HEM | CHD-C4C-C3C | 2.17 | 128.86 | 125.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | E | 500 | HEM | C4A-CHB-C1B | 2.17 | 131.34 | 126.25 |
| 2 | G | 500 | HEM | C3B-C2B-C1B | -2.15 | 104.79 | 106.41 |
| 2 | F | 500 | HEM | C4D-ND-C1D | 2.14 | 107.75 | 105.21 |
| 2 | C | 500 | HEM | C4A-CHB-C1B | 2.14 | 131.28 | 126.25 |
| 2 | D | 500 | HEM | O2A-CGA-CBA | 2.13 | 120.74 | 114.00 |
| 2 | F | 500 | HEM | C4C-C3C-C2C | -2.13 | 104.97 | 106.81 |
| 2 | C | 500 | HEM | O2A-CGA-CBA | 2.12 | 120.69 | 114.00 |
| 2 | E | 500 | HEM | C3B-C2B-C1B | -2.11 | 104.83 | 106.41 |
| 2 | B | 500 | HEM | O2A-CGA-CBA | 2.08 | 120.57 | 114.00 |
| 2 | E | 500 | HEM | C4D-C3D-C2D | -2.07 | 103.89 | 106.89 |
| 2 | C | 500 | HEM | C3B-C4B-NB | 2.06 | 110.94 | 109.47 |
| 2 | B | 500 | HEM | C3B-C4B-NB | 2.04 | 110.93 | 109.47 |

There are no chirality outliers.

All (45) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 500 | HEM | C2C-C3C-CAC-CBC |
| 2 | C | 500 | HEM | C2C-C3C-CAC-CBC |
| 2 | C | 500 | HEM | C4C-C3C-CAC-CBC |
| 2 | D | 500 | HEM | C2C-C3C-CAC-CBC |
| 2 | E | 500 | HEM | C2B-C3B-CAB-CBB |
| 2 | E | 500 | HEM | C4B-C3B-CAB-CBB |
| 2 | F | 500 | HEM | C2C-C3C-CAC-CBC |
| 2 | F | 500 | HEM | C4C-C3C-CAC-CBC |
| 2 | B | 500 | HEM | C2C-C3C-CAC-CBC |
| 2 | A | 500 | HEM | C4C-C3C-CAC-CBC |
| 2 | B | 500 | HEM | C4C-C3C-CAC-CBC |
| 2 | D | 500 | HEM | C4C-C3C-CAC-CBC |
| 2 | E | 500 | HEM | C2C-C3C-CAC-CBC |
| 2 | F | 500 | HEM | C2B-C3B-CAB-CBB |
| 2 | G | 500 | HEM | C2C-C3C-CAC-CBC |
| 2 | E | 500 | HEM | C4C-C3C-CAC-CBC |
| 2 | G | 500 | HEM | C4C-C3C-CAC-CBC |
| 2 | A | 500 | HEM | CAA-CBA-CGA-O2A |
| 2 | C | 500 | HEM | CAA-CBA-CGA-O1A |
| 2 | D | 500 | HEM | CAA-CBA-CGA-O1A |
| 2 | D | 500 | HEM | CAA-CBA-CGA-O2A |
| 2 | G | 500 | HEM | CAA-CBA-CGA-O1A |
| 2 | C | 500 | HEM | CAA-CBA-CGA-O2A |
| 2 | E | 500 | HEM | CAA-CBA-CGA-O1A |
| 2 | E | 500 | HEM | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 500 | HEM | CAA-CBA-CGA-O1A |
| 2 | G | 500 | HEM | CAA-CBA-CGA-O2A |
| 2 | E | 500 | HEM | CAD-CBD-CGD-O2D |
| 2 | F | 500 | HEM | CAA-CBA-CGA-O1A |
| 2 | F | 500 | HEM | CAA-CBA-CGA-O2A |
| 2 | B | 500 | HEM | CAD-CBD-CGD-O2D |
| 2 | E | 500 | HEM | CAD-CBD-CGD-O1D |
| 2 | C | 500 | HEM | C4B-C3B-CAB-CBB |
| 2 | F | 500 | HEM | C4B-C3B-CAB-CBB |
| 2 | G | 500 | HEM | C4B-C3B-CAB-CBB |
| 2 | B | 500 | HEM | CAA-CBA-CGA-O2A |
| 2 | B | 500 | HEM | CAD-CBD-CGD-O1D |
| 2 | B | 500 | HEM | CAA-CBA-CGA-O1A |
| 2 | F | 500 | HEM | CAD-CBD-CGD-O1D |
| 2 | F | 500 | HEM | CAD-CBD-CGD-O2D |
| 2 | G | 500 | HEM | CAD-CBD-CGD-O2D |
| 2 | A | 500 | HEM | CAD-CBD-CGD-O2D |
| 2 | C | 500 | HEM | C2B-C3B-CAB-CBB |
| 2 | G | 500 | HEM | C2B-C3B-CAB-CBB |
| 2 | G | 500 | HEM | CAD-CBD-CGD-O1D |

There are no ring outliers.

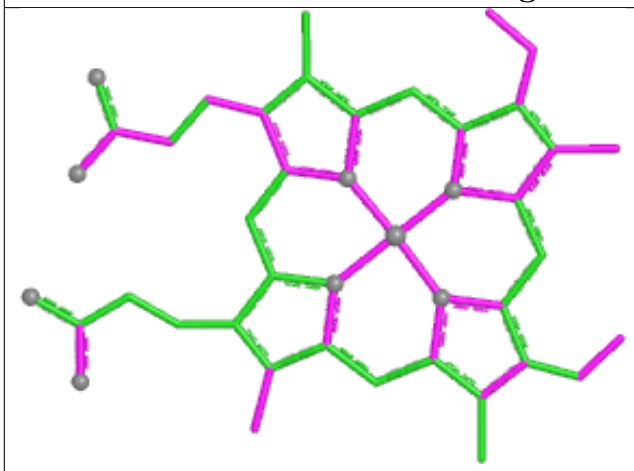
14 monomers are involved in 48 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | G | 500 | HEM | 4 | 0 |
| 2 | F | 500 | HEM | 7 | 0 |
| 3 | C | 501 | 1CI | 3 | 0 |
| 3 | G | 501 | 1CI | 4 | 0 |
| 2 | C | 500 | HEM | 4 | 0 |
| 2 | A | 500 | HEM | 2 | 0 |
| 3 | F | 501 | 1CI | 3 | 0 |
| 3 | B | 501 | 1CI | 3 | 0 |
| 2 | D | 500 | HEM | 6 | 0 |
| 3 | E | 501 | 1CI | 1 | 0 |
| 3 | A | 501 | 1CI | 1 | 0 |
| 2 | E | 500 | HEM | 8 | 0 |
| 3 | D | 501 | 1CI | 2 | 0 |
| 2 | B | 500 | HEM | 3 | 0 |

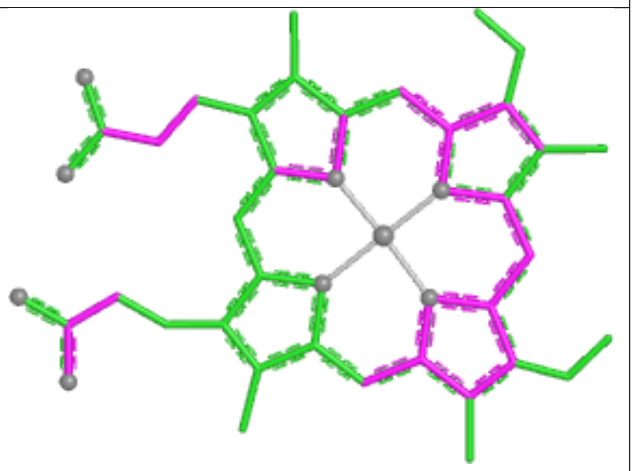
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

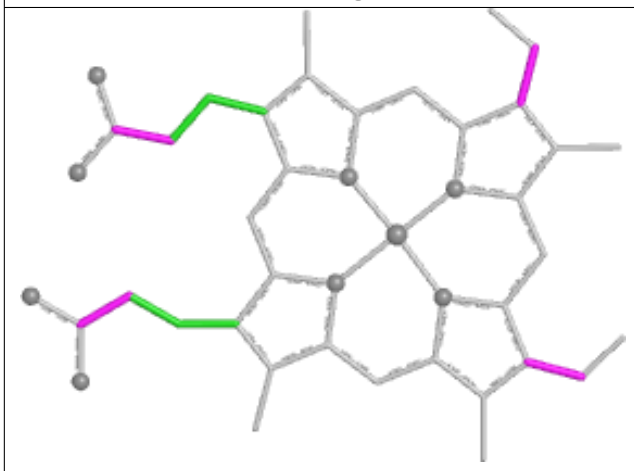
**Ligand HEM G 500**



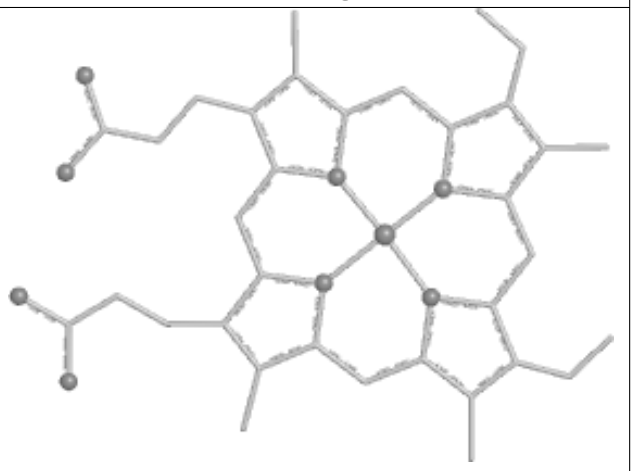
**Bond lengths**



**Bond angles**

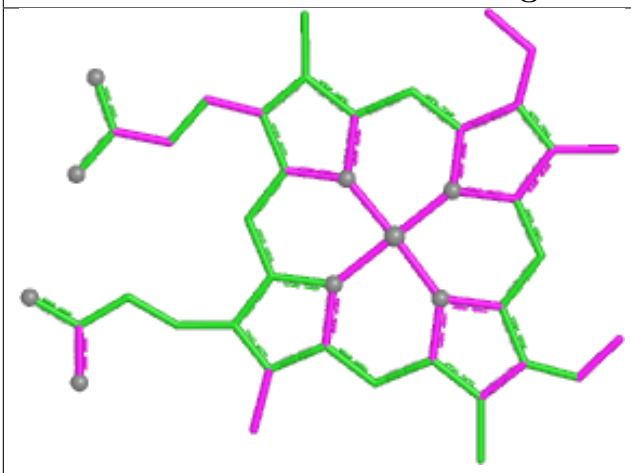


**Torsions**

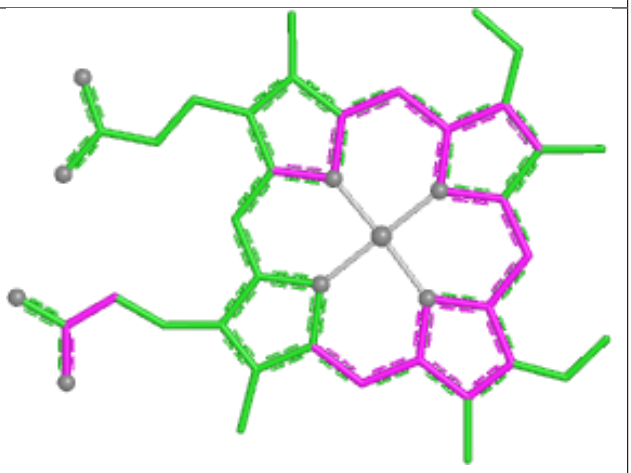


**Rings**

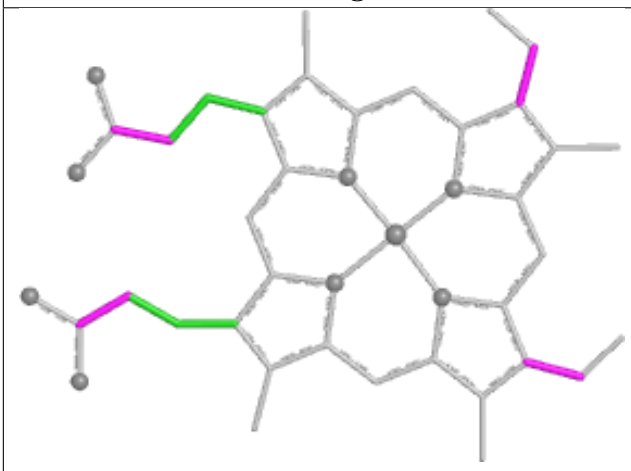
**Ligand HEM F 500**



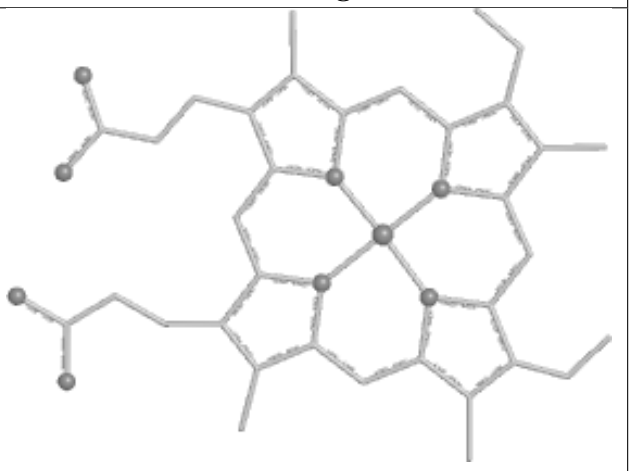
**Bond lengths**



**Bond angles**

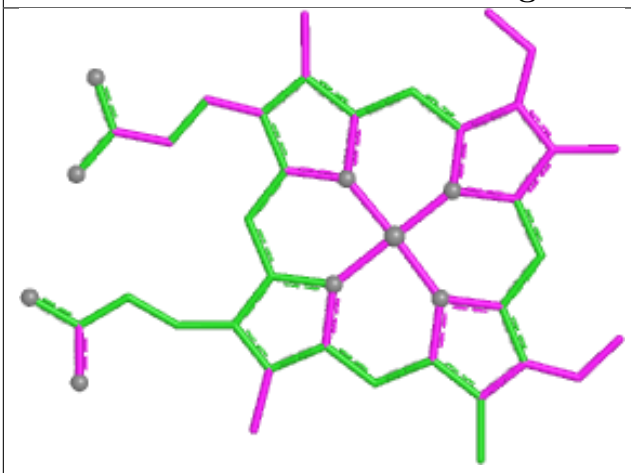


**Torsions**

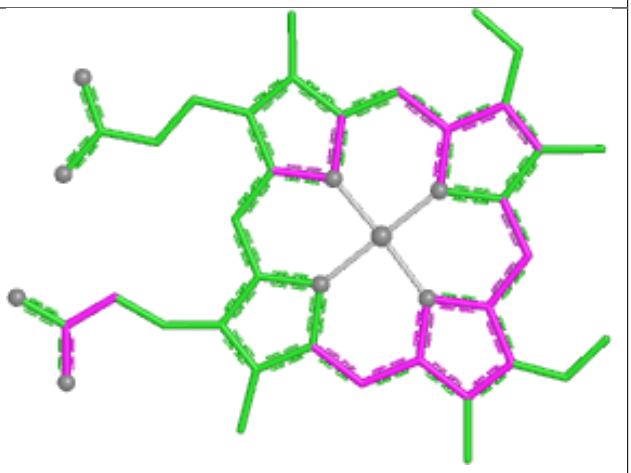


**Rings**

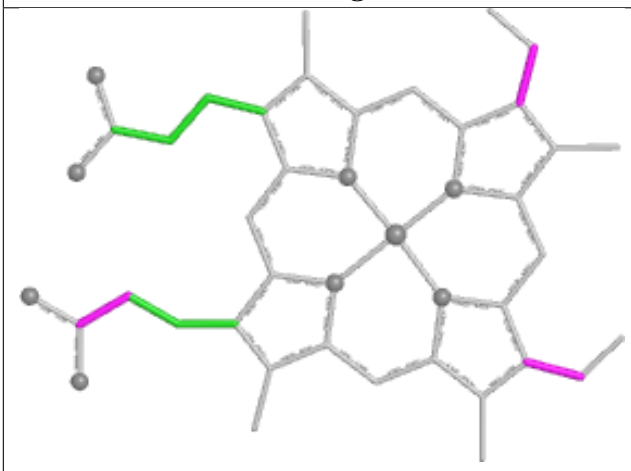
**Ligand HEM C 500**



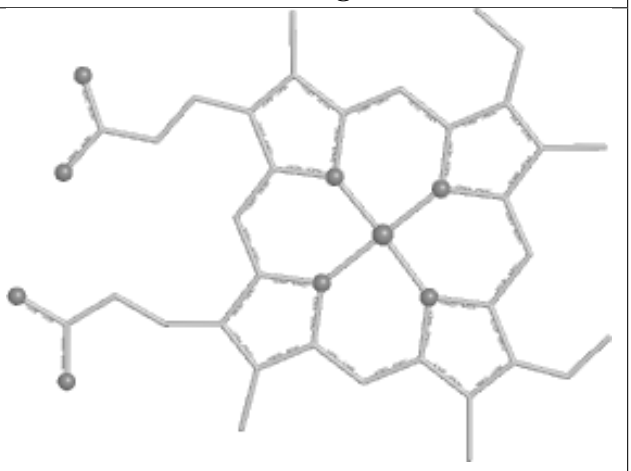
**Bond lengths**



**Bond angles**

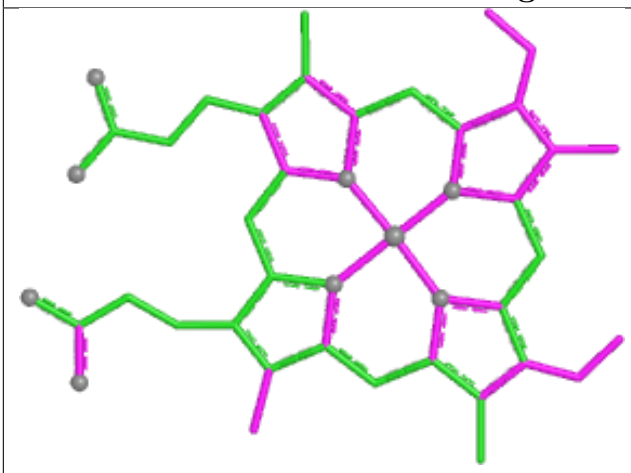


**Torsions**

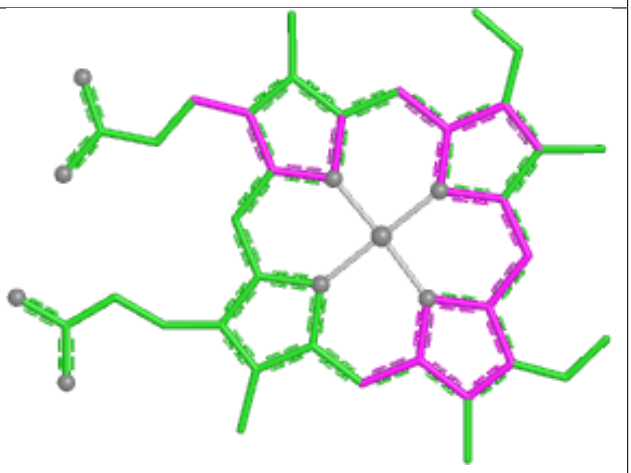


**Rings**

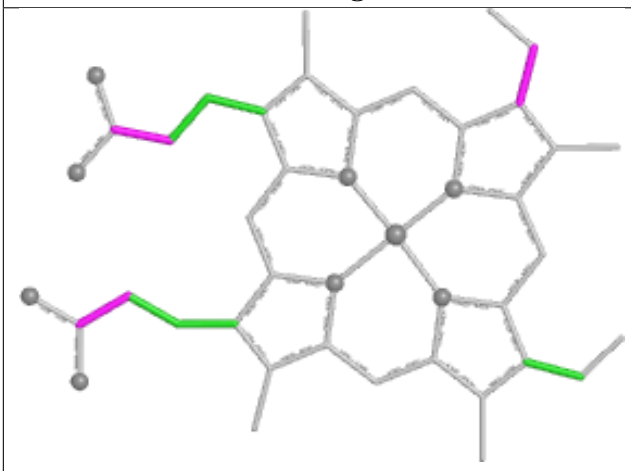
**Ligand HEM A 500**



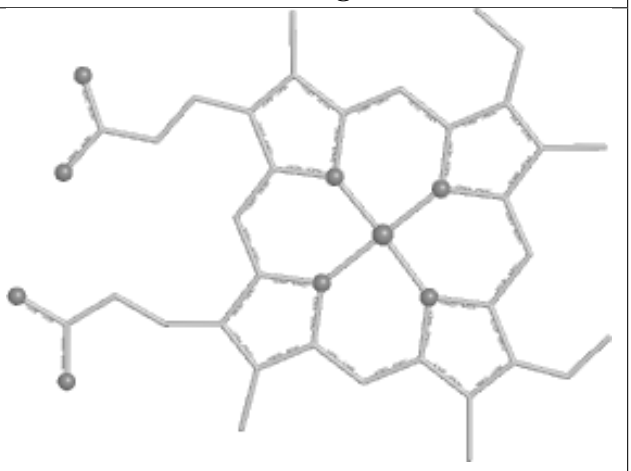
**Bond lengths**



**Bond angles**

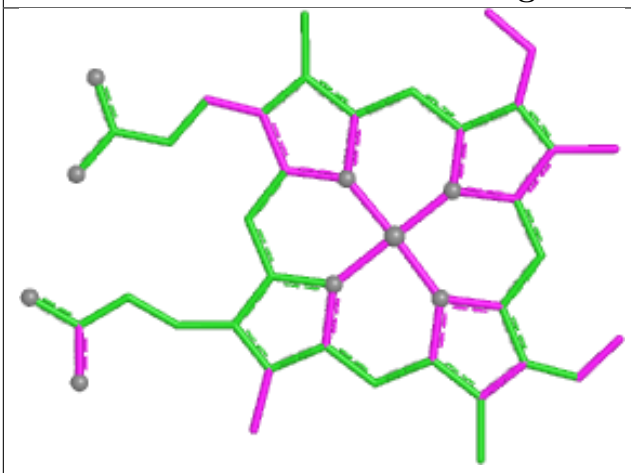


**Torsions**

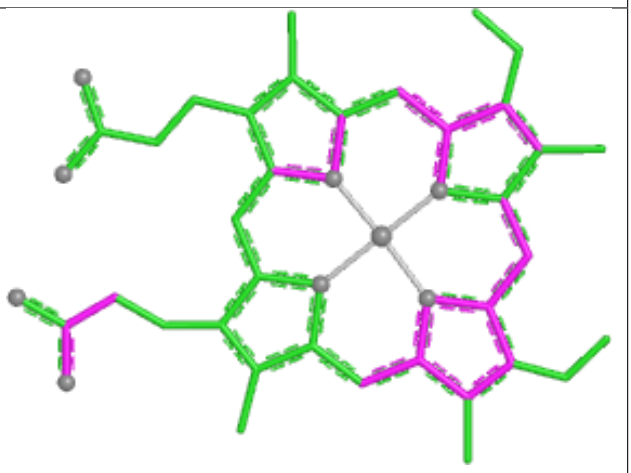


**Rings**

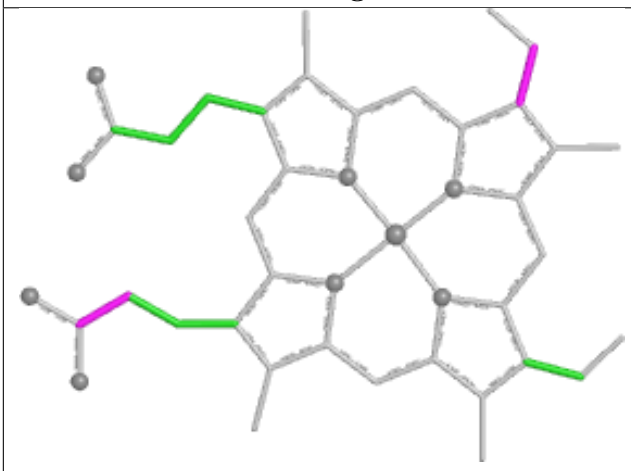
**Ligand HEM D 500**



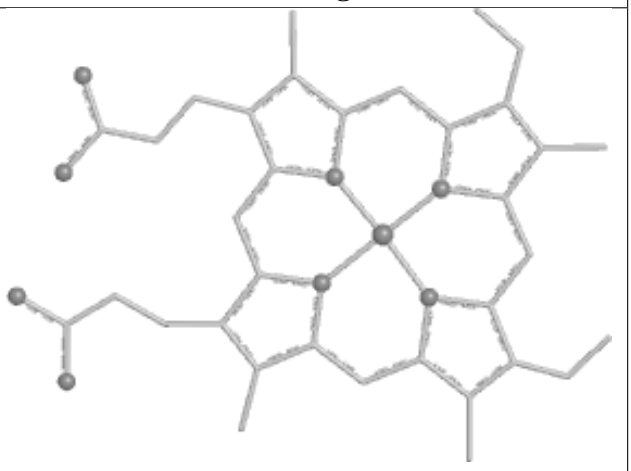
**Bond lengths**



**Bond angles**

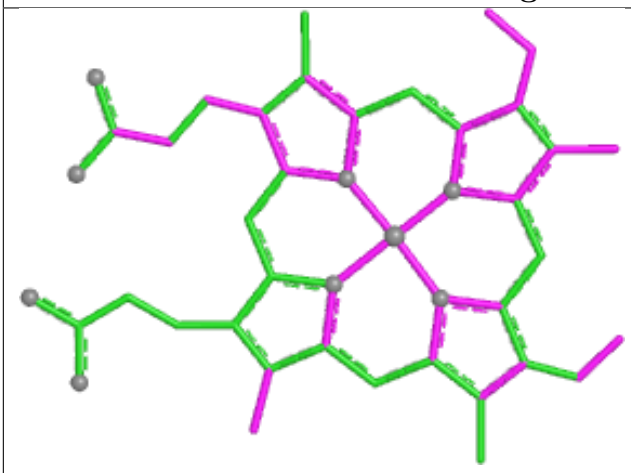


**Torsions**

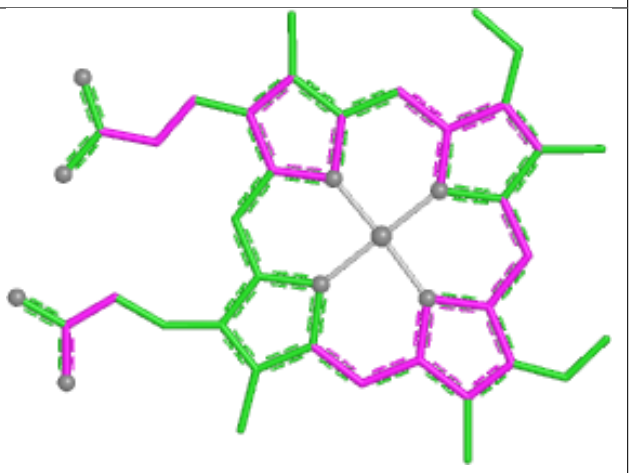


**Rings**

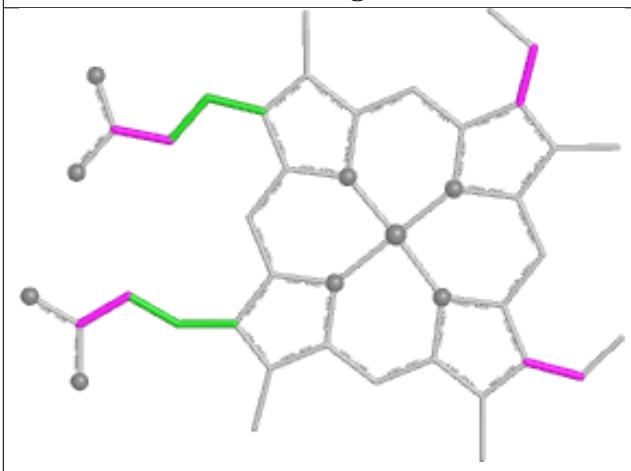
**Ligand HEM E 500**



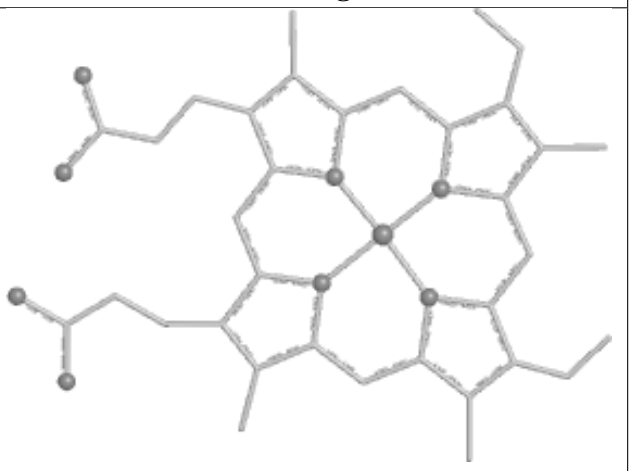
**Bond lengths**



**Bond angles**

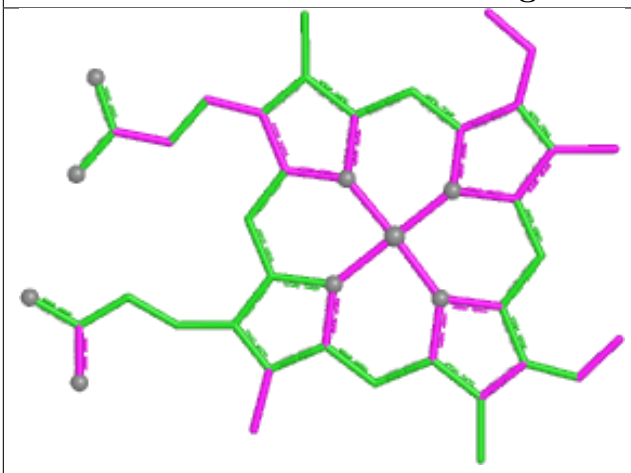


**Torsions**

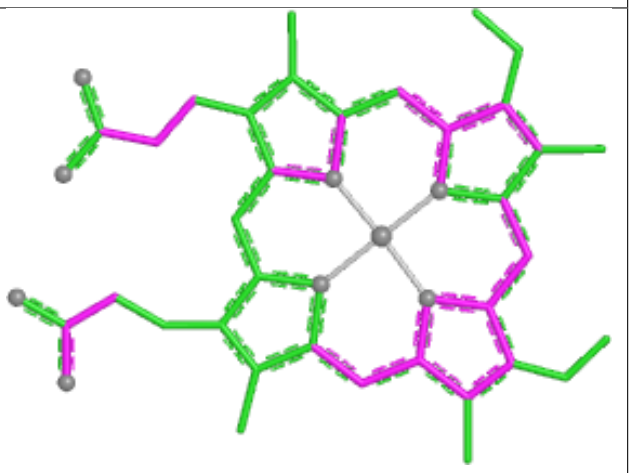


**Rings**

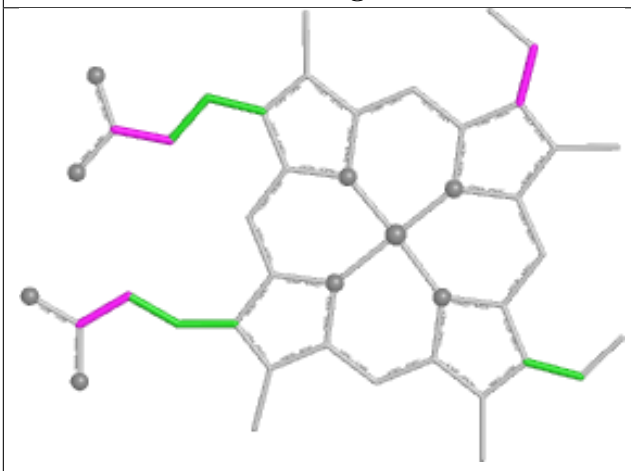
**Ligand HEM B 500**



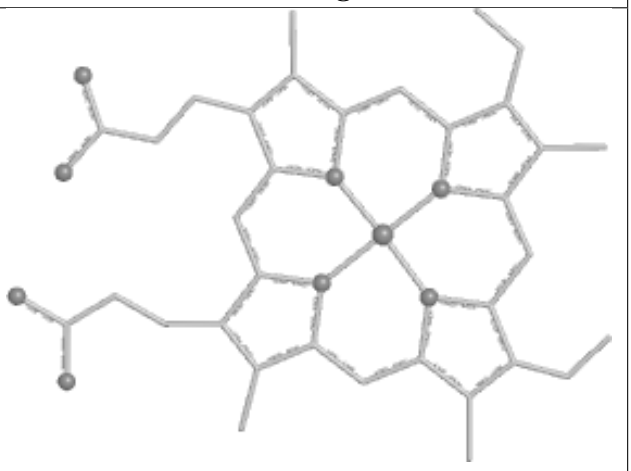
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 | 465/478 (97%) | -0.10 | 2 (0%) | 88 | 79 | 48, 86, 120, 169 | 0 |
| 1 | B | 465/478 (97%) | -0.02 | 4 (0%) | 81 | 64 | 70, 103, 144, 202 | 0 |
| 1 | C | 465/478 (97%) | -0.06 | 3 (0%) | 85 | 73 | 64, 112, 156, 186 | 0 |
| 1 | D | 465/478 (97%) | -0.06 | 4 (0%) | 81 | 64 | 64, 100, 144, 202 | 0 |
| 1 | E | 465/478 (97%) | 0.06 | 3 (0%) | 85 | 73 | 62, 115, 158, 202 | 0 |
| 1 | F | 465/478 (97%) | 0.05 | 4 (0%) | 81 | 64 | 70, 119, 165, 197 | 0 |
| 1 | G | 465/478 (97%) | 0.05 | 8 (1%) | 69 | 49 | 63, 119, 173, 202 | 0 |
| All | All | 3255/3346 (97%) | -0.01 | 28 (0%) | 81 | 64 | 48, 108, 160, 202 | 0 |

All (28) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 393 | SER | 3.4 |
| 1 | C | 67 | THR | 3.3 |
| 1 | G | 299 | GLY | 3.1 |
| 1 | B | 301 | GLU | 3.1 |
| 1 | E | 362 | LEU | 3.0 |
| 1 | F | 95 | PHE | 2.9 |
| 1 | G | 178 | ILE | 2.8 |
| 1 | D | 305 | THR | 2.7 |
| 1 | E | 462 | PRO | 2.7 |
| 1 | G | 104 | VAL | 2.6 |
| 1 | E | 284 | HIS | 2.5 |
| 1 | G | 56 | LEU | 2.5 |
| 1 | F | 492 | HIS | 2.5 |
| 1 | D | 270 | LEU | 2.4 |
| 1 | B | 181 | SER | 2.4 |
| 1 | G | 355 | GLU | 2.4 |
| 1 | C | 113 | VAL | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 299 | GLY | 2.3 |
| 1 | D | 303 | THR | 2.3 |
| 1 | D | 200 | ASP | 2.2 |
| 1 | F | 436 | CYS | 2.2 |
| 1 | B | 459 | ILE | 2.2 |
| 1 | B | 310 | GLY | 2.2 |
| 1 | G | 185 | GLY | 2.1 |
| 1 | G | 177 | ASN | 2.1 |
| 1 | F | 121 | TRP | 2.1 |
| 1 | C | 174 | ILE | 2.0 |
| 1 | G | 179 | ILE | 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)

There are no oligosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | 1CI | E | 501 | 12/12 | 0.62 | 0.20 | 107,107,107,107 | 0 |
| 3 | 1CI | G | 501 | 12/12 | 0.66 | 0.17 | 107,107,107,107 | 0 |
| 3 | 1CI | A | 501 | 12/12 | 0.75 | 0.17 | 107,107,107,107 | 0 |
| 3 | 1CI | B | 501 | 12/12 | 0.75 | 0.19 | 107,107,107,107 | 0 |
| 3 | 1CI | F | 501 | 12/12 | 0.77 | 0.16 | 107,107,107,107 | 0 |
| 3 | 1CI | D | 501 | 12/12 | 0.81 | 0.15 | 107,107,107,107 | 0 |
| 3 | 1CI | C | 501 | 12/12 | 0.82 | 0.14 | 107,107,107,107 | 0 |
| 2 | HEM | G | 500 | 43/43 | 0.91 | 0.12 | 109,109,109,109 | 0 |
| 2 | HEM | F | 500 | 43/43 | 0.92 | 0.14 | 111,111,111,111 | 0 |
| 2 | HEM | E | 500 | 43/43 | 0.93 | 0.11 | 69,69,69,69 | 0 |
| 2 | HEM | B | 500 | 43/43 | 0.93 | 0.12 | 78,78,78,78 | 0 |
| 2 | HEM | C | 500 | 43/43 | 0.94 | 0.10 | 93,93,93,93 | 0 |

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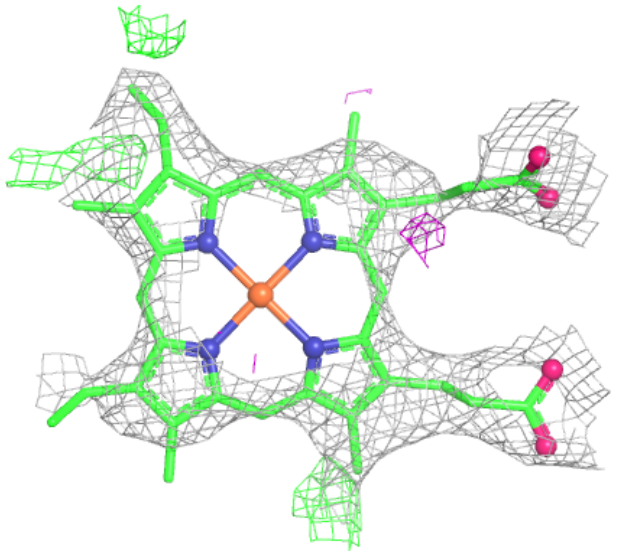
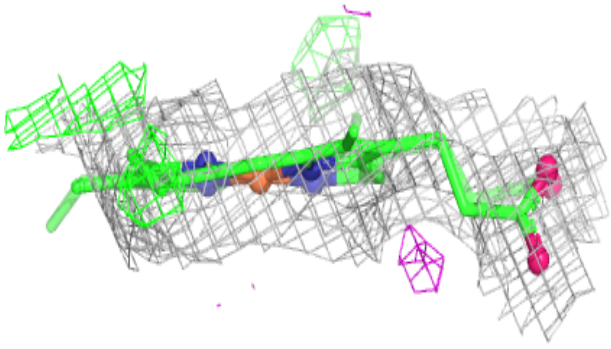
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | HEM | D | 500 | 43/43 | 0.94 | 0.12 | 102,102,102,102 | 0 |
| 2 | HEM | A | 500 | 43/43 | 0.95 | 0.10 | 78,78,78,78 | 0 |

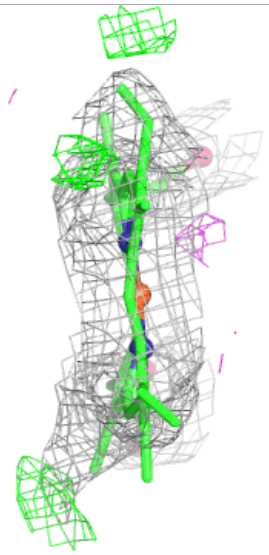
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around HEM G 500:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

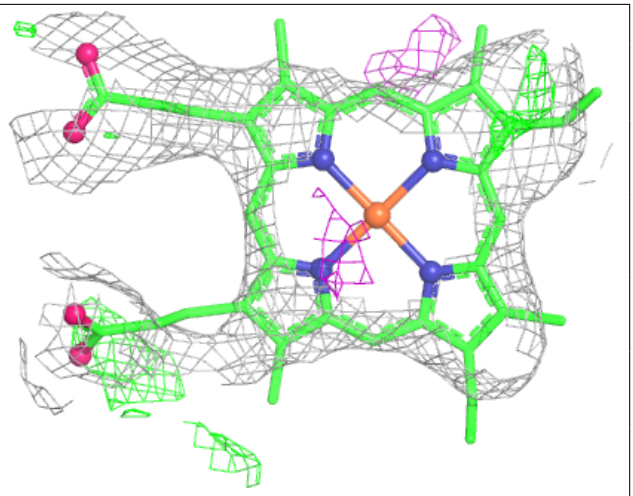


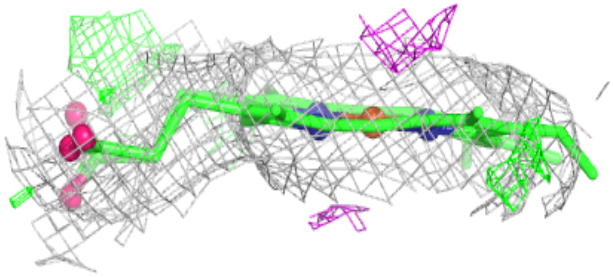


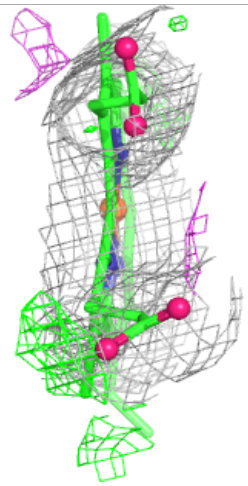


**Electron density around HEM F 500:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

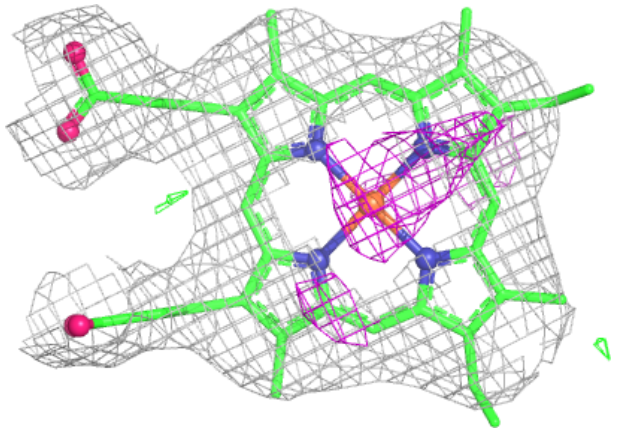


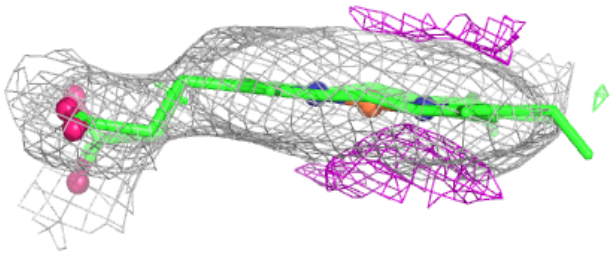


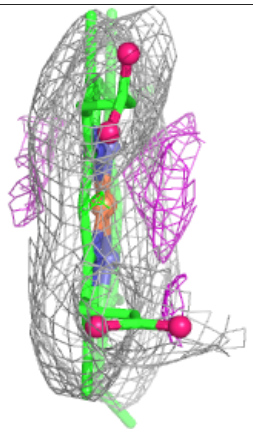


**Electron density around HEM E 500:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

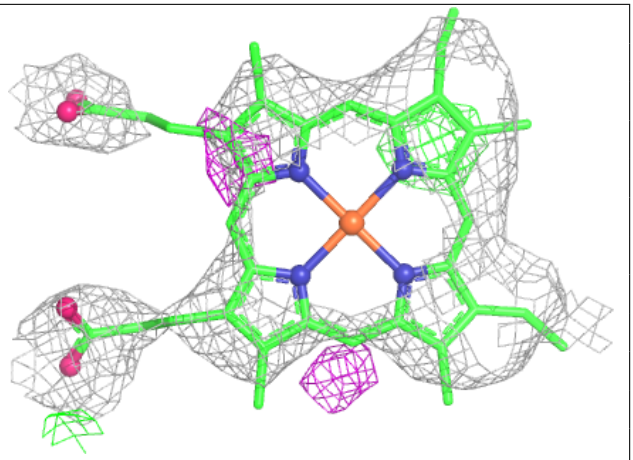


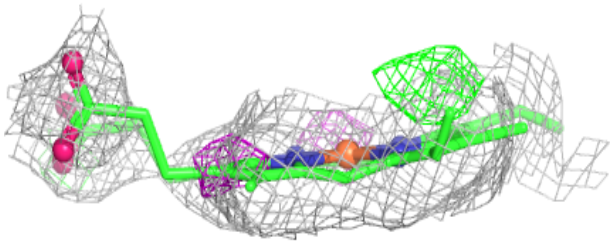


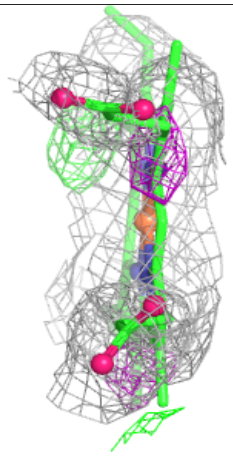


**Electron density around HEM B 500:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

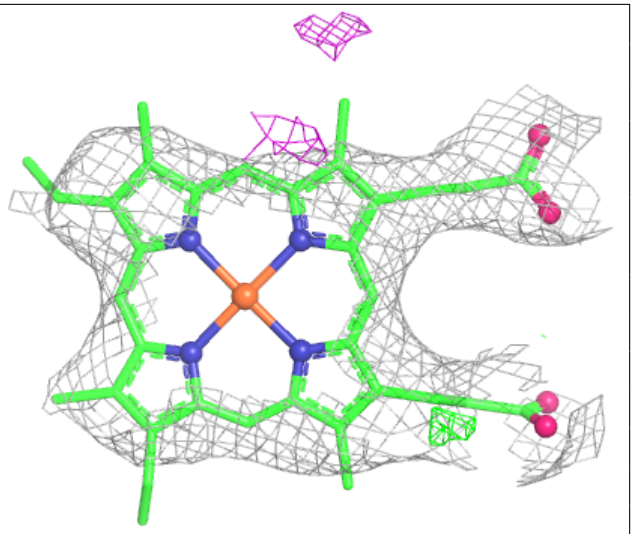


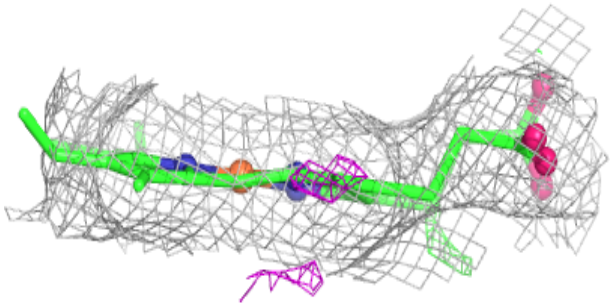


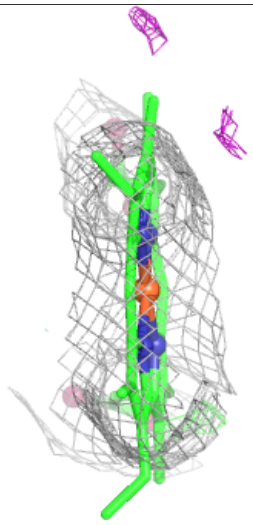


**Electron density around HEM C 500:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

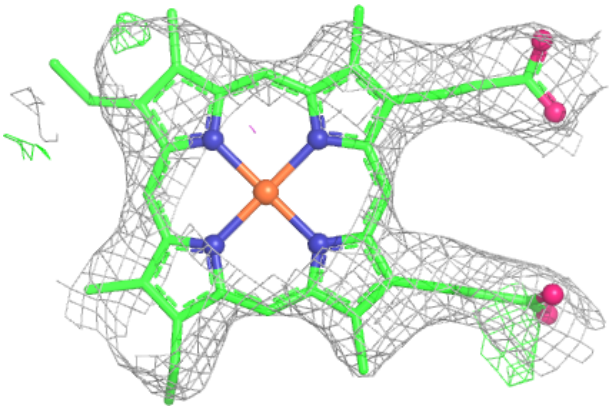


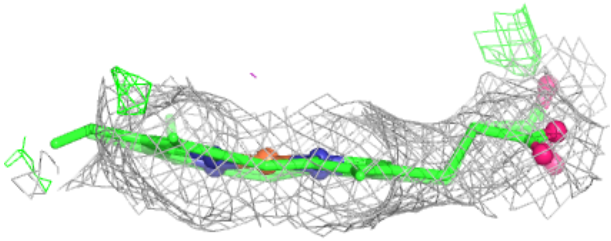


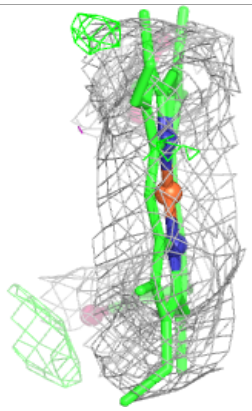


**Electron density around HEM D 500:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

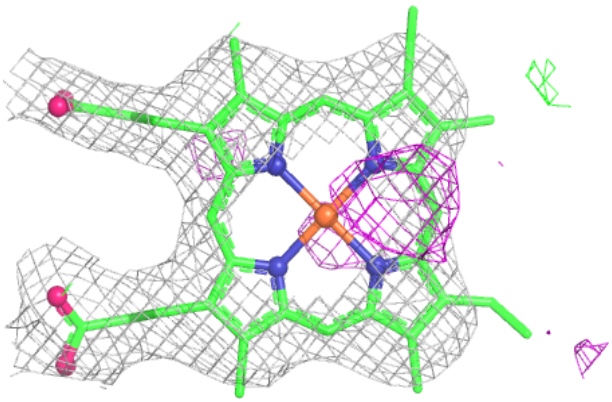


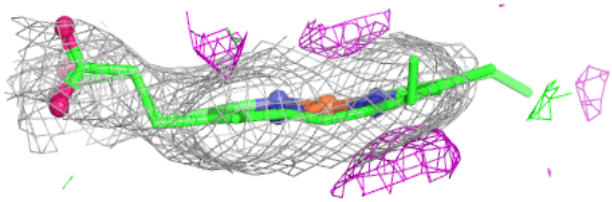


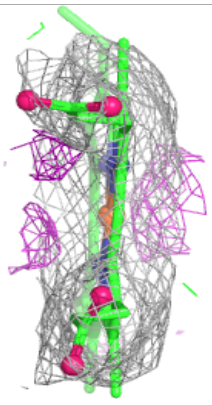


**Electron density around HEM A 500:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)







## 6.5 Other polymers (i)

There are no such residues in this entry.