



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

PDB ID : 3RYO
Title : Crystal Structure of Enhanced Intracellular Survival (Eis) Protein from Mycobacterium tuberculosis with Acetyl CoA
Authors : Kim, K.H.; An, D.R.; Yoon, J.Y.; Kim, H.S.; Yoon, H.J.; Song, J.; Im, H.N.; Kim, J.; Kim, D.J.; Lee, S.J.; Kim, H.J.; Lee, J.Y.; Suh, S.W.
Deposited on : 2011-05-11
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

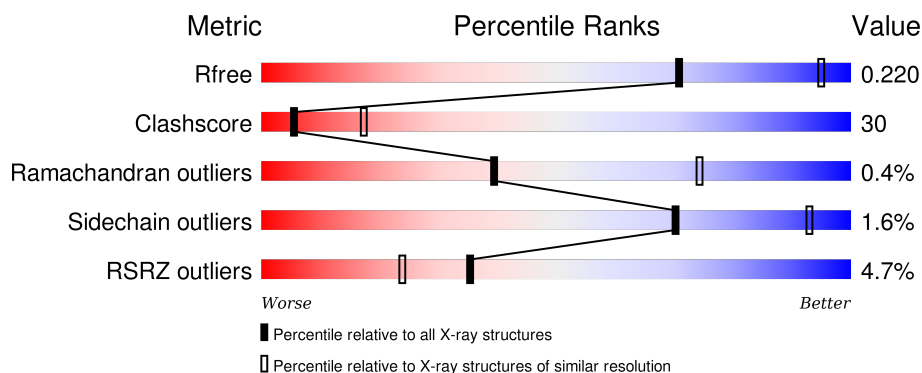
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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} | 91344 | 2393 (2.80-2.80) |
| Clashscore | 102246 | 2827 (2.80-2.80) |
| Ramachandran outliers | 100387 | 2782 (2.80-2.80) |
| Sidechain outliers | 100360 | 2784 (2.80-2.80) |
| RSRZ outliers | 91569 | 2404 (2.80-2.80) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 428 | <div> <div>3%</div> <div>60% 32% 7%</div> </div> |
| 1 | B | 428 | <div> <div>3%</div> <div>61% 32% 7%</div> </div> |
| 1 | C | 428 | <div> <div>5%</div> <div>60% 32% 7%</div> </div> |
| 1 | D | 428 | <div> <div>3%</div> <div>57% 35% 7%</div> </div> |
| 1 | E | 428 | <div> <div>4%</div> <div>57% 34% 7%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | F | 428 | |
| 1 | G | 428 | |
| 1 | H | 428 | |
| 1 | I | 428 | |
| 1 | J | 428 | |
| 1 | K | 428 | |
| 1 | L | 428 | |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37731 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 Enhanced intracellular survival protein.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1 | A | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | B | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | C | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | D | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | E | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | F | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | G | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | H | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | I | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | J | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | K | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |
| 1 | L | 396 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3053 | 1921 | 560 | 560 | 5 | 7 | | | |

There are 240 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -19 | MSE | - | EXPRESSION TAG | UNP P71727 |
| A | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| A | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| A | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| A | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| A | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
| A | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| A | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| A | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| A | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| A | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| A | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| A | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| A | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| A | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| A | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| A | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| A | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| A | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
| B | -19 | MSE | - | EXPRESSION TAG | UNP P71727 |
| B | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| B | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| B | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| B | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| B | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| B | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
| B | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| B | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| B | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| B | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| B | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| B | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| B | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| B | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| B | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| B | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| B | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| B | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| B | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| C | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| C | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| C | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| C | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| C | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| C | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| C | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| C | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| C | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| C | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| C | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| C | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| C | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| C | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| C | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| C | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| C | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| C | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
| D | -19 | MSE | - | EXPRESSION TAG | UNP P71727 |
| D | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| D | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| D | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| D | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| D | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| D | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
| D | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| D | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| D | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| D | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| D | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| D | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| D | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| D | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| D | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| D | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| D | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| D | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| D | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| E | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| E | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| E | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| E | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| E | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| E | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
| E | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| E | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| E | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| E | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| E | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| E | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| E | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| E | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| E | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| E | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| E | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| E | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| E | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| F | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| F | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| F | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
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| F | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| F | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| F | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| F | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| F | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| F | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| F | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| F | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| F | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| F | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| F | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| F | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| G | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| G | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| G | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| G | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| G | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| G | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
| G | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| G | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| G | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| G | -9 | SER | - | EXPRESSION TAG | UNP P71727 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
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| G | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
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| G | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| G | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| G | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| G | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| G | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| G | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
| H | -19 | MSE | - | EXPRESSION TAG | UNP P71727 |
| H | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| H | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| H | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| H | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| H | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| H | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
| H | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| H | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| H | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| H | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| H | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| H | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| H | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| H | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| H | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| H | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| H | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| H | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
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| I | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| I | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| I | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| I | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| I | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| I | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
| I | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| I | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| I | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| I | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |

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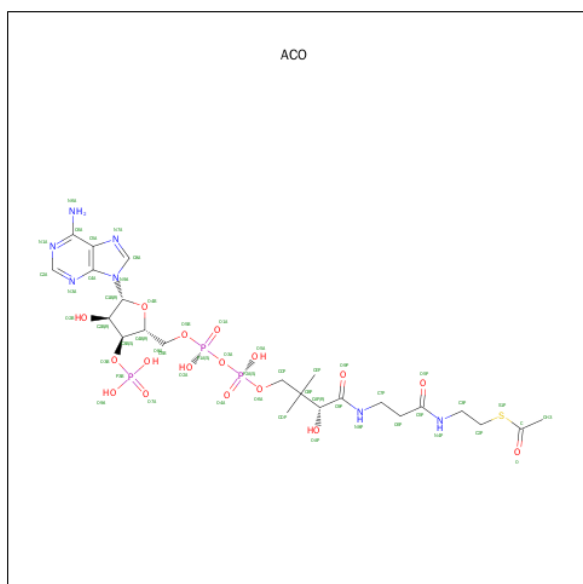
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
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| I | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| I | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| I | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| I | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
| J | -19 | MSE | - | EXPRESSION TAG | UNP P71727 |
| J | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| J | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| J | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| J | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| J | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| J | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| J | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| J | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| J | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| J | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| J | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| J | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| J | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| J | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| J | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| J | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| J | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| J | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
| K | -19 | MSE | - | EXPRESSION TAG | UNP P71727 |
| K | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| K | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| K | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| K | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| K | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
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| K | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| K | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| K | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| K | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| K | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| K | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| K | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| K | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| K | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| K | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| K | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| K | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| K | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |
| L | -19 | MSE | - | EXPRESSION TAG | UNP P71727 |
| L | -18 | GLY | - | EXPRESSION TAG | UNP P71727 |
| L | -17 | SER | - | EXPRESSION TAG | UNP P71727 |
| L | -16 | SER | - | EXPRESSION TAG | UNP P71727 |
| L | -15 | HIS | - | EXPRESSION TAG | UNP P71727 |
| L | -14 | HIS | - | EXPRESSION TAG | UNP P71727 |
| L | -13 | HIS | - | EXPRESSION TAG | UNP P71727 |
| L | -12 | HIS | - | EXPRESSION TAG | UNP P71727 |
| L | -11 | HIS | - | EXPRESSION TAG | UNP P71727 |
| L | -10 | HIS | - | EXPRESSION TAG | UNP P71727 |
| L | -9 | SER | - | EXPRESSION TAG | UNP P71727 |
| L | -8 | SER | - | EXPRESSION TAG | UNP P71727 |
| L | -7 | GLY | - | EXPRESSION TAG | UNP P71727 |
| L | -6 | LEU | - | EXPRESSION TAG | UNP P71727 |
| L | -5 | VAL | - | EXPRESSION TAG | UNP P71727 |
| L | -4 | PRO | - | EXPRESSION TAG | UNP P71727 |
| L | -3 | ARG | - | EXPRESSION TAG | UNP P71727 |
| L | -2 | GLY | - | EXPRESSION TAG | UNP P71727 |
| L | -1 | SER | - | EXPRESSION TAG | UNP P71727 |
| L | 0 | HIS | - | EXPRESSION TAG | UNP P71727 |

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | B | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | C | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | D | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | E | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | F | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | G | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | H | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | I | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | J | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | K | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |
| 2 | L | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | | |

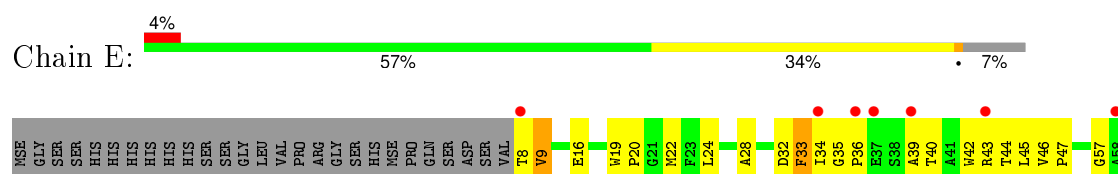
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | A | 46 | Total | O | 0 | 0 |
| | | | 46 | 46 | | |
| 3 | B | 74 | Total | O | 0 | 0 |
| | | | 74 | 74 | | |
| 3 | C | 54 | Total | O | 0 | 0 |
| | | | 54 | 54 | | |
| 3 | D | 51 | Total | O | 0 | 0 |
| | | | 51 | 51 | | |
| 3 | E | 47 | Total | O | 0 | 0 |
| | | | 47 | 47 | | |
| 3 | F | 48 | Total | O | 0 | 0 |
| | | | 48 | 48 | | |
| 3 | G | 31 | Total | O | 0 | 0 |
| | | | 31 | 31 | | |
| 3 | H | 39 | Total | O | 0 | 0 |
| | | | 39 | 39 | | |

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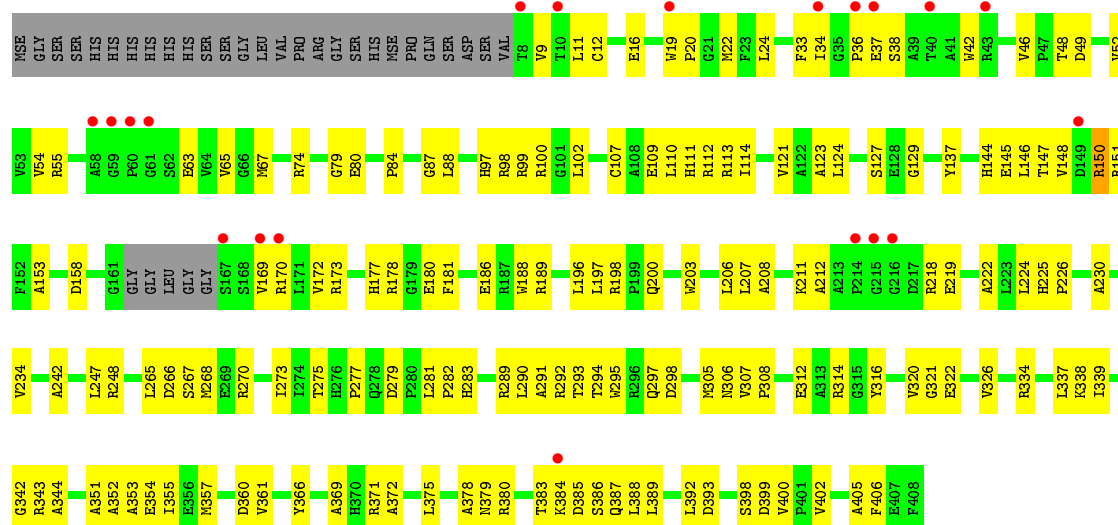
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3 | I | 17 | Total 17 | O 17 | 0 | 0 |
| 3 | J | 9 | Total 9 | O 9 | 0 | 0 |
| 3 | K | 29 | Total 29 | O 29 | 0 | 0 |
| 3 | L | 38 | Total 38 | O 38 | 0 | 0 |



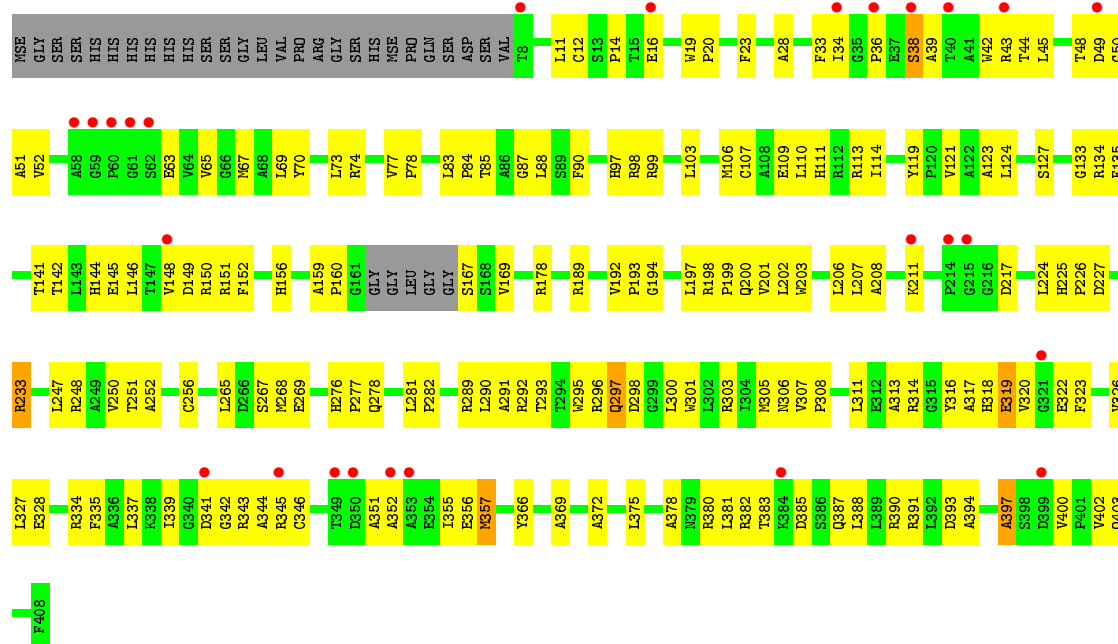




• Molecule 1: Enhanced intracellular survival protein

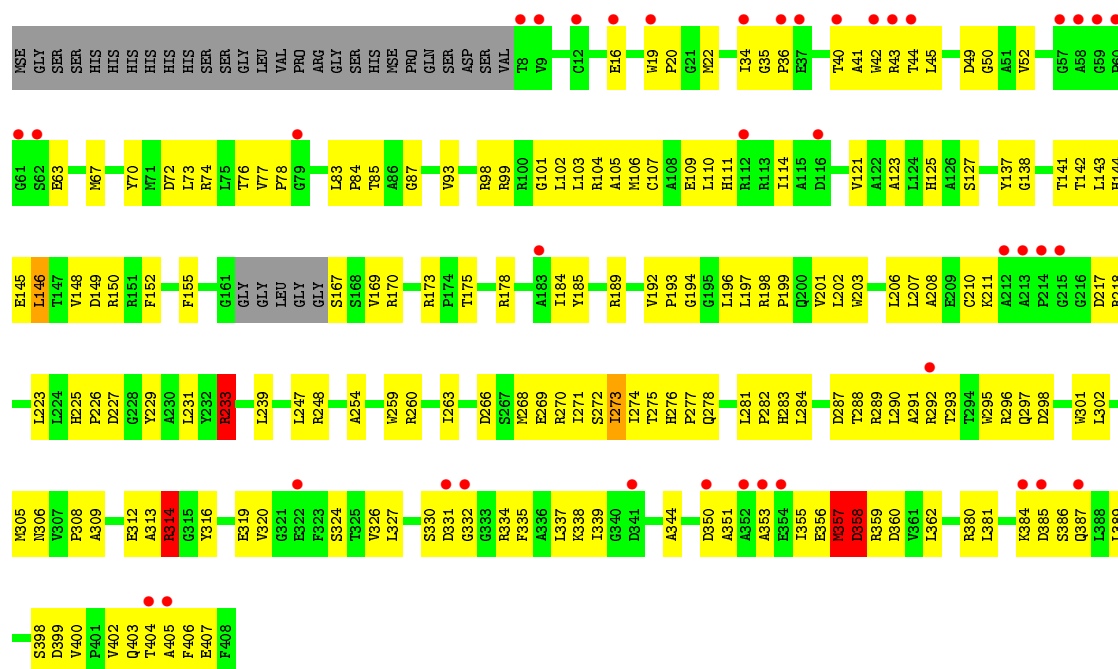


• Molecule 1: Enhanced intracellular survival protein



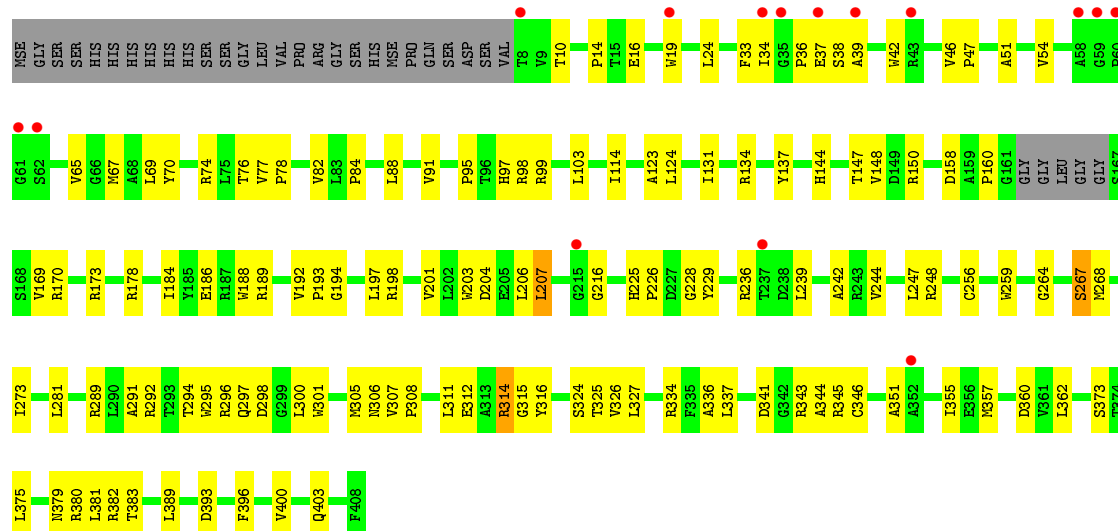
• Molecule 1: Enhanced intracellular survival protein





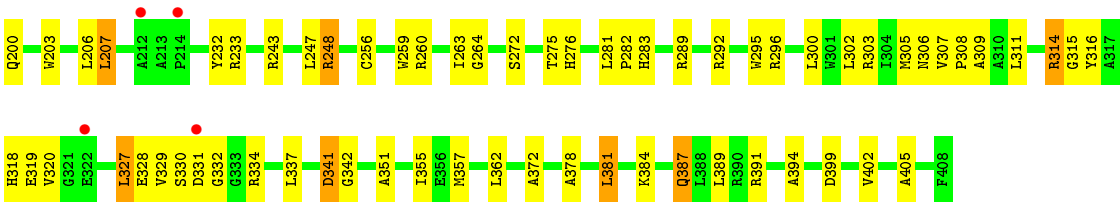
- Molecule 1: Enhanced intracellular survival protein

Chain K: 4% 62% 29% 7%



- Molecule 1: Enhanced intracellular survival protein

Chain L: 3% 66% 24% 7%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 108.13Å 150.19Å 184.38Å 90.00° 103.05° 90.00° | Depositor |
| Resolution (Å) | 29.94 – 2.80 29.94 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 93.4 (29.94-2.80) 95.2 (29.94-2.80) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 5.87 (at 2.80Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.6.4_486) | Depositor |
| R, R_{free} | 0.192 , 0.248 0.223 , 0.220 | Depositor DCC |
| R_{free} test set | 13782 reflections (11.38%) | DCC |
| Wilson B-factor (Å ²) | 40.1 | Xtriage |
| Anisotropy | 0.343 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.38 , 46.1 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 0 of 138028 reflections | Xtriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 37731 | wwPDB-VP |
| Average B, all atoms (Å ²) | 40.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.44 | 0/3115 | 0.63 | 0/4226 |
| 1 | B | 0.41 | 0/3115 | 0.62 | 0/4226 |
| 1 | C | 0.41 | 0/3115 | 0.61 | 0/4226 |
| 1 | D | 0.41 | 0/3115 | 0.63 | 1/4226 (0.0%) |
| 1 | E | 0.41 | 0/3115 | 0.62 | 0/4226 |
| 1 | F | 0.43 | 0/3115 | 0.62 | 1/4226 (0.0%) |
| 1 | G | 0.39 | 0/3115 | 0.59 | 0/4226 |
| 1 | H | 0.39 | 0/3115 | 0.57 | 0/4226 |
| 1 | I | 0.35 | 0/3115 | 0.58 | 0/4226 |
| 1 | J | 0.37 | 0/3115 | 0.59 | 0/4226 |
| 1 | K | 0.37 | 0/3115 | 0.57 | 0/4226 |
| 1 | L | 0.41 | 0/3115 | 0.62 | 1/4226 (0.0%) |
| All | All | 0.40 | 0/37380 | 0.60 | 3/50712 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | C | 0 | 1 |
| 1 | F | 0 | 1 |
| 1 | J | 0 | 2 |
| All | All | 0 | 5 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1 | F | 88 | LEU | CA-CB-CG | 5.76 | 128.56 | 115.30 |
| 1 | L | 35 | GLY | N-CA-C | 5.63 | 127.18 | 113.10 |
| 1 | D | 337 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 296 | ARG | Sidechain |
| 1 | C | 150 | ARG | Sidechain |
| 1 | F | 380 | ARG | Sidechain |
| 1 | J | 233 | ARG | Sidechain |
| 1 | J | 314 | ARG | Sidechain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3053 | 0 | 3020 | 157 | 0 |
| 1 | B | 3053 | 0 | 3020 | 173 | 0 |
| 1 | C | 3053 | 0 | 3020 | 199 | 0 |
| 1 | D | 3053 | 0 | 3020 | 214 | 0 |
| 1 | E | 3053 | 0 | 3020 | 204 | 2 |
| 1 | F | 3053 | 0 | 3020 | 235 | 0 |
| 1 | G | 3053 | 0 | 3020 | 182 | 0 |
| 1 | H | 3053 | 0 | 3020 | 239 | 0 |
| 1 | I | 3053 | 0 | 3020 | 250 | 0 |
| 1 | J | 3053 | 0 | 3020 | 219 | 1 |
| 1 | K | 3053 | 0 | 3020 | 164 | 1 |
| 1 | L | 3053 | 0 | 3018 | 84 | 2 |
| 2 | A | 51 | 0 | 34 | 6 | 0 |
| 2 | B | 51 | 0 | 33 | 4 | 0 |
| 2 | C | 51 | 0 | 34 | 12 | 0 |
| 2 | D | 51 | 0 | 33 | 2 | 0 |
| 2 | E | 51 | 0 | 34 | 8 | 0 |
| 2 | F | 51 | 0 | 33 | 5 | 0 |
| 2 | G | 51 | 0 | 33 | 6 | 0 |
| 2 | H | 51 | 0 | 33 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | I | 51 | 0 | 34 | 7 | 0 |
| 2 | J | 51 | 0 | 34 | 3 | 0 |
| 2 | K | 51 | 0 | 34 | 10 | 0 |
| 2 | L | 51 | 0 | 33 | 5 | 0 |
| 3 | A | 46 | 0 | 0 | 2 | 0 |
| 3 | B | 74 | 0 | 0 | 6 | 0 |
| 3 | C | 54 | 0 | 0 | 6 | 0 |
| 3 | D | 51 | 0 | 0 | 5 | 0 |
| 3 | E | 47 | 0 | 0 | 2 | 0 |
| 3 | F | 48 | 0 | 0 | 2 | 0 |
| 3 | G | 31 | 0 | 0 | 3 | 0 |
| 3 | H | 39 | 0 | 0 | 4 | 0 |
| 3 | I | 17 | 0 | 0 | 1 | 0 |
| 3 | J | 9 | 0 | 0 | 6 | 0 |
| 3 | K | 29 | 0 | 0 | 4 | 0 |
| 3 | L | 38 | 0 | 0 | 3 | 0 |
| All | All | 37731 | 0 | 36640 | 2186 | 3 |

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 30.

All (2186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:22:MSE:HE2 | 1:F:42:TRP:CH2 | 1.32 | 1.64 |
| 1:F:357:MSE:HE2 | 1:F:381:LEU:CD1 | 1.27 | 1.57 |
| 1:C:357:MSE:HE2 | 1:C:381:LEU:CD1 | 1.21 | 1.57 |
| 1:D:148:VAL:CG2 | 1:D:291:ALA:HA | 1.31 | 1.55 |
| 1:H:354:GLU:HA | 1:H:384:LYS:NZ | 1.18 | 1.51 |
| 1:F:22:MSE:CE | 1:F:42:TRP:CH2 | 1.88 | 1.49 |
| 1:I:357:MSE:CE | 1:I:381:LEU:HD13 | 1.39 | 1.48 |
| 1:C:148:VAL:CG2 | 1:C:291:ALA:HA | 1.44 | 1.48 |
| 1:F:144:HIS:NE2 | 1:F:296:ARG:NH1 | 1.66 | 1.44 |
| 1:F:42:TRP:CE2 | 1:F:69:LEU:CD2 | 2.02 | 1.41 |
| 1:C:148:VAL:HG22 | 1:C:291:ALA:CA | 1.51 | 1.40 |
| 1:D:148:VAL:HG22 | 1:D:291:ALA:CA | 1.50 | 1.39 |
| 1:F:42:TRP:NE1 | 1:F:69:LEU:HD22 | 1.38 | 1.38 |
| 1:E:148:VAL:CG2 | 1:E:291:ALA:HA | 1.56 | 1.35 |
| 1:K:244:VAL:CG2 | 1:K:273:ILE:HD11 | 1.58 | 1.34 |
| 1:F:42:TRP:CZ2 | 1:F:69:LEU:HD23 | 1.61 | 1.33 |
| 1:C:357:MSE:CE | 1:C:381:LEU:CD1 | 2.06 | 1.33 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:357:MSE:HE2 | 1:I:381:LEU:CD1 | 1.58 | 1.31 |
| 1:H:180:GLU:OE2 | 1:H:224:LEU:HD21 | 1.20 | 1.29 |
| 1:G:40:THR:O | 1:G:44:THR:HG22 | 1.30 | 1.28 |
| 1:B:85:THR:HG23 | 1:B:121:VAL:O | 1.18 | 1.28 |
| 1:I:44:THR:O | 1:I:45:LEU:HD23 | 1.31 | 1.28 |
| 1:K:244:VAL:HG21 | 1:K:273:ILE:CD1 | 1.63 | 1.28 |
| 1:K:244:VAL:HB | 1:K:273:ILE:CG1 | 1.63 | 1.27 |
| 1:I:357:MSE:CE | 1:I:381:LEU:CD1 | 2.10 | 1.26 |
| 1:A:180:GLU:OE2 | 1:A:224:LEU:HD21 | 1.21 | 1.26 |
| 1:C:52:VAL:CG2 | 1:C:110:LEU:HD11 | 1.67 | 1.24 |
| 1:E:148:VAL:HG22 | 1:E:291:ALA:CA | 1.67 | 1.23 |
| 1:H:34:ILE:HB | 1:H:37:GLU:CG | 1.66 | 1.23 |
| 1:H:354:GLU:CA | 1:H:384:LYS:NZ | 2.03 | 1.22 |
| 1:H:169:VAL:HG13 | 1:H:224:LEU:O | 1.12 | 1.22 |
| 1:K:244:VAL:CB | 1:K:273:ILE:HG12 | 1.69 | 1.21 |
| 1:G:150:ARG:HD3 | 1:G:268:MSE:O | 1.34 | 1.21 |
| 1:G:11:LEU:HD11 | 1:G:52:VAL:CG2 | 1.69 | 1.21 |
| 1:C:106:MSE:O | 1:C:110:LEU:HD13 | 1.37 | 1.20 |
| 1:I:34:ILE:HG22 | 1:I:36:PRO:HD2 | 1.18 | 1.18 |
| 1:C:52:VAL:HG21 | 1:C:110:LEU:CD1 | 1.72 | 1.18 |
| 1:D:150:ARG:NH2 | 1:D:266:ASP:HA | 1.59 | 1.18 |
| 1:B:180:GLU:OE2 | 1:B:224:LEU:HD21 | 1.44 | 1.16 |
| 1:H:169:VAL:HG13 | 1:H:224:LEU:C | 1.62 | 1.16 |
| 1:F:22:MSE:CE | 1:F:42:TRP:CZ2 | 2.28 | 1.16 |
| 1:F:357:MSE:CE | 1:F:381:LEU:CD1 | 2.24 | 1.16 |
| 1:E:146:LEU:HD12 | 1:E:275:THR:CG2 | 1.76 | 1.15 |
| 1:E:327:LEU:HD11 | 1:E:357:MSE:HE3 | 1.18 | 1.15 |
| 1:K:244:VAL:HG11 | 1:K:273:ILE:HD13 | 1.24 | 1.15 |
| 1:D:40:THR:O | 1:D:44:THR:HG22 | 1.44 | 1.14 |
| 1:D:34:ILE:HG22 | 1:D:36:PRO:HD2 | 1.26 | 1.14 |
| 1:L:34:ILE:HG22 | 1:L:36:PRO:HD2 | 1.28 | 1.14 |
| 1:H:34:ILE:HB | 1:H:37:GLU:HG2 | 1.14 | 1.14 |
| 1:B:150:ARG:HD3 | 1:B:268:MSE:O | 1.47 | 1.14 |
| 1:G:11:LEU:HD11 | 1:G:52:VAL:HG21 | 1.27 | 1.13 |
| 1:I:148:VAL:HG22 | 1:I:291:ALA:HA | 1.25 | 1.13 |
| 1:H:385:ASP:OD2 | 1:H:387:GLN:HG2 | 1.45 | 1.13 |
| 1:G:222:ALA:HB2 | 1:G:231:LEU:HD23 | 1.27 | 1.13 |
| 1:C:357:MSE:CE | 1:C:381:LEU:HD13 | 1.73 | 1.13 |
| 1:I:323:PHE:HB2 | 1:I:391:ARG:NH1 | 1.64 | 1.12 |
| 1:F:121:VAL:HG12 | 1:F:304:ILE:HA | 1.30 | 1.12 |
| 1:F:22:MSE:HE1 | 1:F:42:TRP:CZ2 | 1.84 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:106:MSE:O | 1:C:110:LEU:CD1 | 1.98 | 1.12 |
| 1:E:146:LEU:CD1 | 1:E:275:THR:HG21 | 1.80 | 1.12 |
| 1:C:145:GLU:CB | 1:C:295:TRP:HB3 | 1.81 | 1.11 |
| 1:I:149:ASP:OD2 | 1:I:152:PHE:HE1 | 1.30 | 1.11 |
| 1:C:357:MSE:HE2 | 1:C:381:LEU:HD11 | 1.29 | 1.11 |
| 1:D:146:LEU:HD21 | 1:D:148:VAL:CG2 | 1.80 | 1.10 |
| 1:I:148:VAL:CG2 | 1:I:291:ALA:HA | 1.79 | 1.10 |
| 1:F:121:VAL:HA | 1:F:305:MSE:HG2 | 1.32 | 1.10 |
| 1:J:203:TRP:O | 1:J:207:LEU:HD13 | 1.51 | 1.10 |
| 1:C:357:MSE:HE2 | 1:C:381:LEU:CG | 1.82 | 1.10 |
| 1:D:146:LEU:HD21 | 1:D:148:VAL:HG23 | 1.13 | 1.10 |
| 1:H:178:ARG:NH1 | 1:H:207:LEU:CD1 | 2.15 | 1.10 |
| 1:I:148:VAL:HG13 | 1:I:290:LEU:O | 1.51 | 1.10 |
| 1:K:327:LEU:HD11 | 1:K:357:MSE:HE3 | 1.35 | 1.09 |
| 1:D:33:PHE:HE1 | 1:D:38:SER:OG | 1.36 | 1.09 |
| 1:C:145:GLU:HB2 | 1:C:295:TRP:HB3 | 1.22 | 1.09 |
| 1:D:146:LEU:CD2 | 1:D:148:VAL:HG23 | 1.81 | 1.08 |
| 1:E:44:THR:HG21 | 1:E:201:VAL:HG11 | 1.35 | 1.08 |
| 1:C:178:ARG:HD2 | 1:C:207:LEU:HD11 | 1.33 | 1.08 |
| 1:H:169:VAL:CG1 | 1:H:224:LEU:O | 2.01 | 1.08 |
| 1:D:10:THR:HG21 | 1:H:384:LYS:HD2 | 1.36 | 1.08 |
| 1:F:150:ARG:HD3 | 1:F:268:MSE:O | 1.52 | 1.07 |
| 1:J:357:MSE:HE1 | 1:J:362:LEU:HB2 | 1.25 | 1.07 |
| 1:D:148:VAL:HG13 | 1:D:290:LEU:C | 1.75 | 1.07 |
| 1:F:42:TRP:CZ2 | 1:F:69:LEU:CD2 | 2.32 | 1.06 |
| 1:I:149:ASP:OD2 | 1:I:152:PHE:CE1 | 2.06 | 1.06 |
| 1:F:42:TRP:NE1 | 1:F:69:LEU:CD2 | 2.12 | 1.06 |
| 1:C:357:MSE:HE2 | 1:C:381:LEU:HD13 | 1.09 | 1.06 |
| 1:G:222:ALA:HB2 | 1:G:231:LEU:CD2 | 1.85 | 1.06 |
| 1:F:357:MSE:CE | 1:F:381:LEU:HD13 | 1.84 | 1.05 |
| 1:H:354:GLU:CA | 1:H:384:LYS:HZ1 | 1.64 | 1.05 |
| 1:G:150:ARG:CD | 1:G:268:MSE:O | 2.04 | 1.05 |
| 1:J:74:ARG:HD3 | 1:J:84:PRO:HA | 1.39 | 1.05 |
| 1:E:327:LEU:CD1 | 1:E:357:MSE:HE3 | 1.86 | 1.04 |
| 1:H:178:ARG:NH1 | 1:H:207:LEU:HD12 | 1.73 | 1.04 |
| 1:K:327:LEU:CD1 | 1:K:357:MSE:HE3 | 1.87 | 1.04 |
| 1:G:44:THR:HG21 | 1:G:201:VAL:HG11 | 1.39 | 1.04 |
| 1:F:357:MSE:HE2 | 1:F:381:LEU:HD11 | 1.07 | 1.04 |
| 1:D:193:PRO:HD3 | 1:D:400:VAL:HG21 | 1.38 | 1.04 |
| 1:H:109:GLU:O | 1:H:112:ARG:HG2 | 1.57 | 1.04 |
| 1:H:34:ILE:CB | 1:H:37:GLU:HG2 | 1.87 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:104:ARG:NH2 | 2:G:501:ACO:O8A | 1.91 | 1.03 |
| 1:H:33:PHE:CE1 | 1:H:38:SER:OG | 2.10 | 1.03 |
| 1:C:121:VAL:HA | 1:C:305:MSE:HG2 | 1.37 | 1.03 |
| 1:C:178:ARG:HD2 | 1:C:207:LEU:CD1 | 1.88 | 1.03 |
| 1:C:107:CYS:O | 1:C:111:HIS:ND1 | 1.91 | 1.03 |
| 1:E:295:TRP:HZ2 | 1:E:297:GLN:NE2 | 1.54 | 1.02 |
| 1:F:72:ASP:C | 1:F:73:LEU:HD12 | 1.79 | 1.02 |
| 1:J:34:ILE:HG22 | 1:J:36:PRO:HD2 | 1.09 | 1.02 |
| 1:G:175:THR:HA | 1:G:207:LEU:HD11 | 1.34 | 1.02 |
| 1:I:169:VAL:HG22 | 1:I:225:HIS:HB2 | 1.38 | 1.01 |
| 1:C:357:MSE:HB3 | 1:C:381:LEU:HD13 | 1.41 | 1.01 |
| 1:J:34:ILE:HG22 | 1:J:36:PRO:CD | 1.90 | 1.01 |
| 1:J:43:ARG:HH11 | 1:J:43:ARG:HA | 1.23 | 1.01 |
| 1:B:42:TRP:NE1 | 1:B:90:PHE:CE2 | 2.29 | 1.01 |
| 1:G:11:LEU:CD1 | 1:G:52:VAL:CG2 | 2.38 | 1.01 |
| 1:E:146:LEU:HD12 | 1:E:275:THR:HG21 | 1.06 | 1.01 |
| 1:A:355:ILE:HD11 | 1:A:381:LEU:HD13 | 1.41 | 1.01 |
| 1:H:34:ILE:HB | 1:H:37:GLU:CD | 1.80 | 1.00 |
| 1:F:34:ILE:HG22 | 1:F:36:PRO:HD2 | 1.37 | 1.00 |
| 1:K:314:ARG:NH1 | 1:K:315:GLY:O | 1.93 | 1.00 |
| 1:F:357:MSE:HE2 | 1:F:381:LEU:HD13 | 1.06 | 1.00 |
| 1:E:295:TRP:CZ2 | 1:E:297:GLN:NE2 | 2.30 | 1.00 |
| 1:F:356:GLU:O | 1:F:381:LEU:HD12 | 1.62 | 1.00 |
| 1:C:357:MSE:CE | 1:C:381:LEU:HD11 | 1.81 | 1.00 |
| 1:C:34:ILE:HG22 | 1:C:36:PRO:HD2 | 1.43 | 1.00 |
| 1:K:244:VAL:CB | 1:K:273:ILE:CD1 | 2.39 | 1.00 |
| 1:L:34:ILE:CG2 | 1:L:36:PRO:HD2 | 1.92 | 1.00 |
| 1:A:73:LEU:CD1 | 1:A:87:GLY:HA3 | 1.91 | 1.00 |
| 1:I:323:PHE:HB2 | 1:I:391:ARG:HH11 | 1.18 | 0.99 |
| 1:F:22:MSE:CE | 1:F:42:TRP:HH2 | 1.48 | 0.99 |
| 1:D:178:ARG:HG3 | 1:D:207:LEU:HD11 | 1.42 | 0.99 |
| 1:C:357:MSE:HE2 | 1:C:381:LEU:CD2 | 1.93 | 0.99 |
| 1:H:150:ARG:HD3 | 1:H:151:ARG:N | 1.78 | 0.99 |
| 1:H:295:TRP:CZ2 | 1:H:297:GLN:NE2 | 2.30 | 0.99 |
| 1:F:357:MSE:CE | 1:F:381:LEU:HD11 | 1.88 | 0.98 |
| 1:E:358:ASP:O | 1:E:361:VAL:HG12 | 1.60 | 0.98 |
| 1:I:357:MSE:HE3 | 1:I:381:LEU:CD1 | 1.91 | 0.98 |
| 1:C:104:ARG:NH2 | 3:C:635:HOH:O | 1.95 | 0.98 |
| 1:D:148:VAL:CG2 | 1:D:291:ALA:CA | 2.24 | 0.98 |
| 1:H:180:GLU:OE2 | 1:H:224:LEU:CD2 | 2.11 | 0.97 |
| 1:B:85:THR:CG2 | 1:B:121:VAL:O | 2.12 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:148:VAL:HG13 | 1:E:290:LEU:C | 1.84 | 0.97 |
| 1:C:150:ARG:HH21 | 1:C:266:ASP:HA | 1.29 | 0.97 |
| 1:E:156:HIS:CE1 | 1:F:380:ARG:NH1 | 2.33 | 0.97 |
| 1:B:45:LEU:HD11 | 1:B:199:PRO:HG2 | 1.43 | 0.97 |
| 1:I:45:LEU:HD11 | 1:I:199:PRO:HG2 | 1.46 | 0.97 |
| 1:J:189:ARG:HH11 | 1:J:197:LEU:HD13 | 1.28 | 0.97 |
| 1:F:42:TRP:CE2 | 1:F:69:LEU:HD21 | 1.98 | 0.96 |
| 1:H:295:TRP:HZ2 | 1:H:297:GLN:NE2 | 1.63 | 0.96 |
| 1:J:405:ALA:HB3 | 3:J:602:HOH:O | 1.64 | 0.96 |
| 1:K:144:HIS:NE2 | 1:K:296:ARG:NH1 | 2.13 | 0.96 |
| 1:J:227:ASP:OD2 | 3:J:603:HOH:O | 1.84 | 0.96 |
| 1:K:244:VAL:HG11 | 1:K:273:ILE:CD1 | 1.95 | 0.96 |
| 1:C:144:HIS:CD2 | 1:C:277:PRO:HG3 | 2.01 | 0.95 |
| 1:G:303:ARG:NH1 | 1:G:305:MSE:SE | 2.49 | 0.95 |
| 1:E:297:GLN:HG3 | 1:F:289:ARG:HD3 | 1.47 | 0.95 |
| 1:E:34:ILE:HG22 | 1:E:36:PRO:HD2 | 1.48 | 0.95 |
| 1:H:354:GLU:HA | 1:H:384:LYS:HZ2 | 1.29 | 0.95 |
| 1:A:85:THR:HG23 | 1:A:121:VAL:O | 1.66 | 0.95 |
| 1:A:178:ARG:HG3 | 1:A:207:LEU:HD11 | 1.46 | 0.95 |
| 1:I:34:ILE:CG2 | 1:I:36:PRO:HD2 | 1.96 | 0.94 |
| 1:E:93:VAL:O | 1:E:98:ARG:NH2 | 2.00 | 0.94 |
| 1:B:148:VAL:HG22 | 1:B:291:ALA:HA | 1.47 | 0.94 |
| 1:D:8:THR:N | 1:H:353:ALA:H | 1.64 | 0.94 |
| 1:A:320:VAL:CG2 | 1:A:394:ALA:HB1 | 1.97 | 0.94 |
| 1:H:98:ARG:HH21 | 1:H:99:ARG:NH2 | 1.64 | 0.94 |
| 1:F:121:VAL:CG1 | 1:F:304:ILE:HA | 1.97 | 0.94 |
| 1:G:9:VAL:CG1 | 1:G:54:VAL:CG1 | 2.46 | 0.94 |
| 1:J:295:TRP:HZ2 | 1:J:297:GLN:NE2 | 1.67 | 0.93 |
| 1:C:357:MSE:CE | 1:C:381:LEU:CD2 | 2.46 | 0.93 |
| 1:C:178:ARG:CD | 1:C:207:LEU:HD11 | 1.98 | 0.93 |
| 1:H:385:ASP:CG | 1:H:387:GLN:HG2 | 1.87 | 0.93 |
| 1:I:356:GLU:O | 1:I:381:LEU:HD12 | 1.67 | 0.93 |
| 1:K:193:PRO:HD3 | 1:K:400:VAL:HG11 | 1.51 | 0.93 |
| 1:J:34:ILE:CG2 | 1:J:36:PRO:HD2 | 1.98 | 0.92 |
| 1:K:193:PRO:CD | 1:K:400:VAL:CG1 | 2.48 | 0.92 |
| 1:C:355:ILE:HD11 | 1:C:381:LEU:HD21 | 1.48 | 0.92 |
| 1:I:193:PRO:HD3 | 1:I:400:VAL:HG21 | 1.49 | 0.92 |
| 1:G:355:ILE:HD11 | 1:G:381:LEU:HD21 | 1.52 | 0.92 |
| 1:K:244:VAL:CG1 | 1:K:273:ILE:HD13 | 1.98 | 0.92 |
| 1:H:146:LEU:HD23 | 1:H:275:THR:HG22 | 1.50 | 0.92 |
| 1:E:193:PRO:HD3 | 1:E:400:VAL:HG21 | 1.50 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:357:MSE:HE3 | 1:I:381:LEU:HD11 | 1.51 | 0.91 |
| 1:D:145:GLU:HB3 | 1:D:295:TRP:HB3 | 1.49 | 0.91 |
| 1:H:178:ARG:HH11 | 1:H:207:LEU:CD1 | 1.81 | 0.91 |
| 1:F:42:TRP:HE1 | 1:F:69:LEU:HD22 | 1.35 | 0.91 |
| 1:H:385:ASP:OD2 | 1:H:387:GLN:CG | 2.17 | 0.91 |
| 1:I:327:LEU:HD23 | 1:I:328:GLU:N | 1.85 | 0.91 |
| 1:G:44:THR:CG2 | 1:G:201:VAL:HG11 | 2.00 | 0.91 |
| 1:D:193:PRO:CD | 1:D:400:VAL:CG2 | 2.48 | 0.91 |
| 1:J:40:THR:O | 1:J:44:THR:HG22 | 1.71 | 0.91 |
| 1:C:357:MSE:HB3 | 1:C:381:LEU:CD1 | 2.00 | 0.91 |
| 1:H:144:HIS:CD2 | 1:H:277:PRO:HG3 | 2.05 | 0.91 |
| 1:I:193:PRO:CD | 1:I:400:VAL:HG23 | 2.00 | 0.90 |
| 1:A:73:LEU:O | 1:A:85:THR:N | 2.04 | 0.90 |
| 1:B:145:GLU:HB3 | 1:B:295:TRP:HB3 | 1.51 | 0.90 |
| 1:C:121:VAL:HG12 | 1:C:304:ILE:HA | 1.50 | 0.90 |
| 1:J:203:TRP:O | 1:J:207:LEU:CD1 | 2.20 | 0.90 |
| 1:H:178:ARG:HH12 | 1:H:207:LEU:HD12 | 1.33 | 0.90 |
| 1:E:193:PRO:CD | 1:E:400:VAL:HG23 | 2.01 | 0.90 |
| 1:K:244:VAL:CB | 1:K:273:ILE:CG1 | 2.36 | 0.90 |
| 1:I:323:PHE:CB | 1:I:391:ARG:NH1 | 2.34 | 0.90 |
| 1:I:289:ARG:HD3 | 1:J:297:GLN:HG3 | 1.53 | 0.89 |
| 1:J:206:LEU:HD23 | 1:J:206:LEU:O | 1.72 | 0.89 |
| 1:D:10:THR:OG1 | 1:H:384:LYS:HD3 | 1.72 | 0.89 |
| 1:F:199:PRO:HD2 | 1:F:202:LEU:HD12 | 1.55 | 0.89 |
| 1:J:144:HIS:NE2 | 1:J:296:ARG:NH1 | 2.21 | 0.89 |
| 1:D:42:TRP:NE1 | 1:D:90:PHE:CZ | 2.41 | 0.89 |
| 1:I:52:VAL:HG13 | 1:I:110:LEU:HD21 | 1.53 | 0.89 |
| 1:K:148:VAL:HG22 | 1:K:291:ALA:HA | 1.54 | 0.89 |
| 1:F:98:ARG:HG2 | 1:F:99:ARG:HG2 | 1.54 | 0.89 |
| 1:D:65:VAL:HG11 | 1:D:97:HIS:CE1 | 2.06 | 0.89 |
| 1:G:65:VAL:HG11 | 1:G:97:HIS:CE1 | 2.08 | 0.88 |
| 1:K:314:ARG:NH2 | 1:K:396:PHE:O | 2.06 | 0.88 |
| 1:F:357:MSE:HB3 | 1:F:381:LEU:HD13 | 1.53 | 0.88 |
| 1:J:405:ALA:CB | 3:J:602:HOH:O | 2.20 | 0.88 |
| 1:I:193:PRO:HD3 | 1:I:400:VAL:CG2 | 2.03 | 0.88 |
| 1:J:295:TRP:CZ2 | 1:J:297:GLN:NE2 | 2.41 | 0.88 |
| 1:B:144:HIS:NE2 | 1:B:296:ARG:NH1 | 2.22 | 0.88 |
| 1:E:144:HIS:HE1 | 1:E:296:ARG:HE | 1.22 | 0.88 |
| 1:A:73:LEU:HD11 | 1:A:87:GLY:HA3 | 1.53 | 0.88 |
| 1:A:144:HIS:NE2 | 1:A:296:ARG:NH1 | 2.22 | 0.88 |
| 1:G:144:HIS:NE2 | 1:G:296:ARG:NH1 | 2.22 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:193:PRO:CD | 1:K:400:VAL:HG11 | 2.04 | 0.87 |
| 1:B:144:HIS:CE1 | 1:B:296:ARG:HH11 | 1.91 | 0.87 |
| 1:E:146:LEU:CD1 | 1:E:275:THR:CG2 | 2.46 | 0.87 |
| 1:E:206:LEU:HD23 | 1:E:206:LEU:O | 1.74 | 0.87 |
| 1:I:289:ARG:HD3 | 1:J:297:GLN:CG | 2.05 | 0.87 |
| 1:B:233:ARG:NH1 | 3:B:627:HOH:O | 2.01 | 0.87 |
| 1:A:180:GLU:OE2 | 1:A:224:LEU:CD2 | 2.17 | 0.87 |
| 1:I:52:VAL:HG13 | 1:I:110:LEU:CD2 | 2.05 | 0.87 |
| 1:K:206:LEU:O | 1:K:206:LEU:HD23 | 1.73 | 0.87 |
| 1:E:109:GLU:OE1 | 1:E:112:ARG:NH2 | 2.07 | 0.86 |
| 1:A:314:ARG:NH2 | 1:A:396:PHE:O | 2.08 | 0.86 |
| 1:F:22:MSE:HE3 | 1:F:42:TRP:CH2 | 2.05 | 0.86 |
| 1:F:22:MSE:HE3 | 1:F:42:TRP:HH2 | 1.36 | 0.86 |
| 1:I:327:LEU:C | 1:I:327:LEU:HD23 | 1.94 | 0.86 |
| 1:A:34:ILE:HG22 | 1:A:36:PRO:HD2 | 1.55 | 0.86 |
| 1:J:357:MSE:HE1 | 1:J:362:LEU:CB | 2.05 | 0.86 |
| 1:F:98:ARG:HG3 | 1:F:99:ARG:NH1 | 1.90 | 0.86 |
| 1:H:196:LEU:HB2 | 1:H:406:PHE:CE2 | 2.11 | 0.86 |
| 1:J:193:PRO:HD3 | 1:J:400:VAL:HG21 | 1.58 | 0.86 |
| 1:F:206:LEU:HD23 | 1:F:206:LEU:O | 1.73 | 0.86 |
| 1:G:148:VAL:HG22 | 1:G:291:ALA:HA | 1.56 | 0.86 |
| 1:E:193:PRO:CD | 1:E:400:VAL:CG2 | 2.54 | 0.86 |
| 1:F:208:ALA:O | 1:F:211:LYS:HG2 | 1.74 | 0.86 |
| 1:I:148:VAL:HG22 | 1:I:291:ALA:CA | 2.05 | 0.86 |
| 1:G:222:ALA:CB | 1:G:231:LEU:HD23 | 2.06 | 0.86 |
| 1:K:244:VAL:CG1 | 1:K:273:ILE:CD1 | 2.54 | 0.85 |
| 1:H:178:ARG:NH1 | 1:H:207:LEU:HD11 | 1.90 | 0.85 |
| 1:B:40:THR:O | 1:B:44:THR:HG23 | 1.76 | 0.85 |
| 1:D:43:ARG:HA | 1:D:43:ARG:HH11 | 1.40 | 0.85 |
| 1:K:244:VAL:CG2 | 1:K:273:ILE:CG1 | 2.53 | 0.85 |
| 1:E:357:MSE:HB2 | 1:E:361:VAL:HG11 | 1.58 | 0.85 |
| 1:E:206:LEU:HD23 | 1:E:206:LEU:C | 1.96 | 0.85 |
| 1:C:356:GLU:O | 1:C:381:LEU:HD12 | 1.77 | 0.85 |
| 1:H:206:LEU:HD23 | 1:H:206:LEU:O | 1.76 | 0.85 |
| 1:I:193:PRO:CD | 1:I:400:VAL:CG2 | 2.54 | 0.85 |
| 1:A:34:ILE:HD12 | 1:A:37:GLU:OE1 | 1.77 | 0.85 |
| 1:H:150:ARG:C | 1:H:150:ARG:HH11 | 1.80 | 0.85 |
| 1:E:297:GLN:CG | 1:F:289:ARG:HD3 | 2.06 | 0.85 |
| 1:F:71:MSE:HB2 | 1:F:73:LEU:HD11 | 1.55 | 0.85 |
| 1:J:206:LEU:HD23 | 1:J:206:LEU:C | 1.97 | 0.85 |
| 1:D:150:ARG:NH2 | 1:D:266:ASP:CA | 2.39 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:193:PRO:HB2 | 1:C:402:VAL:HG22 | 1.59 | 0.84 |
| 1:D:10:THR:HG21 | 1:H:384:LYS:CD | 2.06 | 0.84 |
| 1:A:72:ASP:OD1 | 1:A:119:TYR:OH | 1.92 | 0.84 |
| 1:I:206:LEU:C | 1:I:206:LEU:HD23 | 1.97 | 0.84 |
| 1:G:248:ARG:NH2 | 1:G:405:ALA:O | 2.09 | 0.84 |
| 1:J:357:MSE:HE3 | 1:J:358:ASP:O | 1.77 | 0.84 |
| 1:D:193:PRO:HD3 | 1:D:400:VAL:CG2 | 2.06 | 0.84 |
| 1:I:44:THR:O | 1:I:45:LEU:CD2 | 2.23 | 0.84 |
| 1:H:196:LEU:HB2 | 1:H:406:PHE:HE2 | 1.43 | 0.84 |
| 1:C:148:VAL:CG2 | 1:C:291:ALA:CA | 2.29 | 0.84 |
| 1:B:123:ALA:HB1 | 1:B:300:LEU:HD11 | 1.58 | 0.84 |
| 1:F:188:TRP:CH2 | 1:F:248:ARG:NH1 | 2.46 | 0.84 |
| 1:J:208:ALA:O | 1:J:211:LYS:HG2 | 1.77 | 0.84 |
| 1:H:109:GLU:OE1 | 1:H:112:ARG:HD3 | 1.77 | 0.84 |
| 1:A:145:GLU:HB3 | 1:A:295:TRP:HB3 | 1.59 | 0.84 |
| 1:I:206:LEU:HD23 | 1:I:206:LEU:O | 1.77 | 0.84 |
| 1:E:193:PRO:HD3 | 1:E:400:VAL:CG2 | 2.07 | 0.84 |
| 1:I:267:SER:O | 1:I:268:MSE:HE2 | 1.78 | 0.84 |
| 1:F:357:MSE:HB3 | 1:F:381:LEU:CD1 | 2.08 | 0.83 |
| 1:I:323:PHE:CB | 1:I:391:ARG:HH11 | 1.90 | 0.83 |
| 1:F:34:ILE:HG22 | 1:F:36:PRO:CD | 2.08 | 0.83 |
| 1:G:327:LEU:HD23 | 1:G:328:GLU:N | 1.92 | 0.83 |
| 1:I:23:PHE:HE1 | 1:I:38:SER:HG | 1.24 | 0.83 |
| 1:K:244:VAL:CG2 | 1:K:273:ILE:CD1 | 2.31 | 0.83 |
| 1:D:40:THR:O | 1:D:44:THR:CG2 | 2.25 | 0.83 |
| 1:G:303:ARG:HH11 | 1:G:305:MSE:SE | 2.08 | 0.83 |
| 1:K:337:LEU:HD12 | 1:K:345:ARG:O | 1.78 | 0.83 |
| 1:E:145:GLU:CB | 1:E:295:TRP:HB3 | 2.08 | 0.83 |
| 1:G:188:TRP:CH2 | 1:G:248:ARG:NH1 | 2.47 | 0.82 |
| 1:F:303:ARG:NH1 | 1:F:359:ARG:HH11 | 1.76 | 0.82 |
| 1:G:11:LEU:CD1 | 1:G:52:VAL:HG22 | 2.07 | 0.82 |
| 1:I:200:GLN:HE21 | 1:I:200:GLN:HA | 1.44 | 0.82 |
| 1:H:34:ILE:N | 1:H:37:GLU:OE1 | 2.12 | 0.82 |
| 1:D:193:PRO:CD | 1:D:400:VAL:HG23 | 2.10 | 0.82 |
| 1:D:144:HIS:CD2 | 1:D:277:PRO:HG3 | 2.15 | 0.82 |
| 1:K:193:PRO:HD2 | 1:K:400:VAL:HG13 | 1.61 | 0.82 |
| 1:K:289:ARG:NH2 | 1:L:126:ALA:O | 2.13 | 0.81 |
| 1:F:206:LEU:HD23 | 1:F:206:LEU:C | 2.01 | 0.81 |
| 1:A:178:ARG:CG | 1:A:207:LEU:HD11 | 2.11 | 0.80 |
| 1:F:192:VAL:HG11 | 1:F:403:GLN:HB2 | 1.63 | 0.80 |
| 1:F:150:ARG:CD | 1:F:268:MSE:O | 2.30 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:42:TRP:HZ2 | 1:B:90:PHE:CE1 | 1.99 | 0.80 |
| 1:I:98:ARG:HG2 | 1:I:99:ARG:HG2 | 1.63 | 0.80 |
| 1:C:206:LEU:O | 1:C:206:LEU:HD23 | 1.80 | 0.80 |
| 1:G:327:LEU:C | 1:G:327:LEU:HD23 | 2.01 | 0.80 |
| 1:K:244:VAL:HB | 1:K:273:ILE:HG12 | 0.84 | 0.80 |
| 1:D:145:GLU:CB | 1:D:295:TRP:HB3 | 2.10 | 0.80 |
| 1:G:381:LEU:C | 1:G:381:LEU:HD23 | 2.01 | 0.80 |
| 1:J:78:PRO:HG2 | 1:J:314:ARG:HH21 | 1.47 | 0.80 |
| 1:E:145:GLU:HB3 | 1:E:295:TRP:HB3 | 1.62 | 0.80 |
| 1:G:9:VAL:HG13 | 1:G:54:VAL:HG12 | 1.63 | 0.80 |
| 1:B:169:VAL:CG2 | 1:B:225:HIS:HD2 | 1.93 | 0.80 |
| 1:E:44:THR:CG2 | 1:E:201:VAL:HG11 | 2.10 | 0.80 |
| 1:H:206:LEU:HD23 | 1:H:206:LEU:C | 2.02 | 0.79 |
| 1:D:145:GLU:OE2 | 1:D:295:TRP:CB | 2.30 | 0.79 |
| 1:G:34:ILE:HG22 | 1:G:36:PRO:HD2 | 1.62 | 0.79 |
| 1:J:271:ILE:N | 1:J:271:ILE:HD12 | 1.96 | 0.79 |
| 1:G:43:ARG:HH11 | 1:G:43:ARG:HA | 1.47 | 0.79 |
| 1:B:169:VAL:CG2 | 1:B:225:HIS:CD2 | 2.65 | 0.79 |
| 1:C:150:ARG:NH2 | 1:C:266:ASP:HA | 1.96 | 0.79 |
| 1:K:193:PRO:HD2 | 1:K:400:VAL:CG1 | 2.12 | 0.79 |
| 1:E:144:HIS:CE1 | 1:E:296:ARG:HE | 2.00 | 0.79 |
| 1:F:14:PRO:HD2 | 1:F:51:ALA:O | 1.82 | 0.79 |
| 1:I:34:ILE:HG22 | 1:I:36:PRO:CD | 2.09 | 0.79 |
| 1:E:144:HIS:HE1 | 1:E:296:ARG:NE | 1.80 | 0.79 |
| 1:A:327:LEU:HD13 | 1:A:355:ILE:HG23 | 1.64 | 0.79 |
| 1:E:144:HIS:CE1 | 1:E:296:ARG:HG3 | 2.18 | 0.79 |
| 1:I:107:CYS:O | 1:I:111:HIS:ND1 | 2.15 | 0.79 |
| 1:H:169:VAL:CG2 | 1:H:225:HIS:HB2 | 2.12 | 0.79 |
| 1:E:148:VAL:HG13 | 1:E:290:LEU:O | 1.82 | 0.78 |
| 1:I:45:LEU:CD1 | 1:I:199:PRO:HG2 | 2.12 | 0.78 |
| 1:F:71:MSE:CB | 1:F:73:LEU:HD11 | 2.13 | 0.78 |
| 1:H:169:VAL:HG22 | 1:H:225:HIS:HB2 | 1.65 | 0.78 |
| 1:F:303:ARG:CZ | 1:F:359:ARG:HH11 | 1.96 | 0.78 |
| 1:K:206:LEU:C | 1:K:206:LEU:HD23 | 2.04 | 0.78 |
| 1:E:314:ARG:NH2 | 1:E:396:PHE:O | 2.17 | 0.78 |
| 1:I:144:HIS:NE2 | 1:I:296:ARG:NH1 | 2.31 | 0.78 |
| 1:K:381:LEU:HD23 | 1:K:382:ARG:N | 1.98 | 0.78 |
| 1:F:98:ARG:HE | 1:F:99:ARG:NH2 | 1.82 | 0.78 |
| 1:F:65:VAL:HG11 | 1:F:97:HIS:CE1 | 2.18 | 0.78 |
| 1:G:218:ARG:NH2 | 1:G:239:LEU:HD21 | 1.97 | 0.78 |
| 1:C:146:LEU:HD11 | 1:C:291:ALA:C | 2.04 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:42:TRP:CD1 | 1:F:46:VAL:HG21 | 2.19 | 0.78 |
| 1:D:148:VAL:HG21 | 1:D:291:ALA:HA | 1.59 | 0.78 |
| 1:C:178:ARG:HH11 | 1:C:207:LEU:HD12 | 1.50 | 0.78 |
| 1:H:98:ARG:NH2 | 1:H:99:ARG:NH2 | 2.31 | 0.78 |
| 1:H:121:VAL:HA | 1:H:305:MSE:HG2 | 1.66 | 0.77 |
| 1:L:318:HIS:CE1 | 1:L:342:GLY:HA3 | 2.19 | 0.77 |
| 1:J:78:PRO:HG2 | 1:J:314:ARG:NH2 | 2.00 | 0.77 |
| 1:K:65:VAL:HG11 | 1:K:97:HIS:CE1 | 2.20 | 0.77 |
| 1:D:146:LEU:HD23 | 1:D:147:THR:N | 1.98 | 0.77 |
| 1:H:146:LEU:HD23 | 1:H:275:THR:CG2 | 2.14 | 0.77 |
| 1:F:34:ILE:HB | 1:F:37:GLU:HG2 | 1.66 | 0.77 |
| 1:E:192:VAL:HG11 | 1:E:403:GLN:HB2 | 1.65 | 0.77 |
| 1:B:206:LEU:HD23 | 1:B:206:LEU:O | 1.85 | 0.77 |
| 1:H:383:THR:HG21 | 1:H:389:LEU:HB2 | 1.66 | 0.77 |
| 1:D:148:VAL:HG13 | 1:D:290:LEU:O | 1.83 | 0.77 |
| 1:E:334:ARG:HD3 | 1:E:353:ALA:HB2 | 1.67 | 0.77 |
| 1:F:34:ILE:CG2 | 1:F:36:PRO:HD2 | 2.13 | 0.77 |
| 1:B:144:HIS:CD2 | 1:B:277:PRO:HG3 | 2.20 | 0.77 |
| 1:E:307:VAL:HB | 1:E:308:PRO:HD3 | 1.66 | 0.77 |
| 1:K:98:ARG:HG2 | 1:K:99:ARG:HG2 | 1.66 | 0.76 |
| 1:H:169:VAL:HG22 | 1:H:225:HIS:CB | 2.16 | 0.76 |
| 1:B:14:PRO:HD2 | 1:B:51:ALA:O | 1.84 | 0.76 |
| 1:G:9:VAL:HG13 | 1:G:54:VAL:CG1 | 2.16 | 0.76 |
| 1:I:38:SER:HB2 | 1:I:42:TRP:CZ2 | 2.19 | 0.76 |
| 1:D:44:THR:HG21 | 1:D:201:VAL:HG21 | 1.67 | 0.76 |
| 1:D:34:ILE:CG2 | 1:D:36:PRO:HD2 | 2.11 | 0.76 |
| 1:C:52:VAL:HG21 | 1:C:110:LEU:HD11 | 0.83 | 0.76 |
| 1:D:169:VAL:HG22 | 1:D:225:HIS:HB2 | 1.67 | 0.76 |
| 1:D:206:LEU:HD23 | 1:D:206:LEU:O | 1.84 | 0.76 |
| 1:F:22:MSE:HE2 | 1:F:42:TRP:CZ3 | 2.14 | 0.76 |
| 1:A:73:LEU:HB2 | 1:A:85:THR:O | 1.86 | 0.76 |
| 1:F:330:SER:O | 3:F:629:HOH:O | 2.02 | 0.76 |
| 1:C:145:GLU:HG2 | 1:C:274:ILE:CD1 | 2.15 | 0.76 |
| 1:J:150:ARG:HD3 | 1:J:268:MSE:O | 1.86 | 0.76 |
| 1:B:169:VAL:HG13 | 1:B:224:LEU:C | 2.06 | 0.76 |
| 1:A:320:VAL:HG21 | 1:A:394:ALA:CB | 2.16 | 0.76 |
| 1:I:43:ARG:HA | 1:I:43:ARG:HH11 | 1.49 | 0.76 |
| 1:G:40:THR:O | 1:G:44:THR:CG2 | 2.24 | 0.75 |
| 1:E:144:HIS:CE1 | 1:E:296:ARG:NE | 2.54 | 0.75 |
| 1:B:24:LEU:HD13 | 1:D:173:ARG:HG2 | 1.68 | 0.75 |
| 1:C:355:ILE:HD11 | 1:C:381:LEU:CD2 | 2.15 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:169:VAL:HG22 | 1:B:225:HIS:CB | 2.17 | 0.75 |
| 1:H:109:GLU:O | 1:H:112:ARG:CG | 2.33 | 0.75 |
| 1:C:121:VAL:CA | 1:C:305:MSE:HG2 | 2.16 | 0.75 |
| 1:A:178:ARG:HH11 | 1:A:207:LEU:HD12 | 1.51 | 0.75 |
| 1:A:320:VAL:HG22 | 1:A:394:ALA:HB1 | 1.68 | 0.75 |
| 1:C:326:VAL:CG1 | 1:C:353:ALA:HA | 2.16 | 0.75 |
| 1:A:73:LEU:HD12 | 1:A:87:GLY:CA | 2.17 | 0.75 |
| 1:J:44:THR:HG21 | 1:J:201:VAL:HG21 | 1.68 | 0.75 |
| 1:A:65:VAL:HG11 | 1:A:97:HIS:CE1 | 2.21 | 0.75 |
| 1:C:134:ARG:NH1 | 2:C:501:ACO:H1B | 2.00 | 0.75 |
| 1:A:42:TRP:CD1 | 1:A:69:LEU:HD21 | 2.21 | 0.75 |
| 1:B:169:VAL:HG23 | 1:B:225:HIS:HD2 | 1.52 | 0.75 |
| 1:I:169:VAL:HG22 | 1:I:225:HIS:CB | 2.17 | 0.75 |
| 1:J:193:PRO:CD | 1:J:400:VAL:HG23 | 2.16 | 0.75 |
| 1:B:150:ARG:CD | 1:B:268:MSE:O | 2.31 | 0.75 |
| 1:J:74:ARG:CD | 1:J:84:PRO:HA | 2.17 | 0.75 |
| 1:D:355:ILE:HD11 | 1:D:381:LEU:HD13 | 1.68 | 0.75 |
| 1:D:10:THR:CG2 | 1:H:384:LYS:HD2 | 2.14 | 0.75 |
| 1:J:193:PRO:HD3 | 1:J:400:VAL:CG2 | 2.16 | 0.75 |
| 1:C:357:MSE:CB | 1:C:381:LEU:HD13 | 2.17 | 0.75 |
| 1:I:355:ILE:HD11 | 1:I:381:LEU:CG | 2.17 | 0.75 |
| 1:I:148:VAL:CG1 | 1:I:290:LEU:O | 2.31 | 0.75 |
| 1:C:144:HIS:NE2 | 1:C:277:PRO:HG3 | 2.02 | 0.75 |
| 1:J:270:ARG:C | 1:J:271:ILE:HD12 | 2.07 | 0.74 |
| 1:G:126:ALA:O | 1:H:289:ARG:NH2 | 2.21 | 0.74 |
| 1:F:98:ARG:NE | 1:F:99:ARG:CZ | 2.50 | 0.74 |
| 1:E:360:ASP:OD2 | 1:E:380:ARG:NH2 | 2.20 | 0.74 |
| 1:B:169:VAL:HG13 | 1:B:224:LEU:O | 1.86 | 0.74 |
| 1:D:74:ARG:HD3 | 1:D:84:PRO:HA | 1.69 | 0.74 |
| 1:B:144:HIS:HB3 | 1:B:146:LEU:HD11 | 1.69 | 0.74 |
| 1:E:83:LEU:HD21 | 1:E:313:ALA:HB1 | 1.68 | 0.74 |
| 1:B:380:ARG:O | 3:B:604:HOH:O | 2.06 | 0.74 |
| 1:I:320:VAL:HG23 | 1:J:319:GLU:HB3 | 1.69 | 0.74 |
| 1:I:289:ARG:CD | 1:J:297:GLN:HG3 | 2.17 | 0.74 |
| 1:C:127:SER:HB3 | 2:C:501:ACO:H22 | 1.68 | 0.74 |
| 1:C:357:MSE:HE3 | 1:C:381:LEU:HD11 | 1.68 | 0.74 |
| 1:K:355:ILE:HD11 | 1:K:381:LEU:HD21 | 1.70 | 0.74 |
| 1:J:355:ILE:HD11 | 1:J:381:LEU:HD13 | 1.70 | 0.74 |
| 1:A:365:LEU:HD21 | 1:A:375:LEU:HD12 | 1.70 | 0.74 |
| 1:I:169:VAL:HG13 | 1:I:224:LEU:O | 1.87 | 0.74 |
| 1:B:206:LEU:C | 1:B:206:LEU:HD23 | 2.07 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:339:ILE:HG12 | 1:J:344:ALA:HB2 | 1.70 | 0.74 |
| 1:J:193:PRO:CG | 1:J:400:VAL:HG23 | 2.18 | 0.73 |
| 1:C:70:TYR:HA | 1:C:87:GLY:O | 1.87 | 0.73 |
| 1:C:206:LEU:HD23 | 1:C:206:LEU:C | 2.08 | 0.73 |
| 1:B:145:GLU:CB | 1:B:295:TRP:HB3 | 2.17 | 0.73 |
| 1:A:145:GLU:CB | 1:A:295:TRP:HB3 | 2.17 | 0.73 |
| 1:G:175:THR:CA | 1:G:207:LEU:HD11 | 2.16 | 0.73 |
| 1:J:43:ARG:NH1 | 1:J:43:ARG:HA | 2.02 | 0.73 |
| 1:A:121:VAL:HG13 | 1:A:303:ARG:O | 1.88 | 0.73 |
| 1:D:145:GLU:OE2 | 1:D:295:TRP:HB2 | 1.86 | 0.73 |
| 1:G:44:THR:HG21 | 1:G:201:VAL:CG1 | 2.18 | 0.73 |
| 1:D:193:PRO:CD | 1:D:400:VAL:HG21 | 2.12 | 0.73 |
| 1:E:33:PHE:C | 1:E:33:PHE:CD1 | 2.62 | 0.73 |
| 1:J:178:ARG:HD2 | 1:J:207:LEU:CD2 | 2.19 | 0.73 |
| 1:E:156:HIS:CE1 | 1:F:380:ARG:HH12 | 2.07 | 0.73 |
| 1:I:148:VAL:HG13 | 1:I:290:LEU:C | 2.09 | 0.72 |
| 1:I:38:SER:O | 1:I:42:TRP:CD1 | 2.41 | 0.72 |
| 1:J:85:THR:HG23 | 1:J:121:VAL:HG23 | 1.71 | 0.72 |
| 1:G:169:VAL:HG22 | 1:G:225:HIS:HB2 | 1.71 | 0.72 |
| 1:L:31:THR:HG23 | 3:L:621:HOH:O | 1.88 | 0.72 |
| 1:I:307:VAL:HB | 1:I:308:PRO:HD3 | 1.70 | 0.72 |
| 1:H:48:THR:O | 1:H:49:ASP:OD1 | 2.08 | 0.72 |
| 1:C:314:ARG:NH1 | 1:C:366:TYR:O | 2.22 | 0.72 |
| 1:F:303:ARG:HH12 | 1:F:359:ARG:NH1 | 1.86 | 0.72 |
| 1:C:120:PRO:O | 1:C:305:MSE:HB2 | 1.88 | 0.72 |
| 1:K:98:ARG:HG3 | 1:K:99:ARG:NH1 | 2.04 | 0.72 |
| 1:H:107:CYS:O | 1:H:111:HIS:ND1 | 2.21 | 0.72 |
| 1:C:357:MSE:CE | 1:C:381:LEU:HD22 | 2.20 | 0.72 |
| 1:J:178:ARG:HD2 | 1:J:207:LEU:HD21 | 1.69 | 0.72 |
| 1:I:200:GLN:NE2 | 1:I:200:GLN:HA | 2.04 | 0.72 |
| 1:I:327:LEU:O | 1:I:335:PHE:N | 2.22 | 0.72 |
| 1:E:156:HIS:NE2 | 1:F:380:ARG:NH1 | 2.38 | 0.72 |
| 1:H:98:ARG:HG2 | 1:H:99:ARG:HG2 | 1.72 | 0.72 |
| 1:E:150:ARG:HD3 | 1:E:268:MSE:O | 1.90 | 0.72 |
| 1:I:357:MSE:HE2 | 1:I:381:LEU:HD13 | 0.72 | 0.71 |
| 1:B:42:TRP:O | 1:B:46:VAL:HB | 1.89 | 0.71 |
| 1:I:337:LEU:HD12 | 1:I:345:ARG:O | 1.89 | 0.71 |
| 1:H:322:GLU:OE1 | 1:H:338:LYS:HE2 | 1.90 | 0.71 |
| 1:F:326:VAL:HG12 | 1:F:353:ALA:HA | 1.72 | 0.71 |
| 1:F:98:ARG:HE | 1:F:99:ARG:CZ | 2.03 | 0.71 |
| 1:I:276:HIS:HD2 | 1:I:278:GLN:H | 1.37 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:355:ILE:CD1 | 1:I:381:LEU:HD11 | 2.20 | 0.71 |
| 1:F:303:ARG:NH1 | 1:F:359:ARG:NH1 | 2.37 | 0.71 |
| 1:D:146:LEU:HD11 | 1:D:291:ALA:HB1 | 1.71 | 0.71 |
| 1:E:297:GLN:HG3 | 1:F:289:ARG:CD | 2.19 | 0.71 |
| 1:D:206:LEU:HD23 | 1:D:206:LEU:C | 2.11 | 0.71 |
| 1:I:83:LEU:HD21 | 1:I:313:ALA:HB1 | 1.71 | 0.71 |
| 1:K:201:VAL:O | 1:K:204:ASP:HB2 | 1.89 | 0.71 |
| 1:H:178:ARG:HH11 | 1:H:207:LEU:HD11 | 1.50 | 0.71 |
| 1:D:146:LEU:HD23 | 1:D:146:LEU:C | 2.10 | 0.71 |
| 1:J:110:LEU:O | 1:J:114:ILE:HG13 | 1.91 | 0.71 |
| 1:B:178:ARG:NH1 | 1:B:207:LEU:HD12 | 2.06 | 0.71 |
| 1:E:358:ASP:O | 1:E:361:VAL:CG1 | 2.38 | 0.71 |
| 1:G:289:ARG:NH1 | 1:H:298:ASP:OD2 | 2.23 | 0.71 |
| 1:A:320:VAL:HG21 | 1:A:394:ALA:HB1 | 1.69 | 0.71 |
| 1:F:16:GLU:HA | 1:F:19:TRP:CD1 | 2.26 | 0.71 |
| 1:C:319:GLU:O | 1:D:319:GLU:O | 2.08 | 0.71 |
| 1:D:150:ARG:CZ | 1:D:266:ASP:HA | 2.19 | 0.71 |
| 1:E:127:SER:HB3 | 2:E:501:ACO:H22 | 1.71 | 0.71 |
| 1:I:169:VAL:CG2 | 1:I:225:HIS:HB2 | 2.19 | 0.71 |
| 1:C:148:VAL:HG21 | 1:C:291:ALA:CB | 2.21 | 0.71 |
| 1:E:297:GLN:OE1 | 1:F:289:ARG:CD | 2.38 | 0.71 |
| 1:I:289:ARG:CG | 1:J:298:ASP:OD1 | 2.39 | 0.71 |
| 1:D:18:ASP:OD2 | 1:D:55:ARG:NH2 | 2.24 | 0.71 |
| 1:K:244:VAL:HG21 | 1:K:273:ILE:HD11 | 0.77 | 0.71 |
| 1:J:193:PRO:CD | 1:J:400:VAL:CG2 | 2.69 | 0.71 |
| 1:C:110:LEU:HD12 | 1:C:110:LEU:H | 1.56 | 0.70 |
| 1:D:33:PHE:CE1 | 1:D:38:SER:CB | 2.73 | 0.70 |
| 1:A:320:VAL:CG2 | 1:A:394:ALA:CB | 2.68 | 0.70 |
| 1:C:407:GLU:HB2 | 3:C:636:HOH:O | 1.91 | 0.70 |
| 1:I:65:VAL:HG11 | 1:I:97:HIS:CE1 | 2.26 | 0.70 |
| 1:D:33:PHE:CE1 | 1:D:38:SER:OG | 2.22 | 0.70 |
| 1:A:73:LEU:CD1 | 1:A:87:GLY:CA | 2.67 | 0.70 |
| 1:B:314:ARG:NH1 | 1:B:366:TYR:O | 2.24 | 0.70 |
| 1:C:334:ARG:HD3 | 1:C:351:ALA:O | 1.91 | 0.70 |
| 1:J:337:LEU:HD11 | 1:J:339:ILE:HD11 | 1.72 | 0.70 |
| 1:C:357:MSE:SE | 1:C:381:LEU:HD13 | 2.41 | 0.70 |
| 1:G:33:PHE:O | 1:G:34:ILE:HG13 | 1.92 | 0.70 |
| 1:F:121:VAL:HG12 | 1:F:304:ILE:CA | 2.16 | 0.70 |
| 1:D:52:VAL:HG13 | 1:D:110:LEU:HD21 | 1.74 | 0.70 |
| 1:E:65:VAL:HG11 | 1:E:97:HIS:CE1 | 2.26 | 0.70 |
| 1:I:148:VAL:HG21 | 1:I:291:ALA:HA | 1.71 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:197:LEU:O | 1:J:199:PRO:HD3 | 1.90 | 0.70 |
| 1:J:44:THR:HG21 | 1:J:201:VAL:HG11 | 1.72 | 0.70 |
| 1:C:85:THR:HG23 | 1:C:121:VAL:O | 1.91 | 0.70 |
| 1:A:73:LEU:HD12 | 1:A:87:GLY:HA3 | 1.74 | 0.70 |
| 1:B:127:SER:HB3 | 2:B:501:ACO:H22 | 1.71 | 0.70 |
| 1:B:48:THR:O | 1:B:49:ASP:CG | 2.30 | 0.70 |
| 1:I:217:ASP:OD1 | 1:I:233:ARG:NH1 | 2.24 | 0.70 |
| 1:I:355:ILE:HG12 | 1:I:356:GLU:N | 2.07 | 0.70 |
| 1:D:217:ASP:HB3 | 1:D:233:ARG:HD2 | 1.72 | 0.70 |
| 1:H:354:GLU:HA | 1:H:384:LYS:HZ1 | 0.83 | 0.69 |
| 1:K:123:ALA:HB1 | 1:K:300:LEU:HD11 | 1.73 | 0.69 |
| 1:G:50:GLY:HA2 | 1:G:70:TYR:CE1 | 2.27 | 0.69 |
| 1:G:16:GLU:O | 1:G:19:TRP:HD1 | 1.75 | 0.69 |
| 1:J:149:ASP:OD2 | 1:J:152:PHE:CE1 | 2.44 | 0.69 |
| 1:C:357:MSE:HE1 | 1:C:381:LEU:CD2 | 2.20 | 0.69 |
| 1:D:8:THR:HG23 | 1:D:9:VAL:N | 2.05 | 0.69 |
| 1:L:256:CYS:O | 1:L:260:ARG:HG3 | 1.91 | 0.69 |
| 1:G:281:LEU:HB3 | 1:G:282:PRO:HD3 | 1.73 | 0.69 |
| 1:I:355:ILE:HD11 | 1:I:381:LEU:HD11 | 1.73 | 0.69 |
| 1:C:148:VAL:CG2 | 1:C:291:ALA:CB | 2.69 | 0.69 |
| 1:G:98:ARG:HD2 | 1:L:264:GLY:CA | 2.23 | 0.69 |
| 1:K:178:ARG:NH1 | 1:K:207:LEU:HD23 | 2.06 | 0.69 |
| 1:D:48:THR:O | 1:D:49:ASP:CG | 2.30 | 0.69 |
| 1:A:248:ARG:NH2 | 1:A:405:ALA:O | 2.22 | 0.69 |
| 1:K:314:ARG:HD3 | 1:K:316:TYR:CE2 | 2.27 | 0.69 |
| 1:G:149:ASP:OD2 | 1:G:152:PHE:CE2 | 2.45 | 0.69 |
| 1:B:221:PHE:CE2 | 1:E:28:ALA:HA | 2.28 | 0.69 |
| 1:C:34:ILE:CG2 | 1:C:36:PRO:HD2 | 2.21 | 0.69 |
| 1:D:178:ARG:CG | 1:D:207:LEU:HD11 | 2.19 | 0.69 |
| 1:B:178:ARG:HG3 | 1:B:207:LEU:HD11 | 1.73 | 0.69 |
| 1:C:146:LEU:HD11 | 1:C:291:ALA:O | 1.92 | 0.69 |
| 1:I:44:THR:HG22 | 1:I:44:THR:O | 1.91 | 0.69 |
| 1:D:150:ARG:NH2 | 1:D:266:ASP:O | 2.26 | 0.69 |
| 1:G:149:ASP:OD2 | 1:G:152:PHE:HE2 | 1.74 | 0.69 |
| 1:E:127:SER:H | 2:E:501:ACO:H21 | 1.58 | 0.69 |
| 1:C:178:ARG:HH21 | 1:C:200:GLN:NE2 | 1.90 | 0.69 |
| 1:D:8:THR:HG23 | 1:D:9:VAL:H | 1.57 | 0.69 |
| 1:L:372:ALA:HB1 | 1:L:381:LEU:HD21 | 1.75 | 0.69 |
| 1:I:327:LEU:CD2 | 1:I:327:LEU:C | 2.61 | 0.69 |
| 1:E:42:TRP:CH2 | 1:E:67:MSE:HE1 | 2.27 | 0.69 |
| 1:K:34:ILE:HG22 | 1:K:36:PRO:HD2 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:266:ASP:OD1 | 1:I:98:ARG:HD2 | 1.92 | 0.68 |
| 1:K:14:PRO:HD2 | 1:K:51:ALA:O | 1.93 | 0.68 |
| 1:I:355:ILE:HG12 | 1:I:356:GLU:H | 1.58 | 0.68 |
| 1:J:357:MSE:CE | 1:J:362:LEU:HB2 | 2.14 | 0.68 |
| 1:B:327:LEU:HD11 | 1:B:357:MSE:HE3 | 1.73 | 0.68 |
| 1:K:216:GLY:HA2 | 1:K:236:ARG:HE | 1.57 | 0.68 |
| 1:A:121:VAL:HG12 | 1:A:122:ALA:N | 2.08 | 0.68 |
| 1:I:114:ILE:CG2 | 1:I:305:MSE:HE2 | 2.24 | 0.68 |
| 1:B:380:ARG:NE | 3:B:633:HOH:O | 2.26 | 0.68 |
| 1:K:188:TRP:CZ2 | 1:K:248:ARG:NH1 | 2.61 | 0.68 |
| 1:J:149:ASP:OD2 | 1:J:152:PHE:HE1 | 1.76 | 0.68 |
| 1:G:44:THR:HG21 | 1:G:201:VAL:HG21 | 1.76 | 0.68 |
| 1:B:169:VAL:HG22 | 1:B:225:HIS:HB2 | 1.76 | 0.68 |
| 1:D:10:THR:OG1 | 1:H:384:LYS:CD | 2.41 | 0.68 |
| 1:H:203:TRP:O | 1:H:207:LEU:HG | 1.93 | 0.68 |
| 1:I:98:ARG:HG3 | 1:I:99:ARG:NH1 | 2.09 | 0.68 |
| 1:L:34:ILE:HG22 | 1:L:36:PRO:CD | 2.17 | 0.68 |
| 1:I:198:ARG:HG2 | 1:I:203:TRP:CD1 | 2.29 | 0.68 |
| 1:A:373:SER:HB3 | 1:A:393:ASP:OD2 | 1.94 | 0.68 |
| 1:K:311:LEU:HD21 | 1:K:362:LEU:HD11 | 1.75 | 0.67 |
| 1:E:193:PRO:HD2 | 1:E:400:VAL:HG23 | 1.74 | 0.67 |
| 1:H:385:ASP:OD1 | 1:H:387:GLN:N | 2.26 | 0.67 |
| 1:H:197:LEU:HD12 | 1:H:198:ARG:N | 2.09 | 0.67 |
| 1:F:188:TRP:CZ2 | 1:F:248:ARG:NH1 | 2.62 | 0.67 |
| 1:G:295:TRP:HZ2 | 1:G:297:GLN:NE2 | 1.91 | 0.67 |
| 1:G:300:LEU:HD21 | 1:G:302:LEU:HD21 | 1.76 | 0.67 |
| 1:G:355:ILE:CD1 | 1:G:381:LEU:HD21 | 2.23 | 0.67 |
| 1:D:73:LEU:O | 1:D:85:THR:N | 2.15 | 0.67 |
| 1:I:339:ILE:HD13 | 1:I:344:ALA:HB2 | 1.74 | 0.67 |
| 1:C:144:HIS:CD2 | 1:C:277:PRO:CG | 2.76 | 0.67 |
| 1:G:120:PRO:O | 1:G:305:MSE:HB2 | 1.94 | 0.67 |
| 1:I:107:CYS:C | 1:I:111:HIS:HD1 | 1.98 | 0.67 |
| 1:I:337:LEU:HD13 | 1:I:346:CYS:HB2 | 1.76 | 0.67 |
| 1:H:399:ASP:OD2 | 3:H:619:HOH:O | 2.11 | 0.67 |
| 1:C:357:MSE:CE | 1:C:381:LEU:HD21 | 2.24 | 0.67 |
| 1:F:22:MSE:HE2 | 1:F:42:TRP:HH2 | 1.09 | 0.67 |
| 1:D:150:ARG:HH21 | 1:D:266:ASP:C | 1.96 | 0.67 |
| 1:K:327:LEU:HD13 | 1:K:357:MSE:HE3 | 1.73 | 0.67 |
| 1:G:146:LEU:HD22 | 1:G:275:THR:HG21 | 1.75 | 0.67 |
| 1:K:189:ARG:NH1 | 1:K:197:LEU:HD13 | 2.10 | 0.67 |
| 1:E:148:VAL:HA | 1:E:290:LEU:O | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:121:VAL:HB | 1:F:303:ARG:O | 1.95 | 0.67 |
| 1:D:193:PRO:HD2 | 1:D:400:VAL:HG23 | 1.75 | 0.67 |
| 1:I:289:ARG:HD3 | 1:J:297:GLN:CD | 2.15 | 0.67 |
| 1:J:41:ALA:HA | 1:J:44:THR:CG2 | 2.25 | 0.67 |
| 1:D:217:ASP:HB3 | 1:D:233:ARG:CD | 2.24 | 0.67 |
| 1:D:247:LEU:HD23 | 1:D:247:LEU:C | 2.15 | 0.67 |
| 1:E:40:THR:O | 1:E:44:THR:HG22 | 1.95 | 0.66 |
| 1:F:73:LEU:HD12 | 1:F:73:LEU:N | 2.09 | 0.66 |
| 1:B:14:PRO:HD3 | 1:B:52:VAL:HA | 1.75 | 0.66 |
| 1:H:385:ASP:OD1 | 1:H:387:GLN:HG2 | 1.96 | 0.66 |
| 1:E:297:GLN:OE1 | 1:F:289:ARG:HD3 | 1.96 | 0.66 |
| 1:D:104:ARG:HG3 | 1:D:135:PHE:HE1 | 1.59 | 0.66 |
| 1:B:149:ASP:OD2 | 1:B:152:PHE:CE2 | 2.49 | 0.66 |
| 1:K:312:GLU:OE1 | 1:K:346:CYS:N | 2.27 | 0.66 |
| 1:H:196:LEU:HD13 | 1:H:406:PHE:CZ | 2.31 | 0.66 |
| 1:B:40:THR:O | 1:B:44:THR:CG2 | 2.42 | 0.66 |
| 1:B:109:GLU:OE1 | 1:B:112:ARG:HD3 | 1.95 | 0.66 |
| 1:G:295:TRP:CZ2 | 1:G:297:GLN:NE2 | 2.64 | 0.66 |
| 1:K:267:SER:O | 1:K:268:MSE:HE2 | 1.96 | 0.66 |
| 1:G:307:VAL:HG13 | 1:G:311:LEU:HD11 | 1.76 | 0.66 |
| 1:D:49:ASP:C | 1:D:49:ASP:OD1 | 2.34 | 0.66 |
| 1:A:177:HIS:O | 1:A:181:PHE:CD2 | 2.49 | 0.66 |
| 1:A:48:THR:O | 1:A:49:ASP:OD1 | 2.13 | 0.66 |
| 1:K:188:TRP:CE2 | 1:K:248:ARG:NH1 | 2.64 | 0.66 |
| 1:J:206:LEU:C | 1:J:206:LEU:CD2 | 2.64 | 0.66 |
| 1:F:295:TRP:CZ2 | 1:F:297:GLN:HB3 | 2.31 | 0.66 |
| 1:J:381:LEU:HD11 | 1:J:389:LEU:HD21 | 1.76 | 0.66 |
| 1:E:156:HIS:NE2 | 1:F:380:ARG:CZ | 2.58 | 0.66 |
| 1:A:8:THR:HA | 1:A:57:GLY:HA2 | 1.78 | 0.66 |
| 1:K:381:LEU:HD23 | 1:K:381:LEU:C | 2.16 | 0.66 |
| 1:E:206:LEU:CD2 | 1:E:206:LEU:C | 2.64 | 0.66 |
| 1:H:146:LEU:HD13 | 1:H:293:THR:HA | 1.77 | 0.66 |
| 1:A:73:LEU:N | 1:A:85:THR:O | 2.29 | 0.65 |
| 1:I:178:ARG:HD2 | 1:I:207:LEU:CD1 | 2.26 | 0.65 |
| 1:C:306:ASN:OD1 | 1:C:308:PRO:HD2 | 1.95 | 0.65 |
| 1:F:365:LEU:HD21 | 1:F:375:LEU:HD12 | 1.77 | 0.65 |
| 1:B:247:LEU:HD23 | 1:B:248:ARG:N | 2.11 | 0.65 |
| 1:I:124:LEU:HD12 | 1:I:301:TRP:HB2 | 1.77 | 0.65 |
| 1:C:106:MSE:O | 1:C:110:LEU:HD12 | 1.93 | 0.65 |
| 1:I:45:LEU:HD11 | 1:I:199:PRO:CG | 2.24 | 0.65 |
| 1:B:169:VAL:HG22 | 1:B:225:HIS:CD2 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:148:VAL:HA | 1:D:290:LEU:O | 1.96 | 0.65 |
| 1:C:178:ARG:CG | 1:C:207:LEU:HD11 | 2.26 | 0.65 |
| 1:B:42:TRP:CZ2 | 1:B:90:PHE:CE1 | 2.85 | 0.65 |
| 1:I:193:PRO:HD2 | 1:I:400:VAL:HG23 | 1.79 | 0.65 |
| 1:G:327:LEU:C | 1:G:327:LEU:CD2 | 2.65 | 0.65 |
| 1:E:314:ARG:HD3 | 1:E:316:TYR:CZ | 2.32 | 0.65 |
| 1:G:98:ARG:CD | 1:L:264:GLY:HA2 | 2.27 | 0.65 |
| 1:B:292:ARG:NH1 | 1:B:294:THR:HG22 | 2.12 | 0.65 |
| 1:H:198:ARG:HD2 | 1:H:203:TRP:CE2 | 2.31 | 0.65 |
| 1:F:150:ARG:NH2 | 1:F:266:ASP:OD1 | 2.29 | 0.65 |
| 1:J:189:ARG:NH1 | 1:J:197:LEU:HD13 | 2.08 | 0.65 |
| 1:G:170:ARG:HD2 | 1:I:63:GLU:OE1 | 1.97 | 0.65 |
| 1:C:357:MSE:HE1 | 1:C:381:LEU:HD21 | 1.79 | 0.65 |
| 1:I:355:ILE:HD11 | 1:I:381:LEU:CD1 | 2.26 | 0.65 |
| 1:C:146:LEU:HD21 | 1:C:291:ALA:HB1 | 1.78 | 0.65 |
| 1:D:67:MSE:HE2 | 1:D:90:PHE:HB3 | 1.78 | 0.65 |
| 1:I:198:ARG:HD2 | 1:I:203:TRP:CE2 | 2.32 | 0.65 |
| 1:I:206:LEU:C | 1:I:206:LEU:CD2 | 2.65 | 0.65 |
| 1:I:337:LEU:HD11 | 1:I:344:ALA:HB1 | 1.79 | 0.65 |
| 1:G:69:LEU:HD12 | 1:G:69:LEU:C | 2.17 | 0.65 |
| 1:L:34:ILE:CG2 | 1:L:36:PRO:CD | 2.73 | 0.65 |
| 1:H:178:ARG:HG3 | 1:H:207:LEU:HD11 | 1.77 | 0.65 |
| 1:C:326:VAL:HG11 | 1:C:353:ALA:HA | 1.77 | 0.65 |
| 1:H:342:GLY:O | 1:H:343:ARG:HD2 | 1.97 | 0.65 |
| 1:G:178:ARG:HH21 | 1:G:200:GLN:NE2 | 1.94 | 0.65 |
| 1:J:74:ARG:CZ | 1:J:84:PRO:HB3 | 2.26 | 0.65 |
| 1:F:16:GLU:HA | 1:F:19:TRP:NE1 | 2.11 | 0.65 |
| 1:C:48:THR:O | 1:C:49:ASP:OD1 | 2.14 | 0.65 |
| 1:B:292:ARG:HH11 | 1:B:294:THR:HG22 | 1.61 | 0.65 |
| 1:F:103:LEU:HD22 | 2:F:501:ACO:H121 | 1.79 | 0.65 |
| 1:L:178:ARG:HH21 | 1:L:200:GLN:NE2 | 1.95 | 0.65 |
| 1:E:44:THR:HG21 | 1:E:201:VAL:CG1 | 2.20 | 0.64 |
| 1:A:121:VAL:HG22 | 1:A:304:ILE:HA | 1.78 | 0.64 |
| 1:G:9:VAL:CG1 | 1:G:54:VAL:HG13 | 2.25 | 0.64 |
| 1:K:192:VAL:HG11 | 1:K:403:GLN:HB2 | 1.79 | 0.64 |
| 1:I:23:PHE:HE1 | 1:I:38:SER:OG | 1.80 | 0.64 |
| 1:I:217:ASP:CG | 1:I:233:ARG:NH1 | 2.50 | 0.64 |
| 1:H:354:GLU:CA | 1:H:384:LYS:HZ3 | 2.03 | 0.64 |
| 1:C:148:VAL:HG13 | 1:C:290:LEU:C | 2.17 | 0.64 |
| 1:B:85:THR:HG23 | 1:B:121:VAL:C | 2.14 | 0.64 |
| 1:H:146:LEU:HD22 | 1:H:146:LEU:N | 2.11 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:246:GLU:OE1 | 1:D:248:ARG:NE | 2.19 | 0.64 |
| 1:B:246:GLU:OE1 | 1:B:248:ARG:NE | 2.22 | 0.64 |
| 1:A:123:ALA:HB1 | 1:A:300:LEU:HD11 | 1.79 | 0.64 |
| 1:G:250:VAL:HG12 | 1:G:250:VAL:O | 1.95 | 0.64 |
| 1:L:319:GLU:N | 1:L:319:GLU:OE1 | 2.30 | 0.64 |
| 1:E:148:VAL:HG22 | 1:E:291:ALA:HA | 0.72 | 0.64 |
| 1:I:320:VAL:HA | 1:J:319:GLU:O | 1.98 | 0.64 |
| 1:J:72:ASP:OD1 | 1:J:74:ARG:NH1 | 2.30 | 0.64 |
| 1:F:35:GLY:N | 1:F:36:PRO:HD2 | 2.11 | 0.64 |
| 1:D:197:LEU:HD12 | 3:D:608:HOH:O | 1.98 | 0.64 |
| 1:E:227:ASP:HB3 | 1:E:250:VAL:HG22 | 1.78 | 0.64 |
| 1:J:43:ARG:HH11 | 1:J:43:ARG:CA | 2.04 | 0.64 |
| 1:J:44:THR:CG2 | 1:J:201:VAL:HG11 | 2.27 | 0.64 |
| 1:I:103:LEU:HD22 | 2:I:501:ACO:H121 | 1.79 | 0.64 |
| 1:H:34:ILE:CB | 1:H:37:GLU:CD | 2.63 | 0.64 |
| 1:J:227:ASP:HB2 | 1:J:254:ALA:HB2 | 1.80 | 0.64 |
| 1:C:148:VAL:HG21 | 1:C:291:ALA:HB2 | 1.80 | 0.64 |
| 1:E:145:GLU:HB2 | 1:E:295:TRP:HB3 | 1.78 | 0.64 |
| 1:I:127:SER:HB3 | 2:I:501:ACO:H22 | 1.80 | 0.64 |
| 1:D:259:TRP:O | 1:D:263:ILE:HG12 | 1.97 | 0.64 |
| 1:C:355:ILE:CD1 | 1:C:381:LEU:HD21 | 2.24 | 0.64 |
| 1:J:143:LEU:HD21 | 1:J:404:THR:HG21 | 1.77 | 0.64 |
| 1:A:34:ILE:HB | 1:A:37:GLU:HG2 | 1.78 | 0.64 |
| 1:B:381:LEU:HD23 | 1:B:381:LEU:C | 2.18 | 0.64 |
| 1:H:34:ILE:HG22 | 1:H:36:PRO:HD2 | 1.79 | 0.64 |
| 1:F:98:ARG:HG3 | 1:F:99:ARG:HH11 | 1.63 | 0.64 |
| 1:K:247:LEU:HD23 | 1:K:248:ARG:N | 2.11 | 0.64 |
| 1:A:42:TRP:CD1 | 1:A:69:LEU:CD2 | 2.81 | 0.64 |
| 1:D:72:ASP:O | 1:D:73:LEU:HD23 | 1.98 | 0.64 |
| 1:C:54:VAL:HG11 | 1:C:102:LEU:HD22 | 1.79 | 0.64 |
| 1:K:193:PRO:CD | 1:K:400:VAL:HG13 | 2.18 | 0.63 |
| 1:B:107:CYS:O | 1:B:111:HIS:ND1 | 2.26 | 0.63 |
| 1:D:139:PRO:HB2 | 3:D:627:HOH:O | 1.97 | 0.63 |
| 1:H:148:VAL:HG22 | 1:H:291:ALA:HA | 1.80 | 0.63 |
| 1:I:303:ARG:HH11 | 1:I:305:MSE:SE | 2.31 | 0.63 |
| 1:D:98:ARG:HD2 | 1:E:264:GLY:CA | 2.28 | 0.63 |
| 1:B:85:THR:HG22 | 1:B:86:ALA:N | 2.14 | 0.63 |
| 1:D:72:ASP:OD1 | 1:D:74:ARG:NH1 | 2.30 | 0.63 |
| 1:J:194:GLY:O | 1:J:405:ALA:HB2 | 1.99 | 0.63 |
| 1:H:312:GLU:HG2 | 1:H:344:ALA:O | 1.99 | 0.63 |
| 1:F:74:ARG:HB3 | 1:F:82:VAL:CG1 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:146:LEU:O | 1:E:272:SER:HA | 1.97 | 0.63 |
| 1:A:121:VAL:CG1 | 1:A:122:ALA:N | 2.62 | 0.63 |
| 1:K:188:TRP:NE1 | 1:K:403:GLN:OE1 | 2.30 | 0.63 |
| 1:D:144:HIS:NE2 | 1:D:296:ARG:NH1 | 2.47 | 0.63 |
| 1:C:110:LEU:HD12 | 1:C:110:LEU:N | 2.13 | 0.63 |
| 1:F:34:ILE:HB | 1:F:37:GLU:CG | 2.28 | 0.63 |
| 1:J:196:LEU:HG | 1:J:405:ALA:CB | 2.29 | 0.63 |
| 1:I:375:LEU:HD21 | 1:J:283:HIS:CE1 | 2.34 | 0.63 |
| 1:D:42:TRP:NE1 | 1:D:90:PHE:CE2 | 2.65 | 0.63 |
| 1:A:98:ARG:HH11 | 1:A:99:ARG:NH2 | 1.97 | 0.63 |
| 1:I:73:LEU:HB2 | 1:I:85:THR:O | 1.98 | 0.63 |
| 1:J:45:LEU:HD11 | 1:J:199:PRO:HG2 | 1.80 | 0.63 |
| 1:H:306:ASN:OD1 | 1:H:308:PRO:HD2 | 1.98 | 0.63 |
| 1:C:404:THR:HG22 | 1:C:405:ALA:O | 1.99 | 0.63 |
| 1:C:178:ARG:NH1 | 1:C:207:LEU:HD12 | 2.12 | 0.62 |
| 1:C:121:VAL:CG1 | 1:C:304:ILE:HA | 2.28 | 0.62 |
| 1:J:312:GLU:HG2 | 1:J:344:ALA:O | 1.98 | 0.62 |
| 1:C:247:LEU:HD13 | 3:C:650:HOH:O | 1.98 | 0.62 |
| 1:B:145:GLU:OE2 | 1:B:295:TRP:CB | 2.47 | 0.62 |
| 1:I:150:ARG:HG2 | 1:I:269:GLU:O | 1.99 | 0.62 |
| 1:F:355:ILE:HD11 | 1:F:381:LEU:HD21 | 1.81 | 0.62 |
| 1:I:199:PRO:HB2 | 1:I:201:VAL:HG12 | 1.80 | 0.62 |
| 1:E:127:SER:HB3 | 2:E:501:ACO:C2P | 2.29 | 0.62 |
| 1:I:148:VAL:HG22 | 1:I:290:LEU:O | 2.00 | 0.62 |
| 1:D:373:SER:HB3 | 1:D:393:ASP:OD2 | 2.00 | 0.62 |
| 1:F:98:ARG:CG | 1:F:99:ARG:NH1 | 2.62 | 0.62 |
| 1:B:45:LEU:CD1 | 1:B:199:PRO:HG2 | 2.26 | 0.62 |
| 1:I:38:SER:HB2 | 1:I:42:TRP:CE2 | 2.35 | 0.62 |
| 1:E:355:ILE:HD11 | 1:E:381:LEU:HD13 | 1.80 | 0.62 |
| 1:C:127:SER:CB | 2:C:501:ACO:H22 | 2.29 | 0.62 |
| 1:J:98:ARG:HD2 | 1:K:264:GLY:CA | 2.29 | 0.62 |
| 1:D:114:ILE:HG22 | 1:D:305:MSE:HE2 | 1.80 | 0.62 |
| 1:I:247:LEU:HD23 | 1:I:248:ARG:N | 2.13 | 0.62 |
| 1:A:74:ARG:O | 1:A:196:LEU:HD23 | 1.98 | 0.62 |
| 1:K:314:ARG:HD3 | 1:K:316:TYR:CZ | 2.35 | 0.62 |
| 1:I:52:VAL:CG1 | 1:I:110:LEU:HD21 | 2.29 | 0.62 |
| 1:D:54:VAL:HG11 | 1:D:102:LEU:HD13 | 1.81 | 0.62 |
| 1:F:334:ARG:HD3 | 1:F:351:ALA:O | 1.99 | 0.62 |
| 1:K:244:VAL:CG2 | 1:K:273:ILE:HG12 | 2.25 | 0.62 |
| 1:B:240:LYS:HB3 | 1:B:269:GLU:HB2 | 1.81 | 0.62 |
| 2:C:501:ACO:H141 | 2:C:501:ACO:O5P | 1.98 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:314:ARG:HH11 | 1:K:314:ARG:CG | 2.13 | 0.62 |
| 1:E:314:ARG:NH1 | 1:E:315:GLY:O | 2.31 | 0.62 |
| 1:D:144:HIS:HD2 | 1:D:277:PRO:HG3 | 1.64 | 0.62 |
| 1:I:306:ASN:OD1 | 1:I:308:PRO:HD2 | 2.00 | 0.62 |
| 1:L:387:GLN:HE22 | 1:L:391:ARG:NH2 | 1.97 | 0.62 |
| 1:G:167:SER:N | 3:G:603:HOH:O | 2.33 | 0.62 |
| 1:I:107:CYS:HB3 | 1:I:111:HIS:CE1 | 2.34 | 0.61 |
| 1:G:325:THR:O | 1:G:337:LEU:N | 2.26 | 0.61 |
| 1:J:247:LEU:HD23 | 1:J:248:ARG:N | 2.15 | 0.61 |
| 1:B:381:LEU:HD23 | 1:B:382:ARG:N | 2.15 | 0.61 |
| 1:B:98:ARG:HD2 | 1:D:264:GLY:CA | 2.30 | 0.61 |
| 1:F:110:LEU:O | 1:F:114:ILE:HG13 | 1.99 | 0.61 |
| 1:G:381:LEU:C | 1:G:381:LEU:CD2 | 2.68 | 0.61 |
| 1:E:247:LEU:HD23 | 1:E:248:ARG:N | 2.14 | 0.61 |
| 1:I:169:VAL:HG13 | 1:I:224:LEU:C | 2.21 | 0.61 |
| 1:B:23:PHE:HE1 | 1:B:42:TRP:HZ3 | 1.47 | 0.61 |
| 1:H:145:GLU:HB3 | 1:H:295:TRP:HB3 | 1.81 | 0.61 |
| 1:G:121:VAL:HG12 | 1:G:304:ILE:HA | 1.82 | 0.61 |
| 1:I:52:VAL:CG1 | 1:I:110:LEU:CD2 | 2.76 | 0.61 |
| 1:A:144:HIS:CE1 | 1:A:296:ARG:NH1 | 2.68 | 0.61 |
| 1:G:218:ARG:HH21 | 1:G:239:LEU:HD21 | 1.65 | 0.61 |
| 1:A:173:ARG:HG3 | 1:C:24:LEU:HD13 | 1.82 | 0.61 |
| 1:G:100:ARG:NH1 | 1:L:167:SER:OG | 2.34 | 0.61 |
| 1:E:144:HIS:CD2 | 1:E:277:PRO:HG3 | 2.35 | 0.61 |
| 1:F:206:LEU:CD2 | 1:F:206:LEU:C | 2.68 | 0.61 |
| 1:H:354:GLU:CB | 1:H:384:LYS:NZ | 2.63 | 0.61 |
| 1:F:303:ARG:NH2 | 1:F:359:ARG:NH1 | 2.49 | 0.61 |
| 1:F:242:ALA:HB2 | 1:F:268:MSE:HG3 | 1.82 | 0.61 |
| 1:I:289:ARG:CD | 1:J:297:GLN:CD | 2.69 | 0.61 |
| 1:K:247:LEU:C | 1:K:247:LEU:HD23 | 2.20 | 0.61 |
| 1:E:144:HIS:CE1 | 1:E:296:ARG:CD | 2.83 | 0.61 |
| 1:B:383:THR:CG2 | 1:B:389:LEU:HD21 | 2.30 | 0.61 |
| 1:K:76:THR:O | 1:K:193:PRO:HA | 1.99 | 0.61 |
| 1:F:14:PRO:CD | 1:F:51:ALA:O | 2.48 | 0.61 |
| 1:G:123:ALA:HB2 | 1:G:302:LEU:CD2 | 2.30 | 0.61 |
| 1:B:149:ASP:OD2 | 1:B:152:PHE:HE2 | 1.83 | 0.61 |
| 1:E:19:TRP:N | 1:E:20:PRO:HD2 | 2.16 | 0.61 |
| 1:J:289:ARG:O | 1:J:292:ARG:HG3 | 1.99 | 0.61 |
| 1:J:203:TRP:C | 1:J:207:LEU:HD13 | 2.19 | 0.61 |
| 1:C:101:GLY:HA2 | 2:C:501:ACO:O2A | 2.01 | 0.61 |
| 1:B:49:ASP:C | 1:B:49:ASP:OD1 | 2.38 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:107:CYS:O | 1:E:111:HIS:ND1 | 2.34 | 0.61 |
| 1:H:19:TRP:N | 1:H:20:PRO:HD2 | 2.16 | 0.61 |
| 1:C:295:TRP:CZ2 | 1:C:297:GLN:NE2 | 2.69 | 0.61 |
| 1:I:293:THR:O | 3:I:608:HOH:O | 2.17 | 0.61 |
| 1:B:109:GLU:O | 1:B:112:ARG:HG2 | 2.01 | 0.61 |
| 1:G:302:LEU:HD11 | 1:G:367:LEU:HD11 | 1.83 | 0.61 |
| 1:G:311:LEU:HD22 | 1:G:346:CYS:SG | 2.40 | 0.61 |
| 1:D:177:HIS:HB3 | 1:D:180:GLU:HG3 | 1.81 | 0.61 |
| 1:D:16:GLU:HA | 1:D:19:TRP:CD1 | 2.36 | 0.61 |
| 1:A:45:LEU:HD13 | 1:A:71:MSE:HE2 | 1.83 | 0.61 |
| 1:I:289:ARG:CD | 1:J:297:GLN:OE1 | 2.48 | 0.60 |
| 1:B:198:ARG:HD2 | 1:B:203:TRP:CE2 | 2.36 | 0.60 |
| 1:G:77:VAL:HB | 1:G:78:PRO:HD2 | 1.82 | 0.60 |
| 1:E:103:LEU:HD22 | 2:E:501:ACO:H142 | 1.83 | 0.60 |
| 1:B:42:TRP:HZ2 | 1:B:90:PHE:CD1 | 2.20 | 0.60 |
| 1:G:289:ARG:HH11 | 1:H:298:ASP:CG | 2.03 | 0.60 |
| 1:G:34:ILE:CG2 | 1:G:36:PRO:HD2 | 2.31 | 0.60 |
| 1:I:247:LEU:C | 1:I:247:LEU:HD23 | 2.21 | 0.60 |
| 1:D:177:HIS:ND1 | 1:D:180:GLU:OE1 | 2.20 | 0.60 |
| 1:H:150:ARG:NH1 | 1:H:150:ARG:O | 2.33 | 0.60 |
| 1:H:146:LEU:CD2 | 1:H:275:THR:HG22 | 2.26 | 0.60 |
| 1:I:167:SER:OG | 1:L:100:ARG:NH1 | 2.33 | 0.60 |
| 1:D:148:VAL:CG1 | 1:D:290:LEU:HB3 | 2.32 | 0.60 |
| 1:C:106:MSE:C | 1:C:110:LEU:HD13 | 2.19 | 0.60 |
| 1:H:267:SER:C | 1:H:268:MSE:HE2 | 2.22 | 0.60 |
| 1:G:303:ARG:HH12 | 1:G:305:MSE:SE | 2.32 | 0.60 |
| 1:F:357:MSE:SE | 1:F:381:LEU:HD13 | 2.51 | 0.60 |
| 1:H:169:VAL:CG1 | 1:H:224:LEU:C | 2.55 | 0.60 |
| 1:H:107:CYS:C | 1:H:111:HIS:HD1 | 2.04 | 0.60 |
| 1:F:170:ARG:O | 1:F:172:VAL:HG13 | 2.02 | 0.60 |
| 1:I:289:ARG:NH1 | 1:J:298:ASP:OD2 | 2.35 | 0.60 |
| 1:K:206:LEU:C | 1:K:206:LEU:CD2 | 2.70 | 0.60 |
| 1:B:246:GLU:CD | 1:B:248:ARG:HE | 2.03 | 0.60 |
| 1:K:184:ILE:HG21 | 1:K:228:GLY:HA2 | 1.82 | 0.60 |
| 1:B:34:ILE:HB | 1:B:37:GLU:HG2 | 1.82 | 0.60 |
| 1:H:34:ILE:CB | 1:H:37:GLU:OE1 | 2.50 | 0.60 |
| 1:D:33:PHE:CE1 | 1:D:38:SER:HB2 | 2.36 | 0.60 |
| 1:L:381:LEU:C | 1:L:381:LEU:HD12 | 2.21 | 0.60 |
| 1:B:34:ILE:HG22 | 1:B:36:PRO:HD2 | 1.82 | 0.60 |
| 1:H:314:ARG:NH1 | 1:H:366:TYR:O | 2.35 | 0.60 |
| 1:K:337:LEU:HD13 | 1:K:346:CYS:HB2 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:98:ARG:HH11 | 1:F:99:ARG:NH2 | 2.00 | 0.60 |
| 1:F:121:VAL:HA | 1:F:305:MSE:CG | 2.20 | 0.59 |
| 1:J:35:GLY:N | 1:J:36:PRO:HD2 | 2.17 | 0.59 |
| 1:J:193:PRO:HG2 | 1:J:400:VAL:HG23 | 1.82 | 0.59 |
| 1:F:303:ARG:HH22 | 1:F:359:ARG:NH1 | 2.00 | 0.59 |
| 1:A:178:ARG:NH1 | 1:A:207:LEU:HD12 | 2.16 | 0.59 |
| 1:E:296:ARG:HB3 | 1:F:293:THR:HB | 1.84 | 0.59 |
| 1:E:319:GLU:O | 1:F:320:VAL:HA | 2.02 | 0.59 |
| 1:H:65:VAL:HG11 | 1:H:97:HIS:CE1 | 2.37 | 0.59 |
| 1:D:10:THR:CG2 | 1:H:384:LYS:CD | 2.77 | 0.59 |
| 1:C:297:GLN:OE1 | 1:D:289:ARG:CZ | 2.50 | 0.59 |
| 1:B:383:THR:HG22 | 1:B:389:LEU:HD21 | 1.83 | 0.59 |
| 1:K:19:TRP:HZ3 | 1:K:42:TRP:HE3 | 1.50 | 0.59 |
| 1:E:33:PHE:CD1 | 1:E:34:ILE:N | 2.70 | 0.59 |
| 1:J:270:ARG:NH1 | 1:J:270:ARG:HB2 | 2.17 | 0.59 |
| 1:J:271:ILE:N | 1:J:271:ILE:CD1 | 2.65 | 0.59 |
| 1:B:131:ILE:HG12 | 2:B:501:ACO:C6A | 2.32 | 0.59 |
| 1:F:303:ARG:NH2 | 1:F:359:ARG:HH11 | 2.01 | 0.59 |
| 1:H:150:ARG:HD3 | 1:H:150:ARG:C | 2.22 | 0.59 |
| 1:A:132:TYR:OH | 2:A:501:ACO:H31 | 2.03 | 0.59 |
| 1:E:114:ILE:CG2 | 1:E:119:TYR:HB2 | 2.33 | 0.59 |
| 1:H:206:LEU:C | 1:H:206:LEU:CD2 | 2.70 | 0.59 |
| 1:A:314:ARG:NH1 | 1:A:316:TYR:CD2 | 2.71 | 0.59 |
| 1:I:99:ARG:NH1 | 2:I:501:ACO:O5A | 2.35 | 0.59 |
| 1:D:234:VAL:HG23 | 3:D:626:HOH:O | 2.03 | 0.59 |
| 1:B:16:GLU:HA | 1:B:19:TRP:CD1 | 2.37 | 0.59 |
| 1:D:247:LEU:HD23 | 1:D:248:ARG:N | 2.18 | 0.59 |
| 1:I:250:VAL:HG23 | 1:I:251:THR:HG23 | 1.85 | 0.59 |
| 1:B:169:VAL:CG2 | 1:B:225:HIS:HB2 | 2.32 | 0.59 |
| 1:H:385:ASP:OD1 | 1:H:386:SER:N | 2.36 | 0.59 |
| 1:I:225:HIS:CE1 | 1:I:226:PRO:HD2 | 2.38 | 0.59 |
| 1:C:16:GLU:HA | 1:C:19:TRP:CD1 | 2.38 | 0.59 |
| 1:D:10:THR:HG21 | 1:H:384:LYS:CE | 2.33 | 0.59 |
| 1:I:289:ARG:HD3 | 1:J:297:GLN:OE1 | 2.02 | 0.59 |
| 1:D:52:VAL:HG13 | 1:D:110:LEU:CD2 | 2.32 | 0.59 |
| 1:D:98:ARG:HD2 | 1:E:264:GLY:HA2 | 1.85 | 0.59 |
| 1:H:34:ILE:HG13 | 1:H:37:GLU:OE1 | 2.03 | 0.58 |
| 1:A:42:TRP:NE1 | 1:A:69:LEU:HD21 | 2.18 | 0.58 |
| 1:B:169:VAL:HG22 | 1:B:225:HIS:CG | 2.38 | 0.58 |
| 1:F:71:MSE:O | 1:F:73:LEU:HD13 | 2.03 | 0.58 |
| 1:E:142:THR:HG22 | 1:E:144:HIS:CD2 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:69:LEU:HD12 | 1:G:69:LEU:O | 2.02 | 0.58 |
| 1:E:247:LEU:HD23 | 1:E:247:LEU:C | 2.24 | 0.58 |
| 1:H:127:SER:HB3 | 2:H:501:ACO:H22 | 1.84 | 0.58 |
| 1:L:329:VAL:O | 1:L:332:GLY:N | 2.30 | 0.58 |
| 1:B:167:SER:N | 3:B:621:HOH:O | 2.35 | 0.58 |
| 1:L:330:SER:O | 1:L:331:ASP:HB2 | 2.03 | 0.58 |
| 1:C:107:CYS:C | 1:C:111:HIS:HD1 | 1.98 | 0.58 |
| 1:A:173:ARG:HB2 | 1:A:176:GLU:OE1 | 2.03 | 0.58 |
| 1:C:355:ILE:HG12 | 1:C:381:LEU:HD11 | 1.85 | 0.58 |
| 1:D:150:ARG:NH2 | 1:D:266:ASP:C | 2.55 | 0.58 |
| 1:G:9:VAL:HG11 | 1:G:54:VAL:CG1 | 2.32 | 0.58 |
| 1:F:326:VAL:CG1 | 1:F:353:ALA:HA | 2.32 | 0.58 |
| 1:A:16:GLU:HA | 1:A:19:TRP:CD1 | 2.38 | 0.58 |
| 1:E:148:VAL:CG2 | 1:E:291:ALA:CA | 2.48 | 0.58 |
| 1:A:34:ILE:HG22 | 1:A:36:PRO:CD | 2.32 | 0.58 |
| 1:G:33:PHE:O | 1:G:34:ILE:CG1 | 2.51 | 0.58 |
| 1:J:247:LEU:C | 1:J:247:LEU:HD23 | 2.23 | 0.58 |
| 1:A:306:ASN:OD1 | 1:A:308:PRO:HD2 | 2.02 | 0.58 |
| 1:E:44:THR:HG23 | 1:E:45:LEU:HG | 1.86 | 0.58 |
| 1:J:52:VAL:CG1 | 1:J:110:LEU:HD21 | 2.34 | 0.58 |
| 1:I:19:TRP:N | 1:I:20:PRO:HD2 | 2.18 | 0.58 |
| 1:H:34:ILE:CG2 | 1:H:36:PRO:HD2 | 2.33 | 0.58 |
| 1:C:150:ARG:O | 1:C:150:ARG:NH1 | 2.36 | 0.58 |
| 1:K:188:TRP:CH2 | 1:K:248:ARG:NH1 | 2.71 | 0.58 |
| 1:A:187:ARG:O | 1:A:191:GLN:HG3 | 2.04 | 0.58 |
| 1:J:98:ARG:CD | 1:K:264:GLY:HA2 | 2.34 | 0.58 |
| 1:F:320:VAL:HG11 | 1:F:395:ALA:HA | 1.86 | 0.58 |
| 1:H:79:GLY:O | 1:H:80:GLU:HB2 | 2.02 | 0.58 |
| 1:I:355:ILE:HD11 | 1:I:381:LEU:HG | 1.84 | 0.58 |
| 1:A:327:LEU:CD1 | 1:A:355:ILE:HG23 | 2.33 | 0.58 |
| 1:H:150:ARG:NH2 | 1:H:266:ASP:OD1 | 2.37 | 0.58 |
| 1:I:193:PRO:CG | 1:I:400:VAL:HG23 | 2.33 | 0.58 |
| 2:I:501:ACO:O8A | 2:I:501:ACO:H4B | 2.04 | 0.58 |
| 1:D:218:ARG:HH21 | 1:D:239:LEU:HD21 | 1.69 | 0.58 |
| 1:J:273:ILE:HG12 | 1:J:274:ILE:N | 2.18 | 0.57 |
| 1:E:199:PRO:HD2 | 1:E:202:LEU:HD12 | 1.85 | 0.57 |
| 1:F:242:ALA:HB3 | 1:F:271:ILE:CD1 | 2.35 | 0.57 |
| 1:J:400:VAL:HG23 | 1:J:400:VAL:O | 2.04 | 0.57 |
| 1:H:107:CYS:HB3 | 1:H:111:HIS:CE1 | 2.39 | 0.57 |
| 1:E:8:THR:O | 1:E:57:GLY:N | 2.37 | 0.57 |
| 1:D:145:GLU:OE2 | 1:D:295:TRP:HB3 | 2.02 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:146:LEU:HD13 | 1:A:275:THR:HG22 | 1.85 | 0.57 |
| 1:G:225:HIS:CG | 1:G:226:PRO:HD2 | 2.38 | 0.57 |
| 1:K:69:LEU:HD12 | 1:K:69:LEU:O | 2.03 | 0.57 |
| 1:J:102:LEU:O | 1:J:103:LEU:C | 2.42 | 0.57 |
| 1:D:33:PHE:O | 1:D:34:ILE:HD13 | 2.04 | 0.57 |
| 1:C:198:ARG:HD2 | 1:C:203:TRP:CE2 | 2.39 | 0.57 |
| 1:J:16:GLU:HA | 1:J:19:TRP:CD1 | 2.39 | 0.57 |
| 1:C:110:LEU:CD1 | 1:C:110:LEU:H | 2.17 | 0.57 |
| 1:E:156:HIS:NE2 | 1:F:380:ARG:NH2 | 2.52 | 0.57 |
| 1:H:326:VAL:HG21 | 1:H:352:ALA:O | 2.04 | 0.57 |
| 1:A:361:VAL:HG13 | 1:A:375:LEU:HD13 | 1.85 | 0.57 |
| 1:I:225:HIS:ND1 | 1:I:226:PRO:HD2 | 2.18 | 0.57 |
| 1:E:144:HIS:CE1 | 1:E:296:ARG:CG | 2.88 | 0.57 |
| 1:K:131:ILE:HG12 | 2:K:501:ACO:C6A | 2.34 | 0.57 |
| 1:I:149:ASP:OD2 | 1:I:152:PHE:CD1 | 2.55 | 0.57 |
| 1:E:69:LEU:O | 1:E:69:LEU:HD12 | 2.04 | 0.57 |
| 1:H:225:HIS:CG | 1:H:226:PRO:HD2 | 2.40 | 0.57 |
| 1:C:52:VAL:CG2 | 1:C:110:LEU:CD1 | 2.55 | 0.57 |
| 1:F:71:MSE:C | 1:F:73:LEU:CD1 | 2.72 | 0.57 |
| 1:G:16:GLU:HA | 1:G:19:TRP:CD1 | 2.39 | 0.57 |
| 1:B:77:VAL:HB | 1:B:78:PRO:HD2 | 1.86 | 0.57 |
| 1:F:250:VAL:HG23 | 1:F:251:THR:HG23 | 1.86 | 0.57 |
| 1:I:357:MSE:HE2 | 1:I:381:LEU:CG | 2.31 | 0.57 |
| 1:G:65:VAL:CG1 | 1:G:97:HIS:CE1 | 2.86 | 0.57 |
| 1:C:134:ARG:NH1 | 2:C:501:ACO:C1B | 2.67 | 0.57 |
| 1:D:18:ASP:O | 1:D:22:MSE:HG3 | 2.05 | 0.57 |
| 1:K:198:ARG:HG2 | 1:K:203:TRP:CD1 | 2.40 | 0.57 |
| 1:I:375:LEU:O | 1:I:380:ARG:HB2 | 2.05 | 0.57 |
| 1:B:247:LEU:C | 1:B:247:LEU:HD23 | 2.25 | 0.57 |
| 1:H:148:VAL:HG21 | 1:H:281:LEU:HD21 | 1.86 | 0.57 |
| 1:B:193:PRO:O | 1:B:402:VAL:HG23 | 2.05 | 0.57 |
| 1:E:387:GLN:HE22 | 1:E:391:ARG:NH2 | 2.03 | 0.57 |
| 1:D:127:SER:H | 2:D:501:ACO:H21 | 1.69 | 0.57 |
| 1:G:242:ALA:HB2 | 1:G:268:MSE:HG3 | 1.86 | 0.56 |
| 1:H:169:VAL:HG21 | 1:H:225:HIS:HB2 | 1.86 | 0.56 |
| 1:H:197:LEU:HD12 | 1:H:198:ARG:H | 1.69 | 0.56 |
| 1:K:355:ILE:CD1 | 1:K:381:LEU:HD21 | 2.34 | 0.56 |
| 1:F:34:ILE:HB | 1:F:37:GLU:CD | 2.24 | 0.56 |
| 1:A:34:ILE:HB | 1:A:37:GLU:OE1 | 2.05 | 0.56 |
| 1:G:311:LEU:N | 1:G:311:LEU:HD12 | 2.20 | 0.56 |
| 1:D:16:GLU:O | 1:D:19:TRP:HD1 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:43:ARG:HH11 | 1:B:43:ARG:HA | 1.69 | 0.56 |
| 1:A:50:GLY:HA2 | 1:A:70:TYR:CE2 | 2.40 | 0.56 |
| 1:K:158:ASP:OD2 | 3:K:604:HOH:O | 2.17 | 0.56 |
| 1:G:222:ALA:HA | 1:G:230:ALA:O | 2.04 | 0.56 |
| 1:F:242:ALA:HB3 | 1:F:271:ILE:HD13 | 1.88 | 0.56 |
| 1:H:109:GLU:CD | 1:H:112:ARG:HD3 | 2.26 | 0.56 |
| 1:K:292:ARG:CG | 3:K:605:HOH:O | 2.54 | 0.56 |
| 1:A:83:LEU:HD21 | 1:A:313:ALA:HB1 | 1.86 | 0.56 |
| 1:K:242:ALA:HB2 | 1:K:268:MSE:SE | 2.55 | 0.56 |
| 1:A:381:LEU:C | 1:A:381:LEU:HD12 | 2.26 | 0.56 |
| 1:G:34:ILE:HB | 1:G:37:GLU:HG2 | 1.87 | 0.56 |
| 1:J:217:ASP:HB3 | 1:J:233:ARG:HD2 | 1.87 | 0.56 |
| 1:I:323:PHE:CG | 1:I:391:ARG:HD3 | 2.39 | 0.56 |
| 1:D:193:PRO:CG | 1:D:400:VAL:CG2 | 2.84 | 0.56 |
| 1:E:193:PRO:CG | 1:E:400:VAL:HG23 | 2.35 | 0.56 |
| 1:J:41:ALA:C | 1:J:44:THR:HG22 | 2.26 | 0.56 |
| 1:J:142:THR:O | 1:J:277:PRO:HD3 | 2.05 | 0.56 |
| 1:I:225:HIS:CG | 1:I:226:PRO:HD2 | 2.40 | 0.56 |
| 1:A:85:THR:HG23 | 1:A:121:VAL:C | 2.25 | 0.56 |
| 1:J:41:ALA:CA | 1:J:44:THR:HG22 | 2.36 | 0.56 |
| 1:B:144:HIS:CE1 | 1:B:296:ARG:NH1 | 2.63 | 0.56 |
| 1:I:342:GLY:O | 1:I:343:ARG:CG | 2.54 | 0.56 |
| 1:I:342:GLY:O | 1:I:343:ARG:HG3 | 2.05 | 0.56 |
| 1:J:107:CYS:O | 1:J:111:HIS:ND1 | 2.38 | 0.56 |
| 1:K:324:SER:O | 1:K:325:THR:HB | 2.04 | 0.56 |
| 1:C:267:SER:O | 1:C:268:MSE:HE2 | 2.06 | 0.56 |
| 1:H:196:LEU:HD12 | 1:H:406:PHE:CE2 | 2.41 | 0.56 |
| 1:I:150:ARG:HD3 | 1:I:268:MSE:O | 2.06 | 0.56 |
| 1:D:193:PRO:O | 1:D:402:VAL:HG23 | 2.06 | 0.55 |
| 1:B:83:LEU:HD21 | 1:B:313:ALA:HB1 | 1.87 | 0.55 |
| 1:I:48:THR:O | 1:I:49:ASP:OD1 | 2.24 | 0.55 |
| 1:J:127:SER:HB3 | 2:J:501:ACO:H22 | 1.89 | 0.55 |
| 1:I:296:ARG:HD3 | 1:J:293:THR:OG1 | 2.05 | 0.55 |
| 1:B:52:VAL:CG1 | 1:B:113:ARG:NH1 | 2.70 | 0.55 |
| 1:C:83:LEU:HD21 | 1:C:313:ALA:HB1 | 1.89 | 0.55 |
| 1:B:38:SER:O | 1:B:39:ALA:C | 2.45 | 0.55 |
| 1:D:58:ALA:CB | 1:H:384:LYS:HG3 | 2.37 | 0.55 |
| 1:A:355:ILE:HD11 | 1:A:381:LEU:CD1 | 2.28 | 0.55 |
| 1:D:43:ARG:NH1 | 1:D:43:ARG:HA | 2.16 | 0.55 |
| 1:J:314:ARG:HD3 | 1:J:316:TYR:CZ | 2.41 | 0.55 |
| 1:K:134:ARG:NH1 | 2:K:501:ACO:H1B | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:178:ARG:O | 1:E:182:GLU:HG3 | 2.07 | 0.55 |
| 1:E:43:ARG:HH11 | 1:E:43:ARG:HA | 1.69 | 0.55 |
| 1:E:208:ALA:O | 1:E:211:LYS:HG2 | 2.06 | 0.55 |
| 1:E:221:PHE:O | 1:E:232:TYR:CD1 | 2.59 | 0.55 |
| 1:C:356:GLU:C | 1:C:381:LEU:HD12 | 2.26 | 0.55 |
| 1:I:356:GLU:OE2 | 1:I:382:ARG:NE | 2.32 | 0.55 |
| 1:L:33:PHE:O | 1:L:34:ILE:HG12 | 2.06 | 0.55 |
| 1:K:400:VAL:O | 1:K:400:VAL:HG13 | 2.07 | 0.55 |
| 1:A:134:ARG:NH1 | 2:A:501:ACO:H1B | 2.21 | 0.55 |
| 1:L:259:TRP:O | 1:L:263:ILE:HG12 | 2.05 | 0.55 |
| 1:A:109:GLU:OE2 | 1:A:112:ARG:NH2 | 2.39 | 0.55 |
| 1:H:208:ALA:O | 1:H:211:LYS:HG2 | 2.06 | 0.55 |
| 1:F:42:TRP:CD2 | 1:F:69:LEU:HD21 | 2.40 | 0.55 |
| 1:C:153:ALA:HA | 1:C:290:LEU:CD1 | 2.36 | 0.55 |
| 1:B:23:PHE:CE1 | 1:B:42:TRP:HZ3 | 2.24 | 0.55 |
| 1:K:34:ILE:HB | 1:K:37:GLU:HG2 | 1.88 | 0.55 |
| 1:C:247:LEU:HD23 | 1:C:247:LEU:C | 2.26 | 0.55 |
| 1:F:43:ARG:HH11 | 1:F:43:ARG:HA | 1.71 | 0.55 |
| 1:F:259:TRP:CE2 | 1:F:281:LEU:HD22 | 2.42 | 0.55 |
| 1:K:192:VAL:CG1 | 1:K:403:GLN:HB2 | 2.36 | 0.55 |
| 1:G:355:ILE:HD11 | 1:G:381:LEU:CD2 | 2.33 | 0.55 |
| 1:D:206:LEU:CD2 | 1:D:206:LEU:C | 2.75 | 0.55 |
| 1:B:150:ARG:CZ | 1:B:266:ASP:HA | 2.37 | 0.55 |
| 1:C:144:HIS:NE2 | 1:C:296:ARG:NH1 | 2.54 | 0.55 |
| 1:D:327:LEU:O | 1:D:335:PHE:N | 2.39 | 0.55 |
| 1:C:160:PRO:HG2 | 1:C:256:CYS:SG | 2.46 | 0.55 |
| 1:C:178:ARG:HG3 | 1:C:207:LEU:HD11 | 1.89 | 0.55 |
| 1:A:35:GLY:N | 1:A:36:PRO:HD2 | 2.22 | 0.55 |
| 1:K:297:GLN:CG | 1:L:289:ARG:HD3 | 2.36 | 0.55 |
| 1:F:123:ALA:HB1 | 1:F:300:LEU:HD11 | 1.89 | 0.55 |
| 1:H:146:LEU:CD2 | 1:H:275:THR:CG2 | 2.84 | 0.55 |
| 1:J:196:LEU:HG | 1:J:405:ALA:HB1 | 1.88 | 0.55 |
| 1:K:192:VAL:HG11 | 1:K:403:GLN:CG | 2.36 | 0.55 |
| 1:D:148:VAL:HG21 | 1:D:291:ALA:CB | 2.36 | 0.55 |
| 1:J:50:GLY:HA2 | 1:J:70:TYR:CE1 | 2.41 | 0.55 |
| 1:H:22:MSE:HE2 | 1:H:42:TRP:CZ3 | 2.42 | 0.54 |
| 1:K:160:PRO:HG2 | 1:K:256:CYS:CB | 2.37 | 0.54 |
| 1:C:206:LEU:C | 1:C:206:LEU:CD2 | 2.75 | 0.54 |
| 1:A:123:ALA:HA | 1:A:301:TRP:O | 2.07 | 0.54 |
| 1:E:175:THR:HA | 1:E:207:LEU:HD11 | 1.90 | 0.54 |
| 1:C:199:PRO:HB2 | 1:C:201:VAL:HG12 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:334:ARG:NH1 | 1:J:350:ASP:O | 2.40 | 0.54 |
| 1:C:88:LEU:HD12 | 1:C:88:LEU:N | 2.22 | 0.54 |
| 1:J:326:VAL:O | 1:J:355:ILE:HG22 | 2.06 | 0.54 |
| 1:D:400:VAL:O | 1:D:400:VAL:HG23 | 2.07 | 0.54 |
| 1:H:196:LEU:CD1 | 1:H:406:PHE:CE2 | 2.90 | 0.54 |
| 1:I:39:ALA:O | 1:I:43:ARG:HG2 | 2.07 | 0.54 |
| 1:L:381:LEU:HD12 | 1:L:381:LEU:O | 2.07 | 0.54 |
| 1:H:212:ALA:HB2 | 1:H:219:GLU:N | 2.21 | 0.54 |
| 1:H:188:TRP:CH2 | 1:H:248:ARG:NH1 | 2.75 | 0.54 |
| 1:H:198:ARG:HG2 | 1:H:203:TRP:CD1 | 2.43 | 0.54 |
| 1:I:52:VAL:HG13 | 1:I:110:LEU:HD23 | 1.86 | 0.54 |
| 1:A:34:ILE:CG2 | 1:A:36:PRO:HD2 | 2.33 | 0.54 |
| 1:C:367:LEU:O | 1:C:402:VAL:HG21 | 2.08 | 0.54 |
| 1:H:19:TRP:HZ3 | 1:H:42:TRP:HE3 | 1.55 | 0.54 |
| 1:J:101:GLY:O | 1:J:104:ARG:HB3 | 2.08 | 0.54 |
| 1:H:34:ILE:HB | 1:H:37:GLU:OE1 | 2.05 | 0.54 |
| 1:G:9:VAL:HG11 | 1:G:102:LEU:HD21 | 1.90 | 0.54 |
| 1:F:330:SER:O | 1:F:331:ASP:HB2 | 2.07 | 0.54 |
| 1:D:186:GLU:O | 1:D:190:GLN:HG3 | 2.06 | 0.54 |
| 1:F:77:VAL:HB | 1:F:78:PRO:HD2 | 1.90 | 0.54 |
| 1:D:148:VAL:HG13 | 1:D:290:LEU:HB3 | 1.90 | 0.54 |
| 1:J:98:ARG:NH2 | 1:J:99:ARG:NH2 | 2.56 | 0.54 |
| 1:D:10:THR:CB | 1:H:384:LYS:CD | 2.86 | 0.54 |
| 1:A:34:ILE:HB | 1:A:37:GLU:CG | 2.37 | 0.54 |
| 1:K:373:SER:HB3 | 1:K:393:ASP:OD2 | 2.08 | 0.54 |
| 1:D:314:ARG:O | 1:D:316:TYR:CE1 | 2.61 | 0.54 |
| 1:K:77:VAL:HB | 1:K:78:PRO:HD2 | 1.90 | 0.54 |
| 1:G:385:ASP:C | 1:G:385:ASP:OD1 | 2.46 | 0.54 |
| 1:C:148:VAL:HG13 | 1:C:290:LEU:HB3 | 1.90 | 0.54 |
| 1:F:144:HIS:CE1 | 1:F:296:ARG:HH12 | 2.23 | 0.54 |
| 1:D:44:THR:HG21 | 1:D:201:VAL:HG11 | 1.90 | 0.54 |
| 1:G:103:LEU:HD22 | 2:G:501:ACO:H133 | 1.90 | 0.54 |
| 1:B:41:ALA:O | 1:B:45:LEU:N | 2.35 | 0.54 |
| 1:A:98:ARG:HD3 | 1:F:264:GLY:HA2 | 1.89 | 0.54 |
| 1:E:248:ARG:NH2 | 1:E:405:ALA:O | 2.41 | 0.54 |
| 1:G:74:ARG:HD3 | 1:G:84:PRO:HA | 1.89 | 0.54 |
| 1:D:304:ILE:O | 1:D:359:ARG:NH1 | 2.40 | 0.54 |
| 1:B:107:CYS:C | 1:B:111:HIS:HD1 | 2.11 | 0.54 |
| 1:C:247:LEU:HD23 | 1:C:248:ARG:N | 2.23 | 0.54 |
| 1:A:297:GLN:HG3 | 1:B:289:ARG:HD3 | 1.88 | 0.54 |
| 1:C:145:GLU:HB3 | 1:C:295:TRP:HB3 | 1.82 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:42:TRP:N | 1:I:42:TRP:CD1 | 2.74 | 0.54 |
| 1:E:192:VAL:HG11 | 1:E:403:GLN:CB | 2.35 | 0.54 |
| 1:K:203:TRP:O | 1:K:207:LEU:HD22 | 2.07 | 0.54 |
| 1:B:19:TRP:N | 1:B:20:PRO:HD2 | 2.23 | 0.54 |
| 1:H:247:LEU:HD23 | 1:H:248:ARG:N | 2.23 | 0.54 |
| 1:L:123:ALA:HB1 | 1:L:300:LEU:HD11 | 1.88 | 0.54 |
| 1:D:146:LEU:CD2 | 1:D:146:LEU:C | 2.76 | 0.53 |
| 1:H:34:ILE:O | 1:H:37:GLU:HG2 | 2.08 | 0.53 |
| 1:E:22:MSE:HE2 | 1:E:67:MSE:HE3 | 1.88 | 0.53 |
| 1:H:247:LEU:HD12 | 1:H:273:ILE:CD1 | 2.38 | 0.53 |
| 1:J:72:ASP:O | 1:J:73:LEU:HD23 | 2.07 | 0.53 |
| 1:J:77:VAL:HB | 1:J:78:PRO:HD2 | 1.89 | 0.53 |
| 1:G:311:LEU:HD12 | 1:G:311:LEU:H | 1.73 | 0.53 |
| 1:B:98:ARG:HD2 | 1:D:264:GLY:HA3 | 1.90 | 0.53 |
| 1:A:45:LEU:CD1 | 1:A:71:MSE:CE | 2.85 | 0.53 |
| 1:F:192:VAL:CG1 | 1:F:403:GLN:HB2 | 2.36 | 0.53 |
| 1:D:225:HIS:CE1 | 1:D:226:PRO:HD2 | 2.44 | 0.53 |
| 1:I:192:VAL:HG11 | 1:I:403:GLN:HB2 | 1.90 | 0.53 |
| 1:E:387:GLN:NE2 | 1:E:391:ARG:NH2 | 2.57 | 0.53 |
| 1:B:85:THR:CG2 | 1:B:86:ALA:N | 2.72 | 0.53 |
| 1:B:42:TRP:NE1 | 1:B:90:PHE:CD2 | 2.70 | 0.53 |
| 1:I:293:THR:HB | 1:J:296:ARG:HB3 | 1.89 | 0.53 |
| 1:B:206:LEU:CD2 | 1:B:206:LEU:C | 2.75 | 0.53 |
| 1:K:169:VAL:HG22 | 1:K:225:HIS:HB2 | 1.91 | 0.53 |
| 1:E:74:ARG:HD3 | 1:E:84:PRO:HA | 1.90 | 0.53 |
| 1:E:146:LEU:HB2 | 1:E:273:ILE:HG23 | 1.90 | 0.53 |
| 1:E:297:GLN:CD | 1:F:289:ARG:HD3 | 2.28 | 0.53 |
| 1:F:197:LEU:O | 1:F:199:PRO:HD3 | 2.09 | 0.53 |
| 1:G:188:TRP:CZ2 | 1:G:248:ARG:NH1 | 2.77 | 0.53 |
| 1:D:381:LEU:HD11 | 1:D:389:LEU:HD21 | 1.90 | 0.53 |
| 1:D:121:VAL:HG12 | 1:D:304:ILE:HA | 1.91 | 0.53 |
| 1:B:178:ARG:HH11 | 1:B:207:LEU:HD12 | 1.71 | 0.53 |
| 2:G:501:ACO:O8A | 2:G:501:ACO:H4B | 2.08 | 0.53 |
| 1:H:144:HIS:HD2 | 1:H:277:PRO:HG3 | 1.66 | 0.53 |
| 1:E:355:ILE:HG13 | 1:E:382:ARG:O | 2.09 | 0.53 |
| 1:D:16:GLU:HA | 1:D:19:TRP:NE1 | 2.24 | 0.53 |
| 1:G:259:TRP:O | 1:G:263:ILE:HG12 | 2.09 | 0.53 |
| 1:K:244:VAL:HB | 1:K:273:ILE:CD1 | 2.15 | 0.53 |
| 1:G:40:THR:C | 1:G:44:THR:HG22 | 2.21 | 0.53 |
| 1:E:144:HIS:HE1 | 1:E:296:ARG:CD | 2.20 | 0.53 |
| 1:D:259:TRP:CE2 | 1:D:281:LEU:HD22 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:48:THR:O | 1:L:49:ASP:OD1 | 2.26 | 0.53 |
| 1:C:259:TRP:CE2 | 1:C:281:LEU:HD22 | 2.44 | 0.53 |
| 1:D:181:PHE:HD1 | 1:D:229:TYR:CG | 2.26 | 0.53 |
| 1:B:100:ARG:NH2 | 1:D:167:SER:OG | 2.42 | 0.53 |
| 1:E:297:GLN:HG2 | 1:E:298:ASP:N | 2.24 | 0.53 |
| 1:H:98:ARG:NE | 1:H:99:ARG:CZ | 2.71 | 0.53 |
| 1:E:107:CYS:HB3 | 1:E:111:HIS:CE1 | 2.44 | 0.53 |
| 1:B:23:PHE:HE1 | 1:B:42:TRP:CZ3 | 2.26 | 0.53 |
| 1:I:289:ARG:CD | 1:J:297:GLN:CG | 2.80 | 0.53 |
| 1:I:114:ILE:HG22 | 1:I:305:MSE:HE2 | 1.90 | 0.53 |
| 1:C:89:SER:O | 1:C:90:PHE:HB2 | 2.09 | 0.53 |
| 1:L:145:GLU:HB3 | 1:L:295:TRP:HB3 | 1.89 | 0.53 |
| 1:E:143:LEU:HD21 | 1:E:404:THR:CB | 2.39 | 0.53 |
| 1:I:44:THR:O | 1:I:44:THR:CG2 | 2.56 | 0.53 |
| 1:J:34:ILE:HG22 | 1:J:36:PRO:CG | 2.38 | 0.53 |
| 1:F:43:ARG:HH11 | 1:F:43:ARG:CA | 2.22 | 0.53 |
| 1:G:192:VAL:HG11 | 1:G:403:GLN:HB2 | 1.90 | 0.53 |
| 1:F:314:ARG:O | 1:F:316:TYR:CE1 | 2.62 | 0.53 |
| 1:L:34:ILE:HG23 | 1:L:36:PRO:HD2 | 1.89 | 0.52 |
| 1:G:372:ALA:HB1 | 1:G:381:LEU:HD13 | 1.91 | 0.52 |
| 1:F:77:VAL:HB | 1:F:78:PRO:CD | 2.39 | 0.52 |
| 1:F:198:ARG:HD2 | 1:F:203:TRP:CE2 | 2.44 | 0.52 |
| 1:J:330:SER:O | 1:J:331:ASP:HB2 | 2.09 | 0.52 |
| 1:F:22:MSE:HE1 | 1:F:42:TRP:HZ2 | 1.65 | 0.52 |
| 1:G:150:ARG:HG2 | 1:G:269:GLU:O | 2.09 | 0.52 |
| 1:I:289:ARG:HG3 | 1:J:298:ASP:OD1 | 2.09 | 0.52 |
| 1:I:400:VAL:O | 1:I:400:VAL:HG23 | 2.08 | 0.52 |
| 1:B:355:ILE:HD11 | 1:B:381:LEU:HD21 | 1.90 | 0.52 |
| 1:D:98:ARG:CD | 1:E:264:GLY:HA2 | 2.39 | 0.52 |
| 1:B:98:ARG:HD2 | 1:D:264:GLY:HA2 | 1.92 | 0.52 |
| 1:A:199:PRO:HD2 | 1:A:202:LEU:HD12 | 1.90 | 0.52 |
| 1:A:45:LEU:HD12 | 1:A:71:MSE:CE | 2.39 | 0.52 |
| 1:J:19:TRP:N | 1:J:20:PRO:HD2 | 2.24 | 0.52 |
| 1:F:39:ALA:O | 1:F:43:ARG:HG2 | 2.08 | 0.52 |
| 1:I:390:ARG:HD3 | 1:J:399:ASP:OD2 | 2.08 | 0.52 |
| 1:I:372:ALA:HB3 | 1:I:393:ASP:OD1 | 2.09 | 0.52 |
| 1:A:127:SER:HB3 | 2:A:501:ACO:H22 | 1.89 | 0.52 |
| 1:D:8:THR:N | 1:H:353:ALA:HB3 | 2.24 | 0.52 |
| 1:I:289:ARG:CZ | 1:J:297:GLN:OE1 | 2.57 | 0.52 |
| 1:J:193:PRO:CG | 1:J:400:VAL:CG2 | 2.86 | 0.52 |
| 1:E:381:LEU:HD12 | 1:E:381:LEU:O | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:146:LEU:HD12 | 1:C:292:ARG:O | 2.10 | 0.52 |
| 1:B:145:GLU:OE2 | 1:B:295:TRP:HB3 | 2.08 | 0.52 |
| 1:A:42:TRP:HA | 1:A:46:VAL:HG23 | 1.92 | 0.52 |
| 1:A:156:HIS:CE1 | 1:B:380:ARG:NH1 | 2.78 | 0.52 |
| 1:B:326:VAL:HB | 1:B:354:GLU:H | 1.75 | 0.52 |
| 1:K:307:VAL:HB | 1:K:308:PRO:HD3 | 1.92 | 0.52 |
| 1:J:207:LEU:HD12 | 1:J:207:LEU:N | 2.24 | 0.52 |
| 1:F:71:MSE:O | 1:F:73:LEU:CD1 | 2.58 | 0.52 |
| 1:F:192:VAL:HG11 | 1:F:403:GLN:CB | 2.39 | 0.52 |
| 1:K:98:ARG:HE | 1:K:99:ARG:NH2 | 2.08 | 0.52 |
| 1:B:69:LEU:HD12 | 1:B:69:LEU:C | 2.30 | 0.52 |
| 1:G:123:ALA:CB | 1:G:302:LEU:HD23 | 2.39 | 0.52 |
| 1:H:339:ILE:HG12 | 1:H:344:ALA:HB2 | 1.90 | 0.52 |
| 1:E:110:LEU:O | 1:E:114:ILE:HG13 | 2.09 | 0.52 |
| 1:G:406:PHE:O | 3:G:629:HOH:O | 2.18 | 0.52 |
| 1:C:170:ARG:HD2 | 1:F:63:GLU:CD | 2.29 | 0.52 |
| 1:D:63:GLU:OE1 | 1:E:170:ARG:HD2 | 2.10 | 0.52 |
| 2:E:501:ACO:O8A | 2:E:501:ACO:H4B | 2.08 | 0.52 |
| 1:K:311:LEU:O | 1:K:316:TYR:OH | 2.13 | 0.52 |
| 1:H:145:GLU:OE2 | 1:H:295:TRP:CB | 2.58 | 0.52 |
| 1:I:293:THR:OG1 | 1:J:296:ARG:HD3 | 2.10 | 0.52 |
| 1:I:198:ARG:NH1 | 1:I:206:LEU:CD1 | 2.73 | 0.52 |
| 1:F:361:VAL:HG13 | 1:F:375:LEU:HD13 | 1.90 | 0.52 |
| 1:C:180:GLU:O | 1:C:184:ILE:HG13 | 2.09 | 0.52 |
| 1:H:385:ASP:OD1 | 1:H:385:ASP:C | 2.48 | 0.52 |
| 1:A:121:VAL:HA | 1:A:305:MSE:HG2 | 1.90 | 0.52 |
| 1:F:98:ARG:HH11 | 1:F:99:ARG:HH21 | 1.57 | 0.52 |
| 1:I:267:SER:C | 1:I:268:MSE:HE2 | 2.29 | 0.52 |
| 1:J:52:VAL:HG12 | 1:J:110:LEU:HD21 | 1.90 | 0.52 |
| 2:B:501:ACO:H4B | 2:B:501:ACO:O8A | 2.10 | 0.52 |
| 1:E:196:LEU:HD12 | 1:E:405:ALA:HB3 | 1.91 | 0.52 |
| 1:D:107:CYS:O | 1:D:111:HIS:ND1 | 2.39 | 0.52 |
| 1:F:73:LEU:N | 1:F:73:LEU:CD1 | 2.73 | 0.52 |
| 1:C:316:TYR:O | 1:C:342:GLY:HA2 | 2.10 | 0.52 |
| 1:F:133:GLY:HA2 | 1:F:137:TYR:O | 2.10 | 0.52 |
| 1:F:120:PRO:O | 1:F:305:MSE:HB2 | 2.10 | 0.52 |
| 1:D:402:VAL:HG12 | 3:D:621:HOH:O | 2.09 | 0.52 |
| 1:G:289:ARG:NH1 | 1:H:298:ASP:CG | 2.62 | 0.52 |
| 1:B:197:LEU:O | 1:B:199:PRO:HD3 | 2.09 | 0.52 |
| 1:I:52:VAL:CG1 | 1:I:110:LEU:HD23 | 2.39 | 0.52 |
| 1:G:98:ARG:HD2 | 1:L:264:GLY:HA2 | 1.88 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:141:THR:HG22 | 1:E:402:VAL:HG11 | 1.93 | 0.52 |
| 1:I:200:GLN:CA | 1:I:200:GLN:HE21 | 2.15 | 0.51 |
| 1:I:178:ARG:HD2 | 1:I:207:LEU:HD11 | 1.92 | 0.51 |
| 1:B:155:PHE:CZ | 1:B:260:ARG:HA | 2.44 | 0.51 |
| 1:H:144:HIS:CD2 | 1:H:277:PRO:CG | 2.88 | 0.51 |
| 1:B:24:LEU:HD13 | 1:D:173:ARG:CG | 2.37 | 0.51 |
| 1:G:98:ARG:HD2 | 1:L:264:GLY:HA3 | 1.90 | 0.51 |
| 1:B:330:SER:O | 1:B:331:ASP:HB2 | 2.09 | 0.51 |
| 1:A:276:HIS:HB2 | 1:A:277:PRO:HD2 | 1.92 | 0.51 |
| 1:D:250:VAL:HG12 | 1:D:250:VAL:O | 2.09 | 0.51 |
| 1:C:357:MSE:CG | 1:C:381:LEU:HD13 | 2.40 | 0.51 |
| 1:I:23:PHE:CE1 | 1:I:38:SER:OG | 2.56 | 0.51 |
| 1:G:43:ARG:NH1 | 1:G:43:ARG:HA | 2.21 | 0.51 |
| 1:B:178:ARG:CG | 1:B:207:LEU:HD11 | 2.40 | 0.51 |
| 1:K:225:HIS:CG | 1:K:226:PRO:HD2 | 2.46 | 0.51 |
| 1:B:219:GLU:HG3 | 3:B:623:HOH:O | 2.09 | 0.51 |
| 1:I:323:PHE:CD2 | 1:I:391:ARG:HD3 | 2.45 | 0.51 |
| 1:A:381:LEU:O | 1:A:381:LEU:HD12 | 2.11 | 0.51 |
| 1:K:314:ARG:HH11 | 1:K:314:ARG:HG2 | 1.74 | 0.51 |
| 1:E:156:HIS:HE2 | 1:F:380:ARG:NH2 | 2.08 | 0.51 |
| 1:H:98:ARG:NE | 1:H:99:ARG:NH1 | 2.57 | 0.51 |
| 1:A:314:ARG:HG2 | 1:A:315:GLY:O | 2.10 | 0.51 |
| 1:E:181:PHE:HD1 | 1:E:229:TYR:CG | 2.29 | 0.51 |
| 1:C:74:ARG:HD3 | 1:C:84:PRO:HA | 1.93 | 0.51 |
| 1:I:208:ALA:O | 1:I:211:LYS:HG2 | 2.10 | 0.51 |
| 1:I:355:ILE:HD11 | 1:I:381:LEU:HD21 | 1.93 | 0.51 |
| 1:I:323:PHE:CE2 | 1:I:391:ARG:HB3 | 2.45 | 0.51 |
| 1:F:72:ASP:O | 1:F:73:LEU:HD12 | 2.11 | 0.51 |
| 1:F:247:LEU:HD23 | 1:F:248:ARG:N | 2.25 | 0.51 |
| 1:L:314:ARG:HD3 | 1:L:315:GLY:O | 2.11 | 0.51 |
| 1:B:200:GLN:HA | 1:B:200:GLN:NE2 | 2.25 | 0.51 |
| 1:D:150:ARG:NE | 1:D:265:LEU:O | 2.44 | 0.51 |
| 1:D:208:ALA:O | 1:D:211:LYS:HG2 | 2.10 | 0.51 |
| 1:D:148:VAL:HG22 | 1:D:291:ALA:HA | 0.56 | 0.51 |
| 1:B:42:TRP:CZ2 | 1:B:90:PHE:CD1 | 2.99 | 0.51 |
| 1:C:150:ARG:HH21 | 1:C:266:ASP:CA | 2.13 | 0.51 |
| 1:H:107:CYS:HB3 | 1:H:111:HIS:HE1 | 1.76 | 0.51 |
| 1:C:340:GLY:O | 1:C:341:ASP:HB2 | 2.11 | 0.51 |
| 1:J:178:ARG:CD | 1:J:207:LEU:HD21 | 2.38 | 0.51 |
| 1:G:289:ARG:NE | 1:H:297:GLN:OE1 | 2.43 | 0.51 |
| 1:A:98:ARG:CD | 1:F:264:GLY:HA2 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:45:LEU:CD1 | 1:A:71:MSE:HE2 | 2.40 | 0.51 |
| 1:B:34:ILE:HB | 1:B:37:GLU:OE1 | 2.11 | 0.51 |
| 1:C:327:LEU:O | 1:C:335:PHE:N | 2.44 | 0.51 |
| 1:G:284:LEU:HD23 | 1:H:378:ALA:HB1 | 1.92 | 0.51 |
| 1:H:354:GLU:CB | 1:H:384:LYS:HZ1 | 2.20 | 0.51 |
| 1:F:144:HIS:CD2 | 1:F:296:ARG:NH1 | 2.68 | 0.51 |
| 1:F:39:ALA:O | 1:F:43:ARG:CG | 2.59 | 0.51 |
| 1:I:317:ALA:HB3 | 1:I:394:ALA:O | 2.11 | 0.51 |
| 1:G:184:ILE:HG21 | 1:G:228:GLY:HA2 | 1.91 | 0.51 |
| 1:F:260:ARG:HH11 | 1:F:260:ARG:HG2 | 1.76 | 0.51 |
| 1:I:355:ILE:HG13 | 1:I:383:THR:HB | 1.92 | 0.51 |
| 1:E:128:GLU:HA | 1:F:289:ARG:NH2 | 2.26 | 0.51 |
| 1:J:41:ALA:CA | 1:J:44:THR:CG2 | 2.89 | 0.51 |
| 1:I:178:ARG:CG | 1:I:207:LEU:HD11 | 2.41 | 0.51 |
| 1:C:357:MSE:HB3 | 1:C:381:LEU:HD12 | 1.90 | 0.50 |
| 1:G:93:VAL:HG23 | 2:G:501:ACO:H132 | 1.93 | 0.50 |
| 1:B:144:HIS:HB3 | 1:B:146:LEU:CD1 | 2.39 | 0.50 |
| 1:I:114:ILE:HG23 | 1:I:119:TYR:HB2 | 1.92 | 0.50 |
| 1:I:197:LEU:HD12 | 1:I:198:ARG:H | 1.77 | 0.50 |
| 1:I:311:LEU:HD13 | 1:I:337:LEU:HD22 | 1.93 | 0.50 |
| 1:B:247:LEU:O | 1:B:248:ARG:HD3 | 2.11 | 0.50 |
| 2:K:501:ACO:H52A | 3:K:622:HOH:O | 2.10 | 0.50 |
| 1:E:341:ASP:OD2 | 1:E:343:ARG:NH2 | 2.44 | 0.50 |
| 1:I:369:ALA:HB2 | 1:I:402:VAL:HG11 | 1.93 | 0.50 |
| 1:G:375:LEU:HD21 | 1:H:283:HIS:CE1 | 2.46 | 0.50 |
| 1:J:263:ILE:O | 1:J:263:ILE:HG22 | 2.11 | 0.50 |
| 1:G:104:ARG:HG3 | 1:G:135:PHE:HE1 | 1.77 | 0.50 |
| 1:F:34:ILE:HG22 | 1:F:36:PRO:CG | 2.40 | 0.50 |
| 1:G:289:ARG:HG3 | 1:H:129:GLY:HA3 | 1.91 | 0.50 |
| 1:F:16:GLU:O | 1:F:19:TRP:CD1 | 2.64 | 0.50 |
| 1:K:198:ARG:HD2 | 1:K:203:TRP:CE2 | 2.47 | 0.50 |
| 1:F:127:SER:HB3 | 2:F:501:ACO:H22 | 1.94 | 0.50 |
| 1:G:250:VAL:CG1 | 1:G:250:VAL:O | 2.59 | 0.50 |
| 1:B:34:ILE:HB | 1:B:37:GLU:CG | 2.41 | 0.50 |
| 1:F:379:ASN:ND2 | 1:F:382:ARG:HD3 | 2.26 | 0.50 |
| 1:D:148:VAL:CG2 | 1:D:291:ALA:CB | 2.88 | 0.50 |
| 1:J:98:ARG:HD2 | 1:K:264:GLY:HA3 | 1.93 | 0.50 |
| 1:E:156:HIS:HE2 | 1:F:380:ARG:HH22 | 1.59 | 0.50 |
| 1:C:198:ARG:NH1 | 1:C:206:LEU:CD1 | 2.75 | 0.50 |
| 1:I:217:ASP:CG | 1:I:233:ARG:HH11 | 2.14 | 0.50 |
| 1:K:16:GLU:HA | 1:K:19:TRP:CD1 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:385:ASP:OD1 | 1:G:387:GLN:N | 2.45 | 0.50 |
| 1:J:405:ALA:N | 3:J:602:HOH:O | 2.09 | 0.50 |
| 1:C:373:SER:HB3 | 1:C:393:ASP:OD2 | 2.11 | 0.50 |
| 1:L:334:ARG:HD2 | 1:L:351:ALA:O | 2.11 | 0.50 |
| 1:C:293:THR:N | 3:C:604:HOH:O | 2.03 | 0.50 |
| 1:C:295:TRP:HZ2 | 1:C:297:GLN:NE2 | 2.08 | 0.50 |
| 1:C:178:ARG:HH21 | 1:C:200:GLN:HE21 | 1.57 | 0.50 |
| 1:J:297:GLN:HG2 | 1:J:298:ASP:N | 2.26 | 0.50 |
| 1:K:192:VAL:HG11 | 1:K:403:GLN:CB | 2.42 | 0.50 |
| 1:E:192:VAL:HG11 | 1:E:403:GLN:CG | 2.42 | 0.50 |
| 1:F:16:GLU:O | 1:F:19:TRP:HD1 | 1.95 | 0.50 |
| 1:E:187:ARG:NH2 | 1:E:250:VAL:HG21 | 2.27 | 0.50 |
| 1:H:247:LEU:O | 1:H:248:ARG:HD3 | 2.11 | 0.50 |
| 1:D:181:PHE:HD1 | 1:D:229:TYR:CD2 | 2.30 | 0.50 |
| 1:E:341:ASP:O | 1:E:341:ASP:OD1 | 2.30 | 0.50 |
| 1:J:225:HIS:CG | 1:J:226:PRO:HD2 | 2.46 | 0.50 |
| 1:G:9:VAL:HG12 | 1:G:54:VAL:HG13 | 1.92 | 0.50 |
| 1:I:107:CYS:HB3 | 1:I:111:HIS:HE1 | 1.75 | 0.50 |
| 1:J:339:ILE:HG12 | 1:J:344:ALA:CB | 2.40 | 0.50 |
| 1:L:178:ARG:HG3 | 1:L:207:LEU:HD21 | 1.94 | 0.50 |
| 1:I:141:THR:HG22 | 1:I:402:VAL:HG21 | 1.92 | 0.50 |
| 1:L:327:LEU:C | 1:L:327:LEU:CD2 | 2.79 | 0.50 |
| 1:G:172:VAL:HB | 1:G:177:HIS:CD2 | 2.47 | 0.50 |
| 1:H:34:ILE:O | 1:H:37:GLU:CG | 2.60 | 0.50 |
| 1:F:148:VAL:HG13 | 1:F:271:ILE:HB | 1.94 | 0.50 |
| 1:H:98:ARG:HD2 | 1:J:266:ASP:OD2 | 2.12 | 0.50 |
| 1:G:9:VAL:HG11 | 1:G:54:VAL:HG11 | 1.93 | 0.50 |
| 1:C:326:VAL:HG21 | 1:C:352:ALA:O | 2.11 | 0.50 |
| 1:E:85:THR:HG23 | 1:E:121:VAL:HG23 | 1.93 | 0.50 |
| 1:H:145:GLU:C | 1:H:146:LEU:HD22 | 2.32 | 0.49 |
| 1:G:381:LEU:O | 1:G:381:LEU:CD2 | 2.59 | 0.49 |
| 1:E:400:VAL:O | 1:E:400:VAL:HG23 | 2.11 | 0.49 |
| 1:C:325:THR:OG1 | 1:C:326:VAL:N | 2.45 | 0.49 |
| 1:G:16:GLU:HA | 1:G:19:TRP:NE1 | 2.27 | 0.49 |
| 1:D:48:THR:O | 1:D:49:ASP:OD1 | 2.30 | 0.49 |
| 1:H:42:TRP:CH2 | 1:H:67:MSE:HE1 | 2.47 | 0.49 |
| 1:K:334:ARG:HD2 | 1:K:351:ALA:O | 2.12 | 0.49 |
| 1:B:266:ASP:H | 1:E:98:ARG:HH11 | 1.59 | 0.49 |
| 1:K:381:LEU:CD2 | 1:K:381:LEU:C | 2.79 | 0.49 |
| 1:D:178:ARG:NH1 | 1:D:207:LEU:HD12 | 2.27 | 0.49 |
| 1:F:98:ARG:NE | 1:F:99:ARG:NH2 | 2.55 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:77:VAL:HB | 1:I:78:PRO:CD | 2.42 | 0.49 |
| 1:A:336:ALA:O | 1:A:346:CYS:HA | 2.12 | 0.49 |
| 1:G:48:THR:O | 1:G:49:ASP:OD1 | 2.30 | 0.49 |
| 1:L:182:GLU:HA | 1:L:203:TRP:CZ2 | 2.47 | 0.49 |
| 1:E:88:LEU:HD12 | 1:E:88:LEU:N | 2.27 | 0.49 |
| 1:A:73:LEU:CB | 1:A:85:THR:O | 2.59 | 0.49 |
| 1:C:266:ASP:OD2 | 1:F:98:ARG:HD2 | 2.12 | 0.49 |
| 1:A:173:ARG:CG | 1:C:24:LEU:HD13 | 2.42 | 0.49 |
| 1:F:259:TRP:CZ2 | 1:F:281:LEU:HD22 | 2.48 | 0.49 |
| 1:H:188:TRP:CZ2 | 1:H:248:ARG:NH1 | 2.80 | 0.49 |
| 1:B:307:VAL:HB | 1:B:308:PRO:HD3 | 1.94 | 0.49 |
| 1:H:292:ARG:HA | 3:H:605:HOH:O | 2.13 | 0.49 |
| 1:F:225:HIS:HD1 | 1:F:227:ASP:H | 1.60 | 0.49 |
| 1:C:145:GLU:HG2 | 1:C:274:ILE:HD13 | 1.95 | 0.49 |
| 1:H:145:GLU:CB | 1:H:295:TRP:HB3 | 2.41 | 0.49 |
| 1:J:76:THR:O | 1:J:193:PRO:HA | 2.12 | 0.49 |
| 1:C:326:VAL:HB | 1:C:354:GLU:H | 1.76 | 0.49 |
| 1:F:19:TRP:N | 1:F:20:PRO:HD2 | 2.26 | 0.49 |
| 1:I:355:ILE:HD11 | 1:I:381:LEU:CD2 | 2.42 | 0.49 |
| 1:I:323:PHE:HB3 | 1:I:391:ARG:NH1 | 2.25 | 0.49 |
| 1:F:121:VAL:HG12 | 1:F:305:MSE:H | 1.76 | 0.49 |
| 1:I:276:HIS:HD2 | 1:I:278:GLN:N | 2.08 | 0.49 |
| 1:K:169:VAL:HG12 | 1:K:170:ARG:N | 2.27 | 0.49 |
| 1:J:83:LEU:HD11 | 1:J:313:ALA:CB | 2.42 | 0.49 |
| 1:A:79:GLY:O | 1:A:80:GLU:HB2 | 2.12 | 0.49 |
| 1:F:42:TRP:CD1 | 1:F:69:LEU:HD22 | 2.34 | 0.49 |
| 1:H:34:ILE:CB | 1:H:37:GLU:CG | 2.58 | 0.49 |
| 1:L:381:LEU:HD11 | 1:L:389:LEU:HD21 | 1.95 | 0.49 |
| 1:D:172:VAL:HB | 1:D:177:HIS:CD2 | 2.48 | 0.49 |
| 1:L:150:ARG:NH1 | 1:L:263:ILE:O | 2.43 | 0.49 |
| 1:F:141:THR:HG22 | 1:F:402:VAL:HG11 | 1.93 | 0.49 |
| 1:K:10:THR:O | 1:K:54:VAL:HA | 2.12 | 0.49 |
| 1:D:223:LEU:HD13 | 1:D:261:ALA:HB1 | 1.95 | 0.49 |
| 1:K:51:ALA:HA | 1:K:69:LEU:HB3 | 1.94 | 0.49 |
| 1:G:123:ALA:HB2 | 1:G:302:LEU:HD23 | 1.95 | 0.49 |
| 1:H:147:THR:OG1 | 1:H:294:THR:HG21 | 2.12 | 0.49 |
| 1:B:231:LEU:HB2 | 1:B:245:SER:OG | 2.11 | 0.49 |
| 1:C:155:PHE:CE2 | 1:C:260:ARG:HA | 2.47 | 0.49 |
| 1:D:148:VAL:HG13 | 1:D:290:LEU:CB | 2.42 | 0.49 |
| 1:F:303:ARG:HD3 | 1:F:305:MSE:SE | 2.62 | 0.49 |
| 1:F:35:GLY:N | 1:F:36:PRO:CD | 2.75 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:295:TRP:CH2 | 1:H:297:GLN:NE2 | 2.66 | 0.49 |
| 1:G:98:ARG:CD | 1:L:264:GLY:CA | 2.86 | 0.49 |
| 1:J:98:ARG:HD2 | 1:K:264:GLY:HA2 | 1.93 | 0.49 |
| 1:E:16:GLU:HA | 1:E:19:TRP:CD1 | 2.46 | 0.49 |
| 1:E:72:ASP:O | 1:E:73:LEU:HD23 | 2.12 | 0.49 |
| 1:D:150:ARG:NE | 1:D:268:MSE:O | 2.46 | 0.49 |
| 1:F:150:ARG:CZ | 1:F:266:ASP:HA | 2.43 | 0.49 |
| 1:H:33:PHE:CZ | 1:H:38:SER:OG | 2.55 | 0.49 |
| 1:A:320:VAL:HG21 | 1:A:394:ALA:HB3 | 1.94 | 0.49 |
| 1:E:198:ARG:CZ | 1:E:206:LEU:HD12 | 2.43 | 0.49 |
| 1:A:314:ARG:HH22 | 1:A:396:PHE:C | 2.15 | 0.49 |
| 1:G:54:VAL:HG11 | 1:G:102:LEU:HD22 | 1.95 | 0.49 |
| 1:B:145:GLU:OE2 | 1:B:295:TRP:HB2 | 2.12 | 0.49 |
| 1:C:50:GLY:HA2 | 1:C:70:TYR:CE1 | 2.48 | 0.49 |
| 1:F:295:TRP:HZ2 | 1:F:297:GLN:NE2 | 2.11 | 0.49 |
| 1:I:178:ARG:HG3 | 1:I:207:LEU:HD11 | 1.95 | 0.49 |
| 1:E:114:ILE:HG22 | 1:E:119:TYR:HB2 | 1.94 | 0.49 |
| 1:J:169:VAL:HG11 | 1:J:223:LEU:HB3 | 1.95 | 0.49 |
| 1:F:311:LEU:HD21 | 1:F:362:LEU:HD11 | 1.95 | 0.49 |
| 1:J:357:MSE:HE1 | 1:J:362:LEU:CA | 2.42 | 0.48 |
| 1:J:43:ARG:NH1 | 1:J:43:ARG:CA | 2.69 | 0.48 |
| 1:B:42:TRP:HD1 | 1:B:71:MSE:HE3 | 1.78 | 0.48 |
| 1:H:297:GLN:HG2 | 1:H:298:ASP:N | 2.28 | 0.48 |
| 1:H:144:HIS:NE2 | 1:H:277:PRO:HG3 | 2.27 | 0.48 |
| 1:D:144:HIS:CD2 | 1:D:277:PRO:CG | 2.92 | 0.48 |
| 1:E:314:ARG:HD3 | 1:E:316:TYR:CE2 | 2.48 | 0.48 |
| 1:C:134:ARG:CZ | 2:C:501:ACO:H1B | 2.43 | 0.48 |
| 1:K:360:ASP:OD2 | 1:K:380:ARG:NH2 | 2.45 | 0.48 |
| 1:L:311:LEU:HD21 | 1:L:362:LEU:HD11 | 1.95 | 0.48 |
| 1:H:170:ARG:O | 1:H:172:VAL:HG13 | 2.11 | 0.48 |
| 1:A:125:HIS:HE1 | 3:A:618:HOH:O | 1.94 | 0.48 |
| 1:G:11:LEU:HD12 | 1:G:52:VAL:CG2 | 2.37 | 0.48 |
| 1:C:200:GLN:NE2 | 1:C:200:GLN:HA | 2.28 | 0.48 |
| 1:G:114:ILE:HG22 | 1:G:305:MSE:HE2 | 1.94 | 0.48 |
| 1:K:229:TYR:N | 1:K:248:ARG:O | 2.45 | 0.48 |
| 2:B:501:ACO:H141 | 2:B:501:ACO:O5P | 2.13 | 0.48 |
| 1:G:307:VAL:HB | 1:G:308:PRO:HD3 | 1.95 | 0.48 |
| 1:I:178:ARG:CD | 1:I:207:LEU:HD11 | 2.42 | 0.48 |
| 1:K:297:GLN:HG3 | 1:L:289:ARG:HD3 | 1.94 | 0.48 |
| 1:F:46:VAL:CG2 | 1:F:69:LEU:HD13 | 2.44 | 0.48 |
| 1:D:148:VAL:HG21 | 1:D:291:ALA:CA | 2.26 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:148:VAL:HG21 | 1:E:281:LEU:HD21 | 1.95 | 0.48 |
| 1:B:148:VAL:HG13 | 1:B:290:LEU:O | 2.14 | 0.48 |
| 1:B:48:THR:O | 1:B:49:ASP:OD1 | 2.30 | 0.48 |
| 1:I:227:ASP:HB3 | 1:I:250:VAL:HG22 | 1.95 | 0.48 |
| 1:K:103:LEU:HB2 | 2:K:501:ACO:O6A | 2.14 | 0.48 |
| 1:B:65:VAL:HG11 | 1:B:97:HIS:CE1 | 2.48 | 0.48 |
| 1:I:70:TYR:HB3 | 1:I:88:LEU:HD23 | 1.94 | 0.48 |
| 1:K:383:THR:HG21 | 1:K:389:LEU:HG | 1.94 | 0.48 |
| 1:J:146:LEU:O | 1:J:272:SER:HA | 2.13 | 0.48 |
| 1:J:184:ILE:HG21 | 1:J:229:TYR:HD1 | 1.78 | 0.48 |
| 1:H:34:ILE:CG1 | 1:H:37:GLU:OE1 | 2.61 | 0.48 |
| 1:K:316:TYR:CE1 | 1:K:344:ALA:HB2 | 2.48 | 0.48 |
| 1:C:239:LEU:O | 1:C:268:MSE:HE1 | 2.13 | 0.48 |
| 1:A:145:GLU:HB3 | 1:A:295:TRP:CB | 2.38 | 0.48 |
| 1:J:77:VAL:HB | 1:J:78:PRO:CD | 2.43 | 0.48 |
| 1:E:381:LEU:HD12 | 1:E:381:LEU:C | 2.34 | 0.48 |
| 1:G:140:ALA:O | 1:G:369:ALA:HB2 | 2.13 | 0.48 |
| 1:G:222:ALA:CB | 1:G:231:LEU:CD2 | 2.75 | 0.48 |
| 1:C:155:PHE:CZ | 1:C:260:ARG:HA | 2.48 | 0.48 |
| 1:D:137:TYR:O | 1:D:360:ASP:HB2 | 2.13 | 0.48 |
| 1:F:144:HIS:CE1 | 1:F:296:ARG:NH1 | 2.67 | 0.48 |
| 1:D:33:PHE:O | 1:D:34:ILE:CD1 | 2.62 | 0.48 |
| 1:H:145:GLU:OE2 | 1:H:295:TRP:HB3 | 2.14 | 0.48 |
| 1:C:150:ARG:HD3 | 1:C:265:LEU:O | 2.13 | 0.48 |
| 1:J:295:TRP:CZ2 | 1:J:297:GLN:HB3 | 2.49 | 0.48 |
| 1:C:307:VAL:HB | 1:C:308:PRO:HD3 | 1.96 | 0.48 |
| 1:B:326:VAL:CG1 | 1:B:353:ALA:HA | 2.44 | 0.48 |
| 1:B:42:TRP:NE1 | 1:B:90:PHE:CZ | 2.72 | 0.48 |
| 1:J:404:THR:HG22 | 1:J:405:ALA:O | 2.14 | 0.48 |
| 1:D:9:VAL:O | 1:H:352:ALA:HB1 | 2.14 | 0.48 |
| 1:E:144:HIS:NE2 | 1:E:277:PRO:HG3 | 2.29 | 0.48 |
| 1:F:74:ARG:HB3 | 1:F:82:VAL:HG11 | 1.95 | 0.48 |
| 1:B:98:ARG:CD | 1:D:264:GLY:HA2 | 2.43 | 0.48 |
| 1:I:70:TYR:HA | 1:I:87:GLY:O | 2.14 | 0.48 |
| 1:F:139:PRO:HD3 | 1:F:301:TRP:CZ3 | 2.49 | 0.48 |
| 1:G:133:GLY:HA2 | 1:G:137:TYR:O | 2.13 | 0.48 |
| 1:A:144:HIS:HB3 | 1:A:146:LEU:HD11 | 1.95 | 0.48 |
| 1:D:247:LEU:CD2 | 1:D:247:LEU:C | 2.80 | 0.48 |
| 1:D:19:TRP:N | 1:D:20:PRO:HD2 | 2.28 | 0.48 |
| 1:B:34:ILE:CG2 | 1:B:36:PRO:HD2 | 2.44 | 0.48 |
| 1:D:88:LEU:HD11 | 1:D:137:TYR:OH | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:360:ASP:OD2 | 1:G:380:ARG:NH2 | 2.46 | 0.48 |
| 1:F:306:ASN:HB3 | 1:F:309:ALA:HB3 | 1.95 | 0.48 |
| 1:B:371:ARG:NH2 | 3:B:652:HOH:O | 2.46 | 0.48 |
| 1:A:263:ILE:HG22 | 1:A:263:ILE:O | 2.13 | 0.48 |
| 1:F:71:MSE:HB2 | 1:F:73:LEU:CD1 | 2.37 | 0.48 |
| 1:J:338:LYS:O | 1:J:344:ALA:HA | 2.13 | 0.48 |
| 1:D:63:GLU:CD | 1:E:170:ARG:HD2 | 2.34 | 0.48 |
| 1:D:400:VAL:CG2 | 1:D:400:VAL:O | 2.62 | 0.48 |
| 1:I:134:ARG:CZ | 2:I:501:ACO:H1B | 2.44 | 0.48 |
| 1:J:141:THR:HG22 | 1:J:402:VAL:HG21 | 1.95 | 0.48 |
| 1:L:307:VAL:HB | 1:L:308:PRO:HD3 | 1.95 | 0.48 |
| 1:H:34:ILE:CA | 1:H:37:GLU:HG2 | 2.43 | 0.47 |
| 1:I:148:VAL:CB | 1:I:290:LEU:O | 2.62 | 0.47 |
| 1:C:303:ARG:HH11 | 1:C:305:MSE:SE | 2.47 | 0.47 |
| 1:I:296:ARG:HB3 | 1:J:293:THR:HB | 1.95 | 0.47 |
| 1:F:74:ARG:HD3 | 1:F:84:PRO:HA | 1.95 | 0.47 |
| 1:F:367:LEU:O | 1:F:402:VAL:CG2 | 2.62 | 0.47 |
| 1:G:379:ASN:OD1 | 1:G:382:ARG:HG2 | 2.14 | 0.47 |
| 1:D:334:ARG:HD3 | 1:D:351:ALA:O | 2.14 | 0.47 |
| 1:C:148:VAL:HG13 | 1:C:290:LEU:O | 2.15 | 0.47 |
| 1:I:44:THR:HG21 | 1:I:201:VAL:HB | 1.96 | 0.47 |
| 1:B:145:GLU:C | 1:B:146:LEU:HD12 | 2.34 | 0.47 |
| 1:K:103:LEU:HD22 | 2:K:501:ACO:H121 | 1.95 | 0.47 |
| 1:A:184:ILE:HG21 | 1:A:228:GLY:HA2 | 1.96 | 0.47 |
| 1:G:8:THR:O | 1:G:57:GLY:N | 2.46 | 0.47 |
| 1:J:155:PHE:CZ | 1:J:260:ARG:HA | 2.49 | 0.47 |
| 1:L:33:PHE:CD1 | 1:L:34:ILE:N | 2.82 | 0.47 |
| 1:K:314:ARG:NH1 | 1:K:314:ARG:CG | 2.72 | 0.47 |
| 1:D:8:THR:N | 1:H:353:ALA:N | 2.47 | 0.47 |
| 1:J:145:GLU:HB3 | 1:J:295:TRP:HB3 | 1.96 | 0.47 |
| 1:D:225:HIS:ND1 | 1:D:226:PRO:HD2 | 2.29 | 0.47 |
| 1:B:381:LEU:C | 1:B:381:LEU:CD2 | 2.83 | 0.47 |
| 1:C:281:LEU:HB3 | 1:C:282:PRO:HD3 | 1.96 | 0.47 |
| 1:A:21:GLY:HA3 | 1:A:64:VAL:CG2 | 2.44 | 0.47 |
| 1:I:14:PRO:HD2 | 1:I:51:ALA:O | 2.14 | 0.47 |
| 1:D:10:THR:CG2 | 1:H:384:LYS:HE3 | 2.44 | 0.47 |
| 1:D:8:THR:N | 1:H:353:ALA:CB | 2.78 | 0.47 |
| 1:H:98:ARG:HH21 | 1:H:99:ARG:HH21 | 1.52 | 0.47 |
| 1:I:289:ARG:HG2 | 1:J:298:ASP:OD1 | 2.13 | 0.47 |
| 1:E:192:VAL:CG1 | 1:E:403:GLN:HB2 | 2.39 | 0.47 |
| 1:H:247:LEU:HD23 | 1:H:247:LEU:C | 2.34 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:218:ARG:HH21 | 1:J:239:LEU:HD21 | 1.79 | 0.47 |
| 1:F:357:MSE:HB3 | 1:F:381:LEU:HD12 | 1.90 | 0.47 |
| 1:B:150:ARG:NH2 | 1:B:266:ASP:OD1 | 2.48 | 0.47 |
| 1:D:42:TRP:NE1 | 1:D:90:PHE:CE1 | 2.77 | 0.47 |
| 1:K:98:ARG:NE | 1:K:99:ARG:CZ | 2.78 | 0.47 |
| 1:A:326:VAL:HG21 | 1:A:351:ALA:HB3 | 1.95 | 0.47 |
| 1:H:137:TYR:O | 1:H:360:ASP:HB2 | 2.14 | 0.47 |
| 1:F:109:GLU:O | 1:F:113:ARG:HG3 | 2.14 | 0.47 |
| 1:G:171:LEU:HD21 | 1:I:28:ALA:CB | 2.45 | 0.47 |
| 1:D:65:VAL:CG1 | 1:D:97:HIS:CE1 | 2.88 | 0.47 |
| 1:E:314:ARG:O | 1:E:316:TYR:CE1 | 2.67 | 0.47 |
| 1:G:218:ARG:HD2 | 1:G:234:VAL:HB | 1.96 | 0.47 |
| 1:E:360:ASP:CG | 1:E:380:ARG:HH22 | 2.17 | 0.47 |
| 1:D:16:GLU:O | 1:D:19:TRP:CD1 | 2.67 | 0.47 |
| 1:J:169:VAL:CG1 | 1:J:223:LEU:HB3 | 2.44 | 0.47 |
| 1:J:146:LEU:HD22 | 1:J:275:THR:HG21 | 1.97 | 0.47 |
| 1:C:225:HIS:CG | 1:C:226:PRO:HD2 | 2.50 | 0.47 |
| 1:C:355:ILE:HD11 | 1:C:381:LEU:CG | 2.44 | 0.47 |
| 1:D:193:PRO:CG | 1:D:400:VAL:HG23 | 2.44 | 0.47 |
| 1:H:109:GLU:OE1 | 1:H:112:ARG:CD | 2.56 | 0.47 |
| 1:I:193:PRO:CG | 1:I:400:VAL:CG2 | 2.92 | 0.47 |
| 1:C:198:ARG:NH1 | 1:C:206:LEU:HD12 | 2.30 | 0.47 |
| 1:I:318:HIS:C | 1:I:320:VAL:H | 2.18 | 0.47 |
| 1:E:111:HIS:CD2 | 1:E:303:ARG:HD3 | 2.49 | 0.47 |
| 1:D:314:ARG:HG3 | 1:D:316:TYR:CZ | 2.49 | 0.47 |
| 1:G:158:ASP:HB3 | 1:H:379:ASN:O | 2.14 | 0.47 |
| 1:G:131:ILE:O | 1:G:134:ARG:HG2 | 2.14 | 0.47 |
| 1:B:264:GLY:O | 1:E:98:ARG:NE | 2.43 | 0.47 |
| 1:J:45:LEU:CD1 | 1:J:199:PRO:HG2 | 2.43 | 0.47 |
| 1:J:35:GLY:N | 1:J:36:PRO:CD | 2.78 | 0.47 |
| 1:K:336:ALA:O | 1:K:346:CYS:HA | 2.15 | 0.47 |
| 1:D:225:HIS:CG | 1:D:226:PRO:HD2 | 2.49 | 0.47 |
| 1:D:15:THR:HG23 | 1:D:55:ARG:HH22 | 1.80 | 0.47 |
| 1:F:93:VAL:HG23 | 2:F:501:ACO:H132 | 1.97 | 0.47 |
| 1:D:114:ILE:CG2 | 1:D:305:MSE:HE2 | 2.45 | 0.47 |
| 1:F:43:ARG:HB3 | 1:F:43:ARG:NH1 | 2.29 | 0.47 |
| 1:J:109:GLU:OE2 | 1:J:109:GLU:HA | 2.15 | 0.47 |
| 1:H:150:ARG:HH21 | 1:H:266:ASP:HA | 1.80 | 0.47 |
| 1:D:294:THR:O | 1:D:295:TRP:HB2 | 2.14 | 0.47 |
| 1:A:314:ARG:NH2 | 1:A:396:PHE:C | 2.68 | 0.47 |
| 1:B:51:ALA:CB | 1:B:69:LEU:HB3 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:250:VAL:HG23 | 1:E:251:THR:HG23 | 1.96 | 0.47 |
| 1:H:281:LEU:O | 1:H:282:PRO:C | 2.54 | 0.47 |
| 1:D:98:ARG:HD2 | 1:E:264:GLY:HA3 | 1.95 | 0.47 |
| 1:J:150:ARG:HB3 | 1:J:271:ILE:HD13 | 1.97 | 0.47 |
| 1:I:318:HIS:O | 1:I:320:VAL:N | 2.44 | 0.47 |
| 1:K:239:LEU:O | 1:K:268:MSE:HE1 | 2.15 | 0.47 |
| 1:G:307:VAL:CG1 | 1:G:311:LEU:HD11 | 2.45 | 0.47 |
| 1:A:276:HIS:HB2 | 1:A:277:PRO:CD | 2.44 | 0.47 |
| 1:J:155:PHE:CE1 | 1:J:260:ARG:HA | 2.50 | 0.47 |
| 1:J:218:ARG:NH2 | 1:J:239:LEU:HD21 | 2.30 | 0.47 |
| 1:H:360:ASP:OD2 | 1:H:380:ARG:NH2 | 2.47 | 0.47 |
| 1:D:387:GLN:HG3 | 1:D:390:ARG:HH21 | 1.80 | 0.47 |
| 1:I:74:ARG:HD3 | 1:I:84:PRO:HA | 1.97 | 0.47 |
| 1:H:11:LEU:HD11 | 1:H:52:VAL:HG22 | 1.96 | 0.47 |
| 1:G:314:ARG:NH1 | 1:G:366:TYR:O | 2.47 | 0.47 |
| 1:K:259:TRP:CZ2 | 1:K:281:LEU:HD22 | 2.49 | 0.47 |
| 1:G:44:THR:HG21 | 1:G:201:VAL:CG2 | 2.43 | 0.46 |
| 1:F:289:ARG:O | 1:F:291:ALA:N | 2.47 | 0.46 |
| 1:G:355:ILE:HG13 | 1:G:383:THR:HB | 1.98 | 0.46 |
| 1:E:314:ARG:CG | 1:E:314:ARG:HH11 | 2.29 | 0.46 |
| 1:I:320:VAL:O | 1:I:320:VAL:HG13 | 2.15 | 0.46 |
| 1:E:114:ILE:HG23 | 1:E:119:TYR:HB2 | 1.98 | 0.46 |
| 1:F:392:LEU:O | 1:F:393:ASP:C | 2.53 | 0.46 |
| 1:J:332:GLY:O | 1:J:335:PHE:CE1 | 2.68 | 0.46 |
| 1:A:145:GLU:C | 1:A:146:LEU:HD12 | 2.36 | 0.46 |
| 1:H:100:ARG:N | 3:H:601:HOH:O | 2.09 | 0.46 |
| 1:H:361:VAL:HG13 | 1:H:375:LEU:HD13 | 1.95 | 0.46 |
| 1:C:120:PRO:C | 1:C:305:MSE:HB2 | 2.35 | 0.46 |
| 1:A:121:VAL:CG1 | 1:A:122:ALA:H | 2.27 | 0.46 |
| 1:B:198:ARG:NH1 | 1:B:206:LEU:HD12 | 2.30 | 0.46 |
| 1:E:77:VAL:HG11 | 1:E:83:LEU:HD12 | 1.97 | 0.46 |
| 1:B:327:LEU:CD1 | 1:B:357:MSE:HE3 | 2.44 | 0.46 |
| 1:I:251:THR:O | 1:I:252:ALA:C | 2.52 | 0.46 |
| 1:E:221:PHE:O | 1:E:232:TYR:CE1 | 2.68 | 0.46 |
| 1:D:314:ARG:NH1 | 1:D:366:TYR:O | 2.48 | 0.46 |
| 1:G:385:ASP:OD1 | 1:G:386:SER:N | 2.48 | 0.46 |
| 1:H:369:ALA:HB2 | 1:H:402:VAL:HG11 | 1.97 | 0.46 |
| 1:C:379:ASN:HB2 | 1:D:160:PRO:HD3 | 1.97 | 0.46 |
| 1:G:372:ALA:HB1 | 1:G:381:LEU:CD1 | 2.45 | 0.46 |
| 1:I:198:ARG:CD | 1:I:203:TRP:CE2 | 2.99 | 0.46 |
| 1:B:109:GLU:O | 1:B:112:ARG:CG | 2.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:247:LEU:C | 1:I:247:LEU:CD2 | 2.83 | 0.46 |
| 1:E:259:TRP:O | 1:E:263:ILE:HG12 | 2.14 | 0.46 |
| 1:L:275:THR:OG1 | 1:L:276:HIS:N | 2.47 | 0.46 |
| 1:H:169:VAL:HG22 | 1:H:225:HIS:CA | 2.45 | 0.46 |
| 1:F:121:VAL:CA | 1:F:305:MSE:HG2 | 2.22 | 0.46 |
| 1:H:98:ARG:CZ | 1:H:99:ARG:CZ | 2.93 | 0.46 |
| 1:B:146:LEU:HD12 | 1:B:146:LEU:N | 2.30 | 0.46 |
| 1:C:314:ARG:HD2 | 1:C:366:TYR:CE1 | 2.51 | 0.46 |
| 1:A:192:VAL:HG12 | 1:A:193:PRO:O | 2.15 | 0.46 |
| 1:J:385:ASP:OD1 | 1:J:386:SER:N | 2.48 | 0.46 |
| 1:K:379:ASN:HB2 | 1:L:160:PRO:HD3 | 1.98 | 0.46 |
| 1:C:126:ALA:HB1 | 1:C:128:GLU:O | 2.16 | 0.46 |
| 1:A:186:GLU:HA | 1:A:186:GLU:OE1 | 2.15 | 0.46 |
| 1:E:128:GLU:CA | 1:F:289:ARG:NH2 | 2.79 | 0.46 |
| 1:I:38:SER:O | 1:I:42:TRP:CG | 2.68 | 0.46 |
| 1:I:318:HIS:CE1 | 1:I:342:GLY:HA3 | 2.50 | 0.46 |
| 1:I:342:GLY:C | 1:I:343:ARG:HG3 | 2.36 | 0.46 |
| 1:H:42:TRP:HA | 1:H:46:VAL:HG23 | 1.98 | 0.46 |
| 1:K:292:ARG:HG3 | 3:K:605:HOH:O | 2.16 | 0.46 |
| 1:E:47:PRO:HG2 | 1:E:70:TYR:CE1 | 2.51 | 0.46 |
| 1:D:10:THR:CB | 1:H:384:LYS:HD2 | 2.45 | 0.46 |
| 1:G:381:LEU:O | 1:G:381:LEU:HD23 | 2.16 | 0.46 |
| 1:G:33:PHE:C | 1:G:34:ILE:HG13 | 2.35 | 0.46 |
| 1:B:109:GLU:O | 1:B:113:ARG:HG3 | 2.16 | 0.46 |
| 1:G:297:GLN:CG | 1:G:298:ASP:N | 2.79 | 0.46 |
| 1:K:19:TRP:HZ3 | 1:K:42:TRP:CE3 | 2.33 | 0.46 |
| 1:A:127:SER:H | 2:A:501:ACO:H21 | 1.80 | 0.46 |
| 1:K:77:VAL:HB | 1:K:78:PRO:CD | 2.46 | 0.46 |
| 1:J:63:GLU:OE1 | 1:K:170:ARG:HD2 | 2.16 | 0.46 |
| 1:G:379:ASN:O | 1:H:158:ASP:HB3 | 2.16 | 0.46 |
| 1:H:218:ARG:HD2 | 1:H:234:VAL:HB | 1.98 | 0.46 |
| 2:L:501:ACO:O5P | 2:L:501:ACO:H141 | 2.16 | 0.46 |
| 1:I:281:LEU:HB3 | 1:I:282:PRO:HD3 | 1.98 | 0.46 |
| 1:D:145:GLU:HB2 | 1:D:295:TRP:HE3 | 1.80 | 0.46 |
| 1:L:327:LEU:HD23 | 1:L:328:GLU:N | 2.31 | 0.46 |
| 1:L:131:ILE:HG12 | 2:L:501:ACO:C6A | 2.46 | 0.46 |
| 1:D:199:PRO:O | 1:D:200:GLN:C | 2.54 | 0.46 |
| 1:L:146:LEU:O | 1:L:272:SER:HA | 2.16 | 0.46 |
| 1:E:128:GLU:HA | 1:F:289:ARG:HH21 | 1.80 | 0.46 |
| 1:B:144:HIS:NE2 | 1:B:277:PRO:HG3 | 2.29 | 0.46 |
| 1:D:304:ILE:HG13 | 1:D:362:LEU:HD23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:233:ARG:HD2 | 3:D:612:HOH:O | 2.14 | 0.46 |
| 1:H:339:ILE:HG12 | 1:H:344:ALA:CB | 2.46 | 0.46 |
| 1:H:19:TRP:N | 1:H:20:PRO:CD | 2.79 | 0.46 |
| 1:A:18:ASP:O | 1:A:19:TRP:C | 2.54 | 0.46 |
| 1:C:42:TRP:NE1 | 1:C:90:PHE:CE2 | 2.80 | 0.46 |
| 1:K:375:LEU:HD21 | 1:L:283:HIS:CE1 | 2.51 | 0.46 |
| 1:F:49:ASP:OD1 | 1:F:49:ASP:C | 2.54 | 0.46 |
| 1:L:70:TYR:HB3 | 1:L:88:LEU:HD23 | 1.97 | 0.46 |
| 1:D:33:PHE:CZ | 1:D:38:SER:CB | 2.99 | 0.46 |
| 1:A:34:ILE:CD1 | 1:A:37:GLU:OE1 | 2.56 | 0.46 |
| 1:F:247:LEU:HD23 | 1:F:247:LEU:C | 2.35 | 0.46 |
| 1:C:188:TRP:CH2 | 1:C:248:ARG:NH1 | 2.84 | 0.46 |
| 1:J:185:TYR:CE2 | 1:J:198:ARG:HB2 | 2.51 | 0.46 |
| 1:K:38:SER:O | 1:K:39:ALA:C | 2.55 | 0.46 |
| 1:K:312:GLU:HG2 | 1:K:344:ALA:O | 2.16 | 0.45 |
| 1:J:288:THR:HG23 | 3:J:606:HOH:O | 2.16 | 0.45 |
| 1:I:378:ALA:HB1 | 1:J:284:LEU:HD23 | 1.98 | 0.45 |
| 1:J:287:ASP:HB3 | 1:J:290:LEU:HD12 | 1.97 | 0.45 |
| 1:I:146:LEU:HA | 1:I:292:ARG:O | 2.16 | 0.45 |
| 1:H:354:GLU:CB | 1:H:384:LYS:HZ3 | 2.28 | 0.45 |
| 1:J:381:LEU:O | 1:J:381:LEU:HD12 | 2.16 | 0.45 |
| 1:J:149:ASP:OD2 | 1:J:152:PHE:CD1 | 2.70 | 0.45 |
| 1:H:281:LEU:HB3 | 1:H:282:PRO:HD3 | 1.98 | 0.45 |
| 1:A:98:ARG:O | 1:A:99:ARG:HB2 | 2.16 | 0.45 |
| 1:H:380:ARG:HD2 | 1:H:380:ARG:HA | 1.81 | 0.45 |
| 1:H:11:LEU:HD12 | 1:H:12:CYS:N | 2.30 | 0.45 |
| 1:H:196:LEU:CD1 | 1:H:406:PHE:CZ | 2.98 | 0.45 |
| 1:J:314:ARG:HD3 | 1:J:316:TYR:CE2 | 2.52 | 0.45 |
| 1:E:289:ARG:HD3 | 1:F:297:GLN:HG3 | 1.99 | 0.45 |
| 1:I:16:GLU:HA | 1:I:19:TRP:CD1 | 2.51 | 0.45 |
| 1:E:8:THR:O | 1:E:57:GLY:HA2 | 2.16 | 0.45 |
| 1:D:194:GLY:HA3 | 1:D:403:GLN:O | 2.16 | 0.45 |
| 1:J:206:LEU:HD21 | 1:J:231:LEU:HD11 | 1.98 | 0.45 |
| 1:G:248:ARG:HH22 | 1:G:405:ALA:HA | 1.82 | 0.45 |
| 1:I:150:ARG:HG3 | 1:I:151:ARG:N | 2.32 | 0.45 |
| 1:I:134:ARG:NH1 | 2:I:501:ACO:H1B | 2.31 | 0.45 |
| 1:A:69:LEU:HD12 | 1:A:69:LEU:C | 2.37 | 0.45 |
| 1:I:308:PRO:HA | 1:I:346:CYS:SG | 2.57 | 0.45 |
| 1:L:123:ALA:HB2 | 1:L:302:LEU:HD23 | 1.98 | 0.45 |
| 1:I:67:MSE:N | 1:I:106:MSE:SE | 3.00 | 0.45 |
| 1:L:306:ASN:ND2 | 1:L:309:ALA:HB2 | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:274:ILE:HD13 | 1:D:274:ILE:N | 2.31 | 0.45 |
| 1:G:185:TYR:C | 1:G:185:TYR:CD1 | 2.89 | 0.45 |
| 1:A:385:ASP:C | 1:A:385:ASP:OD1 | 2.54 | 0.45 |
| 1:F:67:MSE:HE2 | 1:F:90:PHE:HB3 | 1.98 | 0.45 |
| 1:G:150:ARG:HG3 | 1:G:151:ARG:N | 2.31 | 0.45 |
| 1:F:104:ARG:NH2 | 2:F:501:ACO:O8A | 2.49 | 0.45 |
| 1:F:182:GLU:HG2 | 1:F:203:TRP:CE2 | 2.51 | 0.45 |
| 1:K:281:LEU:HD12 | 1:K:281:LEU:O | 2.16 | 0.45 |
| 1:B:322:GLU:HA | 1:B:339:ILE:O | 2.17 | 0.45 |
| 1:J:125:HIS:CE1 | 1:J:407:GLU:HA | 2.50 | 0.45 |
| 1:K:173:ARG:HG2 | 1:K:173:ARG:HH11 | 1.82 | 0.45 |
| 1:D:202:LEU:HD23 | 1:D:202:LEU:HA | 1.69 | 0.45 |
| 1:C:178:ARG:HH11 | 1:C:207:LEU:CD1 | 2.25 | 0.45 |
| 1:C:144:HIS:HD2 | 1:C:277:PRO:HG3 | 1.70 | 0.45 |
| 1:E:142:THR:HG21 | 1:E:144:HIS:NE2 | 2.32 | 0.45 |
| 2:C:501:ACO:O5P | 2:C:501:ACO:N8P | 2.49 | 0.45 |
| 1:A:98:ARG:NH1 | 1:A:99:ARG:NH2 | 2.65 | 0.45 |
| 1:B:34:ILE:HB | 1:B:37:GLU:CD | 2.37 | 0.45 |
| 1:A:16:GLU:HA | 1:A:19:TRP:NE1 | 2.32 | 0.45 |
| 1:E:39:ALA:O | 1:E:43:ARG:HG2 | 2.17 | 0.45 |
| 1:H:173:ARG:HG2 | 1:K:24:LEU:HD13 | 1.99 | 0.45 |
| 1:K:67:MSE:HB2 | 1:K:67:MSE:HE3 | 1.94 | 0.45 |
| 1:F:34:ILE:HG22 | 1:F:36:PRO:HG2 | 1.98 | 0.45 |
| 1:D:85:THR:HG23 | 1:D:121:VAL:O | 2.16 | 0.45 |
| 1:K:389:LEU:HA | 1:K:389:LEU:HD23 | 1.78 | 0.45 |
| 1:J:259:TRP:CE2 | 1:J:281:LEU:HD22 | 2.52 | 0.45 |
| 1:H:222:ALA:HA | 1:H:230:ALA:O | 2.17 | 0.45 |
| 1:A:259:TRP:CZ2 | 1:A:281:LEU:HD22 | 2.52 | 0.45 |
| 1:H:153:ALA:HA | 1:H:290:LEU:CD1 | 2.47 | 0.45 |
| 1:D:123:ALA:HB2 | 1:D:302:LEU:HD23 | 1.99 | 0.45 |
| 1:F:55:ARG:HB3 | 1:F:62:SER:HB2 | 1.98 | 0.45 |
| 1:H:265:LEU:HD23 | 1:K:95:PRO:HB3 | 1.98 | 0.45 |
| 1:C:153:ALA:HA | 1:C:290:LEU:HD13 | 1.98 | 0.45 |
| 1:H:98:ARG:NH2 | 1:H:99:ARG:CZ | 2.79 | 0.45 |
| 1:H:98:ARG:HG3 | 1:H:99:ARG:NH1 | 2.31 | 0.45 |
| 1:K:247:LEU:CD2 | 1:K:247:LEU:C | 2.85 | 0.45 |
| 1:A:145:GLU:HB2 | 1:A:295:TRP:HB3 | 1.98 | 0.45 |
| 1:J:106:MSE:O | 1:J:110:LEU:HG | 2.17 | 0.45 |
| 1:J:83:LEU:HD21 | 1:J:313:ALA:HB1 | 1.98 | 0.45 |
| 2:L:501:ACO:O5P | 2:L:501:ACO:N8P | 2.48 | 0.45 |
| 1:I:148:VAL:CG2 | 1:I:290:LEU:O | 2.65 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:297:GLN:OE1 | 1:F:289:ARG:NE | 2.49 | 0.45 |
| 1:K:98:ARG:CG | 1:K:99:ARG:NH1 | 2.77 | 0.45 |
| 1:I:318:HIS:HA | 1:I:341:ASP:OD1 | 2.16 | 0.45 |
| 1:E:107:CYS:HB3 | 1:E:111:HIS:HE1 | 1.82 | 0.45 |
| 1:J:50:GLY:CA | 1:J:70:TYR:CE1 | 3.00 | 0.45 |
| 1:H:188:TRP:HH2 | 1:H:405:ALA:HB2 | 1.81 | 0.45 |
| 1:B:125:HIS:CE1 | 1:B:407:GLU:HA | 2.51 | 0.45 |
| 1:L:281:LEU:HB3 | 1:L:282:PRO:HD3 | 1.99 | 0.45 |
| 1:K:74:ARG:HD3 | 1:K:84:PRO:HA | 1.98 | 0.45 |
| 1:H:270:ARG:NH1 | 3:H:620:HOH:O | 2.34 | 0.45 |
| 1:B:150:ARG:HG2 | 1:B:269:GLU:C | 2.37 | 0.45 |
| 1:L:318:HIS:CE1 | 1:L:341:ASP:O | 2.70 | 0.45 |
| 1:I:43:ARG:HH11 | 1:I:43:ARG:CA | 2.25 | 0.45 |
| 1:I:276:HIS:CD2 | 1:I:278:GLN:H | 2.27 | 0.45 |
| 1:D:52:VAL:CG1 | 1:D:110:LEU:CD2 | 2.95 | 0.45 |
| 1:F:307:VAL:HB | 1:F:308:PRO:HD3 | 1.99 | 0.45 |
| 1:A:169:VAL:HG22 | 1:A:170:ARG:N | 2.30 | 0.45 |
| 1:J:327:LEU:HD12 | 1:J:355:ILE:HG23 | 1.98 | 0.44 |
| 1:J:297:GLN:CG | 1:J:298:ASP:N | 2.80 | 0.44 |
| 1:B:145:GLU:HB2 | 1:B:295:TRP:HE3 | 1.83 | 0.44 |
| 1:A:142:THR:HG21 | 1:A:296:ARG:NH2 | 2.32 | 0.44 |
| 2:I:501:ACO:H141 | 2:I:501:ACO:O5P | 2.17 | 0.44 |
| 1:G:380:ARG:NH1 | 1:H:158:ASP:OD2 | 2.48 | 0.44 |
| 1:H:87:GLY:HA2 | 1:H:123:ALA:O | 2.16 | 0.44 |
| 1:K:70:TYR:HB3 | 1:K:88:LEU:HD23 | 1.98 | 0.44 |
| 1:C:380:ARG:NH1 | 1:D:158:ASP:OD2 | 2.45 | 0.44 |
| 1:F:42:TRP:CD1 | 1:F:46:VAL:CG2 | 2.96 | 0.44 |
| 1:H:146:LEU:CD2 | 1:H:146:LEU:N | 2.78 | 0.44 |
| 1:I:194:GLY:HA3 | 1:I:403:GLN:O | 2.16 | 0.44 |
| 1:J:247:LEU:C | 1:J:247:LEU:CD2 | 2.84 | 0.44 |
| 1:H:16:GLU:HA | 1:H:19:TRP:CD1 | 2.51 | 0.44 |
| 1:F:198:ARG:HD2 | 1:F:203:TRP:CZ2 | 2.51 | 0.44 |
| 1:A:289:ARG:HG3 | 1:B:129:GLY:HA3 | 1.99 | 0.44 |
| 1:I:145:GLU:HB3 | 1:I:295:TRP:HB3 | 1.99 | 0.44 |
| 1:B:114:ILE:HG22 | 1:B:305:MSE:HE2 | 1.98 | 0.44 |
| 1:K:400:VAL:CG1 | 1:K:400:VAL:O | 2.65 | 0.44 |
| 1:D:218:ARG:HD2 | 1:D:234:VAL:HB | 1.99 | 0.44 |
| 1:K:103:LEU:N | 2:K:501:ACO:O2A | 2.47 | 0.44 |
| 1:A:70:TYR:O | 1:A:70:TYR:CD1 | 2.70 | 0.44 |
| 1:I:67:MSE:HE2 | 1:I:90:PHE:HB3 | 1.99 | 0.44 |
| 1:D:50:GLY:HA2 | 1:D:70:TYR:CE2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:334:ARG:HD3 | 1:I:351:ALA:O | 2.17 | 0.44 |
| 1:H:242:ALA:HB2 | 1:H:268:MSE:HG3 | 1.99 | 0.44 |
| 2:C:501:ACO:H4B | 2:C:501:ACO:O8A | 2.17 | 0.44 |
| 1:I:65:VAL:CG1 | 1:I:97:HIS:CE1 | 2.99 | 0.44 |
| 1:G:16:GLU:HA | 1:G:19:TRP:HE1 | 1.82 | 0.44 |
| 1:F:123:ALA:HB2 | 1:F:302:LEU:HD23 | 1.99 | 0.44 |
| 1:F:178:ARG:O | 1:F:182:GLU:HG3 | 2.17 | 0.44 |
| 1:J:327:LEU:CD1 | 1:J:355:ILE:HG23 | 2.48 | 0.44 |
| 1:J:74:ARG:CD | 1:J:84:PRO:CA | 2.93 | 0.44 |
| 1:K:194:GLY:HA3 | 1:K:403:GLN:O | 2.17 | 0.44 |
| 1:J:400:VAL:O | 1:J:400:VAL:CG2 | 2.66 | 0.44 |
| 1:A:134:ARG:CZ | 2:A:501:ACO:H1B | 2.48 | 0.44 |
| 1:J:184:ILE:HG21 | 1:J:229:TYR:CD1 | 2.53 | 0.44 |
| 1:L:134:ARG:CZ | 2:L:501:ACO:H1B | 2.48 | 0.44 |
| 1:E:9:VAL:O | 1:E:9:VAL:HG12 | 2.16 | 0.44 |
| 1:G:150:ARG:HG2 | 1:G:269:GLU:C | 2.38 | 0.44 |
| 1:E:44:THR:HG21 | 1:E:201:VAL:HG21 | 1.98 | 0.44 |
| 1:G:121:VAL:HA | 1:G:305:MSE:HG2 | 1.99 | 0.44 |
| 1:E:247:LEU:CD2 | 1:E:247:LEU:C | 2.86 | 0.44 |
| 1:L:320:VAL:HG21 | 1:L:394:ALA:CB | 2.47 | 0.44 |
| 1:L:130:GLY:N | 3:L:628:HOH:O | 2.47 | 0.44 |
| 1:C:292:ARG:HG2 | 1:C:293:THR:O | 2.18 | 0.44 |
| 1:H:34:ILE:C | 1:H:37:GLU:HG2 | 2.38 | 0.44 |
| 1:H:198:ARG:NH1 | 1:H:206:LEU:HD12 | 2.33 | 0.44 |
| 1:C:121:VAL:HB | 1:C:303:ARG:O | 2.17 | 0.44 |
| 1:I:198:ARG:NH1 | 1:I:206:LEU:HD12 | 2.33 | 0.44 |
| 1:C:206:LEU:HD21 | 1:C:231:LEU:CD1 | 2.47 | 0.44 |
| 1:C:170:ARG:HD2 | 1:F:63:GLU:OE2 | 2.18 | 0.44 |
| 1:F:146:LEU:HD22 | 1:F:275:THR:HG21 | 2.00 | 0.44 |
| 1:F:181:PHE:HE1 | 1:F:224:LEU:HD13 | 1.83 | 0.44 |
| 1:H:9:VAL:HB | 1:H:55:ARG:O | 2.17 | 0.44 |
| 1:I:289:ARG:NH1 | 1:J:297:GLN:OE1 | 2.50 | 0.44 |
| 1:K:188:TRP:CG | 1:K:248:ARG:HD2 | 2.52 | 0.44 |
| 1:L:320:VAL:CG2 | 1:L:394:ALA:HB1 | 2.48 | 0.44 |
| 1:J:305:MSE:HA | 1:J:359:ARG:HH21 | 1.83 | 0.44 |
| 1:G:63:GLU:OE1 | 1:L:170:ARG:HD2 | 2.17 | 0.44 |
| 1:J:326:VAL:CG1 | 1:J:353:ALA:HA | 2.48 | 0.44 |
| 1:C:296:ARG:HD3 | 1:D:293:THR:OG1 | 2.18 | 0.44 |
| 1:J:41:ALA:HA | 1:J:44:THR:HG21 | 2.00 | 0.44 |
| 1:D:23:PHE:CE1 | 1:D:42:TRP:CZ3 | 3.06 | 0.44 |
| 1:H:337:LEU:HD11 | 1:H:344:ALA:HB1 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:501:ACO:H62 | 2:A:501:ACO:O9P | 2.18 | 0.44 |
| 1:G:48:THR:O | 1:G:49:ASP:CG | 2.56 | 0.44 |
| 1:H:88:LEU:HB2 | 1:H:124:LEU:HB3 | 2.00 | 0.44 |
| 1:G:147:THR:OG1 | 1:G:294:THR:HG21 | 2.17 | 0.44 |
| 1:F:42:TRP:O | 1:F:46:VAL:HB | 2.18 | 0.43 |
| 1:F:295:TRP:CZ2 | 1:F:297:GLN:CB | 3.01 | 0.43 |
| 1:A:45:LEU:HD21 | 1:A:199:PRO:HG2 | 1.99 | 0.43 |
| 1:B:222:ALA:HB2 | 1:B:231:LEU:HD23 | 1.99 | 0.43 |
| 1:A:360:ASP:CG | 1:A:380:ARG:HH22 | 2.21 | 0.43 |
| 1:I:160:PRO:HG2 | 1:I:256:CYS:CB | 2.47 | 0.43 |
| 1:E:225:HIS:CG | 1:E:226:PRO:HD2 | 2.53 | 0.43 |
| 1:F:329:VAL:HB | 1:F:332:GLY:HA3 | 2.00 | 0.43 |
| 1:J:85:THR:CG2 | 1:J:121:VAL:HG23 | 2.44 | 0.43 |
| 1:K:34:ILE:CG2 | 1:K:36:PRO:HD2 | 2.44 | 0.43 |
| 1:A:41:ALA:O | 1:A:45:LEU:HB2 | 2.18 | 0.43 |
| 1:E:69:LEU:C | 1:E:69:LEU:HD12 | 2.39 | 0.43 |
| 1:I:317:ALA:CB | 1:I:394:ALA:O | 2.66 | 0.43 |
| 1:E:46:VAL:HA | 1:E:47:PRO:HD3 | 1.88 | 0.43 |
| 1:H:200:GLN:OE1 | 1:H:200:GLN:HA | 2.18 | 0.43 |
| 1:K:186:GLU:OE1 | 1:K:186:GLU:HA | 2.18 | 0.43 |
| 1:F:150:ARG:HG3 | 1:F:151:ARG:N | 2.33 | 0.43 |
| 1:A:144:HIS:CD2 | 1:A:296:ARG:HG3 | 2.53 | 0.43 |
| 1:B:198:ARG:HD2 | 1:B:203:TRP:CZ2 | 2.53 | 0.43 |
| 1:E:308:PRO:HD3 | 1:E:335:PHE:CE2 | 2.53 | 0.43 |
| 1:J:281:LEU:O | 1:J:282:PRO:C | 2.54 | 0.43 |
| 1:A:281:LEU:N | 1:A:282:PRO:CD | 2.82 | 0.43 |
| 1:D:59:GLY:O | 1:D:60:PRO:C | 2.57 | 0.43 |
| 1:C:72:ASP:O | 1:C:73:LEU:HD23 | 2.18 | 0.43 |
| 1:E:337:LEU:HD13 | 1:E:346:CYS:HB2 | 2.01 | 0.43 |
| 1:L:247:LEU:HD23 | 1:L:248:ARG:N | 2.33 | 0.43 |
| 1:K:193:PRO:CG | 1:K:400:VAL:CG1 | 2.96 | 0.43 |
| 1:D:169:VAL:HG12 | 1:D:170:ARG:N | 2.33 | 0.43 |
| 1:F:19:TRP:HB2 | 1:F:20:PRO:CD | 2.48 | 0.43 |
| 1:G:19:TRP:N | 1:G:20:PRO:HD2 | 2.33 | 0.43 |
| 1:K:326:VAL:CG1 | 1:K:334:ARG:HG2 | 2.49 | 0.43 |
| 1:L:19:TRP:HB2 | 1:L:20:PRO:CD | 2.47 | 0.43 |
| 1:J:202:LEU:CD1 | 1:J:406:PHE:CE2 | 3.01 | 0.43 |
| 1:I:69:LEU:C | 1:I:69:LEU:HD12 | 2.38 | 0.43 |
| 1:B:150:ARG:HG2 | 1:B:269:GLU:O | 2.18 | 0.43 |
| 1:H:295:TRP:CH2 | 1:H:297:GLN:HB3 | 2.53 | 0.43 |
| 1:K:188:TRP:CD2 | 1:K:248:ARG:NH1 | 2.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:198:ARG:HD2 | 1:E:203:TRP:CE2 | 2.53 | 0.43 |
| 1:K:98:ARG:HH21 | 1:K:99:ARG:NH2 | 2.17 | 0.43 |
| 1:C:259:TRP:O | 1:C:263:ILE:HG12 | 2.18 | 0.43 |
| 1:G:125:HIS:HE1 | 3:G:629:HOH:O | 2.00 | 0.43 |
| 1:F:298:ASP:OD2 | 1:F:301:TRP:CZ2 | 2.72 | 0.43 |
| 1:D:334:ARG:CD | 1:D:351:ALA:O | 2.67 | 0.43 |
| 1:C:137:TYR:O | 1:C:360:ASP:HB2 | 2.18 | 0.43 |
| 1:B:153:ALA:CB | 1:B:263:ILE:HD12 | 2.47 | 0.43 |
| 1:D:30:PHE:HB2 | 1:D:33:PHE:HB2 | 1.99 | 0.43 |
| 1:K:327:LEU:HD13 | 1:K:355:ILE:HG23 | 2.00 | 0.43 |
| 1:L:316:TYR:O | 1:L:342:GLY:HA2 | 2.19 | 0.43 |
| 1:E:307:VAL:HB | 1:E:308:PRO:CD | 2.44 | 0.43 |
| 1:D:52:VAL:CG1 | 1:D:110:LEU:HD21 | 2.47 | 0.43 |
| 1:G:282:PRO:O | 1:G:288:THR:HG22 | 2.19 | 0.43 |
| 1:J:93:VAL:HG23 | 2:J:501:ACO:H132 | 1.99 | 0.43 |
| 1:I:393:ASP:O | 1:I:397:ALA:HB2 | 2.19 | 0.43 |
| 1:L:127:SER:HB3 | 2:L:501:ACO:H22 | 2.01 | 0.43 |
| 1:D:123:ALA:HA | 1:D:301:TRP:O | 2.19 | 0.43 |
| 1:I:133:GLY:C | 1:I:135:PHE:H | 2.22 | 0.43 |
| 1:F:44:THR:O | 1:F:45:LEU:HD23 | 2.19 | 0.43 |
| 1:J:137:TYR:O | 1:J:360:ASP:HB2 | 2.19 | 0.43 |
| 1:D:58:ALA:HB2 | 1:H:384:LYS:HG3 | 2.01 | 0.43 |
| 1:J:45:LEU:HD13 | 1:J:73:LEU:HD21 | 2.01 | 0.43 |
| 1:J:324:SER:OG | 1:J:338:LYS:HD2 | 2.19 | 0.43 |
| 1:L:355:ILE:HD11 | 1:L:381:LEU:HD13 | 2.00 | 0.43 |
| 1:G:146:LEU:HD12 | 1:G:146:LEU:HA | 1.79 | 0.43 |
| 1:E:372:ALA:HB1 | 1:E:381:LEU:HD21 | 2.01 | 0.43 |
| 1:B:213:ALA:HA | 1:B:214:PRO:HD2 | 1.86 | 0.43 |
| 1:H:24:LEU:HD13 | 1:J:173:ARG:CG | 2.49 | 0.43 |
| 1:A:148:VAL:HA | 1:A:290:LEU:O | 2.18 | 0.43 |
| 1:L:121:VAL:HA | 1:L:305:MSE:HG2 | 2.01 | 0.43 |
| 1:E:287:ASP:OD1 | 1:F:129:GLY:HA3 | 2.18 | 0.43 |
| 1:D:10:THR:CG2 | 1:H:384:LYS:CE | 2.96 | 0.43 |
| 1:G:289:ARG:HD3 | 1:H:298:ASP:OD1 | 2.19 | 0.43 |
| 1:H:145:GLU:OE2 | 1:H:295:TRP:HB2 | 2.19 | 0.43 |
| 1:E:142:THR:CG2 | 1:E:144:HIS:NE2 | 2.82 | 0.43 |
| 1:G:247:LEU:HD23 | 1:G:248:ARG:N | 2.34 | 0.43 |
| 1:G:225:HIS:O | 1:G:226:PRO:C | 2.56 | 0.43 |
| 1:E:42:TRP:CD1 | 1:E:42:TRP:N | 2.87 | 0.43 |
| 1:K:69:LEU:HD12 | 1:K:69:LEU:C | 2.38 | 0.43 |
| 1:G:297:GLN:HG2 | 1:G:298:ASP:N | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:63:GLU:OE1 | 1:F:170:ARG:HD2 | 2.18 | 0.43 |
| 1:J:123:ALA:HB2 | 1:J:302:LEU:HD23 | 1.99 | 0.43 |
| 1:H:150:ARG:HD3 | 1:H:151:ARG:CA | 2.47 | 0.43 |
| 1:C:266:ASP:C | 1:C:268:MSE:H | 2.22 | 0.43 |
| 1:E:193:PRO:CG | 1:E:400:VAL:CG2 | 2.94 | 0.43 |
| 1:E:193:PRO:HG2 | 1:E:400:VAL:HG23 | 2.00 | 0.43 |
| 1:H:121:VAL:CA | 1:H:305:MSE:HG2 | 2.41 | 0.43 |
| 1:L:49:ASP:O | 1:L:49:ASP:OD1 | 2.37 | 0.43 |
| 1:H:371:ARG:HB3 | 1:H:371:ARG:HE | 1.56 | 0.43 |
| 1:I:385:ASP:OD2 | 1:I:388:LEU:HB2 | 2.19 | 0.43 |
| 1:I:297:GLN:CG | 1:I:298:ASP:N | 2.81 | 0.43 |
| 1:H:169:VAL:CG2 | 1:H:225:HIS:CD2 | 3.02 | 0.43 |
| 1:F:289:ARG:O | 1:F:290:LEU:C | 2.57 | 0.43 |
| 1:A:178:ARG:O | 1:A:182:GLU:HG3 | 2.19 | 0.43 |
| 1:H:196:LEU:CB | 1:H:406:PHE:CE2 | 2.95 | 0.43 |
| 2:H:501:ACO:N8P | 2:H:501:ACO:O5P | 2.52 | 0.43 |
| 1:J:217:ASP:OD2 | 1:J:233:ARG:NH1 | 2.51 | 0.43 |
| 1:J:334:ARG:HD2 | 1:J:351:ALA:O | 2.19 | 0.43 |
| 1:K:306:ASN:OD1 | 1:K:308:PRO:HD2 | 2.19 | 0.43 |
| 1:E:73:LEU:O | 1:E:85:THR:N | 2.33 | 0.43 |
| 1:I:50:GLY:HA2 | 1:I:70:TYR:CE1 | 2.54 | 0.43 |
| 1:F:306:ASN:OD1 | 1:F:308:PRO:HD2 | 2.19 | 0.43 |
| 1:F:322:GLU:HA | 1:F:339:ILE:O | 2.18 | 0.43 |
| 1:J:192:VAL:HG11 | 1:J:403:GLN:HB2 | 2.01 | 0.43 |
| 1:D:45:LEU:HB2 | 1:D:71:MSE:HE2 | 2.01 | 0.43 |
| 1:A:152:PHE:HE1 | 1:D:151:ARG:HB3 | 1.83 | 0.43 |
| 1:G:306:ASN:HB3 | 1:G:309:ALA:HB3 | 2.00 | 0.43 |
| 1:L:378:ALA:O | 3:L:611:HOH:O | 2.21 | 0.43 |
| 1:K:341:ASP:O | 1:K:343:ARG:HG3 | 2.18 | 0.43 |
| 1:A:292:ARG:O | 1:A:294:THR:HG23 | 2.19 | 0.43 |
| 1:H:387:GLN:HG3 | 1:H:388:LEU:N | 2.34 | 0.42 |
| 1:J:381:LEU:C | 1:J:381:LEU:HD12 | 2.40 | 0.42 |
| 1:G:99:ARG:NH1 | 2:G:501:ACO:O5A | 2.52 | 0.42 |
| 1:E:297:GLN:OE1 | 1:F:289:ARG:CZ | 2.67 | 0.42 |
| 1:B:24:LEU:CD1 | 1:D:173:ARG:HG2 | 2.45 | 0.42 |
| 1:A:98:ARG:HD3 | 1:F:264:GLY:CA | 2.49 | 0.42 |
| 1:H:247:LEU:C | 1:H:247:LEU:CD2 | 2.87 | 0.42 |
| 1:H:11:LEU:CD1 | 1:H:52:VAL:HG22 | 2.49 | 0.42 |
| 1:A:76:THR:O | 1:A:193:PRO:HA | 2.20 | 0.42 |
| 1:L:11:LEU:HD12 | 1:L:53:VAL:O | 2.19 | 0.42 |
| 1:H:334:ARG:HD2 | 1:H:351:ALA:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:138:GLY:O | 1:J:301:TRP:HA | 2.18 | 0.42 |
| 1:D:187:ARG:O | 1:D:191:GLN:HG3 | 2.18 | 0.42 |
| 1:F:137:TYR:CD2 | 1:F:303:ARG:HB2 | 2.54 | 0.42 |
| 1:E:145:GLU:HB3 | 1:E:295:TRP:CB | 2.42 | 0.42 |
| 1:J:150:ARG:HG2 | 1:J:269:GLU:O | 2.17 | 0.42 |
| 1:B:247:LEU:C | 1:B:247:LEU:CD2 | 2.87 | 0.42 |
| 2:K:501:ACO:O5P | 2:K:501:ACO:H141 | 2.19 | 0.42 |
| 1:K:225:HIS:O | 1:K:226:PRO:C | 2.56 | 0.42 |
| 1:L:281:LEU:N | 1:L:282:PRO:HD2 | 2.35 | 0.42 |
| 1:C:208:ALA:O | 1:C:211:LYS:HG2 | 2.19 | 0.42 |
| 1:C:200:GLN:HE21 | 1:C:200:GLN:HA | 1.84 | 0.42 |
| 1:A:303:ARG:HH11 | 1:A:305:MSE:SE | 2.53 | 0.42 |
| 1:C:144:HIS:HD2 | 1:C:277:PRO:CD | 2.32 | 0.42 |
| 1:A:69:LEU:HD12 | 1:A:69:LEU:O | 2.19 | 0.42 |
| 1:I:123:ALA:HB1 | 1:I:300:LEU:HD11 | 2.01 | 0.42 |
| 1:I:109:GLU:O | 1:I:113:ARG:HG3 | 2.19 | 0.42 |
| 1:A:359:ARG:NH1 | 3:A:610:HOH:O | 2.53 | 0.42 |
| 1:D:184:ILE:HG21 | 1:D:228:GLY:HA2 | 2.01 | 0.42 |
| 1:K:147:THR:HB | 1:K:294:THR:HG21 | 2.01 | 0.42 |
| 1:H:54:VAL:HG11 | 1:H:102:LEU:HD22 | 2.01 | 0.42 |
| 1:I:33:PHE:CG | 1:I:34:ILE:N | 2.88 | 0.42 |
| 1:E:128:GLU:C | 1:F:289:ARG:NH2 | 2.73 | 0.42 |
| 1:I:289:ARG:NE | 1:J:297:GLN:OE1 | 2.53 | 0.42 |
| 1:I:327:LEU:HD23 | 1:I:328:GLU:CA | 2.49 | 0.42 |
| 1:B:14:PRO:CD | 1:B:51:ALA:O | 2.63 | 0.42 |
| 1:C:314:ARG:O | 1:C:316:TYR:CE1 | 2.72 | 0.42 |
| 1:L:330:SER:O | 1:L:331:ASP:CB | 2.67 | 0.42 |
| 1:L:88:LEU:HA | 1:L:88:LEU:HD23 | 1.78 | 0.42 |
| 1:A:259:TRP:CE2 | 1:A:281:LEU:HD22 | 2.55 | 0.42 |
| 1:A:11:LEU:HD13 | 1:A:54:VAL:HG22 | 2.02 | 0.42 |
| 1:A:185:TYR:CD1 | 1:A:185:TYR:C | 2.92 | 0.42 |
| 1:I:357:MSE:CE | 1:I:381:LEU:CD2 | 2.98 | 0.42 |
| 1:E:148:VAL:HG13 | 1:E:291:ALA:N | 2.32 | 0.42 |
| 1:E:146:LEU:HD12 | 1:E:275:THR:HG22 | 1.85 | 0.42 |
| 1:H:112:ARG:HG3 | 1:H:113:ARG:N | 2.34 | 0.42 |
| 1:C:367:LEU:O | 1:C:402:VAL:CG2 | 2.66 | 0.42 |
| 1:I:83:LEU:HD21 | 1:I:313:ALA:CB | 2.46 | 0.42 |
| 1:A:181:PHE:HD1 | 1:A:229:TYR:CG | 2.38 | 0.42 |
| 1:A:124:LEU:HD12 | 1:A:124:LEU:C | 2.39 | 0.42 |
| 1:E:133:GLY:HA2 | 1:E:137:TYR:O | 2.19 | 0.42 |
| 1:E:134:ARG:N | 3:E:629:HOH:O | 2.45 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:110:LEU:N | 1:C:110:LEU:CD1 | 2.80 | 0.42 |
| 1:E:327:LEU:HD13 | 1:E:357:MSE:HE3 | 1.89 | 0.42 |
| 1:A:136:GLY:O | 1:A:303:ARG:HG3 | 2.20 | 0.42 |
| 1:I:110:LEU:O | 1:I:114:ILE:HG13 | 2.20 | 0.42 |
| 1:A:42:TRP:HA | 1:A:46:VAL:CG2 | 2.50 | 0.42 |
| 1:G:311:LEU:CD1 | 1:G:311:LEU:H | 2.32 | 0.42 |
| 1:L:206:LEU:HD23 | 1:L:207:LEU:HD13 | 2.01 | 0.42 |
| 1:H:279:ASP:O | 1:H:282:PRO:HD2 | 2.18 | 0.42 |
| 1:K:297:GLN:HG2 | 1:K:298:ASP:N | 2.35 | 0.42 |
| 1:B:321:GLY:O | 1:B:322:GLU:C | 2.58 | 0.42 |
| 1:I:11:LEU:HD12 | 1:I:12:CYS:N | 2.34 | 0.42 |
| 1:C:357:MSE:HE1 | 1:C:381:LEU:HD22 | 1.92 | 0.42 |
| 1:E:281:LEU:HD23 | 1:E:291:ALA:HB1 | 2.00 | 0.42 |
| 1:D:44:THR:CG2 | 1:D:201:VAL:HG11 | 2.49 | 0.42 |
| 1:A:314:ARG:NH1 | 1:A:315:GLY:O | 2.52 | 0.42 |
| 1:B:87:GLY:HA2 | 1:B:123:ALA:O | 2.20 | 0.42 |
| 1:C:308:PRO:HA | 1:C:346:CYS:SG | 2.60 | 0.42 |
| 1:A:63:GLU:OE1 | 1:F:170:ARG:HB3 | 2.19 | 0.42 |
| 1:J:102:LEU:O | 1:J:105:ALA:N | 2.53 | 0.42 |
| 2:D:501:ACO:OAP | 1:E:266:ASP:OD2 | 2.38 | 0.42 |
| 1:K:297:GLN:CD | 1:L:289:ARG:HD3 | 2.39 | 0.42 |
| 1:H:188:TRP:CH2 | 1:H:405:ALA:HB2 | 2.54 | 0.42 |
| 1:G:171:LEU:HD11 | 1:G:221:PHE:HB3 | 2.01 | 0.42 |
| 1:H:11:LEU:HD11 | 1:H:52:VAL:CG2 | 2.49 | 0.42 |
| 1:I:156:HIS:CE1 | 1:J:380:ARG:NH1 | 2.88 | 0.42 |
| 1:L:114:ILE:HG22 | 1:L:305:MSE:HE2 | 2.02 | 0.42 |
| 1:G:155:PHE:CZ | 1:G:260:ARG:HA | 2.54 | 0.42 |
| 1:A:25:LEU:O | 1:A:29:SER:HB2 | 2.20 | 0.42 |
| 1:E:127:SER:CB | 2:E:501:ACO:C2P | 2.96 | 0.42 |
| 1:F:303:ARG:HH11 | 1:F:305:MSE:SE | 2.53 | 0.42 |
| 1:A:357:MSE:HE2 | 1:A:381:LEU:HB2 | 2.01 | 0.42 |
| 1:H:326:VAL:CG1 | 1:H:353:ALA:HA | 2.50 | 0.42 |
| 1:G:247:LEU:C | 1:G:247:LEU:HD23 | 2.40 | 0.42 |
| 1:K:134:ARG:CZ | 2:K:501:ACO:H1B | 2.50 | 0.42 |
| 2:J:501:ACO:O8A | 2:J:501:ACO:H4B | 2.20 | 0.42 |
| 1:L:259:TRP:O | 1:L:263:ILE:CG1 | 2.68 | 0.42 |
| 1:K:379:ASN:CB | 1:L:160:PRO:HD3 | 2.49 | 0.42 |
| 1:A:380:ARG:HD2 | 1:B:158:ASP:OD2 | 2.19 | 0.42 |
| 1:K:124:LEU:HD23 | 1:K:137:TYR:CE2 | 2.54 | 0.42 |
| 1:E:235:ASP:HB3 | 1:E:238:ASP:O | 2.19 | 0.42 |
| 1:B:297:GLN:CG | 1:B:298:ASP:N | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:200:GLN:NE2 | 1:F:200:GLN:HA | 2.35 | 0.42 |
| 1:I:148:VAL:HA | 1:I:290:LEU:O | 2.19 | 0.42 |
| 1:I:387:GLN:O | 1:I:391:ARG:HG3 | 2.20 | 0.42 |
| 1:K:327:LEU:HD12 | 1:K:355:ILE:O | 2.20 | 0.42 |
| 1:H:109:GLU:C | 1:H:112:ARG:HG2 | 2.33 | 0.42 |
| 1:C:268:MSE:HE2 | 1:C:268:MSE:HA | 2.02 | 0.42 |
| 1:F:98:ARG:NH1 | 1:F:99:ARG:NH2 | 2.67 | 0.42 |
| 1:J:40:THR:OG1 | 1:J:41:ALA:N | 2.53 | 0.42 |
| 1:C:103:LEU:HD22 | 2:C:501:ACO:H133 | 2.01 | 0.42 |
| 1:H:307:VAL:HB | 1:H:308:PRO:HD3 | 2.02 | 0.42 |
| 1:F:298:ASP:OD2 | 1:F:301:TRP:HZ2 | 2.02 | 0.42 |
| 1:K:173:ARG:HG2 | 1:K:173:ARG:NH1 | 2.35 | 0.42 |
| 1:G:173:ARG:HD2 | 1:G:176:GLU:OE2 | 2.19 | 0.42 |
| 1:C:288:THR:HG23 | 1:C:289:ARG:N | 2.35 | 0.42 |
| 1:H:63:GLU:OE1 | 1:J:170:ARG:HD2 | 2.20 | 0.42 |
| 1:E:45:LEU:HD21 | 1:E:199:PRO:HG2 | 2.02 | 0.42 |
| 1:F:151:ARG:CZ | 1:F:269:GLU:HG3 | 2.50 | 0.42 |
| 1:H:314:ARG:O | 1:H:316:TYR:CE1 | 2.73 | 0.42 |
| 2:K:501:ACO:O5P | 2:K:501:ACO:N8P | 2.53 | 0.42 |
| 1:K:298:ASP:OD2 | 1:K:301:TRP:NE1 | 2.47 | 0.42 |
| 1:L:327:LEU:HG | 1:L:357:MSE:HE3 | 2.02 | 0.42 |
| 1:A:218:ARG:NH2 | 1:A:239:LEU:HD21 | 2.34 | 0.42 |
| 1:C:169:VAL:HG22 | 1:F:96:THR:CG2 | 2.50 | 0.42 |
| 1:G:45:LEU:HD21 | 1:G:199:PRO:HG2 | 2.02 | 0.42 |
| 1:J:384:LYS:HG2 | 1:J:384:LYS:O | 2.20 | 0.42 |
| 1:F:229:TYR:C | 1:F:229:TYR:CD1 | 2.93 | 0.42 |
| 1:K:327:LEU:HD11 | 1:K:357:MSE:CE | 2.26 | 0.41 |
| 1:J:72:ASP:CG | 1:J:74:ARG:HH12 | 2.24 | 0.41 |
| 1:J:42:TRP:O | 1:J:43:ARG:C | 2.58 | 0.41 |
| 1:E:110:LEU:HA | 1:E:110:LEU:HD23 | 1.84 | 0.41 |
| 1:C:74:ARG:HB3 | 1:C:82:VAL:CG1 | 2.49 | 0.41 |
| 1:L:16:GLU:HA | 1:L:19:TRP:CD1 | 2.55 | 0.41 |
| 1:F:213:ALA:HA | 1:F:214:PRO:HD2 | 1.92 | 0.41 |
| 1:I:142:THR:O | 1:I:277:PRO:HD3 | 2.20 | 0.41 |
| 1:H:110:LEU:O | 1:H:114:ILE:HG13 | 2.20 | 0.41 |
| 2:E:501:ACO:H131 | 2:E:501:ACO:O9P | 2.20 | 0.41 |
| 1:K:259:TRP:CE2 | 1:K:281:LEU:HD22 | 2.55 | 0.41 |
| 1:J:360:ASP:OD2 | 1:J:380:ARG:NH2 | 2.53 | 0.41 |
| 1:I:297:GLN:HG3 | 1:I:298:ASP:N | 2.35 | 0.41 |
| 1:B:297:GLN:HG2 | 1:B:298:ASP:N | 2.35 | 0.41 |
| 1:C:169:VAL:HG22 | 1:F:96:THR:HG22 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:232:TYR:HB3 | 1:A:244:VAL:HG22 | 2.02 | 0.41 |
| 1:C:123:ALA:HA | 1:C:301:TRP:O | 2.20 | 0.41 |
| 1:J:148:VAL:HG22 | 1:J:291:ALA:HA | 2.01 | 0.41 |
| 1:D:58:ALA:HB1 | 1:H:384:LYS:HG3 | 2.01 | 0.41 |
| 1:D:44:THR:HG21 | 1:D:201:VAL:CG2 | 2.44 | 0.41 |
| 1:J:405:ALA:CA | 3:J:602:HOH:O | 2.53 | 0.41 |
| 1:I:114:ILE:HG21 | 1:I:305:MSE:HE2 | 2.00 | 0.41 |
| 1:A:47:PRO:O | 1:A:48:THR:C | 2.59 | 0.41 |
| 1:D:281:LEU:O | 1:D:281:LEU:HD12 | 2.20 | 0.41 |
| 1:F:314:ARG:HG3 | 1:F:316:TYR:CE1 | 2.55 | 0.41 |
| 1:J:83:LEU:HD11 | 1:J:313:ALA:HB1 | 2.02 | 0.41 |
| 1:F:181:PHE:CE1 | 1:F:224:LEU:HD13 | 2.55 | 0.41 |
| 1:C:197:LEU:HB3 | 3:C:627:HOH:O | 2.19 | 0.41 |
| 1:L:67:MSE:HE2 | 1:L:90:PHE:HB3 | 2.02 | 0.41 |
| 1:B:86:ALA:O | 1:B:122:ALA:HA | 2.19 | 0.41 |
| 1:E:93:VAL:HG12 | 1:E:94:ALA:O | 2.20 | 0.41 |
| 1:C:297:GLN:HG2 | 1:C:298:ASP:N | 2.35 | 0.41 |
| 1:K:188:TRP:CZ3 | 1:K:248:ARG:NH1 | 2.88 | 0.41 |
| 1:I:276:HIS:ND1 | 1:I:403:GLN:HG2 | 2.35 | 0.41 |
| 1:I:375:LEU:CD2 | 1:J:283:HIS:CE1 | 3.02 | 0.41 |
| 1:K:91:VAL:O | 2:K:501:ACO:N4P | 2.53 | 0.41 |
| 1:I:319:GLU:HB3 | 1:J:320:VAL:HG23 | 2.01 | 0.41 |
| 1:C:14:PRO:HD2 | 1:C:51:ALA:O | 2.20 | 0.41 |
| 1:K:305:MSE:HB3 | 1:K:305:MSE:HE3 | 1.75 | 0.41 |
| 1:G:127:SER:H | 2:G:501:ACO:H21 | 1.84 | 0.41 |
| 1:C:134:ARG:HH12 | 2:C:501:ACO:H1B | 1.82 | 0.41 |
| 1:B:149:ASP:OD2 | 1:B:152:PHE:CD2 | 2.73 | 0.41 |
| 1:G:307:VAL:CG1 | 1:G:311:LEU:CD1 | 2.98 | 0.41 |
| 1:J:169:VAL:HG22 | 1:J:225:HIS:HB2 | 2.02 | 0.41 |
| 1:C:380:ARG:O | 3:C:614:HOH:O | 2.22 | 0.41 |
| 1:L:232:TYR:HA | 1:L:243:ARG:O | 2.21 | 0.41 |
| 1:A:22:MSE:HE3 | 1:A:67:MSE:HE3 | 2.02 | 0.41 |
| 1:H:177:HIS:O | 1:H:181:PHE:CD2 | 2.74 | 0.41 |
| 1:F:85:THR:HG22 | 1:F:86:ALA:N | 2.34 | 0.41 |
| 1:E:148:VAL:CG2 | 1:E:291:ALA:CB | 2.97 | 0.41 |
| 1:H:169:VAL:HG22 | 1:H:225:HIS:HA | 2.01 | 0.41 |
| 1:G:206:LEU:HD21 | 1:G:231:LEU:CD1 | 2.50 | 0.41 |
| 1:C:144:HIS:CE1 | 1:C:296:ARG:NH1 | 2.88 | 0.41 |
| 1:E:387:GLN:O | 1:E:391:ARG:HG3 | 2.20 | 0.41 |
| 1:F:314:ARG:HG3 | 1:F:316:TYR:CZ | 2.56 | 0.41 |
| 1:I:334:ARG:CD | 1:I:351:ALA:O | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:67:MSE:O | 1:L:91:VAL:HA | 2.21 | 0.41 |
| 1:B:134:ARG:HG3 | 1:B:135:PHE:CD1 | 2.56 | 0.41 |
| 1:H:320:VAL:HG22 | 1:H:321:GLY:N | 2.36 | 0.41 |
| 1:C:148:VAL:HA | 1:C:290:LEU:O | 2.20 | 0.41 |
| 1:B:150:ARG:HG3 | 1:B:151:ARG:N | 2.36 | 0.41 |
| 1:J:357:MSE:HB3 | 1:J:381:LEU:CB | 2.50 | 0.41 |
| 1:F:289:ARG:C | 1:F:291:ALA:N | 2.74 | 0.41 |
| 1:E:32:ASP:OD1 | 1:E:33:PHE:N | 2.54 | 0.41 |
| 1:G:54:VAL:HG11 | 1:G:102:LEU:CD2 | 2.49 | 0.41 |
| 1:A:35:GLY:N | 1:A:36:PRO:CD | 2.83 | 0.41 |
| 1:K:33:PHE:CG | 1:K:34:ILE:N | 2.89 | 0.41 |
| 1:D:104:ARG:HG3 | 1:D:135:PHE:CE1 | 2.48 | 0.41 |
| 1:J:98:ARG:NH2 | 1:J:99:ARG:CZ | 2.84 | 0.41 |
| 1:E:169:VAL:HG22 | 1:E:170:ARG:N | 2.34 | 0.41 |
| 1:J:22:MSE:HB3 | 1:J:67:MSE:CE | 2.51 | 0.41 |
| 1:F:373:SER:HA | 1:F:389:LEU:HD22 | 2.02 | 0.41 |
| 1:E:362:LEU:HA | 1:E:362:LEU:HD12 | 1.86 | 0.41 |
| 1:J:276:HIS:CD2 | 1:J:278:GLN:H | 2.39 | 0.41 |
| 1:J:207:LEU:O | 1:J:210:CYS:HB2 | 2.21 | 0.41 |
| 1:I:225:HIS:CG | 1:I:226:PRO:CD | 3.04 | 0.41 |
| 1:F:98:ARG:NE | 1:F:99:ARG:NH1 | 2.68 | 0.41 |
| 1:E:33:PHE:HD1 | 1:E:33:PHE:C | 2.19 | 0.41 |
| 1:I:322:GLU:HA | 1:I:339:ILE:O | 2.20 | 0.41 |
| 1:B:207:LEU:O | 1:B:210:CYS:HB2 | 2.20 | 0.41 |
| 1:B:383:THR:HG21 | 1:B:389:LEU:CD2 | 2.51 | 0.41 |
| 1:B:167:SER:OG | 1:E:100:ARG:NH1 | 2.53 | 0.41 |
| 1:D:213:ALA:HA | 1:D:214:PRO:HD2 | 1.85 | 0.41 |
| 1:C:148:VAL:HG22 | 1:C:291:ALA:HA | 0.56 | 0.41 |
| 1:F:150:ARG:NH2 | 1:F:263:ILE:O | 2.51 | 0.41 |
| 1:F:34:ILE:CG2 | 1:F:36:PRO:HG2 | 2.51 | 0.41 |
| 1:E:34:ILE:HG22 | 1:E:35:GLY:N | 2.34 | 0.41 |
| 1:D:8:THR:CG2 | 1:D:9:VAL:H | 2.19 | 0.41 |
| 1:G:246:GLU:HG2 | 1:G:248:ARG:HG2 | 2.02 | 0.41 |
| 1:B:70:TYR:HA | 1:B:87:GLY:O | 2.21 | 0.41 |
| 1:I:98:ARG:HE | 1:I:99:ARG:NH2 | 2.18 | 0.41 |
| 1:G:33:PHE:CG | 1:G:34:ILE:N | 2.89 | 0.41 |
| 1:B:198:ARG:HG2 | 1:B:203:TRP:CD1 | 2.56 | 0.41 |
| 1:C:70:TYR:CA | 1:C:87:GLY:O | 2.66 | 0.41 |
| 1:G:367:LEU:O | 1:G:402:VAL:CG2 | 2.69 | 0.41 |
| 1:G:141:THR:HG22 | 1:G:402:VAL:HG11 | 2.02 | 0.41 |
| 1:I:300:LEU:HG | 1:I:301:TRP:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:103:LEU:HD22 | 2:F:501:ACO:CCP | 2.50 | 0.41 |
| 1:C:188:TRP:CZ2 | 1:C:248:ARG:NH1 | 2.89 | 0.41 |
| 1:B:167:SER:OG | 1:E:100:ARG:CZ | 2.69 | 0.41 |
| 1:L:49:ASP:OD1 | 1:L:49:ASP:C | 2.59 | 0.41 |
| 1:H:100:ARG:NH1 | 1:J:167:SER:OG | 2.54 | 0.41 |
| 1:J:385:ASP:OD1 | 1:J:387:GLN:N | 2.45 | 0.41 |
| 1:D:198:ARG:HA | 1:D:199:PRO:HD3 | 1.80 | 0.41 |
| 1:F:169:VAL:HG23 | 1:F:224:LEU:O | 2.21 | 0.41 |
| 1:A:290:LEU:HD23 | 1:A:290:LEU:HA | 1.88 | 0.41 |
| 1:I:326:VAL:HG11 | 1:I:352:ALA:O | 2.21 | 0.41 |
| 1:D:126:ALA:HB1 | 1:D:128:GLU:O | 2.21 | 0.41 |
| 1:H:372:ALA:N | 1:H:393:ASP:OD1 | 2.54 | 0.41 |
| 1:E:306:ASN:HB3 | 1:E:309:ALA:HB3 | 2.03 | 0.41 |
| 1:G:274:ILE:N | 1:G:274:ILE:HD13 | 2.36 | 0.41 |
| 1:C:223:LEU:O | 1:C:229:TYR:HA | 2.21 | 0.41 |
| 1:H:186:GLU:OE2 | 1:H:189:ARG:NH1 | 2.52 | 0.41 |
| 1:C:355:ILE:HG13 | 1:C:383:THR:HB | 2.02 | 0.41 |
| 1:F:120:PRO:C | 1:F:121:VAL:HG13 | 2.41 | 0.41 |
| 1:G:328:GLU:HB2 | 1:G:334:ARG:HG3 | 2.03 | 0.41 |
| 1:C:184:ILE:HG21 | 1:C:228:GLY:HA2 | 2.02 | 0.41 |
| 1:J:202:LEU:HD23 | 1:J:202:LEU:HA | 1.86 | 0.41 |
| 1:H:355:ILE:CD1 | 1:H:392:LEU:HD11 | 2.50 | 0.41 |
| 1:I:314:ARG:O | 1:I:316:TYR:CE1 | 2.74 | 0.41 |
| 1:I:357:MSE:HB3 | 1:I:381:LEU:HD12 | 2.03 | 0.40 |
| 1:B:120:PRO:C | 1:B:121:VAL:HG13 | 2.41 | 0.40 |
| 1:B:169:VAL:HG22 | 1:B:225:HIS:CA | 2.51 | 0.40 |
| 1:L:33:PHE:C | 1:L:33:PHE:CD1 | 2.95 | 0.40 |
| 1:E:93:VAL:HG23 | 2:E:501:ACO:H132 | 2.03 | 0.40 |
| 1:H:98:ARG:CG | 1:H:99:ARG:NH1 | 2.84 | 0.40 |
| 1:A:144:HIS:HB3 | 1:A:146:LEU:CD1 | 2.51 | 0.40 |
| 1:I:189:ARG:HH11 | 1:I:197:LEU:HD13 | 1.87 | 0.40 |
| 1:A:124:LEU:HD12 | 1:A:301:TRP:HB2 | 2.02 | 0.40 |
| 1:K:70:TYR:HB3 | 1:K:88:LEU:CD2 | 2.52 | 0.40 |
| 1:I:314:ARG:NH1 | 1:I:366:TYR:O | 2.54 | 0.40 |
| 1:E:180:GLU:O | 1:E:184:ILE:HG13 | 2.21 | 0.40 |
| 1:F:46:VAL:HA | 1:F:47:PRO:HD3 | 1.91 | 0.40 |
| 1:I:356:GLU:C | 1:I:357:MSE:HG2 | 2.42 | 0.40 |
| 1:C:144:HIS:CD2 | 1:C:277:PRO:CD | 3.04 | 0.40 |
| 1:D:144:HIS:CE1 | 1:D:296:ARG:NH1 | 2.89 | 0.40 |
| 1:C:101:GLY:CA | 2:C:501:ACO:O2A | 2.68 | 0.40 |
| 1:G:69:LEU:CD1 | 1:G:69:LEU:C | 2.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:98:ARG:NH1 | 1:A:99:ARG:CZ | 2.85 | 0.40 |
| 1:J:70:TYR:HA | 1:J:87:GLY:O | 2.21 | 0.40 |
| 1:D:250:VAL:CG1 | 1:D:250:VAL:O | 2.69 | 0.40 |
| 1:F:49:ASP:OD1 | 1:F:49:ASP:O | 2.39 | 0.40 |
| 1:B:173:ARG:HG2 | 1:E:24:LEU:HD13 | 2.02 | 0.40 |
| 1:E:234:VAL:HG23 | 3:E:614:HOH:O | 2.21 | 0.40 |
| 1:E:338:LYS:O | 1:E:344:ALA:HA | 2.21 | 0.40 |
| 1:I:202:LEU:HA | 1:I:202:LEU:HD23 | 1.84 | 0.40 |
| 1:G:79:GLY:O | 1:G:80:GLU:HB2 | 2.21 | 0.40 |
| 1:B:42:TRP:HA | 1:B:46:VAL:HG23 | 2.02 | 0.40 |
| 1:H:150:ARG:HD2 | 1:H:268:MSE:O | 2.21 | 0.40 |
| 1:D:145:GLU:HB2 | 1:D:295:TRP:HB3 | 1.99 | 0.40 |
| 1:B:48:THR:O | 1:B:49:ASP:CB | 2.67 | 0.40 |
| 1:I:85:THR:HG23 | 1:I:121:VAL:HG23 | 2.03 | 0.40 |
| 1:C:74:ARG:O | 1:C:196:LEU:HA | 2.21 | 0.40 |
| 1:F:48:THR:O | 1:F:49:ASP:OD1 | 2.39 | 0.40 |
| 1:L:50:GLY:HA2 | 1:L:70:TYR:CE1 | 2.57 | 0.40 |
| 1:H:74:ARG:HD3 | 1:H:84:PRO:HA | 2.03 | 0.40 |
| 1:H:398:SER:OG | 1:H:400:VAL:O | 2.33 | 0.40 |
| 1:F:46:VAL:HG22 | 1:F:69:LEU:HD13 | 2.04 | 0.40 |
| 1:J:45:LEU:HD13 | 1:J:73:LEU:CD2 | 2.52 | 0.40 |
| 1:J:398:SER:OG | 1:J:400:VAL:O | 2.30 | 0.40 |
| 1:C:247:LEU:CD2 | 1:C:247:LEU:C | 2.89 | 0.40 |
| 1:B:298:ASP:O | 1:B:298:ASP:OD1 | 2.39 | 0.40 |
| 1:K:192:VAL:O | 1:K:193:PRO:C | 2.60 | 0.40 |
| 1:G:327:LEU:O | 1:G:335:PHE:N | 2.55 | 0.40 |
| 1:D:48:THR:O | 1:D:49:ASP:CB | 2.70 | 0.40 |
| 1:A:198:ARG:HA | 1:A:199:PRO:HD3 | 1.93 | 0.40 |
| 1:G:77:VAL:HB | 1:G:78:PRO:CD | 2.49 | 0.40 |
| 1:E:319:GLU:HG3 | 3:F:628:HOH:O | 2.21 | 0.40 |
| 1:K:74:ARG:HB3 | 1:K:82:VAL:HG13 | 2.03 | 0.40 |
| 1:I:159:ALA:HA | 1:I:160:PRO:HD2 | 1.83 | 0.40 |
| 1:H:355:ILE:HD11 | 1:H:357:MSE:HE2 | 2.03 | 0.40 |
| 1:K:46:VAL:HA | 1:K:47:PRO:HD3 | 1.96 | 0.40 |
| 1:J:306:ASN:OD1 | 1:J:308:PRO:HD2 | 2.21 | 0.40 |
| 1:L:74:ARG:O | 1:L:196:LEU:HA | 2.21 | 0.40 |
| 1:L:135:PHE:O | 1:L:303:ARG:NE | 2.54 | 0.40 |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:E:9:VAL:CG1 | 1:L:8:THR:OG1[2_545] | 1.66 | 0.54 |
| 1:J:49:ASP:OD1 | 1:K:345:ARG:NH1[2_645] | 1.83 | 0.37 |
| 1:E:9:VAL:O | 1:L:8:THR:OG1[2_545] | 2.14 | 0.06 |

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 | 392/428 (92%) | 375 (96%) | 15 (4%) | 2 (0%) | 34 | 69 |
| 1 | B | 392/428 (92%) | 373 (95%) | 18 (5%) | 1 (0%) | 46 | 79 |
| 1 | C | 392/428 (92%) | 374 (95%) | 18 (5%) | 0 | 100 | 100 |
| 1 | D | 392/428 (92%) | 376 (96%) | 15 (4%) | 1 (0%) | 46 | 79 |
| 1 | E | 392/428 (92%) | 376 (96%) | 16 (4%) | 0 | 100 | 100 |
| 1 | F | 392/428 (92%) | 369 (94%) | 22 (6%) | 1 (0%) | 46 | 79 |
| 1 | G | 392/428 (92%) | 379 (97%) | 12 (3%) | 1 (0%) | 46 | 79 |
| 1 | H | 392/428 (92%) | 377 (96%) | 15 (4%) | 0 | 100 | 100 |
| 1 | I | 392/428 (92%) | 365 (93%) | 23 (6%) | 4 (1%) | 19 | 52 |
| 1 | J | 392/428 (92%) | 357 (91%) | 31 (8%) | 4 (1%) | 19 | 52 |
| 1 | K | 392/428 (92%) | 367 (94%) | 23 (6%) | 2 (0%) | 34 | 69 |
| 1 | L | 392/428 (92%) | 370 (94%) | 21 (5%) | 1 (0%) | 46 | 79 |
| All | All | 4704/5136 (92%) | 4458 (95%) | 229 (5%) | 17 (0%) | 39 | 74 |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | VAL |
| 1 | I | 319 | GLU |
| 1 | I | 357 | MSE |
| 1 | I | 397 | ALA |
| 1 | J | 175 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 309 | ALA |
| 1 | J | 357 | MSE |
| 1 | J | 358 | ASP |
| 1 | B | 62 | SER |
| 1 | F | 290 | LEU |
| 1 | I | 265 | LEU |
| 1 | L | 405 | ALA |
| 1 | A | 62 | SER |
| 1 | D | 319 | GLU |
| 1 | K | 295 | TRP |
| 1 | G | 332 | GLY |
| 1 | K | 114 | ILE |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 311/327 (95%) | 309 (99%) | 2 (1%) | 90 | 98 |
| 1 | B | 311/327 (95%) | 310 (100%) | 1 (0%) | 94 | 99 |
| 1 | C | 311/327 (95%) | 309 (99%) | 2 (1%) | 90 | 98 |
| 1 | D | 311/327 (95%) | 309 (99%) | 2 (1%) | 90 | 98 |
| 1 | E | 311/327 (95%) | 306 (98%) | 5 (2%) | 70 | 93 |
| 1 | F | 311/327 (95%) | 308 (99%) | 3 (1%) | 82 | 96 |
| 1 | G | 311/327 (95%) | 309 (99%) | 2 (1%) | 90 | 98 |
| 1 | H | 311/327 (95%) | 310 (100%) | 1 (0%) | 94 | 99 |
| 1 | I | 311/327 (95%) | 308 (99%) | 3 (1%) | 82 | 96 |
| 1 | J | 311/327 (95%) | 304 (98%) | 7 (2%) | 58 | 88 |
| 1 | K | 311/327 (95%) | 307 (99%) | 4 (1%) | 76 | 94 |
| 1 | L | 311/327 (95%) | 285 (92%) | 26 (8%) | 14 | 37 |
| All | All | 3732/3924 (95%) | 3674 (98%) | 58 (2%) | 70 | 93 |

All (58) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | THR |
| 1 | A | 341 | ASP |
| 1 | B | 106 | MSE |
| 1 | C | 145 | GLU |
| 1 | C | 150 | ARG |
| 1 | D | 38 | SER |
| 1 | D | 180 | GLU |
| 1 | E | 9 | VAL |
| 1 | E | 33 | PHE |
| 1 | E | 98 | ARG |
| 1 | E | 180 | GLU |
| 1 | E | 314 | ARG |
| 1 | F | 106 | MSE |
| 1 | F | 146 | LEU |
| 1 | F | 207 | LEU |
| 1 | G | 146 | LEU |
| 1 | G | 289 | ARG |
| 1 | H | 150 | ARG |
| 1 | I | 38 | SER |
| 1 | I | 233 | ARG |
| 1 | I | 297 | GLN |
| 1 | J | 146 | LEU |
| 1 | J | 233 | ARG |
| 1 | J | 273 | ILE |
| 1 | J | 314 | ARG |
| 1 | J | 356 | GLU |
| 1 | J | 357 | MSE |
| 1 | J | 358 | ASP |
| 1 | K | 150 | ARG |
| 1 | K | 207 | LEU |
| 1 | K | 267 | SER |
| 1 | K | 314 | ARG |
| 1 | L | 9 | VAL |
| 1 | L | 34 | ILE |
| 1 | L | 44 | THR |
| 1 | L | 52 | VAL |
| 1 | L | 85 | THR |
| 1 | L | 98 | ARG |
| 1 | L | 104 | ARG |
| 1 | L | 146 | LEU |
| 1 | L | 148 | VAL |
| 1 | L | 150 | ARG |
| 1 | L | 154 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 169 | VAL |
| 1 | L | 207 | LEU |
| 1 | L | 233 | ARG |
| 1 | L | 248 | ARG |
| 1 | L | 292 | ARG |
| 1 | L | 296 | ARG |
| 1 | L | 314 | ARG |
| 1 | L | 327 | LEU |
| 1 | L | 337 | LEU |
| 1 | L | 341 | ASP |
| 1 | L | 381 | LEU |
| 1 | L | 384 | LYS |
| 1 | L | 387 | GLN |
| 1 | L | 399 | ASP |
| 1 | L | 402 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 125 | HIS |
| 1 | A | 200 | GLN |
| 1 | A | 379 | ASN |
| 1 | B | 125 | HIS |
| 1 | B | 200 | GLN |
| 1 | C | 200 | GLN |
| 1 | C | 255 | HIS |
| 1 | C | 276 | HIS |
| 1 | D | 125 | HIS |
| 1 | E | 144 | HIS |
| 1 | E | 387 | GLN |
| 1 | F | 125 | HIS |
| 1 | F | 200 | GLN |
| 1 | F | 297 | GLN |
| 1 | G | 125 | HIS |
| 1 | G | 200 | GLN |
| 1 | G | 297 | GLN |
| 1 | G | 387 | GLN |
| 1 | H | 144 | HIS |
| 1 | H | 177 | HIS |
| 1 | H | 387 | GLN |
| 1 | I | 200 | GLN |
| 1 | I | 276 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 297 | GLN |
| 1 | I | 318 | HIS |
| 1 | J | 125 | HIS |
| 1 | J | 177 | HIS |
| 1 | J | 283 | HIS |
| 1 | J | 318 | HIS |
| 1 | K | 125 | HIS |
| 1 | K | 200 | GLN |
| 1 | L | 200 | GLN |
| 1 | L | 318 | HIS |
| 1 | L | 387 | GLN |

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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 | ACO | A | 501 | - | 43,53,53 | 1.76 | 6 (13%) | 55,79,79 | 2.46 | 16 (29%) |
| 2 | ACO | B | 501 | - | 43,53,53 | 1.77 | 6 (13%) | 55,79,79 | 2.46 | 17 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | ACO | C | 501 | - | 43,53,53 | 1.68 | 7 (16%) | 55,79,79 | 2.12 | 16 (29%) |
| 2 | ACO | D | 501 | - | 43,53,53 | 1.68 | 7 (16%) | 55,79,79 | 2.62 | 19 (34%) |
| 2 | ACO | E | 501 | - | 43,53,53 | 1.74 | 7 (16%) | 55,79,79 | 2.35 | 16 (29%) |
| 2 | ACO | F | 501 | - | 43,53,53 | 1.79 | 8 (18%) | 55,79,79 | 2.31 | 14 (25%) |
| 2 | ACO | G | 501 | - | 43,53,53 | 1.77 | 7 (16%) | 55,79,79 | 2.20 | 15 (27%) |
| 2 | ACO | H | 501 | - | 43,53,53 | 1.73 | 7 (16%) | 55,79,79 | 2.33 | 18 (32%) |
| 2 | ACO | I | 501 | - | 43,53,53 | 1.74 | 7 (16%) | 55,79,79 | 2.25 | 12 (21%) |
| 2 | ACO | J | 501 | - | 43,53,53 | 1.66 | 6 (13%) | 55,79,79 | 2.38 | 17 (30%) |
| 2 | ACO | K | 501 | - | 43,53,53 | 1.71 | 7 (16%) | 55,79,79 | 2.59 | 20 (36%) |
| 2 | ACO | L | 501 | - | 43,53,53 | 1.78 | 6 (13%) | 55,79,79 | 2.35 | 13 (23%) |

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 | ACO | A | 501 | - | - | 0/47/67/67 | 0/3/3/3 |
| 2 | ACO | B | 501 | - | - | 1/47/67/67 | 0/3/3/3 |
| 2 | ACO | C | 501 | - | - | 1/47/67/67 | 0/3/3/3 |
| 2 | ACO | D | 501 | - | - | 0/47/67/67 | 0/3/3/3 |
| 2 | ACO | E | 501 | - | - | 1/47/67/67 | 0/3/3/3 |
| 2 | ACO | F | 501 | - | - | 0/47/67/67 | 0/3/3/3 |
| 2 | ACO | G | 501 | - | - | 2/47/67/67 | 0/3/3/3 |
| 2 | ACO | H | 501 | - | - | 2/47/67/67 | 0/3/3/3 |
| 2 | ACO | I | 501 | - | - | 1/47/67/67 | 0/3/3/3 |
| 2 | ACO | J | 501 | - | - | 0/47/67/67 | 0/3/3/3 |
| 2 | ACO | K | 501 | - | - | 0/47/67/67 | 0/3/3/3 |
| 2 | ACO | L | 501 | - | - | 2/47/67/67 | 0/3/3/3 |

All (81) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 501 | ACO | C2B-C3B | -4.32 | 1.43 | 1.53 |
| 2 | G | 501 | ACO | C2B-C3B | -4.18 | 1.43 | 1.53 |
| 2 | F | 501 | ACO | C2B-C3B | -4.03 | 1.43 | 1.53 |
| 2 | A | 501 | ACO | C2B-C3B | -4.01 | 1.43 | 1.53 |
| 2 | L | 501 | ACO | C2B-C3B | -4.01 | 1.44 | 1.53 |
| 2 | H | 501 | ACO | C2B-C3B | -3.86 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | C | 501 | ACO | C2B-C3B | -3.58 | 1.44 | 1.53 |
| 2 | I | 501 | ACO | C2B-C3B | -3.47 | 1.45 | 1.53 |
| 2 | K | 501 | ACO | C2B-C3B | -3.45 | 1.45 | 1.53 |
| 2 | E | 501 | ACO | C2B-C3B | -3.39 | 1.45 | 1.53 |
| 2 | J | 501 | ACO | C2B-C3B | -3.31 | 1.45 | 1.53 |
| 2 | D | 501 | ACO | C2B-C3B | -3.30 | 1.45 | 1.53 |
| 2 | L | 501 | ACO | OAP-CAP | -3.23 | 1.35 | 1.42 |
| 2 | D | 501 | ACO | OAP-CAP | -3.04 | 1.36 | 1.42 |
| 2 | B | 501 | ACO | OAP-CAP | -2.93 | 1.36 | 1.42 |
| 2 | H | 501 | ACO | OAP-CAP | -2.75 | 1.36 | 1.42 |
| 2 | F | 501 | ACO | OAP-CAP | -2.73 | 1.36 | 1.42 |
| 2 | G | 501 | ACO | OAP-CAP | -2.71 | 1.36 | 1.42 |
| 2 | K | 501 | ACO | OAP-CAP | -2.67 | 1.36 | 1.42 |
| 2 | I | 501 | ACO | OAP-CAP | -2.62 | 1.37 | 1.42 |
| 2 | A | 501 | ACO | OAP-CAP | -2.57 | 1.37 | 1.42 |
| 2 | E | 501 | ACO | OAP-CAP | -2.56 | 1.37 | 1.42 |
| 2 | C | 501 | ACO | C3B-C4B | -2.55 | 1.45 | 1.52 |
| 2 | F | 501 | ACO | C3B-C4B | -2.54 | 1.45 | 1.52 |
| 2 | I | 501 | ACO | C3B-C4B | -2.47 | 1.45 | 1.52 |
| 2 | E | 501 | ACO | C3B-C4B | -2.42 | 1.45 | 1.52 |
| 2 | H | 501 | ACO | C3B-C4B | -2.38 | 1.46 | 1.52 |
| 2 | K | 501 | ACO | C3B-C4B | -2.38 | 1.46 | 1.52 |
| 2 | G | 501 | ACO | C3B-C4B | -2.37 | 1.46 | 1.52 |
| 2 | J | 501 | ACO | OAP-CAP | -2.37 | 1.37 | 1.42 |
| 2 | C | 501 | ACO | OAP-CAP | -2.27 | 1.37 | 1.42 |
| 2 | E | 501 | ACO | C5B-C4B | -2.26 | 1.44 | 1.51 |
| 2 | J | 501 | ACO | C3B-C4B | -2.23 | 1.46 | 1.52 |
| 2 | A | 501 | ACO | C3B-C4B | -2.20 | 1.46 | 1.52 |
| 2 | B | 501 | ACO | C3B-C4B | -2.19 | 1.46 | 1.52 |
| 2 | H | 501 | ACO | C5B-C4B | -2.16 | 1.44 | 1.51 |
| 2 | I | 501 | ACO | C5B-C4B | -2.10 | 1.44 | 1.51 |
| 2 | G | 501 | ACO | O2B-C2B | -2.08 | 1.38 | 1.43 |
| 2 | F | 501 | ACO | O3B-C3B | -2.05 | 1.37 | 1.44 |
| 2 | D | 501 | ACO | C5B-C4B | -2.04 | 1.45 | 1.51 |
| 2 | D | 501 | ACO | C3B-C4B | -2.03 | 1.47 | 1.52 |
| 2 | C | 501 | ACO | C5B-C4B | -2.02 | 1.45 | 1.51 |
| 2 | F | 501 | ACO | C5B-C4B | -2.01 | 1.45 | 1.51 |
| 2 | L | 501 | ACO | C3B-C4B | -2.01 | 1.47 | 1.52 |
| 2 | K | 501 | ACO | C5B-C4B | -2.00 | 1.45 | 1.51 |
| 2 | B | 501 | ACO | C6A-N6A | 3.45 | 1.45 | 1.34 |
| 2 | G | 501 | ACO | C6A-N6A | 3.50 | 1.45 | 1.34 |
| 2 | F | 501 | ACO | C6A-N6A | 3.51 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | J | 501 | ACO | C6A-N6A | 3.54 | 1.45 | 1.34 |
| 2 | L | 501 | ACO | C6A-N6A | 3.59 | 1.46 | 1.34 |
| 2 | H | 501 | ACO | C6A-N6A | 3.59 | 1.46 | 1.34 |
| 2 | C | 501 | ACO | C6A-N6A | 3.59 | 1.46 | 1.34 |
| 2 | D | 501 | ACO | C6A-N6A | 3.61 | 1.46 | 1.34 |
| 2 | A | 501 | ACO | C6A-N6A | 3.61 | 1.46 | 1.34 |
| 2 | I | 501 | ACO | C6A-N6A | 3.72 | 1.46 | 1.34 |
| 2 | K | 501 | ACO | C6A-N6A | 3.73 | 1.46 | 1.34 |
| 2 | E | 501 | ACO | C6A-N6A | 3.91 | 1.47 | 1.34 |
| 2 | C | 501 | ACO | C5P-N4P | 4.40 | 1.43 | 1.33 |
| 2 | G | 501 | ACO | C5P-N4P | 4.65 | 1.44 | 1.33 |
| 2 | J | 501 | ACO | C5P-N4P | 4.83 | 1.45 | 1.33 |
| 2 | D | 501 | ACO | C5P-N4P | 4.84 | 1.45 | 1.33 |
| 2 | B | 501 | ACO | C5P-N4P | 4.87 | 1.45 | 1.33 |
| 2 | I | 501 | ACO | C5P-N4P | 4.88 | 1.45 | 1.33 |
| 2 | H | 501 | ACO | C5P-N4P | 4.89 | 1.45 | 1.33 |
| 2 | E | 501 | ACO | C5P-N4P | 4.96 | 1.45 | 1.33 |
| 2 | K | 501 | ACO | C5P-N4P | 4.98 | 1.45 | 1.33 |
| 2 | F | 501 | ACO | C5P-N4P | 5.05 | 1.45 | 1.33 |
| 2 | L | 501 | ACO | C5P-N4P | 5.21 | 1.45 | 1.33 |
| 2 | A | 501 | ACO | C5P-N4P | 5.22 | 1.45 | 1.33 |
| 2 | H | 501 | ACO | C9P-N8P | 5.33 | 1.44 | 1.33 |
| 2 | A | 501 | ACO | C9P-N8P | 5.35 | 1.44 | 1.33 |
| 2 | L | 501 | ACO | C9P-N8P | 5.37 | 1.44 | 1.33 |
| 2 | F | 501 | ACO | C9P-N8P | 5.40 | 1.44 | 1.33 |
| 2 | D | 501 | ACO | C9P-N8P | 5.41 | 1.44 | 1.33 |
| 2 | K | 501 | ACO | C9P-N8P | 5.42 | 1.45 | 1.33 |
| 2 | J | 501 | ACO | C9P-N8P | 5.48 | 1.45 | 1.33 |
| 2 | C | 501 | ACO | C9P-N8P | 5.49 | 1.45 | 1.33 |
| 2 | B | 501 | ACO | C9P-N8P | 5.59 | 1.45 | 1.33 |
| 2 | E | 501 | ACO | C9P-N8P | 5.70 | 1.45 | 1.33 |
| 2 | I | 501 | ACO | C9P-N8P | 5.75 | 1.45 | 1.33 |
| 2 | G | 501 | ACO | C9P-N8P | 6.01 | 1.46 | 1.33 |

All (193) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | I | 501 | ACO | N3A-C2A-N1A | -10.49 | 120.86 | 128.89 |
| 2 | A | 501 | ACO | N3A-C2A-N1A | -9.98 | 121.25 | 128.89 |
| 2 | B | 501 | ACO | N3A-C2A-N1A | -9.90 | 121.31 | 128.89 |
| 2 | H | 501 | ACO | N3A-C2A-N1A | -9.84 | 121.36 | 128.89 |
| 2 | K | 501 | ACO | N3A-C2A-N1A | -9.68 | 121.48 | 128.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | E | 501 | ACO | N3A-C2A-N1A | -9.52 | 121.61 | 128.89 |
| 2 | D | 501 | ACO | N3A-C2A-N1A | -9.11 | 121.92 | 128.89 |
| 2 | F | 501 | ACO | N3A-C2A-N1A | -8.94 | 122.05 | 128.89 |
| 2 | G | 501 | ACO | N3A-C2A-N1A | -8.64 | 122.28 | 128.89 |
| 2 | C | 501 | ACO | N3A-C2A-N1A | -8.56 | 122.34 | 128.89 |
| 2 | L | 501 | ACO | N3A-C2A-N1A | -8.50 | 122.38 | 128.89 |
| 2 | J | 501 | ACO | N3A-C2A-N1A | -8.49 | 122.40 | 128.89 |
| 2 | D | 501 | ACO | C1B-N9A-C4A | -5.58 | 118.52 | 126.94 |
| 2 | K | 501 | ACO | C1B-N9A-C4A | -5.09 | 119.26 | 126.94 |
| 2 | A | 501 | ACO | C1B-N9A-C4A | -4.62 | 119.97 | 126.94 |
| 2 | B | 501 | ACO | C2B-C1B-N9A | -4.57 | 107.31 | 114.29 |
| 2 | E | 501 | ACO | C1B-N9A-C4A | -4.56 | 120.06 | 126.94 |
| 2 | K | 501 | ACO | P2A-O3A-P1A | -4.52 | 120.04 | 132.73 |
| 2 | L | 501 | ACO | C2B-C1B-N9A | -4.50 | 107.42 | 114.29 |
| 2 | K | 501 | ACO | C2B-C1B-N9A | -4.44 | 107.51 | 114.29 |
| 2 | J | 501 | ACO | C2B-C1B-N9A | -4.36 | 107.63 | 114.29 |
| 2 | H | 501 | ACO | C1B-N9A-C4A | -4.17 | 120.65 | 126.94 |
| 2 | B | 501 | ACO | C1B-N9A-C4A | -3.99 | 120.92 | 126.94 |
| 2 | I | 501 | ACO | C1B-N9A-C4A | -3.99 | 120.92 | 126.94 |
| 2 | J | 501 | ACO | C1B-N9A-C4A | -3.86 | 121.12 | 126.94 |
| 2 | H | 501 | ACO | P2A-O3A-P1A | -3.79 | 122.09 | 132.73 |
| 2 | J | 501 | ACO | P2A-O3A-P1A | -3.77 | 122.13 | 132.73 |
| 2 | G | 501 | ACO | P2A-O3A-P1A | -3.75 | 122.20 | 132.73 |
| 2 | F | 501 | ACO | C1B-N9A-C4A | -3.74 | 121.31 | 126.94 |
| 2 | C | 501 | ACO | C1B-N9A-C4A | -3.72 | 121.33 | 126.94 |
| 2 | D | 501 | ACO | P2A-O3A-P1A | -3.71 | 122.31 | 132.73 |
| 2 | I | 501 | ACO | P2A-O3A-P1A | -3.68 | 122.40 | 132.73 |
| 2 | L | 501 | ACO | P2A-O3A-P1A | -3.68 | 122.40 | 132.73 |
| 2 | G | 501 | ACO | C2B-C1B-N9A | -3.63 | 108.75 | 114.29 |
| 2 | A | 501 | ACO | C2B-C1B-N9A | -3.59 | 108.80 | 114.29 |
| 2 | A | 501 | ACO | P2A-O3A-P1A | -3.57 | 122.69 | 132.73 |
| 2 | C | 501 | ACO | P2A-O3A-P1A | -3.54 | 122.78 | 132.73 |
| 2 | F | 501 | ACO | C2B-C1B-N9A | -3.41 | 109.08 | 114.29 |
| 2 | F | 501 | ACO | P2A-O3A-P1A | -3.28 | 123.53 | 132.73 |
| 2 | A | 501 | ACO | C7P-N8P-C9P | -3.27 | 116.06 | 122.53 |
| 2 | B | 501 | ACO | O5P-C5P-N4P | -3.24 | 116.50 | 122.94 |
| 2 | E | 501 | ACO | O5P-C5P-N4P | -3.20 | 116.59 | 122.94 |
| 2 | D | 501 | ACO | C3P-N4P-C5P | -3.17 | 116.56 | 122.79 |
| 2 | B | 501 | ACO | C4B-O4B-C1B | -3.11 | 106.31 | 109.72 |
| 2 | D | 501 | ACO | O5P-C5P-N4P | -3.06 | 116.87 | 122.94 |
| 2 | D | 501 | ACO | C2B-C1B-N9A | -3.00 | 109.70 | 114.29 |
| 2 | C | 501 | ACO | C2B-C1B-N9A | -2.97 | 109.76 | 114.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | J | 501 | ACO | C3P-N4P-C5P | -2.93 | 117.04 | 122.79 |
| 2 | H | 501 | ACO | C2B-C1B-N9A | -2.90 | 109.86 | 114.29 |
| 2 | G | 501 | ACO | C1B-N9A-C4A | -2.90 | 122.56 | 126.94 |
| 2 | K | 501 | ACO | C4B-O4B-C1B | -2.83 | 106.61 | 109.72 |
| 2 | H | 501 | ACO | O9P-C9P-N8P | -2.83 | 117.40 | 123.08 |
| 2 | G | 501 | ACO | O5P-C5P-N4P | -2.75 | 117.47 | 122.94 |
| 2 | L | 501 | ACO | C1B-N9A-C4A | -2.75 | 122.80 | 126.94 |
| 2 | C | 501 | ACO | O5P-C5P-N4P | -2.74 | 117.50 | 122.94 |
| 2 | E | 501 | ACO | C7P-N8P-C9P | -2.70 | 117.19 | 122.53 |
| 2 | C | 501 | ACO | C3P-N4P-C5P | -2.69 | 117.50 | 122.79 |
| 2 | E | 501 | ACO | O9P-C9P-N8P | -2.66 | 117.75 | 123.08 |
| 2 | K | 501 | ACO | O5P-C5P-N4P | -2.62 | 117.73 | 122.94 |
| 2 | E | 501 | ACO | P2A-O3A-P1A | -2.59 | 125.45 | 132.73 |
| 2 | H | 501 | ACO | C4B-O4B-C1B | -2.58 | 106.88 | 109.72 |
| 2 | J | 501 | ACO | O9P-C9P-N8P | -2.52 | 118.02 | 123.08 |
| 2 | D | 501 | ACO | C4B-O4B-C1B | -2.39 | 107.09 | 109.72 |
| 2 | F | 501 | ACO | C4B-O4B-C1B | -2.37 | 107.11 | 109.72 |
| 2 | H | 501 | ACO | O5P-C5P-N4P | -2.37 | 118.23 | 122.94 |
| 2 | A | 501 | ACO | O9P-C9P-N8P | -2.35 | 118.37 | 123.08 |
| 2 | L | 501 | ACO | O9P-C9P-N8P | -2.35 | 118.37 | 123.08 |
| 2 | K | 501 | ACO | C5B-C4B-C3B | -2.32 | 105.95 | 114.31 |
| 2 | E | 501 | ACO | C3P-N4P-C5P | -2.29 | 118.29 | 122.79 |
| 2 | J | 501 | ACO | O5P-C5P-N4P | -2.26 | 118.45 | 122.94 |
| 2 | L | 501 | ACO | C4B-O4B-C1B | -2.20 | 107.30 | 109.72 |
| 2 | D | 501 | ACO | C4A-C5A-N7A | -2.19 | 107.46 | 109.48 |
| 2 | L | 501 | ACO | O5P-C5P-N4P | -2.17 | 118.64 | 122.94 |
| 2 | G | 501 | ACO | O9P-C9P-N8P | -2.12 | 118.82 | 123.08 |
| 2 | H | 501 | ACO | C7P-N8P-C9P | -2.10 | 118.38 | 122.53 |
| 2 | A | 501 | ACO | O3B-C3B-C2B | -2.08 | 103.41 | 111.51 |
| 2 | I | 501 | ACO | C2B-C1B-N9A | -2.07 | 111.13 | 114.29 |
| 2 | H | 501 | ACO | C3P-N4P-C5P | -2.02 | 118.81 | 122.79 |
| 2 | B | 501 | ACO | O3B-C3B-C2B | -2.02 | 103.66 | 111.51 |
| 2 | K | 501 | ACO | O9P-C9P-N8P | -2.02 | 119.04 | 123.08 |
| 2 | C | 501 | ACO | C4A-C5A-N7A | -2.01 | 107.63 | 109.48 |
| 2 | F | 501 | ACO | CAP-C9P-N8P | 2.01 | 120.91 | 116.47 |
| 2 | K | 501 | ACO | O4B-C4B-C3B | 2.04 | 109.55 | 104.86 |
| 2 | C | 501 | ACO | C7P-C6P-C5P | 2.04 | 115.67 | 112.31 |
| 2 | A | 501 | ACO | CDP-CBP-CCP | 2.04 | 111.15 | 108.50 |
| 2 | J | 501 | ACO | C6P-C7P-N8P | 2.05 | 116.39 | 111.88 |
| 2 | B | 501 | ACO | CDP-CBP-CCP | 2.06 | 111.17 | 108.50 |
| 2 | E | 501 | ACO | CDP-CBP-CCP | 2.06 | 111.17 | 108.50 |
| 2 | I | 501 | ACO | C2P-C3P-N4P | 2.08 | 116.53 | 112.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | J | 501 | ACO | P3B-O3B-C3B | 2.10 | 126.60 | 121.56 |
| 2 | D | 501 | ACO | C3B-C2B-C1B | 2.13 | 105.10 | 99.98 |
| 2 | D | 501 | ACO | C7P-C6P-C5P | 2.17 | 115.89 | 112.31 |
| 2 | K | 501 | ACO | CDP-CBP-CCP | 2.17 | 111.32 | 108.50 |
| 2 | E | 501 | ACO | C6P-C7P-N8P | 2.21 | 116.72 | 111.88 |
| 2 | D | 501 | ACO | CAP-C9P-N8P | 2.21 | 121.37 | 116.47 |
| 2 | I | 501 | ACO | O3A-P2A-O6A | 2.21 | 108.81 | 102.94 |
| 2 | F | 501 | ACO | O3A-P2A-O6A | 2.21 | 108.81 | 102.94 |
| 2 | C | 501 | ACO | C3B-C2B-C1B | 2.22 | 105.31 | 99.98 |
| 2 | D | 501 | ACO | P3B-O3B-C3B | 2.26 | 126.97 | 121.56 |
| 2 | J | 501 | ACO | O3A-P2A-O6A | 2.27 | 108.97 | 102.94 |
| 2 | J | 501 | ACO | O5B-C5B-C4B | 2.29 | 117.56 | 109.12 |
| 2 | F | 501 | ACO | O5B-C5B-C4B | 2.30 | 117.61 | 109.12 |
| 2 | K | 501 | ACO | C7P-C6P-C5P | 2.35 | 116.18 | 112.31 |
| 2 | H | 501 | ACO | C3P-C2P-S1P | 2.37 | 117.70 | 111.36 |
| 2 | C | 501 | ACO | C6P-C5P-N4P | 2.38 | 120.59 | 116.46 |
| 2 | A | 501 | ACO | C3B-C2B-C1B | 2.39 | 105.70 | 99.98 |
| 2 | B | 501 | ACO | O5B-C5B-C4B | 2.39 | 117.93 | 109.12 |
| 2 | H | 501 | ACO | C3B-C2B-C1B | 2.40 | 105.73 | 99.98 |
| 2 | G | 501 | ACO | C3B-C2B-C1B | 2.41 | 105.75 | 99.98 |
| 2 | G | 501 | ACO | O5B-C5B-C4B | 2.42 | 118.03 | 109.12 |
| 2 | D | 501 | ACO | C3P-C2P-S1P | 2.42 | 117.83 | 111.36 |
| 2 | K | 501 | ACO | C3B-C2B-C1B | 2.42 | 105.78 | 99.98 |
| 2 | A | 501 | ACO | O5B-C5B-C4B | 2.45 | 118.13 | 109.12 |
| 2 | F | 501 | ACO | C6P-C5P-N4P | 2.46 | 120.74 | 116.46 |
| 2 | F | 501 | ACO | CEP-CBP-CCP | 2.46 | 111.70 | 108.50 |
| 2 | I | 501 | ACO | O5B-C5B-C4B | 2.48 | 118.27 | 109.12 |
| 2 | H | 501 | ACO | O3A-P2A-O6A | 2.50 | 109.56 | 102.94 |
| 2 | G | 501 | ACO | O3B-P3B-O7A | 2.50 | 113.36 | 107.11 |
| 2 | I | 501 | ACO | C6P-C5P-N4P | 2.51 | 120.81 | 116.46 |
| 2 | B | 501 | ACO | C3B-C2B-C1B | 2.51 | 106.00 | 99.98 |
| 2 | I | 501 | ACO | C3P-C2P-S1P | 2.52 | 118.12 | 111.36 |
| 2 | C | 501 | ACO | O5B-C5B-C4B | 2.52 | 118.42 | 109.12 |
| 2 | B | 501 | ACO | CAP-C9P-N8P | 2.53 | 122.07 | 116.47 |
| 2 | C | 501 | ACO | C3P-C2P-S1P | 2.58 | 118.27 | 111.36 |
| 2 | B | 501 | ACO | C7P-C6P-C5P | 2.68 | 116.73 | 112.31 |
| 2 | I | 501 | ACO | C3B-C2B-C1B | 2.69 | 106.43 | 99.98 |
| 2 | E | 501 | ACO | C3P-C2P-S1P | 2.72 | 118.63 | 111.36 |
| 2 | J | 501 | ACO | C3B-C2B-C1B | 2.72 | 106.51 | 99.98 |
| 2 | K | 501 | ACO | CAP-C9P-N8P | 2.74 | 122.53 | 116.47 |
| 2 | K | 501 | ACO | O3A-P2A-O6A | 2.75 | 110.22 | 102.94 |
| 2 | K | 501 | ACO | O5B-C5B-C4B | 2.78 | 119.36 | 109.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | E | 501 | ACO | C7P-C6P-C5P | 2.81 | 116.94 | 112.31 |
| 2 | D | 501 | ACO | CDP-CBP-CCP | 2.88 | 112.24 | 108.50 |
| 2 | C | 501 | ACO | C2P-C3P-N4P | 2.91 | 118.17 | 112.36 |
| 2 | K | 501 | ACO | C6P-C5P-N4P | 2.91 | 121.51 | 116.46 |
| 2 | H | 501 | ACO | C6P-C5P-N4P | 2.98 | 121.63 | 116.46 |
| 2 | G | 501 | ACO | CAP-C9P-N8P | 2.99 | 123.09 | 116.47 |
| 2 | A | 501 | ACO | C6P-C5P-N4P | 3.00 | 121.67 | 116.46 |
| 2 | H | 501 | ACO | C6P-C7P-N8P | 3.03 | 118.53 | 111.88 |
| 2 | L | 501 | ACO | CAP-C9P-N8P | 3.07 | 123.27 | 116.47 |
| 2 | C | 501 | ACO | O3A-P2A-O6A | 3.07 | 111.09 | 102.94 |
| 2 | G | 501 | ACO | C3P-C2P-S1P | 3.08 | 119.60 | 111.36 |
| 2 | D | 501 | ACO | O3A-P2A-O6A | 3.09 | 111.14 | 102.94 |
| 2 | J | 501 | ACO | C6P-C5P-N4P | 3.10 | 121.84 | 116.46 |
| 2 | H | 501 | ACO | CAP-C9P-N8P | 3.11 | 123.37 | 116.47 |
| 2 | J | 501 | ACO | CAP-C9P-N8P | 3.13 | 123.41 | 116.47 |
| 2 | K | 501 | ACO | C3P-C2P-S1P | 3.17 | 119.84 | 111.36 |
| 2 | B | 501 | ACO | C6P-C5P-N4P | 3.18 | 121.99 | 116.46 |
| 2 | B | 501 | ACO | O3A-P2A-O6A | 3.27 | 111.61 | 102.94 |
| 2 | E | 501 | ACO | CAP-C9P-N8P | 3.27 | 123.72 | 116.47 |
| 2 | E | 501 | ACO | C6P-C5P-N4P | 3.37 | 122.31 | 116.46 |
| 2 | B | 501 | ACO | C3P-C2P-S1P | 3.38 | 120.40 | 111.36 |
| 2 | L | 501 | ACO | C6P-C5P-N4P | 3.41 | 122.39 | 116.46 |
| 2 | F | 501 | ACO | C3P-C2P-S1P | 3.44 | 120.58 | 111.36 |
| 2 | A | 501 | ACO | CAP-C9P-N8P | 3.45 | 124.11 | 116.47 |
| 2 | K | 501 | ACO | C2P-C3P-N4P | 3.51 | 119.37 | 112.36 |
| 2 | A | 501 | ACO | C2P-C3P-N4P | 3.54 | 119.43 | 112.36 |
| 2 | G | 501 | ACO | O4B-C1B-N9A | 3.58 | 115.59 | 108.10 |
| 2 | L | 501 | ACO | C3P-C2P-S1P | 3.61 | 121.04 | 111.36 |
| 2 | L | 501 | ACO | O4B-C1B-N9A | 3.68 | 115.80 | 108.10 |
| 2 | A | 501 | ACO | C3P-C2P-S1P | 3.68 | 121.22 | 111.36 |
| 2 | E | 501 | ACO | O4B-C1B-N9A | 3.75 | 115.95 | 108.10 |
| 2 | B | 501 | ACO | C2P-C3P-N4P | 3.79 | 119.94 | 112.36 |
| 2 | I | 501 | ACO | O4B-C1B-N9A | 3.86 | 116.19 | 108.10 |
| 2 | J | 501 | ACO | C2P-C3P-N4P | 3.87 | 120.09 | 112.36 |
| 2 | C | 501 | ACO | O6A-CCP-CBP | 3.90 | 116.82 | 110.55 |
| 2 | H | 501 | ACO | C2P-C3P-N4P | 3.95 | 120.26 | 112.36 |
| 2 | E | 501 | ACO | C2P-C3P-N4P | 3.96 | 120.28 | 112.36 |
| 2 | D | 501 | ACO | C6P-C5P-N4P | 4.12 | 123.61 | 116.46 |
| 2 | G | 501 | ACO | C6P-C5P-N4P | 4.17 | 123.71 | 116.46 |
| 2 | H | 501 | ACO | O4B-C1B-N9A | 4.28 | 117.05 | 108.10 |
| 2 | G | 501 | ACO | O6A-CCP-CBP | 4.35 | 117.55 | 110.55 |
| 2 | F | 501 | ACO | O4B-C1B-N9A | 4.36 | 117.22 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | H | 501 | ACO | O6A-CCP-CBP | 4.36 | 117.56 | 110.55 |
| 2 | G | 501 | ACO | C2P-C3P-N4P | 4.44 | 121.23 | 112.36 |
| 2 | C | 501 | ACO | O4B-C1B-N9A | 4.56 | 117.64 | 108.10 |
| 2 | B | 501 | ACO | O4B-C1B-N9A | 4.60 | 117.73 | 108.10 |
| 2 | A | 501 | ACO | O6A-CCP-CBP | 4.63 | 117.98 | 110.55 |
| 2 | K | 501 | ACO | O4B-C1B-N9A | 4.71 | 117.96 | 108.10 |
| 2 | J | 501 | ACO | O4B-C1B-N9A | 4.86 | 118.26 | 108.10 |
| 2 | F | 501 | ACO | O6A-CCP-CBP | 4.86 | 118.35 | 110.55 |
| 2 | D | 501 | ACO | O4B-C1B-N9A | 5.12 | 118.81 | 108.10 |
| 2 | L | 501 | ACO | C2P-C3P-N4P | 5.35 | 123.06 | 112.36 |
| 2 | D | 501 | ACO | C2P-C3P-N4P | 5.39 | 123.14 | 112.36 |
| 2 | A | 501 | ACO | O4B-C1B-N9A | 5.47 | 119.54 | 108.10 |
| 2 | B | 501 | ACO | O6A-CCP-CBP | 5.71 | 119.72 | 110.55 |
| 2 | E | 501 | ACO | O6A-CCP-CBP | 6.30 | 120.68 | 110.55 |
| 2 | I | 501 | ACO | O6A-CCP-CBP | 6.40 | 120.84 | 110.55 |
| 2 | J | 501 | ACO | O6A-CCP-CBP | 6.84 | 121.54 | 110.55 |
| 2 | F | 501 | ACO | C2P-C3P-N4P | 6.97 | 126.30 | 112.36 |
| 2 | L | 501 | ACO | O6A-CCP-CBP | 7.18 | 122.09 | 110.55 |
| 2 | K | 501 | ACO | O6A-CCP-CBP | 7.39 | 122.42 | 110.55 |
| 2 | D | 501 | ACO | O6A-CCP-CBP | 7.73 | 122.97 | 110.55 |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 2 | H | 501 | ACO | CH3-C-S1P-C2P |
| 2 | I | 501 | ACO | O-C-S1P-C2P |
| 2 | H | 501 | ACO | O-C-S1P-C2P |
| 2 | G | 501 | ACO | O-C-S1P-C2P |
| 2 | L | 501 | ACO | CH3-C-S1P-C2P |
| 2 | C | 501 | ACO | O-C-S1P-C2P |
| 2 | B | 501 | ACO | O-C-S1P-C2P |
| 2 | G | 501 | ACO | CH3-C-S1P-C2P |
| 2 | E | 501 | ACO | CH3-C-S1P-C2P |
| 2 | L | 501 | ACO | O-C-S1P-C2P |

There are no ring outliers.

12 monomers are involved in 70 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 501 | ACO | 6 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | B | 501 | ACO | 4 | 0 |
| 2 | C | 501 | ACO | 12 | 0 |
| 2 | D | 501 | ACO | 2 | 0 |
| 2 | E | 501 | ACO | 8 | 0 |
| 2 | F | 501 | ACO | 5 | 0 |
| 2 | G | 501 | ACO | 6 | 0 |
| 2 | H | 501 | ACO | 2 | 0 |
| 2 | I | 501 | ACO | 7 | 0 |
| 2 | J | 501 | ACO | 3 | 0 |
| 2 | K | 501 | ACO | 10 | 0 |
| 2 | L | 501 | ACO | 5 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 | 389/428 (90%) | -0.27 | 14 (3%) | 46 | 34 | 16, 28, 63, 139 | 0 |
| 1 | B | 389/428 (90%) | -0.21 | 14 (3%) | 46 | 34 | 18, 27, 65, 161 | 0 |
| 1 | C | 389/428 (90%) | -0.11 | 21 (5%) | 29 | 19 | 21, 31, 66, 152 | 0 |
| 1 | D | 389/428 (90%) | -0.18 | 12 (3%) | 52 | 40 | 18, 29, 65, 144 | 0 |
| 1 | E | 389/428 (90%) | -0.18 | 16 (4%) | 41 | 29 | 17, 30, 66, 158 | 0 |
| 1 | F | 389/428 (90%) | -0.14 | 15 (3%) | 43 | 31 | 20, 30, 72, 125 | 0 |
| 1 | G | 389/428 (90%) | -0.06 | 17 (4%) | 38 | 26 | 22, 35, 67, 163 | 0 |
| 1 | H | 389/428 (90%) | -0.05 | 20 (5%) | 32 | 21 | 23, 36, 72, 165 | 0 |
| 1 | I | 389/428 (90%) | 0.21 | 26 (6%) | 21 | 12 | 24, 47, 78, 163 | 0 |
| 1 | J | 389/428 (90%) | 0.35 | 40 (10%) | 9 | 4 | 24, 51, 81, 166 | 0 |
| 1 | K | 389/428 (90%) | -0.00 | 15 (3%) | 43 | 31 | 24, 43, 78, 157 | 0 |
| 1 | L | 389/428 (90%) | -0.24 | 11 (2%) | 56 | 44 | 23, 35, 69, 160 | 0 |
| All | All | 4668/5136 (90%) | -0.07 | 221 (4%) | 35 | 24 | 16, 35, 74, 166 | 0 |

All (221) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | H | 60 | PRO | 12.1 |
| 1 | J | 60 | PRO | 11.1 |
| 1 | F | 42 | TRP | 10.9 |
| 1 | K | 61 | GLY | 10.7 |
| 1 | E | 60 | PRO | 10.6 |
| 1 | G | 61 | GLY | 9.7 |
| 1 | I | 60 | PRO | 9.4 |
| 1 | D | 60 | PRO | 8.3 |
| 1 | K | 60 | PRO | 8.0 |
| 1 | E | 58 | ALA | 7.7 |
| 1 | J | 34 | ILE | 7.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | J | 59 | GLY | 7.6 |
| 1 | J | 58 | ALA | 7.3 |
| 1 | G | 60 | PRO | 7.1 |
| 1 | A | 60 | PRO | 7.1 |
| 1 | F | 60 | PRO | 6.9 |
| 1 | I | 61 | GLY | 6.7 |
| 1 | B | 60 | PRO | 6.7 |
| 1 | I | 8 | THR | 6.6 |
| 1 | H | 34 | ILE | 6.4 |
| 1 | D | 8 | THR | 6.0 |
| 1 | A | 59 | GLY | 6.0 |
| 1 | D | 61 | GLY | 5.8 |
| 1 | E | 59 | GLY | 5.8 |
| 1 | K | 34 | ILE | 5.6 |
| 1 | B | 59 | GLY | 5.6 |
| 1 | B | 42 | TRP | 5.5 |
| 1 | K | 59 | GLY | 5.5 |
| 1 | H | 61 | GLY | 5.4 |
| 1 | H | 8 | THR | 5.4 |
| 1 | G | 59 | GLY | 5.3 |
| 1 | C | 60 | PRO | 5.1 |
| 1 | L | 60 | PRO | 5.0 |
| 1 | I | 349 | THR | 5.0 |
| 1 | B | 58 | ALA | 5.0 |
| 1 | E | 36 | PRO | 4.9 |
| 1 | I | 58 | ALA | 4.9 |
| 1 | C | 37 | GLU | 4.8 |
| 1 | C | 61 | GLY | 4.7 |
| 1 | J | 8 | THR | 4.6 |
| 1 | F | 9 | VAL | 4.5 |
| 1 | C | 36 | PRO | 4.5 |
| 1 | K | 43 | ARG | 4.4 |
| 1 | I | 38 | SER | 4.4 |
| 1 | A | 34 | ILE | 4.4 |
| 1 | G | 352 | ALA | 4.4 |
| 1 | J | 352 | ALA | 4.4 |
| 1 | H | 384 | LYS | 4.4 |
| 1 | H | 59 | GLY | 4.3 |
| 1 | A | 58 | ALA | 4.3 |
| 1 | E | 39 | ALA | 4.3 |
| 1 | E | 214 | PRO | 4.2 |
| 1 | H | 43 | ARG | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | J | 62 | SER | 4.2 |
| 1 | C | 43 | ARG | 4.2 |
| 1 | D | 10 | THR | 4.1 |
| 1 | I | 34 | ILE | 4.1 |
| 1 | C | 39 | ALA | 4.1 |
| 1 | J | 384 | LYS | 4.1 |
| 1 | C | 34 | ILE | 4.0 |
| 1 | J | 36 | PRO | 4.0 |
| 1 | C | 58 | ALA | 4.0 |
| 1 | D | 148 | VAL | 3.9 |
| 1 | L | 61 | GLY | 3.8 |
| 1 | I | 341 | ASP | 3.8 |
| 1 | D | 36 | PRO | 3.8 |
| 1 | A | 36 | PRO | 3.8 |
| 1 | J | 19 | TRP | 3.7 |
| 1 | L | 59 | GLY | 3.7 |
| 1 | H | 214 | PRO | 3.7 |
| 1 | C | 384 | LYS | 3.7 |
| 1 | J | 331 | ASP | 3.7 |
| 1 | G | 62 | SER | 3.7 |
| 1 | B | 61 | GLY | 3.6 |
| 1 | J | 405 | ALA | 3.6 |
| 1 | I | 59 | GLY | 3.5 |
| 1 | B | 57 | GLY | 3.5 |
| 1 | K | 19 | TRP | 3.5 |
| 1 | H | 216 | GLY | 3.4 |
| 1 | A | 39 | ALA | 3.4 |
| 1 | G | 57 | GLY | 3.4 |
| 1 | E | 34 | ILE | 3.4 |
| 1 | J | 341 | ASP | 3.4 |
| 1 | E | 61 | GLY | 3.3 |
| 1 | F | 213 | ALA | 3.3 |
| 1 | H | 36 | PRO | 3.3 |
| 1 | B | 34 | ILE | 3.3 |
| 1 | H | 37 | GLU | 3.3 |
| 1 | C | 40 | THR | 3.3 |
| 1 | C | 350 | ASP | 3.3 |
| 1 | G | 43 | ARG | 3.3 |
| 1 | L | 37 | GLU | 3.3 |
| 1 | L | 214 | PRO | 3.3 |
| 1 | L | 36 | PRO | 3.3 |
| 1 | B | 37 | GLU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | I | 384 | LYS | 3.3 |
| 1 | J | 37 | GLU | 3.2 |
| 1 | K | 8 | THR | 3.2 |
| 1 | D | 38 | SER | 3.2 |
| 1 | E | 37 | GLU | 3.2 |
| 1 | G | 214 | PRO | 3.2 |
| 1 | J | 44 | THR | 3.2 |
| 1 | J | 215 | GLY | 3.2 |
| 1 | K | 58 | ALA | 3.1 |
| 1 | A | 73 | LEU | 3.1 |
| 1 | H | 40 | THR | 3.1 |
| 1 | D | 350 | ASP | 3.1 |
| 1 | A | 384 | LYS | 3.1 |
| 1 | I | 321 | GLY | 3.1 |
| 1 | B | 43 | ARG | 3.0 |
| 1 | A | 213 | ALA | 3.0 |
| 1 | B | 8 | THR | 3.0 |
| 1 | F | 8 | THR | 3.0 |
| 1 | K | 39 | ALA | 3.0 |
| 1 | I | 353 | ALA | 3.0 |
| 1 | D | 37 | GLU | 2.9 |
| 1 | G | 58 | ALA | 2.9 |
| 1 | G | 39 | ALA | 2.9 |
| 1 | G | 37 | GLU | 2.9 |
| 1 | C | 214 | PRO | 2.9 |
| 1 | G | 34 | ILE | 2.9 |
| 1 | I | 352 | ALA | 2.9 |
| 1 | J | 112 | ARG | 2.9 |
| 1 | I | 16 | GLU | 2.9 |
| 1 | L | 16 | GLU | 2.9 |
| 1 | J | 61 | GLY | 2.9 |
| 1 | F | 43 | ARG | 2.9 |
| 1 | G | 44 | THR | 2.9 |
| 1 | A | 214 | PRO | 2.8 |
| 1 | I | 62 | SER | 2.8 |
| 1 | I | 148 | VAL | 2.8 |
| 1 | C | 8 | THR | 2.8 |
| 1 | C | 215 | GLY | 2.8 |
| 1 | J | 43 | ARG | 2.8 |
| 1 | E | 144 | HIS | 2.7 |
| 1 | I | 214 | PRO | 2.7 |
| 1 | E | 215 | GLY | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | H | 58 | ALA | 2.7 |
| 1 | A | 352 | ALA | 2.7 |
| 1 | I | 36 | PRO | 2.7 |
| 1 | F | 34 | ILE | 2.7 |
| 1 | J | 57 | GLY | 2.7 |
| 1 | K | 37 | GLU | 2.7 |
| 1 | J | 292 | ARG | 2.7 |
| 1 | F | 19 | TRP | 2.7 |
| 1 | I | 211 | LYS | 2.6 |
| 1 | B | 331 | ASP | 2.6 |
| 1 | L | 322 | GLU | 2.6 |
| 1 | J | 42 | TRP | 2.6 |
| 1 | G | 384 | LYS | 2.6 |
| 1 | C | 19 | TRP | 2.6 |
| 1 | K | 62 | SER | 2.6 |
| 1 | C | 292 | ARG | 2.6 |
| 1 | E | 237 | THR | 2.6 |
| 1 | A | 37 | GLU | 2.6 |
| 1 | F | 57 | GLY | 2.5 |
| 1 | F | 16 | GLU | 2.5 |
| 1 | F | 58 | ALA | 2.5 |
| 1 | H | 215 | GLY | 2.5 |
| 1 | B | 9 | VAL | 2.5 |
| 1 | G | 207 | LEU | 2.5 |
| 1 | J | 116 | ASP | 2.5 |
| 1 | E | 43 | ARG | 2.4 |
| 1 | G | 40 | THR | 2.4 |
| 1 | J | 12 | CYS | 2.4 |
| 1 | I | 40 | THR | 2.4 |
| 1 | A | 40 | THR | 2.4 |
| 1 | K | 237 | THR | 2.4 |
| 1 | H | 167 | SER | 2.4 |
| 1 | K | 215 | GLY | 2.4 |
| 1 | D | 59 | GLY | 2.3 |
| 1 | J | 183 | ALA | 2.3 |
| 1 | C | 148 | VAL | 2.3 |
| 1 | E | 341 | ASP | 2.3 |
| 1 | F | 17 | ASP | 2.3 |
| 1 | L | 17 | ASP | 2.3 |
| 1 | B | 340 | GLY | 2.3 |
| 1 | A | 42 | TRP | 2.3 |
| 1 | J | 212 | ALA | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | L | 212 | ALA | 2.3 |
| 1 | J | 404 | THR | 2.3 |
| 1 | H | 149 | ASP | 2.3 |
| 1 | I | 399 | ASP | 2.3 |
| 1 | L | 331 | ASP | 2.3 |
| 1 | J | 322 | GLU | 2.3 |
| 1 | J | 385 | ASP | 2.2 |
| 1 | E | 213 | ALA | 2.2 |
| 1 | G | 353 | ALA | 2.2 |
| 1 | I | 345 | ARG | 2.2 |
| 1 | J | 214 | PRO | 2.2 |
| 1 | F | 331 | ASP | 2.2 |
| 1 | F | 10 | THR | 2.2 |
| 1 | J | 332 | GLY | 2.2 |
| 1 | C | 318 | HIS | 2.2 |
| 1 | J | 354 | GLU | 2.2 |
| 1 | J | 353 | ALA | 2.2 |
| 1 | J | 350 | ASP | 2.2 |
| 1 | F | 214 | PRO | 2.2 |
| 1 | I | 43 | ARG | 2.2 |
| 1 | I | 350 | ASP | 2.1 |
| 1 | J | 16 | GLU | 2.1 |
| 1 | D | 34 | ILE | 2.1 |
| 1 | J | 387 | GLN | 2.1 |
| 1 | E | 8 | THR | 2.1 |
| 1 | C | 48 | THR | 2.1 |
| 1 | H | 10 | THR | 2.1 |
| 1 | C | 331 | ASP | 2.1 |
| 1 | H | 19 | TRP | 2.1 |
| 1 | H | 169 | VAL | 2.1 |
| 1 | C | 341 | ASP | 2.1 |
| 1 | I | 49 | ASP | 2.1 |
| 1 | J | 40 | THR | 2.1 |
| 1 | B | 36 | PRO | 2.1 |
| 1 | J | 9 | VAL | 2.0 |
| 1 | J | 213 | ALA | 2.0 |
| 1 | J | 79 | GLY | 2.0 |
| 1 | D | 352 | ALA | 2.0 |
| 1 | K | 352 | ALA | 2.0 |
| 1 | I | 215 | GLY | 2.0 |
| 1 | H | 170 | ARG | 2.0 |
| 1 | K | 35 | GLY | 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 2 | ACO | E | 501 | 51/51 | 0.85 | 0.25 | 1.74 | 38,57,82,89 | 0 |
| 2 | ACO | H | 501 | 51/51 | 0.82 | 0.28 | 1.65 | 41,57,73,81 | 0 |
| 2 | ACO | J | 501 | 51/51 | 0.82 | 0.28 | 1.40 | 54,68,82,89 | 0 |
| 2 | ACO | C | 501 | 51/51 | 0.88 | 0.23 | 1.38 | 33,50,71,83 | 0 |
| 2 | ACO | I | 501 | 51/51 | 0.84 | 0.26 | 1.34 | 44,63,78,97 | 0 |
| 2 | ACO | F | 501 | 51/51 | 0.89 | 0.21 | 0.95 | 34,48,66,73 | 0 |
| 2 | ACO | K | 501 | 51/51 | 0.89 | 0.22 | 0.94 | 45,56,70,77 | 0 |
| 2 | ACO | A | 501 | 51/51 | 0.90 | 0.20 | 0.65 | 30,46,67,81 | 0 |
| 2 | ACO | L | 501 | 51/51 | 0.90 | 0.18 | 0.57 | 26,38,61,72 | 0 |
| 2 | ACO | D | 501 | 51/51 | 0.86 | 0.23 | 0.54 | 34,51,70,81 | 0 |
| 2 | ACO | G | 501 | 51/51 | 0.92 | 0.17 | 0.09 | 28,40,60,73 | 0 |
| 2 | ACO | B | 501 | 51/51 | 0.91 | 0.17 | 0.02 | 29,42,54,61 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.