



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2018 – 10:58 am GMT

PDB ID : 1NQT
Title : Crystal structure of bovine Glutamate dehydrogenase-ADP complex
Authors : Banerjee, S.; Schmidt, T.; Fang, J.; Stanley, C.A.; Smith, T.J.
Deposited on : 2003-01-23
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

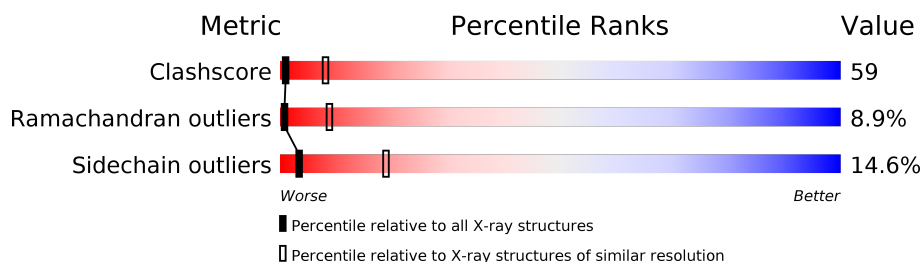
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 122078 | 1485 (3.60-3.40) |
| Ramachandran outliers | 120005 | 1446 (3.60-3.40) |
| Sidechain outliers | 119972 | 1447 (3.60-3.40) |

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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 496 | |
| 1 | B | 496 | |
| 1 | C | 496 | |
| 1 | D | 496 | |
| 1 | E | 496 | |
| 1 | F | 496 | |
| 1 | G | 496 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | H | 496 | <div><div></div><div>30%55%14%</div><div></div></div> |
| 1 | I | 496 | <div><div></div><div>31%52%16%</div><div></div></div> |
| 1 | J | 496 | <div><div></div><div>34%49%15%</div><div></div></div> |
| 1 | K | 496 | <div><div></div><div>24%60%15%</div><div></div></div> |
| 1 | L | 496 | <div><div></div><div>30%54%15%</div><div></div></div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46812 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 Glutamate dehydrogenase 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | B | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | C | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | D | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | E | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | F | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | G | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | H | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | I | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | J | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | K | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |
| 1 | L | 496 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3874 | 2450 | 679 | 726 | 19 | | | |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



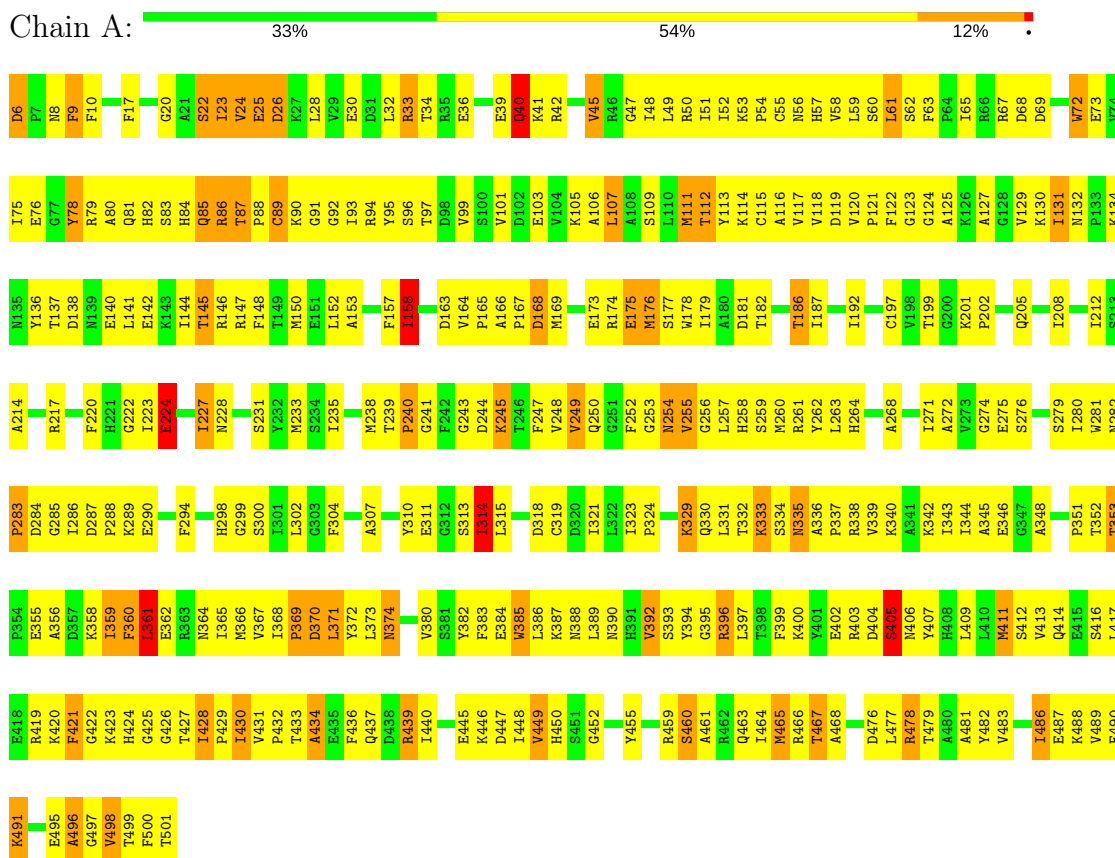
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | I | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | J | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | K | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | L | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

3 Residue-property plots

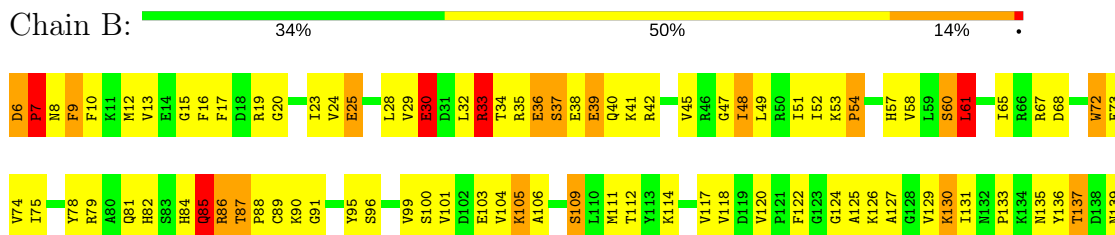
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

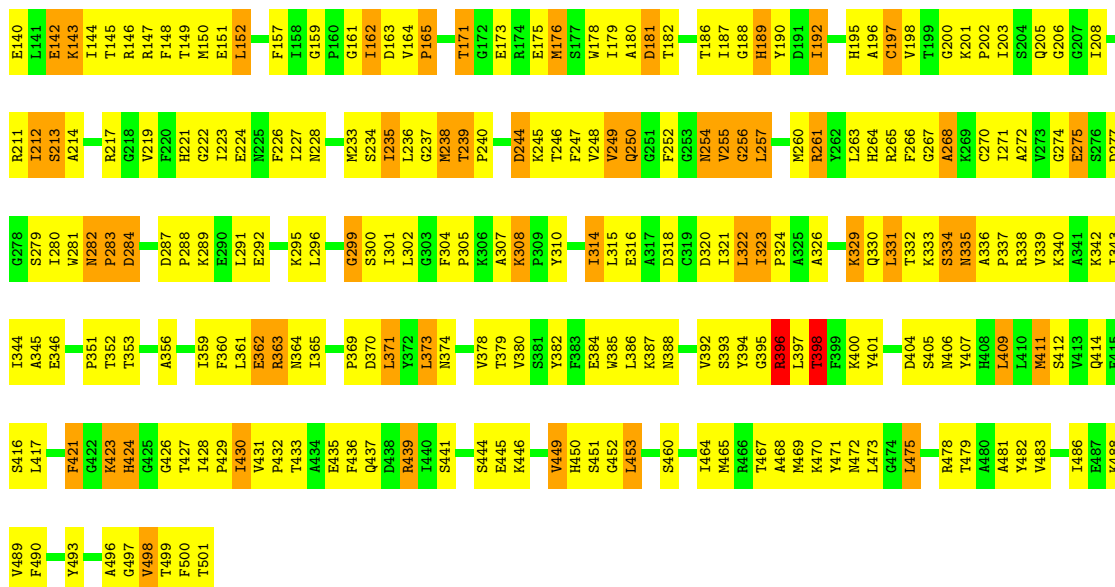
Note EDS was not executed.

• Molecule 1: Glutamate dehydrogenase 1



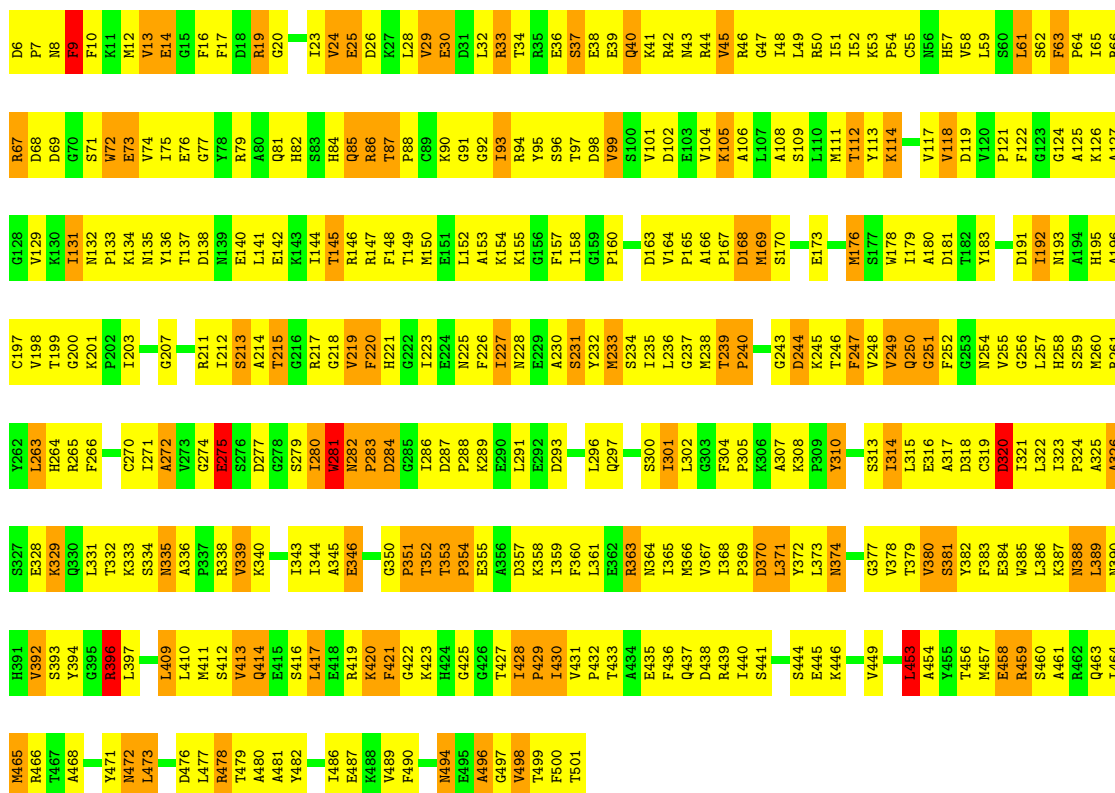
• Molecule 1: Glutamate dehydrogenase 1





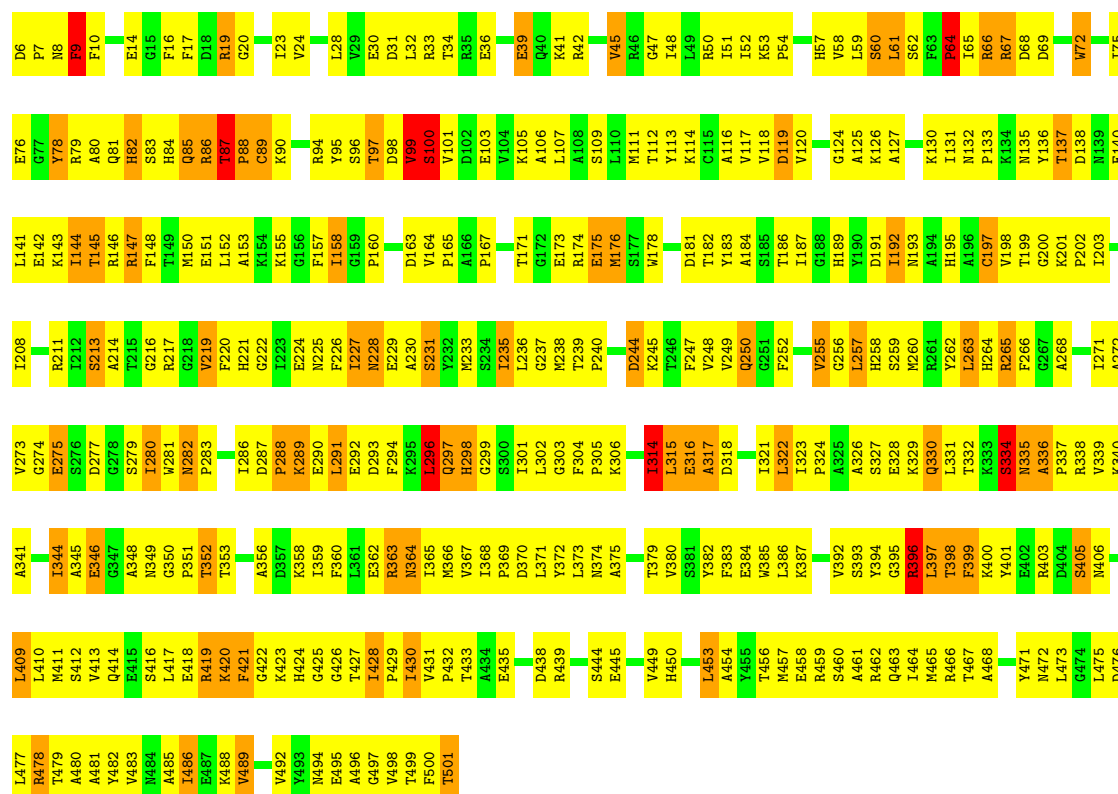
- Molecule 1: Glutamate dehydrogenase 1

Chain C: 26% 54% 18%

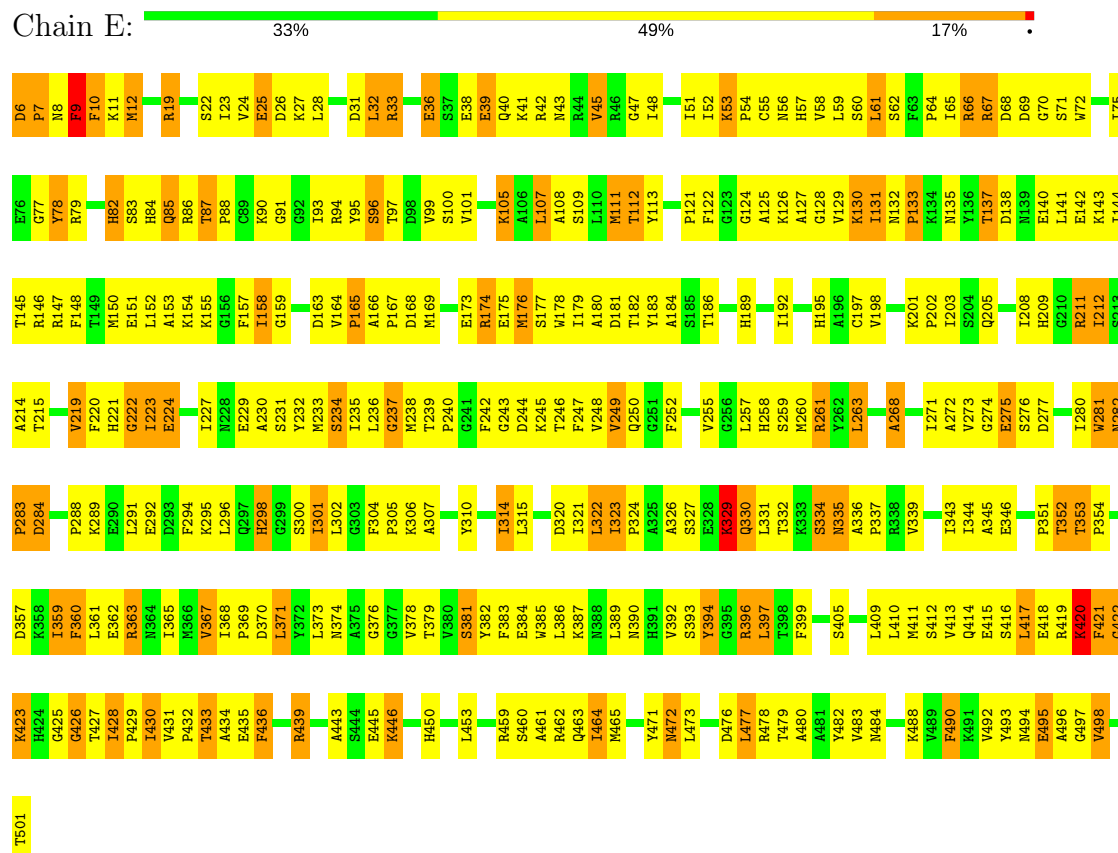


- Molecule 1: Glutamate dehydrogenase 1

Chain D:  29% 55% 15%

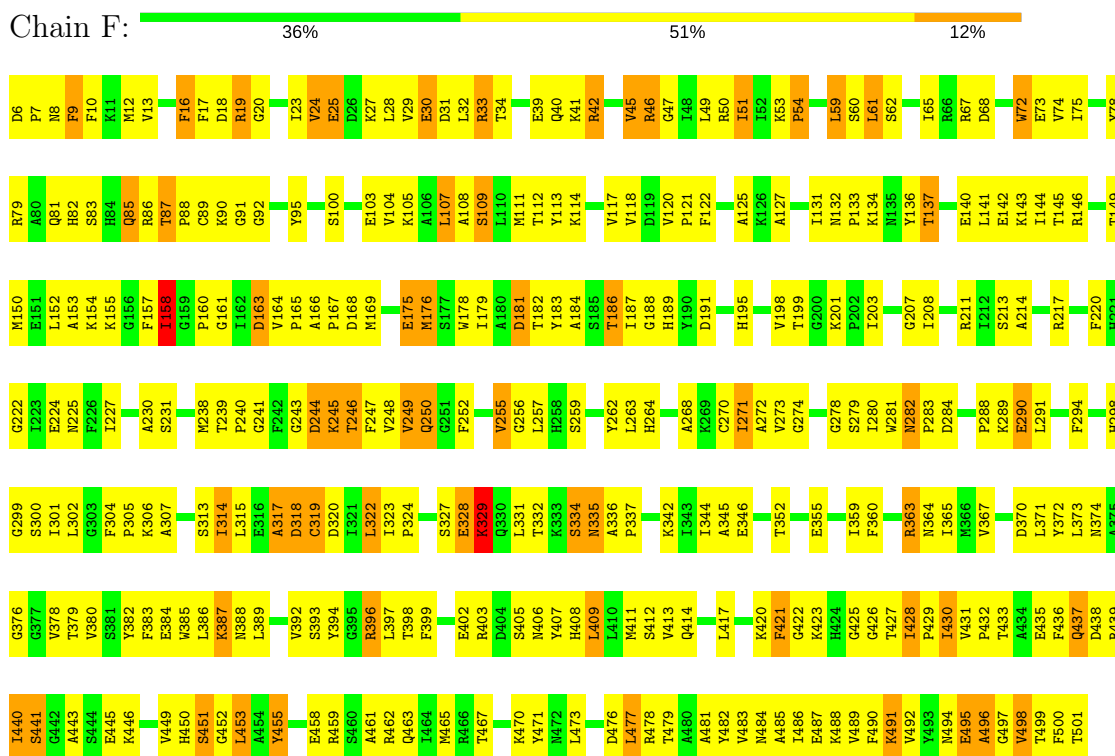


• Molecule 1: Glutamate dehydrogenase 1



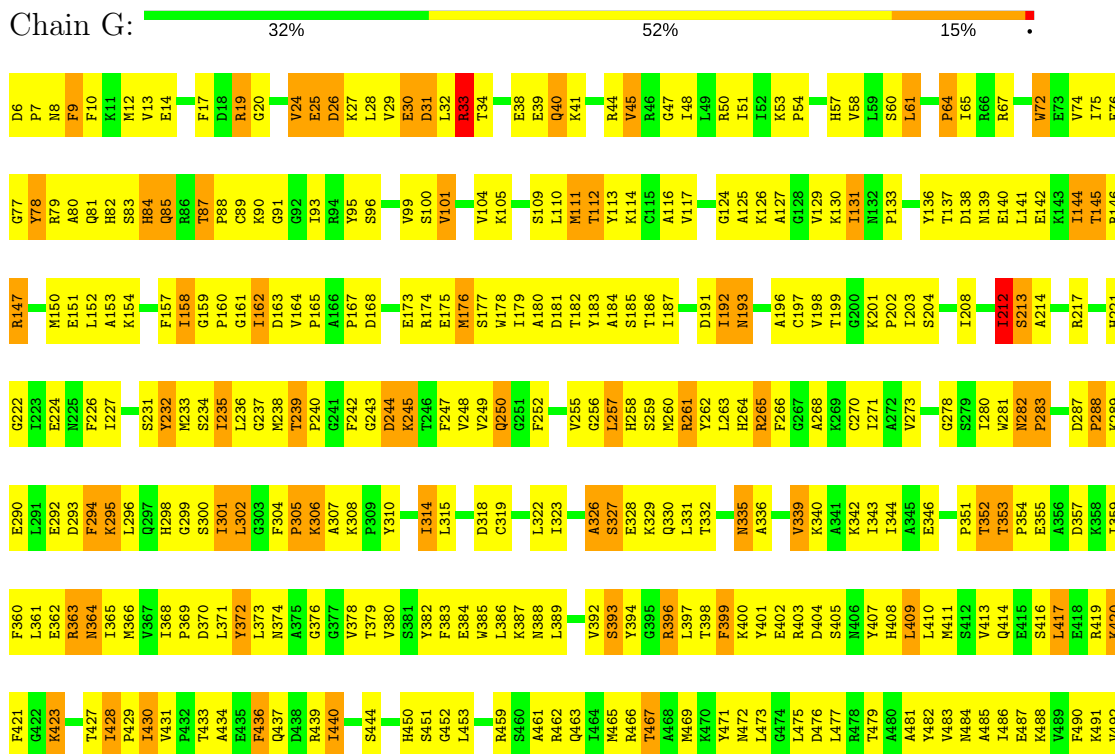
● Molecule 1: Glutamate dehydrogenase 1

Chain F:



● Molecule 1: Glutamate dehydrogenase 1

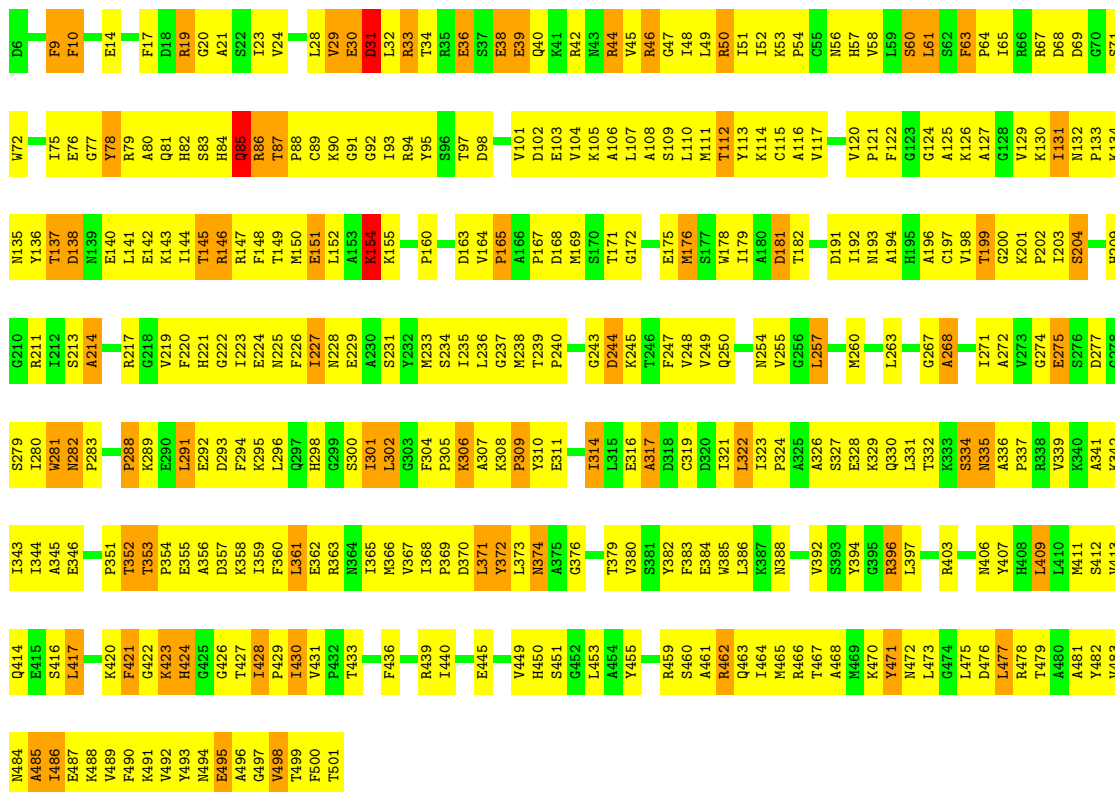
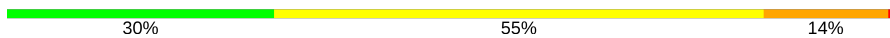
Chain G:





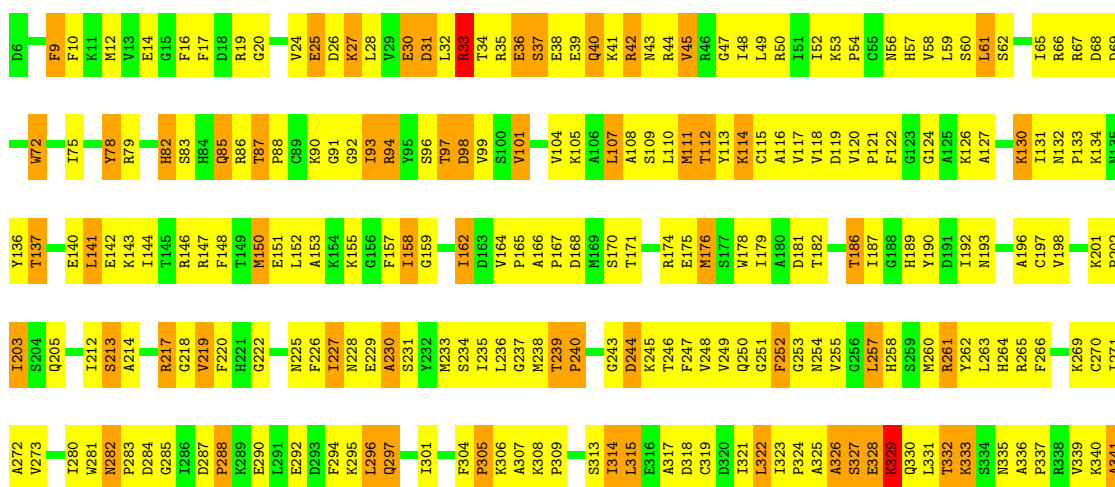
- Molecule 1: Glutamate dehydrogenase 1

Chain H:



- Molecule 1: Glutamate dehydrogenase 1

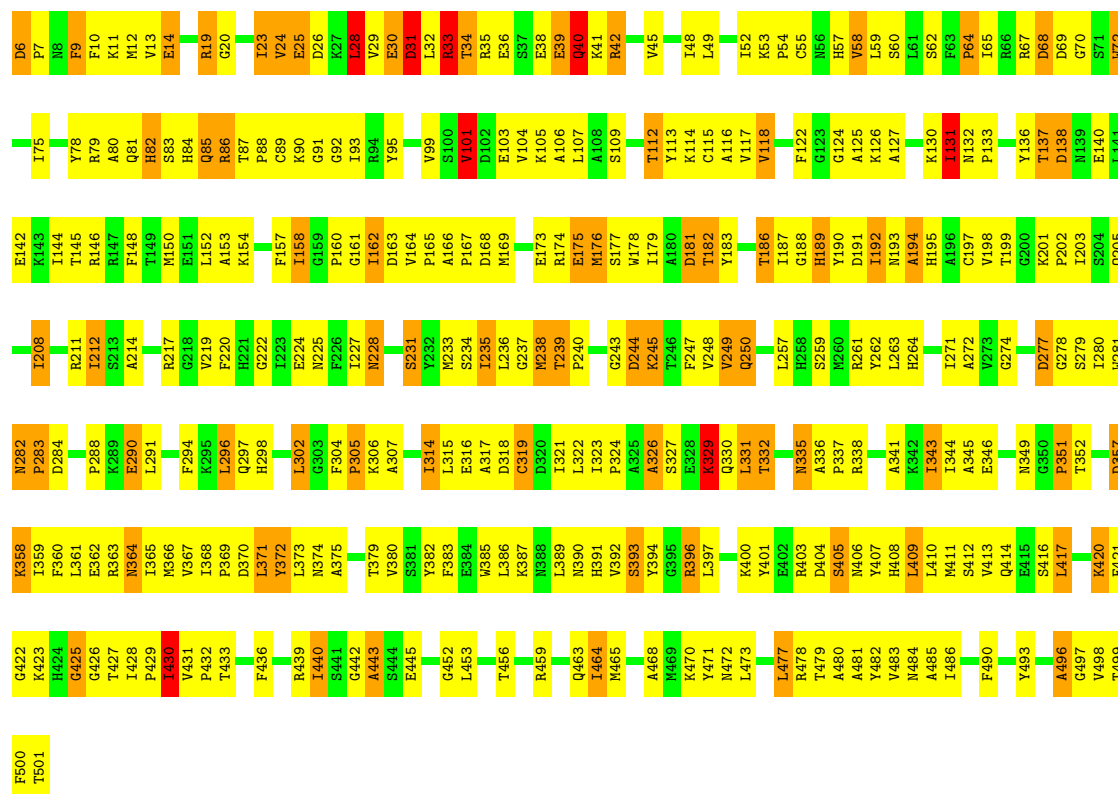
Chain I:





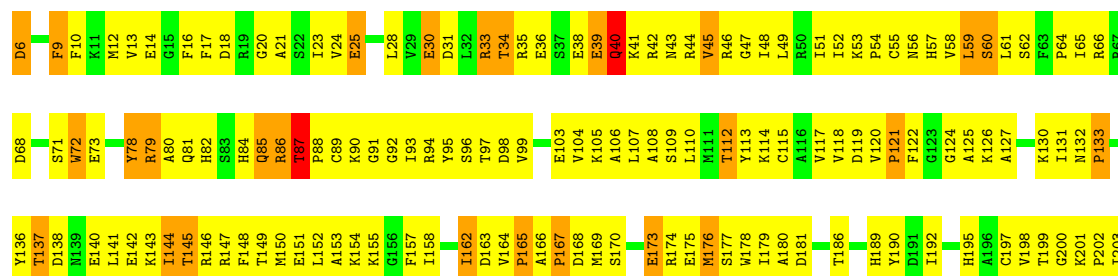
• Molecule 1: Glutamate dehydrogenase 1

Chain J: 34% 49% 15% •



• Molecule 1: Glutamate dehydrogenase 1

Chain K: 24% 60% 15% •





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 96.46 Å 171.93 Å 439.68 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 19.97 – 3.50 | Depositor |
| % Data completeness (in resolution range) | 94.0 (19.97-3.50) | Depositor |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.207 , 0.276 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 46812 | wwPDB-VP |
| Average B, all atoms (Å ²) | 59.0 | wwPDB-VP |

5 Model quality

5.1 Standard geometry

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

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 | 0.70 | 1/3958 (0.0%) | 0.89 | 2/5340 (0.0%) |
| 1 | B | 0.76 | 1/3958 (0.0%) | 0.91 | 2/5340 (0.0%) |
| 1 | C | 0.72 | 1/3958 (0.0%) | 0.91 | 2/5340 (0.0%) |
| 1 | D | 0.69 | 2/3958 (0.1%) | 0.89 | 4/5340 (0.1%) |
| 1 | E | 0.71 | 0/3958 | 0.91 | 2/5340 (0.0%) |
| 1 | F | 0.73 | 0/3958 | 0.89 | 0/5340 |
| 1 | G | 0.79 | 0/3958 | 0.95 | 2/5340 (0.0%) |
| 1 | H | 0.78 | 1/3958 (0.0%) | 0.89 | 1/5340 (0.0%) |
| 1 | I | 0.71 | 1/3958 (0.0%) | 0.88 | 1/5340 (0.0%) |
| 1 | J | 0.74 | 1/3958 (0.0%) | 0.91 | 1/5340 (0.0%) |
| 1 | K | 0.70 | 0/3958 | 0.89 | 2/5340 (0.0%) |
| 1 | L | 0.73 | 2/3958 (0.1%) | 0.88 | 0/5340 |
| All | All | 0.73 | 10/47496 (0.0%) | 0.90 | 19/64080 (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 | E | 0 | 2 |
| 1 | F | 0 | 1 |
| 1 | G | 0 | 1 |
| 1 | H | 0 | 1 |
| All | All | 0 | 5 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | I | 197 | CYS | CB-SG | -7.54 | 1.69 | 1.82 |
| 1 | B | 197 | CYS | CB-SG | -6.96 | 1.70 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | D | 89 | CYS | CB-SG | -6.15 | 1.71 | 1.82 |
| 1 | C | 55 | CYS | CB-SG | -6.08 | 1.72 | 1.82 |
| 1 | L | 89 | CYS | CB-SG | -5.47 | 1.73 | 1.81 |
| 1 | D | 197 | CYS | CB-SG | -5.41 | 1.73 | 1.81 |
| 1 | H | 151 | GLU | CG-CD | 5.32 | 1.59 | 1.51 |
| 1 | J | 101 | VAL | CA-CB | -5.24 | 1.43 | 1.54 |
| 1 | L | 197 | CYS | CB-SG | -5.22 | 1.73 | 1.81 |
| 1 | A | 89 | CYS | CB-SG | -5.03 | 1.73 | 1.81 |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | G | 245 | LYS | CD-CE-NZ | 7.41 | 128.75 | 111.70 |
| 1 | J | 296 | LEU | CA-CB-CG | 6.82 | 130.98 | 115.30 |
| 1 | B | 61 | LEU | CA-CB-CG | 6.37 | 129.94 | 115.30 |
| 1 | D | 87 | THR | N-CA-C | 6.27 | 127.92 | 111.00 |
| 1 | H | 146 | ARG | NE-CZ-NH2 | -6.19 | 117.20 | 120.30 |
| 1 | D | 235 | ILE | N-CA-C | -6.12 | 94.48 | 111.00 |
| 1 | A | 361 | LEU | CA-CB-CG | 5.97 | 129.03 | 115.30 |
| 1 | D | 296 | LEU | CA-CB-CG | 5.88 | 128.81 | 115.30 |
| 1 | G | 239 | THR | N-CA-C | -5.76 | 95.43 | 111.00 |
| 1 | E | 237 | GLY | N-CA-C | -5.67 | 98.93 | 113.10 |
| 1 | E | 420 | LYS | N-CA-C | -5.48 | 96.21 | 111.00 |
| 1 | C | 30 | GLU | N-CA-C | 5.45 | 125.72 | 111.00 |
| 1 | K | 268 | ALA | N-CA-C | -5.29 | 96.72 | 111.00 |
| 1 | D | 489 | VAL | CB-CA-C | -5.23 | 101.47 | 111.40 |
| 1 | B | 299 | GLY | N-CA-C | 5.22 | 126.14 | 113.10 |
| 1 | A | 87 | THR | N-CA-C | 5.09 | 124.75 | 111.00 |
| 1 | K | 299 | GLY | N-CA-C | 5.04 | 125.69 | 113.10 |
| 1 | C | 453 | LEU | CA-CB-CG | 5.03 | 126.88 | 115.30 |
| 1 | I | 322 | LEU | CA-CB-CG | 5.00 | 126.81 | 115.30 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | E | 310 | TYR | Sidechain |
| 1 | E | 490 | PHE | Sidechain |
| 1 | F | 455 | TYR | Sidechain |
| 1 | G | 113 | TYR | Sidechain |
| 1 | H | 310 | TYR | 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 | 3874 | 0 | 3841 | 456 | 0 |
| 1 | B | 3874 | 0 | 3841 | 464 | 0 |
| 1 | C | 3874 | 0 | 3841 | 527 | 0 |
| 1 | D | 3874 | 0 | 3841 | 499 | 0 |
| 1 | E | 3874 | 0 | 3841 | 437 | 0 |
| 1 | F | 3874 | 0 | 3841 | 420 | 0 |
| 1 | G | 3874 | 0 | 3841 | 453 | 0 |
| 1 | H | 3874 | 0 | 3841 | 481 | 0 |
| 1 | I | 3874 | 0 | 3841 | 509 | 0 |
| 1 | J | 3874 | 0 | 3841 | 446 | 0 |
| 1 | K | 3874 | 0 | 3841 | 569 | 0 |
| 1 | L | 3874 | 0 | 3841 | 508 | 0 |
| 2 | A | 27 | 0 | 12 | 6 | 0 |
| 2 | B | 27 | 0 | 12 | 5 | 0 |
| 2 | C | 27 | 0 | 12 | 6 | 0 |
| 2 | D | 27 | 0 | 12 | 5 | 0 |
| 2 | E | 27 | 0 | 12 | 6 | 0 |
| 2 | F | 27 | 0 | 12 | 3 | 0 |
| 2 | G | 27 | 0 | 12 | 4 | 0 |
| 2 | H | 27 | 0 | 12 | 2 | 0 |
| 2 | I | 27 | 0 | 12 | 5 | 0 |
| 2 | J | 27 | 0 | 12 | 3 | 0 |
| 2 | K | 27 | 0 | 12 | 2 | 0 |
| 2 | L | 27 | 0 | 12 | 4 | 0 |
| All | All | 46812 | 0 | 46236 | 5447 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (5447) 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:A:423:LYS:HD3 | 1:A:426:GLY:HA3 | 1.23 | 1.17 |
| 1:B:95:TYR:OH | 1:B:145:THR:HG22 | 1.44 | 1.16 |
| 1:L:57:HIS:CD2 | 1:L:84:HIS:HE1 | 1.62 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:235:ILE:HG22 | 1:C:364:ASN:HD21 | 1.12 | 1.13 |
| 1:C:396:ARG:HH11 | 1:C:396:ARG:HG3 | 1.14 | 1.12 |
| 1:B:336:ALA:HB1 | 1:B:359:ILE:HG21 | 1.22 | 1.11 |
| 1:E:82:HIS:HD2 | 1:E:109:SER:HA | 0.98 | 1.11 |
| 1:B:79:ARG:HD3 | 1:B:127:ALA:HB2 | 1.32 | 1.10 |
| 1:B:33:ARG:HB2 | 1:B:33:ARG:HH11 | 1.05 | 1.10 |
| 1:G:167:PRO:HG3 | 1:G:176:MET:SD | 1.91 | 1.10 |
| 1:E:414:GLN:HB2 | 1:E:429:PRO:HD2 | 1.29 | 1.09 |
| 1:I:186:THR:HG22 | 1:I:187:ILE:H | 1.16 | 1.09 |
| 1:E:314:ILE:H | 1:E:314:ILE:HD13 | 1.16 | 1.09 |
| 1:G:30:GLU:HG3 | 1:G:31:ASP:H | 0.95 | 1.09 |
| 1:C:335:ASN:HB2 | 1:C:338:ARG:HH22 | 1.08 | 1.09 |
| 1:J:212:ILE:HD12 | 1:J:212:ILE:H | 1.16 | 1.08 |
| 1:B:29:VAL:HA | 1:B:33:ARG:HD2 | 1.31 | 1.08 |
| 1:C:65:ILE:HD13 | 1:C:144:ILE:HG12 | 1.34 | 1.08 |
| 1:K:30:GLU:HG3 | 1:K:31:ASP:H | 1.10 | 1.08 |
| 1:C:314:ILE:HD13 | 1:C:314:ILE:H | 1.01 | 1.08 |
| 1:K:40:GLN:HA | 1:K:40:GLN:HE21 | 1.17 | 1.08 |
| 1:C:87:THR:HB | 1:C:88:PRO:HD3 | 1.36 | 1.07 |
| 1:L:250:GLN:HG3 | 1:L:315:LEU:HD11 | 1.32 | 1.07 |
| 1:B:212:ILE:HD12 | 1:B:212:ILE:H | 1.18 | 1.07 |
| 1:L:33:ARG:HB2 | 1:L:33:ARG:NH1 | 1.70 | 1.07 |
| 1:I:82:HIS:CD2 | 1:I:112:THR:HG21 | 1.88 | 1.07 |
| 1:K:20:GLY:O | 1:K:24:VAL:HG23 | 1.55 | 1.07 |
| 1:J:479:THR:O | 1:J:483:VAL:HG23 | 1.52 | 1.06 |
| 1:L:33:ARG:HH11 | 1:L:33:ARG:HB2 | 0.90 | 1.06 |
| 1:L:79:ARG:HD2 | 1:L:127:ALA:HB2 | 1.34 | 1.06 |
| 1:C:52:ILE:HD13 | 1:C:489:VAL:HG12 | 1.36 | 1.06 |
| 1:I:323:ILE:HG22 | 1:I:345:ALA:HB3 | 1.38 | 1.06 |
| 1:L:29:VAL:O | 1:L:33:ARG:HG3 | 1.54 | 1.06 |
| 1:L:118:VAL:HG23 | 1:L:120:VAL:HG23 | 1.37 | 1.06 |
| 1:E:82:HIS:CD2 | 1:E:109:SER:HA | 1.90 | 1.05 |
| 1:H:427:THR:HG22 | 1:H:429:PRO:HD3 | 1.37 | 1.05 |
| 1:A:186:THR:HG22 | 1:A:187:ILE:H | 0.96 | 1.05 |
| 1:C:239:THR:N | 1:C:240:PRO:HD3 | 1.71 | 1.05 |
| 1:I:213:SER:HB2 | 1:I:217:ARG:HD2 | 1.37 | 1.05 |
| 1:B:439:ARG:HG3 | 1:B:439:ARG:HH11 | 1.16 | 1.04 |
| 1:B:261:ARG:HG3 | 1:B:261:ARG:HH11 | 1.22 | 1.04 |
| 1:L:250:GLN:HG2 | 1:L:314:ILE:HD11 | 1.40 | 1.04 |
| 1:K:314:ILE:H | 1:K:314:ILE:HD13 | 1.22 | 1.04 |
| 1:H:332:THR:HG22 | 1:H:353:THR:HG21 | 1.35 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:45:VAL:HG23 | 1:J:72:TRP:HZ3 | 1.22 | 1.03 |
| 1:K:478:ARG:HG2 | 1:K:478:ARG:HH11 | 1.23 | 1.03 |
| 1:B:249:VAL:HB | 1:B:323:ILE:HG12 | 1.41 | 1.03 |
| 1:C:429:PRO:O | 1:C:431:VAL:N | 1.91 | 1.02 |
| 1:F:396:ARG:HH11 | 1:F:396:ARG:HG3 | 1.24 | 1.02 |
| 1:A:323:ILE:HG22 | 1:A:345:ALA:HB3 | 1.42 | 1.01 |
| 1:H:314:ILE:HD13 | 1:H:314:ILE:H | 1.20 | 1.01 |
| 1:D:137:THR:HG23 | 1:D:140:GLU:HG3 | 1.43 | 1.01 |
| 1:C:82:HIS:CD2 | 1:C:112:THR:HG21 | 1.95 | 1.01 |
| 1:K:260:MET:HE3 | 1:K:288:PRO:HA | 1.40 | 1.01 |
| 1:I:93:ILE:HG23 | 1:I:127:ALA:HB3 | 1.42 | 1.01 |
| 1:B:73:GLU:HA | 1:D:50:ARG:HH12 | 1.22 | 1.01 |
| 1:D:336:ALA:HB3 | 1:D:337:PRO:HD3 | 1.40 | 1.01 |
| 1:D:47:GLY:HA2 | 1:D:50:ARG:HG2 | 1.39 | 1.01 |
| 1:H:396:ARG:HH11 | 1:H:396:ARG:HG3 | 1.24 | 1.01 |
| 1:H:498:VAL:HG23 | 1:H:499:THR:H | 1.25 | 1.00 |
| 1:D:19:ARG:HD3 | 1:D:23:ILE:HD11 | 1.43 | 1.00 |
| 1:J:250:GLN:HE21 | 1:J:326:ALA:HB3 | 1.27 | 1.00 |
| 1:F:498:VAL:HG23 | 1:F:499:THR:H | 1.23 | 1.00 |
| 1:A:186:THR:CG2 | 1:A:187:ILE:H | 1.75 | 1.00 |
| 1:G:30:GLU:HG3 | 1:G:31:ASP:N | 1.74 | 1.00 |
| 1:D:286:ILE:HG21 | 1:D:291:LEU:HD12 | 1.42 | 0.99 |
| 1:D:323:ILE:HG22 | 1:D:345:ALA:HB3 | 1.43 | 0.99 |
| 1:A:250:GLN:HG2 | 1:A:314:ILE:HD11 | 1.43 | 0.99 |
| 1:F:423:LYS:HE3 | 1:F:426:GLY:HA3 | 1.44 | 0.99 |
| 1:D:346:GLU:HG2 | 1:D:351:PRO:HG2 | 1.44 | 0.99 |
| 1:E:53:LYS:HB3 | 1:E:54:PRO:HD3 | 1.45 | 0.99 |
| 1:B:186:THR:HG22 | 1:B:187:ILE:HD13 | 1.43 | 0.98 |
| 1:I:219:VAL:HA | 1:I:373:LEU:CD2 | 1.93 | 0.98 |
| 1:I:72:TRP:HE1 | 1:L:498:VAL:HG11 | 1.26 | 0.98 |
| 1:B:137:THR:HG23 | 1:B:140:GLU:HG3 | 1.44 | 0.98 |
| 1:C:498:VAL:HG23 | 1:C:499:THR:H | 1.29 | 0.98 |
| 1:E:65:ILE:HA | 1:E:147:ARG:CZ | 1.94 | 0.98 |
| 1:F:482:TYR:O | 1:F:486:ILE:HG12 | 1.64 | 0.98 |
| 1:G:137:THR:HG22 | 1:G:139:ASN:H | 1.24 | 0.98 |
| 1:C:351:PRO:HG2 | 1:C:352:THR:HG22 | 1.46 | 0.97 |
| 1:L:57:HIS:CD2 | 1:L:84:HIS:CE1 | 2.53 | 0.97 |
| 1:E:329:LYS:NZ | 1:E:329:LYS:HB3 | 1.79 | 0.97 |
| 1:G:47:GLY:HA2 | 1:G:50:ARG:HG2 | 1.46 | 0.97 |
| 1:I:368:ILE:CG2 | 1:I:373:LEU:HD12 | 1.94 | 0.97 |
| 1:L:33:ARG:HH11 | 1:L:33:ARG:CB | 1.76 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:67:ARG:HH11 | 1:D:67:ARG:HB3 | 1.25 | 0.97 |
| 1:G:436:PHE:O | 1:G:440:ILE:HG13 | 1.62 | 0.97 |
| 1:K:107:LEU:HA | 1:K:110:LEU:HD13 | 1.46 | 0.97 |
| 1:K:216:GLY:O | 1:K:219:VAL:HG12 | 1.65 | 0.96 |
| 1:G:112:THR:HG22 | 1:G:124:GLY:HA3 | 1.47 | 0.96 |
| 1:H:9:PHE:HD1 | 1:H:10:PHE:H | 1.03 | 0.96 |
| 1:L:233:MET:HE1 | 1:L:343:ILE:HD11 | 1.45 | 0.96 |
| 1:C:57:HIS:HD2 | 1:C:84:HIS:HE1 | 1.12 | 0.96 |
| 1:A:186:THR:HG22 | 1:A:187:ILE:N | 1.80 | 0.96 |
| 1:G:142:GLU:HG2 | 1:G:146:ARG:HD2 | 1.46 | 0.96 |
| 1:L:239:THR:N | 1:L:240:PRO:HD3 | 1.78 | 0.96 |
| 1:C:496:ALA:HB1 | 1:C:501:THR:OXT | 1.65 | 0.96 |
| 1:L:57:HIS:HD2 | 1:L:84:HIS:CE1 | 1.83 | 0.95 |
| 1:C:314:ILE:H | 1:C:314:ILE:CD1 | 1.80 | 0.95 |
| 1:L:313:SER:HB2 | 1:L:315:LEU:HD13 | 1.45 | 0.95 |
| 1:F:427:THR:HG22 | 1:F:429:PRO:HD3 | 1.46 | 0.95 |
| 1:G:429:PRO:O | 1:G:431:VAL:N | 1.98 | 0.95 |
| 1:I:233:MET:HE1 | 1:I:236:LEU:HD12 | 1.44 | 0.95 |
| 1:B:260:MET:HG2 | 1:B:288:PRO:HG3 | 1.50 | 0.94 |
| 1:I:37:SER:HA | 1:I:42:ARG:NH1 | 1.82 | 0.94 |
| 1:G:30:GLU:CG | 1:G:31:ASP:H | 1.79 | 0.94 |
| 1:L:482:TYR:O | 1:L:486:ILE:HG12 | 1.66 | 0.94 |
| 1:D:150:MET:SD | 1:D:186:THR:HG21 | 2.08 | 0.94 |
| 1:L:314:ILE:HD13 | 1:L:314:ILE:H | 1.32 | 0.94 |
| 1:B:33:ARG:NH1 | 1:B:33:ARG:HB2 | 1.82 | 0.94 |
| 1:I:186:THR:HG22 | 1:I:187:ILE:N | 1.83 | 0.94 |
| 1:K:387:LYS:HE3 | 1:K:445:GLU:OE2 | 1.69 | 0.94 |
| 1:I:118:VAL:HG23 | 1:I:120:VAL:HG23 | 1.50 | 0.93 |
| 1:I:167:PRO:HG3 | 1:I:176:MET:SD | 2.08 | 0.93 |
| 1:L:57:HIS:HD2 | 1:L:84:HIS:HE1 | 0.95 | 0.93 |
| 1:D:87:THR:HG22 | 1:D:88:PRO:HD3 | 1.50 | 0.93 |
| 1:G:260:MET:HG2 | 1:G:288:PRO:HG3 | 1.51 | 0.93 |
| 1:C:335:ASN:HB2 | 1:C:338:ARG:NH2 | 1.83 | 0.93 |
| 1:L:65:ILE:HD13 | 1:L:144:ILE:HG13 | 1.46 | 0.93 |
| 1:I:371:LEU:HD23 | 1:I:481:ALA:HB1 | 1.49 | 0.93 |
| 1:H:57:HIS:ND1 | 1:H:84:HIS:HE1 | 1.65 | 0.93 |
| 1:D:427:THR:HG22 | 1:D:429:PRO:HD3 | 1.50 | 0.93 |
| 1:C:360:PHE:HD1 | 1:C:365:ILE:HG13 | 1.30 | 0.93 |
| 1:D:275:GLU:OE1 | 1:D:301:ILE:HG13 | 1.68 | 0.93 |
| 1:B:227:ILE:HD12 | 1:B:233:MET:SD | 2.08 | 0.92 |
| 1:H:154:LYS:HD2 | 1:K:189:HIS:HD2 | 1.35 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:498:VAL:HG23 | 1:B:499:THR:H | 1.32 | 0.92 |
| 1:G:41:LYS:O | 1:G:44:ARG:HB3 | 1.70 | 0.92 |
| 1:I:219:VAL:HA | 1:I:373:LEU:HD21 | 1.51 | 0.92 |
| 1:F:429:PRO:O | 1:F:431:VAL:N | 2.01 | 0.92 |
| 1:F:47:GLY:HA2 | 1:F:50:ARG:HG2 | 1.52 | 0.92 |
| 1:K:53:LYS:HB3 | 1:K:54:PRO:HD3 | 1.50 | 0.92 |
| 1:G:482:TYR:O | 1:G:486:ILE:HG12 | 1.69 | 0.92 |
| 1:J:432:PRO:HB3 | 1:J:436:PHE:HD1 | 1.36 | 0.91 |
| 1:A:65:ILE:HD13 | 1:A:144:ILE:HG12 | 1.53 | 0.91 |
| 1:H:82:HIS:CD2 | 1:H:109:SER:HA | 2.05 | 0.91 |
| 1:A:260:MET:HE3 | 1:A:288:PRO:HA | 1.52 | 0.91 |
| 1:D:468:ALA:HA | 1:D:473:LEU:HD12 | 1.50 | 0.91 |
| 1:F:414:GLN:OE1 | 1:F:428:ILE:HA | 1.71 | 0.91 |
| 1:K:314:ILE:N | 1:K:314:ILE:HD13 | 1.86 | 0.91 |
| 1:C:314:ILE:HD13 | 1:C:314:ILE:N | 1.86 | 0.91 |
| 1:D:250:GLN:HG2 | 1:D:314:ILE:CD1 | 2.01 | 0.91 |
| 1:F:166:ALA:HB1 | 1:F:167:PRO:HD2 | 1.51 | 0.91 |
| 1:K:414:GLN:HB2 | 1:K:429:PRO:HD2 | 1.51 | 0.91 |
| 1:G:87:THR:HB | 1:G:88:PRO:HD3 | 1.52 | 0.90 |
| 1:I:396:ARG:HG3 | 1:I:396:ARG:HH11 | 1.33 | 0.90 |
| 1:B:24:VAL:HG22 | 1:B:483:VAL:HG13 | 1.51 | 0.90 |
| 1:E:176:MET:HE3 | 1:E:179:ILE:HD12 | 1.53 | 0.90 |
| 1:H:82:HIS:HD2 | 1:H:109:SER:HA | 1.36 | 0.90 |
| 1:J:414:GLN:HG3 | 1:J:429:PRO:HD2 | 1.50 | 0.90 |
| 1:L:112:THR:HB | 1:L:124:GLY:H | 1.36 | 0.90 |
| 1:B:212:ILE:CD1 | 1:B:212:ILE:H | 1.77 | 0.90 |
| 1:B:275:GLU:HB2 | 1:B:301:ILE:HD11 | 1.51 | 0.90 |
| 1:B:331:LEU:HD13 | 1:B:360:PHE:HZ | 1.37 | 0.90 |
| 1:H:233:MET:HE1 | 1:H:236:LEU:HD12 | 1.52 | 0.90 |
| 1:J:250:GLN:NE2 | 1:J:326:ALA:HB3 | 1.86 | 0.90 |
| 1:L:9:PHE:HD1 | 1:L:10:PHE:N | 1.70 | 0.90 |
| 1:C:217:ARG:HH12 | 1:C:221:HIS:HE1 | 1.08 | 0.90 |
| 1:G:29:VAL:HA | 1:G:33:ARG:HD2 | 1.52 | 0.90 |
| 1:J:91:GLY:HA3 | 1:J:125:ALA:O | 1.72 | 0.90 |
| 1:K:239:THR:N | 1:K:240:PRO:HD3 | 1.87 | 0.90 |
| 1:C:181:ASP:OD1 | 1:E:501:THR:HG23 | 1.72 | 0.90 |
| 1:C:65:ILE:HG12 | 1:C:75:ILE:HD11 | 1.54 | 0.90 |
| 1:D:90:LYS:HZ3 | 1:D:199:THR:HG23 | 1.37 | 0.90 |
| 1:A:397:LEU:HD13 | 1:F:394:TYR:HE2 | 1.35 | 0.90 |
| 1:L:96:SER:O | 1:L:99:VAL:HG13 | 1.71 | 0.90 |
| 1:G:82:HIS:CD2 | 1:G:112:THR:HG21 | 2.07 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:498:VAL:HG23 | 1:A:499:THR:H | 1.36 | 0.89 |
| 1:D:332:THR:HG22 | 1:D:353:THR:HG21 | 1.54 | 0.89 |
| 1:I:313:SER:HB2 | 1:I:315:LEU:HD13 | 1.53 | 0.89 |
| 1:K:174:ARG:HG3 | 1:K:175:GLU:H | 1.35 | 0.89 |
| 1:C:396:ARG:O | 1:C:396:ARG:HD3 | 1.73 | 0.89 |
| 1:J:212:ILE:H | 1:J:212:ILE:CD1 | 1.82 | 0.89 |
| 1:K:88:PRO:HA | 1:K:162:ILE:O | 1.72 | 0.89 |
| 1:A:59:LEU:CD2 | 1:A:61:LEU:HD21 | 2.01 | 0.89 |
| 1:C:280:ILE:HG22 | 1:C:281:TRP:H | 1.35 | 0.89 |
| 1:K:59:LEU:HD21 | 1:K:61:LEU:HD21 | 1.54 | 0.89 |
| 1:K:314:ILE:H | 1:K:314:ILE:CD1 | 1.83 | 0.89 |
| 1:H:331:LEU:HD22 | 1:H:360:PHE:HZ | 1.37 | 0.89 |
| 1:D:99:VAL:HG22 | 1:D:130:LYS:HD3 | 1.55 | 0.88 |
| 1:K:107:LEU:HD13 | 1:K:126:LYS:HE2 | 1.55 | 0.88 |
| 1:K:40:GLN:HA | 1:K:40:GLN:NE2 | 1.87 | 0.88 |
| 1:D:82:HIS:ND1 | 1:D:109:SER:HA | 1.88 | 0.88 |
| 1:J:29:VAL:O | 1:J:33:ARG:HB2 | 1.73 | 0.88 |
| 1:L:150:MET:HE1 | 1:L:186:THR:HG21 | 1.55 | 0.88 |
| 1:D:99:VAL:HG23 | 1:D:100:SER:N | 1.86 | 0.88 |
| 1:G:19:ARG:NH1 | 1:G:479:THR:HG21 | 1.88 | 0.88 |
| 1:L:281:TRP:NE1 | 1:L:283:PRO:HD3 | 1.88 | 0.88 |
| 1:B:429:PRO:O | 1:B:431:VAL:N | 2.06 | 0.88 |
| 1:C:239:THR:H | 1:C:240:PRO:HD3 | 1.38 | 0.88 |
| 1:G:47:GLY:O | 1:G:51:ILE:HG13 | 1.72 | 0.88 |
| 1:G:208:ILE:HG13 | 1:G:387:LYS:HD2 | 1.56 | 0.88 |
| 1:K:30:GLU:HA | 1:K:34:THR:HG23 | 1.54 | 0.88 |
| 1:A:247:PHE:HB2 | 1:A:321:ILE:HG22 | 1.53 | 0.88 |
| 1:H:19:ARG:HD3 | 1:H:23:ILE:HD11 | 1.56 | 0.88 |
| 1:F:59:LEU:HD21 | 1:F:61:LEU:HD21 | 1.54 | 0.88 |
| 1:K:301:ILE:HD12 | 1:K:302:LEU:HD12 | 1.56 | 0.88 |
| 1:H:368:ILE:HG21 | 1:H:373:LEU:HD13 | 1.56 | 0.88 |
| 1:H:414:GLN:OE1 | 1:H:430:ILE:HG12 | 1.74 | 0.88 |
| 1:C:280:ILE:O | 1:C:281:TRP:HB2 | 1.72 | 0.88 |
| 1:D:98:ASP:N | 1:D:130:LYS:HE3 | 1.88 | 0.88 |
| 1:A:106:ALA:O | 1:A:109:SER:HB3 | 1.73 | 0.88 |
| 1:B:277:ASP:HB2 | 1:B:302:LEU:HD11 | 1.54 | 0.88 |
| 1:E:332:THR:HA | 1:E:353:THR:CG2 | 2.04 | 0.87 |
| 1:B:52:ILE:HD13 | 1:B:489:VAL:HG12 | 1.57 | 0.87 |
| 1:D:186:THR:HG22 | 1:D:187:ILE:N | 1.89 | 0.87 |
| 1:G:47:GLY:HA2 | 1:G:50:ARG:CG | 2.04 | 0.87 |
| 1:H:346:GLU:HG2 | 1:H:351:PRO:HG2 | 1.54 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:42:ARG:O | 1:J:45:VAL:HG12 | 1.74 | 0.87 |
| 1:A:479:THR:O | 1:A:483:VAL:HG23 | 1.75 | 0.87 |
| 1:L:338:ARG:HB3 | 1:L:338:ARG:NH1 | 1.88 | 0.87 |
| 1:C:360:PHE:HB3 | 1:C:365:ILE:HB | 1.56 | 0.87 |
| 1:L:9:PHE:HD1 | 1:L:10:PHE:H | 0.89 | 0.87 |
| 1:B:20:GLY:O | 1:B:24:VAL:HG23 | 1.75 | 0.87 |
| 1:B:65:ILE:HA | 1:B:147:ARG:NH1 | 1.89 | 0.87 |
| 1:C:168:ASP:O | 1:C:170:SER:N | 2.07 | 0.87 |
| 1:A:386:LEU:HD13 | 1:B:392:VAL:HG21 | 1.57 | 0.87 |
| 1:C:49:LEU:H | 1:C:49:LEU:HD12 | 1.38 | 0.87 |
| 1:L:6:ASP:HB2 | 1:L:329:LYS:HD2 | 1.55 | 0.87 |
| 1:L:82:HIS:CD2 | 1:L:112:THR:HG21 | 2.09 | 0.87 |
| 1:H:308:LYS:HD2 | 1:H:309:PRO:HD2 | 1.54 | 0.86 |
| 1:C:106:ALA:O | 1:C:109:SER:HB3 | 1.74 | 0.86 |
| 1:A:186:THR:HG22 | 1:A:187:ILE:HG12 | 1.54 | 0.86 |
| 1:I:30:GLU:HG3 | 1:I:31:ASP:H | 1.40 | 0.86 |
| 1:C:235:ILE:HG22 | 1:C:364:ASN:ND2 | 1.90 | 0.86 |
| 1:C:275:GLU:HB2 | 1:C:301:ILE:HD11 | 1.58 | 0.86 |
| 1:D:314:ILE:H | 1:D:314:ILE:HD13 | 1.38 | 0.86 |
| 1:J:344:ILE:HB | 1:J:367:VAL:HG22 | 1.58 | 0.86 |
| 1:D:239:THR:N | 1:D:240:PRO:HD3 | 1.88 | 0.86 |
| 1:C:176:MET:CE | 1:C:179:ILE:HD12 | 2.04 | 0.86 |
| 1:C:387:LYS:HE3 | 1:C:445:GLU:OE2 | 1.75 | 0.86 |
| 1:C:79:ARG:HD2 | 1:C:127:ALA:HB2 | 1.57 | 0.86 |
| 1:J:33:ARG:HA | 1:J:33:ARG:CZ | 2.06 | 0.86 |
| 1:H:291:LEU:O | 1:H:291:LEU:HD12 | 1.76 | 0.85 |
| 1:L:396:ARG:HG3 | 1:L:396:ARG:HH11 | 1.38 | 0.85 |
| 1:K:233:MET:HE1 | 1:K:343:ILE:HD11 | 1.57 | 0.85 |
| 1:G:50:ARG:HH12 | 1:K:73:GLU:HA | 1.40 | 0.85 |
| 1:G:212:ILE:H | 1:G:212:ILE:HD12 | 1.38 | 0.85 |
| 1:F:478:ARG:HG3 | 1:F:478:ARG:HH11 | 1.38 | 0.85 |
| 1:E:12:MET:HE3 | 1:E:353:THR:HA | 1.59 | 0.85 |
| 1:H:45:VAL:HG23 | 1:J:72:TRP:CZ3 | 2.10 | 0.85 |
| 1:A:130:LYS:O | 1:A:131:ILE:HD12 | 1.76 | 0.85 |
| 1:C:19:ARG:NE | 1:C:479:THR:HG21 | 1.91 | 0.85 |
| 1:D:186:THR:HG22 | 1:D:187:ILE:H | 1.39 | 0.85 |
| 1:D:316:GLU:HA | 1:D:316:GLU:OE1 | 1.76 | 0.85 |
| 1:H:496:ALA:HB1 | 1:H:501:THR:OXT | 1.77 | 0.85 |
| 1:C:316:GLU:HG3 | 1:C:338:ARG:HH21 | 1.39 | 0.85 |
| 1:B:482:TYR:O | 1:B:486:ILE:HG12 | 1.77 | 0.84 |
| 1:H:429:PRO:O | 1:H:431:VAL:N | 2.09 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:186:THR:CG2 | 1:I:187:ILE:N | 2.40 | 0.84 |
| 1:A:55:CYS:SG | 1:A:105:LYS:HG2 | 2.17 | 0.84 |
| 1:E:137:THR:HG23 | 1:E:140:GLU:HG3 | 1.59 | 0.84 |
| 1:B:65:ILE:HD13 | 1:B:144:ILE:HD11 | 1.60 | 0.84 |
| 1:A:397:LEU:HD13 | 1:F:394:TYR:CE2 | 2.11 | 0.84 |
| 1:F:79:ARG:HD2 | 1:F:127:ALA:HB2 | 1.58 | 0.84 |
| 1:K:131:ILE:HG12 | 1:K:136:TYR:HE2 | 1.42 | 0.84 |
| 1:K:87:THR:HB | 1:K:88:PRO:HD3 | 1.58 | 0.84 |
| 1:C:338:ARG:HB3 | 1:C:338:ARG:NH1 | 1.93 | 0.84 |
| 1:C:93:ILE:HD11 | 1:C:165:PRO:HB3 | 1.58 | 0.84 |
| 1:H:500:PHE:HB3 | 1:L:142:GLU:OE1 | 1.78 | 0.84 |
| 1:B:255:VAL:HG13 | 1:B:256:GLY:H | 1.42 | 0.84 |
| 1:D:501:THR:OXT | 1:E:146:ARG:NH2 | 2.10 | 0.84 |
| 1:L:19:ARG:O | 1:L:23:ILE:HG13 | 1.77 | 0.84 |
| 1:L:260:MET:HG2 | 1:L:288:PRO:HG3 | 1.59 | 0.84 |
| 1:A:423:LYS:CD | 1:A:426:GLY:HA3 | 2.06 | 0.84 |
| 1:C:300:SER:O | 1:C:302:LEU:N | 2.10 | 0.84 |
| 1:C:233:MET:HA | 1:C:236:LEU:HD12 | 1.58 | 0.84 |
| 1:I:131:ILE:HG23 | 1:I:136:TYR:CE2 | 2.12 | 0.84 |
| 1:I:107:LEU:HD13 | 1:I:126:LYS:HE3 | 1.60 | 0.83 |
| 1:I:269:LYS:HD3 | 1:I:285:GLY:HA3 | 1.59 | 0.83 |
| 1:K:30:GLU:HG3 | 1:K:31:ASP:N | 1.92 | 0.83 |
| 1:C:52:ILE:CD1 | 1:C:489:VAL:HG12 | 2.08 | 0.83 |
| 1:E:33:ARG:HB2 | 1:E:36:GLU:OE1 | 1.78 | 0.83 |
| 1:G:335:ASN:HD22 | 1:G:336:ALA:N | 1.75 | 0.83 |
| 1:H:36:GLU:CD | 1:H:42:ARG:HH12 | 1.82 | 0.83 |
| 1:H:42:ARG:O | 1:H:45:VAL:HG12 | 1.77 | 0.83 |
| 1:I:260:MET:HE3 | 1:I:288:PRO:HA | 1.57 | 0.83 |
| 1:A:482:TYR:O | 1:A:486:ILE:HG12 | 1.78 | 0.83 |
| 1:C:498:VAL:HG11 | 1:F:72:TRP:NE1 | 1.93 | 0.83 |
| 1:E:79:ARG:HH11 | 1:E:127:ALA:HB2 | 1.44 | 0.83 |
| 1:H:9:PHE:HD1 | 1:H:10:PHE:N | 1.76 | 0.83 |
| 1:K:336:ALA:HB3 | 1:K:359:ILE:HD12 | 1.59 | 0.83 |
| 1:C:82:HIS:CG | 1:C:112:THR:HG21 | 2.13 | 0.83 |
| 1:E:339:VAL:HG21 | 1:E:360:PHE:HE1 | 1.43 | 0.83 |
| 1:H:314:ILE:CD1 | 1:H:314:ILE:H | 1.91 | 0.83 |
| 1:L:293:ASP:O | 1:L:297:GLN:HG3 | 1.78 | 0.83 |
| 1:C:52:ILE:HD13 | 1:C:489:VAL:CG1 | 2.08 | 0.83 |
| 1:F:396:ARG:HG3 | 1:F:396:ARG:NH1 | 1.87 | 0.83 |
| 1:J:192:ILE:HG12 | 1:J:192:ILE:O | 1.79 | 0.83 |
| 1:B:57:HIS:CE1 | 1:D:155:LYS:HE2 | 2.14 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:249:VAL:HG13 | 1:F:273:VAL:HG22 | 1.59 | 0.83 |
| 1:J:177:SER:OG | 1:J:205:GLN:HG3 | 1.79 | 0.83 |
| 1:E:53:LYS:HB3 | 1:E:54:PRO:CD | 2.07 | 0.83 |
| 1:K:274:GLY:HA3 | 1:K:314:ILE:HD12 | 1.60 | 0.83 |
| 1:B:212:ILE:HD12 | 1:B:212:ILE:N | 1.93 | 0.82 |
| 1:B:291:LEU:HD11 | 1:B:301:ILE:HG22 | 1.61 | 0.82 |
| 1:E:19:ARG:HH11 | 1:E:19:ARG:HG3 | 1.44 | 0.82 |
| 1:E:39:GLU:HB3 | 1:E:41:LYS:HG3 | 1.59 | 0.82 |
| 1:G:192:ILE:O | 1:G:192:ILE:HG12 | 1.78 | 0.82 |
| 1:J:82:HIS:CG | 1:J:112:THR:HG21 | 2.14 | 0.82 |
| 1:I:445:GLU:O | 1:I:449:VAL:HG23 | 1.78 | 0.82 |
| 1:B:396:ARG:HG3 | 1:B:396:ARG:HH11 | 1.44 | 0.82 |
| 1:C:414:GLN:OE1 | 1:C:430:ILE:HG12 | 1.79 | 0.82 |
| 1:H:247:PHE:HB3 | 1:H:321:ILE:HG13 | 1.60 | 0.82 |
| 1:B:414:GLN:OE1 | 1:B:430:ILE:HG12 | 1.79 | 0.82 |
| 1:H:321:ILE:HG22 | 1:H:343:ILE:HB | 1.59 | 0.82 |
| 1:J:346:GLU:OE2 | 1:J:352:THR:HG22 | 1.80 | 0.82 |
| 1:C:118:VAL:HG12 | 1:C:456:THR:HG22 | 1.62 | 0.82 |
| 1:C:57:HIS:CD2 | 1:C:84:HIS:HE1 | 1.97 | 0.82 |
| 1:J:212:ILE:HD12 | 1:J:212:ILE:N | 1.94 | 0.82 |
| 1:K:346:GLU:OE1 | 1:K:369:PRO:HA | 1.78 | 0.82 |
| 1:C:335:ASN:CB | 1:C:338:ARG:HH22 | 1.91 | 0.82 |
| 1:D:90:LYS:NZ | 1:D:199:THR:HG23 | 1.94 | 0.82 |
| 1:I:236:LEU:HD22 | 1:I:342:LYS:HB3 | 1.62 | 0.81 |
| 1:A:57:HIS:ND1 | 1:A:84:HIS:HE1 | 1.77 | 0.81 |
| 1:H:501:THR:O | 1:L:146:ARG:NH1 | 2.13 | 0.81 |
| 1:L:82:HIS:CG | 1:L:112:THR:HG21 | 2.15 | 0.81 |
| 1:L:85:GLN:HE22 | 1:L:489:VAL:HG22 | 1.44 | 0.81 |
| 1:B:423:LYS:HG2 | 1:B:426:GLY:H | 1.45 | 0.81 |
| 1:D:411:MET:HA | 1:D:430:ILE:HG22 | 1.61 | 0.81 |
| 1:E:346:GLU:OE1 | 1:E:478:ARG:NH2 | 2.14 | 0.81 |
| 1:L:427:THR:C | 1:L:428:ILE:HD13 | 2.01 | 0.81 |
| 1:F:345:ALA:HB1 | 1:F:373:LEU:HD21 | 1.61 | 0.81 |
| 1:G:82:HIS:HD2 | 1:G:112:THR:HG21 | 1.44 | 0.81 |
| 1:G:33:ARG:HB2 | 1:G:33:ARG:HH11 | 1.44 | 0.81 |
| 1:H:121:PRO:HD2 | 1:H:382:TYR:CE2 | 2.16 | 0.81 |
| 1:B:336:ALA:CB | 1:B:359:ILE:HG21 | 2.08 | 0.81 |
| 1:C:217:ARG:HB3 | 1:C:217:ARG:HH11 | 1.43 | 0.81 |
| 1:C:392:VAL:HG22 | 1:E:386:LEU:HD22 | 1.61 | 0.81 |
| 1:F:428:ILE:N | 1:F:428:ILE:HD13 | 1.96 | 0.81 |
| 1:F:53:LYS:HB3 | 1:F:54:PRO:HD3 | 1.63 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:501:THR:OXT | 1:K:146:ARG:NH2 | 2.12 | 0.81 |
| 1:L:280:ILE:HG23 | 1:L:307:ALA:HB1 | 1.63 | 0.81 |
| 1:B:176:MET:HE3 | 1:B:179:ILE:HD12 | 1.63 | 0.81 |
| 1:F:19:ARG:HD3 | 1:F:23:ILE:HD11 | 1.63 | 0.81 |
| 1:J:20:GLY:O | 1:J:24:VAL:HG22 | 1.79 | 0.81 |
| 1:J:368:ILE:HG21 | 1:J:373:LEU:HD13 | 1.62 | 0.81 |
| 1:K:220:PHE:HD1 | 1:K:221:HIS:N | 1.79 | 0.81 |
| 1:B:439:ARG:CG | 1:B:439:ARG:HH11 | 1.91 | 0.80 |
| 1:C:217:ARG:HH12 | 1:C:221:HIS:CE1 | 1.95 | 0.80 |
| 1:H:67:ARG:HH11 | 1:H:67:ARG:HB3 | 1.46 | 0.80 |
| 1:I:344:ILE:HD11 | 1:I:360:PHE:CE1 | 2.16 | 0.80 |
| 1:C:396:ARG:HH11 | 1:C:396:ARG:CG | 1.92 | 0.80 |
| 1:E:6:ASP:N | 1:E:7:PRO:HD3 | 1.96 | 0.80 |
| 1:J:30:GLU:HA | 1:J:34:THR:HG23 | 1.63 | 0.80 |
| 1:A:72:TRP:HE1 | 1:E:498:VAL:HG21 | 1.45 | 0.80 |
| 1:A:501:THR:OG1 | 1:B:146:ARG:NH2 | 2.13 | 0.80 |
| 1:C:414:GLN:HB2 | 1:C:429:PRO:HD2 | 1.63 | 0.80 |
| 1:D:249:VAL:HG23 | 1:D:323:ILE:O | 1.82 | 0.80 |
| 1:F:30:GLU:HG3 | 1:F:31:ASP:H | 1.44 | 0.80 |
| 1:I:159:GLY:HA3 | 1:I:162:ILE:HD12 | 1.62 | 0.80 |
| 1:I:252:PHE:HE2 | 1:I:260:MET:HE1 | 1.46 | 0.80 |
| 1:E:167:PRO:HG3 | 1:E:176:MET:SD | 2.22 | 0.80 |
| 1:I:57:HIS:CD2 | 1:L:155:LYS:HE3 | 2.17 | 0.80 |
| 1:I:96:SER:O | 1:I:99:VAL:HG13 | 1.82 | 0.80 |
| 1:L:339:VAL:HG21 | 1:L:360:PHE:HE1 | 1.47 | 0.80 |
| 1:A:437:GLN:NE2 | 1:H:423:LYS:HG2 | 1.96 | 0.80 |
| 1:B:19:ARG:O | 1:B:23:ILE:HG13 | 1.82 | 0.80 |
| 1:E:346:GLU:HG2 | 1:E:351:PRO:HG2 | 1.64 | 0.80 |
| 1:J:85:GLN:HG2 | 1:J:86:ARG:N | 1.97 | 0.80 |
| 1:K:49:LEU:H | 1:K:49:LEU:HD12 | 1.47 | 0.80 |
| 1:A:227:ILE:O | 1:A:233:MET:HG3 | 1.82 | 0.80 |
| 1:E:429:PRO:O | 1:E:431:VAL:N | 2.14 | 0.80 |
| 1:J:336:ALA:HB3 | 1:J:337:PRO:HD3 | 1.63 | 0.80 |
| 1:K:291:LEU:HD11 | 1:K:301:ILE:HG22 | 1.63 | 0.80 |
| 1:K:436:PHE:O | 1:K:440:ILE:HG13 | 1.82 | 0.80 |
| 1:C:39:GLU:HG2 | 1:C:41:LYS:HG2 | 1.61 | 0.80 |
| 1:I:72:TRP:NE1 | 1:L:498:VAL:HG11 | 1.96 | 0.80 |
| 1:J:500:PHE:HB3 | 1:K:142:GLU:OE1 | 1.81 | 0.80 |
| 1:A:429:PRO:O | 1:A:431:VAL:N | 2.15 | 0.79 |
| 1:C:411:MET:SD | 1:C:430:ILE:HG21 | 2.22 | 0.79 |
| 1:J:90:LYS:HZ3 | 1:J:199:THR:HG23 | 1.46 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:96:SER:O | 1:C:99:VAL:HG22 | 1.81 | 0.79 |
| 1:K:131:ILE:HG12 | 1:K:136:TYR:CE2 | 2.17 | 0.79 |
| 1:L:21:ALA:O | 1:L:24:VAL:HG23 | 1.83 | 0.79 |
| 1:A:403:ARG:HG3 | 1:A:440:ILE:CG2 | 2.12 | 0.79 |
| 1:C:87:THR:CB | 1:C:88:PRO:HD3 | 2.12 | 0.79 |
| 1:E:433:THR:CG2 | 1:E:436:PHE:HB2 | 2.12 | 0.79 |
| 1:G:414:GLN:OE1 | 1:G:430:ILE:HG12 | 1.82 | 0.79 |
| 2:G:502:ADP:H3' | 2:G:502:ADP:O1A | 1.82 | 0.79 |
| 1:I:24:VAL:HG12 | 1:I:28:LEU:HD22 | 1.64 | 0.79 |
| 1:A:239:THR:N | 1:A:240:PRO:HD3 | 1.95 | 0.79 |
| 1:D:227:ILE:HA | 1:D:233:MET:SD | 2.22 | 0.79 |
| 1:B:346:GLU:OE1 | 1:B:370:ASP:N | 2.15 | 0.79 |
| 1:B:339:VAL:HG21 | 1:B:360:PHE:HE1 | 1.47 | 0.79 |
| 1:C:322:LEU:HD22 | 1:C:323:ILE:H | 1.46 | 0.79 |
| 1:D:250:GLN:HG2 | 1:D:314:ILE:HD11 | 1.64 | 0.79 |
| 1:E:291:LEU:O | 1:E:291:LEU:HG | 1.81 | 0.79 |
| 1:J:150:MET:SD | 1:J:186:THR:HG21 | 2.23 | 0.79 |
| 1:K:227:ILE:O | 1:K:227:ILE:CG2 | 2.29 | 0.79 |
| 1:C:346:GLU:HG3 | 1:C:368:ILE:O | 1.82 | 0.79 |
| 1:H:220:PHE:HD2 | 1:H:263:LEU:HD23 | 1.48 | 0.79 |
| 1:A:201:LYS:NZ | 1:A:388:ASN:HD21 | 1.80 | 0.79 |
| 1:D:67:ARG:CB | 1:D:67:ARG:HH11 | 1.95 | 0.79 |
| 1:A:91:GLY:HA3 | 1:A:125:ALA:O | 1.82 | 0.79 |
| 1:C:316:GLU:CG | 1:C:338:ARG:HE | 1.95 | 0.79 |
| 1:C:372:TYR:CD2 | 1:C:464:ILE:HD11 | 2.18 | 0.79 |
| 1:C:79:ARG:CD | 1:C:127:ALA:HB2 | 2.13 | 0.79 |
| 1:D:371:LEU:HD22 | 1:D:482:TYR:CD2 | 2.18 | 0.79 |
| 1:A:167:PRO:HG3 | 1:A:176:MET:SD | 2.23 | 0.79 |
| 1:D:57:HIS:HD2 | 1:D:84:HIS:NE2 | 1.81 | 0.79 |
| 1:G:142:GLU:HG3 | 1:G:178:TRP:CD2 | 2.17 | 0.79 |
| 1:K:227:ILE:O | 1:K:227:ILE:HG23 | 1.82 | 0.79 |
| 1:K:336:ALA:CB | 1:K:359:ILE:HD12 | 2.13 | 0.78 |
| 1:G:142:GLU:OE1 | 1:L:500:PHE:HB3 | 1.82 | 0.78 |
| 1:C:420:LYS:O | 1:C:420:LYS:HG2 | 1.81 | 0.78 |
| 1:G:462:ARG:HB3 | 1:G:466:ARG:NH1 | 1.98 | 0.78 |
| 1:H:430:ILE:O | 1:H:430:ILE:HG13 | 1.83 | 0.78 |
| 1:L:336:ALA:HB3 | 1:L:337:PRO:HD3 | 1.65 | 0.78 |
| 1:D:280:ILE:HD11 | 1:D:304:PHE:HB3 | 1.65 | 0.78 |
| 1:G:250:GLN:HG2 | 1:G:314:ILE:HD11 | 1.63 | 0.78 |
| 1:C:192:ILE:HG12 | 1:C:192:ILE:O | 1.83 | 0.78 |
| 1:G:27:LYS:O | 1:G:32:LEU:HD12 | 1.82 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:250:GLN:HG2 | 1:H:314:ILE:HD11 | 1.64 | 0.78 |
| 1:K:414:GLN:CB | 1:K:429:PRO:HD2 | 2.12 | 0.78 |
| 1:F:40:GLN:HG3 | 1:F:40:GLN:O | 1.83 | 0.78 |
| 1:I:24:VAL:CG1 | 1:I:28:LEU:HD22 | 2.14 | 0.78 |
| 1:J:48:ILE:O | 1:J:52:ILE:HG13 | 1.83 | 0.78 |
| 1:A:336:ALA:HB3 | 1:A:337:PRO:HD3 | 1.66 | 0.78 |
| 1:A:59:LEU:HD21 | 1:A:61:LEU:HD21 | 1.65 | 0.78 |
| 1:L:201:LYS:O | 1:L:211:ARG:NH1 | 2.17 | 0.78 |
| 1:L:411:MET:HA | 1:L:430:ILE:HG22 | 1.65 | 0.78 |
| 1:A:118:VAL:HG23 | 1:A:120:VAL:HG23 | 1.64 | 0.78 |
| 1:J:90:LYS:NZ | 1:J:164:VAL:HG12 | 1.98 | 0.78 |
| 1:L:498:VAL:HG23 | 1:L:499:THR:H | 1.48 | 0.78 |
| 2:A:1:ADP:H3' | 2:A:1:ADP:O1A | 1.84 | 0.78 |
| 1:E:433:THR:HG23 | 1:E:436:PHE:HB2 | 1.65 | 0.78 |
| 1:A:428:ILE:HG21 | 1:H:428:ILE:HG21 | 1.66 | 0.78 |
| 1:L:91:GLY:HA3 | 1:L:125:ALA:O | 1.83 | 0.78 |
| 1:A:85:GLN:OE1 | 2:A:1:ADP:N1 | 2.17 | 0.78 |
| 1:C:360:PHE:CD1 | 1:C:365:ILE:HG13 | 2.18 | 0.78 |
| 1:H:90:LYS:HE2 | 1:H:199:THR:HG21 | 1.66 | 0.78 |
| 1:J:90:LYS:HE2 | 1:J:199:THR:HG21 | 1.65 | 0.78 |
| 1:B:52:ILE:HD13 | 1:B:489:VAL:CG1 | 2.13 | 0.78 |
| 1:C:90:LYS:HZ3 | 1:C:164:VAL:HG12 | 1.49 | 0.78 |
| 1:J:95:TYR:OH | 1:J:145:THR:HG22 | 1.83 | 0.78 |
| 1:A:500:PHE:O | 1:A:501:THR:O | 2.02 | 0.77 |
| 1:C:75:ILE:HD12 | 1:C:75:ILE:N | 2.00 | 0.77 |
| 1:H:314:ILE:HD13 | 1:H:314:ILE:N | 1.98 | 0.77 |
| 1:H:346:GLU:HG2 | 1:H:351:PRO:CG | 2.13 | 0.77 |
| 1:L:65:ILE:HD13 | 1:L:144:ILE:CG1 | 2.15 | 0.77 |
| 1:L:294:PHE:HA | 1:L:297:GLN:NE2 | 1.98 | 0.77 |
| 1:L:33:ARG:NH1 | 1:L:33:ARG:CB | 2.38 | 0.77 |
| 1:B:137:THR:HG23 | 1:B:140:GLU:CG | 2.14 | 0.77 |
| 1:C:57:HIS:HD2 | 1:C:84:HIS:CE1 | 1.99 | 0.77 |
| 1:H:106:ALA:O | 1:H:109:SER:HB3 | 1.83 | 0.77 |
| 1:J:420:LYS:HZ2 | 1:J:420:LYS:HB3 | 1.49 | 0.77 |
| 1:K:48:ILE:HG13 | 1:K:490:PHE:HE1 | 1.49 | 0.77 |
| 1:D:387:LYS:HE3 | 1:D:445:GLU:OE2 | 1.85 | 0.77 |
| 1:D:428:ILE:H | 1:D:428:ILE:HD13 | 1.49 | 0.77 |
| 1:D:366:MET:HB2 | 1:D:475:LEU:HD23 | 1.66 | 0.77 |
| 1:E:414:GLN:CB | 1:E:429:PRO:HD2 | 2.13 | 0.77 |
| 1:I:323:ILE:CG2 | 1:I:345:ALA:HB3 | 2.13 | 0.77 |
| 1:H:91:GLY:HA3 | 1:H:125:ALA:O | 1.85 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:9:PHE:HD1 | 1:I:10:PHE:H | 1.30 | 0.77 |
| 1:B:65:ILE:HG12 | 1:B:75:ILE:HD11 | 1.64 | 0.77 |
| 1:D:87:THR:HG22 | 1:D:88:PRO:CD | 2.14 | 0.77 |
| 1:F:95:TYR:OH | 1:F:145:THR:HG22 | 1.83 | 0.77 |
| 1:J:414:GLN:NE2 | 1:J:430:ILE:HG12 | 1.99 | 0.77 |
| 1:A:372:TYR:CD2 | 1:A:464:ILE:HD11 | 2.20 | 0.77 |
| 1:B:330:GLN:O | 1:B:331:LEU:HD23 | 1.84 | 0.77 |
| 1:I:37:SER:HA | 1:I:42:ARG:CZ | 2.14 | 0.77 |
| 1:K:436:PHE:CE2 | 1:K:440:ILE:HD11 | 2.19 | 0.77 |
| 1:A:52:ILE:HD13 | 1:A:489:VAL:HG12 | 1.67 | 0.77 |
| 1:A:59:LEU:HD23 | 1:A:61:LEU:HD21 | 1.67 | 0.77 |
| 1:B:45:VAL:HG13 | 1:B:45:VAL:O | 1.84 | 0.77 |
| 1:G:95:TYR:OH | 1:G:145:THR:HG22 | 1.84 | 0.77 |
| 1:L:68:ASP:OD2 | 1:L:140:GLU:HG3 | 1.85 | 0.77 |
| 1:A:24:VAL:CG1 | 1:A:28:LEU:HD22 | 2.15 | 0.77 |
| 1:C:436:PHE:O | 1:C:440:ILE:HG13 | 1.85 | 0.77 |
| 1:B:176:MET:CE | 1:B:179:ILE:HD12 | 2.15 | 0.77 |
| 1:B:222:GLY:HA3 | 1:B:373:LEU:HD13 | 1.65 | 0.77 |
| 1:B:222:GLY:HA3 | 1:B:373:LEU:CD1 | 2.15 | 0.77 |
| 1:J:386:LEU:HD13 | 1:K:392:VAL:HG11 | 1.65 | 0.77 |
| 1:L:186:THR:HG22 | 1:L:187:ILE:N | 1.99 | 0.77 |
| 1:C:396:ARG:HG3 | 1:C:396:ARG:NH1 | 1.95 | 0.76 |
| 1:L:17:PHE:CE1 | 1:L:486:ILE:HD12 | 2.20 | 0.76 |
| 1:D:274:GLY:O | 1:D:275:GLU:HB2 | 1.83 | 0.76 |
| 1:K:52:ILE:HG12 | 1:K:493:TYR:CE2 | 2.20 | 0.76 |
| 1:L:29:VAL:HA | 1:L:33:ARG:HD2 | 1.67 | 0.76 |
| 1:B:336:ALA:HB1 | 1:B:359:ILE:CG2 | 2.11 | 0.76 |
| 1:J:7:PRO:O | 1:J:329:LYS:HE2 | 1.86 | 0.76 |
| 1:J:32:LEU:O | 1:J:33:ARG:HG2 | 1.86 | 0.76 |
| 1:I:147:ARG:CZ | 1:L:499:THR:HB | 2.14 | 0.76 |
| 1:A:332:THR:H | 1:A:335:ASN:HD21 | 1.30 | 0.76 |
| 1:C:240:PRO:HD2 | 1:C:245:LYS:NZ | 2.00 | 0.76 |
| 2:D:4:ADP:O1A | 2:D:4:ADP:H3' | 1.85 | 0.76 |
| 1:I:236:LEU:HD13 | 1:I:238:MET:HG3 | 1.67 | 0.76 |
| 1:B:95:TYR:HH | 1:B:145:THR:HG22 | 1.48 | 0.76 |
| 1:J:414:GLN:HA | 1:J:429:PRO:HG2 | 1.68 | 0.76 |
| 1:K:220:PHE:CD1 | 1:K:221:HIS:N | 2.53 | 0.76 |
| 1:G:396:ARG:HH11 | 1:G:396:ARG:HG3 | 1.49 | 0.76 |
| 1:H:239:THR:N | 1:H:240:PRO:HD3 | 2.00 | 0.76 |
| 1:J:459:ARG:O | 1:J:463:GLN:HG3 | 1.85 | 0.76 |
| 1:K:87:THR:CB | 1:K:88:PRO:HD3 | 2.15 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:82:HIS:ND1 | 1:A:109:SER:HA | 2.01 | 0.76 |
| 1:B:73:GLU:HA | 1:D:50:ARG:NH1 | 2.01 | 0.76 |
| 1:H:44:ARG:HH11 | 1:H:44:ARG:CB | 1.98 | 0.76 |
| 1:B:65:ILE:O | 1:B:65:ILE:HG13 | 1.83 | 0.76 |
| 1:I:219:VAL:HA | 1:I:373:LEU:HD23 | 1.68 | 0.76 |
| 1:L:167:PRO:HG3 | 1:L:176:MET:HG2 | 1.68 | 0.76 |
| 1:C:414:GLN:HA | 1:C:429:PRO:HG2 | 1.68 | 0.76 |
| 1:I:146:ARG:NH2 | 1:K:501:THR:OXT | 2.13 | 0.76 |
| 1:B:379:THR:HG21 | 1:B:453:LEU:HD23 | 1.68 | 0.76 |
| 1:D:394:TYR:HB2 | 1:D:445:GLU:HG3 | 1.67 | 0.76 |
| 1:I:281:TRP:CD1 | 1:I:283:PRO:HD3 | 2.21 | 0.76 |
| 2:E:5:ADP:H3' | 2:E:5:ADP:O1A | 1.86 | 0.75 |
| 1:I:75:ILE:CG1 | 1:I:131:ILE:HD11 | 2.16 | 0.75 |
| 1:J:432:PRO:HB3 | 1:J:436:PHE:CD1 | 2.20 | 0.75 |
| 1:J:68:ASP:OD1 | 1:J:140:GLU:HG3 | 1.87 | 0.75 |
| 1:K:339:VAL:HG21 | 1:K:360:PHE:HE1 | 1.50 | 0.75 |
| 1:E:19:ARG:O | 1:E:23:ILE:HG13 | 1.85 | 0.75 |
| 1:G:45:VAL:HG13 | 1:G:45:VAL:O | 1.87 | 0.75 |
| 1:A:427:THR:HG22 | 1:A:429:PRO:HD3 | 1.68 | 0.75 |
| 1:F:20:GLY:O | 1:F:24:VAL:HG22 | 1.86 | 0.75 |
| 1:D:296:LEU:HD13 | 1:D:297:GLN:N | 2.02 | 0.75 |
| 1:B:65:ILE:HG12 | 1:B:75:ILE:CD1 | 2.17 | 0.75 |
| 1:E:370:ASP:OD1 | 1:E:371:LEU:N | 2.19 | 0.75 |
| 1:G:150:MET:SD | 1:G:186:THR:HG21 | 2.27 | 0.75 |
| 1:K:286:ILE:HG21 | 1:K:291:LEU:HD22 | 1.68 | 0.75 |
| 1:A:142:GLU:O | 1:A:146:ARG:HG3 | 1.86 | 0.75 |
| 1:E:164:VAL:HG13 | 1:E:197:CYS:O | 1.85 | 0.75 |
| 1:E:396:ARG:HG3 | 1:E:396:ARG:HH11 | 1.50 | 0.75 |
| 1:L:428:ILE:O | 1:L:431:VAL:HG12 | 1.87 | 0.75 |
| 1:C:325:ALA:O | 1:C:326:ALA:HB2 | 1.85 | 0.75 |
| 1:D:250:GLN:HG2 | 1:D:314:ILE:HD13 | 1.68 | 0.75 |
| 1:G:90:LYS:HD2 | 1:G:164:VAL:HB | 1.66 | 0.75 |
| 1:H:331:LEU:O | 1:H:353:THR:HG23 | 1.86 | 0.75 |
| 1:H:52:ILE:HD13 | 1:H:489:VAL:HG12 | 1.68 | 0.75 |
| 1:I:239:THR:N | 1:I:240:PRO:HD3 | 2.02 | 0.75 |
| 1:A:403:ARG:HG3 | 1:A:440:ILE:HG22 | 1.68 | 0.75 |
| 1:B:315:LEU:HD11 | 1:B:330:GLN:HG2 | 1.68 | 0.75 |
| 1:C:217:ARG:HB3 | 1:C:217:ARG:NH1 | 2.02 | 0.75 |
| 1:D:20:GLY:O | 1:D:24:VAL:HG23 | 1.87 | 0.75 |
| 1:J:145:THR:HG21 | 1:J:175:GLU:HG2 | 1.66 | 0.75 |
| 1:J:176:MET:HE3 | 1:J:198:VAL:HG21 | 1.67 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:219:VAL:HG22 | 1:L:373:LEU:HD21 | 1.68 | 0.75 |
| 1:A:222:GLY:HA3 | 1:A:373:LEU:HD12 | 1.67 | 0.75 |
| 1:B:33:ARG:CB | 1:B:33:ARG:HH11 | 1.94 | 0.75 |
| 1:D:233:MET:HE1 | 1:D:236:LEU:HD12 | 1.67 | 0.75 |
| 1:A:498:VAL:HG11 | 1:E:72:TRP:HE1 | 1.52 | 0.75 |
| 1:J:82:HIS:CD2 | 1:J:112:THR:HG21 | 2.22 | 0.75 |
| 1:J:343:ILE:HD11 | 1:J:366:MET:HE2 | 1.66 | 0.75 |
| 1:A:175:GLU:HA | 1:A:178:TRP:CE3 | 2.22 | 0.74 |
| 1:C:72:TRP:NE1 | 1:F:498:VAL:HG11 | 2.02 | 0.74 |
| 1:J:24:VAL:HG13 | 1:J:483:VAL:CG1 | 2.17 | 0.74 |
| 1:K:52:ILE:HD13 | 1:K:489:VAL:HG12 | 1.69 | 0.74 |
| 1:L:192:ILE:HG12 | 1:L:192:ILE:O | 1.87 | 0.74 |
| 1:C:240:PRO:HD2 | 1:C:245:LYS:HZ2 | 1.52 | 0.74 |
| 1:K:360:PHE:HD1 | 1:K:365:ILE:HD12 | 1.52 | 0.74 |
| 1:B:148:PHE:O | 1:B:152:LEU:HB2 | 1.88 | 0.74 |
| 1:B:53:LYS:HB3 | 1:B:54:PRO:HD3 | 1.70 | 0.74 |
| 1:E:236:LEU:HB2 | 1:E:238:MET:HG3 | 1.67 | 0.74 |
| 1:B:147:ARG:CZ | 1:D:499:THR:OG1 | 2.35 | 0.74 |
| 1:E:314:ILE:H | 1:E:314:ILE:CD1 | 1.97 | 0.74 |
| 1:H:67:ARG:HB3 | 1:H:67:ARG:NH1 | 2.01 | 0.74 |
| 1:K:118:VAL:HG11 | 1:K:375:ALA:HB1 | 1.68 | 0.74 |
| 1:E:8:ASN:O | 1:E:10:PHE:N | 2.21 | 0.74 |
| 1:F:145:THR:HG21 | 1:F:175:GLU:HG2 | 1.68 | 0.74 |
| 1:B:501:THR:HG23 | 1:F:181:ASP:OD1 | 1.85 | 0.74 |
| 1:I:332:THR:HG22 | 1:I:353:THR:HG21 | 1.69 | 0.74 |
| 1:K:87:THR:HB | 1:K:88:PRO:CD | 2.15 | 0.74 |
| 1:A:24:VAL:HG11 | 1:A:28:LEU:HD22 | 1.69 | 0.74 |
| 1:E:212:ILE:HG22 | 1:E:258:HIS:HE1 | 1.51 | 0.74 |
| 1:F:387:LYS:HE3 | 1:F:445:GLU:OE2 | 1.87 | 0.74 |
| 1:G:112:THR:HG22 | 1:G:124:GLY:CA | 2.17 | 0.74 |
| 1:G:78:TYR:CE2 | 1:G:101:VAL:HG22 | 2.22 | 0.74 |
| 1:D:195:HIS:O | 1:D:201:LYS:HE3 | 1.87 | 0.74 |
| 1:E:130:LYS:O | 1:E:131:ILE:HD12 | 1.87 | 0.74 |
| 1:E:249:VAL:HG13 | 1:E:273:VAL:HG22 | 1.69 | 0.74 |
| 1:I:136:TYR:HB2 | 1:I:141:LEU:HD23 | 1.68 | 0.74 |
| 1:A:332:THR:HA | 1:A:353:THR:CG2 | 2.18 | 0.74 |
| 1:B:424:HIS:CD2 | 1:B:424:HIS:H | 2.05 | 0.74 |
| 1:C:380:VAL:HG12 | 1:C:381:SER:N | 2.01 | 0.74 |
| 1:E:277:ASP:O | 1:E:302:LEU:HD21 | 1.88 | 0.74 |
| 1:J:337:PRO:HA | 1:J:363:ARG:HE | 1.51 | 0.74 |
| 1:L:25:GLU:O | 1:L:29:VAL:HG23 | 1.88 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:57:HIS:CD2 | 1:C:84:HIS:CE1 | 2.75 | 0.74 |
| 1:D:346:GLU:HG2 | 1:D:351:PRO:CG | 2.17 | 0.74 |
| 1:L:177:SER:OG | 1:L:205:GLN:HG3 | 1.87 | 0.74 |
| 1:C:360:PHE:CD1 | 1:C:365:ILE:HG21 | 2.23 | 0.73 |
| 1:J:239:THR:N | 1:J:240:PRO:HD3 | 2.01 | 0.73 |
| 1:J:420:LYS:HB3 | 1:J:420:LYS:NZ | 2.03 | 0.73 |
| 1:K:384:GLU:O | 1:K:388:ASN:ND2 | 2.21 | 0.73 |
| 1:K:93:ILE:HD11 | 1:K:165:PRO:HB3 | 1.70 | 0.73 |
| 1:B:42:ARG:O | 1:B:45:VAL:HG12 | 1.88 | 0.73 |
| 1:D:459:ARG:O | 1:D:463:GLN:HG3 | 1.87 | 0.73 |
| 1:K:212:ILE:CD1 | 1:K:213:SER:H | 2.00 | 0.73 |
| 1:G:17:PHE:HE2 | 1:G:53:LYS:HB2 | 1.54 | 0.73 |
| 1:H:428:ILE:O | 1:H:431:VAL:HG12 | 1.87 | 0.73 |
| 1:J:150:MET:O | 1:J:154:LYS:HG3 | 1.86 | 0.73 |
| 1:G:423:LYS:HE2 | 1:G:423:LYS:HA | 1.68 | 0.73 |
| 1:G:437:GLN:HA | 1:G:440:ILE:HD12 | 1.71 | 0.73 |
| 1:I:368:ILE:HG21 | 1:I:373:LEU:HD12 | 1.70 | 0.73 |
| 1:K:219:VAL:HG11 | 1:K:259:SER:OG | 1.88 | 0.73 |
| 1:I:181:ASP:OD1 | 1:K:501:THR:OXT | 2.06 | 0.73 |
| 1:L:246:THR:N | 1:L:320:ASP:OD2 | 2.22 | 0.73 |
| 1:B:162:ILE:N | 1:B:162:ILE:HD12 | 2.04 | 0.73 |
| 1:C:114:LYS:HE2 | 1:C:374:ASN:ND2 | 2.03 | 0.73 |
| 1:F:473:LEU:HD22 | 1:F:479:THR:OG1 | 1.88 | 0.73 |
| 1:H:19:ARG:HH22 | 1:H:358:LYS:NZ | 1.87 | 0.73 |
| 1:B:217:ARG:HG2 | 1:B:221:HIS:HE1 | 1.54 | 0.73 |
| 1:B:249:VAL:HB | 1:B:323:ILE:CG1 | 2.16 | 0.73 |
| 1:E:19:ARG:HG3 | 1:E:19:ARG:NH1 | 2.03 | 0.73 |
| 1:J:498:VAL:N | 1:J:501:THR:HB | 2.04 | 0.73 |
| 1:L:252:PHE:CE2 | 1:L:260:MET:HE1 | 2.23 | 0.73 |
| 1:L:321:ILE:HG22 | 1:L:343:ILE:CG2 | 2.17 | 0.73 |
| 1:A:146:ARG:NH2 | 1:F:501:THR:OXT | 2.18 | 0.73 |
| 1:G:250:GLN:HG2 | 1:G:314:ILE:CD1 | 2.19 | 0.73 |
| 1:G:34:THR:O | 1:G:34:THR:HG22 | 1.88 | 0.73 |
| 1:J:112:THR:HG22 | 1:J:124:GLY:HA3 | 1.69 | 0.73 |
| 1:L:260:MET:CE | 1:L:288:PRO:HA | 2.18 | 0.73 |
| 1:C:316:GLU:HG2 | 1:C:338:ARG:HE | 1.54 | 0.73 |
| 1:E:329:LYS:HB3 | 1:E:329:LYS:HZ2 | 1.53 | 0.73 |
| 1:F:131:ILE:HD11 | 1:F:136:TYR:CE2 | 2.23 | 0.73 |
| 1:I:427:THR:HG22 | 1:I:429:PRO:HD3 | 1.71 | 0.73 |
| 1:D:247:PHE:CE1 | 1:D:263:LEU:HB3 | 2.23 | 0.73 |
| 1:D:53:LYS:HB3 | 1:D:54:PRO:HD3 | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:291:LEU:HD11 | 1:H:301:ILE:CG2 | 2.18 | 0.73 |
| 1:L:355:GLU:O | 1:L:359:ILE:HD13 | 1.88 | 0.73 |
| 1:B:314:ILE:HD13 | 1:B:314:ILE:H | 1.53 | 0.73 |
| 1:I:79:ARG:HD2 | 1:I:127:ALA:HB2 | 1.68 | 0.73 |
| 1:L:93:ILE:HD11 | 1:L:165:PRO:HB3 | 1.71 | 0.73 |
| 1:A:28:LEU:HD12 | 1:A:32:LEU:HD22 | 1.70 | 0.72 |
| 1:H:332:THR:H | 1:H:335:ASN:HD21 | 1.37 | 0.72 |
| 1:H:382:TYR:CE1 | 1:H:386:LEU:HD11 | 2.24 | 0.72 |
| 1:L:394:TYR:HB2 | 1:L:445:GLU:HG3 | 1.71 | 0.72 |
| 1:D:286:ILE:CG2 | 1:D:291:LEU:HD12 | 2.19 | 0.72 |
| 1:D:358:LYS:O | 1:D:362:GLU:HG3 | 1.89 | 0.72 |
| 1:D:498:VAL:HG23 | 1:D:499:THR:H | 1.55 | 0.72 |
| 1:F:9:PHE:CE1 | 1:F:103:GLU:HA | 2.24 | 0.72 |
| 1:K:30:GLU:HA | 1:K:34:THR:CG2 | 2.18 | 0.72 |
| 1:K:331:LEU:N | 1:K:331:LEU:HD23 | 2.04 | 0.72 |
| 1:L:17:PHE:HE1 | 1:L:486:ILE:HD12 | 1.54 | 0.72 |
| 1:F:344:ILE:HB | 1:F:367:VAL:HG22 | 1.71 | 0.72 |
| 1:A:146:ARG:HH12 | 1:F:501:THR:C | 1.92 | 0.72 |
| 1:H:459:ARG:O | 1:H:463:GLN:HG3 | 1.89 | 0.72 |
| 1:I:236:LEU:CD2 | 1:I:342:LYS:HB3 | 2.19 | 0.72 |
| 1:L:366:MET:HE3 | 1:L:368:ILE:HD11 | 1.70 | 0.72 |
| 1:B:332:THR:N | 1:B:335:ASN:HD21 | 1.87 | 0.72 |
| 1:C:9:PHE:HD1 | 1:C:10:PHE:N | 1.88 | 0.72 |
| 1:E:396:ARG:O | 1:E:396:ARG:HD3 | 1.89 | 0.72 |
| 1:H:154:LYS:HD2 | 1:K:189:HIS:CD2 | 2.20 | 0.72 |
| 1:H:90:LYS:HE2 | 1:H:199:THR:CG2 | 2.20 | 0.72 |
| 1:J:146:ARG:HG2 | 1:J:182:THR:OG1 | 1.88 | 0.72 |
| 1:J:250:GLN:HB2 | 1:J:314:ILE:HD11 | 1.71 | 0.72 |
| 1:K:274:GLY:HA3 | 1:K:314:ILE:CD1 | 2.20 | 0.72 |
| 1:D:250:GLN:HG3 | 1:D:315:LEU:HD13 | 1.71 | 0.72 |
| 1:H:223:ILE:HD12 | 1:H:263:LEU:HD21 | 1.72 | 0.72 |
| 1:J:234:SER:O | 1:J:237:GLY:N | 2.22 | 0.72 |
| 1:H:501:THR:HG23 | 1:L:181:ASP:OD1 | 1.88 | 0.72 |
| 1:L:20:GLY:O | 1:L:24:VAL:HG22 | 1.90 | 0.72 |
| 1:F:239:THR:N | 1:F:240:PRO:HD3 | 2.04 | 0.72 |
| 1:H:154:LYS:HB3 | 1:K:189:HIS:NE2 | 2.04 | 0.72 |
| 1:H:24:VAL:HG23 | 1:H:483:VAL:HG22 | 1.70 | 0.72 |
| 1:J:305:PRO:O | 1:J:307:ALA:N | 2.22 | 0.72 |
| 2:J:502:ADP:H3' | 2:J:502:ADP:O1A | 1.87 | 0.72 |
| 1:B:471:TYR:O | 1:B:473:LEU:HD23 | 1.89 | 0.72 |
| 1:I:392:VAL:HG13 | 1:K:382:TYR:OH | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:158:ILE:HD12 | 1:K:165:PRO:CD | 2.20 | 0.72 |
| 1:A:109:SER:O | 1:A:112:THR:HG23 | 1.90 | 0.72 |
| 1:C:271:ILE:O | 1:C:272:ALA:HB2 | 1.90 | 0.72 |
| 1:D:137:THR:HG23 | 1:D:140:GLU:CG | 2.20 | 0.72 |
| 1:E:329:LYS:HZ3 | 1:E:329:LYS:HB3 | 1.55 | 0.72 |
| 1:G:501:THR:OXT | 1:H:181:ASP:HB3 | 1.90 | 0.72 |
| 1:H:396:ARG:NH1 | 1:H:396:ARG:HG3 | 2.00 | 0.72 |
| 1:H:61:LEU:HD12 | 1:H:77:GLY:O | 1.90 | 0.72 |
| 1:J:167:PRO:HG3 | 1:J:176:MET:HG2 | 1.69 | 0.72 |
| 1:L:9:PHE:O | 1:L:12:MET:HB2 | 1.89 | 0.72 |
| 1:B:323:ILE:O | 1:B:323:ILE:HG13 | 1.89 | 0.72 |
| 1:C:289:LYS:HE2 | 1:C:293:ASP:OD2 | 1.89 | 0.72 |
| 1:F:498:VAL:HG23 | 1:F:499:THR:N | 2.03 | 0.72 |
| 1:G:271:ILE:HD11 | 1:G:283:PRO:HA | 1.72 | 0.72 |
| 1:H:137:THR:HG23 | 1:H:140:GLU:HB2 | 1.72 | 0.72 |
| 1:J:38:GLU:O | 1:J:40:GLN:N | 2.23 | 0.72 |
| 1:G:392:VAL:HG21 | 1:L:386:LEU:HD13 | 1.71 | 0.72 |
| 1:H:436:PHE:CE1 | 1:L:409:LEU:HD22 | 2.25 | 0.72 |
| 1:A:476:ASP:OD1 | 1:A:479:THR:HG23 | 1.90 | 0.71 |
| 1:E:65:ILE:HA | 1:E:147:ARG:NH2 | 2.05 | 0.71 |
| 1:G:61:LEU:HD12 | 1:G:77:GLY:O | 1.90 | 0.71 |
| 1:G:495:GLU:OE1 | 1:H:204:SER:HB3 | 1.90 | 0.71 |
| 1:H:280:ILE:HD12 | 1:H:301:ILE:HD12 | 1.70 | 0.71 |
| 1:K:68:ASP:OD2 | 1:K:137:THR:HG21 | 1.90 | 0.71 |
| 1:A:90:LYS:HB2 | 1:A:122:PHE:CD1 | 2.24 | 0.71 |
| 1:B:249:VAL:CB | 1:B:323:ILE:HG12 | 2.18 | 0.71 |
| 1:B:99:VAL:HA | 1:B:103:GLU:OE2 | 1.90 | 0.71 |
| 1:D:337:PRO:HA | 1:D:363:ARG:HE | 1.54 | 0.71 |
| 1:G:260:MET:HE3 | 1:G:288:PRO:HA | 1.71 | 0.71 |
| 1:I:251:GLY:O | 1:I:253:GLY:N | 2.23 | 0.71 |
| 1:I:42:ARG:O | 1:I:45:VAL:HG12 | 1.90 | 0.71 |
| 1:L:360:PHE:HB3 | 1:L:365:ILE:HB | 1.72 | 0.71 |
| 1:B:397:LEU:O | 1:B:398:THR:HG23 | 1.90 | 0.71 |
| 1:E:153:ALA:HA | 1:E:158:ILE:HG22 | 1.70 | 0.71 |
| 1:E:246:THR:HG22 | 1:E:320:ASP:OD1 | 1.90 | 0.71 |
| 1:B:501:THR:C | 1:F:146:ARG:HH22 | 1.94 | 0.71 |
| 1:G:250:GLN:HA | 1:G:314:ILE:HD11 | 1.71 | 0.71 |
| 1:I:48:ILE:HG21 | 1:I:490:PHE:HD1 | 1.54 | 0.71 |
| 1:L:219:VAL:HG11 | 1:L:259:SER:OG | 1.90 | 0.71 |
| 1:C:104:VAL:HG23 | 1:C:105:LYS:N | 2.04 | 0.71 |
| 1:C:501:THR:HG23 | 1:D:181:ASP:OD1 | 1.91 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:9:PHE:HD1 | 1:E:10:PHE:H | 1.39 | 0.71 |
| 1:E:335:ASN:HD22 | 1:E:336:ALA:N | 1.87 | 0.71 |
| 1:G:411:MET:HA | 1:G:430:ILE:HG22 | 1.72 | 0.71 |
| 1:I:371:LEU:HD23 | 1:I:481:ALA:CB | 2.19 | 0.71 |
| 1:K:104:VAL:HG23 | 1:K:105:LYS:N | 2.05 | 0.71 |
| 1:H:110:LEU:HD12 | 1:H:110:LEU:O | 1.90 | 0.71 |
| 1:A:150:MET:SD | 1:A:186:THR:HG21 | 2.31 | 0.71 |
| 1:B:114:LYS:O | 1:B:117:VAL:HB | 1.89 | 0.71 |
| 1:C:238:MET:O | 1:C:239:THR:HG22 | 1.90 | 0.71 |
| 1:C:277:ASP:CB | 1:C:302:LEU:HD11 | 2.21 | 0.71 |
| 1:H:82:HIS:CG | 1:H:112:THR:HG21 | 2.26 | 0.71 |
| 1:L:9:PHE:CD1 | 1:L:10:PHE:N | 2.50 | 0.71 |
| 1:C:47:GLY:HA2 | 1:C:50:ARG:HD3 | 1.72 | 0.71 |
| 1:F:19:ARG:HG3 | 1:F:19:ARG:HH11 | 1.55 | 0.71 |
| 1:L:227:ILE:O | 1:L:227:ILE:HG12 | 1.90 | 0.71 |
| 1:A:499:THR:OG1 | 1:E:147:ARG:HD3 | 1.90 | 0.71 |
| 1:E:314:ILE:HD13 | 1:E:314:ILE:N | 2.00 | 0.71 |
| 1:H:332:THR:HG22 | 1:H:353:THR:CG2 | 2.17 | 0.71 |
| 2:H:502:ADP:H3' | 2:H:502:ADP:O1A | 1.91 | 0.71 |
| 1:C:257:LEU:HA | 1:C:260:MET:HE2 | 1.71 | 0.71 |
| 1:D:106:ALA:O | 1:D:109:SER:HB3 | 1.91 | 0.71 |
| 1:E:6:ASP:N | 1:E:6:ASP:OD2 | 2.23 | 0.71 |
| 1:J:436:PHE:CD2 | 1:K:408:HIS:HB3 | 2.26 | 0.71 |
| 1:K:174:ARG:HG3 | 1:K:175:GLU:N | 2.06 | 0.71 |
| 1:A:53:LYS:HB3 | 1:A:54:PRO:HD3 | 1.72 | 0.71 |
| 1:C:226:PHE:CD1 | 1:C:366:MET:HE3 | 2.25 | 0.71 |
| 1:E:257:LEU:HD11 | 1:E:292:GLU:OE1 | 1.91 | 0.71 |
| 1:F:315:LEU:HD23 | 1:F:331:LEU:CD1 | 2.21 | 0.71 |
| 1:K:173:GLU:HB2 | 1:K:202:PRO:HG3 | 1.71 | 0.71 |
| 1:K:229:GLU:OE1 | 1:K:229:GLU:HA | 1.89 | 0.71 |
| 1:L:316:GLU:HB3 | 1:L:338:ARG:HH21 | 1.55 | 0.71 |
| 1:F:250:GLN:HA | 1:F:314:ILE:HD11 | 1.72 | 0.70 |
| 1:H:281:TRP:CD1 | 1:H:283:PRO:HD3 | 2.25 | 0.70 |
| 1:I:332:THR:O | 1:I:336:ALA:HB2 | 1.91 | 0.70 |
| 1:J:318:ASP:O | 1:J:319:CYS:HB3 | 1.91 | 0.70 |
| 1:J:331:LEU:HD22 | 1:J:360:PHE:CZ | 2.26 | 0.70 |
| 1:J:414:GLN:CG | 1:J:429:PRO:HD2 | 2.20 | 0.70 |
| 1:A:414:GLN:OE1 | 1:A:430:ILE:HG12 | 1.91 | 0.70 |
| 1:C:67:ARG:HD2 | 1:C:73:GLU:OE1 | 1.91 | 0.70 |
| 1:L:90:LYS:HB2 | 1:L:122:PHE:CD1 | 2.26 | 0.70 |
| 1:F:224:GLU:HA | 1:F:227:ILE:HG22 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:104:VAL:HG23 | 1:H:105:LYS:N | 2.06 | 0.70 |
| 1:K:13:VAL:HG21 | 1:K:110:LEU:HD11 | 1.73 | 0.70 |
| 1:K:162:ILE:HG22 | 1:K:163:ASP:N | 2.06 | 0.70 |
| 1:K:203:ILE:HD12 | 1:K:209:HIS:CE1 | 2.27 | 0.70 |
| 1:A:75:ILE:HG23 | 1:A:131:ILE:HD13 | 1.74 | 0.70 |
| 1:B:9:PHE:HD1 | 1:B:10:PHE:H | 1.38 | 0.70 |
| 1:C:351:PRO:HG2 | 1:C:352:THR:H | 1.55 | 0.70 |
| 1:C:61:LEU:HD12 | 1:C:77:GLY:O | 1.91 | 0.70 |
| 1:E:208:ILE:HG13 | 1:E:445:GLU:OE2 | 1.91 | 0.70 |
| 1:F:274:GLY:N | 1:F:314:ILE:HD12 | 2.05 | 0.70 |
| 1:I:236:LEU:HB3 | 1:I:238:MET:HG2 | 1.73 | 0.70 |
| 1:I:368:ILE:HG22 | 1:I:373:LEU:HD12 | 1.73 | 0.70 |
| 1:A:314:ILE:N | 1:A:314:ILE:HD13 | 2.06 | 0.70 |
| 1:A:346:GLU:OE2 | 1:A:478:ARG:NH2 | 2.24 | 0.70 |
| 1:C:437:GLN:HA | 1:C:440:ILE:HD12 | 1.73 | 0.70 |
| 1:F:315:LEU:HD23 | 1:F:331:LEU:HD12 | 1.73 | 0.70 |
| 1:H:75:ILE:N | 1:H:75:ILE:HD12 | 2.07 | 0.70 |
| 1:L:53:LYS:HB3 | 1:L:54:PRO:HD3 | 1.71 | 0.70 |
| 1:C:248:VAL:HG12 | 1:C:249:VAL:N | 2.06 | 0.70 |
| 1:C:392:VAL:CG2 | 1:E:386:LEU:HD22 | 2.21 | 0.70 |
| 1:G:429:PRO:C | 1:G:431:VAL:H | 1.95 | 0.70 |
| 1:G:492:VAL:HG21 | 2:G:502:ADP:C2 | 2.26 | 0.70 |
| 1:H:72:TRP:HE1 | 1:J:498:VAL:HG11 | 1.55 | 0.70 |
| 1:I:459:ARG:NH2 | 2:I:502:ADP:O3B | 2.25 | 0.70 |
| 1:J:414:GLN:HE22 | 1:J:430:ILE:HG12 | 1.56 | 0.70 |
| 1:K:236:LEU:HA | 1:K:342:LYS:NZ | 2.06 | 0.70 |
| 1:C:370:ASP:OD2 | 1:C:370:ASP:N | 2.23 | 0.70 |
| 1:F:131:ILE:HD11 | 1:F:136:TYR:HE2 | 1.56 | 0.70 |
| 1:I:101:VAL:HG13 | 1:I:105:LYS:HE3 | 1.73 | 0.70 |
| 1:A:163:ASP:O | 1:A:165:PRO:HD3 | 1.90 | 0.70 |
| 1:A:52:ILE:CD1 | 1:A:489:VAL:HG12 | 2.21 | 0.70 |
| 1:L:112:THR:HG22 | 1:L:124:GLY:HA3 | 1.74 | 0.70 |
| 1:C:322:LEU:HD22 | 1:C:323:ILE:N | 2.05 | 0.70 |
| 1:F:478:ARG:NH1 | 1:F:478:ARG:HG3 | 2.02 | 0.70 |
| 1:L:250:GLN:HG3 | 1:L:315:LEU:CD1 | 2.17 | 0.70 |
| 1:E:86:ARG:NH1 | 1:E:492:VAL:CG2 | 2.55 | 0.70 |
| 1:H:471:TYR:HB2 | 1:H:473:LEU:HD11 | 1.74 | 0.70 |
| 1:K:250:GLN:HG2 | 1:K:314:ILE:HD11 | 1.74 | 0.70 |
| 1:A:393:SER:HB3 | 2:F:502:ADP:O3A | 1.91 | 0.69 |
| 1:A:498:VAL:O | 1:A:501:THR:HG22 | 1.91 | 0.69 |
| 1:F:160:PRO:HG3 | 1:F:191:ASP:OD1 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:181:ASP:OD1 | 1:F:501:THR:HG23 | 1.92 | 0.69 |
| 1:H:239:THR:O | 1:H:239:THR:HG23 | 1.92 | 0.69 |
| 1:H:57:HIS:CE1 | 1:H:84:HIS:HE1 | 2.09 | 0.69 |
| 1:I:38:GLU:HB2 | 1:I:42:ARG:HH21 | 1.56 | 0.69 |
| 1:B:331:LEU:HD13 | 1:B:360:PHE:CZ | 2.24 | 0.69 |
| 1:E:421:PHE:HE1 | 1:E:423:LYS:HG3 | 1.58 | 0.69 |
| 1:G:240:PRO:HG2 | 1:G:244:ASP:O | 1.91 | 0.69 |
| 1:L:239:THR:N | 1:L:240:PRO:CD | 2.54 | 0.69 |
| 1:A:137:THR:HG23 | 1:A:140:GLU:HG3 | 1.73 | 0.69 |
| 1:B:277:ASP:HB2 | 1:B:302:LEU:CD1 | 2.21 | 0.69 |
| 1:C:380:VAL:O | 1:C:383:PHE:N | 2.22 | 0.69 |
| 1:D:96:SER:O | 1:D:99:VAL:HG13 | 1.90 | 0.69 |
| 1:G:250:GLN:CG | 1:G:314:ILE:HD11 | 2.22 | 0.69 |
| 1:L:153:ALA:HA | 1:L:158:ILE:HG22 | 1.73 | 0.69 |
| 1:A:39:GLU:O | 1:A:41:LYS:HG3 | 1.92 | 0.69 |
| 1:F:318:ASP:O | 1:F:319:CYS:HB3 | 1.93 | 0.69 |
| 1:H:220:PHE:CD2 | 1:H:263:LEU:HD23 | 2.27 | 0.69 |
| 1:G:397:LEU:HD22 | 1:L:394:TYR:CE2 | 2.28 | 0.69 |
| 1:B:424:HIS:CD2 | 1:B:424:HIS:N | 2.59 | 0.69 |
| 1:F:386:LEU:O | 1:F:389:LEU:N | 2.25 | 0.69 |
| 1:H:498:VAL:HG23 | 1:H:499:THR:N | 2.03 | 0.69 |
| 2:I:502:ADP:O1A | 2:I:502:ADP:H3' | 1.92 | 0.69 |
| 1:L:471:TYR:O | 1:L:473:LEU:N | 2.26 | 0.69 |
| 1:A:260:MET:CE | 1:A:288:PRO:HA | 2.21 | 0.69 |
| 1:B:9:PHE:CZ | 1:B:103:GLU:HG3 | 2.26 | 0.69 |
| 1:B:292:GLU:O | 1:B:296:LEU:HG | 1.93 | 0.69 |
| 1:B:9:PHE:CE2 | 1:B:103:GLU:HG3 | 2.27 | 0.69 |
| 1:C:284:ASP:OD2 | 1:C:284:ASP:N | 2.25 | 0.69 |
| 1:C:310:TYR:C | 1:C:310:TYR:CD2 | 2.66 | 0.69 |
| 1:C:353:THR:HB | 1:C:354:PRO:CD | 2.23 | 0.69 |
| 1:F:250:GLN:HG2 | 1:F:314:ILE:CD1 | 2.23 | 0.69 |
| 1:H:300:SER:HB3 | 1:H:302:LEU:HD22 | 1.75 | 0.69 |
| 1:H:79:ARG:HH11 | 1:H:127:ALA:HB2 | 1.56 | 0.69 |
| 1:I:181:ASP:OD1 | 1:K:501:THR:HG23 | 1.93 | 0.69 |
| 1:J:264:HIS:CD2 | 1:J:288:PRO:HD3 | 2.26 | 0.69 |
| 1:J:281:TRP:NE1 | 1:J:283:PRO:HD3 | 2.08 | 0.69 |
| 1:I:143:LYS:HG3 | 1:K:500:PHE:HE2 | 1.57 | 0.69 |
| 1:L:250:GLN:CG | 1:L:314:ILE:HD11 | 2.19 | 0.69 |
| 1:A:360:PHE:O | 1:A:365:ILE:HB | 1.91 | 0.69 |
| 1:B:239:THR:N | 1:B:240:PRO:HD3 | 2.07 | 0.69 |
| 1:C:344:ILE:HD11 | 1:C:360:PHE:CE1 | 2.28 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:3:ADP:O1A | 2:C:3:ADP:H3' | 1.93 | 0.69 |
| 1:C:19:ARG:CZ | 1:C:479:THR:HG21 | 2.21 | 0.69 |
| 1:I:40:GLN:O | 1:I:40:GLN:HG3 | 1.93 | 0.69 |
| 1:I:444:SER:HB2 | 1:I:446:LYS:HG2 | 1.75 | 0.69 |
| 1:I:83:SER:OG | 1:I:85:GLN:NE2 | 2.26 | 0.69 |
| 1:J:370:ASP:OD1 | 1:J:371:LEU:N | 2.25 | 0.69 |
| 1:B:81:GLN:HG3 | 1:B:157:PHE:CE1 | 2.27 | 0.69 |
| 1:C:101:VAL:O | 1:C:104:VAL:HG22 | 1.93 | 0.69 |
| 1:K:500:PHE:CE1 | 1:L:500:PHE:HZ | 2.09 | 0.69 |
| 1:B:118:VAL:HG23 | 1:B:120:VAL:HG23 | 1.75 | 0.69 |
| 1:B:57:HIS:ND1 | 1:D:155:LYS:HE2 | 2.08 | 0.69 |
| 1:E:95:TYR:OH | 1:E:145:THR:HG22 | 1.93 | 0.69 |
| 1:F:104:VAL:HG23 | 1:F:105:LYS:N | 2.06 | 0.69 |
| 1:F:250:GLN:HG3 | 1:F:315:LEU:HD11 | 1.74 | 0.69 |
| 1:F:250:GLN:HG3 | 1:F:315:LEU:CD1 | 2.23 | 0.69 |
| 1:J:331:LEU:HD22 | 1:J:360:PHE:HZ | 1.55 | 0.69 |
| 1:J:411:MET:HA | 1:J:430:ILE:CG2 | 2.22 | 0.69 |
| 1:K:195:HIS:O | 1:K:201:LYS:HE3 | 1.93 | 0.69 |
| 1:A:280:ILE:HG23 | 1:A:307:ALA:HB1 | 1.74 | 0.69 |
| 1:C:240:PRO:CD | 1:C:245:LYS:HZ2 | 2.04 | 0.69 |
| 1:D:114:LYS:HG3 | 1:D:371:LEU:O | 1.92 | 0.69 |
| 1:D:192:ILE:HG12 | 1:D:192:ILE:O | 1.92 | 0.69 |
| 1:D:249:VAL:HG23 | 1:D:323:ILE:HG13 | 1.74 | 0.69 |
| 1:E:61:LEU:N | 1:E:61:LEU:HD23 | 2.06 | 0.69 |
| 2:F:502:ADP:O1A | 2:F:502:ADP:H3' | 1.93 | 0.69 |
| 1:H:482:TYR:O | 1:H:486:ILE:HG12 | 1.93 | 0.69 |
| 1:K:346:GLU:OE2 | 1:K:351:PRO:HD2 | 1.93 | 0.69 |
| 1:B:129:VAL:O | 1:B:131:ILE:HG22 | 1.92 | 0.69 |
| 1:E:250:GLN:HG3 | 1:E:315:LEU:HD11 | 1.75 | 0.69 |
| 1:L:247:PHE:CB | 1:L:321:ILE:HG13 | 2.23 | 0.69 |
| 1:B:295:LYS:O | 1:B:295:LYS:HG2 | 1.92 | 0.68 |
| 1:D:24:VAL:HG12 | 1:D:28:LEU:HD22 | 1.75 | 0.68 |
| 1:G:65:ILE:HD13 | 1:G:144:ILE:HG12 | 1.75 | 0.68 |
| 1:J:233:MET:HE1 | 1:J:236:LEU:HD12 | 1.74 | 0.68 |
| 1:L:260:MET:HE2 | 1:L:288:PRO:HA | 1.74 | 0.68 |
| 1:L:371:LEU:HD22 | 1:L:482:TYR:CD2 | 2.28 | 0.68 |
| 1:C:319:CYS:SG | 1:C:320:ASP:N | 2.65 | 0.68 |
| 1:E:67:ARG:NH2 | 1:E:135:ASN:O | 2.25 | 0.68 |
| 1:G:368:ILE:HG21 | 1:G:373:LEU:HD13 | 1.74 | 0.68 |
| 1:H:147:ARG:HH11 | 1:H:147:ARG:HG3 | 1.58 | 0.68 |
| 1:H:233:MET:HE1 | 1:H:236:LEU:CD1 | 2.22 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:57:HIS:HD2 | 1:L:155:LYS:HE3 | 1.56 | 0.68 |
| 1:K:158:ILE:HG23 | 1:K:158:ILE:O | 1.93 | 0.68 |
| 1:L:248:VAL:HG22 | 1:L:271:ILE:HG22 | 1.76 | 0.68 |
| 1:G:409:LEU:HD13 | 1:L:436:PHE:CE1 | 2.28 | 0.68 |
| 1:B:248:VAL:HG13 | 1:B:272:ALA:O | 1.94 | 0.68 |
| 1:B:271:ILE:HG13 | 1:B:283:PRO:HA | 1.75 | 0.68 |
| 1:F:244:ASP:OD1 | 1:F:245:LYS:HG3 | 1.93 | 0.68 |
| 1:J:250:GLN:OE1 | 1:J:330:GLN:HG2 | 1.93 | 0.68 |
| 1:K:291:LEU:CD1 | 1:K:301:ILE:HG22 | 2.23 | 0.68 |
| 1:L:314:ILE:N | 1:L:314:ILE:HD13 | 2.08 | 0.68 |
| 1:A:411:MET:HG2 | 1:A:430:ILE:CG2 | 2.23 | 0.68 |
| 1:C:359:ILE:H | 1:C:359:ILE:HD12 | 1.59 | 0.68 |
| 1:E:246:THR:HG22 | 1:E:320:ASP:CG | 2.14 | 0.68 |
| 1:I:27:LYS:HG2 | 1:I:31:ASP:OD2 | 1.93 | 0.68 |
| 1:I:478:ARG:O | 1:I:479:THR:C | 2.30 | 0.68 |
| 1:K:252:PHE:HB3 | 1:K:275:GLU:OE1 | 1.93 | 0.68 |
| 1:B:196:ALA:HA | 1:B:388:ASN:HD22 | 1.59 | 0.68 |
| 1:D:337:PRO:O | 1:D:363:ARG:NH2 | 2.26 | 0.68 |
| 1:F:414:GLN:OE1 | 1:F:430:ILE:HG12 | 1.93 | 0.68 |
| 1:G:39:GLU:O | 1:G:41:LYS:N | 2.26 | 0.68 |
| 1:H:339:VAL:HG21 | 1:H:360:PHE:HE1 | 1.59 | 0.68 |
| 1:J:429:PRO:O | 1:J:431:VAL:N | 2.25 | 0.68 |
| 1:J:87:THR:HG22 | 1:J:88:PRO:N | 2.08 | 0.68 |
| 1:K:394:TYR:HB2 | 1:K:445:GLU:HG3 | 1.76 | 0.68 |
| 1:L:217:ARG:HH11 | 1:L:217:ARG:HB3 | 1.58 | 0.68 |
| 1:A:433:THR:HG23 | 1:B:412:SER:OG | 1.92 | 0.68 |
| 1:B:257:LEU:HD21 | 1:B:292:GLU:HG3 | 1.76 | 0.68 |
| 1:B:49:LEU:HD12 | 1:B:49:LEU:H | 1.58 | 0.68 |
| 1:G:17:PHE:CE1 | 1:G:486:ILE:HD12 | 2.28 | 0.68 |
| 1:G:19:ARG:HH11 | 1:G:479:THR:HG21 | 1.57 | 0.68 |
| 1:K:93:ILE:CD1 | 1:K:165:PRO:HB3 | 2.24 | 0.68 |
| 1:A:34:THR:O | 1:A:34:THR:HG22 | 1.92 | 0.68 |
| 1:D:213:SER:HB2 | 1:D:217:ARG:HD2 | 1.75 | 0.68 |
| 1:H:355:GLU:O | 1:H:359:ILE:HD13 | 1.94 | 0.68 |
| 1:K:150:MET:O | 1:K:154:LYS:HG3 | 1.93 | 0.68 |
| 1:A:186:THR:CG2 | 1:A:187:ILE:HG12 | 2.24 | 0.68 |
| 1:A:24:VAL:HG12 | 1:A:28:LEU:HB2 | 1.74 | 0.68 |
| 1:B:261:ARG:NH1 | 1:B:261:ARG:HG3 | 2.01 | 0.68 |
| 1:B:346:GLU:OE2 | 1:B:478:ARG:NH2 | 2.26 | 0.68 |
| 1:B:424:HIS:H | 1:B:424:HIS:HD2 | 1.41 | 0.68 |
| 1:C:176:MET:HG3 | 1:C:198:VAL:HG21 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:335:ASN:HA | 1:C:338:ARG:HH12 | 1.59 | 0.68 |
| 1:C:49:LEU:N | 1:C:49:LEU:HD12 | 2.08 | 0.68 |
| 1:J:281:TRP:CD1 | 1:J:283:PRO:HD3 | 2.29 | 0.68 |
| 1:C:239:THR:N | 1:C:240:PRO:CD | 2.45 | 0.68 |
| 1:I:68:ASP:OD1 | 1:I:140:GLU:HG3 | 1.93 | 0.68 |
| 1:I:412:SER:HA | 1:K:433:THR:HG22 | 1.76 | 0.68 |
| 2:L:502:ADP:H3' | 2:L:502:ADP:O1A | 1.92 | 0.68 |
| 1:A:417:LEU:HD11 | 1:F:417:LEU:CD2 | 2.23 | 0.68 |
| 1:C:142:GLU:OE1 | 1:C:178:TRP:CE2 | 2.46 | 0.68 |
| 1:C:239:THR:HG23 | 1:C:239:THR:O | 1.94 | 0.68 |
| 1:D:501:THR:C | 1:E:146:ARG:HH22 | 1.97 | 0.68 |
| 1:F:281:TRP:CZ2 | 1:F:283:PRO:HG3 | 2.29 | 0.68 |
| 1:G:260:MET:CE | 1:G:288:PRO:HA | 2.24 | 0.68 |
| 1:I:75:ILE:HG13 | 1:I:131:ILE:HD11 | 1.76 | 0.68 |
| 1:J:33:ARG:O | 1:J:35:ARG:N | 2.27 | 0.68 |
| 2:K:502:ADP:O1A | 2:K:502:ADP:H3' | 1.93 | 0.68 |
| 1:C:346:GLU:C | 1:C:373:LEU:HD23 | 2.15 | 0.67 |
| 1:D:403:ARG:HG2 | 1:D:403:ARG:HH11 | 1.59 | 0.67 |
| 1:E:432:PRO:HB3 | 1:E:436:PHE:CD1 | 2.29 | 0.67 |
| 1:H:274:GLY:O | 1:H:301:ILE:HD11 | 1.94 | 0.67 |
| 1:J:314:ILE:HD13 | 1:J:314:ILE:N | 2.10 | 0.67 |
| 1:J:436:PHE:CZ | 1:J:440:ILE:HD11 | 2.29 | 0.67 |
| 1:K:239:THR:HG23 | 1:K:239:THR:O | 1.93 | 0.67 |
| 1:K:478:ARG:HG2 | 1:K:478:ARG:NH1 | 1.99 | 0.67 |
| 1:L:16:PHE:CE2 | 1:L:478:ARG:HD2 | 2.28 | 0.67 |
| 1:L:167:PRO:CG | 1:L:176:MET:HG2 | 2.23 | 0.67 |
| 1:L:316:GLU:HB3 | 1:L:338:ARG:NH2 | 2.09 | 0.67 |
| 1:C:53:LYS:HB3 | 1:C:54:PRO:HD3 | 1.76 | 0.67 |
| 1:G:193:ASN:OD1 | 1:G:389:LEU:HD23 | 1.94 | 0.67 |
| 1:J:363:ARG:O | 1:J:365:ILE:HG12 | 1.95 | 0.67 |
| 1:K:199:THR:HA | 1:K:384:GLU:OE1 | 1.93 | 0.67 |
| 1:K:335:ASN:HA | 1:K:338:ARG:HD3 | 1.76 | 0.67 |
| 1:L:436:PHE:O | 1:L:440:ILE:HG13 | 1.94 | 0.67 |
| 1:C:87:THR:HB | 1:C:88:PRO:CD | 2.20 | 0.67 |
| 1:F:142:GLU:HG3 | 1:F:178:TRP:CD2 | 2.29 | 0.67 |
| 1:F:246:THR:HG23 | 1:F:320:ASP:OD1 | 1.93 | 0.67 |
| 1:G:459:ARG:O | 1:G:463:GLN:HG3 | 1.94 | 0.67 |
| 1:I:227:ILE:CD1 | 1:I:343:ILE:HD12 | 2.23 | 0.67 |
| 1:A:339:VAL:HG21 | 1:A:360:PHE:HE1 | 1.58 | 0.67 |
| 1:E:33:ARG:HH11 | 1:E:33:ARG:HB2 | 1.60 | 0.67 |
| 1:I:327:SER:OG | 1:I:330:GLN:NE2 | 2.26 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:323:ILE:HG23 | 1:K:345:ALA:HB3 | 1.76 | 0.67 |
| 1:K:354:PRO:O | 1:K:357:ASP:HB2 | 1.95 | 0.67 |
| 1:K:360:PHE:HB3 | 1:K:365:ILE:HB | 1.76 | 0.67 |
| 1:L:335:ASN:HD22 | 1:L:335:ASN:N | 1.93 | 0.67 |
| 1:A:348:ALA:O | 1:A:351:PRO:HD3 | 1.94 | 0.67 |
| 1:B:175:GLU:HA | 1:B:178:TRP:CE3 | 2.29 | 0.67 |
| 1:C:344:ILE:HD11 | 1:C:365:ILE:HG21 | 1.76 | 0.67 |
| 1:D:393:SER:OG | 1:D:396:ARG:HB2 | 1.94 | 0.67 |
| 1:E:371:LEU:HD22 | 1:E:482:TYR:CE2 | 2.30 | 0.67 |
| 1:G:201:LYS:NZ | 1:G:388:ASN:HD21 | 1.93 | 0.67 |
| 1:H:29:VAL:O | 1:H:30:GLU:O | 2.12 | 0.67 |
| 1:H:436:PHE:CZ | 1:L:409:LEU:HD22 | 2.29 | 0.67 |
| 1:I:212:ILE:HD12 | 1:I:212:ILE:N | 2.10 | 0.67 |
| 1:I:386:LEU:HD13 | 1:J:392:VAL:HG21 | 1.75 | 0.67 |
| 1:J:501:THR:OXT | 1:K:181:ASP:OD1 | 2.12 | 0.67 |
| 1:K:141:LEU:O | 1:K:145:THR:CG2 | 2.43 | 0.67 |
| 1:L:315:LEU:H | 1:L:315:LEU:HD12 | 1.60 | 0.67 |
| 1:B:498:VAL:HG23 | 1:B:499:THR:N | 2.08 | 0.67 |
| 1:C:280:ILE:HG22 | 1:C:281:TRP:N | 2.10 | 0.67 |
| 1:D:213:SER:HB2 | 1:D:217:ARG:CD | 2.24 | 0.67 |
| 1:F:329:LYS:HZ2 | 1:F:329:LYS:H | 1.41 | 0.67 |
| 1:H:121:PRO:CG | 1:H:382:TYR:HE2 | 2.07 | 0.67 |
| 1:I:33:ARG:HD3 | 1:I:33:ARG:O | 1.95 | 0.67 |
| 1:A:250:GLN:HG2 | 1:A:314:ILE:CD1 | 2.21 | 0.67 |
| 1:A:387:LYS:HE3 | 1:A:445:GLU:OE2 | 1.95 | 0.67 |
| 1:B:316:GLU:OE2 | 1:B:338:ARG:HB3 | 1.95 | 0.67 |
| 1:D:99:VAL:HG23 | 1:D:100:SER:H | 1.59 | 0.67 |
| 1:D:371:LEU:HD23 | 1:D:481:ALA:CB | 2.24 | 0.67 |
| 1:E:223:ILE:HD12 | 1:E:263:LEU:HD21 | 1.76 | 0.67 |
| 1:E:479:THR:O | 1:E:483:VAL:HG23 | 1.94 | 0.67 |
| 1:G:331:LEU:O | 1:G:353:THR:HG23 | 1.94 | 0.67 |
| 1:I:217:ARG:HB3 | 1:I:217:ARG:HH11 | 1.59 | 0.67 |
| 1:K:52:ILE:HG12 | 1:K:493:TYR:HE2 | 1.60 | 0.67 |
| 1:K:79:ARG:HD2 | 1:K:127:ALA:HB2 | 1.77 | 0.67 |
| 1:A:164:VAL:HA | 1:A:197:CYS:O | 1.94 | 0.67 |
| 1:A:498:VAL:HG23 | 1:A:499:THR:N | 2.09 | 0.67 |
| 1:B:137:THR:CG2 | 1:B:140:GLU:HG3 | 2.24 | 0.67 |
| 1:B:75:ILE:HG12 | 1:B:144:ILE:CD1 | 2.25 | 0.67 |
| 1:D:371:LEU:HD23 | 1:D:481:ALA:HB1 | 1.77 | 0.67 |
| 1:D:59:LEU:HD21 | 1:D:61:LEU:HD22 | 1.75 | 0.67 |
| 1:E:336:ALA:HB3 | 1:E:337:PRO:HD3 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:421:PHE:CD1 | 1:J:422:GLY:N | 2.63 | 0.67 |
| 1:K:356:ALA:HB1 | 1:K:360:PHE:HE2 | 1.59 | 0.67 |
| 1:B:394:TYR:HB2 | 1:B:445:GLU:HG3 | 1.77 | 0.67 |
| 1:C:498:VAL:HG23 | 1:C:499:THR:N | 2.08 | 0.67 |
| 1:G:17:PHE:CE2 | 1:G:53:LYS:HB2 | 2.30 | 0.67 |
| 1:H:87:THR:HB | 1:H:88:PRO:HD3 | 1.77 | 0.67 |
| 1:I:59:LEU:HB2 | 1:I:157:PHE:CE2 | 2.30 | 0.67 |
| 1:J:99:VAL:HG23 | 1:J:130:LYS:HD3 | 1.76 | 0.67 |
| 1:K:360:PHE:HA | 1:K:365:ILE:HG13 | 1.77 | 0.67 |
| 1:L:219:VAL:HG22 | 1:L:373:LEU:CD2 | 2.25 | 0.67 |
| 1:G:181:ASP:OD1 | 1:L:501:THR:HG23 | 1.94 | 0.66 |
| 1:K:411:MET:HG2 | 1:K:430:ILE:HG22 | 1.77 | 0.66 |
| 1:K:99:VAL:HG23 | 1:K:130:LYS:HG3 | 1.76 | 0.66 |
| 1:B:79:ARG:HH22 | 1:B:165:PRO:HA | 1.60 | 0.66 |
| 1:A:501:THR:OG1 | 1:B:181:ASP:OD1 | 2.12 | 0.66 |
| 1:B:257:LEU:HD12 | 1:B:257:LEU:C | 2.14 | 0.66 |
| 1:E:221:HIS:O | 1:E:222:GLY:C | 2.34 | 0.66 |
| 1:E:90:LYS:HD2 | 1:E:164:VAL:O | 1.95 | 0.66 |
| 1:F:332:THR:N | 1:F:335:ASN:HD21 | 1.93 | 0.66 |
| 1:K:248:VAL:O | 1:K:322:LEU:HD23 | 1.95 | 0.66 |
| 1:B:217:ARG:HG2 | 1:B:221:HIS:CE1 | 2.30 | 0.66 |
| 1:B:280:ILE:CG2 | 1:B:281:TRP:N | 2.57 | 0.66 |
| 1:C:410:LEU:O | 1:C:413:VAL:HG23 | 1.95 | 0.66 |
| 1:D:453:LEU:HD23 | 1:D:457:MET:HG2 | 1.76 | 0.66 |
| 1:E:239:THR:O | 1:E:239:THR:HG23 | 1.95 | 0.66 |
| 1:F:331:LEU:HD23 | 1:F:360:PHE:CZ | 2.30 | 0.66 |
| 1:F:90:LYS:HE2 | 1:F:199:THR:CG2 | 2.25 | 0.66 |
| 1:H:175:GLU:O | 1:H:179:ILE:HG12 | 1.95 | 0.66 |
| 1:I:296:LEU:HD13 | 1:I:297:GLN:N | 2.10 | 0.66 |
| 1:J:498:VAL:HG23 | 1:J:499:THR:N | 2.10 | 0.66 |
| 2:B:2:ADP:O1A | 2:B:2:ADP:H3' | 1.96 | 0.66 |
| 1:E:176:MET:HE3 | 1:E:179:ILE:CD1 | 2.25 | 0.66 |
| 1:E:238:MET:O | 1:E:239:THR:C | 2.33 | 0.66 |
| 1:G:233:MET:HE1 | 1:G:236:LEU:HD12 | 1.78 | 0.66 |
| 1:H:57:HIS:ND1 | 1:H:84:HIS:CE1 | 2.57 | 0.66 |
| 1:J:304:PHE:CD1 | 1:J:305:PRO:HD2 | 2.30 | 0.66 |
| 1:H:72:TRP:NE1 | 1:J:498:VAL:HG11 | 2.10 | 0.66 |
| 1:K:59:LEU:CD2 | 1:K:61:LEU:HD21 | 2.26 | 0.66 |
| 1:L:101:VAL:O | 1:L:104:VAL:HG22 | 1.94 | 0.66 |
| 1:A:281:TRP:HD1 | 1:A:282:ASN:H | 1.43 | 0.66 |
| 1:C:220:PHE:CD1 | 1:C:221:HIS:N | 2.63 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:345:ALA:HB1 | 1:E:373:LEU:CD2 | 2.26 | 0.66 |
| 1:G:57:HIS:HD2 | 1:G:84:HIS:CE1 | 2.13 | 0.66 |
| 1:I:92:GLY:HA2 | 1:I:166:ALA:O | 1.93 | 0.66 |
| 1:I:485:ALA:O | 1:I:489:VAL:HG23 | 1.95 | 0.66 |
| 1:J:346:GLU:OE2 | 1:J:351:PRO:HD2 | 1.95 | 0.66 |
| 1:K:219:VAL:O | 1:K:220:PHE:O | 2.14 | 0.66 |
| 1:K:497:GLY:O | 1:K:498:VAL:HG13 | 1.95 | 0.66 |
| 1:L:104:VAL:HG23 | 1:L:105:LYS:N | 2.10 | 0.66 |
| 1:A:96:SER:O | 1:A:99:VAL:HG13 | 1.95 | 0.66 |
| 1:D:294:PHE:CZ | 1:D:304:PHE:HA | 2.29 | 0.66 |
| 1:F:92:GLY:HA2 | 1:F:166:ALA:O | 1.96 | 0.66 |
| 1:G:212:ILE:H | 1:G:212:ILE:CD1 | 2.00 | 0.66 |
| 1:B:250:GLN:HG2 | 1:B:314:ILE:HD11 | 1.77 | 0.66 |
| 1:B:314:ILE:CD1 | 1:B:314:ILE:H | 2.09 | 0.66 |
| 1:C:90:LYS:NZ | 1:C:164:VAL:HG12 | 2.10 | 0.66 |
| 1:E:332:THR:HA | 1:E:353:THR:HG21 | 1.78 | 0.66 |
| 1:H:257:LEU:HD12 | 1:H:257:LEU:C | 2.16 | 0.66 |
| 1:H:281:TRP:NE1 | 1:H:283:PRO:HD3 | 2.11 | 0.66 |
| 1:I:406:ASN:HD22 | 1:J:409:LEU:CD2 | 2.08 | 0.66 |
| 1:I:417:LEU:HD11 | 1:K:417:LEU:HD23 | 1.77 | 0.66 |
| 1:I:410:LEU:HD21 | 1:J:409:LEU:CD1 | 2.26 | 0.66 |
| 1:J:65:ILE:HG12 | 1:J:75:ILE:HD11 | 1.78 | 0.66 |
| 1:K:203:ILE:HD12 | 1:K:209:HIS:ND1 | 2.11 | 0.66 |
| 1:L:39:GLU:CB | 1:L:41:LYS:HG3 | 2.26 | 0.66 |
| 1:A:396:ARG:HG3 | 1:A:396:ARG:HH11 | 1.60 | 0.66 |
| 1:E:137:THR:HG23 | 1:E:140:GLU:CG | 2.24 | 0.66 |
| 1:I:396:ARG:HD3 | 1:I:396:ARG:O | 1.96 | 0.66 |
| 1:K:118:VAL:HG11 | 1:K:375:ALA:CB | 2.26 | 0.66 |
| 1:A:20:GLY:O | 1:A:24:VAL:HG23 | 1.96 | 0.66 |
| 2:A:1:ADP:O1B | 1:B:396:ARG:NH1 | 2.29 | 0.66 |
| 1:D:500:PHE:HB3 | 1:E:142:GLU:OE2 | 1.95 | 0.66 |
| 1:E:143:LYS:NZ | 1:E:147:ARG:HH21 | 1.94 | 0.66 |
| 1:F:239:THR:O | 1:F:239:THR:HG23 | 1.96 | 0.66 |
| 1:I:32:LEU:O | 1:I:33:ARG:CB | 2.44 | 0.66 |
| 1:K:87:THR:CB | 1:K:88:PRO:CD | 2.71 | 0.66 |
| 1:A:274:GLY:HA3 | 1:A:314:ILE:HD12 | 1.76 | 0.66 |
| 1:A:28:LEU:HD12 | 1:A:32:LEU:CD2 | 2.26 | 0.66 |
| 1:A:386:LEU:CD1 | 1:B:392:VAL:HG21 | 2.26 | 0.66 |
| 1:C:155:LYS:NZ | 1:F:81:GLN:OE1 | 2.26 | 0.66 |
| 1:C:346:GLU:O | 1:C:373:LEU:HD23 | 1.96 | 0.66 |
| 1:D:316:GLU:O | 1:D:317:ALA:O | 2.13 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:263:LEU:O | 1:E:268:ALA:HB3 | 1.95 | 0.66 |
| 1:K:118:VAL:HG23 | 1:K:120:VAL:HG23 | 1.78 | 0.66 |
| 1:L:223:ILE:O | 1:L:227:ILE:HG22 | 1.96 | 0.66 |
| 1:B:471:TYR:CE2 | 1:B:483:VAL:HG11 | 2.31 | 0.65 |
| 1:C:118:VAL:HG12 | 1:C:456:THR:CG2 | 2.26 | 0.65 |
| 1:C:43:ASN:O | 1:C:46:ARG:HG2 | 1.94 | 0.65 |
| 1:D:421:PHE:CD2 | 1:D:422:GLY:N | 2.64 | 0.65 |
| 1:E:390:ASN:O | 1:E:392:VAL:HG23 | 1.95 | 0.65 |
| 1:I:114:LYS:HG3 | 1:I:371:LEU:O | 1.96 | 0.65 |
| 1:J:81:GLN:HG2 | 1:J:89:CYS:SG | 2.36 | 0.65 |
| 1:K:153:ALA:HA | 1:K:158:ILE:HG22 | 1.78 | 0.65 |
| 1:K:17:PHE:HE2 | 1:K:53:LYS:HB2 | 1.61 | 0.65 |
| 1:L:335:ASN:N | 1:L:335:ASN:ND2 | 2.44 | 0.65 |
| 1:L:39:GLU:HB2 | 1:L:41:LYS:HG3 | 1.77 | 0.65 |
| 1:C:280:ILE:O | 1:C:281:TRP:CB | 2.44 | 0.65 |
| 1:E:246:THR:HG23 | 1:E:320:ASP:H | 1.61 | 0.65 |
| 1:E:86:ARG:NH1 | 1:E:492:VAL:HG22 | 2.11 | 0.65 |
| 1:H:274:GLY:HA3 | 1:H:314:ILE:HD12 | 1.77 | 0.65 |
| 1:H:476:ASP:OD2 | 1:H:479:THR:OG1 | 2.13 | 0.65 |
| 1:K:141:LEU:O | 1:K:145:THR:HG23 | 1.96 | 0.65 |
| 1:K:345:ALA:HB1 | 1:K:373:LEU:HD21 | 1.78 | 0.65 |
| 1:L:92:GLY:HA2 | 1:L:166:ALA:O | 1.96 | 0.65 |
| 1:L:300:SER:OG | 1:L:301:ILE:N | 2.29 | 0.65 |
| 1:A:201:LYS:HD3 | 1:A:205:GLN:O | 1.96 | 0.65 |
| 1:C:12:MET:O | 1:C:16:PHE:HD1 | 1.80 | 0.65 |
| 1:C:274:GLY:O | 1:C:275:GLU:HB2 | 1.96 | 0.65 |
| 1:G:250:GLN:HE21 | 1:G:314:ILE:CD1 | 2.10 | 0.65 |
| 1:G:416:SER:OG | 1:L:431:VAL:HG13 | 1.96 | 0.65 |
| 1:C:201:LYS:NZ | 1:C:388:ASN:HD21 | 1.93 | 0.65 |
| 1:D:19:ARG:O | 1:D:23:ILE:HG13 | 1.96 | 0.65 |
| 1:D:47:GLY:HA2 | 1:D:50:ARG:CG | 2.20 | 0.65 |
| 1:E:281:TRP:O | 1:E:282:ASN:HB2 | 1.96 | 0.65 |
| 1:E:280:ILE:HG23 | 1:E:307:ALA:HB1 | 1.78 | 0.65 |
| 1:H:50:ARG:CZ | 1:H:50:ARG:HB2 | 2.25 | 0.65 |
| 1:I:9:PHE:HA | 1:I:12:MET:HE2 | 1.79 | 0.65 |
| 1:I:337:PRO:O | 1:I:363:ARG:NH2 | 2.29 | 0.65 |
| 1:J:421:PHE:CE1 | 1:J:423:LYS:HB2 | 2.31 | 0.65 |
| 1:K:318:ASP:O | 1:K:319:CYS:HB3 | 1.95 | 0.65 |
| 1:K:344:ILE:HD11 | 1:K:365:ILE:HG21 | 1.78 | 0.65 |
| 1:A:201:LYS:HG2 | 1:A:384:GLU:OE1 | 1.97 | 0.65 |
| 1:A:411:MET:HA | 1:A:430:ILE:HG22 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:72:TRP:NE1 | 1:E:498:VAL:HG21 | 2.12 | 0.65 |
| 1:B:386:LEU:HD13 | 1:F:392:VAL:HG21 | 1.77 | 0.65 |
| 1:F:315:LEU:HD12 | 1:F:315:LEU:H | 1.62 | 0.65 |
| 1:F:497:GLY:CA | 1:F:501:THR:HA | 2.27 | 0.65 |
| 1:H:260:MET:HE3 | 1:H:288:PRO:HA | 1.77 | 0.65 |
| 1:J:432:PRO:HA | 1:K:412:SER:OG | 1.96 | 0.65 |
| 1:J:501:THR:HG23 | 1:K:181:ASP:OD1 | 1.96 | 0.65 |
| 1:B:363:ARG:O | 1:B:365:ILE:HG12 | 1.96 | 0.65 |
| 1:D:414:GLN:OE1 | 1:D:430:ILE:HG12 | 1.96 | 0.65 |
| 1:H:343:ILE:HG12 | 1:H:366:MET:HB3 | 1.79 | 0.65 |
| 1:H:368:ILE:CG2 | 1:H:373:LEU:HD13 | 2.27 | 0.65 |
| 1:J:131:ILE:HD11 | 1:J:136:TYR:OH | 1.97 | 0.65 |
| 1:J:497:GLY:HA3 | 1:J:501:THR:HA | 1.78 | 0.65 |
| 1:K:229:GLU:HG3 | 1:K:231:SER:OG | 1.95 | 0.65 |
| 1:L:339:VAL:HG21 | 1:L:360:PHE:CE1 | 2.31 | 0.65 |
| 1:A:433:THR:O | 1:A:436:PHE:N | 2.29 | 0.65 |
| 1:C:344:ILE:HD12 | 1:C:367:VAL:HG22 | 1.77 | 0.65 |
| 1:C:420:LYS:O | 1:C:420:LYS:CG | 2.44 | 0.65 |
| 1:C:482:TYR:O | 1:C:486:ILE:HG12 | 1.97 | 0.65 |
| 1:D:396:ARG:HH11 | 1:D:396:ARG:HG2 | 1.62 | 0.65 |
| 1:E:75:ILE:HG23 | 1:E:131:ILE:HD13 | 1.78 | 0.65 |
| 1:G:208:ILE:HG13 | 1:G:387:LYS:CD | 2.26 | 0.65 |
| 1:D:86:ARG:NH2 | 2:D:4:ADP:O4' | 2.29 | 0.65 |
| 1:D:47:GLY:CA | 1:D:50:ARG:HG2 | 2.21 | 0.65 |
| 1:E:150:MET:SD | 1:E:186:THR:HG21 | 2.36 | 0.65 |
| 1:G:176:MET:CE | 1:G:179:ILE:HD12 | 2.27 | 0.65 |
| 1:I:477:LEU:HD22 | 1:I:477:LEU:H | 1.61 | 0.65 |
| 1:K:301:ILE:CD1 | 1:K:302:LEU:HD12 | 2.27 | 0.65 |
| 1:B:423:LYS:HG2 | 1:B:426:GLY:N | 2.11 | 0.65 |
| 1:C:227:ILE:O | 1:C:233:MET:HG3 | 1.96 | 0.65 |
| 1:C:32:LEU:O | 1:C:33:ARG:HB3 | 1.97 | 0.65 |
| 1:G:165:PRO:O | 1:G:198:VAL:HG23 | 1.97 | 0.65 |
| 1:J:259:SER:O | 1:J:263:LEU:HB2 | 1.97 | 0.65 |
| 1:K:146:ARG:O | 1:K:149:THR:N | 2.29 | 0.65 |
| 1:K:332:THR:O | 1:K:336:ALA:HB2 | 1.97 | 0.65 |
| 1:C:119:ASP:OD1 | 2:C:3:ADP:H2' | 1.97 | 0.65 |
| 1:D:498:VAL:N | 1:D:501:THR:HB | 2.12 | 0.65 |
| 1:G:33:ARG:CB | 1:G:33:ARG:HH11 | 2.10 | 0.65 |
| 1:H:68:ASP:OD2 | 1:H:137:THR:HG21 | 1.97 | 0.65 |
| 1:I:406:ASN:ND2 | 1:J:409:LEU:HD23 | 2.12 | 0.65 |
| 1:K:264:HIS:O | 1:K:266:PHE:N | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:49:LEU:N | 1:K:49:LEU:HD12 | 2.12 | 0.65 |
| 1:L:247:PHE:HZ | 1:L:260:MET:HG3 | 1.60 | 0.65 |
| 1:B:75:ILE:HG12 | 1:B:144:ILE:HD13 | 1.78 | 0.64 |
| 1:C:217:ARG:NH1 | 1:C:221:HIS:HE1 | 1.90 | 0.64 |
| 1:D:396:ARG:HH11 | 1:D:396:ARG:CG | 2.10 | 0.64 |
| 1:F:19:ARG:O | 1:F:23:ILE:HG13 | 1.97 | 0.64 |
| 1:G:61:LEU:HD12 | 1:G:61:LEU:H | 1.62 | 0.64 |
| 1:H:94:ARG:HB2 | 1:H:168:ASP:OD2 | 1.97 | 0.64 |
| 1:H:45:VAL:O | 1:H:45:VAL:HG13 | 1.97 | 0.64 |
| 1:J:332:THR:O | 1:J:336:ALA:HB2 | 1.97 | 0.64 |
| 1:J:90:LYS:HZ3 | 1:J:164:VAL:HG12 | 1.62 | 0.64 |
| 1:C:20:GLY:O | 1:C:24:VAL:HG23 | 1.97 | 0.64 |
| 1:E:82:HIS:CG | 1:E:112:THR:HG21 | 2.32 | 0.64 |
| 1:F:250:GLN:HG2 | 1:F:314:ILE:HD11 | 1.79 | 0.64 |
| 1:I:238:MET:HE1 | 1:I:342:LYS:HG3 | 1.79 | 0.64 |
| 1:J:387:LYS:HE3 | 1:J:393:SER:HA | 1.80 | 0.64 |
| 1:K:174:ARG:HG3 | 1:K:175:GLU:OE1 | 1.97 | 0.64 |
| 1:A:429:PRO:C | 1:A:431:VAL:H | 2.01 | 0.64 |
| 1:B:396:ARG:HG3 | 1:B:396:ARG:NH1 | 2.07 | 0.64 |
| 1:H:85:GLN:HG3 | 1:H:492:VAL:HG21 | 1.79 | 0.64 |
| 1:K:168:ASP:O | 1:K:170:SER:N | 2.29 | 0.64 |
| 1:L:252:PHE:HE2 | 1:L:260:MET:HE1 | 1.63 | 0.64 |
| 1:L:294:PHE:HE2 | 1:L:301:ILE:C | 1.99 | 0.64 |
| 1:L:42:ARG:O | 1:L:45:VAL:HG12 | 1.97 | 0.64 |
| 1:B:335:ASN:HD22 | 1:B:336:ALA:H | 1.45 | 0.64 |
| 1:C:200:GLY:N | 1:C:384:GLU:OE1 | 2.29 | 0.64 |
| 1:D:39:GLU:HB3 | 1:D:41:LYS:HG2 | 1.78 | 0.64 |
| 1:F:47:GLY:CA | 1:F:50:ARG:HG2 | 2.24 | 0.64 |
| 1:H:305:PRO:O | 1:H:306:LYS:HB2 | 1.96 | 0.64 |
| 1:I:280:ILE:HG23 | 1:I:307:ALA:HB1 | 1.77 | 0.64 |
| 1:I:37:SER:O | 1:I:38:GLU:HG3 | 1.97 | 0.64 |
| 1:J:181:ASP:O | 1:J:182:THR:C | 2.34 | 0.64 |
| 1:B:497:GLY:CA | 1:B:501:THR:HA | 2.27 | 0.64 |
| 1:C:13:VAL:HG12 | 1:C:14:GLU:N | 2.13 | 0.64 |
| 1:C:371:LEU:HD23 | 1:C:481:ALA:HB1 | 1.78 | 0.64 |
| 1:D:281:TRP:O | 1:D:282:ASN:HB2 | 1.98 | 0.64 |
| 1:E:143:LYS:HE3 | 1:E:147:ARG:HH21 | 1.62 | 0.64 |
| 1:A:428:ILE:CG2 | 1:H:428:ILE:HG21 | 2.28 | 0.64 |
| 1:I:175:GLU:HA | 1:I:178:TRP:CE3 | 2.32 | 0.64 |
| 1:I:217:ARG:HG2 | 1:I:262:TYR:CE2 | 2.32 | 0.64 |
| 1:I:250:GLN:HG3 | 1:I:315:LEU:HD11 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:85:GLN:OE1 | 2:J:502:ADP:N1 | 2.31 | 0.64 |
| 1:B:250:GLN:HG2 | 1:B:314:ILE:CD1 | 2.28 | 0.64 |
| 1:I:436:PHE:O | 1:I:440:ILE:HG13 | 1.97 | 0.64 |
| 1:I:75:ILE:HG12 | 1:I:131:ILE:HD11 | 1.79 | 0.64 |
| 1:K:226:PHE:O | 1:K:228:ASN:N | 2.26 | 0.64 |
| 1:L:414:GLN:OE1 | 1:L:428:ILE:HA | 1.97 | 0.64 |
| 1:A:353:THR:HG23 | 1:A:356:ALA:H | 1.61 | 0.64 |
| 1:B:433:THR:HG23 | 1:F:412:SER:OG | 1.97 | 0.64 |
| 1:B:65:ILE:HD13 | 1:B:144:ILE:CD1 | 2.28 | 0.64 |
| 1:D:227:ILE:HD11 | 1:D:321:ILE:HD11 | 1.78 | 0.64 |
| 1:E:420:LYS:NZ | 1:E:420:LYS:O | 2.19 | 0.64 |
| 1:F:431:VAL:HG13 | 1:F:431:VAL:O | 1.98 | 0.64 |
| 1:H:274:GLY:O | 1:H:275:GLU:HB2 | 1.96 | 0.64 |
| 1:H:248:VAL:HG11 | 1:H:314:ILE:HB | 1.80 | 0.64 |
| 1:I:484:ASN:ND2 | 1:I:488:LYS:HE3 | 2.13 | 0.64 |
| 1:K:227:ILE:HD11 | 1:K:321:ILE:HD11 | 1.79 | 0.64 |
| 1:K:280:ILE:HG22 | 1:K:281:TRP:N | 2.13 | 0.64 |
| 1:C:42:ARG:O | 1:C:45:VAL:HG12 | 1.97 | 0.64 |
| 1:D:301:ILE:HD12 | 1:D:301:ILE:C | 2.18 | 0.64 |
| 1:E:111:MET:HB3 | 1:E:124:GLY:HA2 | 1.79 | 0.64 |
| 1:H:356:ALA:O | 1:H:360:PHE:CD2 | 2.51 | 0.64 |
| 1:I:148:PHE:O | 1:I:152:LEU:HB2 | 1.98 | 0.64 |
| 1:J:349:ASN:OD1 | 1:J:374:ASN:ND2 | 2.31 | 0.64 |
| 1:J:428:ILE:O | 1:J:428:ILE:HG22 | 1.97 | 0.64 |
| 1:K:465:MET:O | 1:K:468:ALA:N | 2.31 | 0.64 |
| 1:A:345:ALA:HB1 | 1:A:373:LEU:HD21 | 1.80 | 0.64 |
| 1:C:331:LEU:HD23 | 1:C:335:ASN:HD21 | 1.61 | 0.64 |
| 1:C:429:PRO:C | 1:C:431:VAL:H | 1.94 | 0.64 |
| 1:F:68:ASP:N | 1:F:140:GLU:OE2 | 2.29 | 0.64 |
| 1:I:261:ARG:NH1 | 1:I:292:GLU:OE1 | 2.31 | 0.64 |
| 1:J:68:ASP:OD2 | 1:J:137:THR:HG21 | 1.97 | 0.64 |
| 1:J:379:THR:O | 1:J:382:TYR:HB3 | 1.97 | 0.64 |
| 1:K:13:VAL:HG21 | 1:K:110:LEU:CD1 | 2.28 | 0.64 |
| 1:L:176:MET:HE3 | 1:L:179:ILE:HD12 | 1.80 | 0.64 |
| 1:L:423:LYS:HG3 | 1:L:425:GLY:H | 1.63 | 0.64 |
| 1:L:428:ILE:HD13 | 1:L:428:ILE:N | 2.12 | 0.64 |
| 1:A:65:ILE:HD13 | 1:A:144:ILE:CG1 | 2.27 | 0.64 |
| 1:C:131:ILE:HG13 | 1:C:136:TYR:CE2 | 2.33 | 0.64 |
| 1:D:314:ILE:CD1 | 1:D:314:ILE:H | 2.11 | 0.64 |
| 1:B:147:ARG:NE | 1:D:499:THR:OG1 | 2.31 | 0.64 |
| 1:D:98:ASP:CA | 1:D:130:LYS:HE3 | 2.26 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:33:ARG:HH12 | 1:F:45:VAL:HG11 | 1.62 | 0.64 |
| 1:I:202:PRO:HD2 | 1:I:205:GLN:HB2 | 1.80 | 0.64 |
| 1:I:339:VAL:HG21 | 1:I:360:PHE:HE1 | 1.61 | 0.64 |
| 1:I:501:THR:HG23 | 1:J:181:ASP:OD1 | 1.97 | 0.64 |
| 1:A:331:LEU:O | 1:A:353:THR:HG22 | 1.98 | 0.63 |
| 1:D:360:PHE:HD1 | 1:D:365:ILE:HG21 | 1.63 | 0.63 |
| 1:F:414:GLN:HE22 | 1:F:430:ILE:CD1 | 2.11 | 0.63 |
| 1:G:232:TYR:H | 1:G:232:TYR:HD1 | 1.45 | 0.63 |
| 1:G:281:TRP:CZ2 | 1:G:283:PRO:HG3 | 2.33 | 0.63 |
| 1:I:484:ASN:HD21 | 1:I:488:LYS:NZ | 1.96 | 0.63 |
| 1:L:239:THR:O | 1:L:239:THR:HG23 | 1.97 | 0.63 |
| 1:B:65:ILE:HA | 1:B:147:ARG:CZ | 2.28 | 0.63 |
| 1:D:352:THR:HG23 | 1:D:478:ARG:NH2 | 2.13 | 0.63 |
| 1:B:498:VAL:HG11 | 1:D:72:TRP:NE1 | 2.13 | 0.63 |
| 1:E:79:ARG:NH1 | 1:E:127:ALA:HB2 | 2.12 | 0.63 |
| 1:E:378:VAL:HA | 1:E:381:SER:OG | 1.98 | 0.63 |
| 1:F:252:PHE:CE2 | 1:F:257:LEU:HB2 | 2.33 | 0.63 |
| 1:G:61:LEU:HD12 | 1:G:61:LEU:N | 2.13 | 0.63 |
| 1:I:238:MET:CE | 1:I:342:LYS:HG3 | 2.28 | 0.63 |
| 1:I:322:LEU:HD12 | 1:I:344:ILE:HG23 | 1.79 | 0.63 |
| 1:I:93:ILE:HG23 | 1:I:127:ALA:CB | 2.23 | 0.63 |
| 1:J:101:VAL:O | 1:J:104:VAL:HG22 | 1.98 | 0.63 |
| 1:K:45:VAL:C | 1:K:47:GLY:H | 2.02 | 0.63 |
| 1:A:261:ARG:HG3 | 1:A:261:ARG:HH11 | 1.63 | 0.63 |
| 1:B:24:VAL:CG2 | 1:B:483:VAL:HG13 | 2.27 | 0.63 |
| 1:H:487:GLU:O | 1:H:490:PHE:HB3 | 1.99 | 0.63 |
| 1:L:233:MET:HA | 1:L:236:LEU:HD12 | 1.81 | 0.63 |
| 1:B:271:ILE:HD11 | 1:B:283:PRO:HG3 | 1.80 | 0.63 |
| 1:B:439:ARG:HG3 | 1:B:439:ARG:NH1 | 1.97 | 0.63 |
| 1:C:498:VAL:HG11 | 1:F:72:TRP:HE1 | 1.61 | 0.63 |
| 1:E:164:VAL:HG13 | 1:E:197:CYS:C | 2.19 | 0.63 |
| 1:G:322:LEU:HB3 | 1:G:344:ILE:HD13 | 1.80 | 0.63 |
| 1:I:229:GLU:O | 1:I:230:ALA:C | 2.37 | 0.63 |
| 1:J:10:PHE:HD1 | 1:J:106:ALA:HB2 | 1.63 | 0.63 |
| 1:K:96:SER:HA | 1:K:131:ILE:O | 1.99 | 0.63 |
| 1:L:315:LEU:CD1 | 1:L:315:LEU:H | 2.11 | 0.63 |
| 1:A:437:GLN:HG2 | 1:H:423:LYS:HD3 | 1.80 | 0.63 |
| 1:B:171:THR:HG22 | 1:B:175:GLU:OE2 | 1.99 | 0.63 |
| 1:C:217:ARG:CB | 1:C:217:ARG:HH11 | 2.12 | 0.63 |
| 1:D:249:VAL:CG2 | 1:D:323:ILE:HG13 | 2.29 | 0.63 |
| 1:E:463:GLN:HE22 | 1:E:488:LYS:NZ | 1.97 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:332:THR:H | 1:G:335:ASN:HD21 | 1.45 | 0.63 |
| 1:I:414:GLN:OE1 | 1:I:428:ILE:HA | 1.99 | 0.63 |
| 1:K:255:VAL:HG13 | 1:K:256:GLY:N | 2.14 | 0.63 |
| 1:L:336:ALA:O | 1:L:339:VAL:HG22 | 1.97 | 0.63 |
| 1:A:313:SER:O | 1:A:315:LEU:N | 2.32 | 0.63 |
| 1:C:310:TYR:C | 1:C:310:TYR:HD2 | 2.02 | 0.63 |
| 1:E:24:VAL:CG2 | 1:E:483:VAL:HG13 | 2.28 | 0.63 |
| 1:G:212:ILE:N | 1:G:212:ILE:HD12 | 2.11 | 0.63 |
| 1:I:78:TYR:CD2 | 1:I:101:VAL:HG23 | 2.33 | 0.63 |
| 1:L:223:ILE:CD1 | 1:L:263:LEU:HD21 | 2.29 | 0.63 |
| 1:B:13:VAL:HA | 1:B:16:PHE:HD1 | 1.63 | 0.63 |
| 1:B:432:PRO:HB3 | 1:B:436:PHE:CD1 | 2.34 | 0.63 |
| 1:B:87:THR:OG1 | 1:B:88:PRO:CD | 2.47 | 0.63 |
| 1:C:277:ASP:HB2 | 1:C:302:LEU:HD11 | 1.81 | 0.63 |
| 1:D:59:LEU:HG | 1:D:61:LEU:HD23 | 1.81 | 0.63 |
| 1:E:94:ARG:HD2 | 1:E:168:ASP:OD1 | 1.99 | 0.63 |
| 1:F:252:PHE:HD1 | 1:F:301:ILE:HG21 | 1.64 | 0.63 |
| 1:H:217:ARG:HD2 | 1:H:450:HIS:CE1 | 2.33 | 0.63 |
| 1:J:360:PHE:HB3 | 1:J:365:ILE:HB | 1.81 | 0.63 |
| 1:J:501:THR:C | 1:K:146:ARG:HH22 | 2.01 | 0.63 |
| 1:J:386:LEU:HD13 | 1:K:392:VAL:CG1 | 2.28 | 0.63 |
| 1:L:248:VAL:HG13 | 1:L:272:ALA:O | 1.98 | 0.63 |
| 1:D:479:THR:O | 1:D:483:VAL:HG23 | 1.99 | 0.63 |
| 1:E:219:VAL:HG22 | 1:E:373:LEU:HG | 1.80 | 0.63 |
| 1:F:423:LYS:CE | 1:F:426:GLY:HA3 | 2.25 | 0.63 |
| 1:G:30:GLU:HA | 1:G:34:THR:OG1 | 1.98 | 0.63 |
| 1:G:414:GLN:CB | 1:G:429:PRO:HD2 | 2.29 | 0.63 |
| 1:G:500:PHE:HZ | 1:J:500:PHE:HZ | 1.46 | 0.63 |
| 1:G:88:PRO:HA | 1:G:162:ILE:O | 1.98 | 0.63 |
| 1:I:109:SER:O | 1:I:113:TYR:CD2 | 2.52 | 0.63 |
| 1:I:14:GLU:HG3 | 1:I:53:LYS:HZ2 | 1.63 | 0.63 |
| 1:J:217:ARG:HG3 | 1:J:262:TYR:CE2 | 2.33 | 0.63 |
| 1:L:121:PRO:O | 1:L:122:PHE:HD2 | 1.80 | 0.63 |
| 1:L:274:GLY:O | 1:L:275:GLU:HB2 | 1.98 | 0.63 |
| 1:A:186:THR:CG2 | 1:A:187:ILE:N | 2.43 | 0.63 |
| 1:A:287:ASP:OD2 | 1:A:290:GLU:HG3 | 1.98 | 0.63 |
| 1:D:225:ASN:ND2 | 1:D:458:GLU:HA | 2.13 | 0.63 |
| 1:D:79:ARG:HG2 | 1:D:157:PHE:HB3 | 1.80 | 0.63 |
| 1:E:232:TYR:CE1 | 1:E:465:MET:HG2 | 2.33 | 0.63 |
| 1:E:24:VAL:CG1 | 1:E:28:LEU:HD13 | 2.28 | 0.63 |
| 1:E:368:ILE:HG22 | 1:E:373:LEU:HB2 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:142:GLU:HG2 | 1:H:146:ARG:HD2 | 1.81 | 0.63 |
| 1:J:222:GLY:HA3 | 1:J:373:LEU:CD1 | 2.29 | 0.63 |
| 1:K:85:GLN:CG | 1:K:492:VAL:HG11 | 2.28 | 0.63 |
| 1:L:335:ASN:ND2 | 1:L:335:ASN:H | 1.95 | 0.63 |
| 1:L:396:ARG:NH1 | 1:L:396:ARG:HG3 | 2.10 | 0.63 |
| 1:B:159:GLY:HA3 | 1:B:162:ILE:HD13 | 1.80 | 0.62 |
| 1:C:176:MET:HG3 | 1:C:198:VAL:CG2 | 2.29 | 0.62 |
| 1:C:117:VAL:HG21 | 1:C:371:LEU:HG | 1.80 | 0.62 |
| 1:F:217:ARG:HG3 | 1:F:262:TYR:CE2 | 2.34 | 0.62 |
| 1:I:329:LYS:H | 1:I:329:LYS:HD3 | 1.63 | 0.62 |
| 1:K:371:LEU:HD22 | 1:K:482:TYR:CE2 | 2.33 | 0.62 |
| 1:B:34:THR:HG23 | 1:B:35:ARG:NH2 | 2.13 | 0.62 |
| 1:B:342:LYS:HA | 1:B:365:ILE:HD12 | 1.81 | 0.62 |
| 1:B:453:LEU:O | 1:B:453:LEU:HD22 | 1.99 | 0.62 |
| 1:C:176:MET:CE | 1:C:176:MET:HA | 2.30 | 0.62 |
| 1:D:238:MET:HE2 | 1:D:238:MET:HA | 1.80 | 0.62 |
| 1:D:398:THR:O | 1:D:400:LYS:N | 2.32 | 0.62 |
| 1:G:414:GLN:OE1 | 1:G:428:ILE:HA | 1.99 | 0.62 |
| 1:H:260:MET:CE | 1:H:288:PRO:HA | 2.28 | 0.62 |
| 1:L:321:ILE:HG22 | 1:L:343:ILE:HG22 | 1.80 | 0.62 |
| 1:B:280:ILE:HG22 | 1:B:281:TRP:N | 2.14 | 0.62 |
| 1:B:53:LYS:O | 1:B:82:HIS:HE1 | 1.82 | 0.62 |
| 1:F:313:SER:HB2 | 1:F:315:LEU:HD13 | 1.80 | 0.62 |
| 1:F:360:PHE:HB3 | 1:F:365:ILE:HB | 1.79 | 0.62 |
| 1:F:403:ARG:HH21 | 1:G:242:PHE:HD1 | 1.45 | 0.62 |
| 1:F:437:GLN:HG2 | 1:G:244:ASP:HB2 | 1.80 | 0.62 |
| 1:G:280:ILE:CG2 | 1:G:307:ALA:HB1 | 2.29 | 0.62 |
| 1:H:280:ILE:HD11 | 1:H:301:ILE:O | 2.00 | 0.62 |
| 1:H:24:VAL:O | 1:H:28:LEU:HB2 | 1.97 | 0.62 |
| 1:J:281:TRP:HZ3 | 1:J:317:ALA:HB1 | 1.64 | 0.62 |
| 1:K:500:PHE:HE1 | 1:L:500:PHE:HZ | 1.46 | 0.62 |
| 1:D:371:LEU:HD22 | 1:D:482:TYR:CE2 | 2.34 | 0.62 |
| 1:E:75:ILE:HG23 | 1:E:131:ILE:CD1 | 2.30 | 0.62 |
| 1:H:321:ILE:CG2 | 1:H:343:ILE:HB | 2.28 | 0.62 |
| 1:I:9:PHE:HA | 1:I:12:MET:CE | 2.29 | 0.62 |
| 1:J:386:LEU:HA | 1:J:389:LEU:HD12 | 1.80 | 0.62 |
| 1:J:90:LYS:CE | 1:J:199:THR:HG21 | 2.30 | 0.62 |
| 1:K:248:VAL:HG22 | 1:K:272:ALA:H | 1.64 | 0.62 |
| 1:A:335:ASN:HD22 | 1:A:336:ALA:N | 1.98 | 0.62 |
| 1:B:201:LYS:CE | 1:B:388:ASN:HD21 | 2.11 | 0.62 |
| 1:C:65:ILE:HD13 | 1:C:144:ILE:CG1 | 2.22 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:142:GLU:O | 1:E:146:ARG:HG3 | 2.00 | 0.62 |
| 1:F:331:LEU:CB | 1:F:352:THR:HG22 | 2.29 | 0.62 |
| 1:K:95:TYR:OH | 1:K:145:THR:HB | 1.99 | 0.62 |
| 1:K:371:LEU:CD2 | 1:K:481:ALA:HB1 | 2.30 | 0.62 |
| 1:L:275:GLU:HG3 | 1:L:301:ILE:HG12 | 1.81 | 0.62 |
| 1:A:360:PHE:HB3 | 1:A:365:ILE:HB | 1.81 | 0.62 |
| 1:C:414:GLN:CB | 1:C:429:PRO:HD2 | 2.30 | 0.62 |
| 1:C:421:PHE:HE1 | 1:C:423:LYS:HB3 | 1.65 | 0.62 |
| 1:E:47:GLY:O | 1:E:51:ILE:HG13 | 1.99 | 0.62 |
| 1:K:217:ARG:O | 1:K:220:PHE:HB3 | 2.00 | 0.62 |
| 1:K:239:THR:N | 1:K:240:PRO:CD | 2.62 | 0.62 |
| 1:L:203:ILE:HD12 | 1:L:209:HIS:CE1 | 2.34 | 0.62 |
| 1:B:13:VAL:HA | 1:B:16:PHE:CD1 | 2.35 | 0.62 |
| 1:D:476:ASP:O | 1:D:477:LEU:C | 2.38 | 0.62 |
| 1:D:492:VAL:HG21 | 2:D:4:ADP:H2 | 1.63 | 0.62 |
| 1:E:497:GLY:CA | 1:E:501:THR:HA | 2.29 | 0.62 |
| 1:F:104:VAL:CG2 | 1:F:105:LYS:N | 2.62 | 0.62 |
| 1:J:53:LYS:HB3 | 1:J:54:PRO:HD3 | 1.80 | 0.62 |
| 1:K:316:GLU:HG3 | 1:K:338:ARG:O | 1.98 | 0.62 |
| 1:K:467:THR:O | 1:K:467:THR:HG22 | 2.00 | 0.62 |
| 1:L:61:LEU:HD12 | 1:L:63:PHE:HD2 | 1.64 | 0.62 |
| 1:A:24:VAL:O | 1:A:25:GLU:C | 2.38 | 0.62 |
| 1:D:346:GLU:CD | 1:D:478:ARG:HH22 | 2.03 | 0.62 |
| 1:E:371:LEU:HD22 | 1:E:482:TYR:CD2 | 2.34 | 0.62 |
| 1:E:78:TYR:OH | 1:E:130:LYS:NZ | 2.28 | 0.62 |
| 1:E:95:TYR:CE2 | 1:E:129:VAL:HG21 | 2.35 | 0.62 |
| 1:H:131:ILE:CD1 | 1:H:144:ILE:HD13 | 2.30 | 0.62 |
| 1:H:248:VAL:CG2 | 1:H:271:ILE:HG23 | 2.29 | 0.62 |
| 1:H:424:HIS:N | 1:H:424:HIS:ND1 | 2.48 | 0.62 |
| 1:H:58:VAL:HG22 | 1:H:80:ALA:CB | 2.30 | 0.62 |
| 1:I:411:MET:HA | 1:I:430:ILE:HG22 | 1.80 | 0.62 |
| 1:J:368:ILE:CG2 | 1:J:373:LEU:HD13 | 2.30 | 0.62 |
| 1:K:142:GLU:O | 1:K:146:ARG:HG3 | 2.00 | 0.62 |
| 1:L:167:PRO:HG3 | 1:L:176:MET:SD | 2.39 | 0.62 |
| 1:A:201:LYS:CD | 1:A:205:GLN:O | 2.48 | 0.62 |
| 1:A:371:LEU:HD22 | 1:A:482:TYR:CD2 | 2.34 | 0.62 |
| 1:C:112:THR:HB | 1:C:124:GLY:H | 1.65 | 0.62 |
| 1:D:90:LYS:HD2 | 1:D:164:VAL:O | 2.00 | 0.62 |
| 1:E:143:LYS:CE | 1:E:147:ARG:HH21 | 2.12 | 0.62 |
| 1:E:57:HIS:ND1 | 1:E:84:HIS:CE1 | 2.68 | 0.62 |
| 1:J:249:VAL:HB | 1:J:323:ILE:HG23 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:411:MET:SD | 1:J:430:ILE:HG21 | 2.40 | 0.62 |
| 1:K:81:GLN:HG3 | 1:K:157:PHE:HE1 | 1.65 | 0.62 |
| 1:K:380:VAL:O | 1:K:383:PHE:N | 2.33 | 0.62 |
| 1:A:238:MET:O | 1:A:239:THR:HG22 | 2.00 | 0.62 |
| 1:C:203:ILE:HG22 | 2:E:5:ADP:H5'2 | 1.82 | 0.62 |
| 1:C:378:VAL:O | 1:C:381:SER:HB3 | 2.00 | 0.62 |
| 1:F:355:GLU:O | 1:F:359:ILE:HD13 | 2.00 | 0.62 |
| 1:F:421:PHE:CE1 | 1:F:423:LYS:HD3 | 2.35 | 0.62 |
| 1:F:88:PRO:HG2 | 1:F:122:PHE:HD2 | 1.64 | 0.62 |
| 1:G:346:GLU:OE2 | 1:G:352:THR:HG23 | 1.99 | 0.62 |
| 1:H:201:LYS:NZ | 1:H:388:ASN:HD21 | 1.97 | 0.62 |
| 1:I:213:SER:CB | 1:I:217:ARG:HD2 | 2.24 | 0.62 |
| 1:I:477:LEU:O | 1:I:478:ARG:O | 2.18 | 0.62 |
| 1:J:88:PRO:HG2 | 1:J:122:PHE:HD2 | 1.65 | 0.62 |
| 1:K:137:THR:OG1 | 1:K:140:GLU:HG3 | 2.00 | 0.62 |
| 1:K:45:VAL:O | 1:K:48:ILE:HG12 | 2.00 | 0.62 |
| 1:C:30:GLU:O | 1:C:34:THR:HB | 2.00 | 0.61 |
| 1:D:140:GLU:O | 1:D:144:ILE:HD12 | 2.00 | 0.61 |
| 1:D:314:ILE:N | 1:D:314:ILE:HD13 | 2.13 | 0.61 |
| 1:H:370:ASP:OD2 | 1:H:371:LEU:N | 2.32 | 0.61 |
| 1:J:30:GLU:HA | 1:J:34:THR:CG2 | 2.29 | 0.61 |
| 1:J:371:LEU:HD23 | 1:J:481:ALA:HB1 | 1.80 | 0.61 |
| 1:K:219:VAL:CG1 | 1:K:220:PHE:N | 2.62 | 0.61 |
| 1:B:444:SER:OG | 1:B:446:LYS:HG2 | 2.00 | 0.61 |
| 1:C:281:TRP:O | 1:C:282:ASN:HB2 | 2.00 | 0.61 |
| 1:C:223:ILE:HD11 | 1:C:345:ALA:CB | 2.29 | 0.61 |
| 1:I:260:MET:CE | 1:I:288:PRO:HA | 2.30 | 0.61 |
| 1:I:360:PHE:HB3 | 1:I:365:ILE:HB | 1.82 | 0.61 |
| 1:J:281:TRP:CZ3 | 1:J:317:ALA:HB1 | 2.35 | 0.61 |
| 1:K:6:ASP:OD2 | 1:K:6:ASP:C | 2.38 | 0.61 |
| 1:B:332:THR:H | 1:B:335:ASN:HD21 | 1.47 | 0.61 |
| 1:C:142:GLU:HA | 1:C:178:TRP:CZ3 | 2.34 | 0.61 |
| 1:C:461:ALA:HA | 1:C:464:ILE:HD12 | 1.81 | 0.61 |
| 1:C:494:ASN:HD22 | 1:C:494:ASN:C | 2.03 | 0.61 |
| 1:D:117:VAL:HG21 | 1:D:371:LEU:HG | 1.81 | 0.61 |
| 1:E:428:ILE:N | 1:E:428:ILE:HD13 | 2.15 | 0.61 |
| 1:E:86:ARG:HH11 | 1:E:492:VAL:HG21 | 1.64 | 0.61 |
| 1:G:371:LEU:HD23 | 1:G:481:ALA:HB1 | 1.83 | 0.61 |
| 1:K:106:ALA:O | 1:K:109:SER:HB3 | 2.01 | 0.61 |
| 1:L:29:VAL:O | 1:L:30:GLU:O | 2.18 | 0.61 |
| 1:A:201:LYS:NZ | 1:A:388:ASN:ND2 | 2.48 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:186:THR:HG23 | 1:E:186:THR:HG23 | 1.82 | 0.61 |
| 1:B:201:LYS:NZ | 1:B:388:ASN:HD21 | 1.98 | 0.61 |
| 1:C:215:THR:HG23 | 1:C:377:GLY:HA3 | 1.81 | 0.61 |
| 1:D:344:ILE:HG22 | 1:D:344:ILE:O | 1.99 | 0.61 |
| 1:D:90:LYS:HZ3 | 1:D:164:VAL:HG12 | 1.66 | 0.61 |
| 1:D:95:TYR:OH | 1:D:145:THR:HB | 2.00 | 0.61 |
| 1:E:345:ALA:HB1 | 1:E:373:LEU:HD21 | 1.83 | 0.61 |
| 1:E:386:LEU:HB2 | 1:E:394:TYR:OH | 2.00 | 0.61 |
| 1:F:280:ILE:HD11 | 1:F:301:ILE:O | 2.00 | 0.61 |
| 1:I:82:HIS:CD2 | 1:I:112:THR:CG2 | 2.76 | 0.61 |
| 1:I:94:ARG:HG2 | 1:I:94:ARG:HH11 | 1.64 | 0.61 |
| 1:K:142:GLU:HG3 | 1:K:178:TRP:CD2 | 2.34 | 0.61 |
| 1:K:85:GLN:HG3 | 1:K:492:VAL:HG11 | 1.80 | 0.61 |
| 1:L:186:THR:HG22 | 1:L:187:ILE:H | 1.65 | 0.61 |
| 1:A:371:LEU:HD22 | 1:A:482:TYR:CE2 | 2.36 | 0.61 |
| 1:A:436:PHE:CE2 | 1:A:440:ILE:HD11 | 2.36 | 0.61 |
| 1:B:234:SER:O | 1:B:236:LEU:N | 2.33 | 0.61 |
| 1:C:338:ARG:CZ | 1:C:338:ARG:HB3 | 2.30 | 0.61 |
| 1:C:498:VAL:CG2 | 1:C:499:THR:H | 2.10 | 0.61 |
| 1:D:382:TYR:CE2 | 1:D:386:LEU:HD21 | 2.35 | 0.61 |
| 1:E:271:ILE:HD11 | 1:E:283:PRO:HG3 | 1.82 | 0.61 |
| 1:E:389:LEU:HD23 | 1:E:389:LEU:N | 2.15 | 0.61 |
| 1:E:421:PHE:CE1 | 1:E:423:LYS:HG3 | 2.36 | 0.61 |
| 1:E:86:ARG:HH12 | 1:E:492:VAL:HG22 | 1.66 | 0.61 |
| 1:J:88:PRO:HG2 | 1:J:122:PHE:CD2 | 2.35 | 0.61 |
| 1:L:167:PRO:HG3 | 1:L:176:MET:CG | 2.30 | 0.61 |
| 1:L:234:SER:O | 1:L:236:LEU:N | 2.27 | 0.61 |
| 1:L:338:ARG:CZ | 1:L:338:ARG:HB3 | 2.31 | 0.61 |
| 1:A:487:GLU:O | 1:A:490:PHE:HB3 | 2.01 | 0.61 |
| 1:A:53:LYS:HB3 | 1:A:54:PRO:CD | 2.30 | 0.61 |
| 1:B:233:MET:HE2 | 1:B:236:LEU:HD12 | 1.81 | 0.61 |
| 1:C:252:PHE:CE2 | 1:C:260:MET:HE1 | 2.35 | 0.61 |
| 1:D:225:ASN:HD21 | 1:D:458:GLU:HA | 1.65 | 0.61 |
| 1:D:249:VAL:CB | 1:D:323:ILE:HG13 | 2.31 | 0.61 |
| 1:H:104:VAL:CG2 | 1:H:105:LYS:N | 2.63 | 0.61 |
| 1:H:44:ARG:HH11 | 1:H:44:ARG:HB3 | 1.64 | 0.61 |
| 1:J:79:ARG:HG3 | 1:J:127:ALA:HB2 | 1.81 | 0.61 |
| 1:A:403:ARG:HG3 | 1:A:440:ILE:HG21 | 1.83 | 0.61 |
| 1:B:195:HIS:O | 1:B:201:LYS:HE3 | 2.00 | 0.61 |
| 1:B:414:GLN:HB2 | 1:B:429:PRO:HD2 | 1.82 | 0.61 |
| 1:D:141:LEU:O | 1:D:145:THR:HG23 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:411:MET:SD | 1:D:430:ILE:HG21 | 2.41 | 0.61 |
| 1:E:275:GLU:OE2 | 1:E:276:SER:N | 2.33 | 0.61 |
| 1:F:294:PHE:CE1 | 1:F:298:HIS:HE1 | 2.18 | 0.61 |
| 1:H:497:GLY:HA3 | 1:H:501:THR:HA | 1.82 | 0.61 |
| 1:I:137:THR:HG23 | 1:I:140:GLU:HG3 | 1.83 | 0.61 |
| 1:I:213:SER:O | 1:I:217:ARG:HG3 | 2.00 | 0.61 |
| 1:J:331:LEU:CD2 | 1:J:360:PHE:HZ | 2.14 | 0.61 |
| 1:K:371:LEU:HD21 | 1:K:481:ALA:HB1 | 1.83 | 0.61 |
| 1:L:315:LEU:HD12 | 1:L:315:LEU:N | 2.16 | 0.61 |
| 1:C:146:ARG:HH22 | 1:E:501:THR:C | 2.04 | 0.61 |
| 1:C:272:ALA:HB1 | 1:C:314:ILE:HG21 | 1.83 | 0.61 |
| 1:D:131:ILE:HG13 | 1:D:136:TYR:CE2 | 2.36 | 0.61 |
| 1:D:186:THR:CG2 | 1:D:187:ILE:N | 2.60 | 0.61 |
| 1:E:239:THR:N | 1:E:240:PRO:HD3 | 2.14 | 0.61 |
| 1:C:392:VAL:HG22 | 1:E:386:LEU:CD2 | 2.30 | 0.61 |
| 1:A:58:VAL:HG12 | 1:E:60:SER:HB2 | 1.82 | 0.61 |
| 1:E:82:HIS:ND1 | 1:E:82:HIS:C | 2.54 | 0.61 |
| 1:B:469:MET:O | 1:G:308:LYS:HD2 | 2.00 | 0.61 |
| 1:J:346:GLU:HG2 | 1:J:351:PRO:CG | 2.31 | 0.61 |
| 1:J:24:VAL:HG13 | 1:J:483:VAL:HG13 | 1.83 | 0.61 |
| 1:L:274:GLY:HA3 | 1:L:314:ILE:HD12 | 1.82 | 0.61 |
| 1:A:73:GLU:OE1 | 1:A:136:TYR:OH | 2.17 | 0.61 |
| 1:B:332:THR:O | 1:B:336:ALA:HB2 | 2.00 | 0.61 |
| 1:D:132:ASN:HB3 | 1:D:135:ASN:HD22 | 1.65 | 0.61 |
| 1:B:57:HIS:ND1 | 1:D:155:LYS:CE | 2.63 | 0.61 |
| 1:E:143:LYS:NZ | 1:E:147:ARG:NH2 | 2.49 | 0.61 |
| 1:F:34:THR:HG22 | 1:F:34:THR:O | 2.01 | 0.61 |
| 1:H:497:GLY:CA | 1:H:501:THR:HA | 2.31 | 0.61 |
| 1:I:38:GLU:H | 1:I:42:ARG:CZ | 2.14 | 0.61 |
| 1:J:358:LYS:O | 1:J:362:GLU:HG3 | 2.00 | 0.61 |
| 1:J:497:GLY:CA | 1:J:501:THR:HA | 2.31 | 0.61 |
| 1:K:315:LEU:HG | 1:K:331:LEU:HD21 | 1.83 | 0.61 |
| 1:A:346:GLU:CD | 1:A:478:ARG:NH2 | 2.55 | 0.61 |
| 1:B:91:GLY:HA3 | 1:B:125:ALA:O | 2.00 | 0.61 |
| 1:C:432:PRO:HB3 | 1:C:436:PHE:CD1 | 2.35 | 0.61 |
| 1:D:428:ILE:H | 1:D:428:ILE:CD1 | 2.13 | 0.61 |
| 1:E:208:ILE:O | 1:E:208:ILE:HG23 | 2.00 | 0.61 |
| 1:E:334:SER:O | 1:E:337:PRO:HD2 | 2.01 | 0.61 |
| 1:F:90:LYS:HE2 | 1:F:199:THR:HG21 | 1.82 | 0.61 |
| 1:I:14:GLU:CG | 1:I:53:LYS:NZ | 2.64 | 0.61 |
| 1:J:234:SER:O | 1:J:235:ILE:C | 2.39 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:14:GLU:HG3 | 1:J:53:LYS:HE2 | 1.82 | 0.61 |
| 1:L:153:ALA:CA | 1:L:158:ILE:HG22 | 2.31 | 0.61 |
| 1:L:260:MET:CE | 1:L:291:LEU:HD23 | 2.31 | 0.61 |
| 1:C:332:THR:HG22 | 1:C:353:THR:HG21 | 1.81 | 0.60 |
| 1:C:17:PHE:CE1 | 1:C:486:ILE:HD12 | 2.35 | 0.60 |
| 1:C:497:GLY:CA | 1:C:501:THR:HA | 2.31 | 0.60 |
| 1:D:214:ALA:HB1 | 1:D:380:VAL:HG21 | 1.83 | 0.60 |
| 1:D:335:ASN:HD22 | 1:D:335:ASN:N | 1.98 | 0.60 |
| 1:D:79:ARG:HD2 | 1:D:127:ALA:HB2 | 1.82 | 0.60 |
| 1:F:324:PRO:HD2 | 1:F:345:ALA:O | 2.01 | 0.60 |
| 1:B:439:ARG:NH2 | 1:F:405:SER:OG | 2.32 | 0.60 |
| 1:G:72:TRP:HE1 | 1:K:498:VAL:HG11 | 1.66 | 0.60 |
| 1:G:79:ARG:HG2 | 1:G:157:PHE:HB3 | 1.83 | 0.60 |
| 1:H:423:LYS:HE2 | 1:H:423:LYS:HA | 1.83 | 0.60 |
| 1:H:44:ARG:NH1 | 1:H:44:ARG:HB3 | 2.16 | 0.60 |
| 1:H:468:ALA:HA | 1:H:473:LEU:CD1 | 2.31 | 0.60 |
| 1:K:497:GLY:HA3 | 1:K:501:THR:HA | 1.83 | 0.60 |
| 1:B:342:LYS:HA | 1:B:365:ILE:CD1 | 2.31 | 0.60 |
| 1:C:374:ASN:CG | 1:C:374:ASN:O | 2.39 | 0.60 |
| 1:F:9:PHE:CD1 | 1:F:10:PHE:N | 2.69 | 0.60 |
| 1:F:372:TYR:OH | 1:F:461:ALA:HB2 | 2.01 | 0.60 |
| 1:F:83:SER:OG | 1:F:85:GLN:NE2 | 2.35 | 0.60 |
| 1:H:214:ALA:HB1 | 1:H:380:VAL:HG21 | 1.81 | 0.60 |
| 1:H:379:THR:HG21 | 1:H:453:LEU:HD23 | 1.82 | 0.60 |
| 1:I:201:LYS:HB2 | 1:I:202:PRO:CD | 2.31 | 0.60 |
| 1:J:233:MET:HE2 | 1:J:233:MET:HA | 1.83 | 0.60 |
| 1:L:90:LYS:HB2 | 1:L:122:PHE:HD1 | 1.65 | 0.60 |
| 1:A:281:TRP:CD1 | 1:A:283:PRO:HD3 | 2.36 | 0.60 |
| 1:C:355:GLU:O | 1:C:359:ILE:HD12 | 2.01 | 0.60 |
| 1:C:226:PHE:HB3 | 1:C:366:MET:HE1 | 1.83 | 0.60 |
| 1:C:497:GLY:O | 1:C:498:VAL:HG13 | 2.01 | 0.60 |
| 1:G:117:VAL:HG11 | 1:G:372:TYR:HB2 | 1.83 | 0.60 |
| 1:H:439:ARG:HH12 | 1:L:405:SER:CA | 2.14 | 0.60 |
| 1:I:205:GLN:NE2 | 1:K:495:GLU:HB2 | 2.17 | 0.60 |
| 1:I:42:ARG:C | 1:I:44:ARG:H | 2.04 | 0.60 |
| 1:I:87:THR:HB | 1:I:88:PRO:HD3 | 1.83 | 0.60 |
| 1:I:9:PHE:HD1 | 1:I:10:PHE:N | 1.98 | 0.60 |
| 1:A:114:LYS:O | 1:A:117:VAL:HB | 2.01 | 0.60 |
| 1:D:346:GLU:OE1 | 1:D:478:ARG:NH2 | 2.35 | 0.60 |
| 1:A:499:THR:OG1 | 1:E:147:ARG:CD | 2.49 | 0.60 |
| 1:G:404:ASP:O | 1:G:405:SER:C | 2.39 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:436:PHE:O | 1:G:439:ARG:HB3 | 2.00 | 0.60 |
| 1:G:9:PHE:HD1 | 1:G:10:PHE:H | 1.48 | 0.60 |
| 1:K:107:LEU:CA | 1:K:110:LEU:HD13 | 2.28 | 0.60 |
| 1:K:153:ALA:HA | 1:K:158:ILE:CG2 | 2.32 | 0.60 |
| 1:K:497:GLY:CA | 1:K:501:THR:HA | 2.31 | 0.60 |
| 1:A:384:GLU:O | 1:A:385:TRP:C | 2.39 | 0.60 |
| 1:D:78:TYR:HE1 | 1:D:99:VAL:HG21 | 1.66 | 0.60 |
| 1:E:274:GLY:HA3 | 1:E:314:ILE:HD12 | 1.82 | 0.60 |
| 1:F:497:GLY:HA3 | 1:F:501:THR:HA | 1.83 | 0.60 |
| 1:G:44:ARG:HD2 | 1:K:71:SER:HA | 1.84 | 0.60 |
| 1:G:471:TYR:O | 1:G:473:LEU:N | 2.34 | 0.60 |
| 1:H:379:THR:O | 1:H:382:TYR:HB3 | 2.01 | 0.60 |
| 1:I:484:ASN:HD21 | 1:I:488:LYS:HE3 | 1.66 | 0.60 |
| 1:J:239:THR:CG2 | 1:J:239:THR:O | 2.49 | 0.60 |
| 1:K:113:TYR:O | 1:K:117:VAL:HG23 | 2.01 | 0.60 |
| 1:K:17:PHE:CE1 | 1:K:486:ILE:HD12 | 2.36 | 0.60 |
| 1:A:52:ILE:HD13 | 1:A:489:VAL:CG1 | 2.30 | 0.60 |
| 1:A:84:HIS:HD2 | 1:A:89:CYS:SG | 2.25 | 0.60 |
| 1:B:224:GLU:HA | 1:B:227:ILE:HG22 | 1.84 | 0.60 |
| 1:B:247:PHE:HZ | 1:B:260:MET:HG3 | 1.67 | 0.60 |
| 1:C:113:TYR:O | 1:C:117:VAL:HG23 | 2.01 | 0.60 |
| 1:D:322:LEU:O | 1:D:324:PRO:HD3 | 2.02 | 0.60 |
| 1:E:224:GLU:O | 1:E:227:ILE:HG22 | 2.01 | 0.60 |
| 1:H:294:PHE:CG | 1:H:298:HIS:NE2 | 2.64 | 0.60 |
| 1:H:321:ILE:HG22 | 1:H:343:ILE:CB | 2.31 | 0.60 |
| 1:I:118:VAL:HA | 1:I:460:SER:OG | 2.02 | 0.60 |
| 1:I:382:TYR:OH | 1:J:392:VAL:HG22 | 2.00 | 0.60 |
| 1:G:60:SER:HB2 | 1:K:58:VAL:HG13 | 1.81 | 0.60 |
| 1:L:234:SER:O | 1:L:237:GLY:N | 2.34 | 0.60 |
| 1:D:144:ILE:HG22 | 1:D:145:THR:N | 2.16 | 0.60 |
| 1:G:142:GLU:O | 1:G:146:ARG:HG3 | 2.02 | 0.60 |
| 1:G:407:TYR:O | 1:G:411:MET:HB2 | 2.01 | 0.60 |
| 1:H:429:PRO:O | 1:H:431:VAL:HG12 | 2.01 | 0.60 |
| 1:I:390:ASN:O | 1:I:391:HIS:HB2 | 2.01 | 0.60 |
| 1:I:427:THR:O | 1:I:428:ILE:HD13 | 2.01 | 0.60 |
| 1:I:399:PHE:CE2 | 1:I:448:ILE:HD11 | 2.37 | 0.60 |
| 1:L:130:LYS:O | 1:L:131:ILE:HD12 | 2.01 | 0.60 |
| 1:L:260:MET:HE3 | 1:L:291:LEU:HD23 | 1.82 | 0.60 |
| 1:B:331:LEU:CD1 | 1:B:360:PHE:HZ | 2.13 | 0.60 |
| 1:C:287:ASP:OD2 | 1:C:289:LYS:HB3 | 2.02 | 0.60 |
| 1:E:433:THR:HG23 | 1:E:436:PHE:H | 1.65 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:382:TYR:O | 1:G:385:TRP:HB3 | 2.02 | 0.60 |
| 1:G:409:LEU:HD13 | 1:L:436:PHE:HE1 | 1.64 | 0.60 |
| 1:H:248:VAL:CG1 | 1:H:272:ALA:HB3 | 2.31 | 0.60 |
| 1:I:339:VAL:HG21 | 1:I:360:PHE:CE1 | 2.36 | 0.60 |
| 1:J:58:VAL:HG23 | 1:J:80:ALA:CB | 2.32 | 0.60 |
| 1:A:201:LYS:HZ2 | 1:A:388:ASN:HD21 | 1.49 | 0.60 |
| 1:B:359:ILE:CG2 | 1:B:360:PHE:N | 2.64 | 0.60 |
| 1:B:359:ILE:HG22 | 1:B:360:PHE:H | 1.67 | 0.60 |
| 1:D:8:ASN:ND2 | 1:D:10:PHE:HB3 | 2.17 | 0.60 |
| 1:B:501:THR:C | 1:F:146:ARG:HH12 | 2.04 | 0.60 |
| 1:F:429:PRO:C | 1:F:431:VAL:H | 2.03 | 0.60 |
| 1:G:293:ASP:O | 1:G:294:PHE:C | 2.40 | 0.60 |
| 1:I:167:PRO:CG | 1:I:176:MET:SD | 2.87 | 0.60 |
| 1:I:313:SER:HB2 | 1:I:315:LEU:CD1 | 2.30 | 0.60 |
| 1:K:176:MET:CE | 1:K:179:ILE:HD12 | 2.31 | 0.60 |
| 1:C:9:PHE:CD1 | 1:C:10:PHE:N | 2.68 | 0.60 |
| 1:D:336:ALA:HB3 | 1:D:337:PRO:CD | 2.24 | 0.60 |
| 1:J:337:PRO:C | 1:J:363:ARG:HH21 | 2.05 | 0.60 |
| 1:J:371:LEU:HD23 | 1:J:481:ALA:CB | 2.32 | 0.60 |
| 1:K:478:ARG:O | 1:K:481:ALA:HB3 | 2.02 | 0.60 |
| 1:K:53:LYS:HB3 | 1:K:54:PRO:CD | 2.29 | 0.60 |
| 1:A:331:LEU:HB2 | 1:A:352:THR:HG22 | 1.84 | 0.59 |
| 1:A:394:TYR:HB2 | 1:A:445:GLU:HG3 | 1.84 | 0.59 |
| 1:C:114:LYS:HE2 | 1:C:374:ASN:HD21 | 1.65 | 0.59 |
| 1:C:59:LEU:HB2 | 1:C:157:PHE:CE2 | 2.37 | 0.59 |
| 1:F:141:LEU:O | 1:F:145:THR:HG23 | 2.01 | 0.59 |
| 1:H:176:MET:CE | 1:H:179:ILE:HG13 | 2.32 | 0.59 |
| 1:I:353:THR:HB | 1:I:354:PRO:CD | 2.32 | 0.59 |
| 1:I:399:PHE:HB2 | 1:K:455:TYR:CE2 | 2.37 | 0.59 |
| 1:H:155:LYS:HD2 | 1:J:157:PHE:CE2 | 2.37 | 0.59 |
| 1:J:239:THR:O | 1:J:239:THR:HG23 | 2.00 | 0.59 |
| 1:J:421:PHE:CD1 | 1:J:423:LYS:HB2 | 2.37 | 0.59 |
| 1:K:398:THR:O | 1:K:399:PHE:C | 2.39 | 0.59 |
| 1:K:94:ARG:HG2 | 1:K:94:ARG:HH11 | 1.66 | 0.59 |
| 1:L:244:ASP:O | 1:L:245:LYS:HG3 | 2.02 | 0.59 |
| 1:A:271:ILE:HD11 | 1:A:283:PRO:HG3 | 1.83 | 0.59 |
| 1:A:332:THR:HA | 1:A:353:THR:HG22 | 1.83 | 0.59 |
| 1:B:234:SER:O | 1:B:237:GLY:N | 2.35 | 0.59 |
| 1:B:87:THR:OG1 | 1:B:88:PRO:HD2 | 2.01 | 0.59 |
| 1:C:338:ARG:O | 1:C:339:VAL:HG13 | 2.02 | 0.59 |
| 1:E:219:VAL:HG11 | 1:E:259:SER:OG | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:414:GLN:CB | 1:F:429:PRO:HD2 | 2.32 | 0.59 |
| 1:F:59:LEU:HD21 | 1:F:61:LEU:CD2 | 2.31 | 0.59 |
| 1:G:197:CYS:SG | 1:G:198:VAL:HG12 | 2.42 | 0.59 |
| 1:G:222:GLY:HA3 | 1:G:373:LEU:HD12 | 1.84 | 0.59 |
| 1:C:19:ARG:HG3 | 1:C:19:ARG:HH11 | 1.66 | 0.59 |
| 1:C:271:ILE:O | 1:C:272:ALA:CB | 2.50 | 0.59 |
| 1:C:322:LEU:C | 1:C:322:LEU:HD13 | 2.23 | 0.59 |
| 1:C:328:GLU:O | 1:C:329:LYS:HG2 | 2.02 | 0.59 |
| 1:C:75:ILE:CD1 | 1:C:75:ILE:N | 2.65 | 0.59 |
| 1:D:335:ASN:ND2 | 1:D:335:ASN:N | 2.50 | 0.59 |
| 1:E:87:THR:HB | 1:E:88:PRO:CD | 2.32 | 0.59 |
| 1:H:414:GLN:OE1 | 1:H:428:ILE:HA | 2.01 | 0.59 |
| 1:I:484:ASN:HD21 | 1:I:488:LYS:CE | 2.14 | 0.59 |
| 1:K:252:PHE:O | 1:K:253:GLY:O | 2.20 | 0.59 |
| 1:L:8:ASN:O | 1:L:9:PHE:C | 2.40 | 0.59 |
| 1:C:281:TRP:CH2 | 1:C:283:PRO:HG3 | 2.36 | 0.59 |
| 1:C:367:VAL:O | 1:C:477:LEU:HB2 | 2.01 | 0.59 |
| 1:C:498:VAL:N | 1:C:501:THR:HB | 2.17 | 0.59 |
| 1:D:97:THR:C | 1:D:130:LYS:HE3 | 2.22 | 0.59 |
| 1:D:344:ILE:HB | 1:D:367:VAL:HG22 | 1.84 | 0.59 |
| 1:F:19:ARG:NH1 | 1:F:19:ARG:HG3 | 2.16 | 0.59 |
| 1:H:38:GLU:C | 1:H:39:GLU:HG3 | 2.23 | 0.59 |
| 1:I:202:PRO:O | 1:I:205:GLN:N | 2.31 | 0.59 |
| 1:K:330:GLN:C | 1:K:331:LEU:HD23 | 2.22 | 0.59 |
| 1:L:100:SER:O | 1:L:101:VAL:C | 2.39 | 0.59 |
| 1:C:360:PHE:HD1 | 1:C:365:ILE:CG1 | 2.10 | 0.59 |
| 1:D:118:VAL:HG23 | 1:D:120:VAL:HG23 | 1.85 | 0.59 |
| 1:D:67:ARG:NH1 | 1:D:140:GLU:OE2 | 2.35 | 0.59 |
| 1:G:414:GLN:HB2 | 1:G:429:PRO:HD2 | 1.84 | 0.59 |
| 1:I:213:SER:HB2 | 1:I:217:ARG:CD | 2.23 | 0.59 |
| 1:J:436:PHE:CE1 | 1:J:440:ILE:HD11 | 2.37 | 0.59 |
| 1:K:9:PHE:CE1 | 1:K:103:GLU:HA | 2.36 | 0.59 |
| 1:K:323:ILE:CG2 | 1:K:345:ALA:HB3 | 2.31 | 0.59 |
| 1:K:81:GLN:HG3 | 1:K:157:PHE:CE1 | 2.38 | 0.59 |
| 1:C:72:TRP:HE1 | 1:F:498:VAL:HG11 | 1.67 | 0.59 |
| 1:I:101:VAL:CG1 | 1:I:105:LYS:HE3 | 2.32 | 0.59 |
| 1:J:244:ASP:C | 1:J:245:LYS:HG3 | 2.22 | 0.59 |
| 1:A:437:GLN:HE22 | 1:H:426:GLY:HA2 | 1.68 | 0.59 |
| 1:B:239:THR:O | 1:B:239:THR:HG23 | 2.02 | 0.59 |
| 1:C:453:LEU:O | 1:C:457:MET:HG2 | 2.02 | 0.59 |
| 1:C:498:VAL:HG21 | 1:F:72:TRP:HE1 | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:501:THR:O | 1:D:146:ARG:NH2 | 2.34 | 0.59 |
| 1:D:497:GLY:HA3 | 1:D:501:THR:HA | 1.84 | 0.59 |
| 1:E:446:LYS:HG3 | 1:E:450:HIS:CE1 | 2.37 | 0.59 |
| 1:E:87:THR:HB | 1:E:88:PRO:HD3 | 1.84 | 0.59 |
| 1:H:335:ASN:HD22 | 1:H:335:ASN:N | 2.00 | 0.59 |
| 1:H:462:ARG:HB3 | 1:H:466:ARG:HH12 | 1.66 | 0.59 |
| 1:I:281:TRP:CD1 | 1:I:282:ASN:N | 2.69 | 0.59 |
| 1:I:321:ILE:N | 1:I:321:ILE:HD12 | 2.17 | 0.59 |
| 1:I:249:VAL:HG23 | 1:I:323:ILE:HG13 | 1.84 | 0.59 |
| 1:I:330:GLN:HA | 1:I:330:GLN:OE1 | 2.01 | 0.59 |
| 1:I:318:ASP:HA | 1:I:340:LYS:HG3 | 1.85 | 0.59 |
| 1:I:34:THR:O | 1:I:35:ARG:HG3 | 2.02 | 0.59 |
| 1:I:17:PHE:CE2 | 1:I:53:LYS:HB2 | 2.38 | 0.59 |
| 1:J:498:VAL:HG23 | 1:J:499:THR:H | 1.68 | 0.59 |
| 1:L:429:PRO:O | 1:L:431:VAL:N | 2.35 | 0.59 |
| 1:L:47:GLY:O | 1:L:51:ILE:HG13 | 2.03 | 0.59 |
| 1:B:369:PRO:CG | 1:B:478:ARG:HA | 2.32 | 0.59 |
| 1:C:277:ASP:HB3 | 1:C:302:LEU:HD11 | 1.83 | 0.59 |
| 1:F:322:LEU:HD22 | 1:F:322:LEU:C | 2.23 | 0.59 |
| 1:F:322:LEU:HD22 | 1:F:323:ILE:N | 2.17 | 0.59 |
| 1:F:411:MET:SD | 1:F:430:ILE:HG21 | 2.43 | 0.59 |
| 1:F:453:LEU:O | 1:F:453:LEU:HD22 | 2.03 | 0.59 |
| 1:H:411:MET:HA | 1:H:430:ILE:HG22 | 1.84 | 0.59 |
| 1:J:195:HIS:O | 1:J:201:LYS:HE2 | 2.03 | 0.59 |
| 1:G:500:PHE:CZ | 1:J:500:PHE:HZ | 2.20 | 0.59 |
| 1:J:65:ILE:HD13 | 1:J:144:ILE:CG1 | 2.33 | 0.59 |
| 1:K:175:GLU:O | 1:K:178:TRP:N | 2.35 | 0.59 |
| 1:K:371:LEU:HD22 | 1:K:482:TYR:CD2 | 2.37 | 0.59 |
| 1:L:234:SER:C | 1:L:236:LEU:H | 2.04 | 0.59 |
| 1:L:396:ARG:O | 1:L:396:ARG:HD3 | 2.03 | 0.59 |
| 1:A:36:GLU:OE1 | 1:A:42:ARG:NH2 | 2.36 | 0.59 |
| 1:B:142:GLU:OE2 | 1:B:178:TRP:NE1 | 2.34 | 0.59 |
| 1:B:274:GLY:HA2 | 1:B:279:SER:HA | 1.84 | 0.59 |
| 1:B:33:ARG:NH1 | 1:B:33:ARG:CB | 2.59 | 0.59 |
| 1:D:259:SER:O | 1:D:263:LEU:HB2 | 2.03 | 0.59 |
| 1:D:489:VAL:O | 1:D:489:VAL:HG12 | 2.03 | 0.59 |
| 1:E:414:GLN:O | 1:E:418:GLU:HG3 | 2.03 | 0.59 |
| 1:H:69:ASP:OD1 | 1:H:71:SER:N | 2.30 | 0.59 |
| 1:I:94:ARG:HG2 | 1:I:94:ARG:NH1 | 2.17 | 0.59 |
| 1:K:38:GLU:HG2 | 1:K:42:ARG:NH2 | 2.18 | 0.59 |
| 1:I:405:SER:OG | 1:K:439:ARG:NH2 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:161:GLY:C | 1:B:162:ILE:HD12 | 2.22 | 0.59 |
| 1:C:286:ILE:N | 1:C:286:ILE:HD12 | 2.18 | 0.59 |
| 1:D:360:PHE:CD1 | 1:D:365:ILE:HG21 | 2.36 | 0.59 |
| 1:E:227:ILE:HD12 | 1:E:233:MET:HE3 | 1.85 | 0.59 |
| 1:B:436:PHE:CZ | 1:F:409:LEU:HD22 | 2.38 | 0.59 |
| 1:G:201:LYS:HB2 | 1:G:202:PRO:HD2 | 1.85 | 0.59 |
| 1:H:332:THR:CG2 | 1:H:353:THR:HG21 | 2.22 | 0.59 |
| 1:I:433:THR:HG22 | 1:J:412:SER:HA | 1.85 | 0.59 |
| 1:L:497:GLY:CA | 1:L:501:THR:HA | 2.33 | 0.59 |
| 1:B:227:ILE:HD13 | 1:B:343:ILE:CD1 | 2.32 | 0.58 |
| 1:D:138:ASP:O | 1:D:141:LEU:HB2 | 2.03 | 0.58 |
| 1:D:237:GLY:O | 1:D:238:MET:HE3 | 2.03 | 0.58 |
| 1:E:346:GLU:HG2 | 1:E:351:PRO:CG | 2.32 | 0.58 |
| 1:E:439:ARG:HG2 | 1:E:439:ARG:O | 2.03 | 0.58 |
| 1:H:468:ALA:HA | 1:H:473:LEU:HD13 | 1.84 | 0.58 |
| 1:I:158:ILE:HG23 | 1:I:158:ILE:O | 2.04 | 0.58 |
| 1:I:176:MET:HE3 | 1:I:179:ILE:HD12 | 1.84 | 0.58 |
| 1:L:429:PRO:C | 1:L:431:VAL:H | 2.07 | 0.58 |
| 1:A:496:ALA:C | 1:A:501:THR:C | 2.62 | 0.58 |
| 1:B:90:LYS:NZ | 1:B:164:VAL:O | 2.34 | 0.58 |
| 1:C:114:LYS:CE | 1:C:374:ASN:HD21 | 2.17 | 0.58 |
| 1:E:250:GLN:HG3 | 1:E:315:LEU:CD1 | 2.33 | 0.58 |
| 1:E:336:ALA:O | 1:E:339:VAL:HG22 | 2.03 | 0.58 |
| 1:F:259:SER:O | 1:F:263:LEU:HB2 | 2.03 | 0.58 |
| 1:H:33:ARG:HB2 | 1:H:36:GLU:OE2 | 2.02 | 0.58 |
| 1:H:376:GLY:O | 1:H:380:VAL:HG23 | 2.03 | 0.58 |
| 1:J:281:TRP:O | 1:J:282:ASN:HB2 | 2.03 | 0.58 |
| 1:J:401:TYR:O | 1:J:404:ASP:HB2 | 2.03 | 0.58 |
| 1:A:281:TRP:HD1 | 1:A:282:ASN:N | 2.01 | 0.58 |
| 1:C:314:ILE:N | 1:C:314:ILE:CD1 | 2.54 | 0.58 |
| 1:C:316:GLU:HG3 | 1:C:338:ARG:NH2 | 2.15 | 0.58 |
| 1:C:328:GLU:C | 1:C:329:LYS:HG2 | 2.23 | 0.58 |
| 1:C:93:ILE:HD11 | 1:C:165:PRO:CB | 2.31 | 0.58 |
| 1:G:131:ILE:HG12 | 1:G:136:TYR:CE2 | 2.39 | 0.58 |
| 1:G:305:PRO:O | 1:G:307:ALA:N | 2.36 | 0.58 |
| 1:H:165:PRO:O | 1:H:198:VAL:HG23 | 2.03 | 0.58 |
| 1:I:244:ASP:C | 1:I:245:LYS:HG3 | 2.23 | 0.58 |
| 1:I:219:VAL:CA | 1:I:373:LEU:HD21 | 2.31 | 0.58 |
| 1:K:12:MET:O | 1:K:16:PHE:HD1 | 1.86 | 0.58 |
| 1:K:147:ARG:HG3 | 1:K:147:ARG:HH11 | 1.66 | 0.58 |
| 1:K:336:ALA:HB3 | 1:K:337:PRO:HD3 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:313:SER:CB | 1:L:315:LEU:HD13 | 2.28 | 0.58 |
| 1:L:356:ALA:O | 1:L:360:PHE:HD2 | 1.86 | 0.58 |
| 1:A:437:GLN:CD | 1:H:423:LYS:HG2 | 2.23 | 0.58 |
| 1:C:24:VAL:O | 1:C:25:GLU:C | 2.42 | 0.58 |
| 1:I:271:ILE:HG13 | 1:I:283:PRO:HA | 1.84 | 0.58 |
| 1:J:142:GLU:HG2 | 1:J:146:ARG:HD2 | 1.85 | 0.58 |
| 1:J:81:GLN:OE1 | 1:J:84:HIS:HE1 | 1.86 | 0.58 |
| 1:K:467:THR:CG2 | 1:K:467:THR:O | 2.51 | 0.58 |
| 1:K:473:LEU:HD13 | 1:K:480:ALA:HB2 | 1.84 | 0.58 |
| 1:K:94:ARG:HG2 | 1:K:94:ARG:NH1 | 2.18 | 0.58 |
| 1:A:289:LYS:HG3 | 1:A:289:LYS:O | 2.04 | 0.58 |
| 1:A:343:ILE:HG12 | 1:A:366:MET:HE2 | 1.85 | 0.58 |
| 1:C:25:GLU:O | 1:C:29:VAL:HG23 | 2.04 | 0.58 |
| 1:C:386:LEU:HD13 | 1:D:392:VAL:HG21 | 1.86 | 0.58 |
| 1:C:396:ARG:CG | 1:C:396:ARG:NH1 | 2.57 | 0.58 |
| 1:D:6:ASP:O | 1:D:6:ASP:OD2 | 2.22 | 0.58 |
| 1:A:498:VAL:HG11 | 1:E:72:TRP:NE1 | 2.19 | 0.58 |
| 1:F:131:ILE:CG1 | 1:F:136:TYR:CE2 | 2.86 | 0.58 |
| 1:F:394:TYR:HB2 | 1:F:445:GLU:HG3 | 1.85 | 0.58 |
| 1:G:461:ALA:O | 1:G:465:MET:HG3 | 2.04 | 0.58 |
| 1:I:38:GLU:HB2 | 1:I:42:ARG:NH2 | 2.18 | 0.58 |
| 1:I:501:THR:OXT | 1:J:146:ARG:NH2 | 2.28 | 0.58 |
| 1:J:173:GLU:HB2 | 1:J:202:PRO:HG3 | 1.85 | 0.58 |
| 1:J:414:GLN:NE2 | 1:J:430:ILE:CG2 | 2.67 | 0.58 |
| 1:J:414:GLN:CD | 1:J:430:ILE:HG12 | 2.24 | 0.58 |
| 1:K:212:ILE:HD12 | 1:K:213:SER:H | 1.69 | 0.58 |
| 1:K:280:ILE:HG22 | 1:K:281:TRP:H | 1.68 | 0.58 |
| 1:K:117:VAL:HG21 | 1:K:371:LEU:HG | 1.84 | 0.58 |
| 1:H:501:THR:C | 1:L:146:ARG:HH22 | 2.06 | 0.58 |
| 1:A:358:LYS:O | 1:A:361:LEU:HB3 | 2.03 | 0.58 |
| 1:C:133:PRO:O | 1:C:135:ASN:N | 2.37 | 0.58 |
| 1:C:40:GLN:O | 1:C:40:GLN:NE2 | 2.32 | 0.58 |
| 1:C:466:ARG:HB2 | 1:C:466:ARG:NH1 | 2.19 | 0.58 |
| 1:D:189:HIS:CE1 | 1:F:154:LYS:HD3 | 2.39 | 0.58 |
| 1:D:498:VAL:HG23 | 1:D:499:THR:N | 2.18 | 0.58 |
| 1:E:460:SER:O | 1:E:463:GLN:HB2 | 2.02 | 0.58 |
| 1:F:331:LEU:HD23 | 1:F:360:PHE:CE2 | 2.39 | 0.58 |
| 1:F:488:LYS:O | 1:F:492:VAL:HG23 | 2.03 | 0.58 |
| 1:G:141:LEU:O | 1:G:145:THR:HG23 | 2.04 | 0.58 |
| 1:G:239:THR:O | 1:G:239:THR:HG23 | 2.03 | 0.58 |
| 1:H:146:ARG:O | 1:H:149:THR:HB | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:294:PHE:CE2 | 1:H:304:PHE:HA | 2.39 | 0.58 |
| 1:H:24:VAL:CG2 | 1:H:483:VAL:HG22 | 2.32 | 0.58 |
| 1:I:212:ILE:HD12 | 1:I:212:ILE:H | 1.68 | 0.58 |
| 1:I:39:GLU:O | 1:I:41:LYS:N | 2.36 | 0.58 |
| 1:K:226:PHE:C | 1:K:228:ASN:H | 2.05 | 0.58 |
| 1:A:411:MET:HG2 | 1:A:430:ILE:HG22 | 1.85 | 0.58 |
| 1:B:24:VAL:HG12 | 1:B:28:LEU:HB2 | 1.85 | 0.58 |
| 1:C:239:THR:HA | 1:C:245:LYS:HZ2 | 1.69 | 0.58 |
| 1:G:359:ILE:HA | 1:G:362:GLU:HG3 | 1.85 | 0.58 |
| 1:I:16:PHE:O | 1:I:19:ARG:HB3 | 2.04 | 0.58 |
| 1:I:370:ASP:N | 1:I:370:ASP:OD2 | 2.36 | 0.58 |
| 1:I:371:LEU:CD2 | 1:I:481:ALA:HB1 | 2.30 | 0.58 |
| 1:L:420:LYS:HZ2 | 1:L:420:LYS:HB3 | 1.69 | 0.58 |
| 1:L:85:GLN:HE21 | 1:L:489:VAL:HA | 1.68 | 0.58 |
| 1:B:314:ILE:HD13 | 1:B:314:ILE:N | 2.19 | 0.58 |
| 1:B:7:PRO:O | 1:B:329:LYS:HD3 | 2.03 | 0.58 |
| 1:D:363:ARG:O | 1:D:365:ILE:HG12 | 2.04 | 0.58 |
| 1:F:160:PRO:HG2 | 1:F:161:GLY:H | 1.69 | 0.58 |
| 1:G:176:MET:HE3 | 1:G:179:ILE:HD12 | 1.84 | 0.58 |
| 1:G:20:GLY:O | 1:G:24:VAL:HG23 | 2.03 | 0.58 |
| 1:G:250:GLN:HE21 | 1:G:314:ILE:HD13 | 1.67 | 0.58 |
| 1:G:339:VAL:HG21 | 1:G:360:PHE:HE1 | 1.69 | 0.58 |
| 1:I:250:GLN:CB | 1:I:314:ILE:HD11 | 2.34 | 0.58 |
| 1:I:48:ILE:HG21 | 1:I:490:PHE:CD1 | 2.38 | 0.58 |
| 1:J:238:MET:O | 1:J:239:THR:C | 2.41 | 0.58 |
| 1:J:79:ARG:HH11 | 1:J:127:ALA:HB2 | 1.69 | 0.58 |
| 1:K:180:ALA:HA | 1:K:197:CYS:SG | 2.44 | 0.58 |
| 1:K:370:ASP:O | 1:K:372:TYR:N | 2.37 | 0.58 |
| 1:K:416:SER:HA | 1:K:419:ARG:CZ | 2.33 | 0.58 |
| 1:L:100:SER:O | 1:L:103:GLU:HB3 | 2.04 | 0.58 |
| 1:L:330:GLN:O | 1:L:331:LEU:HD23 | 2.04 | 0.58 |
| 1:A:248:VAL:O | 1:A:323:ILE:HG12 | 2.04 | 0.58 |
| 1:B:111:MET:O | 1:B:112:THR:C | 2.41 | 0.58 |
| 1:B:291:LEU:HD11 | 1:B:301:ILE:CG2 | 2.32 | 0.58 |
| 1:E:24:VAL:HG12 | 1:E:28:LEU:HB2 | 1.86 | 0.58 |
| 1:E:428:ILE:HG22 | 1:E:430:ILE:HG12 | 1.85 | 0.58 |
| 1:F:248:VAL:CG1 | 1:F:314:ILE:HG13 | 2.33 | 0.58 |
| 1:F:47:GLY:HA2 | 1:F:50:ARG:HH11 | 1.69 | 0.58 |
| 1:G:96:SER:HB3 | 1:G:99:VAL:HG13 | 1.85 | 0.58 |
| 1:I:111:MET:O | 1:I:112:THR:C | 2.42 | 0.58 |
| 1:J:335:ASN:HD22 | 1:J:335:ASN:C | 2.07 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:260:MET:CE | 1:K:288:PRO:HA | 2.24 | 0.58 |
| 1:G:413:VAL:HG22 | 1:L:413:VAL:HG11 | 1.86 | 0.58 |
| 1:A:141:LEU:O | 1:A:145:THR:HG23 | 2.03 | 0.58 |
| 1:A:247:PHE:CB | 1:A:321:ILE:HG22 | 2.29 | 0.58 |
| 1:B:332:THR:HG22 | 1:B:353:THR:HG21 | 1.86 | 0.58 |
| 1:C:47:GLY:HA2 | 1:C:50:ARG:CD | 2.34 | 0.58 |
| 1:D:258:HIS:O | 1:D:262:TYR:HD2 | 1.86 | 0.58 |
| 1:E:327:SER:HB2 | 1:E:330:GLN:OE1 | 2.03 | 0.58 |
| 1:C:64:PRO:CB | 1:F:51:ILE:HD11 | 2.33 | 0.58 |
| 1:G:65:ILE:CD1 | 1:G:75:ILE:HD11 | 2.33 | 0.58 |
| 1:J:482:TYR:O | 1:J:486:ILE:HG12 | 2.04 | 0.58 |
| 1:K:346:GLU:HG2 | 1:K:351:PRO:HG3 | 1.85 | 0.58 |
| 1:C:414:GLN:HE22 | 1:C:430:ILE:HD13 | 1.67 | 0.57 |
| 1:G:232:TYR:HD1 | 1:G:232:TYR:N | 2.02 | 0.57 |
| 1:H:291:LEU:HD11 | 1:H:301:ILE:HG22 | 1.86 | 0.57 |
| 1:H:380:VAL:HG13 | 1:H:449:VAL:CG1 | 2.34 | 0.57 |
| 1:J:192:ILE:CG1 | 1:J:192:ILE:O | 2.51 | 0.57 |
| 1:J:343:ILE:HD11 | 1:J:366:MET:CE | 2.34 | 0.57 |
| 1:J:58:VAL:HG23 | 1:J:80:ALA:HB2 | 1.85 | 0.57 |
| 1:K:482:TYR:O | 1:K:486:ILE:HG12 | 2.03 | 0.57 |
| 1:L:114:LYS:NZ | 1:L:374:ASN:HD22 | 2.03 | 0.57 |
| 1:L:222:GLY:HA3 | 1:L:373:LEU:CD1 | 2.34 | 0.57 |
| 1:L:359:ILE:O | 1:L:363:ARG:HG2 | 2.03 | 0.57 |
| 1:L:85:GLN:NE2 | 1:L:489:VAL:HA | 2.18 | 0.57 |
| 1:A:55:CYS:SG | 1:A:105:LYS:CG | 2.90 | 0.57 |
| 1:B:321:ILE:HG23 | 1:B:343:ILE:HB | 1.86 | 0.57 |
| 1:E:184:ALA:O | 1:E:189:HIS:HA | 2.04 | 0.57 |
| 1:E:19:ARG:NH1 | 1:E:479:THR:HG21 | 2.18 | 0.57 |
| 1:E:6:ASP:N | 1:E:7:PRO:CD | 2.67 | 0.57 |
| 1:I:247:PHE:CZ | 1:I:270:CYS:HB2 | 2.38 | 0.57 |
| 1:K:12:MET:O | 1:K:16:PHE:CD1 | 2.57 | 0.57 |
| 1:K:158:ILE:HD12 | 1:K:165:PRO:HD2 | 1.86 | 0.57 |
| 1:K:248:VAL:CG1 | 1:K:272:ALA:HB3 | 2.34 | 0.57 |
| 1:L:103:GLU:HG2 | 1:L:104:VAL:N | 2.16 | 0.57 |
| 1:L:229:GLU:O | 1:L:230:ALA:C | 2.41 | 0.57 |
| 1:I:45:VAL:HG23 | 1:L:72:TRP:CZ3 | 2.38 | 0.57 |
| 1:C:112:THR:HG22 | 1:C:124:GLY:HA3 | 1.85 | 0.57 |
| 1:F:113:TYR:O | 1:F:117:VAL:HG23 | 2.03 | 0.57 |
| 1:F:164:VAL:HG13 | 1:F:198:VAL:HA | 1.86 | 0.57 |
| 1:H:28:LEU:HA | 1:H:32:LEU:HD12 | 1.85 | 0.57 |
| 1:I:497:GLY:CA | 1:I:501:THR:HA | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:379:THR:CG2 | 1:K:456:THR:HG21 | 2.34 | 0.57 |
| 1:A:192:ILE:HG12 | 1:A:192:ILE:O | 2.03 | 0.57 |
| 1:C:370:ASP:O | 1:C:372:TYR:N | 2.37 | 0.57 |
| 1:C:225:ASN:ND2 | 1:C:458:GLU:HA | 2.19 | 0.57 |
| 1:D:30:GLU:O | 1:D:31:ASP:HB2 | 2.04 | 0.57 |
| 1:G:264:HIS:C | 1:G:266:PHE:H | 2.07 | 0.57 |
| 1:G:295:LYS:HD3 | 1:G:301:ILE:HG22 | 1.85 | 0.57 |
| 1:H:17:PHE:CE2 | 1:H:53:LYS:HB2 | 2.39 | 0.57 |
| 1:I:56:ASN:C | 1:I:57:HIS:HD1 | 2.07 | 0.57 |
| 1:J:182:THR:O | 1:J:186:THR:OG1 | 2.17 | 0.57 |
| 1:K:137:THR:HG23 | 1:K:140:GLU:CD | 2.24 | 0.57 |
| 1:K:416:SER:HA | 1:K:419:ARG:NH2 | 2.19 | 0.57 |
| 1:L:257:LEU:HD12 | 1:L:257:LEU:C | 2.24 | 0.57 |
| 1:L:356:ALA:O | 1:L:360:PHE:CD2 | 2.58 | 0.57 |
| 1:L:420:LYS:HB3 | 1:L:420:LYS:NZ | 2.18 | 0.57 |
| 1:A:332:THR:N | 1:A:335:ASN:HD21 | 2.01 | 0.57 |
| 1:C:104:VAL:CG2 | 1:C:105:LYS:N | 2.68 | 0.57 |
| 1:C:140:GLU:O | 1:C:144:ILE:HG13 | 2.04 | 0.57 |
| 1:C:164:VAL:HG13 | 1:C:198:VAL:HA | 1.85 | 0.57 |
| 1:D:57:HIS:CD2 | 1:D:84:HIS:NE2 | 2.69 | 0.57 |
| 1:E:346:GLU:CD | 1:E:478:ARG:HH22 | 2.07 | 0.57 |
| 1:E:359:ILE:HG22 | 1:E:360:PHE:N | 2.20 | 0.57 |
| 1:F:264:HIS:CD2 | 1:F:288:PRO:HD3 | 2.40 | 0.57 |
| 1:F:436:PHE:O | 1:F:439:ARG:HB3 | 2.03 | 0.57 |
| 1:G:214:ALA:CB | 1:G:380:VAL:HG21 | 2.34 | 0.57 |
| 1:H:248:VAL:HG13 | 1:H:272:ALA:HB3 | 1.85 | 0.57 |
| 1:H:277:ASP:CB | 1:H:302:LEU:HD11 | 2.34 | 0.57 |
| 1:I:164:VAL:HG13 | 1:I:198:VAL:HA | 1.86 | 0.57 |
| 1:I:495:GLU:O | 1:I:496:ALA:HB2 | 2.04 | 0.57 |
| 2:I:502:ADP:H5'2 | 1:J:203:ILE:CG2 | 2.35 | 0.57 |
| 1:A:332:THR:HA | 1:A:353:THR:HG21 | 1.85 | 0.57 |
| 1:B:322:LEU:O | 1:B:324:PRO:HD3 | 2.05 | 0.57 |
| 1:B:335:ASN:HD22 | 1:B:336:ALA:N | 2.03 | 0.57 |
| 1:B:331:LEU:CD1 | 1:B:360:PHE:CZ | 2.87 | 0.57 |
| 1:D:216:GLY:O | 1:D:219:VAL:HG23 | 2.05 | 0.57 |
| 1:D:330:GLN:HE21 | 1:D:330:GLN:CA | 2.17 | 0.57 |
| 1:E:173:GLU:HB2 | 1:E:202:PRO:HD3 | 1.86 | 0.57 |
| 1:F:184:ALA:O | 1:F:189:HIS:HA | 2.04 | 0.57 |
| 1:G:137:THR:HB | 1:G:140:GLU:HG3 | 1.87 | 0.57 |
| 1:G:271:ILE:CD1 | 1:G:283:PRO:HA | 2.35 | 0.57 |
| 1:I:238:MET:C | 1:I:240:PRO:HD3 | 2.24 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:316:GLU:HG2 | 1:J:338:ARG:O | 2.05 | 0.57 |
| 1:J:357:ASP:O | 1:J:358:LYS:C | 2.41 | 0.57 |
| 1:K:247:PHE:CZ | 1:K:270:CYS:HB2 | 2.40 | 0.57 |
| 1:L:232:TYR:O | 1:L:236:LEU:HG | 2.04 | 0.57 |
| 1:B:414:GLN:CB | 1:B:429:PRO:HD2 | 2.35 | 0.57 |
| 1:C:95:TYR:CE2 | 1:C:129:VAL:HG21 | 2.40 | 0.57 |
| 1:C:28:LEU:HD12 | 1:C:32:LEU:HD23 | 1.86 | 0.57 |
| 1:C:272:ALA:HB1 | 1:C:314:ILE:CG2 | 2.35 | 0.57 |
| 1:C:338:ARG:HB3 | 1:C:338:ARG:HH11 | 1.65 | 0.57 |
| 1:E:344:ILE:HD11 | 1:E:360:PHE:CE1 | 2.40 | 0.57 |
| 1:E:86:ARG:NH1 | 1:E:492:VAL:HG21 | 2.19 | 0.57 |
| 1:F:208:ILE:HD11 | 1:F:449:VAL:HG22 | 1.85 | 0.57 |
| 1:F:315:LEU:CD2 | 1:F:331:LEU:HD12 | 2.35 | 0.57 |
| 1:G:248:VAL:HG12 | 1:G:249:VAL:N | 2.19 | 0.57 |
| 1:I:250:GLN:HA | 1:I:314:ILE:HD11 | 1.87 | 0.57 |
| 1:I:360:PHE:CD1 | 1:I:365:ILE:HG21 | 2.39 | 0.57 |
| 1:J:359:ILE:HA | 1:J:362:GLU:HG3 | 1.87 | 0.57 |
| 1:L:186:THR:CG2 | 1:L:187:ILE:H | 2.18 | 0.57 |
| 1:L:114:LYS:NZ | 1:L:374:ASN:ND2 | 2.53 | 0.57 |
| 1:L:81:GLN:HG3 | 1:L:157:PHE:CE1 | 2.39 | 0.57 |
| 1:B:101:VAL:O | 1:B:104:VAL:HG22 | 2.04 | 0.57 |
| 1:C:181:ASP:CG | 1:E:501:THR:HG23 | 2.25 | 0.57 |
| 1:E:244:ASP:O | 1:E:245:LYS:HG3 | 2.04 | 0.57 |
| 1:E:273:VAL:O | 1:E:273:VAL:HG12 | 2.04 | 0.57 |
| 1:E:376:GLY:O | 1:E:379:THR:HB | 2.04 | 0.57 |
| 1:F:421:PHE:CD1 | 1:F:423:LYS:HD3 | 2.40 | 0.57 |
| 1:F:33:ARG:NH1 | 1:F:45:VAL:HG11 | 2.20 | 0.57 |
| 1:G:137:THR:HG22 | 1:G:139:ASN:N | 2.08 | 0.57 |
| 1:H:121:PRO:CD | 1:H:382:TYR:CE2 | 2.87 | 0.57 |
| 1:G:500:PHE:HB3 | 1:H:142:GLU:OE1 | 2.04 | 0.57 |
| 1:I:30:GLU:HG3 | 1:I:31:ASP:N | 2.16 | 0.57 |
| 1:I:233:MET:HE3 | 1:I:343:ILE:HD11 | 1.86 | 0.57 |
| 1:I:34:THR:HG23 | 1:I:37:SER:OG | 2.05 | 0.57 |
| 1:K:18:ASP:O | 1:K:21:ALA:HB3 | 2.05 | 0.57 |
| 1:L:104:VAL:HG23 | 1:L:105:LYS:H | 1.69 | 0.57 |
| 1:L:65:ILE:HG21 | 1:L:144:ILE:HG12 | 1.86 | 0.57 |
| 1:L:387:LYS:HA | 1:L:390:ASN:HD22 | 1.70 | 0.57 |
| 1:B:424:HIS:N | 1:B:424:HIS:HD2 | 2.02 | 0.57 |
| 1:D:331:LEU:O | 1:D:356:ALA:HB2 | 2.05 | 0.57 |
| 1:F:19:ARG:CD | 1:F:23:ILE:HD11 | 2.33 | 0.57 |
| 1:J:153:ALA:HA | 1:J:158:ILE:HG22 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:293:ASP:HB3 | 1:K:297:GLN:NE2 | 2.20 | 0.57 |
| 1:K:465:MET:O | 1:K:468:ALA:HB3 | 2.05 | 0.57 |
| 1:L:281:TRP:CD1 | 1:L:283:PRO:HD3 | 2.39 | 0.57 |
| 1:L:247:PHE:HB2 | 1:L:321:ILE:HG13 | 1.85 | 0.57 |
| 1:A:414:GLN:HG3 | 1:A:429:PRO:HD2 | 1.87 | 0.57 |
| 1:E:471:TYR:O | 1:E:473:LEU:N | 2.38 | 0.57 |
| 1:F:483:VAL:O | 1:F:487:GLU:HG3 | 2.05 | 0.57 |
| 1:G:371:LEU:CD2 | 1:G:481:ALA:HB1 | 2.35 | 0.57 |
| 1:G:492:VAL:CG2 | 2:G:502:ADP:C2 | 2.87 | 0.57 |
| 1:H:52:ILE:CD1 | 1:H:489:VAL:HG12 | 2.34 | 0.57 |
| 1:J:337:PRO:HA | 1:J:363:ARG:HH21 | 1.70 | 0.57 |
| 1:L:112:THR:HB | 1:L:124:GLY:N | 2.15 | 0.57 |
| 1:A:86:ARG:NH2 | 2:A:1:ADP:O4' | 2.38 | 0.56 |
| 1:C:261:ARG:HG2 | 1:C:288:PRO:HB3 | 1.87 | 0.56 |
| 1:D:165:PRO:HD2 | 1:D:197:CYS:O | 2.05 | 0.56 |
| 1:G:346:GLU:HG2 | 1:G:351:PRO:CG | 2.34 | 0.56 |
| 1:G:467:THR:HG21 | 1:G:484:ASN:HB2 | 1.86 | 0.56 |
| 1:K:316:GLU:OE2 | 1:K:338:ARG:HB2 | 2.05 | 0.56 |
| 1:K:321:ILE:HD13 | 1:K:343:ILE:HB | 1.86 | 0.56 |
| 1:L:360:PHE:HD1 | 1:L:365:ILE:HG13 | 1.70 | 0.56 |
| 1:A:148:PHE:O | 1:A:152:LEU:HB2 | 2.04 | 0.56 |
| 1:A:217:ARG:HG3 | 1:A:262:TYR:CE2 | 2.40 | 0.56 |
| 1:B:9:PHE:O | 1:B:13:VAL:HG23 | 2.05 | 0.56 |
| 1:D:90:LYS:NZ | 1:D:164:VAL:HG12 | 2.20 | 0.56 |
| 1:F:89:CYS:O | 1:F:163:ASP:HA | 2.05 | 0.56 |
| 1:F:53:LYS:O | 1:F:82:HIS:HE1 | 1.87 | 0.56 |
| 1:G:232:TYR:N | 1:G:232:TYR:CD1 | 2.73 | 0.56 |
| 1:G:233:MET:CE | 1:G:343:ILE:HD11 | 2.34 | 0.56 |
| 1:K:141:LEU:HA | 1:K:144:ILE:HD12 | 1.86 | 0.56 |
| 1:K:272:ALA:HB1 | 1:K:314:ILE:HG21 | 1.86 | 0.56 |
| 1:K:272:ALA:HB1 | 1:K:314:ILE:CG2 | 2.35 | 0.56 |
| 1:K:68:ASP:OD2 | 1:K:137:THR:CG2 | 2.52 | 0.56 |
| 1:L:338:ARG:HH11 | 1:L:338:ARG:HB3 | 1.66 | 0.56 |
| 1:A:459:ARG:O | 1:A:463:GLN:HG3 | 2.05 | 0.56 |
| 1:C:153:ALA:HB2 | 1:C:158:ILE:CG2 | 2.35 | 0.56 |
| 1:E:153:ALA:CA | 1:E:158:ILE:HG22 | 2.34 | 0.56 |
| 1:F:74:VAL:HG23 | 1:F:74:VAL:O | 2.04 | 0.56 |
| 1:G:414:GLN:HB2 | 1:G:430:ILE:HG23 | 1.86 | 0.56 |
| 1:H:87:THR:CB | 1:H:88:PRO:HD3 | 2.36 | 0.56 |
| 1:I:439:ARG:HH12 | 1:J:404:ASP:CB | 2.18 | 0.56 |
| 1:L:330:GLN:HE21 | 1:L:330:GLN:HA | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:222:GLY:HA3 | 1:A:373:LEU:CD1 | 2.34 | 0.56 |
| 1:C:427:THR:C | 1:C:428:ILE:HD13 | 2.25 | 0.56 |
| 1:D:403:ARG:O | 1:D:406:ASN:HB2 | 2.05 | 0.56 |
| 1:D:67:ARG:HH11 | 1:D:67:ARG:CG | 2.17 | 0.56 |
| 1:E:291:LEU:CG | 1:E:291:LEU:O | 2.50 | 0.56 |
| 1:F:313:SER:HB2 | 1:F:315:LEU:CD1 | 2.35 | 0.56 |
| 1:F:328:GLU:O | 1:F:329:LYS:C | 2.44 | 0.56 |
| 1:A:416:SER:OG | 1:F:429:PRO:HA | 2.06 | 0.56 |
| 1:J:106:ALA:O | 1:J:109:SER:HB3 | 2.06 | 0.56 |
| 1:I:501:THR:H | 1:J:146:ARG:NH2 | 2.03 | 0.56 |
| 1:L:217:ARG:NH1 | 1:L:217:ARG:HB3 | 2.20 | 0.56 |
| 1:H:394:TYR:HE2 | 1:L:397:LEU:HD13 | 1.68 | 0.56 |
| 1:L:75:ILE:HG23 | 1:L:131:ILE:HD13 | 1.87 | 0.56 |
| 1:C:69:ASP:OD2 | 1:C:69:ASP:C | 2.44 | 0.56 |
| 1:D:336:ALA:HB1 | 1:D:359:ILE:HG21 | 1.88 | 0.56 |
| 1:D:118:VAL:HA | 1:D:460:SER:OG | 2.05 | 0.56 |
| 1:E:280:ILE:CG2 | 1:E:307:ALA:HB1 | 2.35 | 0.56 |
| 1:F:89:CYS:HB2 | 1:F:163:ASP:HB2 | 1.86 | 0.56 |
| 1:F:239:THR:O | 1:F:239:THR:CG2 | 2.53 | 0.56 |
| 1:F:485:ALA:O | 1:F:489:VAL:HG23 | 2.05 | 0.56 |
| 1:H:219:VAL:O | 1:H:223:ILE:HG13 | 2.04 | 0.56 |
| 1:H:82:HIS:HD2 | 1:H:109:SER:CA | 2.15 | 0.56 |
| 1:I:30:GLU:CG | 1:I:31:ASP:H | 2.16 | 0.56 |
| 1:I:325:ALA:O | 1:I:326:ALA:HB2 | 2.06 | 0.56 |
| 1:I:14:GLU:HG3 | 1:I:53:LYS:NZ | 2.21 | 0.56 |
| 1:J:371:LEU:HD13 | 1:J:482:TYR:CE1 | 2.39 | 0.56 |
| 1:K:131:ILE:CG1 | 1:K:136:TYR:CE2 | 2.86 | 0.56 |
| 1:K:65:ILE:HD13 | 1:K:144:ILE:HG13 | 1.87 | 0.56 |
| 1:L:32:LEU:O | 1:L:33:ARG:CB | 2.54 | 0.56 |
| 1:L:393:SER:O | 1:L:394:TYR:C | 2.43 | 0.56 |
| 1:B:161:GLY:H | 1:B:162:ILE:HD12 | 1.70 | 0.56 |
| 1:D:244:ASP:C | 1:D:245:LYS:HG3 | 2.26 | 0.56 |
| 1:F:79:ARG:HG2 | 1:F:157:PHE:HB3 | 1.88 | 0.56 |
| 1:G:471:TYR:O | 1:G:473:LEU:CD2 | 2.53 | 0.56 |
| 1:J:9:PHE:N | 1:J:9:PHE:CD2 | 2.72 | 0.56 |
| 1:L:281:TRP:HE1 | 1:L:283:PRO:HD3 | 1.66 | 0.56 |
| 1:L:346:GLU:HG2 | 1:L:351:PRO:CG | 2.35 | 0.56 |
| 1:B:217:ARG:CG | 1:B:221:HIS:HE1 | 2.18 | 0.56 |
| 1:B:497:GLY:HA3 | 1:B:501:THR:HA | 1.87 | 0.56 |
| 1:C:74:VAL:C | 1:C:75:ILE:HD12 | 2.26 | 0.56 |
| 1:D:99:VAL:CG2 | 1:D:100:SER:N | 2.59 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:229:GLU:OE2 | 1:D:229:GLU:HA | 2.04 | 0.56 |
| 1:D:462:ARG:HD3 | 1:D:466:ARG:HH21 | 1.70 | 0.56 |
| 1:B:498:VAL:HG11 | 1:D:72:TRP:HE1 | 1.71 | 0.56 |
| 1:E:208:ILE:O | 1:E:208:ILE:CG2 | 2.53 | 0.56 |
| 1:F:168:ASP:OD1 | 1:F:169:MET:N | 2.36 | 0.56 |
| 1:B:433:THR:HG22 | 1:F:412:SER:HA | 1.86 | 0.56 |
| 1:F:403:ARG:NH1 | 1:F:440:ILE:HB | 2.21 | 0.56 |
| 1:G:104:VAL:CG2 | 1:G:105:LYS:N | 2.68 | 0.56 |
| 1:G:91:GLY:HA3 | 1:G:125:ALA:O | 2.05 | 0.56 |
| 1:G:198:VAL:O | 1:G:201:LYS:CE | 2.53 | 0.56 |
| 1:G:396:ARG:NH1 | 1:G:396:ARG:HG3 | 2.17 | 0.56 |
| 1:H:403:ARG:HG2 | 1:H:403:ARG:HH11 | 1.69 | 0.56 |
| 1:H:23:ILE:O | 1:H:471:TYR:CE1 | 2.59 | 0.56 |
| 1:I:201:LYS:HB2 | 1:I:202:PRO:HD3 | 1.87 | 0.56 |
| 1:I:396:ARG:CG | 1:I:396:ARG:HH11 | 2.11 | 0.56 |
| 1:J:222:GLY:HA3 | 1:J:373:LEU:HD12 | 1.88 | 0.56 |
| 1:K:212:ILE:HD13 | 1:K:213:SER:H | 1.71 | 0.56 |
| 1:K:359:ILE:O | 1:K:362:GLU:HB2 | 2.05 | 0.56 |
| 1:L:260:MET:HE3 | 1:L:288:PRO:HA | 1.88 | 0.56 |
| 1:L:269:LYS:HD2 | 1:L:285:GLY:HA3 | 1.86 | 0.56 |
| 1:A:67:ARG:NH1 | 1:A:140:GLU:OE1 | 2.39 | 0.56 |
| 1:C:322:LEU:HD13 | 1:C:323:ILE:N | 2.20 | 0.56 |
| 1:C:316:GLU:HG2 | 1:C:338:ARG:NE | 2.19 | 0.56 |
| 1:E:315:LEU:O | 1:E:339:VAL:HG12 | 2.05 | 0.56 |
| 1:D:456:THR:CG2 | 1:E:396:ARG:HH21 | 2.18 | 0.56 |
| 1:F:211:ARG:O | 1:F:211:ARG:HG2 | 2.05 | 0.56 |
| 1:F:252:PHE:HE2 | 1:F:257:LEU:HB2 | 1.70 | 0.56 |
| 1:F:414:GLN:HG3 | 1:F:427:THR:O | 2.06 | 0.56 |
| 1:F:414:GLN:HB2 | 1:F:429:PRO:HD2 | 1.88 | 0.56 |
| 1:F:498:VAL:CG2 | 1:F:499:THR:H | 2.07 | 0.56 |
| 1:I:30:GLU:HG3 | 1:I:31:ASP:OD2 | 2.05 | 0.56 |
| 1:J:104:VAL:HG23 | 1:J:105:LYS:N | 2.20 | 0.56 |
| 1:A:153:ALA:HA | 1:A:158:ILE:HG22 | 1.88 | 0.56 |
| 1:C:354:PRO:O | 1:C:357:ASP:HB2 | 2.05 | 0.56 |
| 1:D:372:TYR:OH | 1:D:461:ALA:HB2 | 2.06 | 0.56 |
| 1:D:429:PRO:O | 1:D:431:VAL:N | 2.38 | 0.56 |
| 1:E:165:PRO:C | 1:E:198:VAL:HG23 | 2.26 | 0.56 |
| 1:F:149:THR:OG1 | 1:F:179:ILE:HD13 | 2.06 | 0.56 |
| 1:F:451:SER:OG | 1:F:452:GLY:N | 2.37 | 0.56 |
| 1:H:247:PHE:CB | 1:H:321:ILE:HG13 | 2.31 | 0.56 |
| 1:K:23:ILE:HG22 | 1:K:471:TYR:CD1 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:55:CYS:SG | 1:K:82:HIS:HA | 2.46 | 0.56 |
| 1:L:475:LEU:N | 1:L:475:LEU:HD12 | 2.20 | 0.56 |
| 1:A:24:VAL:HG22 | 1:A:483:VAL:HG13 | 1.87 | 0.56 |
| 1:C:163:ASP:O | 1:C:165:PRO:HD3 | 2.06 | 0.56 |
| 1:C:250:GLN:HE21 | 1:C:314:ILE:CD1 | 2.19 | 0.56 |
| 1:E:484:ASN:O | 1:E:488:LYS:HG3 | 2.06 | 0.56 |
| 1:F:436:PHE:O | 1:F:439:ARG:N | 2.35 | 0.56 |
| 1:H:117:VAL:HG11 | 1:H:372:TYR:HB2 | 1.87 | 0.56 |
| 1:I:24:VAL:CG1 | 1:I:28:LEU:HD13 | 2.35 | 0.56 |
| 1:I:400:LYS:HE2 | 1:I:403:ARG:HH21 | 1.71 | 0.56 |
| 1:J:53:LYS:HB3 | 1:J:54:PRO:CD | 2.36 | 0.56 |
| 1:K:248:VAL:HG11 | 1:K:314:ILE:HB | 1.88 | 0.56 |
| 1:K:236:LEU:HB3 | 1:K:342:LYS:HE3 | 1.87 | 0.56 |
| 1:L:294:PHE:CE2 | 1:L:301:ILE:HA | 2.41 | 0.56 |
| 1:L:353:THR:O | 1:L:356:ALA:HB3 | 2.06 | 0.56 |
| 1:C:108:ALA:O | 1:C:112:THR:HG22 | 2.06 | 0.56 |
| 1:C:233:MET:HE2 | 1:C:236:LEU:HD11 | 1.88 | 0.56 |
| 1:C:500:PHE:HB3 | 1:D:142:GLU:OE1 | 2.05 | 0.56 |
| 1:D:346:GLU:OE2 | 1:D:352:THR:HG23 | 2.06 | 0.56 |
| 1:D:439:ARG:NH2 | 1:E:405:SER:OG | 2.38 | 0.56 |
| 1:D:462:ARG:CD | 1:D:466:ARG:HH21 | 2.19 | 0.56 |
| 1:E:224:GLU:HA | 1:E:227:ILE:HG22 | 1.88 | 0.56 |
| 1:F:79:ARG:NH1 | 1:F:165:PRO:HB3 | 2.21 | 0.56 |
| 1:H:141:LEU:O | 1:H:145:THR:HG23 | 2.06 | 0.56 |
| 1:H:203:ILE:HD12 | 1:H:209:HIS:CD2 | 2.40 | 0.56 |
| 1:H:9:PHE:CD1 | 1:H:10:PHE:N | 2.63 | 0.56 |
| 1:I:91:GLY:HA2 | 1:I:111:MET:CE | 2.36 | 0.56 |
| 1:J:324:PRO:HD2 | 1:J:345:ALA:O | 2.06 | 0.56 |
| 1:K:53:LYS:CB | 1:K:54:PRO:HD3 | 2.32 | 0.56 |
| 1:L:294:PHE:HA | 1:L:297:GLN:CD | 2.26 | 0.56 |
| 1:L:338:ARG:HH11 | 1:L:338:ARG:CB | 2.19 | 0.56 |
| 1:C:497:GLY:HA3 | 1:C:501:THR:HA | 1.87 | 0.55 |
| 1:D:421:PHE:HD2 | 1:D:422:GLY:H | 1.53 | 0.55 |
| 1:F:153:ALA:HA | 1:F:158:ILE:HG22 | 1.88 | 0.55 |
| 1:G:314:ILE:HD13 | 1:G:314:ILE:H | 1.71 | 0.55 |
| 1:H:176:MET:HE2 | 1:H:179:ILE:HG13 | 1.87 | 0.55 |
| 1:I:431:VAL:HG13 | 1:I:431:VAL:O | 2.06 | 0.55 |
| 1:J:459:ARG:NH2 | 2:J:502:ADP:O3B | 2.39 | 0.55 |
| 1:A:239:THR:N | 1:A:240:PRO:CD | 2.68 | 0.55 |
| 1:A:259:SER:O | 1:A:263:LEU:HB2 | 2.06 | 0.55 |
| 1:A:460:SER:O | 1:A:464:ILE:HG13 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:336:ALA:HB3 | 1:B:337:PRO:HD3 | 1.87 | 0.55 |
| 1:C:236:LEU:HD13 | 1:C:343:ILE:HD11 | 1.89 | 0.55 |
| 1:C:28:LEU:HD11 | 1:C:490:PHE:CD2 | 2.42 | 0.55 |
| 1:F:282:ASN:ND2 | 1:F:306:LYS:O | 2.38 | 0.55 |
| 1:G:131:ILE:HD13 | 1:G:144:ILE:HD13 | 1.88 | 0.55 |
| 1:G:6:ASP:OD1 | 1:G:6:ASP:O | 2.23 | 0.55 |
| 1:H:374:ASN:O | 1:H:374:ASN:ND2 | 2.39 | 0.55 |
| 1:I:96:SER:HA | 1:I:131:ILE:O | 2.06 | 0.55 |
| 1:I:282:ASN:O | 1:I:282:ASN:OD1 | 2.24 | 0.55 |
| 1:I:363:ARG:O | 1:I:365:ILE:HG12 | 2.06 | 0.55 |
| 1:K:282:ASN:OD1 | 1:K:284:ASP:HB2 | 2.06 | 0.55 |
| 1:K:38:GLU:O | 1:K:40:GLN:N | 2.39 | 0.55 |
| 1:K:420:LYS:O | 1:K:421:PHE:HB2 | 2.04 | 0.55 |
| 1:K:466:ARG:C | 1:K:468:ALA:H | 2.10 | 0.55 |
| 1:L:244:ASP:C | 1:L:245:LYS:HG3 | 2.27 | 0.55 |
| 1:A:368:ILE:CG2 | 1:A:373:LEU:HD13 | 2.36 | 0.55 |
| 1:C:417:LEU:HD11 | 1:E:417:LEU:HD23 | 1.88 | 0.55 |
| 1:D:17:PHE:CE1 | 1:D:486:ILE:HD13 | 2.41 | 0.55 |
| 1:G:214:ALA:HB2 | 1:G:380:VAL:HG21 | 1.88 | 0.55 |
| 1:I:314:ILE:H | 1:I:314:ILE:HD13 | 1.71 | 0.55 |
| 1:K:258:HIS:HA | 1:K:261:ARG:HB2 | 1.88 | 0.55 |
| 1:L:467:THR:CG2 | 1:L:467:THR:O | 2.54 | 0.55 |
| 1:L:87:THR:OG1 | 1:L:88:PRO:CD | 2.54 | 0.55 |
| 1:A:202:PRO:HD2 | 1:A:205:GLN:HB2 | 1.89 | 0.55 |
| 1:A:22:SER:O | 1:A:23:ILE:C | 2.44 | 0.55 |
| 1:A:285:GLY:C | 1:A:286:ILE:HG13 | 2.25 | 0.55 |
| 1:A:360:PHE:HB3 | 1:A:365:ILE:CG2 | 2.37 | 0.55 |
| 1:B:302:LEU:H | 1:B:302:LEU:HD12 | 1.71 | 0.55 |
| 1:C:164:VAL:HA | 1:C:197:CYS:O | 2.06 | 0.55 |
| 1:C:316:GLU:CG | 1:C:338:ARG:HH21 | 2.16 | 0.55 |
| 1:D:249:VAL:HB | 1:D:323:ILE:HG13 | 1.88 | 0.55 |
| 1:E:476:ASP:OD2 | 1:E:479:THR:OG1 | 2.16 | 0.55 |
| 1:G:281:TRP:O | 1:G:282:ASN:HB2 | 2.05 | 0.55 |
| 1:H:277:ASP:HB3 | 1:H:302:LEU:HD11 | 1.88 | 0.55 |
| 1:H:319:CYS:O | 1:H:341:ALA:HA | 2.07 | 0.55 |
| 1:H:439:ARG:HH12 | 1:L:405:SER:N | 2.05 | 0.55 |
| 1:H:58:VAL:HG22 | 1:H:80:ALA:HB1 | 1.86 | 0.55 |
| 1:I:174:ARG:HG3 | 1:I:175:GLU:H | 1.71 | 0.55 |
| 1:J:314:ILE:N | 1:J:314:ILE:CD1 | 2.69 | 0.55 |
| 1:J:49:LEU:HD12 | 1:J:49:LEU:H | 1.70 | 0.55 |
| 1:K:436:PHE:CZ | 1:K:440:ILE:HD11 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:137:THR:CG2 | 1:A:140:GLU:HG3 | 2.37 | 0.55 |
| 1:A:90:LYS:HD2 | 1:A:164:VAL:O | 2.06 | 0.55 |
| 1:A:427:THR:O | 1:A:428:ILE:HD13 | 2.07 | 0.55 |
| 1:B:308:LYS:HE3 | 1:B:308:LYS:HA | 1.87 | 0.55 |
| 1:C:104:VAL:HG23 | 1:C:105:LYS:H | 1.72 | 0.55 |
| 1:D:100:SER:O | 1:D:103:GLU:N | 2.38 | 0.55 |
| 1:F:114:LYS:HG3 | 1:F:371:LEU:O | 2.06 | 0.55 |
| 1:I:234:SER:C | 1:I:236:LEU:H | 2.09 | 0.55 |
| 1:I:305:PRO:O | 1:I:307:ALA:N | 2.40 | 0.55 |
| 1:I:336:ALA:O | 1:I:339:VAL:HG22 | 2.06 | 0.55 |
| 1:I:24:VAL:HG22 | 1:I:483:VAL:HG13 | 1.87 | 0.55 |
| 1:J:92:GLY:HA2 | 1:J:166:ALA:O | 2.07 | 0.55 |
| 1:J:33:ARG:NE | 1:J:33:ARG:HA | 2.21 | 0.55 |
| 1:J:456:THR:HG23 | 1:K:396:ARG:HH21 | 1.72 | 0.55 |
| 1:K:107:LEU:CD1 | 1:K:126:LYS:HE2 | 2.32 | 0.55 |
| 1:K:96:SER:O | 1:K:98:ASP:N | 2.40 | 0.55 |
| 1:L:163:ASP:O | 1:L:165:PRO:HD3 | 2.07 | 0.55 |
| 1:A:423:LYS:HD3 | 1:A:426:GLY:CA | 2.16 | 0.55 |
| 1:A:62:SER:OG | 1:E:56:ASN:HA | 2.07 | 0.55 |
| 1:B:161:GLY:N | 1:B:162:ILE:HD12 | 2.21 | 0.55 |
| 1:B:186:THR:HG22 | 1:B:187:ILE:N | 2.20 | 0.55 |
| 1:C:19:ARG:HG3 | 1:C:19:ARG:NH1 | 2.21 | 0.55 |
| 1:C:252:PHE:HE2 | 1:C:260:MET:HE1 | 1.72 | 0.55 |
| 1:C:380:VAL:CG1 | 1:C:381:SER:N | 2.70 | 0.55 |
| 1:C:91:GLY:HA3 | 1:C:125:ALA:O | 2.07 | 0.55 |
| 1:D:294:PHE:HZ | 1:D:303:GLY:O | 1.88 | 0.55 |
| 1:E:33:ARG:HG3 | 1:E:33:ARG:O | 2.07 | 0.55 |
| 1:F:158:ILE:O | 1:F:158:ILE:HG23 | 2.06 | 0.55 |
| 1:G:328:GLU:HG2 | 1:G:329:LYS:HG3 | 1.89 | 0.55 |
| 1:G:331:LEU:HD12 | 1:G:352:THR:HG22 | 1.89 | 0.55 |
| 1:I:153:ALA:CA | 1:I:158:ILE:HG22 | 2.37 | 0.55 |
| 1:I:61:LEU:N | 1:I:61:LEU:HD12 | 2.21 | 0.55 |
| 1:K:492:VAL:HG12 | 1:K:493:TYR:N | 2.21 | 0.55 |
| 1:L:81:GLN:HG3 | 1:L:157:PHE:HE1 | 1.72 | 0.55 |
| 1:A:368:ILE:HG21 | 1:A:373:LEU:HD13 | 1.88 | 0.55 |
| 1:A:59:LEU:HD21 | 1:A:61:LEU:CD2 | 2.35 | 0.55 |
| 1:B:100:SER:OG | 1:B:103:GLU:HB2 | 2.07 | 0.55 |
| 1:B:271:ILE:CD1 | 1:B:283:PRO:HA | 2.36 | 0.55 |
| 1:C:248:VAL:CG1 | 1:C:249:VAL:N | 2.69 | 0.55 |
| 1:C:280:ILE:HD11 | 1:C:301:ILE:HB | 1.88 | 0.55 |
| 1:D:113:TYR:O | 1:D:117:VAL:HG23 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:335:ASN:H | 1:D:335:ASN:ND2 | 2.04 | 0.55 |
| 1:C:428:ILE:O | 1:D:416:SER:HB3 | 2.07 | 0.55 |
| 1:H:112:THR:HB | 1:H:124:GLY:H | 1.72 | 0.55 |
| 1:I:153:ALA:HA | 1:I:158:ILE:HG22 | 1.87 | 0.55 |
| 1:I:24:VAL:HG12 | 1:I:28:LEU:HB2 | 1.87 | 0.55 |
| 1:J:431:VAL:HG13 | 1:J:431:VAL:O | 2.07 | 0.55 |
| 1:K:245:LYS:HG3 | 1:K:267:GLY:O | 2.06 | 0.55 |
| 1:K:255:VAL:HG13 | 1:K:256:GLY:H | 1.72 | 0.55 |
| 1:K:59:LEU:HB2 | 1:K:157:PHE:CE2 | 2.42 | 0.55 |
| 1:L:201:LYS:HB2 | 1:L:202:PRO:HD2 | 1.89 | 0.55 |
| 1:A:386:LEU:HD13 | 1:B:392:VAL:CG2 | 2.33 | 0.55 |
| 1:B:36:GLU:HG3 | 1:B:37:SER:N | 2.20 | 0.55 |
| 1:D:497:GLY:CA | 1:D:501:THR:HA | 2.36 | 0.55 |
| 1:E:248:VAL:HG11 | 1:E:314:ILE:HB | 1.89 | 0.55 |
| 1:E:24:VAL:O | 1:E:25:GLU:C | 2.46 | 0.55 |
| 1:E:305:PRO:O | 1:E:306:LYS:HB2 | 2.07 | 0.55 |
| 1:F:6:ASP:N | 1:F:7:PRO:HD3 | 2.20 | 0.55 |
| 1:G:259:SER:O | 1:G:263:LEU:HD23 | 2.07 | 0.55 |
| 1:G:29:VAL:CA | 1:G:33:ARG:HD2 | 2.30 | 0.55 |
| 1:G:427:THR:C | 1:G:428:ILE:HD13 | 2.27 | 0.55 |
| 1:H:167:PRO:HG3 | 1:H:176:MET:SD | 2.47 | 0.55 |
| 1:H:160:PRO:HG3 | 1:H:191:ASP:OD1 | 2.07 | 0.55 |
| 1:G:408:HIS:HB3 | 1:L:436:PHE:CD2 | 2.42 | 0.55 |
| 1:C:358:LYS:O | 1:C:361:LEU:HB2 | 2.06 | 0.55 |
| 1:C:494:ASN:ND2 | 1:C:494:ASN:O | 2.36 | 0.55 |
| 1:D:257:LEU:C | 1:D:257:LEU:HD12 | 2.27 | 0.55 |
| 1:D:34:THR:O | 1:D:34:THR:CG2 | 2.55 | 0.55 |
| 1:H:121:PRO:HG2 | 1:H:382:TYR:HE2 | 1.71 | 0.55 |
| 1:H:111:MET:HB3 | 1:H:124:GLY:HA2 | 1.89 | 0.55 |
| 1:H:56:ASN:HA | 1:J:62:SER:OG | 2.06 | 0.55 |
| 1:I:475:LEU:C | 1:I:477:LEU:HD22 | 2.27 | 0.55 |
| 1:I:479:THR:O | 1:I:480:ALA:C | 2.45 | 0.55 |
| 1:J:314:ILE:H | 1:J:314:ILE:CD1 | 2.20 | 0.55 |
| 1:K:59:LEU:HD22 | 1:K:157:PHE:CD2 | 2.42 | 0.55 |
| 1:K:371:LEU:HD13 | 1:K:482:TYR:CE2 | 2.42 | 0.55 |
| 1:L:281:TRP:O | 1:L:282:ASN:HB2 | 2.07 | 0.55 |
| 1:L:369:PRO:CD | 1:L:477:LEU:HB3 | 2.37 | 0.55 |
| 1:A:58:VAL:HG23 | 1:A:80:ALA:HB2 | 1.89 | 0.55 |
| 1:C:114:LYS:NZ | 1:C:374:ASN:HD21 | 2.05 | 0.55 |
| 1:D:147:ARG:NH1 | 1:D:151:GLU:OE2 | 2.40 | 0.55 |
| 1:E:211:ARG:HG3 | 1:E:211:ARG:HH11 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:52:ILE:HD13 | 1:H:489:VAL:CG1 | 2.36 | 0.55 |
| 1:I:151:GLU:HB3 | 1:L:57:HIS:HE1 | 1.72 | 0.55 |
| 1:I:281:TRP:NE1 | 1:I:283:PRO:HD3 | 2.21 | 0.55 |
| 1:K:379:THR:HG21 | 1:K:456:THR:HG21 | 1.89 | 0.55 |
| 1:L:213:SER:HB2 | 1:L:217:ARG:HD2 | 1.89 | 0.55 |
| 1:B:165:PRO:C | 1:B:198:VAL:HG23 | 2.27 | 0.54 |
| 1:C:247:PHE:CE1 | 1:C:270:CYS:N | 2.75 | 0.54 |
| 1:C:45:VAL:HG23 | 1:F:72:TRP:CZ3 | 2.41 | 0.54 |
| 1:D:158:ILE:HG12 | 1:D:165:PRO:HG2 | 1.88 | 0.54 |
| 1:D:296:LEU:CD1 | 1:D:297:GLN:N | 2.69 | 0.54 |
| 1:D:453:LEU:CD2 | 1:D:457:MET:HG2 | 2.36 | 0.54 |
| 1:D:453:LEU:HD23 | 1:D:453:LEU:C | 2.27 | 0.54 |
| 1:E:219:VAL:HA | 1:E:373:LEU:CD1 | 2.37 | 0.54 |
| 1:F:240:PRO:O | 1:G:431:VAL:HG23 | 2.06 | 0.54 |
| 1:F:45:VAL:C | 1:F:47:GLY:H | 2.08 | 0.54 |
| 1:H:274:GLY:CA | 1:H:314:ILE:HD12 | 2.37 | 0.54 |
| 1:H:34:THR:HG22 | 1:H:34:THR:O | 2.07 | 0.54 |
| 1:I:252:PHE:CE2 | 1:I:260:MET:HE1 | 2.35 | 0.54 |
| 1:J:161:GLY:O | 1:J:162:ILE:HD12 | 2.06 | 0.54 |
| 1:J:498:VAL:CG2 | 1:J:499:THR:H | 2.19 | 0.54 |
| 1:A:446:LYS:HG3 | 1:A:450:HIS:CE1 | 2.42 | 0.54 |
| 1:B:238:MET:O | 1:B:239:THR:C | 2.45 | 0.54 |
| 1:B:281:TRP:O | 1:B:282:ASN:HB2 | 2.07 | 0.54 |
| 1:C:94:ARG:HD3 | 1:C:168:ASP:OD2 | 2.06 | 0.54 |
| 1:D:250:GLN:HE21 | 1:D:274:GLY:HA3 | 1.71 | 0.54 |
| 1:D:30:GLU:O | 1:D:30:GLU:HG3 | 2.07 | 0.54 |
| 1:E:222:GLY:HA3 | 1:E:373:LEU:CD1 | 2.37 | 0.54 |
| 1:C:413:VAL:CG1 | 1:E:413:VAL:HG11 | 2.38 | 0.54 |
| 1:E:69:ASP:OD1 | 1:E:71:SER:N | 2.37 | 0.54 |
| 1:F:335:ASN:HD22 | 1:F:336:ALA:H | 1.54 | 0.54 |
| 1:G:201:LYS:HB2 | 1:G:202:PRO:CD | 2.37 | 0.54 |
| 1:H:219:VAL:HG13 | 1:H:373:LEU:HD21 | 1.89 | 0.54 |
| 1:L:328:GLU:O | 1:L:329:LYS:HB2 | 2.07 | 0.54 |
| 1:B:100:SER:O | 1:B:103:GLU:HB3 | 2.07 | 0.54 |
| 1:B:165:PRO:HD2 | 1:B:197:CYS:O | 2.07 | 0.54 |
| 1:C:142:GLU:HA | 1:C:178:TRP:CE3 | 2.42 | 0.54 |
| 1:C:281:TRP:O | 1:C:282:ASN:CB | 2.55 | 0.54 |
| 1:C:318:ASP:HA | 1:C:340:LYS:HB2 | 1.87 | 0.54 |
| 1:C:30:GLU:HA | 1:C:34:THR:OG1 | 2.07 | 0.54 |
| 1:C:374:ASN:ND2 | 1:C:374:ASN:O | 2.40 | 0.54 |
| 1:C:380:VAL:HG22 | 1:C:449:VAL:CG1 | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:435:GLU:O | 1:C:438:ASP:N | 2.41 | 0.54 |
| 1:D:24:VAL:CG1 | 1:D:28:LEU:HD22 | 2.36 | 0.54 |
| 1:D:335:ASN:HA | 1:D:338:ARG:HD3 | 1.87 | 0.54 |
| 1:E:239:THR:CG2 | 1:E:239:THR:O | 2.54 | 0.54 |
| 1:F:335:ASN:HD22 | 1:F:335:ASN:N | 2.05 | 0.54 |
| 1:H:294:PHE:O | 1:H:298:HIS:CE1 | 2.61 | 0.54 |
| 1:H:57:HIS:CE1 | 1:H:84:HIS:CE1 | 2.94 | 0.54 |
| 1:I:406:ASN:ND2 | 1:J:409:LEU:CD2 | 2.69 | 0.54 |
| 1:J:165:PRO:HD2 | 1:J:197:CYS:O | 2.06 | 0.54 |
| 1:L:247:PHE:HE2 | 1:L:249:VAL:CG1 | 2.21 | 0.54 |
| 1:L:498:VAL:N | 1:L:501:THR:HB | 2.22 | 0.54 |
| 1:L:65:ILE:HG12 | 1:L:75:ILE:HD11 | 1.89 | 0.54 |
| 1:L:65:ILE:HG23 | 1:L:75:ILE:HD13 | 1.88 | 0.54 |
| 1:A:411:MET:HG2 | 1:A:430:ILE:HG21 | 1.88 | 0.54 |
| 1:A:496:ALA:C | 1:A:501:THR:O | 2.46 | 0.54 |
| 1:B:246:THR:O | 1:B:320:ASP:HB2 | 2.08 | 0.54 |
| 1:C:239:THR:CA | 1:C:245:LYS:HZ2 | 2.21 | 0.54 |
| 1:C:249:VAL:O | 1:C:249:VAL:HG22 | 2.07 | 0.54 |
| 1:G:213:SER:HB2 | 1:G:217:ARG:HD2 | 1.90 | 0.54 |
| 1:G:224:GLU:O | 1:G:227:ILE:HG22 | 2.07 | 0.54 |
| 1:J:104:VAL:CG2 | 1:J:105:LYS:N | 2.70 | 0.54 |
| 1:K:360:PHE:CD1 | 1:K:365:ILE:HD12 | 2.37 | 0.54 |
| 1:G:72:TRP:NE1 | 1:K:498:VAL:HG11 | 2.22 | 0.54 |
| 1:K:66:ARG:HG3 | 1:K:72:TRP:CE2 | 2.42 | 0.54 |
| 1:L:6:ASP:CB | 1:L:329:LYS:HD2 | 2.34 | 0.54 |
| 1:A:153:ALA:CA | 1:A:158:ILE:HG22 | 2.36 | 0.54 |
| 1:A:22:SER:OG | 1:A:23:ILE:N | 2.40 | 0.54 |
| 1:B:411:MET:HG2 | 1:B:430:ILE:HG22 | 1.89 | 0.54 |
| 1:C:248:VAL:HG11 | 1:C:314:ILE:HB | 1.90 | 0.54 |
| 1:D:281:TRP:CD1 | 1:D:283:PRO:HD3 | 2.43 | 0.54 |
| 1:B:501:THR:OXT | 1:F:181:ASP:CG | 2.46 | 0.54 |
| 1:F:294:PHE:CE1 | 1:F:298:HIS:CE1 | 2.96 | 0.54 |
| 1:G:221:HIS:O | 1:G:222:GLY:C | 2.46 | 0.54 |
| 1:J:244:ASP:CG | 1:J:245:LYS:HG3 | 2.28 | 0.54 |
| 1:A:496:ALA:O | 1:A:501:THR:O | 2.25 | 0.54 |
| 1:B:162:ILE:N | 1:B:162:ILE:CD1 | 2.71 | 0.54 |
| 1:B:164:VAL:HA | 1:B:197:CYS:O | 2.08 | 0.54 |
| 1:B:213:SER:HB2 | 1:B:217:ARG:HH21 | 1.73 | 0.54 |
| 1:B:295:LYS:HA | 1:B:300:SER:O | 2.07 | 0.54 |
| 1:B:324:PRO:HD2 | 1:B:345:ALA:O | 2.06 | 0.54 |
| 1:C:215:THR:HG23 | 1:C:377:GLY:CA | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:175:GLU:HA | 1:D:178:TRP:CE3 | 2.43 | 0.54 |
| 1:D:274:GLY:HA2 | 1:D:279:SER:HA | 1.90 | 0.54 |
| 1:F:150:MET:SD | 1:F:186:THR:HG21 | 2.48 | 0.54 |
| 1:F:25:GLU:O | 1:F:29:VAL:HG23 | 2.08 | 0.54 |
| 1:F:336:ALA:HB3 | 1:F:337:PRO:HD3 | 1.90 | 0.54 |
| 1:G:7:PRO:O | 1:G:329:LYS:HE3 | 2.07 | 0.54 |
| 1:H:332:THR:HA | 1:H:353:THR:CG2 | 2.37 | 0.54 |
| 1:H:455:TYR:HB2 | 1:L:400:LYS:HB2 | 1.89 | 0.54 |
| 1:J:137:THR:HG22 | 1:J:140:GLU:OE1 | 2.08 | 0.54 |
| 1:K:291:LEU:HD11 | 1:K:301:ILE:CG2 | 2.35 | 0.54 |
| 1:L:459:ARG:O | 1:L:463:GLN:HG3 | 2.08 | 0.54 |
| 1:A:25:GLU:O | 1:A:26:ASP:C | 2.46 | 0.54 |
| 1:B:291:LEU:CD1 | 1:B:301:ILE:HG22 | 2.35 | 0.54 |
| 1:B:117:VAL:HG21 | 1:B:371:LEU:HG | 1.88 | 0.54 |
| 1:C:414:GLN:CA | 1:C:429:PRO:HG2 | 2.37 | 0.54 |
| 1:D:97:THR:C | 1:D:130:LYS:CE | 2.76 | 0.54 |
| 1:D:372:TYR:CD2 | 1:D:464:ILE:CD1 | 2.90 | 0.54 |
| 1:D:53:LYS:N | 1:D:54:PRO:HD2 | 2.23 | 0.54 |
| 1:D:59:LEU:CD2 | 1:D:61:LEU:HD22 | 2.37 | 0.54 |
| 1:E:232:TYR:HE1 | 1:E:465:MET:HG2 | 1.72 | 0.54 |
| 1:F:332:THR:H | 1:F:335:ASN:HD21 | 1.55 | 0.54 |
| 1:A:417:LEU:HD11 | 1:F:417:LEU:HD22 | 1.88 | 0.54 |
| 1:G:392:VAL:HG12 | 1:G:393:SER:O | 2.07 | 0.54 |
| 1:G:487:GLU:O | 1:G:490:PHE:HB3 | 2.07 | 0.54 |
| 1:G:87:THR:HB | 1:G:88:PRO:CD | 2.34 | 0.54 |
| 1:H:229:GLU:HA | 1:H:229:GLU:OE2 | 2.07 | 0.54 |
| 1:H:331:LEU:HD22 | 1:H:360:PHE:CZ | 2.28 | 0.54 |
| 1:I:410:LEU:CD2 | 1:J:409:LEU:CD1 | 2.85 | 0.54 |
| 1:I:414:GLN:CG | 1:I:429:PRO:HD2 | 2.38 | 0.54 |
| 1:I:475:LEU:HD12 | 1:I:475:LEU:N | 2.23 | 0.54 |
| 1:K:248:VAL:HG13 | 1:K:272:ALA:O | 2.08 | 0.54 |
| 1:L:247:PHE:HB3 | 1:L:321:ILE:HG13 | 1.90 | 0.54 |
| 1:B:176:MET:O | 1:B:179:ILE:HB | 2.08 | 0.54 |
| 1:C:410:LEU:HB3 | 1:C:430:ILE:HA | 1.90 | 0.54 |
| 1:E:148:PHE:O | 1:E:152:LEU:HB2 | 2.08 | 0.54 |
| 1:E:369:PRO:HG2 | 1:E:478:ARG:HA | 1.90 | 0.54 |
| 1:F:225:ASN:ND2 | 1:F:458:GLU:HA | 2.23 | 0.54 |
| 1:F:17:PHE:CE2 | 1:F:53:LYS:HB2 | 2.43 | 0.54 |
| 1:H:289:LYS:HG2 | 1:H:293:ASP:OD2 | 2.08 | 0.54 |
| 1:I:92:GLY:CA | 1:I:166:ALA:O | 2.56 | 0.54 |
| 1:K:24:VAL:O | 1:K:25:GLU:C | 2.45 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:165:PRO:HD2 | 1:L:197:CYS:O | 2.08 | 0.54 |
| 1:H:394:TYR:CE2 | 1:L:397:LEU:HD13 | 2.42 | 0.54 |
| 1:L:411:MET:HA | 1:L:430:ILE:CG2 | 2.35 | 0.54 |
| 1:A:158:ILE:HG23 | 1:A:158:ILE:O | 2.06 | 0.54 |
| 1:A:314:ILE:N | 1:A:314:ILE:CD1 | 2.71 | 0.54 |
| 1:B:19:ARG:CZ | 1:B:479:THR:HG21 | 2.38 | 0.54 |
| 1:C:460:SER:O | 1:C:464:ILE:HG13 | 2.07 | 0.54 |
| 1:E:112:THR:HG22 | 1:E:124:GLY:HA3 | 1.89 | 0.54 |
| 1:E:33:ARG:NH1 | 1:E:33:ARG:HB2 | 2.22 | 0.54 |
| 1:F:371:LEU:HD23 | 1:F:481:ALA:CB | 2.38 | 0.54 |
| 1:H:114:LYS:NZ | 1:H:374:ASN:HD21 | 2.06 | 0.54 |
| 1:H:492:VAL:HG23 | 1:H:493:TYR:H | 1.73 | 0.54 |
| 1:H:90:LYS:CE | 1:H:199:THR:HG21 | 2.35 | 0.54 |
| 1:I:250:GLN:HB2 | 1:I:314:ILE:HD11 | 1.89 | 0.54 |
| 1:J:425:GLY:O | 1:J:428:ILE:HD11 | 2.08 | 0.54 |
| 1:K:6:ASP:OD2 | 1:K:329:LYS:HE2 | 2.07 | 0.54 |
| 1:K:93:ILE:HD11 | 1:K:165:PRO:CB | 2.38 | 0.54 |
| 1:L:367:VAL:O | 1:L:367:VAL:HG23 | 2.07 | 0.54 |
| 1:B:104:VAL:HG23 | 1:B:105:LYS:N | 2.23 | 0.54 |
| 1:B:181:ASP:O | 1:B:182:THR:C | 2.45 | 0.54 |
| 1:B:335:ASN:HD22 | 1:B:335:ASN:N | 2.05 | 0.54 |
| 1:B:339:VAL:HG21 | 1:B:360:PHE:CE1 | 2.36 | 0.54 |
| 1:C:351:PRO:CG | 1:C:352:THR:H | 2.20 | 0.54 |
| 1:C:355:GLU:O | 1:C:359:ILE:CD1 | 2.56 | 0.54 |
| 1:G:9:PHE:HA | 1:G:12:MET:CE | 2.38 | 0.54 |
| 1:H:65:ILE:C | 1:H:65:ILE:HD12 | 2.29 | 0.54 |
| 1:I:78:TYR:CE2 | 1:I:101:VAL:HG23 | 2.43 | 0.54 |
| 1:I:315:LEU:H | 1:I:315:LEU:HD12 | 1.72 | 0.54 |
| 1:J:33:ARG:CZ | 1:J:33:ARG:CA | 2.84 | 0.54 |
| 1:J:380:VAL:CG1 | 1:J:380:VAL:O | 2.56 | 0.54 |
| 1:K:248:VAL:HG11 | 1:K:272:ALA:HB3 | 1.89 | 0.54 |
| 1:K:336:ALA:HB3 | 1:K:359:ILE:CD1 | 2.35 | 0.54 |
| 1:K:236:LEU:O | 1:K:342:LYS:HE2 | 2.08 | 0.54 |
| 1:A:208:ILE:O | 1:A:208:ILE:CG2 | 2.56 | 0.53 |
| 1:A:386:LEU:O | 1:A:389:LEU:N | 2.41 | 0.53 |
| 1:B:73:GLU:HG2 | 1:B:74:VAL:N | 2.23 | 0.53 |
| 1:C:61:LEU:HD12 | 1:C:61:LEU:N | 2.22 | 0.53 |
| 1:D:214:ALA:CB | 1:D:380:VAL:HG21 | 2.37 | 0.53 |
| 1:D:249:VAL:HB | 1:D:323:ILE:CG1 | 2.38 | 0.53 |
| 1:E:421:PHE:O | 1:E:422:GLY:C | 2.47 | 0.53 |
| 1:G:90:LYS:NZ | 1:G:199:THR:OG1 | 2.40 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:17:PHE:HE1 | 1:G:486:ILE:HD12 | 1.70 | 0.53 |
| 1:J:244:ASP:OD2 | 1:J:245:LYS:HG3 | 2.08 | 0.53 |
| 1:K:248:VAL:HG22 | 1:K:272:ALA:N | 2.22 | 0.53 |
| 1:L:247:PHE:CE2 | 1:L:249:VAL:HG12 | 2.43 | 0.53 |
| 1:L:386:LEU:O | 1:L:389:LEU:N | 2.42 | 0.53 |
| 1:B:257:LEU:O | 1:B:257:LEU:HD12 | 2.09 | 0.53 |
| 1:D:260:MET:HE3 | 1:D:288:PRO:HA | 1.89 | 0.53 |
| 1:E:173:GLU:OE2 | 1:E:211:ARG:NH2 | 2.41 | 0.53 |
| 1:G:326:ALA:O | 1:G:327:SER:O | 2.26 | 0.53 |
| 1:H:75:ILE:HD12 | 1:H:75:ILE:H | 1.74 | 0.53 |
| 1:I:382:TYR:CE2 | 1:I:386:LEU:HD21 | 2.43 | 0.53 |
| 1:J:174:ARG:HG3 | 1:J:175:GLU:H | 1.73 | 0.53 |
| 1:J:81:GLN:NE2 | 1:J:157:PHE:CD1 | 2.76 | 0.53 |
| 1:K:104:VAL:CG2 | 1:K:105:LYS:N | 2.71 | 0.53 |
| 1:K:49:LEU:H | 1:K:49:LEU:CD1 | 2.20 | 0.53 |
| 1:L:219:VAL:HA | 1:L:373:LEU:HD11 | 1.90 | 0.53 |
| 1:A:132:ASN:OD1 | 1:A:134:LYS:HB2 | 2.09 | 0.53 |
| 1:A:24:VAL:CG2 | 1:A:483:VAL:HG13 | 2.38 | 0.53 |
| 1:B:247:PHE:CE1 | 1:B:263:LEU:HB3 | 2.44 | 0.53 |
| 1:D:20:GLY:HA2 | 1:D:23:ILE:HD12 | 1.90 | 0.53 |
| 1:D:287:ASP:OD1 | 1:D:288:PRO:HD2 | 2.08 | 0.53 |
| 1:D:335:ASN:O | 1:D:336:ALA:C | 2.47 | 0.53 |
| 1:D:19:ARG:NH1 | 1:D:479:THR:HG21 | 2.23 | 0.53 |
| 1:F:263:LEU:O | 1:F:268:ALA:HB3 | 2.07 | 0.53 |
| 1:G:483:VAL:HG12 | 1:G:484:ASN:N | 2.23 | 0.53 |
| 1:J:413:VAL:O | 1:J:417:LEU:HB2 | 2.09 | 0.53 |
| 1:K:162:ILE:CG2 | 1:K:163:ASP:N | 2.66 | 0.53 |
| 1:K:417:LEU:O | 1:K:420:LYS:HG3 | 2.09 | 0.53 |
| 1:L:94:ARG:O | 1:L:128:GLY:HA2 | 2.08 | 0.53 |
| 1:L:223:ILE:HD13 | 1:L:263:LEU:HD21 | 1.90 | 0.53 |
| 1:L:492:VAL:HG21 | 2:L:502:ADP:C2 | 2.43 | 0.53 |
| 1:C:499:THR:HG1 | 1:C:500:PHE:HD1 | 1.54 | 0.53 |
| 1:D:293:ASP:O | 1:D:296:LEU:HB3 | 2.07 | 0.53 |
| 1:D:219:VAL:HG13 | 1:D:373:LEU:HD21 | 1.90 | 0.53 |
| 1:E:368:ILE:CG2 | 1:E:373:LEU:HD22 | 2.39 | 0.53 |
| 1:H:51:ILE:HD13 | 1:J:64:PRO:HG3 | 1.89 | 0.53 |
| 1:I:379:THR:O | 1:I:382:TYR:HB3 | 2.09 | 0.53 |
| 1:I:41:LYS:O | 1:I:44:ARG:HB3 | 2.09 | 0.53 |
| 1:J:343:ILE:CD1 | 1:J:366:MET:HE2 | 2.36 | 0.53 |
| 1:I:499:THR:HG23 | 1:L:147:ARG:CZ | 2.38 | 0.53 |
| 1:L:247:PHE:CZ | 1:L:270:CYS:HB2 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:420:LYS:HB3 | 1:A:420:LYS:NZ | 2.22 | 0.53 |
| 1:A:431:VAL:HG13 | 1:B:416:SER:OG | 2.08 | 0.53 |
| 1:C:168:ASP:O | 1:C:169:MET:C | 2.46 | 0.53 |
| 1:C:114:LYS:CE | 1:C:374:ASN:ND2 | 2.71 | 0.53 |
| 1:C:53:LYS:HB3 | 1:C:54:PRO:CD | 2.37 | 0.53 |
| 1:D:336:ALA:CB | 1:D:337:PRO:HD3 | 2.24 | 0.53 |
| 1:F:88:PRO:HG2 | 1:F:122:PHE:CD2 | 2.42 | 0.53 |
| 1:F:131:ILE:CD1 | 1:F:136:TYR:HE2 | 2.22 | 0.53 |
| 1:F:250:GLN:HG2 | 1:F:314:ILE:HG12 | 1.89 | 0.53 |
| 1:G:244:ASP:OD1 | 1:G:245:LYS:HG3 | 2.08 | 0.53 |
| 1:G:82:HIS:CD2 | 1:G:112:THR:CG2 | 2.85 | 0.53 |
| 1:I:17:PHE:HE2 | 1:I:53:LYS:HB2 | 1.73 | 0.53 |
| 1:I:49:LEU:HA | 1:I:52:ILE:HG13 | 1.90 | 0.53 |
| 1:I:69:ASP:OD1 | 1:I:69:ASP:C | 2.46 | 0.53 |
| 2:I:502:ADP:H5'2 | 1:J:203:ILE:HG22 | 1.90 | 0.53 |
| 1:K:23:ILE:O | 1:K:23:ILE:HG22 | 2.08 | 0.53 |
| 1:K:315:LEU:HD21 | 1:K:330:GLN:HG3 | 1.89 | 0.53 |
| 1:L:142:GLU:HG3 | 1:L:178:TRP:CD2 | 2.44 | 0.53 |
| 1:L:497:GLY:O | 1:L:498:VAL:HG13 | 2.08 | 0.53 |
| 1:B:142:GLU:O | 1:B:145:THR:N | 2.42 | 0.53 |
| 1:B:498:VAL:O | 1:B:501:THR:HB | 2.09 | 0.53 |
| 1:B:52:ILE:CD1 | 1:B:489:VAL:HG12 | 2.32 | 0.53 |
| 1:C:363:ARG:NH1 | 1:C:363:ARG:HB2 | 2.23 | 0.53 |
| 1:C:38:GLU:O | 1:C:39:GLU:HB3 | 2.08 | 0.53 |
| 1:D:294:PHE:CE1 | 1:D:305:PRO:HD3 | 2.44 | 0.53 |
| 1:E:330:GLN:HA | 1:E:330:GLN:NE2 | 2.22 | 0.53 |
| 1:F:131:ILE:CD1 | 1:F:136:TYR:CE2 | 2.92 | 0.53 |
| 1:F:386:LEU:O | 1:F:388:ASN:N | 2.42 | 0.53 |
| 1:G:153:ALA:HA | 1:G:158:ILE:HG23 | 1.90 | 0.53 |
| 1:G:7:PRO:O | 1:G:329:LYS:CE | 2.56 | 0.53 |
| 1:G:451:SER:OG | 1:G:452:GLY:N | 2.40 | 0.53 |
| 1:H:332:THR:HA | 1:H:353:THR:HG23 | 1.89 | 0.53 |
| 1:H:485:ALA:O | 1:H:486:ILE:C | 2.46 | 0.53 |
| 1:I:360:PHE:HD1 | 1:I:365:ILE:HG21 | 1.73 | 0.53 |
| 1:I:394:TYR:HB2 | 1:I:445:GLU:HG3 | 1.91 | 0.53 |
| 1:K:252:PHE:CZ | 1:K:260:MET:HE1 | 2.43 | 0.53 |
| 1:K:17:PHE:CE2 | 1:K:53:LYS:HB2 | 2.42 | 0.53 |
| 1:L:146:ARG:NE | 1:L:182:THR:OG1 | 2.40 | 0.53 |
| 1:A:201:LYS:HZ3 | 1:A:388:ASN:ND2 | 2.07 | 0.53 |
| 1:A:208:ILE:HG13 | 1:A:387:LYS:HD2 | 1.90 | 0.53 |
| 1:A:396:ARG:HD3 | 1:A:396:ARG:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:371:LEU:HD23 | 1:B:481:ALA:HB3 | 1.90 | 0.53 |
| 1:B:38:GLU:O | 1:B:42:ARG:HD3 | 2.08 | 0.53 |
| 1:D:403:ARG:HG2 | 1:D:403:ARG:NH1 | 2.22 | 0.53 |
| 1:E:429:PRO:C | 1:E:431:VAL:H | 2.12 | 0.53 |
| 1:F:160:PRO:HG2 | 1:F:161:GLY:N | 2.24 | 0.53 |
| 1:F:166:ALA:HB1 | 1:F:167:PRO:CD | 2.32 | 0.53 |
| 1:F:271:ILE:HD11 | 1:F:319:CYS:HB2 | 1.91 | 0.53 |
| 1:G:252:PHE:CD2 | 1:G:273:VAL:HG11 | 2.44 | 0.53 |
| 1:G:29:VAL:O | 1:G:30:GLU:O | 2.27 | 0.53 |
| 1:G:39:GLU:O | 1:G:41:LYS:HG3 | 2.09 | 0.53 |
| 1:H:226:PHE:CE2 | 1:H:477:LEU:HD21 | 2.43 | 0.53 |
| 1:H:234:SER:O | 1:H:237:GLY:N | 2.40 | 0.53 |
| 1:H:407:TYR:O | 1:H:411:MET:HB2 | 2.08 | 0.53 |
| 1:H:379:THR:CG2 | 1:H:453:LEU:HD23 | 2.38 | 0.53 |
| 1:H:84:HIS:O | 1:H:85:GLN:C | 2.47 | 0.53 |
| 1:J:498:VAL:CG2 | 1:J:499:THR:N | 2.71 | 0.53 |
| 1:L:336:ALA:HB1 | 1:L:359:ILE:HG21 | 1.91 | 0.53 |
| 1:A:137:THR:OG1 | 1:A:140:GLU:HG3 | 2.08 | 0.53 |
| 1:A:294:PHE:CE2 | 1:A:298:HIS:HE1 | 2.26 | 0.53 |
| 1:B:280:ILE:HD11 | 1:B:304:PHE:HB3 | 1.89 | 0.53 |
| 1:B:359:ILE:HG22 | 1:B:360:PHE:N | 2.22 | 0.53 |
| 1:D:462:ARG:NE | 1:D:466:ARG:HH21 | 2.06 | 0.53 |
| 1:F:280:ILE:HD12 | 1:F:301:ILE:HD12 | 1.91 | 0.53 |
| 1:F:363:ARG:O | 1:F:365:ILE:HG12 | 2.08 | 0.53 |
| 1:G:57:HIS:CD2 | 1:G:84:HIS:CE1 | 2.96 | 0.53 |
| 1:H:211:ARG:HH11 | 1:H:211:ARG:CB | 2.22 | 0.53 |
| 1:I:501:THR:N | 1:J:146:ARG:NH2 | 2.56 | 0.53 |
| 1:J:224:GLU:HG2 | 1:J:225:ASN:N | 2.24 | 0.53 |
| 1:I:394:TYR:CE1 | 1:J:397:LEU:HD23 | 2.43 | 0.53 |
| 1:J:65:ILE:CG1 | 1:J:75:ILE:HD11 | 2.39 | 0.53 |
| 1:K:478:ARG:NH1 | 1:K:478:ARG:CG | 2.67 | 0.53 |
| 1:L:294:PHE:HE2 | 1:L:301:ILE:CA | 2.21 | 0.53 |
| 1:A:386:LEU:O | 1:A:387:LYS:C | 2.47 | 0.53 |
| 1:A:45:VAL:C | 1:A:47:GLY:H | 2.12 | 0.53 |
| 1:C:109:SER:O | 1:C:112:THR:HG23 | 2.09 | 0.53 |
| 1:C:244:ASP:O | 1:C:245:LYS:HD3 | 2.09 | 0.53 |
| 1:D:411:MET:HA | 1:D:430:ILE:CG2 | 2.36 | 0.53 |
| 1:E:9:PHE:HD1 | 1:E:10:PHE:N | 2.03 | 0.53 |
| 1:E:411:MET:HA | 1:E:430:ILE:HG22 | 1.91 | 0.53 |
| 1:F:280:ILE:CG2 | 1:F:307:ALA:HB1 | 2.38 | 0.53 |
| 1:F:396:ARG:CG | 1:F:396:ARG:NH1 | 2.63 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:420:LYS:O | 1:F:421:PHE:HB2 | 2.09 | 0.53 |
| 1:G:89:CYS:N | 1:G:162:ILE:O | 2.42 | 0.53 |
| 1:H:460:SER:O | 1:H:461:ALA:C | 2.46 | 0.53 |
| 1:H:475:LEU:HD12 | 1:H:475:LEU:N | 2.24 | 0.53 |
| 1:I:314:ILE:HD13 | 1:I:314:ILE:N | 2.23 | 0.53 |
| 1:I:339:VAL:O | 1:I:363:ARG:NH2 | 2.41 | 0.53 |
| 1:I:38:GLU:N | 1:I:42:ARG:NH2 | 2.56 | 0.53 |
| 1:I:475:LEU:HD12 | 1:I:475:LEU:H | 1.73 | 0.53 |
| 1:J:115:CYS:O | 1:J:116:ALA:C | 2.48 | 0.53 |
| 1:K:104:VAL:HG23 | 1:K:105:LYS:H | 1.73 | 0.53 |
| 1:L:85:GLN:HG2 | 1:L:86:ARG:N | 2.23 | 0.53 |
| 1:A:300:SER:HB3 | 1:A:302:LEU:HG | 1.91 | 0.53 |
| 1:A:433:THR:O | 1:A:434:ALA:C | 2.47 | 0.53 |
| 1:D:132:ASN:HB3 | 1:D:135:ASN:ND2 | 2.23 | 0.53 |
| 1:E:394:TYR:HB2 | 1:E:445:GLU:HG3 | 1.90 | 0.53 |
| 1:F:334:SER:O | 1:F:337:PRO:HD2 | 2.09 | 0.53 |
| 1:F:420:LYS:O | 1:F:420:LYS:HG2 | 2.10 | 0.53 |
| 1:F:45:VAL:HG13 | 1:F:45:VAL:O | 2.09 | 0.53 |
| 1:G:160:PRO:HG3 | 1:G:191:ASP:OD1 | 2.09 | 0.53 |
| 1:G:382:TYR:CE2 | 1:G:386:LEU:HD21 | 2.43 | 0.53 |
| 1:I:237:GLY:O | 1:I:238:MET:HE2 | 2.09 | 0.53 |
| 1:K:153:ALA:CA | 1:K:158:ILE:CG2 | 2.87 | 0.53 |
| 1:K:210:GLY:HA2 | 1:K:212:ILE:HD11 | 1.91 | 0.53 |
| 1:K:249:VAL:HG12 | 1:K:323:ILE:CD1 | 2.39 | 0.53 |
| 1:K:59:LEU:CB | 1:K:157:PHE:CE2 | 2.92 | 0.53 |
| 1:L:100:SER:O | 1:L:103:GLU:N | 2.37 | 0.53 |
| 1:A:287:ASP:HB3 | 1:A:290:GLU:HG3 | 1.90 | 0.52 |
| 1:A:223:ILE:HD11 | 1:A:345:ALA:CB | 2.39 | 0.52 |
| 1:A:385:TRP:O | 1:A:386:LEU:C | 2.48 | 0.52 |
| 1:C:271:ILE:O | 1:C:271:ILE:HG12 | 2.09 | 0.52 |
| 1:C:17:PHE:HE1 | 1:C:486:ILE:HD12 | 1.72 | 0.52 |
| 1:D:239:THR:O | 1:D:239:THR:HG23 | 2.09 | 0.52 |
| 1:D:281:TRP:HZ3 | 1:D:317:ALA:HB1 | 1.74 | 0.52 |
| 1:E:480:ALA:O | 1:E:483:VAL:HB | 2.09 | 0.52 |
| 1:F:82:HIS:CD2 | 1:F:112:THR:OG1 | 2.62 | 0.52 |
| 1:G:152:LEU:HD23 | 1:G:158:ILE:HB | 1.92 | 0.52 |
| 1:G:265:ARG:O | 1:G:265:ARG:HG2 | 2.08 | 0.52 |
| 1:G:330:GLN:OE1 | 1:G:330:GLN:HA | 2.09 | 0.52 |
| 1:G:335:ASN:C | 1:G:335:ASN:HD22 | 2.04 | 0.52 |
| 1:G:364:ASN:O | 1:G:365:ILE:HD13 | 2.09 | 0.52 |
| 1:H:176:MET:HE2 | 1:H:176:MET:HA | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:421:PHE:CD1 | 1:I:423:LYS:HB2 | 2.43 | 0.52 |
| 1:J:236:LEU:HB2 | 1:J:238:MET:HG3 | 1.91 | 0.52 |
| 1:L:118:VAL:HG23 | 1:L:120:VAL:CG2 | 2.25 | 0.52 |
| 1:H:433:THR:HG23 | 1:L:412:SER:OG | 2.09 | 0.52 |
| 1:A:192:ILE:CG1 | 1:A:192:ILE:O | 2.58 | 0.52 |
| 1:A:396:ARG:HG3 | 1:A:396:ARG:NH1 | 2.25 | 0.52 |
| 1:B:248:VAL:HG13 | 1:B:272:ALA:HB3 | 1.92 | 0.52 |
| 1:C:164:VAL:HG21 | 1:C:385:TRP:CD1 | 2.44 | 0.52 |
| 1:C:218:GLY:O | 1:C:219:VAL:C | 2.46 | 0.52 |
| 1:C:256:GLY:O | 1:C:259:SER:HB2 | 2.09 | 0.52 |
| 1:C:85:GLN:OE1 | 2:C:3:ADP:N1 | 2.42 | 0.52 |
| 1:D:349:ASN:HD21 | 1:D:374:ASN:ND2 | 2.08 | 0.52 |
| 1:E:368:ILE:HG21 | 1:E:373:LEU:HD22 | 1.91 | 0.52 |
| 1:E:387:LYS:HD2 | 1:E:445:GLU:OE2 | 2.09 | 0.52 |
| 1:F:403:ARG:HH12 | 1:F:441:SER:N | 2.08 | 0.52 |
| 1:G:82:HIS:HB3 | 1:G:112:THR:HG21 | 1.91 | 0.52 |
| 1:I:167:PRO:HD3 | 1:I:176:MET:HG2 | 1.91 | 0.52 |
| 1:I:472:ASN:CG | 1:I:472:ASN:O | 2.48 | 0.52 |
| 1:K:252:PHE:CZ | 1:K:260:MET:CE | 2.92 | 0.52 |
| 1:K:48:ILE:O | 1:K:52:ILE:HG13 | 2.08 | 0.52 |
| 1:L:414:GLN:CD | 1:L:430:ILE:HG23 | 2.29 | 0.52 |
| 1:A:461:ALA:O | 1:A:464:ILE:HB | 2.08 | 0.52 |
| 1:B:271:ILE:CG1 | 1:B:283:PRO:HA | 2.39 | 0.52 |
| 1:B:61:LEU:N | 1:B:61:LEU:HD12 | 2.25 | 0.52 |
| 1:D:265:ARG:HG2 | 1:D:266:PHE:CD2 | 2.44 | 0.52 |
| 1:D:280:ILE:HD11 | 1:D:304:PHE:CB | 2.37 | 0.52 |
| 1:E:195:HIS:O | 1:E:201:LYS:HE3 | 2.10 | 0.52 |
| 1:H:439:ARG:HH12 | 1:L:405:SER:HA | 1.73 | 0.52 |
| 1:I:36:GLU:O | 1:I:37:SER:O | 2.27 | 0.52 |
| 1:I:478:ARG:O | 1:I:480:ALA:N | 2.41 | 0.52 |
| 1:I:498:VAL:O | 1:I:501:THR:CG2 | 2.58 | 0.52 |
| 1:J:82:HIS:HD2 | 1:J:83:SER:HB2 | 1.74 | 0.52 |
| 1:L:435:GLU:CD | 1:L:435:GLU:H | 2.12 | 0.52 |
| 1:B:239:THR:O | 1:B:239:THR:CG2 | 2.57 | 0.52 |
| 1:C:148:PHE:O | 1:C:152:LEU:HB2 | 2.09 | 0.52 |
| 1:F:90:LYS:HE2 | 1:F:199:THR:HG23 | 1.92 | 0.52 |
| 1:F:79:ARG:NH2 | 1:F:163:ASP:OD1 | 2.42 | 0.52 |
| 1:G:501:THR:C | 1:H:146:ARG:HH12 | 2.13 | 0.52 |
| 1:H:23:ILE:HG22 | 1:H:23:ILE:O | 2.09 | 0.52 |
| 1:H:267:GLY:O | 1:H:268:ALA:O | 2.28 | 0.52 |
| 1:H:332:THR:O | 1:H:336:ALA:HB2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:79:ARG:HE | 1:J:163:ASP:CG | 2.13 | 0.52 |
| 1:I:143:LYS:CG | 1:K:500:PHE:HE2 | 2.21 | 0.52 |
| 1:L:38:GLU:O | 1:L:39:GLU:HB2 | 2.09 | 0.52 |
| 1:L:53:LYS:HB3 | 1:L:54:PRO:CD | 2.39 | 0.52 |
| 1:B:395:GLY:O | 1:B:397:LEU:N | 2.42 | 0.52 |
| 1:A:439:ARG:HH22 | 1:B:404:ASP:HB2 | 1.75 | 0.52 |
| 1:D:239:THR:N | 1:D:240:PRO:CD | 2.62 | 0.52 |
| 1:D:263:LEU:HD12 | 1:D:268:ALA:CB | 2.40 | 0.52 |
| 1:E:10:PHE:CD1 | 1:E:10:PHE:C | 2.82 | 0.52 |
| 1:E:137:THR:HG23 | 1:E:140:GLU:CD | 2.29 | 0.52 |
| 1:E:428:ILE:HG22 | 1:E:430:ILE:CG1 | 2.38 | 0.52 |
| 1:E:433:THR:HG22 | 1:E:436:PHE:HB2 | 1.90 | 0.52 |
| 1:F:208:ILE:HD11 | 1:F:449:VAL:CG2 | 2.39 | 0.52 |
| 1:G:192:ILE:CG1 | 1:G:192:ILE:O | 2.52 | 0.52 |
| 1:I:322:LEU:O | 1:I:324:PRO:HD3 | 2.10 | 0.52 |
| 1:I:33:ARG:NH1 | 1:I:36:GLU:HG2 | 2.25 | 0.52 |
| 1:I:406:ASN:HD22 | 1:J:409:LEU:HD21 | 1.75 | 0.52 |
| 1:J:294:PHE:CZ | 1:J:298:HIS:CE1 | 2.97 | 0.52 |
| 1:K:496:ALA:C | 1:K:501:THR:O | 2.48 | 0.52 |
| 1:L:259:SER:O | 1:L:263:LEU:HB2 | 2.09 | 0.52 |
| 1:L:332:THR:H | 1:L:335:ASN:HD21 | 1.57 | 0.52 |
| 1:L:483:VAL:HG12 | 1:L:484:ASN:N | 2.25 | 0.52 |
| 1:A:465:MET:O | 1:A:468:ALA:N | 2.36 | 0.52 |
| 1:B:488:LYS:HB3 | 2:B:2:ADP:C2 | 2.45 | 0.52 |
| 1:B:30:GLU:O | 1:B:34:THR:HG22 | 2.10 | 0.52 |
| 1:C:478:ARG:O | 1:C:481:ALA:N | 2.37 | 0.52 |
| 1:D:192:ILE:O | 1:D:192:ILE:CG1 | 2.56 | 0.52 |
| 1:D:176:MET:HG2 | 1:D:199:THR:O | 2.10 | 0.52 |
| 1:D:372:TYR:CD2 | 1:D:464:ILE:HD11 | 2.44 | 0.52 |
| 1:E:378:VAL:O | 1:E:381:SER:OG | 2.27 | 0.52 |
| 1:G:44:ARG:NH1 | 1:K:71:SER:HB3 | 2.25 | 0.52 |
| 1:G:497:GLY:CA | 1:G:501:THR:HA | 2.40 | 0.52 |
| 1:I:359:ILE:HG22 | 1:I:360:PHE:N | 2.25 | 0.52 |
| 1:I:119:ASP:HB2 | 1:J:396:ARG:NH2 | 2.24 | 0.52 |
| 1:J:90:LYS:HE2 | 1:J:199:THR:CG2 | 2.36 | 0.52 |
| 1:K:199:THR:CA | 1:K:384:GLU:OE1 | 2.58 | 0.52 |
| 1:A:67:ARG:O | 1:A:68:ASP:C | 2.48 | 0.52 |
| 1:E:496:ALA:C | 1:E:501:THR:O | 2.47 | 0.52 |
| 1:F:117:VAL:HG21 | 1:F:371:LEU:HG | 1.92 | 0.52 |
| 1:F:459:ARG:NH2 | 2:F:502:ADP:O3B | 2.30 | 0.52 |
| 1:G:191:ASP:C | 1:G:193:ASN:H | 2.12 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:248:VAL:HG11 | 1:G:314:ILE:HB | 1.91 | 0.52 |
| 1:G:428:ILE:O | 1:G:431:VAL:HG12 | 2.10 | 0.52 |
| 1:G:471:TYR:O | 1:G:473:LEU:HD23 | 2.09 | 0.52 |
| 1:H:274:GLY:HA3 | 1:H:314:ILE:CD1 | 2.40 | 0.52 |
| 1:I:480:ALA:O | 1:I:483:VAL:HB | 2.10 | 0.52 |
| 1:A:42:ARG:O | 1:A:45:VAL:HG12 | 2.10 | 0.52 |
| 1:A:95:TYR:CE2 | 1:A:129:VAL:HG21 | 2.44 | 0.52 |
| 1:C:141:LEU:O | 1:C:145:THR:HG22 | 2.10 | 0.52 |
| 1:C:234:SER:C | 1:C:236:LEU:N | 2.63 | 0.52 |
| 1:C:252:PHE:HE2 | 1:C:260:MET:CE | 2.23 | 0.52 |
| 1:C:397:LEU:HD21 | 1:E:383:PHE:CZ | 2.45 | 0.52 |
| 1:C:494:ASN:ND2 | 1:C:494:ASN:C | 2.63 | 0.52 |
| 1:E:150:MET:CE | 1:E:186:THR:HG21 | 2.39 | 0.52 |
| 1:E:219:VAL:HA | 1:E:373:LEU:HD11 | 1.90 | 0.52 |
| 1:E:45:VAL:O | 1:E:45:VAL:HG13 | 2.10 | 0.52 |
| 1:C:146:ARG:NH2 | 1:E:501:THR:OXT | 2.34 | 0.52 |
| 1:F:32:LEU:O | 1:F:33:ARG:HB3 | 2.10 | 0.52 |
| 1:G:137:THR:HG22 | 1:G:138:ASP:N | 2.25 | 0.52 |
| 1:G:248:VAL:CG1 | 1:G:314:ILE:HG13 | 2.40 | 0.52 |
| 1:H:120:VAL:HG22 | 1:H:382:TYR:CD2 | 2.45 | 0.52 |
| 1:I:498:VAL:N | 1:I:501:THR:HB | 2.25 | 0.52 |
| 1:J:93:ILE:HD12 | 1:J:176:MET:HE1 | 1.92 | 0.52 |
| 1:J:49:LEU:HD12 | 1:J:49:LEU:N | 2.25 | 0.52 |
| 1:K:370:ASP:C | 1:K:372:TYR:H | 2.13 | 0.52 |
| 1:L:114:LYS:HZ3 | 1:L:374:ASN:ND2 | 2.07 | 0.52 |
| 1:L:32:LEU:O | 1:L:33:ARG:HB3 | 2.09 | 0.52 |
| 1:A:9:PHE:CE1 | 1:A:103:GLU:HA | 2.45 | 0.52 |
| 1:A:24:VAL:HG12 | 1:A:28:LEU:HD22 | 1.91 | 0.52 |
| 1:B:142:GLU:O | 1:B:144:ILE:N | 2.43 | 0.52 |
| 1:D:140:GLU:O | 1:D:144:ILE:CD1 | 2.57 | 0.52 |
| 1:D:248:VAL:HG13 | 1:D:272:ALA:HB3 | 1.91 | 0.52 |
| 1:D:288:PRO:O | 1:D:289:LYS:C | 2.48 | 0.52 |
| 1:D:78:TYR:CD2 | 1:D:101:VAL:HG22 | 2.45 | 0.52 |
| 1:E:369:PRO:CG | 1:E:478:ARG:HA | 2.40 | 0.52 |
| 1:F:224:GLU:O | 1:F:227:ILE:HG22 | 2.10 | 0.52 |
| 1:F:335:ASN:HD22 | 1:F:336:ALA:N | 2.08 | 0.52 |
| 1:F:53:LYS:HB3 | 1:F:54:PRO:CD | 2.38 | 0.52 |
| 1:H:147:ARG:HG3 | 1:H:147:ARG:NH1 | 2.23 | 0.52 |
| 1:H:499:THR:HG23 | 1:H:500:PHE:N | 2.24 | 0.52 |
| 1:J:82:HIS:ND1 | 1:J:109:SER:HA | 2.25 | 0.52 |
| 1:K:89:CYS:HB3 | 1:K:125:ALA:HB2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:275:GLU:HG3 | 1:K:301:ILE:CG1 | 2.40 | 0.52 |
| 1:L:142:GLU:HA | 1:L:178:TRP:CE3 | 2.45 | 0.52 |
| 1:L:221:HIS:O | 1:L:222:GLY:C | 2.48 | 0.52 |
| 1:L:248:VAL:HG11 | 1:L:314:ILE:HB | 1.92 | 0.52 |
| 1:A:372:TYR:CD2 | 1:A:464:ILE:CD1 | 2.93 | 0.52 |
| 1:B:331:LEU:HB2 | 1:B:352:THR:HG22 | 1.92 | 0.52 |
| 1:C:226:PHE:HD1 | 1:C:368:ILE:CD1 | 2.23 | 0.52 |
| 1:D:330:GLN:HE21 | 1:D:330:GLN:HA | 1.75 | 0.52 |
| 1:F:158:ILE:O | 1:F:158:ILE:CG2 | 2.57 | 0.52 |
| 1:F:331:LEU:HB2 | 1:F:352:THR:HG22 | 1.90 | 0.52 |
| 1:F:376:GLY:O | 1:F:380:VAL:HG23 | 2.10 | 0.52 |
| 1:F:379:THR:O | 1:F:382:TYR:HB3 | 2.10 | 0.52 |
| 1:F:68:ASP:OD2 | 1:F:137:THR:HG21 | 2.10 | 0.52 |
| 1:G:226:PHE:CB | 1:G:366:MET:HE1 | 2.40 | 0.52 |
| 1:H:336:ALA:O | 1:H:339:VAL:HG22 | 2.09 | 0.52 |
| 1:I:146:ARG:HH22 | 1:K:501:THR:C | 2.07 | 0.52 |
| 1:I:65:ILE:HA | 1:I:147:ARG:CZ | 2.39 | 0.52 |
| 1:I:225:ASN:OD1 | 1:I:458:GLU:HA | 2.10 | 0.52 |
| 1:J:168:ASP:OD1 | 1:J:169:MET:N | 2.34 | 0.52 |
| 1:J:380:VAL:HG12 | 1:J:380:VAL:O | 2.09 | 0.52 |
| 1:K:115:CYS:HB3 | 1:K:120:VAL:O | 2.10 | 0.52 |
| 1:K:496:ALA:O | 1:K:501:THR:O | 2.28 | 0.52 |
| 1:I:143:LYS:HG3 | 1:K:500:PHE:CE2 | 2.42 | 0.52 |
| 1:A:138:ASP:O | 1:A:141:LEU:HB2 | 2.10 | 0.51 |
| 1:A:92:GLY:HA2 | 1:A:166:ALA:O | 2.10 | 0.51 |
| 1:A:449:VAL:O | 1:A:450:HIS:C | 2.49 | 0.51 |
| 1:B:429:PRO:C | 1:B:431:VAL:H | 2.14 | 0.51 |
| 1:B:498:VAL:CG2 | 1:D:72:TRP:HZ2 | 2.24 | 0.51 |
| 1:D:289:LYS:O | 1:D:292:GLU:HB3 | 2.10 | 0.51 |
| 1:D:382:TYR:O | 1:D:386:LEU:HG | 2.10 | 0.51 |
| 1:E:33:ARG:CB | 1:E:33:ARG:NH1 | 2.73 | 0.51 |
| 1:G:250:GLN:CA | 1:G:314:ILE:HD11 | 2.38 | 0.51 |
| 1:I:38:GLU:OE1 | 1:I:42:ARG:NH2 | 2.42 | 0.51 |
| 1:I:48:ILE:O | 1:I:52:ILE:HG12 | 2.09 | 0.51 |
| 1:K:490:PHE:O | 1:K:491:LYS:C | 2.48 | 0.51 |
| 1:L:12:MET:O | 1:L:15:GLY:N | 2.42 | 0.51 |
| 1:A:33:ARG:NH2 | 1:A:42:ARG:HD2 | 2.25 | 0.51 |
| 1:B:234:SER:C | 1:B:236:LEU:N | 2.61 | 0.51 |
| 1:B:460:SER:O | 1:B:464:ILE:HG13 | 2.09 | 0.51 |
| 1:C:300:SER:C | 1:C:302:LEU:H | 2.12 | 0.51 |
| 1:C:325:ALA:O | 1:C:326:ALA:CB | 2.52 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:369:PRO:HD3 | 1:C:477:LEU:HB3 | 1.92 | 0.51 |
| 1:D:221:HIS:HA | 1:D:224:GLU:HB3 | 1.92 | 0.51 |
| 1:D:6:ASP:HB2 | 1:D:329:LYS:HD3 | 1.92 | 0.51 |
| 1:F:75:ILE:HD12 | 1:F:144:ILE:HG12 | 1.92 | 0.51 |
| 1:F:331:LEU:HB3 | 1:F:352:THR:HG22 | 1.91 | 0.51 |
| 1:G:368:ILE:CG2 | 1:G:373:LEU:HD13 | 2.40 | 0.51 |
| 1:H:336:ALA:HB3 | 1:H:337:PRO:HD3 | 1.92 | 0.51 |
| 1:H:36:GLU:OE2 | 1:H:42:ARG:NH1 | 2.41 | 0.51 |
| 1:I:26:ASP:C | 1:I:28:LEU:H | 2.13 | 0.51 |
| 1:K:395:GLY:HA2 | 1:K:398:THR:HG23 | 1.91 | 0.51 |
| 1:K:41:LYS:O | 1:K:44:ARG:HB2 | 2.10 | 0.51 |
| 1:K:6:ASP:OD2 | 1:K:6:ASP:O | 2.28 | 0.51 |
| 1:A:345:ALA:HB1 | 1:A:373:LEU:CD2 | 2.41 | 0.51 |
| 1:B:40:GLN:HG3 | 1:B:40:GLN:O | 2.10 | 0.51 |
| 1:C:246:THR:OG1 | 1:C:320:ASP:HB2 | 2.10 | 0.51 |
| 1:E:248:VAL:HG22 | 1:E:272:ALA:H | 1.76 | 0.51 |
| 1:F:142:GLU:OE2 | 1:F:146:ARG:NH1 | 2.42 | 0.51 |
| 1:G:359:ILE:O | 1:G:362:GLU:N | 2.43 | 0.51 |
| 1:H:151:GLU:OE1 | 1:J:57:HIS:CE1 | 2.64 | 0.51 |
| 1:H:244:ASP:C | 1:H:245:LYS:HG3 | 2.31 | 0.51 |
| 1:I:244:ASP:OD1 | 1:I:245:LYS:HE2 | 2.10 | 0.51 |
| 1:J:30:GLU:O | 1:J:32:LEU:N | 2.43 | 0.51 |
| 1:K:176:MET:HE3 | 1:K:179:ILE:HD12 | 1.92 | 0.51 |
| 1:K:51:ILE:O | 1:K:54:PRO:HD2 | 2.10 | 0.51 |
| 1:L:221:HIS:HA | 1:L:224:GLU:HB3 | 1.92 | 0.51 |
| 1:A:82:HIS:CD2 | 1:A:82:HIS:C | 2.84 | 0.51 |
| 1:C:176:MET:HE1 | 1:C:179:ILE:HD12 | 1.90 | 0.51 |
| 1:C:252:PHE:CE2 | 1:C:260:MET:CE | 2.94 | 0.51 |
| 1:C:344:ILE:HD11 | 1:C:360:PHE:CD1 | 2.46 | 0.51 |
| 1:C:67:ARG:CD | 1:C:73:GLU:OE1 | 2.57 | 0.51 |
| 1:D:96:SER:O | 1:D:99:VAL:CG1 | 2.57 | 0.51 |
| 1:E:282:ASN:O | 1:E:284:ASP:N | 2.43 | 0.51 |
| 1:F:491:LYS:O | 1:F:495:GLU:HB2 | 2.10 | 0.51 |
| 1:F:498:VAL:N | 1:F:501:THR:HB | 2.26 | 0.51 |
| 1:G:417:LEU:CD2 | 1:H:417:LEU:HD11 | 2.39 | 0.51 |
| 1:H:243:GLY:O | 1:H:244:ASP:HB3 | 2.10 | 0.51 |
| 1:H:247:PHE:CD2 | 1:H:263:LEU:HD12 | 2.46 | 0.51 |
| 1:I:248:VAL:HG11 | 1:I:314:ILE:HB | 1.92 | 0.51 |
| 1:I:486:ILE:O | 1:I:487:GLU:C | 2.47 | 0.51 |
| 1:K:163:ASP:O | 1:K:165:PRO:HD3 | 2.10 | 0.51 |
| 1:K:30:GLU:CG | 1:K:31:ASP:H | 1.98 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:274:GLY:O | 1:L:275:GLU:CB | 2.58 | 0.51 |
| 1:A:90:LYS:HE2 | 1:A:164:VAL:HG12 | 1.93 | 0.51 |
| 1:A:239:THR:O | 1:A:239:THR:HG23 | 2.09 | 0.51 |
| 1:B:323:ILE:CG1 | 1:B:323:ILE:O | 2.56 | 0.51 |
| 1:B:87:THR:CB | 1:B:88:PRO:CD | 2.89 | 0.51 |
| 1:C:264:HIS:CD2 | 1:C:288:PRO:HD3 | 2.46 | 0.51 |
| 1:C:250:GLN:HG2 | 1:C:314:ILE:HD11 | 1.93 | 0.51 |
| 1:D:176:MET:HG3 | 1:D:198:VAL:CG2 | 2.40 | 0.51 |
| 1:F:248:VAL:CG2 | 1:F:271:ILE:HG13 | 2.41 | 0.51 |
| 1:F:382:TYR:O | 1:F:385:TRP:HB3 | 2.11 | 0.51 |
| 1:F:87:THR:OG1 | 1:F:88:PRO:HD3 | 2.10 | 0.51 |
| 1:G:104:VAL:HG23 | 1:G:105:LYS:N | 2.25 | 0.51 |
| 1:G:7:PRO:O | 1:G:329:LYS:NZ | 2.39 | 0.51 |
| 1:H:90:LYS:HB2 | 1:H:122:PHE:HB3 | 1.92 | 0.51 |
| 1:I:65:ILE:HG21 | 1:I:144:ILE:HG12 | 1.93 | 0.51 |
| 1:I:176:MET:O | 1:I:179:ILE:HB | 2.10 | 0.51 |
| 1:J:28:LEU:HD21 | 1:J:490:PHE:CG | 2.46 | 0.51 |
| 1:K:117:VAL:HG21 | 1:K:371:LEU:O | 2.11 | 0.51 |
| 1:L:343:ILE:HG12 | 1:L:366:MET:HB3 | 1.93 | 0.51 |
| 1:L:368:ILE:HA | 1:L:477:LEU:HD23 | 1.91 | 0.51 |
| 1:L:465:MET:O | 1:L:468:ALA:N | 2.40 | 0.51 |
| 1:A:359:ILE:O | 1:A:362:GLU:N | 2.43 | 0.51 |
| 1:A:407:TYR:CE1 | 1:H:424:HIS:CE1 | 2.99 | 0.51 |
| 1:B:164:VAL:HG13 | 1:B:197:CYS:C | 2.31 | 0.51 |
| 1:B:42:ARG:HD2 | 1:B:42:ARG:N | 2.25 | 0.51 |
| 1:B:497:GLY:N | 1:B:501:THR:HA | 2.25 | 0.51 |
| 1:D:36:GLU:O | 1:D:42:ARG:NH1 | 2.43 | 0.51 |
| 1:D:428:ILE:O | 1:D:428:ILE:HG12 | 2.11 | 0.51 |
| 1:E:294:PHE:HE2 | 1:E:301:ILE:O | 1.93 | 0.51 |
| 1:E:60:SER:HB3 | 1:E:78:TYR:HD2 | 1.75 | 0.51 |
| 2:B:2:ADP:H5'2 | 1:F:203:ILE:CG2 | 2.41 | 0.51 |
| 1:G:129:VAL:O | 1:G:131:ILE:N | 2.43 | 0.51 |
| 1:G:82:HIS:HB3 | 1:G:112:THR:CG2 | 2.40 | 0.51 |
| 1:G:82:HIS:HD2 | 1:G:112:THR:CG2 | 2.20 | 0.51 |
| 1:H:44:ARG:NH1 | 1:H:44:ARG:CB | 2.70 | 0.51 |
| 1:I:38:GLU:N | 1:I:42:ARG:CZ | 2.73 | 0.51 |
| 1:J:181:ASP:O | 1:J:183:TYR:N | 2.44 | 0.51 |
| 1:J:212:ILE:N | 1:J:212:ILE:CD1 | 2.60 | 0.51 |
| 1:J:281:TRP:CD1 | 1:J:282:ASN:N | 2.79 | 0.51 |
| 1:J:390:ASN:O | 1:J:391:HIS:HB2 | 2.11 | 0.51 |
| 1:J:42:ARG:C | 1:J:45:VAL:HG12 | 2.31 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:118:VAL:HG23 | 1:K:120:VAL:CG2 | 2.41 | 0.51 |
| 1:K:65:ILE:HD13 | 1:K:144:ILE:CG1 | 2.41 | 0.51 |
| 1:K:433:THR:O | 1:K:434:ALA:C | 2.47 | 0.51 |
| 1:L:82:HIS:ND1 | 1:L:109:SER:HA | 2.25 | 0.51 |
| 1:L:497:GLY:HA3 | 1:L:501:THR:HA | 1.91 | 0.51 |
| 1:A:465:MET:O | 1:A:466:ARG:C | 2.49 | 0.51 |
| 1:B:208:ILE:HD11 | 1:B:449:VAL:HG22 | 1.91 | 0.51 |
| 1:B:255:VAL:HG13 | 1:B:256:GLY:N | 2.20 | 0.51 |
| 1:B:406:ASN:O | 1:B:409:LEU:HB2 | 2.11 | 0.51 |
| 1:C:227:ILE:HG22 | 1:C:228:ASN:ND2 | 2.26 | 0.51 |
| 1:C:431:VAL:HG11 | 1:D:419:ARG:HH21 | 1.75 | 0.51 |
| 1:E:429:PRO:C | 1:E:431:VAL:N | 2.64 | 0.51 |
| 1:G:245:LYS:HB2 | 1:G:268:ALA:HA | 1.92 | 0.51 |
| 1:G:81:GLN:HG3 | 1:G:157:PHE:CE1 | 2.46 | 0.51 |
| 1:H:45:VAL:O | 1:H:45:VAL:CG1 | 2.58 | 0.51 |
| 1:J:248:VAL:HG13 | 1:J:272:ALA:O | 2.10 | 0.51 |
| 1:K:118:VAL:O | 1:K:118:VAL:HG23 | 2.10 | 0.51 |
| 1:K:166:ALA:HB1 | 1:K:167:PRO:HD2 | 1.93 | 0.51 |
| 1:K:219:VAL:HG13 | 1:K:220:PHE:N | 2.25 | 0.51 |
| 1:K:479:THR:O | 1:K:483:VAL:HG23 | 2.10 | 0.51 |
| 1:K:371:LEU:CD2 | 1:K:481:ALA:CB | 2.88 | 0.51 |
| 1:L:497:GLY:N | 1:L:501:THR:HA | 2.25 | 0.51 |
| 1:G:146:ARG:NH2 | 1:L:501:THR:OXT | 2.36 | 0.51 |
| 1:A:355:GLU:HA | 1:A:358:LYS:CD | 2.40 | 0.51 |
| 1:C:227:ILE:HA | 1:C:233:MET:SD | 2.50 | 0.51 |
| 1:C:363:ARG:HH11 | 1:C:363:ARG:CB | 2.24 | 0.51 |
| 1:C:478:ARG:HG2 | 1:C:478:ARG:HH11 | 1.74 | 0.51 |
| 1:D:158:ILE:HD11 | 1:D:197:CYS:O | 2.11 | 0.51 |
| 1:D:252:PHE:CD2 | 1:D:273:VAL:HG11 | 2.45 | 0.51 |
| 1:D:274:GLY:O | 1:D:275:GLU:CB | 2.57 | 0.51 |
| 1:E:223:ILE:CD1 | 1:E:263:LEU:HD21 | 2.39 | 0.51 |
| 1:E:383:PHE:HA | 1:E:386:LEU:HD12 | 1.93 | 0.51 |
| 1:F:118:VAL:HG23 | 1:F:120:VAL:HG23 | 1.93 | 0.51 |
| 1:F:13:VAL:HG11 | 1:F:109:SER:OG | 2.10 | 0.51 |
| 1:F:181:ASP:O | 1:F:182:THR:C | 2.48 | 0.51 |
| 1:F:459:ARG:O | 1:F:463:GLN:HG3 | 2.10 | 0.51 |
| 1:G:157:PHE:CE2 | 1:K:155:LYS:HD2 | 2.46 | 0.51 |
| 1:I:96:SER:O | 1:I:98:ASP:N | 2.44 | 0.51 |
| 1:K:9:PHE:HD1 | 1:K:10:PHE:N | 2.09 | 0.51 |
| 1:K:293:ASP:HB3 | 1:K:297:GLN:HE21 | 1.76 | 0.51 |
| 1:L:252:PHE:CZ | 1:L:260:MET:HE1 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:39:GLU:OE1 | 1:L:41:LYS:HD2 | 2.10 | 0.51 |
| 1:B:361:LEU:HD23 | 1:B:361:LEU:O | 2.11 | 0.51 |
| 1:A:436:PHE:CZ | 1:B:409:LEU:HD22 | 2.46 | 0.51 |
| 1:C:104:VAL:CG2 | 1:C:105:LYS:H | 2.24 | 0.51 |
| 1:D:213:SER:O | 1:D:217:ARG:HG3 | 2.11 | 0.51 |
| 1:E:323:ILE:HG12 | 1:E:323:ILE:O | 2.10 | 0.51 |
| 1:E:359:ILE:O | 1:E:362:GLU:N | 2.44 | 0.51 |
| 1:F:31:ASP:O | 1:F:32:LEU:HD23 | 2.10 | 0.51 |
| 1:F:414:GLN:CD | 1:F:430:ILE:HG12 | 2.31 | 0.51 |
| 1:G:126:LYS:NZ | 1:G:168:ASP:OD1 | 2.41 | 0.51 |
| 1:G:53:LYS:HB3 | 1:G:54:PRO:HD3 | 1.93 | 0.51 |
| 1:H:461:ALA:O | 1:H:464:ILE:HB | 2.11 | 0.51 |
| 1:I:497:GLY:HA3 | 1:I:501:THR:HA | 1.92 | 0.51 |
| 1:K:286:ILE:CG2 | 1:K:291:LEU:HD22 | 2.40 | 0.51 |
| 1:K:39:GLU:HB2 | 1:K:41:LYS:HG3 | 1.92 | 0.51 |
| 1:L:142:GLU:HA | 1:L:178:TRP:CZ3 | 2.46 | 0.51 |
| 1:L:214:ALA:HB2 | 1:L:380:VAL:HG21 | 1.93 | 0.51 |
| 1:L:386:LEU:O | 1:L:387:LYS:C | 2.49 | 0.51 |
| 1:L:87:THR:OG1 | 1:L:88:PRO:HD3 | 2.11 | 0.51 |
| 1:A:176:MET:CE | 1:A:179:ILE:HD12 | 2.40 | 0.51 |
| 1:A:412:SER:O | 1:A:413:VAL:C | 2.48 | 0.51 |
| 1:B:137:THR:HG22 | 1:B:140:GLU:OE1 | 2.11 | 0.51 |
| 1:B:271:ILE:O | 1:B:271:ILE:HG12 | 2.10 | 0.51 |
| 1:B:277:ASP:OD2 | 1:B:300:SER:HB2 | 2.10 | 0.51 |
| 1:C:248:VAL:HG13 | 1:C:272:ALA:O | 2.10 | 0.51 |
| 1:C:257:LEU:HA | 1:C:260:MET:CE | 2.38 | 0.51 |
| 1:C:32:LEU:O | 1:C:33:ARG:CB | 2.58 | 0.51 |
| 1:C:96:SER:O | 1:C:99:VAL:CG2 | 2.54 | 0.51 |
| 1:D:471:TYR:O | 1:D:473:LEU:HG | 2.11 | 0.51 |
| 1:D:8:ASN:HD21 | 1:D:10:PHE:HB3 | 1.76 | 0.51 |
| 1:E:175:GLU:HA | 1:E:178:TRP:CE3 | 2.46 | 0.51 |
| 1:E:294:PHE:CD1 | 1:E:298:HIS:CE1 | 2.99 | 0.51 |
| 1:F:150:MET:CE | 1:F:186:THR:HG21 | 2.41 | 0.51 |
| 1:F:248:VAL:HG13 | 1:F:272:ALA:O | 2.11 | 0.51 |
| 1:A:416:SER:HB2 | 1:F:428:ILE:O | 2.10 | 0.51 |
| 1:G:111:MET:HB3 | 1:G:124:GLY:HA2 | 1.93 | 0.51 |
| 1:G:33:ARG:HH21 | 1:G:45:VAL:HG11 | 1.74 | 0.51 |
| 1:G:45:VAL:CG1 | 1:G:45:VAL:O | 2.57 | 0.51 |
| 1:H:133:PRO:HB3 | 1:H:141:LEU:HD11 | 1.93 | 0.51 |
| 1:H:164:VAL:HG13 | 1:H:198:VAL:HA | 1.91 | 0.51 |
| 1:H:411:MET:HA | 1:H:430:ILE:CG2 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:115:CYS:O | 1:I:116:ALA:C | 2.49 | 0.51 |
| 1:I:94:ARG:HD2 | 1:I:170:SER:OG | 2.11 | 0.51 |
| 1:I:244:ASP:O | 1:I:245:LYS:HG3 | 2.10 | 0.51 |
| 1:J:294:PHE:CZ | 1:J:298:HIS:HE1 | 2.29 | 0.51 |
| 1:L:346:GLU:HG2 | 1:L:351:PRO:HG2 | 1.92 | 0.51 |
| 1:L:471:TYR:HB2 | 1:L:473:LEU:HD12 | 1.93 | 0.51 |
| 1:A:148:PHE:CE2 | 1:A:152:LEU:HD22 | 2.47 | 0.50 |
| 2:A:1:ADP:O3A | 1:B:393:SER:HB3 | 2.12 | 0.50 |
| 1:B:222:GLY:HA3 | 1:B:373:LEU:HD11 | 1.91 | 0.50 |
| 1:C:45:VAL:C | 1:C:47:GLY:H | 2.14 | 0.50 |
| 1:D:81:GLN:OE1 | 1:D:84:HIS:HE1 | 1.94 | 0.50 |
| 1:E:335:ASN:C | 1:E:335:ASN:HD22 | 2.11 | 0.50 |
| 1:C:409:LEU:HD11 | 1:E:409:LEU:HB3 | 1.93 | 0.50 |
| 1:F:315:LEU:HD12 | 1:F:315:LEU:N | 2.26 | 0.50 |
| 1:G:322:LEU:HD22 | 1:G:344:ILE:HD12 | 1.93 | 0.50 |
| 1:G:428:ILE:N | 1:G:428:ILE:HD13 | 2.27 | 0.50 |
| 1:H:471:TYR:O | 1:H:472:ASN:C | 2.49 | 0.50 |
| 1:K:369:PRO:HB3 | 1:K:478:ARG:HG3 | 1.93 | 0.50 |
| 1:K:81:GLN:NE2 | 1:K:157:PHE:CD1 | 2.79 | 0.50 |
| 1:L:369:PRO:HD3 | 1:L:477:LEU:HB3 | 1.91 | 0.50 |
| 1:A:67:ARG:NE | 1:A:73:GLU:OE2 | 2.44 | 0.50 |
| 1:C:20:GLY:O | 1:C:24:VAL:CG2 | 2.59 | 0.50 |
| 1:C:324:PRO:HD2 | 1:C:345:ALA:O | 2.11 | 0.50 |
| 1:C:344:ILE:CD1 | 1:C:365:ILE:HG21 | 2.39 | 0.50 |
| 1:C:8:ASN:O | 1:C:10:PHE:N | 2.44 | 0.50 |
| 1:D:396:ARG:CG | 1:D:396:ARG:NH1 | 2.71 | 0.50 |
| 1:F:403:ARG:NH1 | 1:F:440:ILE:C | 2.65 | 0.50 |
| 1:F:413:VAL:HG12 | 1:F:413:VAL:O | 2.11 | 0.50 |
| 1:G:116:ALA:O | 1:G:488:LYS:NZ | 2.38 | 0.50 |
| 1:G:295:LYS:HD3 | 1:G:301:ILE:CG2 | 2.42 | 0.50 |
| 1:G:222:GLY:HA3 | 1:G:373:LEU:CD1 | 2.40 | 0.50 |
| 1:H:465:MET:O | 1:H:468:ALA:HB3 | 2.10 | 0.50 |
| 1:I:229:GLU:O | 1:I:231:SER:N | 2.45 | 0.50 |
| 1:J:198:VAL:O | 1:J:201:LYS:HE3 | 2.11 | 0.50 |
| 1:J:404:ASP:O | 1:J:405:SER:C | 2.50 | 0.50 |
| 1:L:146:ARG:NH2 | 1:L:181:ASP:OD1 | 2.45 | 0.50 |
| 1:L:346:GLU:OE2 | 1:L:352:THR:HG23 | 2.11 | 0.50 |
| 1:C:465:MET:O | 1:C:468:ALA:N | 2.35 | 0.50 |
| 1:E:142:GLU:CG | 1:E:146:ARG:HD2 | 2.40 | 0.50 |
| 1:E:79:ARG:HH11 | 1:E:79:ARG:HG3 | 1.76 | 0.50 |
| 1:G:162:ILE:HG22 | 1:G:163:ASP:N | 2.25 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:111:MET:HE1 | 1:G:378:VAL:HG21 | 1.94 | 0.50 |
| 1:G:392:VAL:HG21 | 1:L:386:LEU:CD1 | 2.39 | 0.50 |
| 1:G:65:ILE:HD13 | 1:G:75:ILE:HD11 | 1.93 | 0.50 |
| 1:H:176:MET:CE | 1:H:176:MET:HA | 2.41 | 0.50 |
| 1:H:322:LEU:O | 1:H:324:PRO:HD3 | 2.10 | 0.50 |
| 1:H:117:VAL:HG21 | 1:H:371:LEU:HG | 1.94 | 0.50 |
| 1:I:175:GLU:HG3 | 1:I:178:TRP:CZ3 | 2.46 | 0.50 |
| 1:I:213:SER:HB3 | 1:I:262:TYR:OH | 2.11 | 0.50 |
| 1:K:16:PHE:CE2 | 1:K:478:ARG:NH1 | 2.79 | 0.50 |
| 1:C:239:THR:HA | 1:C:245:LYS:NZ | 2.26 | 0.50 |
| 1:D:116:ALA:HA | 2:D:4:ADP:N6 | 2.27 | 0.50 |
| 1:D:287:ASP:HB3 | 1:D:290:GLU:HG3 | 1.92 | 0.50 |
| 1:E:68:ASP:OD2 | 1:E:140:GLU:HG3 | 2.11 | 0.50 |
| 1:E:65:ILE:O | 1:E:65:ILE:HG13 | 2.10 | 0.50 |
| 1:E:66:ARG:HD3 | 1:E:72:TRP:CH2 | 2.46 | 0.50 |
| 1:B:436:PHE:CD2 | 1:F:408:HIS:HB3 | 2.46 | 0.50 |
| 1:F:67:ARG:HG2 | 1:F:67:ARG:NH1 | 2.25 | 0.50 |
| 1:G:238:MET:O | 1:G:239:THR:HG22 | 2.11 | 0.50 |
| 1:G:74:VAL:O | 1:G:74:VAL:HG23 | 2.11 | 0.50 |
| 1:H:82:HIS:N | 1:H:124:GLY:O | 2.41 | 0.50 |
| 1:H:280:ILE:CG2 | 1:H:307:ALA:HB1 | 2.41 | 0.50 |
| 1:I:165:PRO:O | 1:I:198:VAL:HG23 | 2.12 | 0.50 |
| 1:I:294:PHE:CD1 | 1:I:304:PHE:HD1 | 2.30 | 0.50 |
| 1:I:53:LYS:HB3 | 1:I:54:PRO:HD3 | 1.92 | 0.50 |
| 1:J:30:GLU:O | 1:J:31:ASP:C | 2.49 | 0.50 |
| 1:J:414:GLN:NE2 | 1:J:430:ILE:HG23 | 2.26 | 0.50 |
| 1:K:211:ARG:O | 1:K:214:ALA:HB3 | 2.11 | 0.50 |
| 1:K:417:LEU:O | 1:K:420:LYS:CG | 2.59 | 0.50 |
| 1:K:476:ASP:OD2 | 1:K:479:THR:OG1 | 2.23 | 0.50 |
| 1:K:459:ARG:NH1 | 2:K:502:ADP:O3B | 2.37 | 0.50 |
| 1:A:439:ARG:HG3 | 1:A:439:ARG:HH11 | 1.76 | 0.50 |
| 1:B:282:ASN:O | 1:B:284:ASP:N | 2.43 | 0.50 |
| 1:C:234:SER:O | 1:C:236:LEU:N | 2.45 | 0.50 |
| 1:D:68:ASP:OD1 | 1:D:140:GLU:CG | 2.60 | 0.50 |
| 1:E:164:VAL:HA | 1:E:197:CYS:O | 2.11 | 0.50 |
| 1:E:24:VAL:HG22 | 1:E:483:VAL:HG13 | 1.93 | 0.50 |
| 1:G:271:ILE:CG1 | 1:G:283:PRO:HA | 2.42 | 0.50 |
| 1:H:236:LEU:HB3 | 1:H:342:LYS:HE2 | 1.93 | 0.50 |
| 1:I:409:LEU:O | 1:I:413:VAL:HG23 | 2.11 | 0.50 |
| 1:I:461:ALA:O | 1:I:464:ILE:HB | 2.11 | 0.50 |
| 1:K:344:ILE:HD11 | 1:K:360:PHE:CD1 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:465:MET:O | 1:K:466:ARG:C | 2.50 | 0.50 |
| 1:A:121:PRO:O | 1:A:122:PHE:HD2 | 1.94 | 0.50 |
| 1:A:390:ASN:O | 1:A:392:VAL:HG23 | 2.11 | 0.50 |
| 1:D:327:SER:HB2 | 1:D:330:GLN:OE1 | 2.12 | 0.50 |
| 1:D:9:PHE:CD2 | 1:D:328:GLU:OE1 | 2.64 | 0.50 |
| 1:D:421:PHE:CZ | 1:D:423:LYS:HB2 | 2.47 | 0.50 |
| 1:E:384:GLU:O | 1:E:387:LYS:HB3 | 2.12 | 0.50 |
| 1:F:91:GLY:HA3 | 1:F:125:ALA:O | 2.11 | 0.50 |
| 1:F:250:GLN:HG2 | 1:F:314:ILE:CG1 | 2.41 | 0.50 |
| 1:I:117:VAL:HG23 | 1:I:485:ALA:HB2 | 1.94 | 0.50 |
| 1:K:236:LEU:HA | 1:K:342:LYS:HZ1 | 1.76 | 0.50 |
| 1:L:82:HIS:CB | 1:L:112:THR:HG21 | 2.41 | 0.50 |
| 1:L:413:VAL:O | 1:L:417:LEU:HB2 | 2.11 | 0.50 |
| 1:A:239:THR:H | 1:A:240:PRO:HD3 | 1.73 | 0.50 |
| 1:B:321:ILE:HG23 | 1:B:343:ILE:CG2 | 2.41 | 0.50 |
| 1:C:28:LEU:HD21 | 1:C:490:PHE:CD1 | 2.47 | 0.50 |
| 1:D:144:ILE:H | 1:D:144:ILE:HD12 | 1.77 | 0.50 |
| 1:E:107:LEU:O | 1:E:108:ALA:C | 2.46 | 0.50 |
| 1:F:428:ILE:N | 1:F:428:ILE:CD1 | 2.65 | 0.50 |
| 1:G:252:PHE:HE2 | 1:G:260:MET:HE1 | 1.77 | 0.50 |
| 1:G:17:PHE:CD1 | 1:G:486:ILE:HD12 | 2.46 | 0.50 |
| 1:I:14:GLU:CG | 1:I:53:LYS:HZ2 | 2.25 | 0.50 |
| 1:J:346:GLU:CD | 1:J:478:ARG:HH22 | 2.14 | 0.50 |
| 1:I:439:ARG:HH12 | 1:J:404:ASP:HB2 | 1.76 | 0.50 |
| 1:J:414:GLN:OE1 | 1:J:430:ILE:HG12 | 2.11 | 0.50 |
| 1:K:147:ARG:NH1 | 1:K:151:GLU:OE2 | 2.44 | 0.50 |
| 1:K:175:GLU:HA | 1:K:178:TRP:CE3 | 2.47 | 0.50 |
| 1:B:249:VAL:HB | 1:B:323:ILE:CD1 | 2.42 | 0.50 |
| 1:B:96:SER:O | 1:B:99:VAL:HG13 | 2.12 | 0.50 |
| 1:C:176:MET:HG2 | 1:C:199:THR:O | 2.10 | 0.50 |
| 1:C:471:TYR:O | 1:C:472:ASN:C | 2.51 | 0.50 |
| 1:E:410:LEU:HB3 | 1:E:430:ILE:HA | 1.92 | 0.50 |
| 1:E:399:PHE:CE2 | 1:E:443:ALA:HB1 | 2.47 | 0.50 |
| 1:F:108:ALA:O | 1:F:109:SER:C | 2.50 | 0.50 |
| 1:F:407:TYR:OH | 1:G:242:PHE:HA | 2.12 | 0.50 |
| 1:G:226:PHE:HB3 | 1:G:366:MET:HE1 | 1.92 | 0.50 |
| 1:H:323:ILE:HG22 | 1:H:323:ILE:O | 2.12 | 0.50 |
| 1:H:459:ARG:NH2 | 2:H:502:ADP:O3B | 2.45 | 0.50 |
| 1:I:496:ALA:CA | 1:I:501:THR:O | 2.60 | 0.50 |
| 1:J:167:PRO:HG3 | 1:J:176:MET:CG | 2.38 | 0.50 |
| 1:J:344:ILE:HD12 | 1:J:367:VAL:CG2 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:153:ALA:CA | 1:K:158:ILE:HG22 | 2.41 | 0.50 |
| 1:K:328:GLU:HG3 | 1:K:329:LYS:HG2 | 1.93 | 0.50 |
| 1:L:233:MET:HE1 | 1:L:343:ILE:CD1 | 2.31 | 0.50 |
| 1:L:75:ILE:HG23 | 1:L:131:ILE:CD1 | 2.42 | 0.50 |
| 1:A:91:GLY:O | 1:A:165:PRO:HA | 2.12 | 0.50 |
| 1:A:346:GLU:OE1 | 1:A:478:ARG:NH2 | 2.45 | 0.50 |
| 1:D:111:MET:HB3 | 1:D:124:GLY:HA2 | 1.94 | 0.50 |
| 1:D:428:ILE:CD1 | 1:D:428:ILE:N | 2.74 | 0.50 |
| 1:E:95:TYR:CE2 | 1:E:129:VAL:CG2 | 2.95 | 0.50 |
| 1:E:322:LEU:CD2 | 1:E:323:ILE:N | 2.74 | 0.50 |
| 1:F:322:LEU:HD13 | 1:F:344:ILE:HG23 | 1.94 | 0.50 |
| 1:F:207:GLY:HA2 | 1:F:384:GLU:OE1 | 2.12 | 0.50 |
| 1:F:67:ARG:HG2 | 1:F:67:ARG:HH11 | 1.77 | 0.50 |
| 1:H:165:PRO:C | 1:H:198:VAL:HG23 | 2.32 | 0.50 |
| 1:H:234:SER:O | 1:H:236:LEU:N | 2.44 | 0.50 |
| 1:H:353:THR:HB | 1:H:354:PRO:HD2 | 1.93 | 0.50 |
| 1:I:20:GLY:O | 1:I:24:VAL:HG23 | 2.12 | 0.50 |
| 1:J:371:LEU:HD22 | 1:J:482:TYR:CD2 | 2.47 | 0.50 |
| 1:K:219:VAL:O | 1:K:220:PHE:C | 2.50 | 0.50 |
| 1:J:394:TYR:CE2 | 1:K:397:LEU:HD13 | 2.47 | 0.50 |
| 1:K:48:ILE:HG13 | 1:K:490:PHE:CE1 | 2.39 | 0.50 |
| 1:A:153:ALA:N | 1:A:158:ILE:HG22 | 2.27 | 0.49 |
| 1:B:187:ILE:N | 1:B:187:ILE:HD13 | 2.27 | 0.49 |
| 1:B:252:PHE:HE2 | 1:B:260:MET:HE2 | 1.77 | 0.49 |
| 1:B:255:VAL:O | 1:B:256:GLY:C | 2.48 | 0.49 |
| 1:C:142:GLU:HA | 1:C:145:THR:HG23 | 1.93 | 0.49 |
| 1:C:281:TRP:HB3 | 1:C:308:LYS:O | 2.12 | 0.49 |
| 1:C:328:GLU:HG3 | 1:C:329:LYS:NZ | 2.27 | 0.49 |
| 1:C:388:ASN:O | 1:C:390:ASN:N | 2.45 | 0.49 |
| 1:D:398:THR:O | 1:D:401:TYR:N | 2.45 | 0.49 |
| 1:F:247:PHE:CZ | 1:F:270:CYS:HB2 | 2.47 | 0.49 |
| 1:G:258:HIS:O | 1:G:259:SER:C | 2.49 | 0.49 |
| 1:G:58:VAL:HG23 | 1:G:80:ALA:HB2 | 1.93 | 0.49 |
| 1:H:462:ARG:O | 1:H:463:GLN:C | 2.51 | 0.49 |
| 1:H:61:LEU:H | 1:H:61:LEU:HD12 | 1.77 | 0.49 |
| 1:I:399:PHE:CZ | 1:I:448:ILE:HD11 | 2.47 | 0.49 |
| 1:J:9:PHE:O | 1:J:13:VAL:HG23 | 2.13 | 0.49 |
| 1:K:346:GLU:O | 1:K:373:LEU:HD23 | 2.12 | 0.49 |
| 1:K:87:THR:O | 1:K:88:PRO:C | 2.50 | 0.49 |
| 1:L:201:LYS:NZ | 1:L:388:ASN:HD21 | 2.10 | 0.49 |
| 1:L:403:ARG:NH1 | 1:L:407:TYR:HE2 | 2.10 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:257:LEU:HG | 1:A:258:HIS:N | 2.26 | 0.49 |
| 1:A:497:GLY:CA | 1:A:501:THR:HA | 2.42 | 0.49 |
| 1:B:429:PRO:C | 1:B:431:VAL:N | 2.66 | 0.49 |
| 1:C:95:TYR:OH | 1:C:145:THR:HB | 2.12 | 0.49 |
| 1:C:230:ALA:O | 1:C:231:SER:C | 2.49 | 0.49 |
| 1:E:335:ASN:ND2 | 1:E:335:ASN:C | 2.65 | 0.49 |
| 1:C:72:TRP:HE1 | 1:F:498:VAL:HG21 | 1.75 | 0.49 |
| 1:G:159:GLY:O | 1:G:163:ASP:O | 2.29 | 0.49 |
| 1:H:248:VAL:HG23 | 1:H:271:ILE:HG23 | 1.93 | 0.49 |
| 1:H:280:ILE:HG23 | 1:H:307:ALA:HB1 | 1.94 | 0.49 |
| 1:H:281:TRP:O | 1:H:282:ASN:HB2 | 2.12 | 0.49 |
| 1:H:323:ILE:HG12 | 1:H:345:ALA:HB3 | 1.94 | 0.49 |
| 1:H:394:TYR:HB2 | 1:H:445:GLU:HG3 | 1.93 | 0.49 |
| 1:I:239:THR:O | 1:I:239:THR:HG23 | 2.12 | 0.49 |
| 1:I:336:ALA:HB1 | 1:I:359:ILE:HG21 | 1.94 | 0.49 |
| 1:K:79:ARG:NH2 | 1:K:91:GLY:O | 2.40 | 0.49 |
| 1:L:387:LYS:HD2 | 1:L:445:GLU:OE2 | 2.12 | 0.49 |
| 1:C:226:PHE:HD1 | 1:C:368:ILE:HD13 | 1.77 | 0.49 |
| 1:C:436:PHE:CE1 | 1:D:409:LEU:HD22 | 2.47 | 0.49 |
| 1:D:462:ARG:HD3 | 1:D:466:ARG:NH2 | 2.27 | 0.49 |
| 1:G:278:GLY:HA3 | 1:G:302:LEU:HD21 | 1.94 | 0.49 |
| 1:H:227:ILE:O | 1:H:233:MET:HG3 | 2.13 | 0.49 |
| 1:I:142:GLU:HG2 | 1:I:146:ARG:HD2 | 1.94 | 0.49 |
| 1:I:212:ILE:H | 1:I:212:ILE:CD1 | 2.25 | 0.49 |
| 1:I:321:ILE:CD1 | 1:I:321:ILE:N | 2.75 | 0.49 |
| 1:I:339:VAL:O | 1:I:339:VAL:HG23 | 2.12 | 0.49 |
| 1:J:36:GLU:O | 1:J:36:GLU:CD | 2.50 | 0.49 |
| 1:J:403:ARG:NH1 | 1:J:407:TYR:CZ | 2.80 | 0.49 |
| 1:K:222:GLY:HA3 | 1:K:373:LEU:CD1 | 2.42 | 0.49 |
| 1:L:481:ALA:O | 1:L:484:ASN:N | 2.45 | 0.49 |
| 1:A:56:ASN:HA | 1:E:62:SER:OG | 2.12 | 0.49 |
| 1:A:81:GLN:OE1 | 1:E:155:LYS:HE3 | 2.12 | 0.49 |
| 1:A:90:LYS:CB | 1:A:122:PHE:CD1 | 2.95 | 0.49 |
| 1:C:232:TYR:O | 1:C:236:LEU:HG | 2.12 | 0.49 |
| 1:D:258:HIS:O | 1:D:262:TYR:CD2 | 2.66 | 0.49 |
| 1:D:75:ILE:HG23 | 1:D:131:ILE:HD13 | 1.95 | 0.49 |
| 1:E:168:ASP:OD2 | 1:E:169:MET:N | 2.43 | 0.49 |
| 1:H:148:PHE:CE1 | 1:H:152:LEU:HD11 | 2.47 | 0.49 |
| 1:I:271:ILE:HD11 | 1:I:283:PRO:HG3 | 1.94 | 0.49 |
| 1:I:72:TRP:HE1 | 1:L:498:VAL:CG1 | 2.12 | 0.49 |
| 1:K:321:ILE:CD1 | 1:K:343:ILE:HB | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:351:PRO:C | 1:L:352:THR:HG22 | 2.33 | 0.49 |
| 1:L:398:THR:O | 1:L:399:PHE:C | 2.51 | 0.49 |
| 1:B:233:MET:HB3 | 1:B:238:MET:HB2 | 1.94 | 0.49 |
| 1:D:277:ASP:HB2 | 1:D:302:LEU:HD11 | 1.94 | 0.49 |
| 1:D:47:GLY:O | 1:D:48:ILE:C | 2.51 | 0.49 |
| 1:D:99:VAL:N | 1:D:130:LYS:HE3 | 2.28 | 0.49 |
| 1:F:322:LEU:HD12 | 1:F:344:ILE:HG12 | 1.94 | 0.49 |
| 1:H:211:ARG:NH1 | 1:H:211:ARG:HB3 | 2.27 | 0.49 |
| 1:J:65:ILE:HD13 | 1:J:144:ILE:HG12 | 1.95 | 0.49 |
| 1:J:148:PHE:O | 1:J:152:LEU:HB2 | 2.12 | 0.49 |
| 1:J:208:ILE:HD12 | 1:J:387:LYS:HD2 | 1.94 | 0.49 |
| 1:L:107:LEU:HD13 | 1:L:126:LYS:HE3 | 1.95 | 0.49 |
| 1:L:332:THR:O | 1:L:336:ALA:HB2 | 2.12 | 0.49 |
| 1:A:142:GLU:OE2 | 1:A:146:ARG:NH1 | 2.45 | 0.49 |
| 1:A:59:LEU:CD2 | 1:A:61:LEU:CD2 | 2.86 | 0.49 |
| 1:D:477:LEU:O | 1:D:480:ALA:HB3 | 2.12 | 0.49 |
| 1:D:98:ASP:O | 1:D:99:VAL:O | 2.31 | 0.49 |
| 1:E:494:ASN:C | 1:E:496:ALA:H | 2.16 | 0.49 |
| 1:F:75:ILE:CD1 | 1:F:144:ILE:HG12 | 2.43 | 0.49 |
| 1:G:293:ASP:O | 1:G:296:LEU:N | 2.42 | 0.49 |
| 1:H:257:LEU:O | 1:H:260:MET:HB3 | 2.12 | 0.49 |
| 1:H:60:SER:HA | 1:H:78:TYR:HB3 | 1.93 | 0.49 |
| 1:I:133:PRO:HA | 1:I:141:LEU:HD21 | 1.95 | 0.49 |
| 1:J:343:ILE:CG1 | 1:J:366:MET:HE2 | 2.43 | 0.49 |
| 1:K:95:TYR:OH | 1:K:145:THR:CB | 2.61 | 0.49 |
| 1:L:89:CYS:O | 1:L:163:ASP:HA | 2.12 | 0.49 |
| 1:A:421:PHE:CE1 | 1:A:423:LYS:HE2 | 2.48 | 0.49 |
| 1:B:151:GLU:HB3 | 1:D:57:HIS:HE1 | 1.78 | 0.49 |
| 1:B:379:THR:CG2 | 1:B:453:LEU:HD23 | 2.41 | 0.49 |
| 1:D:146:ARG:NE | 1:D:182:THR:OG1 | 2.45 | 0.49 |
| 1:D:146:ARG:NH2 | 1:D:181:ASP:OD1 | 2.46 | 0.49 |
| 1:E:233:MET:HE1 | 1:E:343:ILE:HD11 | 1.94 | 0.49 |
| 1:E:414:GLN:HB2 | 1:E:429:PRO:CD | 2.21 | 0.49 |
| 1:G:176:MET:HE3 | 1:G:176:MET:HA | 1.95 | 0.49 |
| 1:H:131:ILE:HD13 | 1:H:144:ILE:CD1 | 2.43 | 0.49 |
| 1:H:238:MET:O | 1:H:239:THR:C | 2.50 | 0.49 |
| 1:H:478:ARG:HH11 | 1:H:478:ARG:HG3 | 1.78 | 0.49 |
| 1:H:67:ARG:CB | 1:H:67:ARG:HH11 | 2.20 | 0.49 |
| 1:I:212:ILE:N | 1:I:212:ILE:CD1 | 2.76 | 0.49 |
| 1:I:32:LEU:O | 1:I:33:ARG:HB3 | 2.13 | 0.49 |
| 1:I:93:ILE:HD11 | 1:I:165:PRO:CB | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:178:TRP:O | 1:J:179:ILE:C | 2.51 | 0.49 |
| 1:J:57:HIS:CE1 | 1:J:84:HIS:HE2 | 2.27 | 0.49 |
| 1:L:499:THR:HG23 | 1:L:500:PHE:CD1 | 2.48 | 0.49 |
| 1:A:249:VAL:HG22 | 1:A:249:VAL:O | 2.13 | 0.49 |
| 1:A:499:THR:O | 1:A:499:THR:HG22 | 2.13 | 0.49 |
| 1:B:356:ALA:O | 1:B:360:PHE:CD2 | 2.65 | 0.49 |
| 1:B:411:MET:HG2 | 1:B:430:ILE:CG2 | 2.42 | 0.49 |
| 1:C:234:SER:O | 1:C:237:GLY:N | 2.46 | 0.49 |
| 1:C:345:ALA:HB1 | 1:C:373:LEU:HD21 | 1.94 | 0.49 |
| 1:C:85:GLN:HG2 | 1:C:86:ARG:N | 2.25 | 0.49 |
| 1:D:148:PHE:O | 1:D:152:LEU:HB2 | 2.13 | 0.49 |
| 1:D:165:PRO:O | 1:D:198:VAL:HG23 | 2.12 | 0.49 |
| 1:D:344:ILE:CG2 | 1:D:367:VAL:HG22 | 2.43 | 0.49 |
| 1:D:47:GLY:O | 1:D:50:ARG:N | 2.46 | 0.49 |
| 1:E:300:SER:OG | 1:E:301:ILE:N | 2.44 | 0.49 |
| 1:E:414:GLN:OE1 | 1:E:428:ILE:HA | 2.13 | 0.49 |
| 1:F:239:THR:N | 1:F:240:PRO:CD | 2.75 | 0.49 |
| 1:F:411:MET:HA | 1:F:430:ILE:CG2 | 2.43 | 0.49 |
| 1:G:208:ILE:CG1 | 1:G:387:LYS:HD2 | 2.35 | 0.49 |
| 1:I:252:PHE:CD1 | 1:I:295:LYS:HD3 | 2.47 | 0.49 |
| 1:I:346:GLU:O | 1:I:348:ALA:N | 2.45 | 0.49 |
| 1:I:332:THR:CG2 | 1:I:353:THR:HG21 | 2.41 | 0.49 |
| 1:I:439:ARG:NH2 | 1:J:405:SER:HB2 | 2.28 | 0.49 |
| 1:I:48:ILE:HG13 | 1:I:490:PHE:HE1 | 1.76 | 0.49 |
| 1:J:281:TRP:HZ3 | 1:J:317:ALA:CB | 2.25 | 0.49 |
| 1:J:414:GLN:CB | 1:J:429:PRO:HD2 | 2.41 | 0.49 |
| 1:J:421:PHE:HD1 | 1:J:423:LYS:N | 2.10 | 0.49 |
| 1:J:496:ALA:O | 1:J:501:THR:HA | 2.13 | 0.49 |
| 1:J:14:GLU:HG3 | 1:J:53:LYS:CE | 2.42 | 0.49 |
| 1:K:219:VAL:HG11 | 1:K:259:SER:CB | 2.42 | 0.49 |
| 1:L:275:GLU:HG3 | 1:L:301:ILE:CG1 | 2.42 | 0.49 |
| 1:G:181:ASP:OD1 | 1:L:501:THR:OXT | 2.30 | 0.49 |
| 1:B:315:LEU:HD22 | 1:B:322:LEU:HD11 | 1.94 | 0.49 |
| 1:B:201:LYS:NZ | 1:B:384:GLU:OE1 | 2.43 | 0.49 |
| 1:C:65:ILE:CD1 | 1:C:144:ILE:HG12 | 2.24 | 0.49 |
| 1:C:28:LEU:HD11 | 1:C:490:PHE:CE2 | 2.48 | 0.49 |
| 1:D:167:PRO:HB3 | 1:D:176:MET:SD | 2.53 | 0.49 |
| 1:D:318:ASP:HA | 1:D:340:LYS:HB2 | 1.95 | 0.49 |
| 1:E:107:LEU:HD12 | 1:E:126:LYS:NZ | 2.27 | 0.49 |
| 1:F:85:GLN:HE21 | 1:F:85:GLN:H | 1.60 | 0.49 |
| 1:G:239:THR:O | 1:G:239:THR:CG2 | 2.61 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:234:SER:C | 1:H:236:LEU:N | 2.66 | 0.49 |
| 1:H:339:VAL:HG21 | 1:H:360:PHE:CE1 | 2.45 | 0.49 |
| 1:J:39:GLU:O | 1:J:41:LYS:N | 2.44 | 0.49 |
| 1:J:6:ASP:O | 1:J:6:ASP:OD1 | 2.30 | 0.49 |
| 1:K:118:VAL:O | 1:K:120:VAL:HG23 | 2.12 | 0.49 |
| 1:K:371:LEU:HG | 1:K:371:LEU:O | 2.12 | 0.49 |
| 1:G:58:VAL:HG12 | 1:K:60:SER:HB2 | 1.94 | 0.49 |
| 1:L:343:ILE:HG22 | 1:L:343:ILE:O | 2.13 | 0.49 |
| 1:L:395:GLY:O | 1:L:397:LEU:N | 2.45 | 0.49 |
| 1:A:82:HIS:CG | 1:A:112:THR:HG21 | 2.47 | 0.49 |
| 1:B:396:ARG:HD3 | 1:B:396:ARG:O | 2.13 | 0.49 |
| 1:B:48:ILE:O | 1:B:52:ILE:HG13 | 2.13 | 0.49 |
| 1:B:68:ASP:OD1 | 1:B:140:GLU:HG3 | 2.12 | 0.49 |
| 1:C:149:THR:OG1 | 1:C:179:ILE:HG12 | 2.12 | 0.49 |
| 1:C:33:ARG:HE | 1:C:33:ARG:HB2 | 1.41 | 0.49 |
| 1:D:428:ILE:HD13 | 1:D:428:ILE:N | 2.21 | 0.49 |
| 1:E:247:PHE:HB3 | 1:E:321:ILE:HB | 1.94 | 0.49 |
| 1:G:126:LYS:HG3 | 1:G:127:ALA:N | 2.28 | 0.49 |
| 1:G:335:ASN:HD22 | 1:G:336:ALA:H | 1.59 | 0.49 |
| 1:G:419:ARG:O | 1:G:420:LYS:HB2 | 2.12 | 0.49 |
| 1:G:48:ILE:HG21 | 1:G:490:PHE:CD1 | 2.48 | 0.49 |
| 1:H:164:VAL:CG1 | 1:H:198:VAL:HA | 2.42 | 0.49 |
| 1:I:101:VAL:O | 1:I:104:VAL:HG22 | 2.13 | 0.49 |
| 1:J:163:ASP:O | 1:J:165:PRO:HD3 | 2.13 | 0.49 |
| 1:J:496:ALA:C | 1:J:501:THR:HA | 2.33 | 0.49 |
| 1:A:24:VAL:CG1 | 1:A:28:LEU:HB2 | 2.42 | 0.48 |
| 1:A:33:ARG:HH21 | 1:A:42:ARG:CZ | 2.26 | 0.48 |
| 1:C:264:HIS:O | 1:C:266:PHE:N | 2.45 | 0.48 |
| 1:D:117:VAL:HG11 | 1:D:372:TYR:HB2 | 1.94 | 0.48 |
| 1:D:485:ALA:O | 1:D:488:LYS:N | 2.45 | 0.48 |
| 1:D:59:LEU:HB2 | 1:D:157:PHE:CE2 | 2.47 | 0.48 |
| 1:F:195:HIS:O | 1:F:201:LYS:HE3 | 2.13 | 0.48 |
| 1:F:380:VAL:O | 1:F:383:PHE:HB2 | 2.13 | 0.48 |
| 1:G:235:ILE:HA | 1:G:235:ILE:HD13 | 1.68 | 0.48 |
| 1:G:248:VAL:HG23 | 1:G:319:CYS:SG | 2.52 | 0.48 |
| 1:H:217:ARG:HD2 | 1:H:450:HIS:NE2 | 2.28 | 0.48 |
| 1:H:240:PRO:HD2 | 1:H:244:ASP:O | 2.13 | 0.48 |
| 1:H:295:LYS:HD3 | 1:H:301:ILE:HG23 | 1.95 | 0.48 |
| 1:I:87:THR:HG22 | 1:I:88:PRO:N | 2.28 | 0.48 |
| 1:J:318:ASP:O | 1:J:319:CYS:CB | 2.61 | 0.48 |
| 1:J:337:PRO:HG3 | 1:J:359:ILE:HG21 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:397:LEU:HD21 | 1:K:383:PHE:CD1 | 2.48 | 0.48 |
| 1:L:315:LEU:HD23 | 1:L:331:LEU:CD2 | 2.43 | 0.48 |
| 1:L:338:ARG:CB | 1:L:338:ARG:NH1 | 2.67 | 0.48 |
| 2:A:1:ADP:H5'2 | 1:B:203:ILE:HG22 | 1.93 | 0.48 |
| 1:A:86:ARG:HG2 | 1:A:121:PRO:HA | 1.94 | 0.48 |
| 1:B:497:GLY:O | 1:B:498:VAL:HG13 | 2.14 | 0.48 |
| 1:C:274:GLY:O | 1:C:301:ILE:CD1 | 2.61 | 0.48 |
| 1:C:201:LYS:HZ1 | 1:C:388:ASN:HD21 | 1.58 | 0.48 |
| 1:C:81:GLN:HG3 | 1:C:157:PHE:CE1 | 2.48 | 0.48 |
| 1:D:339:VAL:HG21 | 1:D:360:PHE:HE1 | 1.78 | 0.48 |
| 1:D:406:ASN:O | 1:D:409:LEU:HB2 | 2.13 | 0.48 |
| 1:D:89:CYS:O | 1:D:163:ASP:HA | 2.12 | 0.48 |
| 1:E:261:ARG:HG3 | 1:E:261:ARG:HH11 | 1.78 | 0.48 |
| 1:G:420:LYS:O | 1:G:420:LYS:CE | 2.62 | 0.48 |
| 1:G:414:GLN:CB | 1:G:430:ILE:HG23 | 2.43 | 0.48 |
| 1:G:498:VAL:HG21 | 1:K:72:TRP:NE1 | 2.28 | 0.48 |
| 1:G:47:GLY:CA | 1:G:50:ARG:HG2 | 2.33 | 0.48 |
| 1:G:80:ALA:O | 1:G:125:ALA:HA | 2.13 | 0.48 |
| 1:J:470:LYS:HG2 | 1:J:470:LYS:O | 2.11 | 0.48 |
| 1:K:247:PHE:HD1 | 1:K:268:ALA:HB1 | 1.78 | 0.48 |
| 1:K:372:TYR:OH | 1:K:461:ALA:HB2 | 2.13 | 0.48 |
| 1:L:403:ARG:HH11 | 1:L:403:ARG:HG3 | 1.78 | 0.48 |
| 1:A:174:ARG:O | 1:A:177:SER:HB3 | 2.14 | 0.48 |
| 1:A:233:MET:HA | 1:A:233:MET:CE | 2.43 | 0.48 |
| 1:B:360:PHE:HB3 | 1:B:365:ILE:HB | 1.95 | 0.48 |
| 1:C:150:MET:O | 1:C:154:LYS:HG3 | 2.13 | 0.48 |
| 1:D:189:HIS:ND1 | 1:F:154:LYS:HD3 | 2.29 | 0.48 |
| 1:D:429:PRO:HG3 | 1:E:417:LEU:CD1 | 2.43 | 0.48 |
| 1:C:181:ASP:CG | 1:E:501:THR:OXT | 2.52 | 0.48 |
| 1:F:49:LEU:H | 1:F:49:LEU:HD22 | 1.78 | 0.48 |
| 1:G:203:ILE:HG22 | 2:L:502:ADP:H5'2 | 1.95 | 0.48 |
| 1:G:437:GLN:HA | 1:G:440:ILE:CD1 | 2.41 | 0.48 |
| 1:H:120:VAL:HG12 | 1:H:120:VAL:O | 2.12 | 0.48 |
| 1:H:121:PRO:CG | 1:H:382:TYR:CE2 | 2.94 | 0.48 |
| 1:H:122:PHE:HE1 | 1:H:382:TYR:HA | 1.77 | 0.48 |
| 1:H:260:MET:HG2 | 1:H:288:PRO:HG3 | 1.96 | 0.48 |
| 1:I:219:VAL:HG22 | 1:I:373:LEU:CD2 | 2.43 | 0.48 |
| 1:I:91:GLY:HA2 | 1:I:111:MET:HE2 | 1.96 | 0.48 |
| 1:J:115:CYS:O | 1:J:118:VAL:N | 2.45 | 0.48 |
| 1:J:142:GLU:CG | 1:J:146:ARG:HD2 | 2.43 | 0.48 |
| 1:K:103:GLU:O | 1:K:106:ALA:HB3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:137:THR:HG23 | 1:K:140:GLU:HG3 | 1.94 | 0.48 |
| 1:K:294:PHE:CD2 | 1:K:298:HIS:CE1 | 3.01 | 0.48 |
| 1:K:360:PHE:HD1 | 1:K:365:ILE:CD1 | 2.23 | 0.48 |
| 1:I:392:VAL:HG21 | 1:K:386:LEU:HD13 | 1.96 | 0.48 |
| 1:K:9:PHE:CD1 | 1:K:10:PHE:N | 2.81 | 0.48 |
| 1:L:138:ASP:CG | 1:L:174:ARG:HH12 | 2.17 | 0.48 |
| 1:L:223:ILE:HD12 | 1:L:263:LEU:HD21 | 1.95 | 0.48 |
| 1:A:383:PHE:O | 1:A:384:GLU:C | 2.51 | 0.48 |
| 1:A:486:ILE:O | 1:A:490:PHE:HB2 | 2.14 | 0.48 |
| 1:B:161:GLY:CA | 1:B:162:ILE:HD12 | 2.43 | 0.48 |
| 1:C:322:LEU:CD1 | 1:C:324:PRO:HG3 | 2.42 | 0.48 |
| 1:C:411:MET:HA | 1:C:430:ILE:CG2 | 2.43 | 0.48 |
| 1:D:294:PHE:CZ | 1:D:303:GLY:O | 2.66 | 0.48 |
| 1:D:453:LEU:O | 1:D:456:THR:N | 2.46 | 0.48 |
| 1:G:346:GLU:HG2 | 1:G:351:PRO:HG3 | 1.94 | 0.48 |
| 1:G:384:GLU:O | 1:G:387:LYS:HB3 | 2.13 | 0.48 |
| 1:G:498:VAL:N | 1:G:501:THR:HB | 2.28 | 0.48 |
| 1:K:176:MET:HE2 | 1:K:176:MET:HA | 1.94 | 0.48 |
| 1:K:372:TYR:CD1 | 1:K:372:TYR:C | 2.86 | 0.48 |
| 1:I:58:VAL:CG1 | 1:L:60:SER:HB2 | 2.43 | 0.48 |
| 1:A:414:GLN:CD | 1:A:430:ILE:HG23 | 2.34 | 0.48 |
| 1:D:107:LEU:CD1 | 1:D:107:LEU:N | 2.75 | 0.48 |
| 1:E:220:PHE:C | 1:E:220:PHE:CD1 | 2.86 | 0.48 |
| 1:F:90:LYS:HD2 | 1:F:164:VAL:O | 2.13 | 0.48 |
| 1:F:24:VAL:O | 1:F:25:GLU:C | 2.52 | 0.48 |
| 1:F:380:VAL:HG13 | 1:F:449:VAL:CG1 | 2.43 | 0.48 |
| 1:F:398:THR:O | 1:F:399:PHE:C | 2.50 | 0.48 |
| 1:F:417:LEU:HD23 | 1:F:427:THR:HG21 | 1.95 | 0.48 |
| 1:G:160:PRO:CG | 1:G:191:ASP:OD1 | 2.62 | 0.48 |
| 1:G:304:PHE:CD1 | 1:G:305:PRO:HD2 | 2.47 | 0.48 |
| 1:J:282:ASN:O | 1:J:284:ASP:N | 2.47 | 0.48 |
| 1:K:304:PHE:CD2 | 1:K:305:PRO:O | 2.67 | 0.48 |
| 1:K:368:ILE:HG22 | 1:K:373:LEU:HB2 | 1.96 | 0.48 |
| 1:L:224:GLU:HA | 1:L:227:ILE:CG2 | 2.43 | 0.48 |
| 1:A:249:VAL:HA | 1:A:323:ILE:HG13 | 1.96 | 0.48 |
| 1:A:57:HIS:HE2 | 1:E:151:GLU:HB3 | 1.78 | 0.48 |
| 1:A:94:ARG:NH1 | 1:A:96:SER:CB | 2.77 | 0.48 |
| 1:B:106:ALA:O | 1:B:109:SER:HB3 | 2.13 | 0.48 |
| 1:B:252:PHE:CE2 | 1:B:260:MET:HE2 | 2.49 | 0.48 |
| 1:B:90:LYS:HD3 | 1:B:122:PHE:CE1 | 2.49 | 0.48 |
| 1:C:332:THR:HG22 | 1:C:353:THR:CG2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:497:GLY:N | 1:C:501:THR:HA | 2.29 | 0.48 |
| 1:D:348:ALA:O | 1:D:370:ASP:HB3 | 2.14 | 0.48 |
| 1:D:429:PRO:C | 1:D:431:VAL:H | 2.15 | 0.48 |
| 1:D:492:VAL:HG21 | 2:D:4:ADP:C2 | 2.47 | 0.48 |
| 1:E:238:MET:O | 1:E:239:THR:O | 2.31 | 0.48 |
| 1:E:243:GLY:O | 1:E:244:ASP:HB3 | 2.13 | 0.48 |
| 1:G:89:CYS:O | 1:G:164:VAL:N | 2.46 | 0.48 |
| 1:G:252:PHE:CE2 | 1:G:260:MET:HE1 | 2.48 | 0.48 |
| 1:H:137:THR:O | 1:H:138:ASP:C | 2.51 | 0.48 |
| 1:H:131:ILE:CD1 | 1:H:144:ILE:CD1 | 2.91 | 0.48 |
| 1:I:252:PHE:CZ | 1:I:257:LEU:HD13 | 2.48 | 0.48 |
| 1:I:439:ARG:HH22 | 1:J:405:SER:HB2 | 1.78 | 0.48 |
| 1:J:36:GLU:O | 1:J:36:GLU:OE2 | 2.32 | 0.48 |
| 1:K:346:GLU:HG2 | 1:K:351:PRO:CG | 2.43 | 0.48 |
| 1:L:458:GLU:O | 1:L:459:ARG:C | 2.51 | 0.48 |
| 1:A:231:SER:O | 1:A:235:ILE:HG12 | 2.14 | 0.48 |
| 1:A:360:PHE:HB3 | 1:A:365:ILE:CB | 2.43 | 0.48 |
| 1:B:176:MET:HE1 | 1:B:179:ILE:HD12 | 1.93 | 0.48 |
| 1:B:217:ARG:O | 1:B:221:HIS:ND1 | 2.39 | 0.48 |
| 1:B:234:SER:O | 1:B:235:ILE:C | 2.49 | 0.48 |
| 1:B:24:VAL:O | 1:B:25:GLU:C | 2.52 | 0.48 |
| 1:B:250:GLN:CG | 1:B:314:ILE:HD11 | 2.43 | 0.48 |
| 1:C:379:THR:O | 1:C:380:VAL:C | 2.49 | 0.48 |
| 1:C:75:ILE:HG22 | 1:C:76:GLU:N | 2.28 | 0.48 |
| 1:C:79:ARG:HD3 | 1:C:127:ALA:HB2 | 1.90 | 0.48 |
| 1:D:140:GLU:O | 1:D:143:LYS:HB2 | 2.14 | 0.48 |
| 1:D:260:MET:CE | 1:D:288:PRO:HA | 2.44 | 0.48 |
| 1:D:85:GLN:HG2 | 1:D:492:VAL:HG11 | 1.96 | 0.48 |
| 1:E:85:GLN:HG2 | 1:E:86:ARG:N | 2.24 | 0.48 |
| 1:G:87:THR:CB | 1:G:88:PRO:HD3 | 2.32 | 0.48 |
| 1:H:202:PRO:O | 1:H:203:ILE:C | 2.51 | 0.48 |
| 1:H:332:THR:N | 1:H:335:ASN:HD21 | 2.08 | 0.48 |
| 1:I:414:GLN:HA | 1:I:429:PRO:CG | 2.44 | 0.48 |
| 1:I:88:PRO:HA | 1:I:162:ILE:O | 2.12 | 0.48 |
| 1:J:13:VAL:O | 1:J:14:GLU:C | 2.51 | 0.48 |
| 1:J:237:GLY:O | 1:J:238:MET:HG2 | 2.14 | 0.48 |
| 1:K:467:THR:HG22 | 1:K:480:ALA:O | 2.14 | 0.48 |
| 1:L:467:THR:HG22 | 1:L:467:THR:O | 2.13 | 0.48 |
| 1:A:45:VAL:HG13 | 1:A:45:VAL:O | 2.13 | 0.48 |
| 1:C:439:ARG:HH22 | 1:D:405:SER:HB2 | 1.78 | 0.48 |
| 1:D:137:THR:O | 1:D:138:ASP:C | 2.52 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:501:THR:HG23 | 1:E:181:ASP:OD1 | 2.13 | 0.48 |
| 1:E:246:THR:O | 1:E:246:THR:HG23 | 2.12 | 0.48 |
| 1:E:359:ILE:O | 1:E:360:PHE:C | 2.51 | 0.48 |
| 1:E:490:PHE:CZ | 1:E:494:ASN:HB2 | 2.49 | 0.48 |
| 1:F:103:GLU:O | 1:F:107:LEU:HD12 | 2.12 | 0.48 |
| 1:F:414:GLN:HE22 | 1:F:430:ILE:HD13 | 1.76 | 0.48 |
| 1:G:208:ILE:HD12 | 1:G:387:LYS:HB2 | 1.95 | 0.48 |
| 1:G:492:VAL:CG2 | 2:G:502:ADP:H2 | 2.26 | 0.48 |
| 1:G:53:LYS:O | 1:G:82:HIS:HE1 | 1.97 | 0.48 |
| 1:H:430:ILE:O | 1:H:431:VAL:HB | 2.14 | 0.48 |
| 1:I:90:LYS:HB2 | 1:I:122:PHE:HB3 | 1.96 | 0.48 |
| 1:I:249:VAL:HA | 1:I:323:ILE:HG13 | 1.95 | 0.48 |
| 1:J:24:VAL:O | 1:J:25:GLU:C | 2.52 | 0.48 |
| 1:J:297:GLN:O | 1:J:298:HIS:HB3 | 2.14 | 0.48 |
| 1:J:87:THR:CG2 | 1:J:88:PRO:N | 2.77 | 0.48 |
| 1:K:280:ILE:CG2 | 1:K:281:TRP:H | 2.25 | 0.48 |
| 1:K:39:GLU:O | 1:K:41:LYS:N | 2.46 | 0.48 |
| 1:H:413:VAL:HG11 | 1:L:413:VAL:HG22 | 1.96 | 0.48 |
| 1:A:287:ASP:HA | 1:A:288:PRO:HD3 | 1.74 | 0.48 |
| 1:A:336:ALA:HB1 | 1:A:359:ILE:HG21 | 1.96 | 0.48 |
| 1:A:370:ASP:OD2 | 1:A:371:LEU:N | 2.40 | 0.48 |
| 1:A:498:VAL:N | 1:A:501:THR:HA | 2.29 | 0.48 |
| 1:A:47:GLY:O | 1:A:50:ARG:N | 2.46 | 0.48 |
| 1:B:280:ILE:HG23 | 1:B:307:ALA:HB1 | 1.95 | 0.48 |
| 1:C:133:PRO:C | 1:C:135:ASN:H | 2.17 | 0.48 |
| 1:D:359:ILE:HG22 | 1:D:360:PHE:N | 2.28 | 0.48 |
| 1:D:501:THR:OXT | 1:E:181:ASP:HB3 | 2.14 | 0.48 |
| 1:D:432:PRO:HA | 1:E:412:SER:HB3 | 1.96 | 0.48 |
| 1:F:279:SER:O | 1:F:280:ILE:HG13 | 2.13 | 0.48 |
| 1:G:9:PHE:HA | 1:G:12:MET:HE2 | 1.95 | 0.48 |
| 1:H:236:LEU:HD22 | 1:H:342:LYS:HE3 | 1.95 | 0.48 |
| 1:H:498:VAL:CG2 | 1:H:499:THR:H | 2.08 | 0.48 |
| 1:H:87:THR:HG22 | 1:H:88:PRO:CD | 2.44 | 0.48 |
| 1:I:238:MET:O | 1:I:239:THR:C | 2.51 | 0.48 |
| 1:J:137:THR:O | 1:J:138:ASP:C | 2.51 | 0.48 |
| 1:K:234:SER:O | 1:K:236:LEU:N | 2.47 | 0.48 |
| 1:L:238:MET:O | 1:L:239:THR:HG22 | 2.14 | 0.48 |
| 1:A:65:ILE:CD1 | 1:A:75:ILE:HD11 | 2.44 | 0.48 |
| 1:B:371:LEU:HD23 | 1:B:481:ALA:CB | 2.44 | 0.48 |
| 1:B:437:GLN:O | 1:B:441:SER:HB2 | 2.14 | 0.48 |
| 1:D:200:GLY:HA2 | 1:D:211:ARG:HD2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:244:ASP:C | 1:D:245:LYS:CG | 2.82 | 0.48 |
| 1:D:450:HIS:O | 1:D:453:LEU:HB3 | 2.14 | 0.48 |
| 1:F:335:ASN:ND2 | 1:F:336:ALA:N | 2.61 | 0.48 |
| 1:F:490:PHE:CZ | 1:F:494:ASN:ND2 | 2.82 | 0.48 |
| 1:G:371:LEU:HD23 | 1:G:481:ALA:CB | 2.44 | 0.48 |
| 1:G:471:TYR:CE2 | 1:G:483:VAL:HG11 | 2.49 | 0.48 |
| 1:I:413:VAL:O | 1:I:417:LEU:HB2 | 2.13 | 0.48 |
| 1:J:257:LEU:HD12 | 1:J:257:LEU:O | 2.14 | 0.48 |
| 1:K:280:ILE:HG23 | 1:K:307:ALA:HB1 | 1.95 | 0.48 |
| 1:K:339:VAL:HG21 | 1:K:360:PHE:CE1 | 2.39 | 0.48 |
| 1:L:142:GLU:O | 1:L:145:THR:N | 2.47 | 0.48 |
| 1:L:217:ARG:HG2 | 1:L:262:TYR:CE2 | 2.48 | 0.48 |
| 1:L:226:PHE:C | 1:L:228:ASN:H | 2.16 | 0.48 |
| 1:L:346:GLU:HG2 | 1:L:351:PRO:HD2 | 1.95 | 0.48 |
| 1:A:261:ARG:NH1 | 1:A:261:ARG:HG3 | 2.24 | 0.47 |
| 1:A:25:GLU:O | 1:A:28:LEU:N | 2.47 | 0.47 |
| 1:A:336:ALA:HB3 | 1:A:359:ILE:HD12 | 1.95 | 0.47 |
| 1:A:94:ARG:NH1 | 1:A:96:SER:HB3 | 2.29 | 0.47 |
| 1:B:118:VAL:HG23 | 1:B:120:VAL:CG2 | 2.42 | 0.47 |
| 1:B:53:LYS:HB3 | 1:B:54:PRO:CD | 2.42 | 0.47 |
| 1:C:315:LEU:HD21 | 1:C:322:LEU:HD11 | 1.95 | 0.47 |
| 1:D:274:GLY:HA3 | 1:D:314:ILE:HD12 | 1.96 | 0.47 |
| 1:D:67:ARG:NH1 | 1:D:67:ARG:CG | 2.75 | 0.47 |
| 1:E:150:MET:HE1 | 1:E:186:THR:HG21 | 1.95 | 0.47 |
| 1:E:229:GLU:HG3 | 1:E:465:MET:SD | 2.54 | 0.47 |
| 1:E:69:ASP:OD1 | 1:E:70:GLY:N | 2.46 | 0.47 |
| 1:F:241:GLY:O | 1:G:437:GLN:OE1 | 2.32 | 0.47 |
| 1:G:411:MET:HA | 1:G:430:ILE:CG2 | 2.41 | 0.47 |
| 1:H:50:ARG:O | 1:H:54:PRO:HD2 | 2.13 | 0.47 |
| 1:I:108:ALA:O | 1:I:112:THR:HG22 | 2.14 | 0.47 |
| 1:I:282:ASN:OD1 | 1:I:285:GLY:N | 2.46 | 0.47 |
| 1:J:38:GLU:H | 1:J:42:ARG:HD2 | 1.78 | 0.47 |
| 1:L:121:PRO:C | 1:L:122:PHE:CD2 | 2.88 | 0.47 |
| 1:L:121:PRO:C | 1:L:122:PHE:HD2 | 2.17 | 0.47 |
| 1:L:294:PHE:HE2 | 1:L:301:ILE:HA | 1.77 | 0.47 |
| 1:L:396:ARG:NH1 | 1:L:396:ARG:CG | 2.76 | 0.47 |
| 1:A:412:SER:HB3 | 1:F:432:PRO:HA | 1.96 | 0.47 |
| 1:B:202:PRO:HD2 | 1:B:205:GLN:HB2 | 1.96 | 0.47 |
| 1:B:261:ARG:NH1 | 1:B:261:ARG:CG | 2.67 | 0.47 |
| 1:C:260:MET:HG2 | 1:C:288:PRO:HG3 | 1.95 | 0.47 |
| 1:E:164:VAL:HG12 | 1:E:198:VAL:HA | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:246:THR:HG23 | 1:E:320:ASP:N | 2.29 | 0.47 |
| 1:E:413:VAL:O | 1:E:417:LEU:HB2 | 2.14 | 0.47 |
| 1:G:75:ILE:CD1 | 1:G:144:ILE:HG12 | 2.44 | 0.47 |
| 1:H:44:ARG:HB2 | 1:H:44:ARG:HH11 | 1.75 | 0.47 |
| 1:H:90:LYS:HD2 | 1:H:164:VAL:O | 2.14 | 0.47 |
| 1:I:290:GLU:HB3 | 1:I:304:PHE:HZ | 1.79 | 0.47 |
| 1:J:248:VAL:HG22 | 1:J:271:ILE:HG23 | 1.96 | 0.47 |
| 1:I:406:ASN:HD22 | 1:J:409:LEU:HD23 | 1.69 | 0.47 |
| 1:J:417:LEU:HD21 | 1:K:417:LEU:HD21 | 1.96 | 0.47 |
| 1:J:463:GLN:HB3 | 1:J:484:ASN:HD21 | 1.79 | 0.47 |
| 1:K:140:GLU:HA | 1:K:143:LYS:HD2 | 1.96 | 0.47 |
| 1:K:363:ARG:HB3 | 1:K:363:ARG:HH11 | 1.79 | 0.47 |
| 1:L:106:ALA:O | 1:L:109:SER:HB3 | 2.14 | 0.47 |
| 1:L:363:ARG:HH11 | 1:L:363:ARG:HB3 | 1.79 | 0.47 |
| 1:A:116:ALA:O | 1:A:488:LYS:NZ | 2.40 | 0.47 |
| 1:A:227:ILE:HG22 | 1:A:228:ASN:N | 2.29 | 0.47 |
| 1:A:255:VAL:HG13 | 1:A:256:GLY:H | 1.79 | 0.47 |
| 1:B:34:THR:HG23 | 1:B:35:ARG:CZ | 2.44 | 0.47 |
| 1:B:431:VAL:O | 1:B:431:VAL:HG13 | 2.15 | 0.47 |
| 1:C:146:ARG:O | 1:C:147:ARG:C | 2.50 | 0.47 |
| 1:D:371:LEU:HD23 | 1:D:481:ALA:HB3 | 1.96 | 0.47 |
| 1:D:398:THR:O | 1:D:399:PHE:C | 2.52 | 0.47 |
| 1:D:352:THR:HG23 | 1:D:478:ARG:HH22 | 1.79 | 0.47 |
| 1:D:485:ALA:O | 1:D:486:ILE:C | 2.51 | 0.47 |
| 1:D:48:ILE:HG22 | 1:D:52:ILE:HD11 | 1.96 | 0.47 |
| 1:B:498:VAL:HG21 | 1:D:72:TRP:CZ2 | 2.49 | 0.47 |
| 1:D:78:TYR:HE1 | 1:D:99:VAL:CG2 | 2.27 | 0.47 |
| 1:F:250:GLN:CG | 1:F:314:ILE:HD11 | 2.43 | 0.47 |
| 1:G:34:THR:O | 1:G:34:THR:CG2 | 2.60 | 0.47 |
| 1:G:494:ASN:O | 1:G:496:ALA:N | 2.41 | 0.47 |
| 1:H:263:LEU:HD11 | 1:H:323:ILE:HD11 | 1.95 | 0.47 |
| 1:H:486:ILE:HG12 | 1:H:486:ILE:H | 1.54 | 0.47 |
| 1:H:490:PHE:O | 1:H:491:LYS:C | 2.52 | 0.47 |
| 1:J:167:PRO:CG | 1:J:176:MET:HG2 | 2.41 | 0.47 |
| 1:J:346:GLU:OE2 | 1:J:352:THR:CG2 | 2.56 | 0.47 |
| 1:K:234:SER:O | 1:K:237:GLY:N | 2.48 | 0.47 |
| 1:K:264:HIS:C | 1:K:266:PHE:N | 2.67 | 0.47 |
| 1:K:325:ALA:O | 1:K:326:ALA:HB2 | 2.14 | 0.47 |
| 1:A:498:VAL:O | 1:A:501:THR:CG2 | 2.60 | 0.47 |
| 1:B:275:GLU:HB2 | 1:B:301:ILE:CD1 | 2.35 | 0.47 |
| 1:C:226:PHE:HE2 | 1:C:465:MET:HG2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:84:HIS:C | 1:C:86:ARG:N | 2.67 | 0.47 |
| 1:E:236:LEU:CB | 1:E:238:MET:HG3 | 2.40 | 0.47 |
| 1:E:294:PHE:O | 1:E:294:PHE:CG | 2.66 | 0.47 |
| 1:E:96:SER:O | 1:E:99:VAL:HG13 | 2.15 | 0.47 |
| 1:F:29:VAL:O | 1:F:33:ARG:HG3 | 2.14 | 0.47 |
| 1:G:213:SER:HB2 | 1:G:217:ARG:CD | 2.44 | 0.47 |
| 1:I:150:MET:SD | 1:I:186:THR:HG21 | 2.54 | 0.47 |
| 1:I:59:LEU:CB | 1:I:157:PHE:CE2 | 2.97 | 0.47 |
| 1:I:181:ASP:OD1 | 1:K:501:THR:CG2 | 2.62 | 0.47 |
| 1:I:226:PHE:C | 1:I:228:ASN:H | 2.18 | 0.47 |
| 1:I:367:VAL:O | 1:I:369:PRO:HD3 | 2.14 | 0.47 |
| 1:J:364:ASN:H | 1:J:364:ASN:HD22 | 1.63 | 0.47 |
| 1:K:86:ARG:HG2 | 1:K:121:PRO:HA | 1.97 | 0.47 |
| 1:K:158:ILE:O | 1:K:158:ILE:CG2 | 2.61 | 0.47 |
| 1:K:405:SER:O | 1:K:409:LEU:HD23 | 2.14 | 0.47 |
| 1:K:48:ILE:O | 1:K:51:ILE:HB | 2.14 | 0.47 |
| 1:L:132:ASN:OD1 | 1:L:134:LYS:HB2 | 2.14 | 0.47 |
| 1:L:195:HIS:O | 1:L:201:LYS:HE3 | 2.15 | 0.47 |
| 1:L:24:VAL:O | 1:L:26:ASP:N | 2.48 | 0.47 |
| 1:L:39:GLU:HB3 | 1:L:41:LYS:HG3 | 1.97 | 0.47 |
| 1:L:61:LEU:HD12 | 1:L:63:PHE:CD2 | 2.49 | 0.47 |
| 1:A:112:THR:HB | 1:A:124:GLY:H | 1.80 | 0.47 |
| 1:B:359:ILE:HD12 | 1:B:359:ILE:HA | 1.83 | 0.47 |
| 1:D:99:VAL:O | 1:D:100:SER:CB | 2.62 | 0.47 |
| 1:D:68:ASP:OD1 | 1:D:140:GLU:HG2 | 2.15 | 0.47 |
| 1:D:349:ASN:HD21 | 1:D:374:ASN:HD22 | 1.61 | 0.47 |
| 1:D:392:VAL:HG12 | 1:D:393:SER:N | 2.29 | 0.47 |
| 1:G:318:ASP:HA | 1:G:340:LYS:HB2 | 1.97 | 0.47 |
| 1:G:462:ARG:HG3 | 1:G:462:ARG:HH11 | 1.78 | 0.47 |
| 1:H:172:GLY:N | 1:H:175:GLU:OE1 | 2.42 | 0.47 |
| 1:H:274:GLY:O | 1:H:275:GLU:CB | 2.62 | 0.47 |
| 1:J:428:ILE:O | 1:J:431:VAL:HG12 | 2.14 | 0.47 |
| 1:K:211:ARG:O | 1:K:214:ALA:CB | 2.62 | 0.47 |
| 1:K:252:PHE:HZ | 1:K:260:MET:CE | 2.28 | 0.47 |
| 1:K:220:PHE:CD2 | 1:K:262:TYR:HB3 | 2.49 | 0.47 |
| 1:G:60:SER:HB2 | 1:K:58:VAL:CG1 | 2.44 | 0.47 |
| 1:L:142:GLU:O | 1:L:143:LYS:C | 2.52 | 0.47 |
| 1:L:424:HIS:CD2 | 1:L:424:HIS:H | 2.32 | 0.47 |
| 1:A:321:ILE:O | 1:A:321:ILE:HG22 | 2.15 | 0.47 |
| 1:B:147:ARG:CD | 1:D:499:THR:OG1 | 2.63 | 0.47 |
| 1:C:264:HIS:ND1 | 1:C:264:HIS:C | 2.67 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:95:TYR:OH | 1:D:145:THR:CB | 2.63 | 0.47 |
| 1:D:160:PRO:HD3 | 1:D:183:TYR:CE2 | 2.50 | 0.47 |
| 1:D:226:PHE:CD2 | 1:D:465:MET:HE2 | 2.49 | 0.47 |
| 1:D:350:GLY:N | 1:D:370:ASP:OD1 | 2.43 | 0.47 |
| 1:E:273:VAL:HG11 | 1:E:291:LEU:HD21 | 1.96 | 0.47 |
| 1:E:66:ARG:HG3 | 1:E:72:TRP:CE2 | 2.49 | 0.47 |
| 1:E:8:ASN:ND2 | 1:E:10:PHE:CD2 | 2.82 | 0.47 |
| 1:F:90:LYS:NZ | 1:F:166:ALA:HB2 | 2.29 | 0.47 |
| 1:G:13:VAL:HG11 | 1:G:109:SER:OG | 2.14 | 0.47 |
| 1:G:257:LEU:C | 1:G:257:LEU:HD12 | 2.34 | 0.47 |
| 1:G:79:ARG:HH11 | 1:G:127:ALA:HB2 | 1.78 | 0.47 |
| 1:H:114:LYS:HZ1 | 1:H:374:ASN:HD21 | 1.62 | 0.47 |
| 1:H:294:PHE:CD1 | 1:H:298:HIS:NE2 | 2.76 | 0.47 |
| 1:H:302:LEU:N | 1:H:302:LEU:HD13 | 2.29 | 0.47 |
| 1:H:331:LEU:HD12 | 1:H:352:THR:HG22 | 1.96 | 0.47 |
| 1:H:412:SER:O | 1:H:413:VAL:C | 2.50 | 0.47 |
| 1:H:84:HIS:O | 1:H:86:ARG:N | 2.47 | 0.47 |
| 1:J:274:GLY:HA2 | 1:J:279:SER:HA | 1.96 | 0.47 |
| 1:J:383:PHE:CD2 | 1:J:383:PHE:N | 2.80 | 0.47 |
| 1:L:280:ILE:CG2 | 1:L:307:ALA:HB1 | 2.41 | 0.47 |
| 1:L:366:MET:HE3 | 1:L:368:ILE:CD1 | 2.41 | 0.47 |
| 1:A:113:TYR:O | 1:A:117:VAL:HG23 | 2.14 | 0.47 |
| 1:B:281:TRP:CZ2 | 1:B:283:PRO:HG3 | 2.50 | 0.47 |
| 1:C:48:ILE:O | 1:C:52:ILE:HG13 | 2.13 | 0.47 |
| 1:C:62:SER:HA | 1:C:75:ILE:O | 2.15 | 0.47 |
| 1:D:248:VAL:HG22 | 1:D:271:ILE:HG23 | 1.96 | 0.47 |
| 1:D:294:PHE:CZ | 1:D:305:PRO:HD3 | 2.50 | 0.47 |
| 1:D:411:MET:O | 1:D:414:GLN:HB3 | 2.14 | 0.47 |
| 1:D:432:PRO:O | 1:D:433:THR:C | 2.51 | 0.47 |
| 1:E:145:THR:O | 1:E:148:PHE:N | 2.48 | 0.47 |
| 1:E:192:ILE:O | 1:E:192:ILE:HG12 | 2.14 | 0.47 |
| 1:E:396:ARG:NH1 | 1:E:396:ARG:HG3 | 2.22 | 0.47 |
| 1:F:476:ASP:OD2 | 1:F:479:THR:CG2 | 2.62 | 0.47 |
| 1:H:179:ILE:HB | 1:H:198:VAL:HG11 | 1.97 | 0.47 |
| 1:H:239:THR:O | 1:H:239:THR:CG2 | 2.61 | 0.47 |
| 1:H:322:LEU:CD2 | 1:H:322:LEU:C | 2.83 | 0.47 |
| 1:I:219:VAL:HG12 | 1:I:220:PHE:N | 2.30 | 0.47 |
| 1:I:243:GLY:O | 1:I:245:LYS:N | 2.48 | 0.47 |
| 1:J:9:PHE:HA | 1:J:12:MET:CE | 2.45 | 0.47 |
| 1:L:386:LEU:C | 1:L:390:ASN:ND2 | 2.68 | 0.47 |
| 1:L:407:TYR:O | 1:L:411:MET:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:103:GLU:O | 1:A:106:ALA:HB3 | 2.14 | 0.47 |
| 1:A:114:LYS:NZ | 1:A:374:ASN:HD21 | 2.13 | 0.47 |
| 1:A:336:ALA:O | 1:A:339:VAL:HG22 | 2.14 | 0.47 |
| 1:B:473:LEU:HD23 | 1:B:473:LEU:N | 2.29 | 0.47 |
| 1:B:72:TRP:O | 1:D:50:ARG:NH1 | 2.48 | 0.47 |
| 1:D:248:VAL:HB | 1:D:322:LEU:HD23 | 1.96 | 0.47 |
| 1:D:363:ARG:O | 1:D:364:ASN:C | 2.53 | 0.47 |
| 1:E:152:LEU:HA | 1:E:152:LEU:HD12 | 1.58 | 0.47 |
| 1:E:222:GLY:HA3 | 1:E:373:LEU:HD13 | 1.95 | 0.47 |
| 1:G:58:VAL:O | 1:G:58:VAL:HG13 | 2.14 | 0.47 |
| 1:H:222:GLY:HA3 | 1:H:373:LEU:HD12 | 1.97 | 0.47 |
| 1:H:371:LEU:HD22 | 1:H:482:TYR:CD2 | 2.50 | 0.47 |
| 1:J:176:MET:HE3 | 1:J:179:ILE:HG13 | 1.96 | 0.47 |
| 1:J:322:LEU:HD13 | 1:J:323:ILE:N | 2.30 | 0.47 |
| 1:K:235:ILE:O | 1:K:235:ILE:HG22 | 2.14 | 0.47 |
| 1:K:280:ILE:CG2 | 1:K:281:TRP:N | 2.76 | 0.47 |
| 1:K:87:THR:OG1 | 1:K:88:PRO:HD3 | 2.13 | 0.47 |
| 1:L:219:VAL:O | 1:L:373:LEU:HD11 | 2.15 | 0.47 |
| 1:L:85:GLN:NE2 | 1:L:489:VAL:HG22 | 2.20 | 0.47 |
| 1:A:361:LEU:C | 1:A:361:LEU:HD23 | 2.35 | 0.47 |
| 1:A:446:LYS:HD2 | 1:A:450:HIS:CE1 | 2.50 | 0.47 |
| 1:B:213:SER:CB | 1:B:217:ARG:HH21 | 2.28 | 0.47 |
| 1:B:201:LYS:HG2 | 1:B:384:GLU:OE1 | 2.14 | 0.47 |
| 1:B:84:HIS:O | 1:B:86:ARG:N | 2.48 | 0.47 |
| 1:D:136:TYR:HD1 | 1:D:140:GLU:OE1 | 1.97 | 0.47 |
| 1:D:213:SER:HB2 | 1:D:217:ARG:NE | 2.30 | 0.47 |
| 1:E:33:ARG:NH1 | 1:E:36:GLU:OE1 | 2.41 | 0.47 |
| 1:E:9:PHE:N | 1:E:9:PHE:CD1 | 2.83 | 0.47 |
| 1:F:264:HIS:CD2 | 1:F:288:PRO:CD | 2.98 | 0.47 |
| 1:F:291:LEU:HD11 | 1:F:301:ILE:HB | 1.96 | 0.47 |
| 1:F:501:THR:OXT | 1:F:501:THR:HG23 | 2.15 | 0.47 |
| 1:G:501:THR:HG23 | 1:H:181:ASP:OD1 | 2.14 | 0.47 |
| 1:I:68:ASP:OD1 | 1:I:140:GLU:CG | 2.62 | 0.47 |
| 1:K:459:ARG:O | 1:K:463:GLN:HG3 | 2.15 | 0.47 |
| 1:K:57:HIS:HD2 | 1:K:84:HIS:CE1 | 2.32 | 0.47 |
| 1:L:238:MET:C | 1:L:240:PRO:HD3 | 2.35 | 0.47 |
| 1:L:371:LEU:HD23 | 1:L:481:ALA:HB1 | 1.96 | 0.47 |
| 1:A:416:SER:HB3 | 1:F:431:VAL:CG1 | 2.44 | 0.47 |
| 1:A:436:PHE:CZ | 1:A:440:ILE:HD11 | 2.50 | 0.47 |
| 1:B:148:PHE:CE2 | 1:B:152:LEU:CD2 | 2.98 | 0.47 |
| 1:C:191:ASP:C | 1:C:193:ASN:H | 2.18 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:211:ARG:O | 1:C:211:ARG:HG2 | 2.14 | 0.47 |
| 1:C:335:ASN:HB2 | 1:C:338:ARG:CZ | 2.42 | 0.47 |
| 1:D:176:MET:HG3 | 1:D:198:VAL:HG21 | 1.95 | 0.47 |
| 1:E:250:GLN:OE1 | 1:E:330:GLN:HG2 | 2.15 | 0.47 |
| 1:E:335:ASN:ND2 | 1:E:336:ALA:N | 2.59 | 0.47 |
| 1:E:339:VAL:O | 1:E:363:ARG:NH2 | 2.47 | 0.47 |
| 1:F:243:GLY:O | 1:F:245:LYS:N | 2.48 | 0.47 |
| 1:F:222:GLY:HA3 | 1:F:373:LEU:CD1 | 2.45 | 0.47 |
| 1:F:371:LEU:HD23 | 1:F:481:ALA:HB1 | 1.97 | 0.47 |
| 1:G:255:VAL:HG13 | 1:G:256:GLY:N | 2.29 | 0.47 |
| 1:G:371:LEU:CD2 | 1:G:481:ALA:CB | 2.92 | 0.47 |
| 1:H:234:SER:C | 1:H:236:LEU:H | 2.18 | 0.47 |
| 1:H:214:ALA:CB | 1:H:380:VAL:HG21 | 2.44 | 0.47 |
| 1:H:492:VAL:HG23 | 1:H:493:TYR:N | 2.30 | 0.47 |
| 1:I:153:ALA:HB2 | 1:I:158:ILE:CG2 | 2.45 | 0.47 |
| 1:I:174:ARG:HG3 | 1:I:175:GLU:N | 2.29 | 0.47 |
| 1:I:322:LEU:HB2 | 1:I:341:ALA:CB | 2.45 | 0.47 |
| 1:J:131:ILE:HG13 | 1:J:136:TYR:CE2 | 2.50 | 0.47 |
| 1:J:498:VAL:CA | 1:J:501:THR:HB | 2.45 | 0.47 |
| 1:L:314:ILE:CD1 | 1:L:314:ILE:H | 2.04 | 0.47 |
| 1:L:411:MET:HG2 | 1:L:430:ILE:HG21 | 1.96 | 0.47 |
| 1:A:141:LEU:HD23 | 1:A:141:LEU:HA | 1.74 | 0.47 |
| 1:A:260:MET:HE3 | 1:A:288:PRO:CA | 2.36 | 0.47 |
| 1:B:163:ASP:O | 1:B:165:PRO:HD3 | 2.14 | 0.47 |
| 1:B:280:ILE:CG2 | 1:B:281:TRP:H | 2.27 | 0.47 |
| 1:C:19:ARG:HD2 | 1:C:479:THR:CG2 | 2.45 | 0.47 |
| 1:C:335:ASN:CA | 1:C:338:ARG:HH12 | 2.27 | 0.47 |
| 1:C:346:GLU:OE1 | 1:C:369:PRO:HA | 2.15 | 0.47 |
| 1:D:316:GLU:OE1 | 1:D:339:VAL:HA | 2.15 | 0.47 |
| 1:D:431:VAL:HA | 1:D:432:PRO:HD3 | 1.54 | 0.47 |
| 1:E:142:GLU:O | 1:E:143:LYS:C | 2.54 | 0.47 |
| 1:F:213:SER:HB2 | 1:F:217:ARG:HD2 | 1.97 | 0.47 |
| 1:F:252:PHE:HD1 | 1:F:301:ILE:CG2 | 2.28 | 0.47 |
| 1:F:396:ARG:O | 1:F:396:ARG:HD3 | 2.14 | 0.47 |
| 1:F:414:GLN:OE1 | 1:F:428:ILE:HG22 | 2.14 | 0.47 |
| 1:G:26:ASP:C | 1:G:28:LEU:H | 2.18 | 0.47 |
| 1:H:75:ILE:HG22 | 1:H:76:GLU:N | 2.29 | 0.47 |
| 1:I:220:PHE:HZ | 1:I:266:PHE:CD1 | 2.33 | 0.47 |
| 1:I:246:THR:OG1 | 1:I:246:THR:O | 2.33 | 0.47 |
| 1:I:250:GLN:CA | 1:I:314:ILE:HD11 | 2.45 | 0.47 |
| 1:I:356:ALA:HB1 | 1:I:360:PHE:HE2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:394:TYR:CE1 | 1:J:397:LEU:CD2 | 2.97 | 0.47 |
| 1:J:322:LEU:HD13 | 1:J:322:LEU:C | 2.35 | 0.47 |
| 1:J:346:GLU:HG2 | 1:J:351:PRO:HG2 | 1.97 | 0.47 |
| 1:K:13:VAL:O | 1:K:14:GLU:C | 2.53 | 0.47 |
| 1:K:227:ILE:CD1 | 1:K:321:ILE:HD11 | 2.45 | 0.47 |
| 1:K:356:ALA:HB1 | 1:K:360:PHE:CE2 | 2.45 | 0.47 |
| 1:K:200:GLY:N | 1:K:384:GLU:OE1 | 2.47 | 0.47 |
| 1:L:402:GLU:O | 1:L:403:ARG:C | 2.51 | 0.47 |
| 1:A:367:VAL:O | 1:A:369:PRO:HD3 | 2.15 | 0.46 |
| 1:B:246:THR:O | 1:B:246:THR:OG1 | 2.34 | 0.46 |
| 1:C:232:TYR:HB3 | 1:C:233:MET:HE2 | 1.97 | 0.46 |
| 1:C:359:ILE:N | 1:C:359:ILE:HD12 | 2.28 | 0.46 |
| 1:D:81:GLN:NE2 | 1:D:163:ASP:HB2 | 2.30 | 0.46 |
| 1:D:382:TYR:O | 1:D:385:TRP:HB3 | 2.14 | 0.46 |
| 1:D:418:GLU:C | 1:D:420:LYS:H | 2.18 | 0.46 |
| 1:E:145:THR:O | 1:E:148:PHE:HB3 | 2.15 | 0.46 |
| 1:E:158:ILE:HD13 | 1:E:159:GLY:N | 2.30 | 0.46 |
| 1:E:221:HIS:O | 1:E:223:ILE:N | 2.48 | 0.46 |
| 1:E:88:PRO:HG2 | 1:E:122:PHE:CD2 | 2.49 | 0.46 |
| 1:F:25:GLU:O | 1:F:28:LEU:HB3 | 2.15 | 0.46 |
| 1:F:427:THR:O | 1:F:429:PRO:HD3 | 2.15 | 0.46 |
| 1:G:90:LYS:HD2 | 1:G:164:VAL:O | 2.15 | 0.46 |
| 1:G:9:PHE:HD1 | 1:G:10:PHE:N | 2.13 | 0.46 |
| 1:H:104:VAL:CG2 | 1:H:105:LYS:H | 2.27 | 0.46 |
| 1:H:249:VAL:HG22 | 1:H:250:GLN:N | 2.29 | 0.46 |
| 1:H:28:LEU:O | 1:H:32:LEU:HB2 | 2.15 | 0.46 |
| 1:I:153:ALA:N | 1:I:158:ILE:HG22 | 2.30 | 0.46 |
| 1:I:252:PHE:HE2 | 1:I:260:MET:CE | 2.23 | 0.46 |
| 1:I:40:GLN:CG | 1:I:40:GLN:O | 2.63 | 0.46 |
| 1:I:431:VAL:CG1 | 1:J:416:SER:OG | 2.63 | 0.46 |
| 1:I:117:VAL:HG13 | 1:I:464:ILE:HD11 | 1.96 | 0.46 |
| 1:J:153:ALA:CA | 1:J:158:ILE:HG22 | 2.44 | 0.46 |
| 1:J:160:PRO:HG3 | 1:J:191:ASP:OD1 | 2.15 | 0.46 |
| 1:J:368:ILE:HG22 | 1:J:373:LEU:HB2 | 1.96 | 0.46 |
| 1:K:286:ILE:HG21 | 1:K:291:LEU:CD2 | 2.44 | 0.46 |
| 1:L:164:VAL:HG13 | 1:L:198:VAL:HA | 1.98 | 0.46 |
| 1:L:281:TRP:CD1 | 1:L:282:ASN:N | 2.83 | 0.46 |
| 1:L:45:VAL:O | 1:L:45:VAL:HG13 | 2.15 | 0.46 |
| 1:L:465:MET:O | 1:L:466:ARG:C | 2.53 | 0.46 |
| 1:A:264:HIS:ND1 | 1:A:288:PRO:HG2 | 2.29 | 0.46 |
| 1:A:250:GLN:HG3 | 1:A:315:LEU:HD13 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:395:GLY:HA3 | 1:A:399:PHE:CE1 | 2.51 | 0.46 |
| 1:B:392:VAL:HG12 | 1:B:393:SER:N | 2.31 | 0.46 |
| 1:B:85:GLN:HB3 | 1:B:85:GLN:HE21 | 1.46 | 0.46 |
| 1:C:296:LEU:O | 1:C:297:GLN:C | 2.54 | 0.46 |
| 1:C:479:THR:O | 1:C:480:ALA:C | 2.53 | 0.46 |
| 1:D:274:GLY:CA | 1:D:314:ILE:HD12 | 2.45 | 0.46 |
| 1:D:341:ALA:O | 1:D:365:ILE:HD12 | 2.16 | 0.46 |
| 1:D:368:ILE:HG22 | 1:D:373:LEU:HB2 | 1.97 | 0.46 |
| 1:D:372:TYR:CD2 | 1:D:464:ILE:HD12 | 2.50 | 0.46 |
| 1:D:67:ARG:NH1 | 1:D:67:ARG:HB3 | 2.10 | 0.46 |
| 1:E:133:PRO:HA | 1:E:141:LEU:HD21 | 1.97 | 0.46 |
| 1:E:359:ILE:O | 1:E:361:LEU:N | 2.48 | 0.46 |
| 1:F:248:VAL:HG23 | 1:F:271:ILE:HG13 | 1.97 | 0.46 |
| 1:A:400:LYS:HB2 | 1:F:455:TYR:HB2 | 1.96 | 0.46 |
| 1:G:75:ILE:HG23 | 1:G:131:ILE:HD12 | 1.97 | 0.46 |
| 1:G:471:TYR:O | 1:G:473:LEU:HG | 2.15 | 0.46 |
| 1:H:211:ARG:HH11 | 1:H:211:ARG:HB3 | 1.81 | 0.46 |
| 1:H:331:LEU:HD11 | 1:H:344:ILE:HD13 | 1.96 | 0.46 |
| 1:H:200:GLY:N | 1:H:384:GLU:OE1 | 2.48 | 0.46 |
| 1:J:173:GLU:HB2 | 1:J:202:PRO:HD3 | 1.95 | 0.46 |
| 1:K:142:GLU:HG3 | 1:K:178:TRP:CE2 | 2.50 | 0.46 |
| 1:J:186:THR:CG2 | 1:L:186:THR:HG23 | 2.45 | 0.46 |
| 1:L:498:VAL:HG23 | 1:L:499:THR:N | 2.23 | 0.46 |
| 1:A:330:GLN:C | 1:A:331:LEU:HD12 | 2.36 | 0.46 |
| 1:A:446:LYS:HD2 | 1:A:450:HIS:HE1 | 1.80 | 0.46 |
| 1:B:244:ASP:OD2 | 1:B:245:LYS:HG3 | 2.14 | 0.46 |
| 1:B:51:ILE:HD13 | 1:D:64:PRO:HG3 | 1.96 | 0.46 |
| 1:C:141:LEU:O | 1:C:145:THR:CG2 | 2.64 | 0.46 |
| 1:C:234:SER:C | 1:C:236:LEU:H | 2.17 | 0.46 |
| 1:C:359:ILE:O | 1:C:363:ARG:HG2 | 2.15 | 0.46 |
| 1:C:459:ARG:O | 1:C:463:GLN:HG3 | 2.15 | 0.46 |
| 1:C:478:ARG:O | 1:C:479:THR:C | 2.54 | 0.46 |
| 1:D:445:GLU:O | 1:D:449:VAL:HG23 | 2.15 | 0.46 |
| 1:D:488:LYS:O | 1:D:492:VAL:HG23 | 2.15 | 0.46 |
| 1:E:294:PHE:CE2 | 1:E:304:PHE:HB2 | 2.50 | 0.46 |
| 1:E:65:ILE:HA | 1:E:147:ARG:NH1 | 2.29 | 0.46 |
| 1:F:142:GLU:O | 1:F:143:LYS:C | 2.53 | 0.46 |
| 1:F:164:VAL:HG13 | 1:F:198:VAL:CA | 2.45 | 0.46 |
| 1:F:142:GLU:HG3 | 1:F:178:TRP:CE2 | 2.50 | 0.46 |
| 1:F:244:ASP:C | 1:F:245:LYS:HG2 | 2.35 | 0.46 |
| 1:F:437:GLN:O | 1:F:439:ARG:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:258:HIS:HB3 | 1:G:262:TYR:CE2 | 2.50 | 0.46 |
| 1:G:335:ASN:C | 1:G:335:ASN:ND2 | 2.65 | 0.46 |
| 1:G:414:GLN:CG | 1:G:429:PRO:HD2 | 2.45 | 0.46 |
| 1:G:440:ILE:H | 1:G:440:ILE:HG13 | 1.52 | 0.46 |
| 1:I:45:VAL:HG13 | 1:I:45:VAL:O | 2.15 | 0.46 |
| 1:I:478:ARG:O | 1:I:481:ALA:N | 2.48 | 0.46 |
| 1:J:193:ASN:O | 1:J:194:ALA:C | 2.53 | 0.46 |
| 1:J:222:GLY:HA3 | 1:J:373:LEU:HD11 | 1.96 | 0.46 |
| 1:I:412:SER:CA | 1:K:433:THR:HG22 | 2.44 | 0.46 |
| 1:K:500:PHE:CE1 | 1:L:500:PHE:CZ | 2.98 | 0.46 |
| 1:L:117:VAL:HG11 | 1:L:372:TYR:HB2 | 1.97 | 0.46 |
| 1:L:201:LYS:HB2 | 1:L:202:PRO:CD | 2.45 | 0.46 |
| 1:A:17:PHE:CD1 | 1:A:113:TYR:OH | 2.67 | 0.46 |
| 1:A:208:ILE:O | 1:A:208:ILE:HG23 | 2.14 | 0.46 |
| 1:A:372:TYR:CD1 | 1:A:372:TYR:C | 2.88 | 0.46 |
| 1:A:40:GLN:C | 1:A:42:ARG:H | 2.17 | 0.46 |
| 1:B:248:VAL:CG1 | 1:B:272:ALA:HB3 | 2.45 | 0.46 |
| 1:B:359:ILE:O | 1:B:362:GLU:N | 2.48 | 0.46 |
| 1:C:201:LYS:HZ3 | 1:C:388:ASN:HD21 | 1.60 | 0.46 |
| 1:C:394:TYR:HB2 | 1:C:445:GLU:HG3 | 1.97 | 0.46 |
| 1:D:142:GLU:OE1 | 1:D:146:ARG:NH1 | 2.48 | 0.46 |
| 1:D:238:MET:O | 1:D:239:THR:HG22 | 2.14 | 0.46 |
| 1:E:387:LYS:HE3 | 1:E:393:SER:HA | 1.96 | 0.46 |
| 1:F:141:LEU:HD23 | 1:F:141:LEU:HA | 1.77 | 0.46 |
| 1:F:470:LYS:HD3 | 1:F:471:TYR:HE2 | 1.79 | 0.46 |
| 1:G:462:ARG:HB3 | 1:G:466:ARG:HH11 | 1.74 | 0.46 |
| 1:G:96:SER:HB3 | 1:G:99:VAL:CG1 | 2.45 | 0.46 |
| 1:H:334:SER:O | 1:H:337:PRO:HD2 | 2.16 | 0.46 |
| 1:H:481:ALA:O | 1:H:482:TYR:C | 2.51 | 0.46 |
| 1:H:498:VAL:O | 1:H:501:THR:HB | 2.15 | 0.46 |
| 1:I:218:GLY:O | 1:I:219:VAL:C | 2.53 | 0.46 |
| 1:I:236:LEU:HB3 | 1:I:238:MET:CG | 2.43 | 0.46 |
| 1:I:346:GLU:C | 1:I:348:ALA:H | 2.18 | 0.46 |
| 1:I:387:LYS:HA | 1:I:390:ASN:HD22 | 1.81 | 0.46 |
| 1:J:264:HIS:HD2 | 1:J:288:PRO:HD3 | 1.76 | 0.46 |
| 1:J:471:TYR:O | 1:J:473:LEU:HD23 | 2.15 | 0.46 |
| 1:L:109:SER:O | 1:L:113:TYR:CD2 | 2.69 | 0.46 |
| 1:A:359:ILE:HG22 | 1:A:360:PHE:N | 2.30 | 0.46 |
| 1:B:111:MET:O | 1:B:114:LYS:N | 2.48 | 0.46 |
| 1:B:192:ILE:O | 1:B:192:ILE:CG1 | 2.63 | 0.46 |
| 1:B:40:GLN:C | 1:B:42:ARG:H | 2.18 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:329:LYS:HA | 1:C:351:PRO:O | 2.15 | 0.46 |
| 1:D:435:GLU:O | 1:D:438:ASP:HB2 | 2.16 | 0.46 |
| 1:D:53:LYS:HB3 | 1:D:54:PRO:CD | 2.43 | 0.46 |
| 1:D:59:LEU:HG | 1:D:61:LEU:CD2 | 2.46 | 0.46 |
| 1:F:304:PHE:HA | 1:F:305:PRO:HD3 | 1.70 | 0.46 |
| 1:F:305:PRO:O | 1:F:306:LYS:HB2 | 2.15 | 0.46 |
| 1:F:328:GLU:HG2 | 1:F:328:GLU:H | 1.41 | 0.46 |
| 1:F:384:GLU:O | 1:F:385:TRP:C | 2.53 | 0.46 |
| 1:F:497:GLY:N | 1:F:501:THR:HA | 2.30 | 0.46 |
| 1:G:112:THR:HG22 | 1:G:124:GLY:N | 2.30 | 0.46 |
| 1:G:398:THR:O | 1:G:401:TYR:N | 2.48 | 0.46 |
| 1:G:57:HIS:CD2 | 1:G:84:HIS:NE2 | 2.83 | 0.46 |
| 1:H:36:GLU:O | 1:H:38:GLU:OE1 | 2.34 | 0.46 |
| 1:I:112:THR:H | 1:I:124:GLY:HA3 | 1.80 | 0.46 |
| 1:I:396:ARG:HG3 | 1:I:396:ARG:NH1 | 2.13 | 0.46 |
| 1:K:45:VAL:C | 1:K:47:GLY:N | 2.68 | 0.46 |
| 1:L:280:ILE:HD11 | 1:L:304:PHE:HB3 | 1.97 | 0.46 |
| 1:L:90:LYS:CB | 1:L:122:PHE:HD1 | 2.27 | 0.46 |
| 1:B:473:LEU:HD13 | 1:B:479:THR:OG1 | 2.15 | 0.46 |
| 1:C:372:TYR:CD2 | 1:C:464:ILE:CD1 | 2.96 | 0.46 |
| 1:C:374:ASN:C | 1:C:374:ASN:ND2 | 2.69 | 0.46 |
| 1:C:386:LEU:O | 1:C:387:LYS:C | 2.53 | 0.46 |
| 1:C:87:THR:CB | 1:C:88:PRO:CD | 2.82 | 0.46 |
| 1:D:230:ALA:O | 1:D:231:SER:C | 2.53 | 0.46 |
| 1:D:294:PHE:CE2 | 1:D:304:PHE:HA | 2.51 | 0.46 |
| 1:E:282:ASN:C | 1:E:284:ASP:H | 2.18 | 0.46 |
| 1:E:305:PRO:O | 1:E:306:LYS:CB | 2.62 | 0.46 |
| 1:F:224:GLU:HA | 1:F:227:ILE:CG2 | 2.43 | 0.46 |
| 1:H:431:VAL:HG13 | 1:H:431:VAL:O | 2.16 | 0.46 |
| 1:I:132:ASN:OD1 | 1:I:134:LYS:HB2 | 2.16 | 0.46 |
| 1:I:24:VAL:HG12 | 1:I:28:LEU:CD2 | 2.41 | 0.46 |
| 1:I:496:ALA:C | 1:I:501:THR:O | 2.54 | 0.46 |
| 1:J:132:ASN:HA | 1:J:133:PRO:HD3 | 1.62 | 0.46 |
| 1:J:137:THR:O | 1:J:140:GLU:N | 2.49 | 0.46 |
| 1:J:142:GLU:HA | 1:J:178:TRP:CE3 | 2.50 | 0.46 |
| 1:K:254:ASN:O | 1:K:257:LEU:HB3 | 2.16 | 0.46 |
| 1:K:257:LEU:C | 1:K:257:LEU:HD12 | 2.36 | 0.46 |
| 1:K:274:GLY:HA2 | 1:K:279:SER:HA | 1.96 | 0.46 |
| 1:K:368:ILE:HG21 | 1:K:373:LEU:HD13 | 1.98 | 0.46 |
| 1:L:221:HIS:CD2 | 1:L:224:GLU:OE1 | 2.68 | 0.46 |
| 1:B:129:VAL:O | 1:B:130:LYS:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:467:THR:O | 1:B:470:LYS:HB3 | 2.15 | 0.46 |
| 1:B:475:LEU:CD1 | 1:B:475:LEU:N | 2.78 | 0.46 |
| 1:C:72:TRP:NE1 | 1:F:498:VAL:HG21 | 2.31 | 0.46 |
| 1:D:45:VAL:C | 1:D:47:GLY:N | 2.69 | 0.46 |
| 1:D:497:GLY:C | 1:D:501:THR:HB | 2.36 | 0.46 |
| 1:E:330:GLN:HA | 1:E:330:GLN:HE21 | 1.81 | 0.46 |
| 1:E:85:GLN:HB3 | 1:E:85:GLN:HE21 | 1.33 | 0.46 |
| 1:A:412:SER:OG | 1:F:433:THR:HG23 | 2.15 | 0.46 |
| 1:G:221:HIS:HA | 1:G:224:GLU:HB3 | 1.98 | 0.46 |
| 1:G:264:HIS:C | 1:G:266:PHE:N | 2.68 | 0.46 |
| 1:G:79:ARG:HD2 | 1:G:127:ALA:HB2 | 1.97 | 0.46 |
| 1:G:90:LYS:HE2 | 1:G:164:VAL:CG1 | 2.46 | 0.46 |
| 1:G:9:PHE:CD1 | 1:G:10:PHE:N | 2.82 | 0.46 |
| 1:H:165:PRO:HD2 | 1:H:197:CYS:O | 2.16 | 0.46 |
| 1:H:498:VAL:HG21 | 1:J:72:TRP:HE1 | 1.80 | 0.46 |
| 1:H:61:LEU:N | 1:H:61:LEU:HD12 | 2.31 | 0.46 |
| 1:K:275:GLU:HG3 | 1:K:301:ILE:HG13 | 1.97 | 0.46 |
| 1:K:369:PRO:O | 1:K:370:ASP:C | 2.54 | 0.46 |
| 1:L:461:ALA:O | 1:L:465:MET:HG3 | 2.16 | 0.46 |
| 1:A:404:ASP:O | 1:A:405:SER:C | 2.54 | 0.46 |
| 1:B:129:VAL:O | 1:B:131:ILE:N | 2.48 | 0.46 |
| 1:B:192:ILE:HG12 | 1:B:192:ILE:O | 2.14 | 0.46 |
| 1:B:335:ASN:ND2 | 1:B:335:ASN:N | 2.63 | 0.46 |
| 1:C:160:PRO:HD3 | 1:C:183:TYR:CE2 | 2.50 | 0.46 |
| 1:C:247:PHE:CE2 | 1:C:263:LEU:HB3 | 2.51 | 0.46 |
| 1:D:366:MET:CB | 1:D:475:LEU:HD23 | 2.39 | 0.46 |
| 1:E:131:ILE:HG23 | 1:E:132:ASN:N | 2.31 | 0.46 |
| 1:F:12:MET:HG2 | 1:F:16:PHE:CZ | 2.50 | 0.46 |
| 1:F:17:PHE:O | 1:F:18:ASP:C | 2.53 | 0.46 |
| 1:G:346:GLU:OE2 | 1:G:351:PRO:HD2 | 2.16 | 0.46 |
| 1:G:420:LYS:O | 1:G:420:LYS:HE2 | 2.16 | 0.46 |
| 1:H:428:ILE:O | 1:H:431:VAL:CG1 | 2.61 | 0.46 |
| 1:I:451:SER:OG | 1:I:452:GLY:N | 2.49 | 0.46 |
| 1:J:114:LYS:HD3 | 1:J:375:ALA:HA | 1.98 | 0.46 |
| 1:J:248:VAL:CG2 | 1:J:271:ILE:HG23 | 2.45 | 0.46 |
| 1:J:386:LEU:HB2 | 1:J:394:TYR:OH | 2.16 | 0.46 |
| 1:J:87:THR:HG22 | 1:J:88:PRO:CD | 2.45 | 0.46 |
| 1:K:152:LEU:HD23 | 1:K:158:ILE:HB | 1.97 | 0.46 |
| 1:K:313:SER:C | 1:K:315:LEU:H | 2.19 | 0.46 |
| 1:K:485:ALA:O | 1:K:488:LYS:N | 2.46 | 0.46 |
| 1:L:104:VAL:CG2 | 1:L:105:LYS:N | 2.77 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:318:ASP:OD1 | 1:L:340:LYS:HB3 | 2.15 | 0.46 |
| 1:L:380:VAL:O | 1:L:383:PHE:HB2 | 2.16 | 0.46 |
| 1:A:282:ASN:O | 1:A:284:ASP:N | 2.38 | 0.46 |
| 1:A:433:THR:CG2 | 1:B:412:SER:HA | 2.46 | 0.46 |
| 1:A:84:HIS:CD2 | 1:A:89:CYS:SG | 3.07 | 0.46 |
| 1:B:17:PHE:CE1 | 1:B:486:ILE:HD12 | 2.50 | 0.46 |
| 1:B:279:SER:HB2 | 1:B:310:TYR:HB3 | 1.97 | 0.46 |
| 1:C:101:VAL:HG23 | 1:C:102:ASP:H | 1.81 | 0.46 |
| 1:D:96:SER:O | 1:D:130:LYS:HD2 | 2.16 | 0.46 |
| 1:D:244:ASP:O | 1:D:245:LYS:CG | 2.64 | 0.46 |
| 1:D:423:LYS:HG3 | 1:D:424:HIS:N | 2.31 | 0.46 |
| 1:E:237:GLY:C | 1:E:238:MET:HG2 | 2.36 | 0.46 |
| 1:E:409:LEU:O | 1:E:410:LEU:C | 2.52 | 0.46 |
| 1:F:165:PRO:O | 1:F:198:VAL:HG23 | 2.16 | 0.46 |
| 1:F:436:PHE:O | 1:F:437:GLN:C | 2.54 | 0.46 |
| 1:G:238:MET:O | 1:G:239:THR:O | 2.33 | 0.46 |
| 1:G:114:LYS:HG3 | 1:G:371:LEU:O | 2.16 | 0.46 |
| 1:H:132:ASN:HB3 | 1:H:135:ASN:ND2 | 2.31 | 0.46 |
| 1:H:114:LYS:HA | 1:H:371:LEU:HD12 | 1.97 | 0.46 |
| 1:H:427:THR:O | 1:H:428:ILE:HD13 | 2.16 | 0.46 |
| 1:I:155:LYS:HE3 | 1:L:81:GLN:OE1 | 2.16 | 0.46 |
| 1:I:193:ASN:HB3 | 1:I:389:LEU:HD23 | 1.97 | 0.46 |
| 1:I:344:ILE:CD1 | 1:I:360:PHE:CE1 | 2.95 | 0.46 |
| 1:I:96:SER:OG | 1:I:98:ASP:OD1 | 2.30 | 0.46 |
| 1:J:403:ARG:HG3 | 1:J:440:ILE:HG22 | 1.96 | 0.46 |
| 1:K:148:PHE:O | 1:K:152:LEU:HB2 | 2.15 | 0.46 |
| 1:K:252:PHE:HZ | 1:K:260:MET:HE1 | 1.80 | 0.46 |
| 1:K:17:PHE:HE1 | 1:K:486:ILE:HD12 | 1.77 | 0.46 |
| 1:L:423:LYS:HG2 | 1:L:426:GLY:CA | 2.46 | 0.46 |
| 1:L:460:SER:O | 1:L:461:ALA:C | 2.51 | 0.46 |
| 1:L:470:LYS:HD2 | 1:L:471:TYR:CE2 | 2.51 | 0.46 |
| 1:L:90:LYS:HG3 | 1:L:91:GLY:N | 2.31 | 0.46 |
| 1:A:287:ASP:HB3 | 1:A:290:GLU:CG | 2.46 | 0.46 |
| 1:A:385:TRP:O | 1:A:388:ASN:HB2 | 2.16 | 0.46 |
| 1:C:279:SER:OG | 1:C:280:ILE:N | 2.49 | 0.46 |
| 1:C:344:ILE:CD1 | 1:C:360:PHE:CE1 | 2.97 | 0.46 |
| 1:D:417:LEU:CD2 | 1:E:417:LEU:HD11 | 2.46 | 0.46 |
| 1:F:271:ILE:HG22 | 1:F:283:PRO:HA | 1.98 | 0.46 |
| 1:F:470:LYS:HD3 | 1:F:471:TYR:CE2 | 2.51 | 0.46 |
| 1:F:47:GLY:O | 1:F:50:ARG:HG3 | 2.16 | 0.46 |
| 1:G:288:PRO:O | 1:G:289:LYS:C | 2.53 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:368:ILE:HA | 1:G:369:PRO:HD3 | 1.41 | 0.46 |
| 1:I:166:ALA:HA | 1:I:176:MET:HE2 | 1.98 | 0.46 |
| 1:J:126:LYS:HG3 | 1:J:127:ALA:H | 1.81 | 0.46 |
| 1:J:90:LYS:HZ2 | 1:J:164:VAL:HG12 | 1.78 | 0.46 |
| 1:J:281:TRP:O | 1:J:282:ASN:CB | 2.63 | 0.46 |
| 1:J:346:GLU:OE1 | 1:J:369:PRO:HA | 2.16 | 0.46 |
| 1:J:479:THR:O | 1:J:480:ALA:C | 2.54 | 0.46 |
| 1:J:99:VAL:HG23 | 1:J:99:VAL:O | 2.16 | 0.46 |
| 1:K:232:TYR:HD1 | 1:K:232:TYR:H | 1.62 | 0.46 |
| 1:K:466:ARG:O | 1:K:468:ALA:N | 2.47 | 0.46 |
| 1:K:471:TYR:O | 1:K:473:LEU:N | 2.49 | 0.46 |
| 1:L:234:SER:C | 1:L:236:LEU:N | 2.66 | 0.46 |
| 1:L:248:VAL:HG22 | 1:L:271:ILE:CG2 | 2.44 | 0.46 |
| 1:L:496:ALA:HB1 | 1:L:501:THR:O | 2.15 | 0.46 |
| 1:A:157:PHE:CE2 | 1:E:155:LYS:HD2 | 2.52 | 0.45 |
| 1:A:173:GLU:O | 1:A:174:ARG:C | 2.53 | 0.45 |
| 1:A:256:GLY:O | 1:A:259:SER:N | 2.49 | 0.45 |
| 1:A:495:GLU:O | 1:A:496:ALA:HB2 | 2.16 | 0.45 |
| 1:A:57:HIS:ND1 | 1:A:84:HIS:CE1 | 2.68 | 0.45 |
| 1:B:369:PRO:HG3 | 1:B:478:ARG:HA | 1.96 | 0.45 |
| 1:B:498:VAL:HG21 | 1:D:72:TRP:HZ2 | 1.81 | 0.45 |
| 1:D:244:ASP:OD1 | 1:D:245:LYS:N | 2.49 | 0.45 |
| 1:D:368:ILE:HA | 1:D:369:PRO:HD3 | 1.54 | 0.45 |
| 1:E:159:GLY:O | 1:E:163:ASP:O | 2.34 | 0.45 |
| 1:E:433:THR:HG23 | 1:E:436:PHE:CB | 2.41 | 0.45 |
| 1:H:489:VAL:O | 1:H:492:VAL:HG23 | 2.16 | 0.45 |
| 1:H:75:ILE:N | 1:H:75:ILE:CD1 | 2.77 | 0.45 |
| 1:I:104:VAL:HG23 | 1:I:105:LYS:N | 2.31 | 0.45 |
| 1:I:264:HIS:O | 1:I:266:PHE:N | 2.50 | 0.45 |
| 1:I:48:ILE:HG13 | 1:I:490:PHE:CE1 | 2.51 | 0.45 |
| 1:J:175:GLU:HA | 1:J:178:TRP:CE3 | 2.51 | 0.45 |
| 1:J:337:PRO:HA | 1:J:363:ARG:NE | 2.23 | 0.45 |
| 1:I:410:LEU:HD21 | 1:J:409:LEU:HD13 | 1.95 | 0.45 |
| 1:K:114:LYS:O | 1:K:117:VAL:HB | 2.15 | 0.45 |
| 1:K:150:MET:HB3 | 1:K:150:MET:HE2 | 1.79 | 0.45 |
| 1:K:410:LEU:HB3 | 1:K:430:ILE:HA | 1.98 | 0.45 |
| 1:G:72:TRP:CZ3 | 1:K:45:VAL:HG23 | 2.51 | 0.45 |
| 1:L:152:LEU:HD12 | 1:L:157:PHE:HB2 | 1.99 | 0.45 |
| 1:L:369:PRO:HG3 | 1:L:478:ARG:N | 2.31 | 0.45 |
| 1:L:471:TYR:HB2 | 1:L:473:LEU:CD1 | 2.46 | 0.45 |
| 1:A:281:TRP:CD1 | 1:A:282:ASN:N | 2.83 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:ARG:NH2 | 1:A:42:ARG:CZ | 2.79 | 0.45 |
| 1:B:164:VAL:HG21 | 1:B:385:TRP:NE1 | 2.30 | 0.45 |
| 1:B:449:VAL:O | 1:B:450:HIS:C | 2.53 | 0.45 |
| 1:B:89:CYS:O | 1:B:163:ASP:HA | 2.17 | 0.45 |
| 1:D:101:VAL:O | 1:D:105:LYS:HG3 | 2.17 | 0.45 |
| 1:D:203:ILE:HD13 | 1:D:203:ILE:HA | 1.74 | 0.45 |
| 1:B:500:PHE:CE1 | 1:F:143:LYS:HD3 | 2.52 | 0.45 |
| 1:G:14:GLU:HG3 | 1:G:53:LYS:HE3 | 1.97 | 0.45 |
| 1:G:252:PHE:HD2 | 1:G:273:VAL:HG11 | 1.81 | 0.45 |
| 1:G:78:TYR:CD1 | 1:G:78:TYR:N | 2.84 | 0.45 |
| 1:H:81:GLN:HG2 | 1:H:163:ASP:OD2 | 2.16 | 0.45 |
| 1:H:248:VAL:HG22 | 1:H:271:ILE:HG23 | 1.98 | 0.45 |
| 1:H:305:PRO:O | 1:H:306:LYS:CB | 2.61 | 0.45 |
| 1:I:202:PRO:O | 1:I:203:ILE:C | 2.54 | 0.45 |
| 1:I:382:TYR:O | 1:I:386:LEU:HG | 2.16 | 0.45 |
| 1:I:389:LEU:O | 1:I:391:HIS:CD2 | 2.70 | 0.45 |
| 1:I:39:GLU:O | 1:I:40:GLN:C | 2.55 | 0.45 |
| 1:I:91:GLY:HA2 | 1:I:111:MET:HE3 | 1.98 | 0.45 |
| 1:J:58:VAL:CG2 | 1:J:80:ALA:HB2 | 2.46 | 0.45 |
| 1:K:414:GLN:CG | 1:K:429:PRO:HD2 | 2.46 | 0.45 |
| 1:A:360:PHE:CD1 | 1:A:365:ILE:HG21 | 2.52 | 0.45 |
| 1:B:60:SER:C | 1:B:61:LEU:HD12 | 2.36 | 0.45 |
| 1:C:93:ILE:CD1 | 1:C:165:PRO:HB3 | 2.39 | 0.45 |
| 1:D:87:THR:CG2 | 1:D:88:PRO:CD | 2.91 | 0.45 |
| 1:D:87:THR:HG22 | 1:D:88:PRO:CG | 2.46 | 0.45 |
| 1:E:140:GLU:O | 1:E:144:ILE:HG13 | 2.15 | 0.45 |
| 1:F:132:ASN:HA | 1:F:133:PRO:HD3 | 1.67 | 0.45 |
| 1:F:397:LEU:N | 1:F:397:LEU:HD12 | 2.30 | 0.45 |
| 1:G:114:LYS:HA | 1:G:117:VAL:HG23 | 1.99 | 0.45 |
| 1:G:342:LYS:HA | 1:G:342:LYS:HD2 | 1.79 | 0.45 |
| 1:I:31:ASP:N | 1:I:31:ASP:OD2 | 2.49 | 0.45 |
| 1:I:431:VAL:HG12 | 1:J:416:SER:OG | 2.15 | 0.45 |
| 1:I:492:VAL:HG21 | 2:I:502:ADP:C2 | 2.51 | 0.45 |
| 1:I:87:THR:CB | 1:I:88:PRO:HD3 | 2.45 | 0.45 |
| 1:J:191:ASP:C | 1:J:193:ASN:H | 2.20 | 0.45 |
| 1:J:385:TRP:CE3 | 1:J:386:LEU:HD23 | 2.51 | 0.45 |
| 1:K:95:TYR:O | 1:K:133:PRO:HD3 | 2.16 | 0.45 |
| 1:K:345:ALA:HB1 | 1:K:373:LEU:CD2 | 2.45 | 0.45 |
| 1:K:52:ILE:HD13 | 1:K:489:VAL:CG1 | 2.42 | 0.45 |
| 1:L:82:HIS:HB3 | 1:L:112:THR:HG21 | 1.98 | 0.45 |
| 1:L:65:ILE:HG21 | 1:L:144:ILE:CG1 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:269:LYS:HD2 | 1:L:285:GLY:CA | 2.46 | 0.45 |
| 1:L:431:VAL:O | 1:L:431:VAL:HG13 | 2.16 | 0.45 |
| 1:A:314:ILE:H | 1:A:314:ILE:HD13 | 1.80 | 0.45 |
| 1:A:356:ALA:O | 1:A:360:PHE:CD2 | 2.68 | 0.45 |
| 1:A:414:GLN:CB | 1:A:429:PRO:HD2 | 2.47 | 0.45 |
| 1:B:281:TRP:CZ2 | 1:B:283:PRO:CG | 2.99 | 0.45 |
| 1:B:28:LEU:HD21 | 1:B:490:PHE:CD2 | 2.51 | 0.45 |
| 1:C:213:SER:HA | 1:C:258:HIS:CD2 | 2.51 | 0.45 |
| 1:D:48:ILE:O | 1:D:52:ILE:HG13 | 2.16 | 0.45 |
| 1:E:220:PHE:CD1 | 1:E:221:HIS:N | 2.84 | 0.45 |
| 1:F:32:LEU:O | 1:F:33:ARG:CB | 2.64 | 0.45 |
| 1:G:137:THR:HB | 1:G:140:GLU:H | 1.81 | 0.45 |
| 1:G:6:ASP:HA | 1:G:7:PRO:HD3 | 1.75 | 0.45 |
| 1:H:148:PHE:O | 1:H:149:THR:C | 2.55 | 0.45 |
| 1:H:238:MET:C | 1:H:240:PRO:HD3 | 2.37 | 0.45 |
| 1:H:300:SER:OG | 1:H:302:LEU:HD13 | 2.16 | 0.45 |
| 1:I:107:LEU:O | 1:I:110:LEU:HB3 | 2.16 | 0.45 |
| 1:I:91:GLY:O | 1:I:165:PRO:HA | 2.16 | 0.45 |
| 1:I:328:GLU:O | 1:I:329:LYS:C | 2.55 | 0.45 |
| 1:I:343:ILE:HD13 | 1:I:366:MET:HE2 | 1.99 | 0.45 |
| 1:I:344:ILE:HB | 1:I:367:VAL:HG13 | 1.97 | 0.45 |
| 1:I:417:LEU:HD21 | 1:J:417:LEU:HD21 | 1.99 | 0.45 |
| 1:J:282:ASN:OD1 | 1:J:282:ASN:C | 2.54 | 0.45 |
| 1:K:332:THR:H | 1:K:335:ASN:HD21 | 1.63 | 0.45 |
| 1:I:401:TYR:CD1 | 1:K:448:ILE:HD13 | 2.51 | 0.45 |
| 1:A:329:LYS:HB2 | 1:A:329:LYS:HE3 | 1.67 | 0.45 |
| 1:B:201:LYS:HB2 | 1:B:202:PRO:CD | 2.47 | 0.45 |
| 1:B:323:ILE:HA | 1:B:324:PRO:HD3 | 1.79 | 0.45 |
| 1:C:112:THR:HB | 1:C:124:GLY:N | 2.29 | 0.45 |
| 1:C:389:LEU:HD21 | 1:D:192:ILE:HD11 | 1.99 | 0.45 |
| 1:C:471:TYR:HB2 | 1:C:473:LEU:HD12 | 1.98 | 0.45 |
| 1:C:389:LEU:HD21 | 1:D:192:ILE:CD1 | 2.46 | 0.45 |
| 1:D:222:GLY:HA3 | 1:D:373:LEU:HD12 | 1.98 | 0.45 |
| 1:D:229:GLU:O | 1:D:233:MET:HG2 | 2.17 | 0.45 |
| 1:D:331:LEU:CD1 | 1:D:344:ILE:HD13 | 2.46 | 0.45 |
| 1:E:223:ILE:O | 1:E:224:GLU:C | 2.54 | 0.45 |
| 1:E:410:LEU:HD13 | 1:E:430:ILE:C | 2.36 | 0.45 |
| 1:E:462:ARG:O | 1:E:463:GLN:C | 2.55 | 0.45 |
| 1:E:498:VAL:O | 1:E:501:THR:CG2 | 2.64 | 0.45 |
| 1:F:244:ASP:HB2 | 1:G:437:GLN:HG2 | 1.98 | 0.45 |
| 2:B:2:ADP:O3A | 1:F:393:SER:HB3 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:453:LEU:C | 1:F:453:LEU:HD22 | 2.36 | 0.45 |
| 1:H:142:GLU:O | 1:H:143:LYS:C | 2.54 | 0.45 |
| 1:I:140:GLU:O | 1:I:144:ILE:HG13 | 2.15 | 0.45 |
| 1:I:24:VAL:O | 1:I:25:GLU:C | 2.54 | 0.45 |
| 1:I:369:PRO:CG | 1:I:478:ARG:HA | 2.47 | 0.45 |
| 1:I:219:VAL:HG22 | 1:I:373:LEU:HD22 | 1.99 | 0.45 |
| 1:K:10:PHE:O | 1:K:14:GLU:HG3 | 2.16 | 0.45 |
| 1:K:230:ALA:O | 1:K:231:SER:C | 2.55 | 0.45 |
| 1:K:40:GLN:CA | 1:K:40:GLN:HE21 | 1.96 | 0.45 |
| 1:K:421:PHE:O | 1:K:422:GLY:C | 2.55 | 0.45 |
| 1:K:429:PRO:O | 1:K:431:VAL:N | 2.50 | 0.45 |
| 1:L:448:ILE:O | 1:L:449:VAL:C | 2.53 | 0.45 |
| 1:L:474:GLY:C | 1:L:475:LEU:HD12 | 2.36 | 0.45 |
| 1:A:182:THR:O | 1:A:186:THR:HB | 2.17 | 0.45 |
| 1:A:263:LEU:HD12 | 1:A:263:LEU:HA | 1.85 | 0.45 |
| 1:A:252:PHE:H | 1:A:275:GLU:HG2 | 1.81 | 0.45 |
| 1:A:414:GLN:CG | 1:A:429:PRO:HD2 | 2.47 | 0.45 |
| 1:B:336:ALA:O | 1:B:339:VAL:HG22 | 2.17 | 0.45 |
| 1:B:39:GLU:HB2 | 1:B:41:LYS:HG2 | 1.99 | 0.45 |
| 1:C:180:ALA:HA | 1:C:197:CYS:SG | 2.56 | 0.45 |
| 1:C:382:TYR:O | 1:C:386:LEU:HG | 2.17 | 0.45 |
| 1:C:394:TYR:CE2 | 1:D:397:LEU:HD22 | 2.51 | 0.45 |
| 1:C:466:ARG:HB2 | 1:C:466:ARG:HH11 | 1.82 | 0.45 |
| 1:D:265:ARG:HG2 | 1:D:266:PHE:CE2 | 2.51 | 0.45 |
| 1:D:305:PRO:O | 1:D:306:LYS:HB2 | 2.16 | 0.45 |
| 1:D:324:PRO:HD2 | 1:D:345:ALA:O | 2.17 | 0.45 |
| 1:D:379:THR:O | 1:D:382:TYR:HB3 | 2.16 | 0.45 |
| 1:E:182:THR:HG22 | 1:E:183:TYR:N | 2.30 | 0.45 |
| 1:E:415:GLU:O | 1:E:419:ARG:HG3 | 2.17 | 0.45 |
| 1:E:8:ASN:O | 1:E:11:LYS:N | 2.49 | 0.45 |
| 1:F:342:LYS:HD3 | 1:F:365:ILE:HD13 | 1.99 | 0.45 |
| 1:F:46:ARG:HD3 | 1:F:46:ARG:O | 2.17 | 0.45 |
| 1:G:111:MET:HE2 | 1:G:111:MET:HA | 1.98 | 0.45 |
| 1:G:153:ALA:CA | 1:G:158:ILE:HG23 | 2.46 | 0.45 |
| 1:G:248:VAL:HG12 | 1:G:314:ILE:HG13 | 1.98 | 0.45 |
| 1:G:380:VAL:O | 1:G:383:PHE:HB2 | 2.16 | 0.45 |
| 1:G:431:VAL:HG13 | 1:G:431:VAL:O | 2.16 | 0.45 |
| 1:J:243:GLY:O | 1:J:245:LYS:N | 2.50 | 0.45 |
| 1:J:33:ARG:HH12 | 1:J:36:GLU:HG3 | 1.81 | 0.45 |
| 1:J:337:PRO:CA | 1:J:363:ARG:HH21 | 2.28 | 0.45 |
| 1:J:57:HIS:ND1 | 1:J:84:HIS:NE2 | 2.42 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:226:PHE:C | 1:K:228:ASN:N | 2.67 | 0.45 |
| 1:A:107:LEU:HA | 1:A:107:LEU:HD22 | 1.69 | 0.45 |
| 1:A:404:ASP:O | 1:A:406:ASN:N | 2.49 | 0.45 |
| 1:A:490:PHE:O | 1:A:491:LYS:C | 2.54 | 0.45 |
| 1:B:186:THR:HG22 | 1:B:187:ILE:H | 1.81 | 0.45 |
| 1:C:149:THR:HG23 | 1:C:158:ILE:HD13 | 1.98 | 0.45 |
| 1:C:217:ARG:NH1 | 1:C:221:HIS:CE1 | 2.73 | 0.45 |
| 1:C:335:ASN:O | 1:C:338:ARG:N | 2.50 | 0.45 |
| 1:C:393:SER:HB3 | 2:E:5:ADP:O3A | 2.17 | 0.45 |
| 1:C:457:MET:O | 1:C:458:GLU:C | 2.54 | 0.45 |
| 1:E:248:VAL:HG22 | 1:E:272:ALA:N | 2.31 | 0.45 |
| 1:F:476:ASP:OD2 | 1:F:479:THR:HG23 | 2.17 | 0.45 |
| 1:C:64:PRO:HB3 | 1:F:51:ILE:HD11 | 1.97 | 0.45 |
| 1:G:82:HIS:CG | 1:G:112:THR:HG21 | 2.48 | 0.45 |
| 1:H:244:ASP:OD2 | 1:H:245:LYS:HE2 | 2.17 | 0.45 |
| 1:H:483:VAL:HG12 | 1:H:484:ASN:N | 2.30 | 0.45 |
| 1:H:494:ASN:C | 1:H:496:ALA:H | 2.20 | 0.45 |
| 1:H:89:CYS:O | 1:H:163:ASP:HA | 2.16 | 0.45 |
| 1:I:101:VAL:O | 1:I:105:LYS:HG3 | 2.16 | 0.45 |
| 1:I:34:THR:C | 1:I:35:ARG:HG3 | 2.37 | 0.45 |
| 1:I:47:GLY:O | 1:I:48:ILE:C | 2.55 | 0.45 |
| 1:J:464:ILE:HD13 | 1:J:481:ALA:HB2 | 1.99 | 0.45 |
| 1:K:308:LYS:HA | 1:K:309:PRO:HD3 | 1.72 | 0.45 |
| 1:K:453:LEU:CD2 | 1:K:453:LEU:C | 2.84 | 0.45 |
| 1:K:6:ASP:CG | 1:K:329:LYS:HE2 | 2.37 | 0.45 |
| 1:L:334:SER:O | 1:L:337:PRO:HD2 | 2.16 | 0.45 |
| 1:L:362:GLU:OE1 | 1:L:362:GLU:HA | 2.17 | 0.45 |
| 1:A:271:ILE:CD1 | 1:A:283:PRO:HA | 2.47 | 0.45 |
| 1:A:335:ASN:HD22 | 1:A:336:ALA:H | 1.65 | 0.45 |
| 1:A:411:MET:HA | 1:A:430:ILE:CG2 | 2.46 | 0.45 |
| 1:A:6:ASP:N | 1:A:6:ASP:OD1 | 2.50 | 0.45 |
| 1:B:147:ARG:HD3 | 1:D:499:THR:OG1 | 2.17 | 0.45 |
| 1:B:282:ASN:C | 1:B:282:ASN:OD1 | 2.55 | 0.45 |
| 1:B:335:ASN:ND2 | 1:B:336:ALA:N | 2.64 | 0.45 |
| 1:C:132:ASN:O | 1:C:133:PRO:C | 2.55 | 0.45 |
| 1:C:142:GLU:CA | 1:C:178:TRP:CZ3 | 2.99 | 0.45 |
| 1:C:240:PRO:HD2 | 1:C:245:LYS:HZ3 | 1.81 | 0.45 |
| 1:C:221:HIS:CE1 | 1:C:454:ALA:HB2 | 2.51 | 0.45 |
| 1:D:346:GLU:OE2 | 1:D:352:THR:CG2 | 2.64 | 0.45 |
| 2:C:3:ADP:O3A | 1:D:393:SER:HB3 | 2.17 | 0.45 |
| 1:D:47:GLY:O | 1:D:51:ILE:HG13 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:173:GLU:O | 1:E:202:PRO:HD3 | 2.16 | 0.45 |
| 1:E:344:ILE:HB | 1:E:367:VAL:HG13 | 1.99 | 0.45 |
| 1:F:328:GLU:HB2 | 1:F:329:LYS:NZ | 2.31 | 0.45 |
| 1:G:191:ASP:O | 1:G:193:ASN:N | 2.39 | 0.45 |
| 1:G:328:GLU:HG2 | 1:G:329:LYS:HD2 | 1.99 | 0.45 |
| 1:G:346:GLU:OE1 | 1:G:369:PRO:HA | 2.16 | 0.45 |
| 1:H:220:PHE:CD1 | 1:H:221:HIS:N | 2.85 | 0.45 |
| 1:H:294:PHE:O | 1:H:298:HIS:NE2 | 2.49 | 0.45 |
| 1:H:34:THR:CG2 | 1:H:34:THR:O | 2.65 | 0.45 |
| 1:H:19:ARG:NH2 | 1:H:358:LYS:NZ | 2.62 | 0.45 |
| 1:H:445:GLU:O | 1:H:449:VAL:HG23 | 2.17 | 0.45 |
| 1:J:175:GLU:HG3 | 1:J:178:TRP:CZ3 | 2.52 | 0.45 |
| 1:K:249:VAL:HG12 | 1:K:323:ILE:HG13 | 1.98 | 0.45 |
| 1:K:236:LEU:HD22 | 1:K:342:LYS:O | 2.17 | 0.45 |
| 1:I:392:VAL:CG1 | 1:K:386:LEU:HD11 | 2.47 | 0.45 |
| 1:K:450:HIS:O | 1:K:453:LEU:HB3 | 2.17 | 0.45 |
| 1:K:91:GLY:HA3 | 1:K:125:ALA:O | 2.16 | 0.45 |
| 1:L:282:ASN:O | 1:L:284:ASP:N | 2.49 | 0.45 |
| 1:B:197:CYS:SG | 1:B:198:VAL:N | 2.89 | 0.45 |
| 1:B:201:LYS:HE2 | 1:B:206:GLY:O | 2.17 | 0.45 |
| 1:B:261:ARG:CG | 1:B:261:ARG:HH11 | 2.04 | 0.45 |
| 1:B:68:ASP:OD1 | 1:B:140:GLU:CG | 2.65 | 0.45 |
| 1:C:153:ALA:CA | 1:C:158:ILE:HG22 | 2.47 | 0.45 |
| 1:C:431:VAL:CG1 | 1:D:419:ARG:HH21 | 2.30 | 0.45 |
| 1:D:352:THR:CG2 | 1:D:478:ARG:NH2 | 2.79 | 0.45 |
| 1:E:12:MET:CE | 1:E:354:PRO:HD3 | 2.47 | 0.45 |
| 1:D:456:THR:HG23 | 1:E:396:ARG:HH21 | 1.82 | 0.45 |
| 1:G:239:THR:N | 1:G:240:PRO:HD3 | 2.31 | 0.45 |
| 1:G:485:ALA:O | 1:G:486:ILE:C | 2.56 | 0.45 |
| 1:G:495:GLU:OE1 | 1:H:204:SER:CB | 2.64 | 0.45 |
| 1:G:65:ILE:HD11 | 1:G:75:ILE:HD11 | 1.99 | 0.45 |
| 1:H:421:PHE:CE1 | 1:H:423:LYS:HB2 | 2.52 | 0.45 |
| 1:H:47:GLY:O | 1:H:50:ARG:N | 2.48 | 0.45 |
| 1:H:87:THR:HG22 | 1:H:88:PRO:N | 2.32 | 0.45 |
| 1:I:239:THR:N | 1:I:240:PRO:CD | 2.75 | 0.45 |
| 1:K:203:ILE:HG21 | 1:K:209:HIS:CE1 | 2.52 | 0.45 |
| 1:K:399:PHE:HZ | 1:K:444:SER:O | 2.00 | 0.45 |
| 1:L:214:ALA:CB | 1:L:380:VAL:HG21 | 2.46 | 0.45 |
| 1:A:386:LEU:CD1 | 1:B:392:VAL:CG2 | 2.93 | 0.45 |
| 1:A:63:PHE:CD1 | 1:A:63:PHE:O | 2.70 | 0.45 |
| 1:B:130:LYS:O | 1:B:131:ILE:HB | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:67:ARG:NH2 | 1:B:136:TYR:CZ | 2.85 | 0.45 |
| 1:C:444:SER:OG | 1:C:446:LYS:HG2 | 2.17 | 0.45 |
| 1:C:501:THR:C | 1:D:146:ARG:HH22 | 2.20 | 0.45 |
| 1:D:395:GLY:HA2 | 1:D:398:THR:HG23 | 1.99 | 0.45 |
| 1:D:59:LEU:CD2 | 1:D:61:LEU:CD2 | 2.95 | 0.45 |
| 1:E:412:SER:O | 1:E:413:VAL:C | 2.55 | 0.45 |
| 1:E:83:SER:OG | 1:E:85:GLN:HB3 | 2.17 | 0.45 |
| 1:F:244:ASP:OD2 | 1:F:245:LYS:HE2 | 2.17 | 0.45 |
| 1:F:373:LEU:HD12 | 1:F:373:LEU:HA | 1.79 | 0.45 |
| 1:G:152:LEU:C | 1:G:158:ILE:HG22 | 2.36 | 0.45 |
| 1:H:247:PHE:CE2 | 1:H:263:LEU:HD12 | 2.52 | 0.45 |
| 1:H:427:THR:C | 1:H:428:ILE:HD13 | 2.37 | 0.45 |
| 1:H:468:ALA:O | 1:H:473:LEU:HD12 | 2.16 | 0.45 |
| 1:H:46:ARG:HA | 1:H:49:LEU:HD12 | 1.98 | 0.45 |
| 1:I:137:THR:CG2 | 1:I:140:GLU:HG3 | 2.47 | 0.45 |
| 1:I:238:MET:O | 1:I:240:PRO:N | 2.50 | 0.45 |
| 1:I:257:LEU:HG | 1:I:258:HIS:N | 2.31 | 0.45 |
| 1:I:344:ILE:HD11 | 1:I:360:PHE:CD1 | 2.51 | 0.45 |
| 1:I:47:GLY:O | 1:I:50:ARG:HB2 | 2.17 | 0.45 |
| 1:J:167:PRO:HG3 | 1:J:176:MET:SD | 2.57 | 0.45 |
| 1:J:227:ILE:O | 1:J:227:ILE:HG23 | 2.16 | 0.45 |
| 1:J:19:ARG:O | 1:J:23:ILE:HG13 | 2.17 | 0.45 |
| 1:J:314:ILE:H | 1:J:314:ILE:HD13 | 1.77 | 0.45 |
| 1:J:420:LYS:CB | 1:J:420:LYS:NZ | 2.71 | 0.45 |
| 1:J:501:THR:OXT | 1:J:501:THR:HG23 | 2.17 | 0.45 |
| 1:K:332:THR:HA | 1:K:353:THR:OG1 | 2.17 | 0.45 |
| 1:K:318:ASP:HA | 1:K:340:LYS:HB2 | 1.98 | 0.45 |
| 1:K:417:LEU:HA | 1:K:417:LEU:HD12 | 1.68 | 0.45 |
| 1:L:152:LEU:HA | 1:L:152:LEU:HD12 | 1.77 | 0.45 |
| 1:L:274:GLY:CA | 1:L:314:ILE:HD12 | 2.47 | 0.45 |
| 1:L:90:LYS:HE3 | 1:L:199:THR:CG2 | 2.47 | 0.45 |
| 1:A:147:ARG:HG3 | 1:A:147:ARG:O | 2.17 | 0.44 |
| 1:A:318:ASP:HA | 1:A:340:LYS:HB2 | 1.98 | 0.44 |
| 1:B:281:TRP:CE2 | 1:B:283:PRO:HD3 | 2.52 | 0.44 |
| 1:C:122:PHE:CZ | 1:C:382:TYR:HD2 | 2.34 | 0.44 |
| 1:C:369:PRO:HG3 | 1:C:478:ARG:N | 2.32 | 0.44 |
| 1:C:410:LEU:HD23 | 1:C:410:LEU:HA | 1.69 | 0.44 |
| 1:C:498:VAL:HG11 | 1:F:72:TRP:CE2 | 2.51 | 0.44 |
| 1:D:79:ARG:CD | 1:D:127:ALA:HB2 | 2.47 | 0.44 |
| 1:D:383:PHE:O | 1:D:384:GLU:C | 2.54 | 0.44 |
| 1:E:143:LYS:HZ1 | 1:E:147:ARG:NH2 | 2.15 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:19:ARG:HD3 | 1:E:23:ILE:HD11 | 1.98 | 0.44 |
| 1:F:183:TYR:CE2 | 1:F:188:GLY:HA3 | 2.52 | 0.44 |
| 1:F:282:ASN:OD1 | 1:F:284:ASP:HB2 | 2.17 | 0.44 |
| 1:F:17:PHE:CE1 | 1:F:486:ILE:HD12 | 2.52 | 0.44 |
| 1:I:134:LYS:HA | 1:I:134:LYS:HE3 | 1.99 | 0.44 |
| 1:I:212:ILE:HG23 | 1:I:254:ASN:HD21 | 1.82 | 0.44 |
| 1:K:220:PHE:HD1 | 1:K:221:HIS:CA | 2.30 | 0.44 |
| 1:L:75:ILE:HG12 | 1:L:144:ILE:CD1 | 2.47 | 0.44 |
| 1:A:355:GLU:HA | 1:A:358:LYS:HD2 | 1.99 | 0.44 |
| 1:B:450:HIS:O | 1:B:451:SER:C | 2.53 | 0.44 |
| 1:D:125:ALA:O | 1:D:126:LYS:HB2 | 2.17 | 0.44 |
| 1:D:201:LYS:HB2 | 1:D:202:PRO:HD2 | 1.99 | 0.44 |
| 1:D:256:GLY:O | 1:D:259:SER:HB2 | 2.18 | 0.44 |
| 1:D:344:ILE:HG22 | 1:D:367:VAL:HG13 | 1.99 | 0.44 |
| 1:E:323:ILE:HA | 1:E:324:PRO:HD2 | 1.48 | 0.44 |
| 1:E:498:VAL:O | 1:E:501:THR:HG22 | 2.17 | 0.44 |
| 1:F:91:GLY:O | 1:F:165:PRO:HA | 2.16 | 0.44 |
| 1:F:383:PHE:O | 1:F:386:LEU:HB2 | 2.17 | 0.44 |
| 1:F:387:LYS:HG2 | 1:F:387:LYS:O | 2.17 | 0.44 |
| 1:G:93:ILE:HA | 1:G:127:ALA:HB3 | 1.98 | 0.44 |
| 1:G:89:CYS:O | 1:G:163:ASP:HA | 2.17 | 0.44 |
| 1:G:302:LEU:HA | 1:G:302:LEU:HD12 | 1.80 | 0.44 |
| 1:G:233:MET:HE1 | 1:G:343:ILE:HD11 | 1.98 | 0.44 |
| 1:G:400:LYS:O | 1:G:403:ARG:HB3 | 2.17 | 0.44 |
| 1:G:410:LEU:HB3 | 1:G:430:ILE:HA | 1.99 | 0.44 |
| 1:J:386:LEU:CD1 | 1:K:392:VAL:CG1 | 2.94 | 0.44 |
| 1:J:67:ARG:O | 1:J:70:GLY:N | 2.47 | 0.44 |
| 1:K:12:MET:C | 1:K:16:PHE:HD1 | 2.20 | 0.44 |
| 1:K:254:ASN:HB3 | 1:K:255:VAL:H | 1.63 | 0.44 |
| 1:K:226:PHE:HB3 | 1:K:366:MET:HE1 | 1.99 | 0.44 |
| 1:K:414:GLN:OE1 | 1:K:430:ILE:HG12 | 2.16 | 0.44 |
| 1:K:454:ALA:O | 1:K:455:TYR:C | 2.54 | 0.44 |
| 1:L:17:PHE:CE2 | 1:L:53:LYS:HB2 | 2.53 | 0.44 |
| 1:L:28:LEU:HA | 1:L:28:LEU:HD12 | 1.85 | 0.44 |
| 1:L:367:VAL:O | 1:L:477:LEU:HB2 | 2.16 | 0.44 |
| 1:L:200:GLY:N | 1:L:384:GLU:OE1 | 2.50 | 0.44 |
| 1:L:432:PRO:HB3 | 1:L:436:PHE:CD1 | 2.51 | 0.44 |
| 1:A:181:ASP:OD1 | 1:F:501:THR:OXT | 2.35 | 0.44 |
| 1:A:358:LYS:HA | 1:A:361:LEU:HD13 | 1.99 | 0.44 |
| 1:A:428:ILE:O | 1:A:429:PRO:C | 2.54 | 0.44 |
| 1:A:427:THR:CG2 | 1:A:429:PRO:HD3 | 2.43 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:55:CYS:HA | 1:A:82:HIS:HA | 2.00 | 0.44 |
| 1:B:6:ASP:HB2 | 1:B:329:LYS:HD2 | 1.99 | 0.44 |
| 1:B:407:TYR:O | 1:B:411:MET:HB2 | 2.17 | 0.44 |
| 1:B:451:SER:OG | 1:B:452:GLY:N | 2.51 | 0.44 |
| 1:C:235:ILE:CG2 | 1:C:364:ASN:HD21 | 2.04 | 0.44 |
| 1:D:249:VAL:O | 1:D:249:VAL:HG13 | 2.18 | 0.44 |
| 1:D:417:LEU:HD23 | 1:E:417:LEU:HD11 | 2.00 | 0.44 |
| 1:E:65:ILE:HD13 | 1:E:144:ILE:CG1 | 2.47 | 0.44 |
| 1:E:177:SER:OG | 1:E:205:GLN:HG3 | 2.18 | 0.44 |
| 1:E:28:LEU:HD12 | 1:E:28:LEU:HA | 1.78 | 0.44 |
| 1:D:394:TYR:CE2 | 1:E:397:LEU:HD23 | 2.53 | 0.44 |
| 1:E:82:HIS:CG | 1:E:112:THR:CG2 | 2.99 | 0.44 |
| 1:F:224:GLU:CA | 1:F:227:ILE:HG22 | 2.46 | 0.44 |
| 1:G:346:GLU:HG2 | 1:G:351:PRO:HG2 | 1.99 | 0.44 |
| 1:G:501:THR:OXT | 1:H:181:ASP:CB | 2.61 | 0.44 |
| 1:H:360:PHE:HB3 | 1:H:365:ILE:HB | 1.98 | 0.44 |
| 1:H:374:ASN:ND2 | 1:H:374:ASN:C | 2.69 | 0.44 |
| 1:H:406:ASN:HD22 | 1:H:406:ASN:N | 2.14 | 0.44 |
| 1:K:99:VAL:O | 1:K:130:LYS:HE3 | 2.17 | 0.44 |
| 1:K:398:THR:O | 1:K:401:TYR:N | 2.50 | 0.44 |
| 1:K:39:GLU:O | 1:K:40:GLN:C | 2.55 | 0.44 |
| 1:J:433:THR:N | 1:K:412:SER:OG | 2.49 | 0.44 |
| 1:G:50:ARG:NH1 | 1:K:73:GLU:HA | 2.21 | 0.44 |
| 1:L:233:MET:CE | 1:L:236:LEU:HD11 | 2.47 | 0.44 |
| 1:L:225:ASN:ND2 | 1:L:458:GLU:HA | 2.32 | 0.44 |
| 1:A:83:SER:O | 1:A:123:GLY:HA3 | 2.17 | 0.44 |
| 1:A:247:PHE:O | 1:A:271:ILE:HG22 | 2.17 | 0.44 |
| 1:A:323:ILE:HA | 1:A:324:PRO:HD3 | 1.79 | 0.44 |
| 1:A:356:ALA:HB1 | 1:A:360:PHE:CE2 | 2.53 | 0.44 |
| 1:A:419:ARG:NH2 | 1:F:431:VAL:HG11 | 2.33 | 0.44 |
| 1:A:78:TYR:O | 1:A:127:ALA:HA | 2.17 | 0.44 |
| 1:B:379:THR:O | 1:B:382:TYR:HB3 | 2.18 | 0.44 |
| 1:B:435:GLU:H | 1:B:435:GLU:CD | 2.21 | 0.44 |
| 1:C:280:ILE:CG2 | 1:C:281:TRP:H | 2.19 | 0.44 |
| 1:C:321:ILE:O | 1:C:321:ILE:HG22 | 2.18 | 0.44 |
| 1:C:476:ASP:O | 1:C:477:LEU:C | 2.56 | 0.44 |
| 1:C:85:GLN:OE1 | 1:C:489:VAL:HG22 | 2.18 | 0.44 |
| 1:D:337:PRO:HA | 1:D:363:ARG:NE | 2.28 | 0.44 |
| 1:E:271:ILE:CD1 | 1:E:283:PRO:HA | 2.48 | 0.44 |
| 1:E:247:PHE:CB | 1:E:321:ILE:HB | 2.47 | 0.44 |
| 1:E:12:MET:HE2 | 1:E:354:PRO:HD3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:2:ADP:H5'2 | 1:F:203:ILE:HG23 | 1.98 | 0.44 |
| 1:F:414:GLN:OE1 | 1:F:428:ILE:CA | 2.56 | 0.44 |
| 1:G:141:LEU:HD23 | 1:G:141:LEU:HA | 1.71 | 0.44 |
| 1:H:92:GLY:O | 1:H:126:LYS:HD2 | 2.17 | 0.44 |
| 1:H:131:ILE:HD13 | 1:H:144:ILE:HD13 | 2.00 | 0.44 |
| 1:H:28:LEU:HD21 | 1:H:490:PHE:CD1 | 2.52 | 0.44 |
| 1:H:294:PHE:CD2 | 1:H:304:PHE:HD1 | 2.36 | 0.44 |
| 1:H:30:GLU:HB3 | 1:H:31:ASP:H | 1.32 | 0.44 |
| 1:H:354:PRO:HG2 | 1:H:355:GLU:N | 2.32 | 0.44 |
| 1:I:219:VAL:O | 1:I:222:GLY:N | 2.50 | 0.44 |
| 1:I:269:LYS:HD3 | 1:I:284:ASP:O | 2.17 | 0.44 |
| 1:I:332:THR:HB | 1:I:333:LYS:H | 1.55 | 0.44 |
| 1:I:414:GLN:CB | 1:I:429:PRO:HD2 | 2.46 | 0.44 |
| 1:I:96:SER:O | 1:I:97:THR:C | 2.56 | 0.44 |
| 1:J:248:VAL:HG11 | 1:J:314:ILE:HB | 1.98 | 0.44 |
| 1:J:368:ILE:HA | 1:J:369:PRO:HD3 | 1.47 | 0.44 |
| 1:J:423:LYS:HD2 | 1:J:423:LYS:HA | 1.78 | 0.44 |
| 1:K:264:HIS:ND1 | 1:K:288:PRO:HG2 | 2.33 | 0.44 |
| 1:K:326:ALA:O | 1:K:327:SER:O | 2.35 | 0.44 |
| 1:K:82:HIS:HD2 | 1:K:112:THR:OG1 | 1.99 | 0.44 |
| 1:K:57:HIS:CD2 | 1:K:84:HIS:CE1 | 3.06 | 0.44 |
| 1:L:101:VAL:O | 1:L:104:VAL:CG2 | 2.64 | 0.44 |
| 1:L:26:ASP:C | 1:L:28:LEU:H | 2.20 | 0.44 |
| 1:L:431:VAL:HG22 | 1:L:431:VAL:O | 2.17 | 0.44 |
| 1:A:423:LYS:CE | 1:A:426:GLY:HA3 | 2.47 | 0.44 |
| 1:A:427:THR:HG22 | 1:A:428:ILE:H | 1.82 | 0.44 |
| 1:A:437:GLN:HE22 | 1:H:426:GLY:CA | 2.29 | 0.44 |
| 1:A:45:VAL:O | 1:A:48:ILE:HG12 | 2.17 | 0.44 |
| 1:B:227:ILE:HD13 | 1:B:343:ILE:HD13 | 1.99 | 0.44 |
| 1:B:257:LEU:C | 1:B:257:LEU:CD1 | 2.84 | 0.44 |
| 1:B:346:GLU:HG2 | 1:B:351:PRO:CG | 2.48 | 0.44 |
| 1:C:49:LEU:H | 1:C:49:LEU:CD1 | 2.19 | 0.44 |
| 1:D:256:GLY:O | 1:D:259:SER:N | 2.50 | 0.44 |
| 1:D:414:GLN:OE1 | 1:D:428:ILE:HA | 2.17 | 0.44 |
| 1:D:423:LYS:HG3 | 1:D:424:HIS:H | 1.82 | 0.44 |
| 1:E:64:PRO:O | 1:E:147:ARG:HD2 | 2.17 | 0.44 |
| 1:E:426:GLY:O | 1:E:428:ILE:CD1 | 2.66 | 0.44 |
| 1:E:427:THR:O | 1:E:429:PRO:HD3 | 2.17 | 0.44 |
| 1:E:38:GLU:OE2 | 1:E:42:ARG:HD2 | 2.17 | 0.44 |
| 1:E:459:ARG:O | 1:E:463:GLN:HG3 | 2.17 | 0.44 |
| 1:E:91:GLY:HA3 | 1:E:125:ALA:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:279:SER:C | 1:F:280:ILE:HG13 | 2.38 | 0.44 |
| 1:F:315:LEU:HD23 | 1:F:331:LEU:HD11 | 1.96 | 0.44 |
| 1:B:386:LEU:CD1 | 1:F:392:VAL:CG2 | 2.96 | 0.44 |
| 1:H:107:LEU:O | 1:H:108:ALA:C | 2.54 | 0.44 |
| 1:H:115:CYS:O | 1:H:116:ALA:C | 2.55 | 0.44 |
| 1:H:324:PRO:HD2 | 1:H:345:ALA:O | 2.17 | 0.44 |
| 1:I:130:LYS:O | 1:I:131:ILE:HG13 | 2.17 | 0.44 |
| 1:J:173:GLU:HB2 | 1:J:202:PRO:CG | 2.47 | 0.44 |
| 1:J:188:GLY:O | 1:J:190:TYR:N | 2.50 | 0.44 |
| 1:J:25:GLU:O | 1:J:29:VAL:HG23 | 2.17 | 0.44 |
| 1:J:431:VAL:CG1 | 1:K:419:ARG:HH21 | 2.30 | 0.44 |
| 1:J:28:LEU:HD21 | 1:J:490:PHE:CD2 | 2.52 | 0.44 |
| 1:L:96:SER:HA | 1:L:131:ILE:O | 2.18 | 0.44 |
| 1:L:316:GLU:O | 1:L:317:ALA:C | 2.56 | 0.44 |
| 1:A:101:VAL:O | 1:A:101:VAL:CG1 | 2.64 | 0.44 |
| 1:A:447:ASP:O | 1:A:448:ILE:C | 2.55 | 0.44 |
| 1:B:147:ARG:O | 1:B:151:GLU:HG2 | 2.17 | 0.44 |
| 1:B:304:PHE:CD1 | 1:B:305:PRO:HD2 | 2.53 | 0.44 |
| 1:B:250:GLN:CG | 1:B:315:LEU:HD21 | 2.47 | 0.44 |
| 1:D:220:PHE:HE1 | 1:D:224:GLU:OE1 | 1.99 | 0.44 |
| 1:D:24:VAL:HG22 | 1:D:483:VAL:HG13 | 1.99 | 0.44 |
| 1:D:90:LYS:NZ | 1:D:199:THR:CG2 | 2.75 | 0.44 |
| 1:E:167:PRO:HG3 | 1:E:176:MET:CG | 2.48 | 0.44 |
| 1:D:429:PRO:HA | 1:E:416:SER:CB | 2.47 | 0.44 |
| 1:E:420:LYS:O | 1:E:421:PHE:HB2 | 2.17 | 0.44 |
| 1:E:53:LYS:CB | 1:E:54:PRO:CD | 2.79 | 0.44 |
| 1:F:428:ILE:H | 1:F:428:ILE:HD13 | 1.78 | 0.44 |
| 1:G:142:GLU:OE2 | 1:G:178:TRP:NE1 | 2.50 | 0.44 |
| 1:H:322:LEU:C | 1:H:322:LEU:HD22 | 2.38 | 0.44 |
| 1:H:383:PHE:O | 1:H:384:GLU:C | 2.54 | 0.44 |
| 1:J:90:LYS:CE | 1:J:199:THR:CG2 | 2.95 | 0.44 |
| 1:K:89:CYS:N | 1:K:162:ILE:O | 2.50 | 0.44 |
| 1:K:192:ILE:O | 1:K:192:ILE:HG12 | 2.17 | 0.44 |
| 1:K:318:ASP:HA | 1:K:340:LYS:CB | 2.47 | 0.44 |
| 1:K:46:ARG:HA | 1:K:49:LEU:HD13 | 1.99 | 0.44 |
| 1:G:64:PRO:HG3 | 1:K:51:ILE:HD13 | 2.00 | 0.44 |
| 1:L:476:ASP:O | 1:L:477:LEU:C | 2.56 | 0.44 |
| 1:L:369:PRO:CG | 1:L:477:LEU:HB3 | 2.47 | 0.44 |
| 1:A:114:LYS:CE | 1:A:374:ASN:ND2 | 2.81 | 0.44 |
| 1:A:39:GLU:O | 1:A:41:LYS:N | 2.51 | 0.44 |
| 1:B:233:MET:CE | 1:B:236:LEU:HD12 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:378:VAL:O | 1:B:379:THR:C | 2.56 | 0.44 |
| 1:C:13:VAL:CG1 | 1:C:14:GLU:N | 2.75 | 0.44 |
| 1:C:226:PHE:HE2 | 1:C:465:MET:SD | 2.40 | 0.44 |
| 1:C:396:ARG:O | 1:C:396:ARG:CD | 2.54 | 0.44 |
| 1:C:19:ARG:CD | 1:C:479:THR:HG21 | 2.48 | 0.44 |
| 1:D:80:ALA:O | 1:D:125:ALA:HA | 2.18 | 0.44 |
| 1:F:248:VAL:HG11 | 1:F:314:ILE:HB | 1.98 | 0.44 |
| 1:F:484:ASN:HA | 1:F:487:GLU:OE1 | 2.17 | 0.44 |
| 1:G:147:ARG:NH1 | 1:G:151:GLU:CD | 2.71 | 0.44 |
| 1:G:153:ALA:CA | 1:G:158:ILE:CG2 | 2.96 | 0.44 |
| 1:I:315:LEU:N | 1:I:315:LEU:HD12 | 2.33 | 0.44 |
| 1:I:373:LEU:O | 1:I:373:LEU:HD23 | 2.17 | 0.44 |
| 1:J:465:MET:O | 1:J:468:ALA:N | 2.51 | 0.44 |
| 1:J:65:ILE:CD1 | 1:J:75:ILE:HD11 | 2.48 | 0.44 |
| 1:K:104:VAL:CG2 | 1:K:105:LYS:H | 2.30 | 0.44 |
| 1:G:401:TYR:CE2 | 1:L:439:ARG:NH2 | 2.86 | 0.44 |
| 1:L:475:LEU:CD1 | 1:L:475:LEU:N | 2.81 | 0.44 |
| 1:L:481:ALA:O | 1:L:482:TYR:C | 2.55 | 0.44 |
| 1:A:223:ILE:O | 1:A:224:GLU:C | 2.56 | 0.44 |
| 1:A:90:LYS:HD3 | 1:A:122:PHE:CE1 | 2.53 | 0.44 |
| 1:B:142:GLU:O | 1:B:143:LYS:C | 2.55 | 0.44 |
| 1:B:219:VAL:O | 1:B:223:ILE:HD12 | 2.18 | 0.44 |
| 1:C:459:ARG:CZ | 2:C:3:ADP:O3B | 2.65 | 0.44 |
| 1:D:201:LYS:HB2 | 1:D:202:PRO:CD | 2.47 | 0.44 |
| 1:D:199:THR:HA | 1:D:384:GLU:OE1 | 2.18 | 0.44 |
| 1:E:68:ASP:OD2 | 1:E:140:GLU:CG | 2.66 | 0.44 |
| 1:C:392:VAL:HG13 | 1:E:382:TYR:OH | 2.18 | 0.44 |
| 1:F:328:GLU:O | 1:F:329:LYS:O | 2.36 | 0.44 |
| 1:F:385:TRP:HA | 1:F:388:ASN:HD22 | 1.82 | 0.44 |
| 1:G:314:ILE:HD13 | 1:G:314:ILE:N | 2.31 | 0.44 |
| 1:G:497:GLY:N | 1:G:501:THR:HA | 2.33 | 0.44 |
| 1:H:421:PHE:CD1 | 1:H:423:LYS:HB2 | 2.52 | 0.44 |
| 1:I:9:PHE:CD1 | 1:I:10:PHE:N | 2.82 | 0.44 |
| 1:I:167:PRO:HD3 | 1:I:176:MET:CG | 2.48 | 0.44 |
| 1:I:30:GLU:CG | 1:I:31:ASP:N | 2.80 | 0.44 |
| 1:I:405:SER:O | 1:I:409:LEU:HD23 | 2.17 | 0.44 |
| 1:I:94:ARG:CG | 1:I:94:ARG:HH11 | 2.27 | 0.44 |
| 1:J:280:ILE:HG23 | 1:J:307:ALA:CB | 2.48 | 0.44 |
| 1:K:255:VAL:HG13 | 1:K:325:ALA:HB1 | 2.00 | 0.44 |
| 1:K:465:MET:O | 1:K:468:ALA:CB | 2.65 | 0.44 |
| 1:L:120:VAL:HG21 | 1:L:378:VAL:HG12 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:280:ILE:CG2 | 1:L:281:TRP:N | 2.80 | 0.44 |
| 1:L:300:SER:OG | 1:L:302:LEU:HD13 | 2.17 | 0.44 |
| 1:L:406:ASN:O | 1:L:409:LEU:HB2 | 2.17 | 0.44 |
| 1:A:140:GLU:O | 1:A:144:ILE:HG13 | 2.17 | 0.44 |
| 1:A:336:ALA:HB3 | 1:A:359:ILE:CD1 | 2.47 | 0.44 |
| 1:B:227:ILE:CD1 | 1:B:233:MET:SD | 2.96 | 0.44 |
| 1:C:90:LYS:HB2 | 1:C:122:PHE:CD1 | 2.53 | 0.44 |
| 1:C:90:LYS:HB2 | 1:C:122:PHE:HB3 | 1.99 | 0.44 |
| 1:C:166:ALA:HB1 | 1:C:167:PRO:CD | 2.48 | 0.44 |
| 1:C:291:LEU:HD13 | 1:C:304:PHE:CD2 | 2.53 | 0.44 |
| 1:D:220:PHE:C | 1:D:220:PHE:CD1 | 2.92 | 0.44 |
| 1:D:244:ASP:O | 1:D:245:LYS:HG2 | 2.18 | 0.44 |
| 1:E:88:PRO:HG2 | 1:E:122:PHE:HD2 | 1.83 | 0.44 |
| 1:E:237:GLY:O | 1:E:238:MET:HG2 | 2.18 | 0.44 |
| 1:F:111:MET:O | 1:F:112:THR:C | 2.56 | 0.44 |
| 1:F:65:ILE:HG21 | 1:F:144:ILE:HG12 | 2.00 | 0.44 |
| 1:G:328:GLU:O | 1:G:329:LYS:HB2 | 2.18 | 0.44 |
| 1:H:137:THR:HG23 | 1:H:140:GLU:CB | 2.44 | 0.44 |
| 1:H:149:THR:O | 1:H:150:MET:C | 2.55 | 0.44 |
| 1:H:368:ILE:HG22 | 1:H:373:LEU:HB2 | 2.00 | 0.44 |
| 1:I:198:VAL:O | 1:I:201:LYS:CE | 2.66 | 0.44 |
| 1:I:217:ARG:HB3 | 1:I:217:ARG:NH1 | 2.29 | 0.44 |
| 1:I:248:VAL:HG23 | 1:I:319:CYS:SG | 2.58 | 0.44 |
| 1:I:308:LYS:HA | 1:I:309:PRO:HD3 | 1.75 | 0.44 |
| 1:I:227:ILE:HD11 | 1:I:343:ILE:HD12 | 1.99 | 0.44 |
| 1:I:336:ALA:CB | 1:I:359:ILE:HG21 | 2.48 | 0.44 |
| 1:I:432:PRO:O | 1:I:433:THR:C | 2.56 | 0.44 |
| 1:J:280:ILE:HG23 | 1:J:307:ALA:HB1 | 2.00 | 0.44 |
| 1:K:277:ASP:HB3 | 1:K:302:LEU:HD11 | 2.00 | 0.44 |
| 1:K:481:ALA:O | 1:K:482:TYR:C | 2.56 | 0.44 |
| 1:L:90:LYS:HE2 | 1:L:164:VAL:HG12 | 2.00 | 0.44 |
| 1:L:79:ARG:NH1 | 1:L:165:PRO:HG3 | 2.33 | 0.44 |
| 1:L:244:ASP:HB3 | 1:L:245:LYS:H | 1.70 | 0.44 |
| 1:L:439:ARG:O | 1:L:439:ARG:HG2 | 2.16 | 0.44 |
| 1:B:280:ILE:HG23 | 1:B:281:TRP:H | 1.82 | 0.43 |
| 1:B:282:ASN:O | 1:B:282:ASN:OD1 | 2.36 | 0.43 |
| 1:B:369:PRO:HG3 | 1:B:478:ARG:CA | 2.48 | 0.43 |
| 1:C:335:ASN:HB2 | 1:C:338:ARG:HH12 | 1.82 | 0.43 |
| 1:C:82:HIS:CD2 | 1:C:112:THR:CG2 | 2.86 | 0.43 |
| 1:D:410:LEU:HB3 | 1:D:430:ILE:HA | 1.99 | 0.43 |
| 1:D:453:LEU:O | 1:D:454:ALA:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:90:LYS:HD2 | 1:D:90:LYS:HA | 1.84 | 0.43 |
| 1:E:382:TYR:O | 1:E:385:TRP:HB3 | 2.18 | 0.43 |
| 1:E:426:GLY:O | 1:E:428:ILE:HD13 | 2.19 | 0.43 |
| 1:H:428:ILE:O | 1:H:429:PRO:C | 2.54 | 0.43 |
| 1:H:485:ALA:O | 1:H:488:LYS:N | 2.51 | 0.43 |
| 1:I:227:ILE:HG23 | 1:I:227:ILE:O | 2.18 | 0.43 |
| 1:I:337:PRO:HA | 1:I:363:ARG:HE | 1.83 | 0.43 |
| 1:I:380:VAL:HG23 | 1:I:453:LEU:HG | 2.00 | 0.43 |
| 1:I:65:ILE:HA | 1:I:147:ARG:NH1 | 2.33 | 0.43 |
| 1:J:411:MET:N | 1:J:430:ILE:HG22 | 2.33 | 0.43 |
| 1:K:198:VAL:HG22 | 1:K:199:THR:N | 2.32 | 0.43 |
| 1:K:275:GLU:HB3 | 1:K:276:SER:H | 1.64 | 0.43 |
| 1:K:313:SER:O | 1:K:315:LEU:N | 2.51 | 0.43 |
| 1:K:396:ARG:HH11 | 1:K:396:ARG:HG3 | 1.82 | 0.43 |
| 1:L:353:THR:HB | 1:L:354:PRO:HD2 | 2.00 | 0.43 |
| 1:L:432:PRO:C | 1:L:433:THR:O | 2.54 | 0.43 |
| 1:G:400:LYS:HB2 | 1:L:455:TYR:HB2 | 2.00 | 0.43 |
| 1:L:96:SER:C | 1:L:98:ASP:H | 2.22 | 0.43 |
| 1:A:500:PHE:HB3 | 1:B:142:GLU:OE1 | 2.18 | 0.43 |
| 1:B:52:ILE:HD13 | 1:B:489:VAL:HG11 | 1.96 | 0.43 |
| 1:C:131:ILE:HA | 1:C:131:ILE:HD12 | 1.76 | 0.43 |
| 1:C:198:VAL:HG22 | 1:C:199:THR:N | 2.33 | 0.43 |
| 1:C:274:GLY:O | 1:C:275:GLU:CB | 2.63 | 0.43 |
| 1:C:328:GLU:O | 1:C:329:LYS:CG | 2.65 | 0.43 |
| 1:D:118:VAL:O | 1:D:120:VAL:HG23 | 2.17 | 0.43 |
| 1:D:233:MET:O | 1:D:238:MET:N | 2.47 | 0.43 |
| 1:D:65:ILE:HD13 | 1:D:144:ILE:CD1 | 2.47 | 0.43 |
| 1:D:62:SER:HA | 1:D:75:ILE:O | 2.17 | 0.43 |
| 1:E:497:GLY:HA3 | 1:E:501:THR:HA | 1.99 | 0.43 |
| 1:E:60:SER:C | 1:E:61:LEU:HD23 | 2.38 | 0.43 |
| 1:F:217:ARG:CZ | 1:F:450:HIS:CE1 | 3.01 | 0.43 |
| 1:F:380:VAL:HG13 | 1:F:449:VAL:HG13 | 2.01 | 0.43 |
| 1:F:47:GLY:O | 1:F:50:ARG:CG | 2.66 | 0.43 |
| 1:F:17:PHE:HE2 | 1:F:53:LYS:HB2 | 1.83 | 0.43 |
| 1:G:248:VAL:CG1 | 1:G:249:VAL:N | 2.81 | 0.43 |
| 1:G:305:PRO:O | 1:G:306:LYS:C | 2.56 | 0.43 |
| 1:G:490:PHE:O | 1:G:491:LYS:C | 2.56 | 0.43 |
| 1:H:396:ARG:NH1 | 1:H:396:ARG:CG | 2.74 | 0.43 |
| 1:H:478:ARG:NH1 | 1:H:478:ARG:HG3 | 2.33 | 0.43 |
| 1:I:82:HIS:HD2 | 1:I:112:THR:HG21 | 1.67 | 0.43 |
| 1:I:201:LYS:CB | 1:I:202:PRO:CD | 2.95 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:24:VAL:HG11 | 1:I:28:LEU:HD22 | 1.93 | 0.43 |
| 1:J:12:MET:HB2 | 1:J:12:MET:HE3 | 1.86 | 0.43 |
| 1:K:280:ILE:CG2 | 1:K:307:ALA:HB1 | 2.48 | 0.43 |
| 1:K:363:ARG:CB | 1:K:363:ARG:HH11 | 2.30 | 0.43 |
| 1:K:429:PRO:C | 1:K:431:VAL:H | 2.21 | 0.43 |
| 1:K:85:GLN:HB2 | 1:K:492:VAL:HG11 | 2.01 | 0.43 |
| 1:K:92:GLY:HA2 | 1:K:166:ALA:O | 2.17 | 0.43 |
| 1:L:202:PRO:O | 1:L:207:GLY:N | 2.45 | 0.43 |
| 1:L:334:SER:OG | 1:L:335:ASN:N | 2.51 | 0.43 |
| 1:L:372:TYR:CD1 | 1:L:373:LEU:N | 2.86 | 0.43 |
| 1:G:397:LEU:HD22 | 1:L:394:TYR:CZ | 2.53 | 0.43 |
| 1:A:324:PRO:HD2 | 1:A:345:ALA:O | 2.18 | 0.43 |
| 1:A:478:ARG:O | 1:A:481:ALA:N | 2.51 | 0.43 |
| 1:A:497:GLY:O | 1:A:498:VAL:HG13 | 2.18 | 0.43 |
| 1:A:85:GLN:HE21 | 1:A:85:GLN:HB3 | 1.43 | 0.43 |
| 1:B:282:ASN:C | 1:B:284:ASP:H | 2.22 | 0.43 |
| 1:B:334:SER:O | 1:B:337:PRO:HD2 | 2.17 | 0.43 |
| 1:C:227:ILE:HG22 | 1:C:228:ASN:HD22 | 1.83 | 0.43 |
| 1:C:251:GLY:HA3 | 1:C:325:ALA:O | 2.17 | 0.43 |
| 1:C:346:GLU:HB3 | 1:C:351:PRO:HG3 | 2.01 | 0.43 |
| 1:C:416:SER:HA | 1:C:419:ARG:NH2 | 2.33 | 0.43 |
| 1:D:66:ARG:HD2 | 1:D:72:TRP:CH2 | 2.53 | 0.43 |
| 1:E:250:GLN:HA | 1:E:314:ILE:HD11 | 2.00 | 0.43 |
| 1:E:322:LEU:HD22 | 1:E:323:ILE:N | 2.33 | 0.43 |
| 1:E:421:PHE:CD1 | 1:E:421:PHE:C | 2.91 | 0.43 |
| 1:E:494:ASN:O | 1:E:496:ALA:N | 2.51 | 0.43 |
| 1:E:86:ARG:NH2 | 2:E:5:ADP:O4' | 2.52 | 0.43 |
| 1:F:246:THR:OG1 | 1:F:271:ILE:HD11 | 2.17 | 0.43 |
| 1:F:370:ASP:OD2 | 1:F:371:LEU:N | 2.49 | 0.43 |
| 1:F:496:ALA:C | 1:F:501:THR:O | 2.57 | 0.43 |
| 1:G:201:LYS:CB | 1:G:202:PRO:CD | 2.92 | 0.43 |
| 1:G:261:ARG:NH1 | 1:G:292:GLU:OE1 | 2.46 | 0.43 |
| 1:H:142:GLU:HA | 1:H:178:TRP:CE3 | 2.53 | 0.43 |
| 1:H:482:TYR:O | 1:H:486:ILE:CG1 | 2.65 | 0.43 |
| 1:I:142:GLU:OE2 | 1:I:178:TRP:NE1 | 2.52 | 0.43 |
| 1:I:39:GLU:C | 1:I:41:LYS:N | 2.70 | 0.43 |
| 1:I:93:ILE:HD11 | 1:I:165:PRO:HB3 | 2.01 | 0.43 |
| 1:J:176:MET:CE | 1:J:179:ILE:HG13 | 2.47 | 0.43 |
| 1:K:230:ALA:O | 1:K:233:MET:N | 2.51 | 0.43 |
| 1:K:356:ALA:O | 1:K:360:PHE:HD2 | 2.00 | 0.43 |
| 1:K:43:ASN:O | 1:K:46:ARG:HG2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:392:VAL:CG2 | 1:L:386:LEU:CD1 | 2.97 | 0.43 |
| 1:L:464:ILE:O | 1:L:465:MET:C | 2.56 | 0.43 |
| 1:A:250:GLN:HG3 | 1:A:315:LEU:CD1 | 2.48 | 0.43 |
| 1:B:406:ASN:O | 1:B:409:LEU:N | 2.49 | 0.43 |
| 1:B:431:VAL:HA | 1:B:432:PRO:HD3 | 1.80 | 0.43 |
| 1:B:498:VAL:N | 1:B:501:THR:HB | 2.33 | 0.43 |
| 1:C:195:HIS:O | 1:C:201:LYS:HE3 | 2.18 | 0.43 |
| 1:C:459:ARG:NH2 | 2:C:3:ADP:O3B | 2.52 | 0.43 |
| 1:D:413:VAL:O | 1:D:417:LEU:HB2 | 2.19 | 0.43 |
| 1:E:141:LEU:HD12 | 1:E:174:ARG:NH2 | 2.33 | 0.43 |
| 1:E:492:VAL:HG23 | 2:E:5:ADP:C2 | 2.54 | 0.43 |
| 1:F:317:ALA:O | 1:F:318:ASP:C | 2.56 | 0.43 |
| 1:F:53:LYS:CB | 1:F:54:PRO:CD | 2.97 | 0.43 |
| 1:F:53:LYS:N | 1:F:54:PRO:HD2 | 2.32 | 0.43 |
| 1:G:104:VAL:O | 1:G:105:LYS:C | 2.57 | 0.43 |
| 1:G:51:ILE:HD13 | 1:G:498:VAL:HG11 | 2.00 | 0.43 |
| 1:G:83:SER:OG | 1:G:85:GLN:NE2 | 2.51 | 0.43 |
| 1:H:164:VAL:HG12 | 1:H:164:VAL:O | 2.18 | 0.43 |
| 1:H:294:PHE:CD2 | 1:H:298:HIS:NE2 | 2.86 | 0.43 |
| 1:H:478:ARG:O | 1:H:481:ALA:N | 2.52 | 0.43 |
| 1:J:219:VAL:HG22 | 1:J:373:LEU:CD2 | 2.48 | 0.43 |
| 1:J:40:GLN:C | 1:J:42:ARG:H | 2.20 | 0.43 |
| 1:K:137:THR:HG23 | 1:K:140:GLU:CG | 2.48 | 0.43 |
| 1:K:81:GLN:CD | 1:K:157:PHE:CD1 | 2.92 | 0.43 |
| 1:K:175:GLU:O | 1:K:176:MET:C | 2.57 | 0.43 |
| 1:K:229:GLU:O | 1:K:233:MET:HG2 | 2.17 | 0.43 |
| 1:K:199:THR:HG22 | 1:K:384:GLU:HB3 | 1.99 | 0.43 |
| 1:L:200:GLY:HA2 | 1:L:211:ARG:HD2 | 2.00 | 0.43 |
| 1:L:403:ARG:O | 1:L:406:ASN:HB2 | 2.18 | 0.43 |
| 1:A:368:ILE:HA | 1:A:369:PRO:HD3 | 1.79 | 0.43 |
| 1:A:498:VAL:CG2 | 1:A:499:THR:N | 2.78 | 0.43 |
| 1:B:318:ASP:HA | 1:B:340:LYS:HB2 | 2.01 | 0.43 |
| 1:B:439:ARG:CG | 1:B:439:ARG:NH1 | 2.61 | 0.43 |
| 1:C:81:GLN:OE1 | 1:F:155:LYS:HE3 | 2.19 | 0.43 |
| 1:D:98:ASP:C | 1:D:99:VAL:O | 2.57 | 0.43 |
| 1:E:260:MET:HG2 | 1:E:288:PRO:HG3 | 2.01 | 0.43 |
| 1:F:274:GLY:H | 1:F:314:ILE:HD12 | 1.80 | 0.43 |
| 1:G:224:GLU:HA | 1:G:227:ILE:HG22 | 1.99 | 0.43 |
| 1:G:372:TYR:C | 1:G:372:TYR:CD1 | 2.88 | 0.43 |
| 1:H:14:GLU:O | 1:H:17:PHE:HB3 | 2.18 | 0.43 |
| 1:H:228:ASN:HD22 | 1:H:228:ASN:HA | 1.68 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:413:VAL:HG21 | 1:L:413:VAL:HG21 | 2.00 | 0.43 |
| 1:H:414:GLN:CB | 1:H:429:PRO:HD2 | 2.49 | 0.43 |
| 1:H:65:ILE:HG12 | 1:H:75:ILE:HD11 | 1.99 | 0.43 |
| 1:I:90:LYS:HB2 | 1:I:122:PHE:CG | 2.52 | 0.43 |
| 1:J:109:SER:O | 1:J:113:TYR:CD2 | 2.71 | 0.43 |
| 1:J:145:THR:CG2 | 1:J:175:GLU:HG2 | 2.44 | 0.43 |
| 1:J:173:GLU:HB2 | 1:J:202:PRO:CD | 2.48 | 0.43 |
| 1:J:69:ASP:OD1 | 1:J:69:ASP:C | 2.57 | 0.43 |
| 1:J:436:PHE:CE2 | 1:K:408:HIS:HB3 | 2.52 | 0.43 |
| 1:L:137:THR:H | 1:L:140:GLU:HB2 | 1.82 | 0.43 |
| 1:L:166:ALA:HA | 1:L:167:PRO:HD3 | 1.78 | 0.43 |
| 1:L:113:TYR:CE1 | 1:L:486:ILE:HD13 | 2.53 | 0.43 |
| 1:A:164:VAL:CG1 | 1:A:199:THR:HG23 | 2.48 | 0.43 |
| 1:A:294:PHE:CE2 | 1:A:304:PHE:HA | 2.53 | 0.43 |
| 1:A:339:VAL:HG23 | 1:A:339:VAL:O | 2.19 | 0.43 |
| 1:B:112:THR:H | 1:B:124:GLY:HA3 | 1.84 | 0.43 |
| 1:B:498:VAL:HG11 | 1:D:72:TRP:CE2 | 2.53 | 0.43 |
| 1:C:351:PRO:HG2 | 1:C:352:THR:N | 2.30 | 0.43 |
| 1:C:397:LEU:HD21 | 1:E:383:PHE:CE2 | 2.53 | 0.43 |
| 1:C:41:LYS:HA | 1:C:41:LYS:HD3 | 1.78 | 0.43 |
| 1:C:47:GLY:HA2 | 1:C:50:ARG:CG | 2.49 | 0.43 |
| 1:D:107:LEU:HD12 | 1:D:107:LEU:N | 2.33 | 0.43 |
| 1:D:186:THR:HG22 | 1:D:187:ILE:HG12 | 2.00 | 0.43 |
| 1:D:344:ILE:O | 1:D:344:ILE:CG2 | 2.67 | 0.43 |
| 1:E:252:PHE:HE2 | 1:E:260:MET:HE2 | 1.84 | 0.43 |
| 1:E:248:VAL:CG2 | 1:E:272:ALA:HB3 | 2.48 | 0.43 |
| 1:E:322:LEU:HD23 | 1:E:323:ILE:N | 2.34 | 0.43 |
| 1:F:120:VAL:HG12 | 1:F:122:PHE:CD1 | 2.54 | 0.43 |
| 1:F:250:GLN:HG3 | 1:F:315:LEU:HD12 | 1.98 | 0.43 |
| 1:F:220:PHE:HE2 | 1:F:263:LEU:HA | 1.83 | 0.43 |
| 1:F:40:GLN:CG | 1:F:40:GLN:O | 2.61 | 0.43 |
| 1:F:90:LYS:HZ1 | 1:F:166:ALA:HB2 | 1.83 | 0.43 |
| 1:H:420:LYS:HG2 | 1:H:420:LYS:O | 2.19 | 0.43 |
| 1:H:371:LEU:HD22 | 1:H:482:TYR:CE2 | 2.54 | 0.43 |
| 1:H:53:LYS:HB3 | 1:H:54:PRO:HD3 | 2.00 | 0.43 |
| 1:I:94:ARG:HD3 | 1:I:168:ASP:CG | 2.39 | 0.43 |
| 1:I:414:GLN:CD | 1:I:430:ILE:HG23 | 2.39 | 0.43 |
| 1:J:198:VAL:HG22 | 1:J:199:THR:N | 2.34 | 0.43 |
| 1:J:239:THR:N | 1:J:240:PRO:CD | 2.75 | 0.43 |
| 1:K:234:SER:C | 1:K:236:LEU:N | 2.72 | 0.43 |
| 1:K:264:HIS:C | 1:K:266:PHE:H | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:233:MET:CE | 1:L:236:LEU:CD1 | 2.96 | 0.43 |
| 1:L:444:SER:O | 1:L:447:ASP:HB2 | 2.18 | 0.43 |
| 1:A:130:LYS:O | 1:A:131:ILE:CD1 | 2.57 | 0.43 |
| 1:A:250:GLN:CG | 1:A:314:ILE:HD11 | 2.33 | 0.43 |
| 1:B:449:VAL:O | 1:B:452:GLY:N | 2.52 | 0.43 |
| 1:C:366:MET:HG2 | 1:C:366:MET:O | 2.19 | 0.43 |
| 1:D:141:LEU:O | 1:D:145:THR:CG2 | 2.66 | 0.43 |
| 1:D:281:TRP:NE1 | 1:D:283:PRO:HD3 | 2.34 | 0.43 |
| 1:D:301:ILE:CD1 | 1:D:301:ILE:C | 2.85 | 0.43 |
| 1:E:497:GLY:C | 1:E:501:THR:HB | 2.39 | 0.43 |
| 1:A:62:SER:OG | 1:E:55:CYS:O | 2.31 | 0.43 |
| 1:F:158:ILE:HG12 | 1:F:165:PRO:CG | 2.49 | 0.43 |
| 1:G:453:LEU:HD23 | 1:G:453:LEU:O | 2.17 | 0.43 |
| 1:G:67:ARG:NH1 | 1:G:67:ARG:HG2 | 2.34 | 0.43 |
| 1:I:247:PHE:HZ | 1:I:260:MET:HG3 | 1.83 | 0.43 |
| 1:I:315:LEU:HD23 | 1:I:331:LEU:CD2 | 2.48 | 0.43 |
| 1:I:343:ILE:HD13 | 1:I:366:MET:CE | 2.49 | 0.43 |
| 1:J:85:GLN:HE21 | 1:J:85:GLN:HB3 | 1.35 | 0.43 |
| 1:K:59:LEU:HD22 | 1:K:157:PHE:HD2 | 1.82 | 0.43 |
| 1:K:201:LYS:O | 1:K:207:GLY:HA3 | 2.19 | 0.43 |
| 1:K:78:TYR:O | 1:K:127:ALA:HA | 2.18 | 0.43 |
| 1:K:82:HIS:CD2 | 1:K:112:THR:OG1 | 2.72 | 0.43 |
| 1:K:94:ARG:CG | 1:K:94:ARG:HH11 | 2.32 | 0.43 |
| 1:L:132:ASN:O | 1:L:134:LYS:N | 2.52 | 0.43 |
| 1:L:137:THR:OG1 | 1:L:140:GLU:CD | 2.57 | 0.43 |
| 1:L:304:PHE:HA | 1:L:305:PRO:HD3 | 1.89 | 0.43 |
| 1:L:363:ARG:CB | 1:L:363:ARG:NH1 | 2.82 | 0.43 |
| 1:L:38:GLU:O | 1:L:39:GLU:CB | 2.67 | 0.43 |
| 1:L:75:ILE:HD12 | 1:L:75:ILE:N | 2.34 | 0.43 |
| 1:A:486:ILE:HG12 | 1:A:486:ILE:H | 1.63 | 0.43 |
| 1:B:227:ILE:HD12 | 1:B:227:ILE:HA | 1.83 | 0.43 |
| 1:B:219:VAL:HA | 1:B:373:LEU:CD1 | 2.49 | 0.43 |
| 1:C:164:VAL:HG11 | 1:C:199:THR:HG23 | 2.00 | 0.43 |
| 1:C:264:HIS:CD2 | 1:C:288:PRO:CD | 3.02 | 0.43 |
| 1:C:372:TYR:OH | 1:C:461:ALA:HB2 | 2.18 | 0.43 |
| 1:C:478:ARG:HG2 | 1:C:478:ARG:NH1 | 2.33 | 0.43 |
| 1:D:498:VAL:CG2 | 1:D:499:THR:H | 2.28 | 0.43 |
| 1:D:53:LYS:N | 1:D:54:PRO:CD | 2.81 | 0.43 |
| 1:B:58:VAL:HG12 | 1:D:60:SER:HB2 | 2.01 | 0.43 |
| 1:D:79:ARG:NE | 1:D:163:ASP:OD2 | 2.51 | 0.43 |
| 1:E:397:LEU:HA | 1:E:397:LEU:HD12 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:57:HIS:ND1 | 1:E:84:HIS:HE1 | 2.15 | 0.43 |
| 1:F:153:ALA:CA | 1:F:158:ILE:HG22 | 2.48 | 0.43 |
| 1:F:248:VAL:HG12 | 1:F:314:ILE:HG13 | 1.99 | 0.43 |
| 1:F:399:PHE:CE2 | 1:F:443:ALA:HB1 | 2.53 | 0.43 |
| 1:F:477:LEU:HD13 | 1:F:477:LEU:N | 2.34 | 0.43 |
| 1:F:87:THR:CB | 1:F:88:PRO:CD | 2.97 | 0.43 |
| 1:G:158:ILE:HD12 | 1:G:165:PRO:CD | 2.48 | 0.43 |
| 1:G:335:ASN:ND2 | 1:G:336:ALA:N | 2.55 | 0.43 |
| 1:H:433:THR:CG2 | 1:L:412:SER:HA | 2.48 | 0.43 |
| 1:I:65:ILE:HD13 | 1:I:144:ILE:HG12 | 2.00 | 0.43 |
| 1:I:281:TRP:HD1 | 1:I:282:ASN:N | 2.13 | 0.43 |
| 1:J:264:HIS:CD2 | 1:J:288:PRO:CD | 2.98 | 0.43 |
| 1:J:396:ARG:HH11 | 1:J:396:ARG:HG3 | 1.84 | 0.43 |
| 1:K:110:LEU:HD12 | 1:K:110:LEU:N | 2.34 | 0.43 |
| 1:K:59:LEU:HB3 | 1:K:157:PHE:CE2 | 2.54 | 0.43 |
| 1:K:153:ALA:HB2 | 1:K:158:ILE:HG21 | 2.01 | 0.43 |
| 1:K:257:LEU:O | 1:K:260:MET:HB3 | 2.18 | 0.43 |
| 1:K:296:LEU:HA | 1:K:296:LEU:HD22 | 1.75 | 0.43 |
| 1:L:164:VAL:HG21 | 1:L:385:TRP:NE1 | 2.33 | 0.43 |
| 1:A:253:GLY:O | 1:A:254:ASN:C | 2.56 | 0.43 |
| 1:A:332:THR:O | 1:A:333:LYS:C | 2.57 | 0.43 |
| 1:A:353:THR:HG23 | 1:A:356:ALA:CB | 2.49 | 0.43 |
| 1:A:464:ILE:O | 1:A:465:MET:C | 2.56 | 0.43 |
| 1:C:176:MET:HE3 | 1:C:179:ILE:HD12 | 1.96 | 0.43 |
| 1:C:412:SER:OG | 1:E:433:THR:N | 2.44 | 0.43 |
| 1:C:47:GLY:O | 1:C:51:ILE:HG13 | 2.19 | 0.43 |
| 1:C:66:ARG:HD3 | 1:C:72:TRP:CH2 | 2.53 | 0.43 |
| 1:D:414:GLN:CB | 1:D:429:PRO:HD2 | 2.48 | 0.43 |
| 1:E:234:SER:O | 1:E:235:ILE:C | 2.57 | 0.43 |
| 1:F:134:LYS:HD3 | 1:F:134:LYS:HA | 1.92 | 0.43 |
| 1:F:451:SER:O | 1:F:452:GLY:C | 2.57 | 0.43 |
| 1:F:87:THR:OG1 | 1:F:88:PRO:CD | 2.67 | 0.43 |
| 1:G:133:PRO:HB3 | 1:G:141:LEU:HD11 | 2.01 | 0.43 |
| 1:G:475:LEU:HD12 | 1:G:475:LEU:HA | 1.87 | 0.43 |
| 1:H:78:TYR:CE2 | 1:H:101:VAL:HG22 | 2.54 | 0.43 |
| 1:H:223:ILE:CD1 | 1:H:263:LEU:HD11 | 2.48 | 0.43 |
| 1:H:300:SER:CB | 1:H:302:LEU:HD22 | 2.47 | 0.43 |
| 1:H:272:ALA:HB1 | 1:H:314:ILE:CG2 | 2.49 | 0.43 |
| 1:H:63:PHE:N | 1:H:63:PHE:CD2 | 2.87 | 0.43 |
| 1:I:280:ILE:HD11 | 1:I:301:ILE:O | 2.18 | 0.43 |
| 1:I:368:ILE:CB | 1:I:373:LEU:HD12 | 2.47 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:38:GLU:H | 1:I:42:ARG:NE | 2.16 | 0.43 |
| 1:K:107:LEU:O | 1:K:108:ALA:C | 2.55 | 0.43 |
| 1:K:153:ALA:HB2 | 1:K:158:ILE:CG2 | 2.49 | 0.43 |
| 1:K:363:ARG:CB | 1:K:363:ARG:NH1 | 2.82 | 0.43 |
| 1:K:371:LEU:HD13 | 1:K:482:TYR:CZ | 2.54 | 0.43 |
| 1:L:24:VAL:O | 1:L:25:GLU:C | 2.57 | 0.43 |
| 1:L:274:GLY:HA2 | 1:L:279:SER:HA | 2.01 | 0.43 |
| 1:L:327:SER:HB3 | 1:L:330:GLN:OE1 | 2.17 | 0.43 |
| 1:L:464:ILE:O | 1:L:465:MET:O | 2.35 | 0.43 |
| 1:A:428:ILE:N | 1:A:429:PRO:HD3 | 2.34 | 0.43 |
| 1:A:431:VAL:O | 1:A:431:VAL:HG13 | 2.19 | 0.43 |
| 1:B:226:PHE:C | 1:B:228:ASN:H | 2.23 | 0.43 |
| 1:B:118:VAL:HA | 1:B:460:SER:OG | 2.19 | 0.43 |
| 1:C:339:VAL:HG21 | 1:C:360:PHE:CE1 | 2.54 | 0.43 |
| 1:C:421:PHE:CE1 | 1:C:423:LYS:HB3 | 2.51 | 0.43 |
| 1:D:301:ILE:HD12 | 1:D:302:LEU:N | 2.34 | 0.43 |
| 1:E:79:ARG:HD3 | 1:E:157:PHE:HB3 | 1.99 | 0.43 |
| 1:F:462:ARG:HA | 1:F:465:MET:HE2 | 2.01 | 0.43 |
| 1:G:186:THR:HG22 | 1:G:187:ILE:N | 2.34 | 0.43 |
| 1:I:118:VAL:HG23 | 1:I:118:VAL:O | 2.18 | 0.43 |
| 1:J:281:TRP:HE1 | 1:J:283:PRO:HD3 | 1.80 | 0.43 |
| 1:J:39:GLU:C | 1:J:41:LYS:N | 2.72 | 0.43 |
| 1:J:39:GLU:C | 1:J:41:LYS:H | 2.21 | 0.43 |
| 1:K:224:GLU:O | 1:K:228:ASN:HB2 | 2.19 | 0.43 |
| 1:K:478:ARG:O | 1:K:481:ALA:CB | 2.67 | 0.43 |
| 1:K:85:GLN:HG2 | 1:K:86:ARG:N | 2.34 | 0.43 |
| 1:L:208:ILE:HG13 | 1:L:445:GLU:OE1 | 2.19 | 0.43 |
| 1:A:152:LEU:HG | 1:A:157:PHE:O | 2.18 | 0.42 |
| 1:A:247:PHE:CZ | 1:A:260:MET:HA | 2.54 | 0.42 |
| 1:A:252:PHE:CE2 | 1:A:260:MET:HE2 | 2.54 | 0.42 |
| 1:A:406:ASN:ND2 | 1:B:409:LEU:HD21 | 2.33 | 0.42 |
| 1:A:95:TYR:CE2 | 1:A:129:VAL:CG2 | 3.02 | 0.42 |
| 1:B:214:ALA:HB2 | 1:B:380:VAL:HG21 | 2.00 | 0.42 |
| 1:B:284:ASP:OD2 | 1:B:284:ASP:N | 2.52 | 0.42 |
| 1:C:315:LEU:HA | 1:C:315:LEU:HD23 | 1.76 | 0.42 |
| 1:C:36:GLU:O | 1:C:37:SER:O | 2.37 | 0.42 |
| 1:D:118:VAL:O | 1:D:119:ASP:C | 2.58 | 0.42 |
| 1:D:45:VAL:C | 1:D:47:GLY:H | 2.22 | 0.42 |
| 1:E:227:ILE:HD12 | 1:E:233:MET:CE | 2.49 | 0.42 |
| 1:E:19:ARG:CD | 1:E:23:ILE:HD11 | 2.49 | 0.42 |
| 1:E:288:PRO:O | 1:E:289:LYS:C | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:496:ALA:HB1 | 1:E:501:THR:C | 2.40 | 0.42 |
| 1:G:173:GLU:HG3 | 1:G:174:ARG:N | 2.34 | 0.42 |
| 1:H:9:PHE:CE2 | 1:H:103:GLU:OE2 | 2.72 | 0.42 |
| 1:H:160:PRO:HB3 | 1:H:196:ALA:HB3 | 2.01 | 0.42 |
| 1:H:353:THR:CB | 1:H:354:PRO:HD2 | 2.49 | 0.42 |
| 1:H:82:HIS:ND1 | 1:H:83:SER:HB2 | 2.33 | 0.42 |
| 1:I:356:ALA:O | 1:I:360:PHE:CD2 | 2.72 | 0.42 |
| 1:I:65:ILE:HA | 1:I:147:ARG:NH2 | 2.34 | 0.42 |
| 1:J:211:ARG:N | 1:J:212:ILE:HD12 | 2.34 | 0.42 |
| 1:J:55:CYS:HA | 1:J:82:HIS:HA | 2.01 | 0.42 |
| 1:L:32:LEU:O | 1:L:33:ARG:HG2 | 2.19 | 0.42 |
| 1:L:420:LYS:CB | 1:L:420:LYS:NZ | 2.77 | 0.42 |
| 1:L:496:ALA:CA | 1:L:501:THR:O | 2.67 | 0.42 |
| 1:A:118:VAL:HG23 | 1:A:120:VAL:CG2 | 2.42 | 0.42 |
| 1:A:137:THR:HG23 | 1:A:140:GLU:CG | 2.47 | 0.42 |
| 1:B:180:ALA:O | 1:B:181:ASP:C | 2.57 | 0.42 |
| 1:B:411:MET:HA | 1:B:430:ILE:HG22 | 2.00 | 0.42 |
| 1:B:84:HIS:C | 1:B:86:ARG:N | 2.71 | 0.42 |
| 1:C:223:ILE:HD11 | 1:C:345:ALA:HB1 | 2.01 | 0.42 |
| 1:C:6:ASP:HA | 1:C:7:PRO:HD3 | 1.83 | 0.42 |
| 1:D:184:ALA:O | 1:D:189:HIS:HA | 2.19 | 0.42 |
| 1:E:368:ILE:HA | 1:E:369:PRO:HD3 | 1.61 | 0.42 |
| 1:F:186:THR:HB | 1:F:187:ILE:H | 1.33 | 0.42 |
| 1:F:278:GLY:N | 1:F:302:LEU:HD11 | 2.34 | 0.42 |
| 1:F:378:VAL:HG12 | 1:F:379:THR:N | 2.34 | 0.42 |
| 1:F:371:LEU:HD23 | 1:F:481:ALA:HB3 | 2.00 | 0.42 |
| 1:G:109:SER:OG | 1:G:110:LEU:N | 2.50 | 0.42 |
| 1:G:217:ARG:CZ | 1:G:450:HIS:CE1 | 3.03 | 0.42 |
| 1:G:247:PHE:O | 1:G:270:CYS:HA | 2.19 | 0.42 |
| 1:G:39:GLU:O | 1:G:40:GLN:C | 2.57 | 0.42 |
| 1:H:354:PRO:HG2 | 1:H:355:GLU:H | 1.83 | 0.42 |
| 1:I:271:ILE:HG23 | 1:I:272:ALA:N | 2.34 | 0.42 |
| 1:J:186:THR:HG23 | 1:L:186:THR:HG23 | 2.00 | 0.42 |
| 1:J:25:GLU:HG2 | 1:J:26:ASP:N | 2.33 | 0.42 |
| 1:J:400:LYS:O | 1:J:401:TYR:C | 2.57 | 0.42 |
| 1:J:496:ALA:C | 1:J:501:THR:O | 2.58 | 0.42 |
| 1:K:150:MET:SD | 1:K:186:THR:HG21 | 2.59 | 0.42 |
| 1:K:428:ILE:HG23 | 1:K:430:ILE:HD11 | 2.01 | 0.42 |
| 1:K:399:PHE:CE2 | 1:K:443:ALA:HB1 | 2.54 | 0.42 |
| 1:L:18:ASP:O | 1:L:21:ALA:HB3 | 2.18 | 0.42 |
| 1:L:492:VAL:HG21 | 2:L:502:ADP:H2 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:79:ARG:HH12 | 1:L:165:PRO:HA | 1.83 | 0.42 |
| 1:A:310:TYR:CG | 1:A:311:GLU:N | 2.86 | 0.42 |
| 1:B:267:GLY:O | 1:B:268:ALA:C | 2.57 | 0.42 |
| 1:B:400:LYS:O | 1:B:401:TYR:C | 2.57 | 0.42 |
| 1:B:423:LYS:HG2 | 1:B:426:GLY:CA | 2.50 | 0.42 |
| 1:B:346:GLU:CD | 1:B:478:ARG:HH22 | 2.16 | 0.42 |
| 1:C:23:ILE:O | 1:C:23:ILE:HG22 | 2.18 | 0.42 |
| 1:C:280:ILE:CG2 | 1:C:307:ALA:HB1 | 2.49 | 0.42 |
| 1:C:335:ASN:HB2 | 1:C:338:ARG:NH1 | 2.35 | 0.42 |
| 1:C:318:ASP:HA | 1:C:340:LYS:CB | 2.49 | 0.42 |
| 1:C:420:LYS:O | 1:C:421:PHE:HB2 | 2.19 | 0.42 |
| 1:E:177:SER:HB2 | 1:E:202:PRO:HD2 | 2.01 | 0.42 |
| 1:E:371:LEU:CD2 | 1:E:482:TYR:CD2 | 3.01 | 0.42 |
| 1:F:167:PRO:HB3 | 1:F:176:MET:SD | 2.60 | 0.42 |
| 1:F:255:VAL:O | 1:F:256:GLY:C | 2.56 | 0.42 |
| 1:G:90:LYS:CD | 1:G:164:VAL:HB | 2.43 | 0.42 |
| 1:G:359:ILE:HG22 | 1:G:363:ARG:HD3 | 2.01 | 0.42 |
| 1:I:322:LEU:CD1 | 1:I:344:ILE:HG23 | 2.47 | 0.42 |
| 1:I:57:HIS:CE1 | 1:L:151:GLU:OE1 | 2.72 | 0.42 |
| 1:J:117:VAL:HG11 | 1:J:372:TYR:HB2 | 2.01 | 0.42 |
| 1:J:383:PHE:CD1 | 1:K:397:LEU:HD21 | 2.54 | 0.42 |
| 1:J:414:GLN:CA | 1:J:429:PRO:HG2 | 2.44 | 0.42 |
| 1:K:81:GLN:NE2 | 1:K:157:PHE:HD1 | 2.17 | 0.42 |
| 1:K:239:THR:CG2 | 1:K:239:THR:O | 2.64 | 0.42 |
| 1:K:298:HIS:ND1 | 1:K:298:HIS:O | 2.52 | 0.42 |
| 1:K:491:LYS:HB2 | 1:K:491:LYS:HE3 | 1.78 | 0.42 |
| 1:K:85:GLN:CB | 1:K:492:VAL:HG11 | 2.48 | 0.42 |
| 1:A:248:VAL:HG23 | 1:A:319:CYS:CB | 2.49 | 0.42 |
| 1:A:382:TYR:CE2 | 1:A:386:LEU:HD21 | 2.54 | 0.42 |
| 1:A:49:LEU:HD12 | 1:A:49:LEU:H | 1.84 | 0.42 |
| 1:B:234:SER:C | 1:B:236:LEU:H | 2.23 | 0.42 |
| 1:B:344:ILE:HD11 | 1:B:360:PHE:CE1 | 2.54 | 0.42 |
| 1:C:165:PRO:O | 1:C:198:VAL:HG23 | 2.19 | 0.42 |
| 1:C:385:TRP:CE3 | 1:C:386:LEU:HD23 | 2.55 | 0.42 |
| 1:C:92:GLY:O | 1:C:126:LYS:HD3 | 2.19 | 0.42 |
| 1:E:82:HIS:CD2 | 1:E:112:THR:HG21 | 2.54 | 0.42 |
| 1:E:229:GLU:O | 1:E:230:ALA:C | 2.58 | 0.42 |
| 1:E:59:LEU:HG | 1:E:61:LEU:HD22 | 2.01 | 0.42 |
| 1:F:67:ARG:CG | 1:F:67:ARG:HH11 | 2.31 | 0.42 |
| 1:G:360:PHE:HB3 | 1:G:365:ILE:HB | 2.00 | 0.42 |
| 1:G:398:THR:O | 1:G:399:PHE:C | 2.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:476:ASP:OD2 | 1:G:479:THR:OG1 | 2.34 | 0.42 |
| 1:H:79:ARG:HH11 | 1:H:79:ARG:HG3 | 1.83 | 0.42 |
| 1:I:175:GLU:O | 1:I:179:ILE:HG13 | 2.19 | 0.42 |
| 1:I:182:THR:O | 1:I:186:THR:HB | 2.19 | 0.42 |
| 1:I:85:GLN:H | 1:I:85:GLN:HE21 | 1.68 | 0.42 |
| 1:J:247:PHE:HB3 | 1:J:321:ILE:HB | 2.01 | 0.42 |
| 1:J:24:VAL:CG1 | 1:J:483:VAL:CG1 | 2.94 | 0.42 |
| 1:J:485:ALA:O | 1:J:486:ILE:C | 2.56 | 0.42 |
| 1:K:226:PHE:HB3 | 1:K:366:MET:CE | 2.49 | 0.42 |
| 1:J:386:LEU:CD1 | 1:K:392:VAL:HG11 | 2.44 | 0.42 |
| 1:K:45:VAL:O | 1:K:45:VAL:HG13 | 2.19 | 0.42 |
| 1:L:103:GLU:O | 1:L:106:ALA:HB3 | 2.19 | 0.42 |
| 1:L:157:PHE:O | 1:L:163:ASP:HB3 | 2.20 | 0.42 |
| 1:L:90:LYS:HE2 | 1:L:165:PRO:O | 2.19 | 0.42 |
| 1:A:95:TYR:HE2 | 1:A:129:VAL:HG21 | 1.84 | 0.42 |
| 1:A:201:LYS:HD2 | 1:A:205:GLN:O | 2.20 | 0.42 |
| 1:A:339:VAL:HG21 | 1:A:360:PHE:CE1 | 2.47 | 0.42 |
| 1:B:201:LYS:HA | 1:B:202:PRO:HD3 | 1.86 | 0.42 |
| 1:B:471:TYR:HE2 | 1:B:483:VAL:HG11 | 1.79 | 0.42 |
| 1:B:81:GLN:HG3 | 1:B:157:PHE:HE1 | 1.81 | 0.42 |
| 1:C:24:VAL:HG11 | 1:C:487:GLU:HG2 | 2.00 | 0.42 |
| 1:C:363:ARG:HH11 | 1:C:363:ARG:HB2 | 1.83 | 0.42 |
| 1:C:458:GLU:O | 1:C:461:ALA:N | 2.47 | 0.42 |
| 1:D:19:ARG:CD | 1:D:23:ILE:HD11 | 2.31 | 0.42 |
| 1:D:255:VAL:O | 1:D:259:SER:OG | 2.23 | 0.42 |
| 1:D:87:THR:CG2 | 1:D:88:PRO:HD3 | 2.34 | 0.42 |
| 1:D:88:PRO:O | 1:D:89:CYS:C | 2.57 | 0.42 |
| 1:E:158:ILE:CD1 | 1:E:197:CYS:HB2 | 2.49 | 0.42 |
| 1:E:460:SER:O | 1:E:461:ALA:C | 2.57 | 0.42 |
| 1:E:79:ARG:NH1 | 1:E:79:ARG:HG3 | 2.32 | 0.42 |
| 1:G:79:ARG:HA | 1:G:126:LYS:O | 2.19 | 0.42 |
| 1:G:394:TYR:CE2 | 1:H:397:LEU:HD22 | 2.54 | 0.42 |
| 1:G:417:LEU:HD23 | 1:H:417:LEU:HD11 | 2.00 | 0.42 |
| 1:G:82:HIS:CG | 1:G:109:SER:HA | 2.55 | 0.42 |
| 1:H:409:LEU:HD13 | 1:H:409:LEU:HA | 1.79 | 0.42 |
| 1:H:461:ALA:O | 1:H:464:ILE:N | 2.52 | 0.42 |
| 1:I:498:VAL:O | 1:I:501:THR:HG22 | 2.19 | 0.42 |
| 1:I:501:THR:OXT | 1:J:181:ASP:HB3 | 2.19 | 0.42 |
| 1:J:277:ASP:HB3 | 1:J:302:LEU:HD22 | 2.01 | 0.42 |
| 1:K:339:VAL:O | 1:K:339:VAL:HG23 | 2.19 | 0.42 |
| 1:L:374:ASN:O | 1:L:374:ASN:ND2 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:227:ILE:O | 1:A:233:MET:CG | 2.61 | 0.42 |
| 1:B:88:PRO:HG2 | 1:B:122:PHE:CD2 | 2.54 | 0.42 |
| 1:C:370:ASP:C | 1:C:372:TYR:N | 2.73 | 0.42 |
| 1:C:498:VAL:HG21 | 1:F:72:TRP:NE1 | 2.33 | 0.42 |
| 1:D:257:LEU:O | 1:D:257:LEU:HD12 | 2.19 | 0.42 |
| 1:D:364:ASN:O | 1:D:365:ILE:HD13 | 2.20 | 0.42 |
| 1:D:394:TYR:HB2 | 1:D:445:GLU:CG | 2.43 | 0.42 |
| 1:E:100:SER:O | 1:E:101:VAL:C | 2.56 | 0.42 |
| 1:E:93:ILE:HD12 | 1:E:179:ILE:HD11 | 2.02 | 0.42 |
| 1:E:314:ILE:CD1 | 1:E:314:ILE:N | 2.70 | 0.42 |
| 1:E:48:ILE:HG21 | 1:E:490:PHE:CD1 | 2.54 | 0.42 |
| 1:C:146:ARG:NH2 | 1:E:501:THR:N | 2.68 | 0.42 |
| 1:F:220:PHE:CE2 | 1:F:263:LEU:HA | 2.54 | 0.42 |
| 1:G:175:GLU:HA | 1:G:178:TRP:CE3 | 2.55 | 0.42 |
| 1:G:293:ASP:O | 1:G:294:PHE:O | 2.37 | 0.42 |
| 1:G:433:THR:O | 1:G:434:ALA:C | 2.57 | 0.42 |
| 1:G:87:THR:HG22 | 1:G:161:GLY:O | 2.20 | 0.42 |
| 1:H:109:SER:O | 1:H:112:THR:HG23 | 2.20 | 0.42 |
| 1:H:267:GLY:O | 1:H:268:ALA:C | 2.57 | 0.42 |
| 1:H:345:ALA:HB1 | 1:H:373:LEU:HD21 | 2.01 | 0.42 |
| 1:I:111:MET:O | 1:I:114:LYS:N | 2.53 | 0.42 |
| 1:I:315:LEU:HD23 | 1:I:331:LEU:HD23 | 2.02 | 0.42 |
| 1:I:414:GLN:OE1 | 1:I:430:ILE:HG12 | 2.20 | 0.42 |
| 1:I:477:LEU:HD22 | 1:I:477:LEU:N | 2.30 | 0.42 |
| 1:J:235:ILE:H | 1:J:235:ILE:HG12 | 1.59 | 0.42 |
| 1:L:315:LEU:HD23 | 1:L:331:LEU:HD21 | 2.02 | 0.42 |
| 1:L:400:LYS:O | 1:L:401:TYR:C | 2.58 | 0.42 |
| 1:A:238:MET:CE | 1:A:342:LYS:HG3 | 2.50 | 0.42 |
| 1:A:449:VAL:O | 1:A:452:GLY:N | 2.53 | 0.42 |
| 1:A:87:THR:HG22 | 1:A:88:PRO:CD | 2.49 | 0.42 |
| 1:B:61:LEU:N | 1:B:61:LEU:CD1 | 2.83 | 0.42 |
| 1:C:91:GLY:HA2 | 1:C:111:MET:CE | 2.50 | 0.42 |
| 1:D:109:SER:O | 1:D:113:TYR:CD2 | 2.72 | 0.42 |
| 1:D:316:GLU:O | 1:D:317:ALA:C | 2.57 | 0.42 |
| 1:D:372:TYR:C | 1:D:372:TYR:CD1 | 2.93 | 0.42 |
| 1:D:453:LEU:CD2 | 1:D:453:LEU:C | 2.87 | 0.42 |
| 1:E:112:THR:OG1 | 1:E:113:TYR:N | 2.53 | 0.42 |
| 1:E:378:VAL:O | 1:E:379:THR:C | 2.57 | 0.42 |
| 1:G:282:ASN:ND2 | 1:G:306:LYS:O | 2.50 | 0.42 |
| 1:G:332:THR:H | 1:G:335:ASN:ND2 | 2.16 | 0.42 |
| 1:G:53:LYS:HB3 | 1:G:54:PRO:CD | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:291:LEU:C | 1:H:291:LEU:HD12 | 2.34 | 0.42 |
| 1:I:112:THR:HB | 1:I:124:GLY:H | 1.85 | 0.42 |
| 1:I:281:TRP:HE1 | 1:I:283:PRO:CG | 2.33 | 0.42 |
| 1:I:384:GLU:O | 1:I:387:LYS:HB3 | 2.20 | 0.42 |
| 1:J:249:VAL:HA | 1:J:323:ILE:HG23 | 2.02 | 0.42 |
| 1:J:90:LYS:HZ3 | 1:J:199:THR:CG2 | 2.24 | 0.42 |
| 1:K:17:PHE:CD2 | 1:K:53:LYS:HD2 | 2.55 | 0.42 |
| 1:K:248:VAL:HG23 | 1:K:271:ILE:HG23 | 2.00 | 0.42 |
| 1:K:287:ASP:OD2 | 1:K:289:LYS:HB3 | 2.19 | 0.42 |
| 1:K:370:ASP:C | 1:K:372:TYR:N | 2.72 | 0.42 |
| 1:K:41:LYS:O | 1:K:44:ARG:CB | 2.67 | 0.42 |
| 1:K:498:VAL:N | 1:K:501:THR:HB | 2.35 | 0.42 |
| 1:A:24:VAL:O | 1:A:25:GLU:O | 2.37 | 0.42 |
| 1:A:280:ILE:HG22 | 1:A:281:TRP:N | 2.35 | 0.42 |
| 1:A:53:LYS:CB | 1:A:54:PRO:CD | 2.97 | 0.42 |
| 1:B:137:THR:CG2 | 1:B:140:GLU:CD | 2.88 | 0.42 |
| 1:B:142:GLU:HG2 | 1:B:146:ARG:HD2 | 2.01 | 0.42 |
| 1:B:361:LEU:HD23 | 1:B:361:LEU:C | 2.40 | 0.42 |
| 1:B:344:ILE:HD11 | 1:B:365:ILE:HG21 | 2.01 | 0.42 |
| 1:B:386:LEU:HD13 | 1:F:392:VAL:CG2 | 2.47 | 0.42 |
| 1:B:65:ILE:CG1 | 1:B:75:ILE:HD11 | 2.40 | 0.42 |
| 1:D:99:VAL:HG13 | 1:D:130:LYS:CD | 2.50 | 0.42 |
| 1:D:171:THR:HG22 | 1:D:175:GLU:OE2 | 2.20 | 0.42 |
| 1:D:213:SER:HB2 | 1:D:217:ARG:HE | 1.85 | 0.42 |
| 1:D:280:ILE:CG2 | 1:D:286:ILE:HD13 | 2.49 | 0.42 |
| 1:C:432:PRO:HA | 1:D:412:SER:OG | 2.20 | 0.42 |
| 1:F:40:GLN:C | 1:F:42:ARG:H | 2.22 | 0.42 |
| 1:B:433:THR:CG2 | 1:F:412:SER:HA | 2.49 | 0.42 |
| 1:G:67:ARG:NH1 | 1:G:140:GLU:OE1 | 2.53 | 0.42 |
| 1:G:183:TYR:O | 1:G:185:SER:N | 2.53 | 0.42 |
| 1:G:301:ILE:HG23 | 1:G:301:ILE:H | 1.52 | 0.42 |
| 1:G:497:GLY:HA3 | 1:G:501:THR:HA | 2.01 | 0.42 |
| 1:H:224:GLU:O | 1:H:225:ASN:C | 2.58 | 0.42 |
| 1:H:361:LEU:HA | 1:H:361:LEU:HD12 | 1.82 | 0.42 |
| 1:H:79:ARG:HG3 | 1:H:79:ARG:NH1 | 2.34 | 0.42 |
| 1:I:431:VAL:CG1 | 1:I:431:VAL:O | 2.68 | 0.42 |
| 1:J:228:ASN:HA | 1:J:228:ASN:HD22 | 1.57 | 0.42 |
| 1:J:465:MET:O | 1:J:468:ALA:HB3 | 2.19 | 0.42 |
| 1:J:477:LEU:HD12 | 1:J:477:LEU:HA | 1.91 | 0.42 |
| 1:K:204:SER:HG | 1:K:205:GLN:HE21 | 1.68 | 0.42 |
| 1:K:255:VAL:CG1 | 1:K:256:GLY:N | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:356:ALA:O | 1:K:360:PHE:CD2 | 2.73 | 0.42 |
| 1:J:439:ARG:NH2 | 1:K:405:SER:OG | 2.51 | 0.42 |
| 1:L:158:ILE:HG12 | 1:L:165:PRO:HG2 | 2.01 | 0.42 |
| 1:L:20:GLY:O | 1:L:24:VAL:CG2 | 2.64 | 0.42 |
| 1:L:239:THR:O | 1:L:239:THR:CG2 | 2.66 | 0.42 |
| 1:L:329:LYS:NZ | 1:L:329:LYS:HB2 | 2.34 | 0.42 |
| 1:A:111:MET:HB3 | 1:A:124:GLY:HA2 | 2.02 | 0.42 |
| 1:A:8:ASN:O | 1:A:10:PHE:N | 2.53 | 0.42 |
| 1:B:104:VAL:HG23 | 1:B:105:LYS:H | 1.85 | 0.42 |
| 1:C:101:VAL:HG23 | 1:C:102:ASP:N | 2.35 | 0.42 |
| 1:C:243:GLY:O | 1:C:245:LYS:N | 2.53 | 0.42 |
| 1:C:247:PHE:CD1 | 1:C:247:PHE:N | 2.88 | 0.42 |
| 1:D:331:LEU:O | 1:D:356:ALA:CB | 2.68 | 0.42 |
| 1:E:86:ARG:HG2 | 1:E:121:PRO:HA | 2.01 | 0.42 |
| 1:E:295:LYS:O | 1:E:295:LYS:HG3 | 2.20 | 0.42 |
| 1:F:39:GLU:C | 1:F:41:LYS:N | 2.72 | 0.42 |
| 1:G:142:GLU:CG | 1:G:146:ARG:HD2 | 2.33 | 0.42 |
| 1:G:300:SER:O | 1:G:302:LEU:N | 2.53 | 0.42 |
| 1:H:129:VAL:O | 1:H:131:ILE:N | 2.53 | 0.42 |
| 1:H:227:ILE:HA | 1:H:233:MET:SD | 2.60 | 0.42 |
| 1:H:335:ASN:N | 1:H:335:ASN:ND2 | 2.67 | 0.42 |
| 1:H:95:TYR:CD1 | 1:H:171:THR:HG22 | 2.55 | 0.42 |
| 1:H:95:TYR:OH | 1:H:145:THR:HG22 | 2.19 | 0.42 |
| 1:I:171:THR:HB | 1:I:175:GLU:OE1 | 2.20 | 0.42 |
| 1:I:32:LEU:O | 1:I:33:ARG:HB2 | 2.18 | 0.42 |
| 1:I:479:THR:O | 1:I:483:VAL:HG23 | 2.19 | 0.42 |
| 1:J:153:ALA:HB2 | 1:J:158:ILE:CG2 | 2.50 | 0.42 |
| 1:J:404:ASP:O | 1:J:406:ASN:N | 2.53 | 0.42 |
| 1:I:433:THR:CG2 | 1:J:412:SER:HA | 2.49 | 0.42 |
| 1:K:248:VAL:HG13 | 1:K:272:ALA:C | 2.39 | 0.42 |
| 1:K:336:ALA:N | 1:K:337:PRO:CD | 2.83 | 0.42 |
| 1:K:430:ILE:O | 1:K:432:PRO:HD3 | 2.20 | 0.42 |
| 1:K:499:THR:OG1 | 1:K:500:PHE:HD1 | 2.03 | 0.42 |
| 1:K:90:LYS:HB2 | 1:K:122:PHE:CG | 2.55 | 0.42 |
| 1:L:13:VAL:O | 1:L:14:GLU:C | 2.58 | 0.42 |
| 1:L:219:VAL:HA | 1:L:373:LEU:CD1 | 2.49 | 0.42 |
| 1:A:115:CYS:HB3 | 1:A:120:VAL:O | 2.19 | 0.42 |
| 1:B:201:LYS:HG2 | 1:B:201:LYS:HZ3 | 1.69 | 0.42 |
| 1:D:334:SER:HB2 | 1:D:335:ASN:H | 1.70 | 0.42 |
| 1:F:289:LYS:O | 1:F:290:GLU:C | 2.57 | 0.42 |
| 1:G:176:MET:HE1 | 1:G:179:ILE:HD12 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:177:SER:O | 1:G:180:ALA:HB3 | 2.20 | 0.42 |
| 1:G:160:PRO:HB3 | 1:G:196:ALA:HB3 | 2.02 | 0.42 |
| 1:G:84:HIS:O | 1:G:85:GLN:C | 2.57 | 0.42 |
| 1:H:154:LYS:HB3 | 1:K:189:HIS:CD2 | 2.54 | 0.42 |
| 1:H:192:ILE:HG12 | 1:H:192:ILE:O | 2.20 | 0.42 |
| 1:H:203:ILE:HG21 | 1:H:209:HIS:NE2 | 2.35 | 0.42 |
| 1:H:321:ILE:HG22 | 1:H:343:ILE:CG2 | 2.50 | 0.42 |
| 1:K:222:GLY:O | 1:K:223:ILE:C | 2.58 | 0.42 |
| 1:K:230:ALA:O | 1:K:233:MET:HB2 | 2.20 | 0.42 |
| 1:K:335:ASN:C | 1:K:335:ASN:HD22 | 2.23 | 0.42 |
| 1:K:360:PHE:CA | 1:K:365:ILE:HG13 | 2.49 | 0.42 |
| 1:K:498:VAL:HG23 | 1:K:499:THR:H | 1.85 | 0.42 |
| 1:L:168:ASP:OD1 | 1:L:169:MET:N | 2.53 | 0.42 |
| 1:L:485:ALA:O | 1:L:486:ILE:C | 2.58 | 0.42 |
| 1:L:499:THR:HG23 | 1:L:500:PHE:N | 2.35 | 0.42 |
| 1:A:250:GLN:NE2 | 1:A:274:GLY:O | 2.53 | 0.41 |
| 1:A:314:ILE:H | 1:A:314:ILE:CD1 | 2.32 | 0.41 |
| 1:A:448:ILE:HD13 | 1:B:401:TYR:CD1 | 2.55 | 0.41 |
| 1:A:79:ARG:HA | 1:A:127:ALA:HA | 2.02 | 0.41 |
| 1:C:499:THR:OG1 | 1:C:500:PHE:HD1 | 2.01 | 0.41 |
| 1:A:499:THR:HB | 1:E:147:ARG:CZ | 2.50 | 0.41 |
| 1:E:224:GLU:HA | 1:E:227:ILE:CG2 | 2.49 | 0.41 |
| 1:E:36:GLU:O | 1:E:38:GLU:OE1 | 2.38 | 0.41 |
| 1:E:77:GLY:C | 1:E:78:TYR:CG | 2.93 | 0.41 |
| 1:E:60:SER:CB | 1:E:78:TYR:HD2 | 2.32 | 0.41 |
| 1:F:145:THR:HG21 | 1:F:175:GLU:CG | 2.44 | 0.41 |
| 1:F:392:VAL:CG1 | 1:F:393:SER:N | 2.82 | 0.41 |
| 1:F:39:GLU:O | 1:F:41:LYS:N | 2.53 | 0.41 |
| 1:G:198:VAL:O | 1:G:201:LYS:HE2 | 2.19 | 0.41 |
| 1:G:322:LEU:HD22 | 1:G:344:ILE:CD1 | 2.50 | 0.41 |
| 1:G:484:ASN:O | 1:G:488:LYS:HG3 | 2.20 | 0.41 |
| 1:H:274:GLY:HA2 | 1:H:279:SER:HA | 2.02 | 0.41 |
| 1:H:296:LEU:HD13 | 1:H:296:LEU:C | 2.41 | 0.41 |
| 1:H:403:ARG:HG3 | 1:H:440:ILE:HG23 | 2.02 | 0.41 |
| 1:H:93:ILE:O | 1:H:168:ASP:HB2 | 2.20 | 0.41 |
| 1:I:34:THR:O | 1:I:34:THR:HG22 | 2.19 | 0.41 |
| 1:I:382:TYR:O | 1:I:385:TRP:HB3 | 2.20 | 0.41 |
| 1:I:42:ARG:HG2 | 1:I:42:ARG:H | 1.52 | 0.41 |
| 1:J:329:LYS:HB3 | 1:J:329:LYS:HE3 | 1.87 | 0.41 |
| 1:K:263:LEU:HD12 | 1:K:263:LEU:HA | 1.64 | 0.41 |
| 1:K:360:PHE:HB3 | 1:K:365:ILE:CB | 2.47 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:344:ILE:HD11 | 1:L:360:PHE:CE1 | 2.56 | 0.41 |
| 1:L:346:GLU:HG2 | 1:L:351:PRO:CD | 2.50 | 0.41 |
| 1:L:120:VAL:HG13 | 1:L:382:TYR:HB2 | 2.02 | 0.41 |
| 1:G:401:TYR:HE2 | 1:L:402:GLU:OE1 | 2.03 | 0.41 |
| 1:L:94:ARG:HG3 | 1:L:95:TYR:N | 2.35 | 0.41 |
| 1:A:34:THR:O | 1:A:34:THR:CG2 | 2.63 | 0.41 |
| 1:A:337:PRO:HD3 | 1:A:359:ILE:HD13 | 2.01 | 0.41 |
| 1:A:382:TYR:O | 1:A:385:TRP:HB3 | 2.19 | 0.41 |
| 1:B:17:PHE:CD2 | 1:B:53:LYS:HG3 | 2.55 | 0.41 |
| 1:B:387:LYS:HE3 | 1:B:393:SER:HA | 2.02 | 0.41 |
| 1:C:198:VAL:HG13 | 1:C:198:VAL:O | 2.20 | 0.41 |
| 1:C:233:MET:CE | 1:C:236:LEU:HD11 | 2.50 | 0.41 |
| 1:C:436:PHE:O | 1:C:440:ILE:CG1 | 2.63 | 0.41 |
| 1:C:53:LYS:O | 1:C:82:HIS:HE1 | 2.03 | 0.41 |
| 1:D:315:LEU:HA | 1:D:315:LEU:HD12 | 1.87 | 0.41 |
| 1:D:90:LYS:HZ3 | 1:D:164:VAL:CG1 | 2.31 | 0.41 |
| 1:D:99:VAL:HG13 | 1:D:130:LYS:HD2 | 2.01 | 0.41 |
| 1:E:203:ILE:HG21 | 1:E:209:HIS:HE1 | 1.85 | 0.41 |
| 1:E:257:LEU:O | 1:E:257:LEU:HD12 | 2.20 | 0.41 |
| 1:E:433:THR:O | 1:E:434:ALA:C | 2.58 | 0.41 |
| 1:F:160:PRO:CG | 1:F:161:GLY:N | 2.83 | 0.41 |
| 1:F:420:LYS:NZ | 1:F:420:LYS:O | 2.39 | 0.41 |
| 1:F:496:ALA:CA | 1:F:501:THR:O | 2.68 | 0.41 |
| 1:G:24:VAL:O | 1:G:25:GLU:C | 2.58 | 0.41 |
| 1:G:376:GLY:O | 1:G:379:THR:HB | 2.20 | 0.41 |
| 1:G:420:LYS:HB3 | 1:G:420:LYS:HE2 | 1.92 | 0.41 |
| 1:H:149:THR:HG21 | 1:H:182:THR:HB | 2.02 | 0.41 |
| 1:H:316:GLU:O | 1:H:317:ALA:O | 2.38 | 0.41 |
| 1:H:346:GLU:HG2 | 1:H:351:PRO:HG3 | 2.00 | 0.41 |
| 1:I:264:HIS:C | 1:I:266:PHE:N | 2.72 | 0.41 |
| 1:I:439:ARG:HH12 | 1:J:404:ASP:HB3 | 1.82 | 0.41 |
| 1:J:406:ASN:O | 1:J:409:LEU:N | 2.48 | 0.41 |
| 1:J:371:LEU:HD13 | 1:J:482:TYR:CZ | 2.55 | 0.41 |
| 1:J:59:LEU:HB2 | 1:J:157:PHE:CZ | 2.55 | 0.41 |
| 1:K:141:LEU:O | 1:K:145:THR:HG22 | 2.19 | 0.41 |
| 1:K:308:LYS:HG2 | 1:K:309:PRO:HD2 | 2.01 | 0.41 |
| 1:K:363:ARG:HB2 | 1:K:363:ARG:NH1 | 2.34 | 0.41 |
| 1:K:497:GLY:N | 1:K:501:THR:HA | 2.34 | 0.41 |
| 1:L:227:ILE:HA | 1:L:233:MET:SD | 2.61 | 0.41 |
| 1:G:416:SER:CB | 1:L:429:PRO:HA | 2.50 | 0.41 |
| 1:L:465:MET:HB2 | 1:L:466:ARG:H | 1.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:402:GLU:O | 1:A:403:ARG:C | 2.59 | 0.41 |
| 1:A:352:THR:HG1 | 1:A:478:ARG:HH22 | 1.67 | 0.41 |
| 1:B:28:LEU:HD21 | 1:B:490:PHE:CG | 2.54 | 0.41 |
| 1:B:407:TYR:HD2 | 1:B:407:TYR:H | 1.69 | 0.41 |
| 1:C:219:VAL:O | 1:C:220:PHE:C | 2.57 | 0.41 |
| 1:C:316:GLU:HG3 | 1:C:338:ARG:HE | 1.80 | 0.41 |
| 1:C:63:PHE:CD2 | 1:C:63:PHE:N | 2.88 | 0.41 |
| 1:D:109:SER:O | 1:D:112:THR:HB | 2.21 | 0.41 |
| 1:E:330:GLN:C | 1:E:331:LEU:HD12 | 2.40 | 0.41 |
| 1:E:396:ARG:HD3 | 1:E:396:ARG:C | 2.39 | 0.41 |
| 1:E:477:LEU:HD12 | 1:E:477:LEU:HA | 1.85 | 0.41 |
| 1:E:66:ARG:HD3 | 1:E:72:TRP:CZ2 | 2.54 | 0.41 |
| 1:F:131:ILE:HD12 | 1:F:131:ILE:HA | 1.68 | 0.41 |
| 1:F:131:ILE:HG13 | 1:F:136:TYR:CE2 | 2.55 | 0.41 |
| 1:F:332:THR:O | 1:F:335:ASN:ND2 | 2.53 | 0.41 |
| 1:G:111:MET:HE3 | 1:G:114:LYS:HD2 | 2.03 | 0.41 |
| 1:H:30:GLU:O | 1:H:32:LEU:N | 2.53 | 0.41 |
| 1:H:368:ILE:HA | 1:H:369:PRO:HD3 | 1.72 | 0.41 |
| 1:H:414:GLN:HB2 | 1:H:429:PRO:HD2 | 2.02 | 0.41 |
| 1:I:56:ASN:C | 1:I:57:HIS:ND1 | 2.73 | 0.41 |
| 1:K:12:MET:HG2 | 1:K:16:PHE:HE1 | 1.84 | 0.41 |
| 1:K:210:GLY:HA2 | 1:K:212:ILE:CD1 | 2.50 | 0.41 |
| 1:K:256:GLY:O | 1:K:259:SER:HB2 | 2.20 | 0.41 |
| 1:K:358:LYS:O | 1:K:361:LEU:N | 2.51 | 0.41 |
| 1:K:428:ILE:O | 1:K:431:VAL:HG12 | 2.19 | 0.41 |
| 1:L:280:ILE:CD1 | 1:L:304:PHE:HB3 | 2.50 | 0.41 |
| 1:A:220:PHE:CD1 | 1:A:220:PHE:C | 2.94 | 0.41 |
| 1:A:332:THR:O | 1:A:335:ASN:ND2 | 2.53 | 0.41 |
| 1:A:466:ARG:C | 1:A:468:ALA:H | 2.24 | 0.41 |
| 1:A:48:ILE:O | 1:A:51:ILE:HB | 2.21 | 0.41 |
| 1:B:211:ARG:N | 1:B:212:ILE:HD12 | 2.35 | 0.41 |
| 1:B:264:HIS:C | 1:B:266:PHE:N | 2.73 | 0.41 |
| 1:C:201:LYS:O | 1:C:207:GLY:HA3 | 2.20 | 0.41 |
| 1:D:265:ARG:HG3 | 1:D:265:ARG:O | 2.19 | 0.41 |
| 1:D:219:VAL:O | 1:D:373:LEU:HD11 | 2.20 | 0.41 |
| 1:E:129:VAL:O | 1:E:131:ILE:N | 2.53 | 0.41 |
| 1:E:351:PRO:O | 1:E:352:THR:HG23 | 2.21 | 0.41 |
| 1:E:434:ALA:O | 1:E:435:GLU:C | 2.58 | 0.41 |
| 1:E:497:GLY:N | 1:E:501:THR:HA | 2.35 | 0.41 |
| 1:F:118:VAL:O | 1:F:120:VAL:HG23 | 2.20 | 0.41 |
| 1:F:167:PRO:N | 1:F:176:MET:SD | 2.93 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:176:MET:HG2 | 1:F:199:THR:O | 2.21 | 0.41 |
| 1:F:372:TYR:CD1 | 1:F:373:LEU:N | 2.88 | 0.41 |
| 1:F:122:PHE:HE1 | 1:F:382:TYR:HA | 1.85 | 0.41 |
| 1:F:403:ARG:O | 1:F:406:ASN:HB2 | 2.20 | 0.41 |
| 1:B:433:THR:N | 1:F:412:SER:OG | 2.54 | 0.41 |
| 1:G:181:ASP:O | 1:G:182:THR:C | 2.57 | 0.41 |
| 1:G:19:ARG:HH11 | 1:G:19:ARG:HG3 | 1.85 | 0.41 |
| 1:G:255:VAL:HG13 | 1:G:256:GLY:H | 1.86 | 0.41 |
| 1:G:294:PHE:O | 1:G:296:LEU:N | 2.53 | 0.41 |
| 1:G:33:ARG:CG | 1:G:33:ARG:HH11 | 2.33 | 0.41 |
| 1:G:405:SER:O | 1:G:408:HIS:HB2 | 2.19 | 0.41 |
| 1:H:249:VAL:CG2 | 1:H:250:GLN:N | 2.82 | 0.41 |
| 1:A:437:GLN:CG | 1:H:423:LYS:HD3 | 2.49 | 0.41 |
| 1:I:158:ILE:CG2 | 1:I:158:ILE:O | 2.68 | 0.41 |
| 1:I:378:VAL:O | 1:I:379:THR:C | 2.59 | 0.41 |
| 1:J:131:ILE:O | 1:J:133:PRO:HD3 | 2.20 | 0.41 |
| 1:I:428:ILE:O | 1:J:416:SER:HB3 | 2.20 | 0.41 |
| 1:K:282:ASN:O | 1:K:284:ASP:N | 2.53 | 0.41 |
| 1:K:353:THR:HB | 1:K:354:PRO:CD | 2.51 | 0.41 |
| 1:L:104:VAL:CG2 | 1:L:105:LYS:H | 2.33 | 0.41 |
| 1:L:271:ILE:CG2 | 1:L:272:ALA:N | 2.83 | 0.41 |
| 1:L:304:PHE:CD1 | 1:L:305:PRO:HD2 | 2.56 | 0.41 |
| 1:L:353:THR:HB | 1:L:354:PRO:CD | 2.51 | 0.41 |
| 1:G:146:ARG:HH12 | 1:L:501:THR:C | 2.24 | 0.41 |
| 1:A:465:MET:O | 1:A:468:ALA:HB3 | 2.19 | 0.41 |
| 1:B:173:GLU:HB2 | 1:B:202:PRO:HG3 | 2.02 | 0.41 |
| 1:B:387:LYS:HE3 | 1:B:445:GLU:OE2 | 2.21 | 0.41 |
| 1:B:501:THR:C | 1:F:146:ARG:NH2 | 2.69 | 0.41 |
| 1:C:160:PRO:HD3 | 1:C:183:TYR:HE2 | 1.86 | 0.41 |
| 1:C:433:THR:HG23 | 1:D:412:SER:OG | 2.20 | 0.41 |
| 1:C:16:PHE:HE2 | 1:C:478:ARG:HD3 | 1.85 | 0.41 |
| 1:D:153:ALA:HA | 1:D:158:ILE:HG22 | 2.02 | 0.41 |
| 1:D:281:TRP:O | 1:D:282:ASN:CB | 2.66 | 0.41 |
| 1:D:386:LEU:O | 1:D:387:LYS:C | 2.58 | 0.41 |
| 1:D:429:PRO:HA | 1:E:416:SER:HB3 | 2.01 | 0.41 |
| 1:G:238:MET:O | 1:G:239:THR:C | 2.58 | 0.41 |
| 1:H:32:LEU:HD23 | 1:H:32:LEU:HA | 1.91 | 0.41 |
| 1:G:429:PRO:HA | 1:H:416:SER:CB | 2.50 | 0.41 |
| 1:H:346:GLU:CD | 1:H:478:ARG:HH22 | 2.23 | 0.41 |
| 1:I:192:ILE:HG23 | 1:I:193:ASN:OD1 | 2.20 | 0.41 |
| 1:I:30:GLU:HA | 1:I:34:THR:OG1 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:414:GLN:OE1 | 1:I:429:PRO:HD2 | 2.21 | 0.41 |
| 1:J:277:ASP:HB2 | 1:J:278:GLY:H | 1.67 | 0.41 |
| 1:J:410:LEU:HD23 | 1:J:410:LEU:N | 2.33 | 0.41 |
| 1:K:90:LYS:HD2 | 1:K:164:VAL:HB | 2.02 | 0.41 |
| 1:K:164:VAL:HA | 1:K:197:CYS:O | 2.21 | 0.41 |
| 1:L:297:GLN:H | 1:L:297:GLN:HG3 | 1.64 | 0.41 |
| 1:B:277:ASP:OD2 | 1:B:300:SER:CB | 2.68 | 0.41 |
| 1:B:321:ILE:HG23 | 1:B:343:ILE:CB | 2.49 | 0.41 |
| 1:C:153:ALA:HA | 1:C:158:ILE:HG22 | 2.02 | 0.41 |
| 1:C:250:GLN:HE21 | 1:C:314:ILE:HD11 | 1.85 | 0.41 |
| 1:C:497:GLY:O | 1:C:498:VAL:CG1 | 2.67 | 0.41 |
| 1:D:281:TRP:CG | 1:D:282:ASN:N | 2.89 | 0.41 |
| 1:B:58:VAL:CG1 | 1:D:60:SER:HB2 | 2.50 | 0.41 |
| 1:F:82:HIS:CG | 1:F:109:SER:HA | 2.55 | 0.41 |
| 1:F:244:ASP:CG | 1:F:245:LYS:HG3 | 2.39 | 0.41 |
| 1:F:421:PHE:O | 1:F:423:LYS:N | 2.54 | 0.41 |
| 1:G:191:ASP:C | 1:G:193:ASN:N | 2.74 | 0.41 |
| 1:G:58:VAL:HG23 | 1:G:80:ALA:CB | 2.50 | 0.41 |
| 1:I:364:ASN:O | 1:I:365:ILE:HD13 | 2.21 | 0.41 |
| 1:I:47:GLY:O | 1:I:50:ARG:N | 2.53 | 0.41 |
| 1:J:23:ILE:H | 1:J:23:ILE:HG13 | 1.36 | 0.41 |
| 1:K:80:ALA:O | 1:K:125:ALA:HA | 2.20 | 0.41 |
| 1:K:330:GLN:HB3 | 1:K:331:LEU:HD23 | 2.02 | 0.41 |
| 1:K:52:ILE:CD1 | 1:K:489:VAL:HG12 | 2.46 | 0.41 |
| 1:L:17:PHE:HE2 | 1:L:53:LYS:HB2 | 1.85 | 0.41 |
| 1:L:370:ASP:OD2 | 1:L:371:LEU:N | 2.52 | 0.41 |
| 1:H:439:ARG:NH1 | 1:L:405:SER:HA | 2.35 | 0.41 |
| 1:B:12:MET:O | 1:B:15:GLY:N | 2.54 | 0.41 |
| 1:B:175:GLU:HA | 1:B:178:TRP:HE3 | 1.79 | 0.41 |
| 1:B:247:PHE:CZ | 1:B:270:CYS:HB2 | 2.56 | 0.41 |
| 1:B:264:HIS:O | 1:B:266:PHE:N | 2.54 | 0.41 |
| 1:B:374:ASN:O | 1:B:374:ASN:ND2 | 2.53 | 0.41 |
| 1:C:248:VAL:HB | 1:C:322:LEU:HD23 | 2.03 | 0.41 |
| 1:D:32:LEU:HA | 1:D:32:LEU:HD23 | 1.98 | 0.41 |
| 1:E:167:PRO:HG3 | 1:E:176:MET:HG2 | 2.03 | 0.41 |
| 1:E:28:LEU:HD21 | 1:E:490:PHE:CD2 | 2.56 | 0.41 |
| 1:E:461:ALA:O | 1:E:462:ARG:C | 2.59 | 0.41 |
| 1:G:243:GLY:O | 1:G:245:LYS:N | 2.54 | 0.41 |
| 1:G:258:HIS:HB3 | 1:G:262:TYR:HE2 | 1.83 | 0.41 |
| 1:G:346:GLU:OE1 | 1:G:370:ASP:N | 2.53 | 0.41 |
| 1:H:126:LYS:HD2 | 1:H:127:ALA:H | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:94:ARG:CB | 1:H:168:ASP:OD2 | 2.67 | 0.41 |
| 1:H:20:GLY:O | 1:H:21:ALA:C | 2.59 | 0.41 |
| 1:H:48:ILE:HG12 | 1:H:48:ILE:H | 1.60 | 0.41 |
| 1:H:48:ILE:O | 1:H:52:ILE:HG13 | 2.20 | 0.41 |
| 1:I:247:PHE:CZ | 1:I:260:MET:HA | 2.55 | 0.41 |
| 1:I:287:ASP:HA | 1:I:288:PRO:HD3 | 1.72 | 0.41 |
| 1:I:196:ALA:HB1 | 1:I:385:TRP:CD1 | 2.56 | 0.41 |
| 1:J:93:ILE:HD11 | 1:J:165:PRO:HB3 | 2.03 | 0.41 |
| 1:K:147:ARG:NH1 | 1:K:147:ARG:HG3 | 2.34 | 0.41 |
| 1:K:24:VAL:HG12 | 1:K:28:LEU:HB2 | 2.02 | 0.41 |
| 1:L:58:VAL:HG13 | 1:L:60:SER:HB2 | 2.02 | 0.41 |
| 1:A:497:GLY:N | 1:A:501:THR:C | 2.73 | 0.41 |
| 1:A:90:LYS:CB | 1:A:122:PHE:HD1 | 2.34 | 0.41 |
| 1:B:280:ILE:CD1 | 1:B:304:PHE:HB3 | 2.50 | 0.41 |
| 1:B:47:GLY:O | 1:B:51:ILE:HG13 | 2.21 | 0.41 |
| 1:D:173:GLU:O | 1:D:174:ARG:C | 2.59 | 0.41 |
| 1:D:191:ASP:C | 1:D:193:ASN:H | 2.24 | 0.41 |
| 1:D:226:PHE:O | 1:D:228:ASN:N | 2.54 | 0.41 |
| 1:D:296:LEU:O | 1:D:298:HIS:N | 2.54 | 0.41 |
| 1:D:460:SER:O | 1:D:464:ILE:HG13 | 2.21 | 0.41 |
| 1:D:83:SER:OG | 1:D:84:HIS:N | 2.54 | 0.41 |
| 1:E:339:VAL:CG2 | 1:E:360:PHE:HE1 | 2.25 | 0.41 |
| 1:F:263:LEU:HA | 1:F:263:LEU:HD12 | 1.92 | 0.41 |
| 1:G:346:GLU:O | 1:G:373:LEU:HD23 | 2.21 | 0.41 |
| 1:H:300:SER:O | 1:H:302:LEU:N | 2.53 | 0.41 |
| 1:H:342:LYS:O | 1:H:365:ILE:HG23 | 2.21 | 0.41 |
| 1:H:120:VAL:HG22 | 1:H:382:TYR:HB2 | 2.02 | 0.41 |
| 1:I:233:MET:CE | 1:I:343:ILE:HD11 | 2.49 | 0.41 |
| 1:I:389:LEU:O | 1:I:391:HIS:HD2 | 2.04 | 0.41 |
| 1:I:435:GLU:O | 1:I:438:ASP:N | 2.52 | 0.41 |
| 1:J:193:ASN:O | 1:J:195:HIS:N | 2.54 | 0.41 |
| 1:J:290:GLU:O | 1:J:291:LEU:C | 2.59 | 0.41 |
| 1:J:337:PRO:HA | 1:J:363:ARG:NH2 | 2.35 | 0.41 |
| 1:I:397:LEU:HD13 | 1:K:394:TYR:CE2 | 2.55 | 0.41 |
| 1:L:294:PHE:CA | 1:L:297:GLN:NE2 | 2.77 | 0.41 |
| 1:L:34:THR:HG22 | 1:L:34:THR:O | 2.21 | 0.41 |
| 1:L:463:GLN:O | 1:L:467:THR:HB | 2.21 | 0.41 |
| 1:A:412:SER:O | 1:A:413:VAL:O | 2.39 | 0.41 |
| 1:B:95:TYR:CZ | 1:B:145:THR:HG22 | 2.45 | 0.41 |
| 1:B:150:MET:SD | 1:B:186:THR:HG21 | 2.61 | 0.41 |
| 1:B:307:ALA:O | 1:B:308:LYS:HB2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:75:ILE:HD12 | 1:B:75:ILE:N | 2.36 | 0.41 |
| 1:C:280:ILE:CG2 | 1:C:281:TRP:N | 2.81 | 0.41 |
| 1:D:141:LEU:HD23 | 1:D:141:LEU:HA | 1.70 | 0.41 |
| 1:D:227:ILE:O | 1:D:227:ILE:HG23 | 2.21 | 0.41 |
| 1:D:67:ARG:O | 1:D:68:ASP:C | 2.58 | 0.41 |
| 1:E:105:LYS:HB3 | 1:E:105:LYS:HE2 | 1.55 | 0.41 |
| 1:F:386:LEU:HD12 | 1:F:394:TYR:OH | 2.21 | 0.41 |
| 1:F:497:GLY:HA3 | 1:F:500:PHE:O | 2.20 | 0.41 |
| 1:G:85:GLN:N | 1:G:85:GLN:HE21 | 2.18 | 0.41 |
| 1:H:113:TYR:O | 1:H:114:LYS:C | 2.59 | 0.41 |
| 1:H:137:THR:H | 1:H:137:THR:HG22 | 1.58 | 0.41 |
| 1:H:193:ASN:O | 1:H:194:ALA:C | 2.56 | 0.41 |
| 1:H:29:VAL:HB | 1:H:30:GLU:H | 1.43 | 0.41 |
| 1:H:346:GLU:OE1 | 1:H:478:ARG:NH2 | 2.49 | 0.41 |
| 1:H:369:PRO:CG | 1:H:478:ARG:HA | 2.51 | 0.41 |
| 1:I:148:PHE:CE2 | 1:I:152:LEU:HD22 | 2.56 | 0.41 |
| 1:I:189:HIS:HD2 | 1:I:190:TYR:CE1 | 2.39 | 0.41 |
| 1:I:228:ASN:HA | 1:I:228:ASN:HD22 | 1.71 | 0.41 |
| 1:I:247:PHE:CZ | 1:I:260:MET:HG3 | 2.56 | 0.41 |
| 1:I:263:LEU:HD12 | 1:I:263:LEU:HA | 1.93 | 0.41 |
| 1:I:282:ASN:C | 1:I:282:ASN:OD1 | 2.58 | 0.41 |
| 1:J:369:PRO:CG | 1:J:478:ARG:HA | 2.51 | 0.41 |
| 1:J:417:LEU:HD12 | 1:J:417:LEU:HA | 1.79 | 0.41 |
| 1:J:442:GLY:O | 1:J:443:ALA:C | 2.59 | 0.41 |
| 1:K:212:ILE:HD12 | 1:K:212:ILE:N | 2.36 | 0.41 |
| 1:I:396:ARG:HH21 | 1:K:456:THR:HG23 | 1.86 | 0.41 |
| 1:I:57:HIS:HE1 | 1:L:151:GLU:OE1 | 2.04 | 0.41 |
| 1:A:119:ASP:OD2 | 1:A:459:ARG:NH1 | 2.43 | 0.41 |
| 1:B:501:THR:OXT | 1:B:501:THR:HG23 | 2.21 | 0.41 |
| 1:C:346:GLU:OE1 | 1:C:367:VAL:HG12 | 2.21 | 0.41 |
| 1:C:439:ARG:NH2 | 1:D:405:SER:CB | 2.84 | 0.41 |
| 1:B:189:HIS:CE1 | 1:E:154:LYS:HD3 | 2.55 | 0.41 |
| 1:E:86:ARG:HG2 | 1:E:121:PRO:C | 2.41 | 0.41 |
| 1:F:335:ASN:ND2 | 1:F:335:ASN:N | 2.69 | 0.41 |
| 1:G:294:PHE:O | 1:G:295:LYS:C | 2.59 | 0.41 |
| 1:G:250:GLN:CB | 1:G:314:ILE:HD11 | 2.51 | 0.41 |
| 1:G:355:GLU:O | 1:G:359:ILE:HG13 | 2.21 | 0.41 |
| 1:H:280:ILE:CD1 | 1:H:301:ILE:HD12 | 2.45 | 0.41 |
| 1:H:370:ASP:O | 1:H:372:TYR:N | 2.54 | 0.41 |
| 1:I:335:ASN:O | 1:I:339:VAL:HG13 | 2.21 | 0.41 |
| 1:I:353:THR:HB | 1:I:354:PRO:HD2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:9:PHE:CE1 | 1:J:103:GLU:HG3 | 2.56 | 0.41 |
| 1:J:188:GLY:O | 1:J:189:HIS:C | 2.59 | 0.41 |
| 1:J:335:ASN:ND2 | 1:J:335:ASN:C | 2.73 | 0.41 |
| 1:J:394:TYR:HB2 | 1:J:445:GLU:HG3 | 2.02 | 0.41 |
| 1:K:256:GLY:O | 1:K:257:LEU:C | 2.58 | 0.41 |
| 1:K:416:SER:CA | 1:K:419:ARG:NH2 | 2.83 | 0.41 |
| 1:L:247:PHE:CZ | 1:L:260:MET:HA | 2.56 | 0.41 |
| 1:L:280:ILE:HG22 | 1:L:281:TRP:N | 2.36 | 0.41 |
| 1:A:176:MET:HE3 | 1:A:179:ILE:HD12 | 2.02 | 0.41 |
| 1:A:331:LEU:HD22 | 1:A:344:ILE:HD13 | 2.02 | 0.41 |
| 1:B:90:LYS:HD3 | 1:B:122:PHE:CD1 | 2.56 | 0.41 |
| 1:B:188:GLY:O | 1:B:190:TYR:N | 2.54 | 0.41 |
| 1:B:200:GLY:H | 1:B:384:GLU:CD | 2.24 | 0.41 |
| 1:B:254:ASN:O | 1:B:255:VAL:C | 2.60 | 0.41 |
| 1:D:142:GLU:O | 1:D:143:LYS:C | 2.59 | 0.41 |
| 1:D:501:THR:OXT | 1:E:181:ASP:OD1 | 2.38 | 0.41 |
| 1:E:32:LEU:O | 1:E:33:ARG:HB3 | 2.21 | 0.41 |
| 1:F:29:VAL:O | 1:F:33:ARG:CG | 2.68 | 0.41 |
| 1:F:346:GLU:OE1 | 1:F:370:ASP:N | 2.49 | 0.41 |
| 1:G:48:ILE:O | 1:G:51:ILE:HB | 2.21 | 0.41 |
| 1:H:357:ASP:O | 1:H:358:LYS:C | 2.59 | 0.41 |
| 1:H:382:TYR:O | 1:H:386:LEU:HG | 2.21 | 0.41 |
| 1:I:248:VAL:HG22 | 1:I:271:ILE:HG22 | 2.02 | 0.41 |
| 1:I:397:LEU:HD21 | 1:K:383:PHE:CE1 | 2.55 | 0.41 |
| 1:I:410:LEU:CD2 | 1:J:409:LEU:HD11 | 2.49 | 0.41 |
| 1:I:412:SER:OG | 1:K:433:THR:HG23 | 2.20 | 0.41 |
| 1:I:495:GLU:O | 1:I:496:ALA:CB | 2.67 | 0.41 |
| 1:J:174:ARG:HG3 | 1:J:175:GLU:N | 2.35 | 0.41 |
| 1:J:371:LEU:HD22 | 1:J:482:TYR:CE2 | 2.55 | 0.41 |
| 1:K:232:TYR:CD1 | 1:K:232:TYR:N | 2.89 | 0.41 |
| 1:K:463:GLN:O | 1:K:467:THR:HB | 2.21 | 0.41 |
| 1:K:90:LYS:HD3 | 1:K:122:PHE:CE1 | 2.56 | 0.41 |
| 1:L:374:ASN:O | 1:L:374:ASN:CG | 2.59 | 0.41 |
| 1:L:429:PRO:C | 1:L:431:VAL:N | 2.73 | 0.41 |
| 1:L:48:ILE:HG21 | 1:L:490:PHE:CD1 | 2.55 | 0.41 |
| 1:A:214:ALA:CB | 1:A:380:VAL:HG21 | 2.51 | 0.40 |
| 1:A:79:ARG:NH2 | 1:A:91:GLY:O | 2.53 | 0.40 |
| 1:C:431:VAL:HA | 1:C:432:PRO:HD3 | 1.86 | 0.40 |
| 1:D:16:PHE:HD1 | 1:D:482:TYR:CZ | 2.39 | 0.40 |
| 1:E:45:VAL:C | 1:E:47:GLY:H | 2.25 | 0.40 |
| 1:F:82:HIS:HD2 | 1:F:112:THR:OG1 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:27:LYS:O | 1:F:32:LEU:HD12 | 2.20 | 0.40 |
| 1:G:111:MET:CE | 1:G:378:VAL:HG21 | 2.51 | 0.40 |
| 1:H:163:ASP:O | 1:H:165:PRO:HD3 | 2.21 | 0.40 |
| 1:H:257:LEU:O | 1:H:260:MET:N | 2.54 | 0.40 |
| 1:H:279:SER:C | 1:H:280:ILE:HG13 | 2.42 | 0.40 |
| 1:H:85:GLN:HE21 | 1:H:85:GLN:HB3 | 1.39 | 0.40 |
| 1:I:131:ILE:CD1 | 1:I:144:ILE:HD13 | 2.51 | 0.40 |
| 1:I:198:VAL:O | 1:I:201:LYS:HE3 | 2.21 | 0.40 |
| 1:I:346:GLU:HG2 | 1:I:351:PRO:HG2 | 2.03 | 0.40 |
| 1:I:475:LEU:O | 1:I:477:LEU:HD22 | 2.22 | 0.40 |
| 1:J:126:LYS:HG3 | 1:J:127:ALA:N | 2.36 | 0.40 |
| 1:J:186:THR:HB | 1:J:187:ILE:H | 1.34 | 0.40 |
| 1:J:240:PRO:HD2 | 1:J:244:ASP:O | 2.21 | 0.40 |
| 1:J:319:CYS:O | 1:J:341:ALA:HA | 2.21 | 0.40 |
| 1:J:358:LYS:O | 1:J:362:GLU:CG | 2.68 | 0.40 |
| 1:J:9:PHE:HA | 1:J:12:MET:HE2 | 2.03 | 0.40 |
| 1:K:82:HIS:N | 1:K:124:GLY:O | 2.48 | 0.40 |
| 1:K:142:GLU:O | 1:K:143:LYS:C | 2.58 | 0.40 |
| 1:K:233:MET:CE | 1:K:236:LEU:HD12 | 2.51 | 0.40 |
| 1:I:392:VAL:HG11 | 1:K:386:LEU:HD11 | 2.03 | 0.40 |
| 1:K:414:GLN:OE1 | 1:K:428:ILE:HA | 2.21 | 0.40 |
| 1:K:414:GLN:HG3 | 1:K:427:THR:O | 2.21 | 0.40 |
| 1:K:500:PHE:HE1 | 1:L:500:PHE:CZ | 2.33 | 0.40 |
| 1:G:61:LEU:HA | 1:K:56:ASN:O | 2.21 | 0.40 |
| 1:L:220:PHE:C | 1:L:220:PHE:CD1 | 2.94 | 0.40 |
| 1:L:247:PHE:CZ | 1:L:260:MET:HG3 | 2.47 | 0.40 |
| 1:A:114:LYS:CE | 1:A:374:ASN:HD21 | 2.33 | 0.40 |
| 1:A:93:ILE:O | 1:A:168:ASP:HB3 | 2.22 | 0.40 |
| 1:A:233:MET:HA | 1:A:233:MET:HE1 | 2.04 | 0.40 |
| 1:A:243:GLY:O | 1:A:245:LYS:N | 2.54 | 0.40 |
| 1:A:346:GLU:OE1 | 1:A:369:PRO:HA | 2.21 | 0.40 |
| 1:A:374:ASN:ND2 | 1:A:374:ASN:C | 2.73 | 0.40 |
| 1:C:164:VAL:HG22 | 1:C:196:ALA:O | 2.21 | 0.40 |
| 1:D:264:HIS:O | 1:D:266:PHE:N | 2.54 | 0.40 |
| 1:D:332:THR:O | 1:D:336:ALA:HB2 | 2.20 | 0.40 |
| 1:E:145:THR:OG1 | 1:E:146:ARG:N | 2.54 | 0.40 |
| 1:E:166:ALA:CA | 1:E:176:MET:HE2 | 2.50 | 0.40 |
| 1:E:335:ASN:O | 1:E:336:ALA:C | 2.58 | 0.40 |
| 1:F:73:GLU:OE1 | 1:F:136:TYR:OH | 2.39 | 0.40 |
| 1:G:167:PRO:HG3 | 1:G:176:MET:CG | 2.47 | 0.40 |
| 1:G:17:PHE:CE2 | 1:G:53:LYS:CB | 3.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:234:SER:O | 1:G:237:GLY:N | 2.54 | 0.40 |
| 1:G:9:PHE:HA | 1:G:12:MET:HE3 | 2.02 | 0.40 |
| 1:H:80:ALA:O | 1:H:125:ALA:HA | 2.20 | 0.40 |
| 1:H:300:SER:C | 1:H:302:LEU:H | 2.25 | 0.40 |
| 1:I:90:LYS:HD2 | 1:I:164:VAL:HB | 2.03 | 0.40 |
| 1:I:238:MET:C | 1:I:240:PRO:CD | 2.89 | 0.40 |
| 1:I:497:GLY:N | 1:I:501:THR:HA | 2.35 | 0.40 |
| 1:J:90:LYS:NZ | 1:J:199:THR:HG23 | 2.27 | 0.40 |
| 1:J:244:ASP:O | 1:J:245:LYS:HG3 | 2.21 | 0.40 |
| 1:J:30:GLU:CA | 1:J:34:THR:HG23 | 2.45 | 0.40 |
| 1:J:496:ALA:HB1 | 1:J:501:THR:O | 2.21 | 0.40 |
| 1:A:272:ALA:HB1 | 1:A:314:ILE:CG2 | 2.51 | 0.40 |
| 1:A:272:ALA:HB1 | 1:A:314:ILE:HG21 | 2.04 | 0.40 |
| 1:A:275:GLU:HB3 | 1:A:276:SER:H | 1.69 | 0.40 |
| 1:A:370:ASP:C | 1:A:372:TYR:H | 2.23 | 0.40 |
| 1:A:423:LYS:NZ | 1:A:426:GLY:CA | 2.84 | 0.40 |
| 1:A:68:ASP:O | 1:A:69:ASP:C | 2.60 | 0.40 |
| 1:A:501:THR:HG21 | 1:B:181:ASP:OD1 | 2.21 | 0.40 |
| 1:B:250:GLN:HA | 1:B:314:ILE:HD11 | 2.03 | 0.40 |
| 1:B:250:GLN:CB | 1:B:314:ILE:HD11 | 2.51 | 0.40 |
| 1:B:332:THR:HB | 1:B:333:LYS:H | 1.66 | 0.40 |
| 1:A:455:TYR:HB2 | 1:B:400:LYS:HB2 | 2.03 | 0.40 |
| 1:C:82:HIS:CB | 1:C:112:THR:HG21 | 2.50 | 0.40 |
| 1:C:201:LYS:HZ1 | 1:C:388:ASN:ND2 | 2.18 | 0.40 |
| 1:C:435:GLU:O | 1:C:436:PHE:C | 2.60 | 0.40 |
| 1:D:163:ASP:O | 1:D:165:PRO:HD3 | 2.22 | 0.40 |
| 1:D:255:VAL:O | 1:D:256:GLY:C | 2.57 | 0.40 |
| 1:C:383:PHE:CE2 | 1:D:397:LEU:HD11 | 2.56 | 0.40 |
| 1:D:409:LEU:HA | 1:D:409:LEU:HD22 | 1.89 | 0.40 |
| 1:D:87:THR:HG22 | 1:D:88:PRO:HG3 | 2.04 | 0.40 |
| 1:E:40:GLN:C | 1:E:42:ARG:H | 2.21 | 0.40 |
| 1:E:492:VAL:CG2 | 2:E:5:ADP:C2 | 3.05 | 0.40 |
| 1:E:496:ALA:O | 1:E:501:THR:O | 2.39 | 0.40 |
| 1:E:78:TYR:OH | 1:E:130:LYS:CE | 2.69 | 0.40 |
| 1:F:315:LEU:H | 1:F:315:LEU:CD1 | 2.31 | 0.40 |
| 1:F:323:ILE:HD13 | 1:F:323:ILE:HG21 | 1.79 | 0.40 |
| 1:F:328:GLU:HB2 | 1:F:329:LYS:HZ3 | 1.85 | 0.40 |
| 1:F:476:ASP:OD2 | 1:F:479:THR:OG1 | 2.22 | 0.40 |
| 1:G:287:ASP:HB3 | 1:G:290:GLU:HG3 | 2.03 | 0.40 |
| 1:G:117:VAL:HG21 | 1:G:371:LEU:HG | 2.03 | 0.40 |
| 1:H:470:LYS:C | 1:H:472:ASN:H | 2.25 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:167:PRO:CD | 1:I:176:MET:SD | 3.09 | 0.40 |
| 1:I:52:ILE:O | 1:I:82:HIS:CE1 | 2.75 | 0.40 |
| 1:J:162:ILE:HG22 | 1:J:163:ASP:N | 2.35 | 0.40 |
| 1:J:220:PHE:C | 1:J:220:PHE:CD1 | 2.93 | 0.40 |
| 1:J:84:HIS:O | 1:J:85:GLN:C | 2.60 | 0.40 |
| 1:J:90:LYS:HD3 | 1:J:122:PHE:CE1 | 2.55 | 0.40 |
| 1:K:86:ARG:HG2 | 1:K:121:PRO:C | 2.41 | 0.40 |
| 1:K:213:SER:O | 1:K:214:ALA:C | 2.60 | 0.40 |
| 1:K:290:GLU:HB3 | 1:K:304:PHE:HZ | 1.86 | 0.40 |
| 1:K:368:ILE:HA | 1:K:369:PRO:HD3 | 1.51 | 0.40 |
| 1:K:478:ARG:O | 1:K:481:ALA:N | 2.39 | 0.40 |
| 1:L:301:ILE:H | 1:L:301:ILE:HG13 | 1.74 | 0.40 |
| 1:L:279:SER:HB2 | 1:L:310:TYR:O | 2.22 | 0.40 |
| 1:L:323:ILE:O | 1:L:323:ILE:HG22 | 2.22 | 0.40 |
| 1:A:109:SER:O | 1:A:113:TYR:CD2 | 2.74 | 0.40 |
| 1:A:359:ILE:O | 1:A:361:LEU:N | 2.55 | 0.40 |
| 1:A:117:VAL:HG21 | 1:A:371:LEU:HG | 2.03 | 0.40 |
| 1:A:387:LYS:HE3 | 1:A:393:SER:HA | 2.03 | 0.40 |
| 1:A:432:PRO:HB3 | 1:A:436:PHE:CD1 | 2.56 | 0.40 |
| 1:B:467:THR:O | 1:B:468:ALA:C | 2.59 | 0.40 |
| 1:C:313:SER:O | 1:C:316:GLU:OE2 | 2.40 | 0.40 |
| 1:C:465:MET:O | 1:C:466:ARG:C | 2.58 | 0.40 |
| 1:D:96:SER:HA | 1:D:131:ILE:O | 2.21 | 0.40 |
| 1:D:366:MET:CA | 1:D:475:LEU:HD23 | 2.52 | 0.40 |
| 1:E:464:ILE:HG22 | 1:E:465:MET:N | 2.36 | 0.40 |
| 1:F:230:ALA:O | 1:F:231:SER:C | 2.58 | 0.40 |
| 1:F:45:VAL:C | 1:F:47:GLY:N | 2.74 | 0.40 |
| 1:G:174:ARG:HG3 | 1:G:175:GLU:H | 1.86 | 0.40 |
| 1:G:315:LEU:CD2 | 1:G:331:LEU:HD23 | 2.51 | 0.40 |
| 1:G:67:ARG:NH1 | 1:G:140:GLU:OE2 | 2.54 | 0.40 |
| 1:G:8:ASN:O | 1:G:9:PHE:C | 2.59 | 0.40 |
| 1:H:23:ILE:H | 1:H:23:ILE:HG13 | 1.67 | 0.40 |
| 1:H:250:GLN:HG2 | 1:H:314:ILE:CD1 | 2.44 | 0.40 |
| 1:H:294:PHE:C | 1:H:298:HIS:CE1 | 2.95 | 0.40 |
| 1:H:382:TYR:O | 1:H:385:TRP:HB3 | 2.21 | 0.40 |
| 1:H:382:TYR:HE1 | 1:H:386:LEU:HD11 | 1.76 | 0.40 |
| 1:H:42:ARG:C | 1:H:44:ARG:N | 2.75 | 0.40 |
| 1:H:462:ARG:CG | 1:H:462:ARG:HH11 | 2.35 | 0.40 |
| 1:H:67:ARG:NH2 | 1:H:136:TYR:CD1 | 2.90 | 0.40 |
| 1:H:91:GLY:O | 1:H:165:PRO:HA | 2.22 | 0.40 |
| 1:J:113:TYR:O | 1:J:117:VAL:HG23 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:65:ILE:CD1 | 1:L:144:ILE:HG13 | 2.35 | 0.40 |
| 1:L:226:PHE:CE2 | 1:L:465:MET:CE | 3.05 | 0.40 |
| 1:L:239:THR:H | 1:L:240:PRO:HD3 | 1.73 | 0.40 |
| 1:L:400:LYS:O | 1:L:403:ARG:HB3 | 2.20 | 0.40 |
| 1:A:176:MET:HE1 | 1:A:179:ILE:HD12 | 2.02 | 0.40 |
| 1:B:120:VAL:HG12 | 1:B:122:PHE:CD1 | 2.56 | 0.40 |
| 1:B:126:LYS:HD2 | 1:B:126:LYS:HA | 1.91 | 0.40 |
| 1:C:315:LEU:CD2 | 1:C:322:LEU:HD11 | 2.50 | 0.40 |
| 1:C:322:LEU:HD12 | 1:C:344:ILE:HG23 | 2.04 | 0.40 |
| 1:D:16:PHE:CD2 | 1:D:16:PHE:N | 2.90 | 0.40 |
| 1:D:208:ILE:HG13 | 1:D:445:GLU:OE1 | 2.21 | 0.40 |
| 1:D:294:PHE:CG | 1:D:304:PHE:HD1 | 2.40 | 0.40 |
| 1:D:328:GLU:O | 1:D:329:LYS:HG2 | 2.21 | 0.40 |
| 1:D:383:PHE:N | 1:D:383:PHE:CD2 | 2.89 | 0.40 |
| 1:E:94:ARG:O | 1:E:128:GLY:HA2 | 2.22 | 0.40 |
| 1:E:296:LEU:HD13 | 1:E:296:LEU:HA | 1.86 | 0.40 |
| 1:E:414:GLN:HA | 1:E:429:PRO:HG2 | 2.03 | 0.40 |
| 1:E:52:ILE:O | 1:E:82:HIS:HE1 | 2.04 | 0.40 |
| 1:F:431:VAL:HA | 1:F:432:PRO:HD3 | 1.99 | 0.40 |
| 1:F:53:LYS:N | 1:F:54:PRO:CD | 2.85 | 0.40 |
| 1:G:248:VAL:O | 1:G:323:ILE:HG13 | 2.22 | 0.40 |
| 1:G:87:THR:CB | 1:G:88:PRO:CD | 2.98 | 0.40 |
| 1:H:371:LEU:HD23 | 1:H:481:ALA:CB | 2.52 | 0.40 |
| 1:I:319:CYS:O | 1:I:341:ALA:HA | 2.21 | 0.40 |
| 1:I:346:GLU:OE2 | 1:I:478:ARG:NH2 | 2.51 | 0.40 |
| 1:J:10:PHE:O | 1:J:11:LYS:C | 2.60 | 0.40 |
| 1:K:240:PRO:HD2 | 1:K:244:ASP:O | 2.22 | 0.40 |
| 1:K:383:PHE:N | 1:K:383:PHE:CD2 | 2.87 | 0.40 |
| 1:G:151:GLU:HB3 | 1:K:57:HIS:HE1 | 1.85 | 0.40 |
| 1:L:247:PHE:HE2 | 1:L:249:VAL:HG12 | 1.79 | 0.40 |
| 1:L:217:ARG:HG2 | 1:L:262:TYR:CZ | 2.57 | 0.40 |
| 1:L:33:ARG:CZ | 1:L:33:ARG:CB | 2.99 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 | 494/496 (100%) | 341 (69%) | 109 (22%) | 44 (9%) | 1 | 9 |
| 1 | B | 494/496 (100%) | 359 (73%) | 94 (19%) | 41 (8%) | 1 | 10 |
| 1 | C | 494/496 (100%) | 351 (71%) | 82 (17%) | 61 (12%) | 0 | 5 |
| 1 | D | 494/496 (100%) | 344 (70%) | 105 (21%) | 45 (9%) | 1 | 8 |
| 1 | E | 494/496 (100%) | 352 (71%) | 100 (20%) | 42 (8%) | 1 | 10 |
| 1 | F | 494/496 (100%) | 378 (76%) | 85 (17%) | 31 (6%) | 1 | 16 |
| 1 | G | 494/496 (100%) | 362 (73%) | 94 (19%) | 38 (8%) | 1 | 11 |
| 1 | H | 494/496 (100%) | 341 (69%) | 116 (24%) | 37 (8%) | 1 | 12 |
| 1 | I | 494/496 (100%) | 355 (72%) | 89 (18%) | 50 (10%) | 0 | 7 |
| 1 | J | 494/496 (100%) | 353 (72%) | 99 (20%) | 42 (8%) | 1 | 10 |
| 1 | K | 494/496 (100%) | 328 (66%) | 113 (23%) | 53 (11%) | 0 | 6 |
| 1 | L | 494/496 (100%) | 347 (70%) | 102 (21%) | 45 (9%) | 1 | 8 |
| All | All | 5928/5952 (100%) | 4211 (71%) | 1188 (20%) | 529 (9%) | 1 | 9 |

All (529) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | PHE |
| 1 | A | 25 | GLU |
| 1 | A | 26 | ASP |
| 1 | A | 30 | GLU |
| 1 | A | 33 | ARG |
| 1 | A | 40 | GLN |
| 1 | A | 158 | ILE |
| 1 | A | 240 | PRO |
| 1 | A | 314 | ILE |
| 1 | A | 430 | ILE |
| 1 | A | 496 | ALA |
| 1 | A | 498 | VAL |
| 1 | B | 30 | GLU |
| 1 | B | 33 | ARG |
| 1 | B | 37 | SER |
| 1 | B | 39 | GLU |
| 1 | B | 87 | THR |
| 1 | B | 255 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 283 | PRO |
| 1 | B | 334 | SER |
| 1 | B | 364 | ASN |
| 1 | B | 396 | ARG |
| 1 | B | 430 | ILE |
| 1 | B | 496 | ALA |
| 1 | B | 498 | VAL |
| 1 | C | 9 | PHE |
| 1 | C | 25 | GLU |
| 1 | C | 29 | VAL |
| 1 | C | 33 | ARG |
| 1 | C | 37 | SER |
| 1 | C | 169 | MET |
| 1 | C | 244 | ASP |
| 1 | C | 265 | ARG |
| 1 | C | 272 | ALA |
| 1 | C | 275 | GLU |
| 1 | C | 281 | TRP |
| 1 | C | 282 | ASN |
| 1 | C | 301 | ILE |
| 1 | C | 326 | ALA |
| 1 | C | 334 | SER |
| 1 | C | 371 | LEU |
| 1 | C | 421 | PHE |
| 1 | C | 430 | ILE |
| 1 | C | 498 | VAL |
| 1 | D | 99 | VAL |
| 1 | D | 100 | SER |
| 1 | D | 275 | GLU |
| 1 | D | 282 | ASN |
| 1 | D | 317 | ALA |
| 1 | D | 334 | SER |
| 1 | D | 364 | ASN |
| 1 | D | 399 | PHE |
| 1 | D | 430 | ILE |
| 1 | E | 7 | PRO |
| 1 | E | 9 | PHE |
| 1 | E | 26 | ASP |
| 1 | E | 214 | ALA |
| 1 | E | 329 | LYS |
| 1 | E | 421 | PHE |
| 1 | E | 423 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 430 | ILE |
| 1 | E | 472 | ASN |
| 1 | F | 9 | PHE |
| 1 | F | 30 | GLU |
| 1 | F | 33 | ARG |
| 1 | F | 87 | THR |
| 1 | F | 158 | ILE |
| 1 | F | 214 | ALA |
| 1 | F | 329 | LYS |
| 1 | F | 334 | SER |
| 1 | F | 421 | PHE |
| 1 | F | 430 | ILE |
| 1 | F | 496 | ALA |
| 1 | G | 30 | GLU |
| 1 | G | 31 | ASP |
| 1 | G | 33 | ARG |
| 1 | G | 40 | GLN |
| 1 | G | 130 | LYS |
| 1 | G | 282 | ASN |
| 1 | G | 306 | LYS |
| 1 | G | 327 | SER |
| 1 | G | 399 | PHE |
| 1 | G | 420 | LYS |
| 1 | G | 430 | ILE |
| 1 | G | 472 | ASN |
| 1 | G | 496 | ALA |
| 1 | H | 30 | GLU |
| 1 | H | 31 | ASP |
| 1 | H | 268 | ALA |
| 1 | H | 275 | GLU |
| 1 | H | 317 | ALA |
| 1 | H | 329 | LYS |
| 1 | H | 334 | SER |
| 1 | H | 430 | ILE |
| 1 | I | 33 | ARG |
| 1 | I | 37 | SER |
| 1 | I | 40 | GLN |
| 1 | I | 87 | THR |
| 1 | I | 97 | THR |
| 1 | I | 230 | ALA |
| 1 | I | 240 | PRO |
| 1 | I | 244 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 252 | PHE |
| 1 | I | 306 | LYS |
| 1 | I | 327 | SER |
| 1 | I | 329 | LYS |
| 1 | I | 346 | GLU |
| 1 | I | 478 | ARG |
| 1 | I | 479 | THR |
| 1 | I | 496 | ALA |
| 1 | J | 30 | GLU |
| 1 | J | 31 | ASP |
| 1 | J | 33 | ARG |
| 1 | J | 34 | THR |
| 1 | J | 39 | GLU |
| 1 | J | 244 | ASP |
| 1 | J | 430 | ILE |
| 1 | K | 25 | GLU |
| 1 | K | 30 | GLU |
| 1 | K | 39 | GLU |
| 1 | K | 87 | THR |
| 1 | K | 97 | THR |
| 1 | K | 169 | MET |
| 1 | K | 214 | ALA |
| 1 | K | 220 | PHE |
| 1 | K | 227 | ILE |
| 1 | K | 231 | SER |
| 1 | K | 244 | ASP |
| 1 | K | 253 | GLY |
| 1 | K | 265 | ARG |
| 1 | K | 327 | SER |
| 1 | K | 334 | SER |
| 1 | K | 399 | PHE |
| 1 | K | 421 | PHE |
| 1 | K | 498 | VAL |
| 1 | L | 9 | PHE |
| 1 | L | 25 | GLU |
| 1 | L | 30 | GLU |
| 1 | L | 33 | ARG |
| 1 | L | 87 | THR |
| 1 | L | 165 | PRO |
| 1 | L | 275 | GLU |
| 1 | L | 317 | ALA |
| 1 | L | 327 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 334 | SER |
| 1 | L | 338 | ARG |
| 1 | L | 346 | GLU |
| 1 | L | 430 | ILE |
| 1 | L | 465 | MET |
| 1 | L | 472 | ASN |
| 1 | L | 498 | VAL |
| 1 | A | 169 | MET |
| 1 | A | 244 | ASP |
| 1 | A | 255 | VAL |
| 1 | A | 268 | ALA |
| 1 | A | 299 | GLY |
| 1 | A | 329 | LYS |
| 1 | A | 334 | SER |
| 1 | A | 364 | ASN |
| 1 | A | 369 | PRO |
| 1 | B | 25 | GLU |
| 1 | B | 143 | LYS |
| 1 | B | 268 | ALA |
| 1 | B | 299 | GLY |
| 1 | B | 398 | THR |
| 1 | B | 421 | PHE |
| 1 | C | 87 | THR |
| 1 | C | 134 | LYS |
| 1 | C | 219 | VAL |
| 1 | C | 220 | PHE |
| 1 | C | 231 | SER |
| 1 | C | 254 | ASN |
| 1 | C | 329 | LYS |
| 1 | C | 389 | LEU |
| 1 | C | 414 | GLN |
| 1 | C | 422 | GLY |
| 1 | C | 458 | GLU |
| 1 | C | 478 | ARG |
| 1 | C | 496 | ALA |
| 1 | D | 33 | ARG |
| 1 | D | 82 | HIS |
| 1 | D | 119 | ASP |
| 1 | D | 144 | ILE |
| 1 | D | 231 | SER |
| 1 | D | 265 | ARG |
| 1 | D | 297 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 326 | ALA |
| 1 | D | 421 | PHE |
| 1 | D | 472 | ASN |
| 1 | D | 495 | GLU |
| 1 | E | 27 | LYS |
| 1 | E | 33 | ARG |
| 1 | E | 36 | GLU |
| 1 | E | 130 | LYS |
| 1 | E | 222 | GLY |
| 1 | E | 223 | ILE |
| 1 | E | 283 | PRO |
| 1 | E | 334 | SER |
| 1 | E | 360 | PHE |
| 1 | E | 371 | LEU |
| 1 | E | 420 | LYS |
| 1 | E | 422 | GLY |
| 1 | E | 495 | GLU |
| 1 | F | 387 | LYS |
| 1 | F | 422 | GLY |
| 1 | F | 498 | VAL |
| 1 | G | 184 | ALA |
| 1 | G | 192 | ILE |
| 1 | G | 231 | SER |
| 1 | G | 244 | ASP |
| 1 | G | 294 | PHE |
| 1 | G | 301 | ILE |
| 1 | H | 29 | VAL |
| 1 | H | 130 | LYS |
| 1 | H | 301 | ILE |
| 1 | H | 328 | GLU |
| 1 | H | 371 | LEU |
| 1 | H | 495 | GLU |
| 1 | H | 498 | VAL |
| 1 | I | 25 | GLU |
| 1 | I | 219 | VAL |
| 1 | I | 265 | ARG |
| 1 | I | 297 | GLN |
| 1 | I | 328 | GLU |
| 1 | I | 341 | ALA |
| 1 | I | 364 | ASN |
| 1 | I | 421 | PHE |
| 1 | J | 28 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 40 | GLN |
| 1 | J | 68 | ASP |
| 1 | J | 182 | THR |
| 1 | J | 319 | CYS |
| 1 | J | 364 | ASN |
| 1 | J | 405 | SER |
| 1 | J | 496 | ALA |
| 1 | K | 33 | ARG |
| 1 | K | 40 | GLN |
| 1 | K | 299 | GLY |
| 1 | K | 314 | ILE |
| 1 | K | 319 | CYS |
| 1 | K | 371 | LEU |
| 1 | K | 381 | SER |
| 1 | K | 422 | GLY |
| 1 | K | 467 | THR |
| 1 | K | 472 | ASN |
| 1 | K | 478 | ARG |
| 1 | K | 492 | VAL |
| 1 | L | 224 | GLU |
| 1 | L | 227 | ILE |
| 1 | L | 230 | ALA |
| 1 | L | 235 | ILE |
| 1 | L | 299 | GLY |
| 1 | L | 396 | ARG |
| 1 | L | 422 | GLY |
| 1 | A | 23 | ILE |
| 1 | A | 371 | LEU |
| 1 | A | 421 | PHE |
| 1 | A | 434 | ALA |
| 1 | A | 465 | MET |
| 1 | A | 478 | ARG |
| 1 | A | 491 | LYS |
| 1 | B | 85 | GLN |
| 1 | B | 109 | SER |
| 1 | B | 142 | GLU |
| 1 | B | 181 | ASP |
| 1 | B | 189 | HIS |
| 1 | B | 244 | ASP |
| 1 | B | 254 | ASN |
| 1 | B | 265 | ARG |
| 1 | B | 326 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 329 | LYS |
| 1 | C | 68 | ASP |
| 1 | C | 71 | SER |
| 1 | C | 121 | PRO |
| 1 | C | 240 | PRO |
| 1 | C | 320 | ASP |
| 1 | C | 351 | PRO |
| 1 | C | 472 | ASN |
| 1 | D | 64 | PRO |
| 1 | D | 88 | PRO |
| 1 | D | 244 | ASP |
| 1 | D | 346 | GLU |
| 1 | D | 396 | ARG |
| 1 | D | 419 | ARG |
| 1 | D | 425 | GLY |
| 1 | D | 496 | ALA |
| 1 | E | 87 | THR |
| 1 | E | 224 | GLU |
| 1 | F | 244 | ASP |
| 1 | F | 317 | ALA |
| 1 | F | 319 | CYS |
| 1 | F | 327 | SER |
| 1 | F | 364 | ASN |
| 1 | F | 438 | ASP |
| 1 | F | 491 | LYS |
| 1 | G | 25 | GLU |
| 1 | G | 265 | ARG |
| 1 | G | 299 | GLY |
| 1 | G | 421 | PHE |
| 1 | H | 10 | PHE |
| 1 | H | 154 | LYS |
| 1 | H | 165 | PRO |
| 1 | H | 422 | GLY |
| 1 | I | 36 | GLU |
| 1 | I | 67 | ARG |
| 1 | I | 288 | PRO |
| 1 | I | 317 | ALA |
| 1 | I | 480 | ALA |
| 1 | I | 498 | VAL |
| 1 | J | 189 | HIS |
| 1 | J | 214 | ALA |
| 1 | J | 231 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 282 | ASN |
| 1 | J | 283 | PRO |
| 1 | J | 306 | LYS |
| 1 | J | 315 | LEU |
| 1 | J | 326 | ALA |
| 1 | J | 329 | LYS |
| 1 | J | 358 | LYS |
| 1 | J | 371 | LEU |
| 1 | J | 443 | ALA |
| 1 | K | 36 | GLU |
| 1 | K | 119 | ASP |
| 1 | K | 221 | HIS |
| 1 | K | 235 | ILE |
| 1 | K | 257 | LEU |
| 1 | K | 283 | PRO |
| 1 | K | 341 | ALA |
| 1 | K | 351 | PRO |
| 1 | K | 364 | ASN |
| 1 | K | 425 | GLY |
| 1 | K | 465 | MET |
| 1 | L | 37 | SER |
| 1 | L | 82 | HIS |
| 1 | L | 133 | PRO |
| 1 | L | 236 | LEU |
| 1 | L | 283 | PRO |
| 1 | L | 315 | LEU |
| 1 | L | 449 | VAL |
| 1 | L | 495 | GLU |
| 1 | A | 254 | ASN |
| 1 | A | 359 | ILE |
| 1 | A | 405 | SER |
| 1 | B | 130 | LYS |
| 1 | B | 235 | ILE |
| 1 | B | 282 | ASN |
| 1 | B | 308 | LYS |
| 1 | B | 371 | LEU |
| 1 | C | 26 | ASP |
| 1 | C | 214 | ALA |
| 1 | C | 336 | ALA |
| 1 | C | 354 | PRO |
| 1 | C | 396 | ARG |
| 1 | C | 459 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 465 | MET |
| 1 | D | 69 | ASP |
| 1 | D | 288 | PRO |
| 1 | D | 375 | ALA |
| 1 | D | 453 | LEU |
| 1 | D | 478 | ARG |
| 1 | E | 12 | MET |
| 1 | E | 25 | GLU |
| 1 | E | 39 | GLU |
| 1 | E | 180 | ALA |
| 1 | E | 268 | ALA |
| 1 | E | 282 | ASN |
| 1 | E | 394 | TYR |
| 1 | E | 425 | GLY |
| 1 | F | 16 | PHE |
| 1 | F | 25 | GLU |
| 1 | F | 181 | ASP |
| 1 | G | 9 | PHE |
| 1 | G | 154 | LYS |
| 1 | G | 193 | ASN |
| 1 | G | 295 | LYS |
| 1 | G | 305 | PRO |
| 1 | G | 326 | ALA |
| 1 | H | 33 | ARG |
| 1 | H | 85 | GLN |
| 1 | H | 214 | ALA |
| 1 | H | 244 | ASP |
| 1 | H | 254 | ASN |
| 1 | H | 288 | PRO |
| 1 | H | 326 | ALA |
| 1 | H | 471 | TYR |
| 1 | H | 486 | ILE |
| 1 | I | 214 | ALA |
| 1 | I | 257 | LEU |
| 1 | I | 326 | ALA |
| 1 | I | 433 | THR |
| 1 | J | 23 | ILE |
| 1 | J | 25 | GLU |
| 1 | J | 82 | HIS |
| 1 | J | 181 | ASP |
| 1 | J | 277 | ASP |
| 1 | J | 425 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 62 | SER |
| 1 | L | 31 | ASP |
| 1 | L | 130 | LYS |
| 1 | L | 214 | ALA |
| 1 | L | 244 | ASP |
| 1 | L | 261 | ARG |
| 1 | L | 282 | ASN |
| 1 | L | 496 | ALA |
| 1 | A | 22 | SER |
| 1 | A | 283 | PRO |
| 1 | A | 338 | ARG |
| 1 | A | 360 | PHE |
| 1 | A | 467 | THR |
| 1 | B | 256 | GLY |
| 1 | B | 449 | VAL |
| 1 | C | 233 | MET |
| 1 | C | 251 | GLY |
| 1 | C | 317 | ALA |
| 1 | C | 339 | VAL |
| 1 | C | 346 | GLU |
| 1 | C | 388 | ASN |
| 1 | C | 429 | PRO |
| 1 | D | 7 | PRO |
| 1 | D | 9 | PHE |
| 1 | D | 39 | GLU |
| 1 | D | 314 | ILE |
| 1 | D | 336 | ALA |
| 1 | E | 53 | LYS |
| 1 | E | 67 | ARG |
| 1 | E | 133 | PRO |
| 1 | F | 290 | GLU |
| 1 | F | 318 | ASP |
| 1 | F | 374 | ASN |
| 1 | F | 425 | GLY |
| 1 | F | 437 | GLN |
| 1 | G | 288 | PRO |
| 1 | G | 364 | ASN |
| 1 | G | 495 | GLU |
| 1 | G | 498 | VAL |
| 1 | H | 306 | LYS |
| 1 | H | 421 | PHE |
| 1 | H | 451 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 27 | LYS |
| 1 | I | 82 | HIS |
| 1 | I | 130 | LYS |
| 1 | I | 315 | LEU |
| 1 | J | 131 | ILE |
| 1 | J | 192 | ILE |
| 1 | J | 194 | ALA |
| 1 | J | 290 | GLU |
| 1 | J | 452 | GLY |
| 1 | K | 430 | ILE |
| 1 | L | 7 | PRO |
| 1 | L | 238 | MET |
| 1 | L | 336 | ALA |
| 1 | A | 224 | GLU |
| 1 | A | 385 | TRP |
| 1 | B | 472 | ASN |
| 1 | C | 280 | ILE |
| 1 | C | 283 | PRO |
| 1 | D | 133 | PRO |
| 1 | E | 231 | SER |
| 1 | E | 326 | ALA |
| 1 | E | 359 | ILE |
| 1 | H | 309 | PRO |
| 1 | H | 485 | ALA |
| 1 | I | 150 | MET |
| 1 | I | 282 | ASN |
| 1 | I | 305 | PRO |
| 1 | I | 347 | GLY |
| 1 | K | 144 | ILE |
| 1 | K | 255 | VAL |
| 1 | K | 298 | HIS |
| 1 | L | 101 | VAL |
| 1 | L | 223 | ILE |
| 1 | A | 212 | ILE |
| 1 | A | 422 | GLY |
| 1 | B | 133 | PRO |
| 1 | C | 192 | ILE |
| 1 | C | 239 | THR |
| 1 | D | 192 | ILE |
| 1 | D | 219 | VAL |
| 1 | D | 235 | ILE |
| 1 | E | 165 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 426 | GLY |
| 1 | G | 87 | THR |
| 1 | G | 144 | ILE |
| 1 | G | 212 | ILE |
| 1 | H | 87 | THR |
| 1 | J | 235 | ILE |
| 1 | J | 305 | PRO |
| 1 | K | 121 | PRO |
| 1 | K | 359 | ILE |
| 1 | L | 240 | PRO |
| 1 | B | 165 | PRO |
| 1 | C | 350 | GLY |
| 1 | C | 353 | THR |
| 1 | D | 426 | GLY |
| 1 | E | 464 | ILE |
| 1 | F | 282 | ASN |
| 1 | F | 299 | GLY |
| 1 | G | 162 | ILE |
| 1 | I | 235 | ILE |
| 1 | I | 273 | VAL |
| 1 | I | 426 | GLY |
| 1 | I | 429 | PRO |
| 1 | J | 426 | GLY |
| 1 | K | 162 | ILE |
| 1 | K | 165 | PRO |
| 1 | A | 24 | VAL |
| 1 | A | 241 | GLY |
| 1 | A | 425 | GLY |
| 1 | A | 449 | VAL |
| 1 | E | 212 | ILE |
| 1 | H | 235 | ILE |
| 1 | I | 203 | ILE |
| 1 | K | 133 | PRO |
| 1 | B | 7 | PRO |
| 1 | C | 305 | PRO |
| 1 | C | 425 | GLY |
| 1 | D | 299 | GLY |
| 1 | G | 283 | PRO |
| 1 | H | 64 | PRO |
| 1 | H | 282 | ASN |
| 1 | I | 227 | ILE |
| 1 | I | 239 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 425 | GLY |
| 1 | K | 223 | ILE |
| 1 | K | 376 | GLY |
| 1 | B | 192 | ILE |
| 1 | D | 486 | ILE |
| 1 | J | 64 | PRO |
| 1 | L | 58 | VAL |

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 | 413/413 (100%) | 368 (89%) | 45 (11%) | 7 | 31 |
| 1 | B | 413/413 (100%) | 352 (85%) | 61 (15%) | 3 | 18 |
| 1 | C | 413/413 (100%) | 348 (84%) | 65 (16%) | 3 | 16 |
| 1 | D | 413/413 (100%) | 354 (86%) | 59 (14%) | 3 | 20 |
| 1 | E | 413/413 (100%) | 343 (83%) | 70 (17%) | 2 | 13 |
| 1 | F | 413/413 (100%) | 359 (87%) | 54 (13%) | 4 | 22 |
| 1 | G | 413/413 (100%) | 354 (86%) | 59 (14%) | 3 | 20 |
| 1 | H | 413/413 (100%) | 348 (84%) | 65 (16%) | 3 | 16 |
| 1 | I | 413/413 (100%) | 362 (88%) | 51 (12%) | 5 | 25 |
| 1 | J | 413/413 (100%) | 348 (84%) | 65 (16%) | 3 | 16 |
| 1 | K | 413/413 (100%) | 346 (84%) | 67 (16%) | 2 | 14 |
| 1 | L | 413/413 (100%) | 351 (85%) | 62 (15%) | 3 | 18 |
| All | All | 4956/4956 (100%) | 4233 (85%) | 723 (15%) | 3 | 19 |

All (723) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | ASP |
| 1 | A | 40 | GLN |
| 1 | A | 45 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 60 | SER |
| 1 | A | 61 | LEU |
| 1 | A | 72 | TRP |
| 1 | A | 76 | GLU |
| 1 | A | 78 | TYR |
| 1 | A | 85 | GLN |
| 1 | A | 86 | ARG |
| 1 | A | 97 | THR |
| 1 | A | 107 | LEU |
| 1 | A | 111 | MET |
| 1 | A | 112 | THR |
| 1 | A | 131 | ILE |
| 1 | A | 145 | THR |
| 1 | A | 158 | ILE |
| 1 | A | 168 | ASP |
| 1 | A | 175 | GLU |
| 1 | A | 176 | MET |
| 1 | A | 186 | THR |
| 1 | A | 224 | GLU |
| 1 | A | 227 | ILE |
| 1 | A | 245 | LYS |
| 1 | A | 249 | VAL |
| 1 | A | 279 | SER |
| 1 | A | 314 | ILE |
| 1 | A | 333 | LYS |
| 1 | A | 335 | ASN |
| 1 | A | 353 | THR |
| 1 | A | 361 | LEU |
| 1 | A | 370 | ASP |
| 1 | A | 374 | ASN |
| 1 | A | 392 | VAL |
| 1 | A | 396 | ARG |
| 1 | A | 405 | SER |
| 1 | A | 409 | LEU |
| 1 | A | 411 | MET |
| 1 | A | 424 | HIS |
| 1 | A | 428 | ILE |
| 1 | A | 439 | ARG |
| 1 | A | 460 | SER |
| 1 | A | 467 | THR |
| 1 | A | 477 | LEU |
| 1 | A | 486 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 6 | ASP |
| 1 | B | 7 | PRO |
| 1 | B | 8 | ASN |
| 1 | B | 9 | PHE |
| 1 | B | 30 | GLU |
| 1 | B | 32 | LEU |
| 1 | B | 33 | ARG |
| 1 | B | 36 | GLU |
| 1 | B | 48 | ILE |
| 1 | B | 54 | PRO |
| 1 | B | 60 | SER |
| 1 | B | 61 | LEU |
| 1 | B | 72 | TRP |
| 1 | B | 78 | TYR |
| 1 | B | 85 | GLN |
| 1 | B | 86 | ARG |
| 1 | B | 105 | LYS |
| 1 | B | 135 | ASN |
| 1 | B | 137 | THR |
| 1 | B | 139 | ASN |
| 1 | B | 149 | THR |
| 1 | B | 152 | LEU |
| 1 | B | 162 | ILE |
| 1 | B | 171 | THR |
| 1 | B | 176 | MET |
| 1 | B | 212 | ILE |
| 1 | B | 213 | SER |
| 1 | B | 238 | MET |
| 1 | B | 239 | THR |
| 1 | B | 249 | VAL |
| 1 | B | 250 | GLN |
| 1 | B | 257 | LEU |
| 1 | B | 261 | ARG |
| 1 | B | 275 | GLU |
| 1 | B | 284 | ASP |
| 1 | B | 287 | ASP |
| 1 | B | 289 | LYS |
| 1 | B | 314 | ILE |
| 1 | B | 322 | LEU |
| 1 | B | 323 | ILE |
| 1 | B | 331 | LEU |
| 1 | B | 335 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 362 | GLU |
| 1 | B | 363 | ARG |
| 1 | B | 373 | LEU |
| 1 | B | 396 | ARG |
| 1 | B | 398 | THR |
| 1 | B | 405 | SER |
| 1 | B | 409 | LEU |
| 1 | B | 411 | MET |
| 1 | B | 417 | LEU |
| 1 | B | 421 | PHE |
| 1 | B | 423 | LYS |
| 1 | B | 424 | HIS |
| 1 | B | 427 | THR |
| 1 | B | 428 | ILE |
| 1 | B | 439 | ARG |
| 1 | B | 453 | LEU |
| 1 | B | 465 | MET |
| 1 | B | 475 | LEU |
| 1 | B | 493 | TYR |
| 1 | C | 9 | PHE |
| 1 | C | 13 | VAL |
| 1 | C | 14 | GLU |
| 1 | C | 19 | ARG |
| 1 | C | 24 | VAL |
| 1 | C | 40 | GLN |
| 1 | C | 44 | ARG |
| 1 | C | 45 | VAL |
| 1 | C | 58 | VAL |
| 1 | C | 61 | LEU |
| 1 | C | 63 | PHE |
| 1 | C | 67 | ARG |
| 1 | C | 72 | TRP |
| 1 | C | 73 | GLU |
| 1 | C | 85 | GLN |
| 1 | C | 86 | ARG |
| 1 | C | 93 | ILE |
| 1 | C | 97 | THR |
| 1 | C | 98 | ASP |
| 1 | C | 99 | VAL |
| 1 | C | 105 | LYS |
| 1 | C | 112 | THR |
| 1 | C | 114 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 118 | VAL |
| 1 | C | 131 | ILE |
| 1 | C | 137 | THR |
| 1 | C | 138 | ASP |
| 1 | C | 145 | THR |
| 1 | C | 168 | ASP |
| 1 | C | 173 | GLU |
| 1 | C | 176 | MET |
| 1 | C | 212 | ILE |
| 1 | C | 213 | SER |
| 1 | C | 215 | THR |
| 1 | C | 227 | ILE |
| 1 | C | 247 | PHE |
| 1 | C | 249 | VAL |
| 1 | C | 250 | GLN |
| 1 | C | 255 | VAL |
| 1 | C | 263 | LEU |
| 1 | C | 275 | GLU |
| 1 | C | 281 | TRP |
| 1 | C | 284 | ASP |
| 1 | C | 310 | TYR |
| 1 | C | 314 | ILE |
| 1 | C | 320 | ASP |
| 1 | C | 333 | LYS |
| 1 | C | 335 | ASN |
| 1 | C | 352 | THR |
| 1 | C | 363 | ARG |
| 1 | C | 370 | ASP |
| 1 | C | 374 | ASN |
| 1 | C | 380 | VAL |
| 1 | C | 381 | SER |
| 1 | C | 392 | VAL |
| 1 | C | 396 | ARG |
| 1 | C | 409 | LEU |
| 1 | C | 413 | VAL |
| 1 | C | 417 | LEU |
| 1 | C | 420 | LYS |
| 1 | C | 428 | ILE |
| 1 | C | 441 | SER |
| 1 | C | 453 | LEU |
| 1 | C | 473 | LEU |
| 1 | C | 494 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 9 | PHE |
| 1 | D | 14 | GLU |
| 1 | D | 19 | ARG |
| 1 | D | 45 | VAL |
| 1 | D | 58 | VAL |
| 1 | D | 60 | SER |
| 1 | D | 61 | LEU |
| 1 | D | 64 | PRO |
| 1 | D | 66 | ARG |
| 1 | D | 67 | ARG |
| 1 | D | 72 | TRP |
| 1 | D | 76 | GLU |
| 1 | D | 78 | TYR |
| 1 | D | 85 | GLN |
| 1 | D | 86 | ARG |
| 1 | D | 87 | THR |
| 1 | D | 94 | ARG |
| 1 | D | 97 | THR |
| 1 | D | 99 | VAL |
| 1 | D | 100 | SER |
| 1 | D | 137 | THR |
| 1 | D | 145 | THR |
| 1 | D | 147 | ARG |
| 1 | D | 158 | ILE |
| 1 | D | 175 | GLU |
| 1 | D | 176 | MET |
| 1 | D | 213 | SER |
| 1 | D | 227 | ILE |
| 1 | D | 228 | ASN |
| 1 | D | 250 | GLN |
| 1 | D | 255 | VAL |
| 1 | D | 257 | LEU |
| 1 | D | 263 | LEU |
| 1 | D | 280 | ILE |
| 1 | D | 289 | LYS |
| 1 | D | 291 | LEU |
| 1 | D | 296 | LEU |
| 1 | D | 298 | HIS |
| 1 | D | 314 | ILE |
| 1 | D | 315 | LEU |
| 1 | D | 316 | GLU |
| 1 | D | 322 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 330 | GLN |
| 1 | D | 334 | SER |
| 1 | D | 335 | ASN |
| 1 | D | 344 | ILE |
| 1 | D | 352 | THR |
| 1 | D | 363 | ARG |
| 1 | D | 396 | ARG |
| 1 | D | 397 | LEU |
| 1 | D | 398 | THR |
| 1 | D | 405 | SER |
| 1 | D | 409 | LEU |
| 1 | D | 420 | LYS |
| 1 | D | 428 | ILE |
| 1 | D | 444 | SER |
| 1 | D | 467 | THR |
| 1 | D | 494 | ASN |
| 1 | D | 501 | THR |
| 1 | E | 6 | ASP |
| 1 | E | 9 | PHE |
| 1 | E | 10 | PHE |
| 1 | E | 19 | ARG |
| 1 | E | 22 | SER |
| 1 | E | 31 | ASP |
| 1 | E | 32 | LEU |
| 1 | E | 43 | ASN |
| 1 | E | 45 | VAL |
| 1 | E | 58 | VAL |
| 1 | E | 61 | LEU |
| 1 | E | 66 | ARG |
| 1 | E | 78 | TYR |
| 1 | E | 82 | HIS |
| 1 | E | 85 | GLN |
| 1 | E | 96 | SER |
| 1 | E | 97 | THR |
| 1 | E | 105 | LYS |
| 1 | E | 107 | LEU |
| 1 | E | 111 | MET |
| 1 | E | 112 | THR |
| 1 | E | 131 | ILE |
| 1 | E | 137 | THR |
| 1 | E | 138 | ASP |
| 1 | E | 158 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 174 | ARG |
| 1 | E | 176 | MET |
| 1 | E | 211 | ARG |
| 1 | E | 215 | THR |
| 1 | E | 219 | VAL |
| 1 | E | 234 | SER |
| 1 | E | 242 | PHE |
| 1 | E | 249 | VAL |
| 1 | E | 255 | VAL |
| 1 | E | 261 | ARG |
| 1 | E | 263 | LEU |
| 1 | E | 275 | GLU |
| 1 | E | 281 | TRP |
| 1 | E | 284 | ASP |
| 1 | E | 298 | HIS |
| 1 | E | 301 | ILE |
| 1 | E | 314 | ILE |
| 1 | E | 322 | LEU |
| 1 | E | 323 | ILE |
| 1 | E | 329 | LYS |
| 1 | E | 330 | GLN |
| 1 | E | 335 | ASN |
| 1 | E | 352 | THR |
| 1 | E | 353 | THR |
| 1 | E | 357 | ASP |
| 1 | E | 363 | ARG |
| 1 | E | 365 | ILE |
| 1 | E | 367 | VAL |
| 1 | E | 374 | ASN |
| 1 | E | 381 | SER |
| 1 | E | 396 | ARG |
| 1 | E | 397 | LEU |
| 1 | E | 417 | LEU |
| 1 | E | 420 | LYS |
| 1 | E | 428 | ILE |
| 1 | E | 433 | THR |
| 1 | E | 436 | PHE |
| 1 | E | 439 | ARG |
| 1 | E | 446 | LYS |
| 1 | E | 453 | LEU |
| 1 | E | 472 | ASN |
| 1 | E | 477 | LEU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 493 | TYR |
| 1 | E | 495 | GLU |
| 1 | E | 498 | VAL |
| 1 | F | 8 | ASN |
| 1 | F | 19 | ARG |
| 1 | F | 24 | VAL |
| 1 | F | 42 | ARG |
| 1 | F | 45 | VAL |
| 1 | F | 46 | ARG |
| 1 | F | 51 | ILE |
| 1 | F | 54 | PRO |
| 1 | F | 59 | LEU |
| 1 | F | 60 | SER |
| 1 | F | 61 | LEU |
| 1 | F | 62 | SER |
| 1 | F | 72 | TRP |
| 1 | F | 78 | TYR |
| 1 | F | 85 | GLN |
| 1 | F | 86 | ARG |
| 1 | F | 100 | SER |
| 1 | F | 107 | LEU |
| 1 | F | 109 | SER |
| 1 | F | 121 | PRO |
| 1 | F | 137 | THR |
| 1 | F | 152 | LEU |
| 1 | F | 158 | ILE |
| 1 | F | 163 | ASP |
| 1 | F | 175 | GLU |
| 1 | F | 176 | MET |
| 1 | F | 186 | THR |
| 1 | F | 238 | MET |
| 1 | F | 245 | LYS |
| 1 | F | 246 | THR |
| 1 | F | 249 | VAL |
| 1 | F | 250 | GLN |
| 1 | F | 255 | VAL |
| 1 | F | 271 | ILE |
| 1 | F | 300 | SER |
| 1 | F | 314 | ILE |
| 1 | F | 322 | LEU |
| 1 | F | 328 | GLU |
| 1 | F | 329 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 335 | ASN |
| 1 | F | 363 | ARG |
| 1 | F | 396 | ARG |
| 1 | F | 402 | GLU |
| 1 | F | 409 | LEU |
| 1 | F | 428 | ILE |
| 1 | F | 435 | GLU |
| 1 | F | 440 | ILE |
| 1 | F | 441 | SER |
| 1 | F | 446 | LYS |
| 1 | F | 451 | SER |
| 1 | F | 453 | LEU |
| 1 | F | 467 | THR |
| 1 | F | 477 | LEU |
| 1 | F | 495 | GLU |
| 1 | G | 19 | ARG |
| 1 | G | 24 | VAL |
| 1 | G | 26 | ASP |
| 1 | G | 33 | ARG |
| 1 | G | 38 | GLU |
| 1 | G | 45 | VAL |
| 1 | G | 61 | LEU |
| 1 | G | 64 | PRO |
| 1 | G | 72 | TRP |
| 1 | G | 76 | GLU |
| 1 | G | 78 | TYR |
| 1 | G | 84 | HIS |
| 1 | G | 85 | GLN |
| 1 | G | 100 | SER |
| 1 | G | 101 | VAL |
| 1 | G | 111 | MET |
| 1 | G | 112 | THR |
| 1 | G | 131 | ILE |
| 1 | G | 145 | THR |
| 1 | G | 147 | ARG |
| 1 | G | 158 | ILE |
| 1 | G | 176 | MET |
| 1 | G | 204 | SER |
| 1 | G | 212 | ILE |
| 1 | G | 213 | SER |
| 1 | G | 232 | TYR |
| 1 | G | 235 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 250 | GLN |
| 1 | G | 257 | LEU |
| 1 | G | 261 | ARG |
| 1 | G | 298 | HIS |
| 1 | G | 302 | LEU |
| 1 | G | 310 | TYR |
| 1 | G | 314 | ILE |
| 1 | G | 335 | ASN |
| 1 | G | 339 | VAL |
| 1 | G | 352 | THR |
| 1 | G | 353 | THR |
| 1 | G | 354 | PRO |
| 1 | G | 357 | ASP |
| 1 | G | 361 | LEU |
| 1 | G | 363 | ARG |
| 1 | G | 372 | TYR |
| 1 | G | 374 | ASN |
| 1 | G | 393 | SER |
| 1 | G | 396 | ARG |
| 1 | G | 402 | GLU |
| 1 | G | 409 | LEU |
| 1 | G | 417 | LEU |
| 1 | G | 423 | LYS |
| 1 | G | 428 | ILE |
| 1 | G | 436 | PHE |
| 1 | G | 440 | ILE |
| 1 | G | 444 | SER |
| 1 | G | 467 | THR |
| 1 | G | 469 | MET |
| 1 | G | 477 | LEU |
| 1 | G | 498 | VAL |
| 1 | G | 501 | THR |
| 1 | H | 9 | PHE |
| 1 | H | 19 | ARG |
| 1 | H | 31 | ASP |
| 1 | H | 36 | GLU |
| 1 | H | 38 | GLU |
| 1 | H | 39 | GLU |
| 1 | H | 40 | GLN |
| 1 | H | 44 | ARG |
| 1 | H | 46 | ARG |
| 1 | H | 50 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 60 | SER |
| 1 | H | 61 | LEU |
| 1 | H | 63 | PHE |
| 1 | H | 78 | TYR |
| 1 | H | 85 | GLN |
| 1 | H | 86 | ARG |
| 1 | H | 97 | THR |
| 1 | H | 98 | ASP |
| 1 | H | 102 | ASP |
| 1 | H | 112 | THR |
| 1 | H | 131 | ILE |
| 1 | H | 134 | LYS |
| 1 | H | 137 | THR |
| 1 | H | 138 | ASP |
| 1 | H | 145 | THR |
| 1 | H | 154 | LYS |
| 1 | H | 169 | MET |
| 1 | H | 176 | MET |
| 1 | H | 181 | ASP |
| 1 | H | 199 | THR |
| 1 | H | 204 | SER |
| 1 | H | 213 | SER |
| 1 | H | 227 | ILE |
| 1 | H | 231 | SER |
| 1 | H | 255 | VAL |
| 1 | H | 257 | LEU |
| 1 | H | 281 | TRP |
| 1 | H | 291 | LEU |
| 1 | H | 292 | GLU |
| 1 | H | 302 | LEU |
| 1 | H | 311 | GLU |
| 1 | H | 314 | ILE |
| 1 | H | 322 | LEU |
| 1 | H | 327 | SER |
| 1 | H | 330 | GLN |
| 1 | H | 335 | ASN |
| 1 | H | 352 | THR |
| 1 | H | 353 | THR |
| 1 | H | 361 | LEU |
| 1 | H | 362 | GLU |
| 1 | H | 363 | ARG |
| 1 | H | 367 | VAL |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 372 | TYR |
| 1 | H | 374 | ASN |
| 1 | H | 392 | VAL |
| 1 | H | 396 | ARG |
| 1 | H | 409 | LEU |
| 1 | H | 417 | LEU |
| 1 | H | 423 | LYS |
| 1 | H | 424 | HIS |
| 1 | H | 428 | ILE |
| 1 | H | 462 | ARG |
| 1 | H | 467 | THR |
| 1 | H | 477 | LEU |
| 1 | H | 495 | GLU |
| 1 | I | 9 | PHE |
| 1 | I | 30 | GLU |
| 1 | I | 31 | ASP |
| 1 | I | 33 | ARG |
| 1 | I | 42 | ARG |
| 1 | I | 43 | ASN |
| 1 | I | 45 | VAL |
| 1 | I | 60 | SER |
| 1 | I | 61 | LEU |
| 1 | I | 62 | SER |
| 1 | I | 66 | ARG |
| 1 | I | 72 | TRP |
| 1 | I | 78 | TYR |
| 1 | I | 85 | GLN |
| 1 | I | 86 | ARG |
| 1 | I | 93 | ILE |
| 1 | I | 94 | ARG |
| 1 | I | 98 | ASP |
| 1 | I | 101 | VAL |
| 1 | I | 107 | LEU |
| 1 | I | 111 | MET |
| 1 | I | 112 | THR |
| 1 | I | 114 | LYS |
| 1 | I | 121 | PRO |
| 1 | I | 137 | THR |
| 1 | I | 141 | LEU |
| 1 | I | 158 | ILE |
| 1 | I | 162 | ILE |
| 1 | I | 176 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 186 | THR |
| 1 | I | 213 | SER |
| 1 | I | 217 | ARG |
| 1 | I | 255 | VAL |
| 1 | I | 261 | ARG |
| 1 | I | 296 | LEU |
| 1 | I | 314 | ILE |
| 1 | I | 329 | LYS |
| 1 | I | 332 | THR |
| 1 | I | 333 | LYS |
| 1 | I | 352 | THR |
| 1 | I | 373 | LEU |
| 1 | I | 374 | ASN |
| 1 | I | 392 | VAL |
| 1 | I | 396 | ARG |
| 1 | I | 401 | TYR |
| 1 | I | 409 | LEU |
| 1 | I | 421 | PHE |
| 1 | I | 428 | ILE |
| 1 | I | 444 | SER |
| 1 | I | 453 | LEU |
| 1 | I | 499 | THR |
| 1 | J | 6 | ASP |
| 1 | J | 9 | PHE |
| 1 | J | 14 | GLU |
| 1 | J | 19 | ARG |
| 1 | J | 24 | VAL |
| 1 | J | 28 | LEU |
| 1 | J | 31 | ASP |
| 1 | J | 33 | ARG |
| 1 | J | 40 | GLN |
| 1 | J | 42 | ARG |
| 1 | J | 58 | VAL |
| 1 | J | 60 | SER |
| 1 | J | 72 | TRP |
| 1 | J | 78 | TYR |
| 1 | J | 85 | GLN |
| 1 | J | 86 | ARG |
| 1 | J | 101 | VAL |
| 1 | J | 107 | LEU |
| 1 | J | 112 | THR |
| 1 | J | 118 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 131 | ILE |
| 1 | J | 137 | THR |
| 1 | J | 138 | ASP |
| 1 | J | 158 | ILE |
| 1 | J | 162 | ILE |
| 1 | J | 175 | GLU |
| 1 | J | 176 | MET |
| 1 | J | 186 | THR |
| 1 | J | 208 | ILE |
| 1 | J | 212 | ILE |
| 1 | J | 228 | ASN |
| 1 | J | 231 | SER |
| 1 | J | 238 | MET |
| 1 | J | 239 | THR |
| 1 | J | 245 | LYS |
| 1 | J | 249 | VAL |
| 1 | J | 250 | GLN |
| 1 | J | 261 | ARG |
| 1 | J | 296 | LEU |
| 1 | J | 302 | LEU |
| 1 | J | 314 | ILE |
| 1 | J | 327 | SER |
| 1 | J | 329 | LYS |
| 1 | J | 331 | LEU |
| 1 | J | 332 | THR |
| 1 | J | 335 | ASN |
| 1 | J | 343 | ILE |
| 1 | J | 351 | PRO |
| 1 | J | 357 | ASP |
| 1 | J | 361 | LEU |
| 1 | J | 372 | TYR |
| 1 | J | 393 | SER |
| 1 | J | 396 | ARG |
| 1 | J | 408 | HIS |
| 1 | J | 409 | LEU |
| 1 | J | 417 | LEU |
| 1 | J | 420 | LYS |
| 1 | J | 427 | THR |
| 1 | J | 430 | ILE |
| 1 | J | 440 | ILE |
| 1 | J | 453 | LEU |
| 1 | J | 464 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 472 | ASN |
| 1 | J | 477 | LEU |
| 1 | J | 493 | TYR |
| 1 | K | 6 | ASP |
| 1 | K | 9 | PHE |
| 1 | K | 33 | ARG |
| 1 | K | 34 | THR |
| 1 | K | 35 | ARG |
| 1 | K | 40 | GLN |
| 1 | K | 45 | VAL |
| 1 | K | 59 | LEU |
| 1 | K | 60 | SER |
| 1 | K | 64 | PRO |
| 1 | K | 72 | TRP |
| 1 | K | 78 | TYR |
| 1 | K | 79 | ARG |
| 1 | K | 85 | GLN |
| 1 | K | 86 | ARG |
| 1 | K | 87 | THR |
| 1 | K | 112 | THR |
| 1 | K | 132 | ASN |
| 1 | K | 137 | THR |
| 1 | K | 138 | ASP |
| 1 | K | 145 | THR |
| 1 | K | 167 | PRO |
| 1 | K | 173 | GLU |
| 1 | K | 176 | MET |
| 1 | K | 177 | SER |
| 1 | K | 190 | TYR |
| 1 | K | 204 | SER |
| 1 | K | 212 | ILE |
| 1 | K | 215 | THR |
| 1 | K | 219 | VAL |
| 1 | K | 225 | ASN |
| 1 | K | 227 | ILE |
| 1 | K | 245 | LYS |
| 1 | K | 249 | VAL |
| 1 | K | 257 | LEU |
| 1 | K | 271 | ILE |
| 1 | K | 291 | LEU |
| 1 | K | 294 | PHE |
| 1 | K | 296 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 301 | ILE |
| 1 | K | 314 | ILE |
| 1 | K | 315 | LEU |
| 1 | K | 316 | GLU |
| 1 | K | 322 | LEU |
| 1 | K | 323 | ILE |
| 1 | K | 335 | ASN |
| 1 | K | 344 | ILE |
| 1 | K | 358 | LYS |
| 1 | K | 363 | ARG |
| 1 | K | 368 | ILE |
| 1 | K | 371 | LEU |
| 1 | K | 374 | ASN |
| 1 | K | 396 | ARG |
| 1 | K | 398 | THR |
| 1 | K | 402 | GLU |
| 1 | K | 417 | LEU |
| 1 | K | 420 | LYS |
| 1 | K | 421 | PHE |
| 1 | K | 423 | LYS |
| 1 | K | 433 | THR |
| 1 | K | 435 | GLU |
| 1 | K | 451 | SER |
| 1 | K | 453 | LEU |
| 1 | K | 478 | ARG |
| 1 | K | 494 | ASN |
| 1 | K | 498 | VAL |
| 1 | K | 501 | THR |
| 1 | L | 9 | PHE |
| 1 | L | 19 | ARG |
| 1 | L | 24 | VAL |
| 1 | L | 31 | ASP |
| 1 | L | 33 | ARG |
| 1 | L | 38 | GLU |
| 1 | L | 45 | VAL |
| 1 | L | 58 | VAL |
| 1 | L | 72 | TRP |
| 1 | L | 76 | GLU |
| 1 | L | 78 | TYR |
| 1 | L | 85 | GLN |
| 1 | L | 86 | ARG |
| 1 | L | 94 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 97 | THR |
| 1 | L | 100 | SER |
| 1 | L | 103 | GLU |
| 1 | L | 111 | MET |
| 1 | L | 112 | THR |
| 1 | L | 131 | ILE |
| 1 | L | 137 | THR |
| 1 | L | 147 | ARG |
| 1 | L | 158 | ILE |
| 1 | L | 175 | GLU |
| 1 | L | 176 | MET |
| 1 | L | 212 | ILE |
| 1 | L | 213 | SER |
| 1 | L | 238 | MET |
| 1 | L | 242 | PHE |
| 1 | L | 255 | VAL |
| 1 | L | 257 | LEU |
| 1 | L | 263 | LEU |
| 1 | L | 266 | PHE |
| 1 | L | 309 | PRO |
| 1 | L | 313 | SER |
| 1 | L | 314 | ILE |
| 1 | L | 330 | GLN |
| 1 | L | 335 | ASN |
| 1 | L | 338 | ARG |
| 1 | L | 352 | THR |
| 1 | L | 362 | GLU |
| 1 | L | 363 | ARG |
| 1 | L | 364 | ASN |
| 1 | L | 392 | VAL |
| 1 | L | 393 | SER |
| 1 | L | 396 | ARG |
| 1 | L | 398 | THR |
| 1 | L | 405 | SER |
| 1 | L | 409 | LEU |
| 1 | L | 411 | MET |
| 1 | L | 413 | VAL |
| 1 | L | 417 | LEU |
| 1 | L | 420 | LYS |
| 1 | L | 424 | HIS |
| 1 | L | 428 | ILE |
| 1 | L | 444 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 447 | ASP |
| 1 | L | 451 | SER |
| 1 | L | 453 | LEU |
| 1 | L | 472 | ASN |
| 1 | L | 477 | LEU |
| 1 | L | 478 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (164) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 84 | HIS |
| 1 | A | 85 | GLN |
| 1 | A | 139 | ASN |
| 1 | A | 205 | GLN |
| 1 | A | 282 | ASN |
| 1 | A | 330 | GLN |
| 1 | A | 335 | ASN |
| 1 | A | 374 | ASN |
| 1 | A | 388 | ASN |
| 1 | A | 406 | ASN |
| 1 | A | 437 | GLN |
| 1 | A | 450 | HIS |
| 1 | A | 484 | ASN |
| 1 | B | 82 | HIS |
| 1 | B | 85 | GLN |
| 1 | B | 228 | ASN |
| 1 | B | 250 | GLN |
| 1 | B | 330 | GLN |
| 1 | B | 335 | ASN |
| 1 | B | 374 | ASN |
| 1 | B | 388 | ASN |
| 1 | B | 406 | ASN |
| 1 | B | 424 | HIS |
| 1 | C | 56 | ASN |
| 1 | C | 57 | HIS |
| 1 | C | 82 | HIS |
| 1 | C | 84 | HIS |
| 1 | C | 85 | GLN |
| 1 | C | 135 | ASN |
| 1 | C | 189 | HIS |
| 1 | C | 205 | GLN |
| 1 | C | 221 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 225 | ASN |
| 1 | C | 228 | ASN |
| 1 | C | 250 | GLN |
| 1 | C | 258 | HIS |
| 1 | C | 335 | ASN |
| 1 | C | 374 | ASN |
| 1 | C | 388 | ASN |
| 1 | C | 391 | HIS |
| 1 | C | 406 | ASN |
| 1 | C | 484 | ASN |
| 1 | D | 57 | HIS |
| 1 | D | 85 | GLN |
| 1 | D | 135 | ASN |
| 1 | D | 209 | HIS |
| 1 | D | 225 | ASN |
| 1 | D | 228 | ASN |
| 1 | D | 250 | GLN |
| 1 | D | 282 | ASN |
| 1 | D | 330 | GLN |
| 1 | D | 335 | ASN |
| 1 | D | 349 | ASN |
| 1 | D | 374 | ASN |
| 1 | D | 390 | ASN |
| 1 | D | 391 | HIS |
| 1 | D | 406 | ASN |
| 1 | D | 484 | ASN |
| 1 | D | 494 | ASN |
| 1 | E | 56 | ASN |
| 1 | E | 82 | HIS |
| 1 | E | 84 | HIS |
| 1 | E | 85 | GLN |
| 1 | E | 209 | HIS |
| 1 | E | 254 | ASN |
| 1 | E | 258 | HIS |
| 1 | E | 335 | ASN |
| 1 | E | 374 | ASN |
| 1 | E | 391 | HIS |
| 1 | E | 406 | ASN |
| 1 | E | 463 | GLN |
| 1 | E | 472 | ASN |
| 1 | F | 8 | ASN |
| 1 | F | 82 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 84 | HIS |
| 1 | F | 85 | GLN |
| 1 | F | 139 | ASN |
| 1 | F | 189 | HIS |
| 1 | F | 225 | ASN |
| 1 | F | 228 | ASN |
| 1 | F | 298 | HIS |
| 1 | F | 330 | GLN |
| 1 | F | 335 | ASN |
| 1 | F | 388 | ASN |
| 1 | F | 406 | ASN |
| 1 | F | 437 | GLN |
| 1 | F | 494 | ASN |
| 1 | G | 57 | HIS |
| 1 | G | 82 | HIS |
| 1 | G | 85 | GLN |
| 1 | G | 135 | ASN |
| 1 | G | 139 | ASN |
| 1 | G | 225 | ASN |
| 1 | G | 250 | GLN |
| 1 | G | 335 | ASN |
| 1 | G | 374 | ASN |
| 1 | G | 388 | ASN |
| 1 | G | 406 | ASN |
| 1 | G | 484 | ASN |
| 1 | G | 494 | ASN |
| 1 | H | 84 | HIS |
| 1 | H | 85 | GLN |
| 1 | H | 135 | ASN |
| 1 | H | 189 | HIS |
| 1 | H | 228 | ASN |
| 1 | H | 335 | ASN |
| 1 | H | 374 | ASN |
| 1 | H | 388 | ASN |
| 1 | H | 391 | HIS |
| 1 | H | 437 | GLN |
| 1 | I | 56 | ASN |
| 1 | I | 82 | HIS |
| 1 | I | 85 | GLN |
| 1 | I | 189 | HIS |
| 1 | I | 205 | GLN |
| 1 | I | 228 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 254 | ASN |
| 1 | I | 330 | GLN |
| 1 | I | 364 | ASN |
| 1 | I | 388 | ASN |
| 1 | I | 390 | ASN |
| 1 | I | 406 | ASN |
| 1 | I | 484 | ASN |
| 1 | J | 40 | GLN |
| 1 | J | 85 | GLN |
| 1 | J | 189 | HIS |
| 1 | J | 228 | ASN |
| 1 | J | 298 | HIS |
| 1 | J | 335 | ASN |
| 1 | J | 364 | ASN |
| 1 | J | 388 | ASN |
| 1 | J | 406 | ASN |
| 1 | J | 414 | GLN |
| 1 | J | 494 | ASN |
| 1 | K | 40 | GLN |
| 1 | K | 56 | ASN |
| 1 | K | 57 | HIS |
| 1 | K | 82 | HIS |
| 1 | K | 84 | HIS |
| 1 | K | 85 | GLN |
| 1 | K | 209 | HIS |
| 1 | K | 225 | ASN |
| 1 | K | 297 | GLN |
| 1 | K | 335 | ASN |
| 1 | K | 364 | ASN |
| 1 | K | 374 | ASN |
| 1 | K | 406 | ASN |
| 1 | K | 437 | GLN |
| 1 | L | 57 | HIS |
| 1 | L | 84 | HIS |
| 1 | L | 85 | GLN |
| 1 | L | 205 | GLN |
| 1 | L | 225 | ASN |
| 1 | L | 335 | ASN |
| 1 | L | 349 | ASN |
| 1 | L | 364 | ASN |
| 1 | L | 374 | ASN |
| 1 | L | 388 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 390 | ASN |
| 1 | L | 406 | ASN |
| 1 | L | 424 | HIS |
| 1 | L | 472 | ASN |
| 1 | L | 484 | ASN |
| 1 | L | 494 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 | ADP | A | 1 | - | 25,29,29 | 1.66 | 5 (20%) | 25,45,45 | 2.33 | 3 (12%) |
| 2 | ADP | B | 2 | - | 25,29,29 | 1.28 | 3 (12%) | 25,45,45 | 2.34 | 3 (12%) |
| 2 | ADP | C | 3 | - | 25,29,29 | 1.34 | 4 (16%) | 25,45,45 | 2.27 | 3 (12%) |
| 2 | ADP | D | 4 | - | 25,29,29 | 2.08 | 5 (20%) | 25,45,45 | 2.26 | 3 (12%) |
| 2 | ADP | E | 5 | - | 25,29,29 | 1.99 | 4 (16%) | 25,45,45 | 2.39 | 4 (16%) |
| 2 | ADP | F | 502 | - | 25,29,29 | 1.31 | 3 (12%) | 25,45,45 | 2.30 | 5 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | ADP | G | 502 | - | 25,29,29 | 1.70 | 5 (20%) | 25,45,45 | 2.28 | 3 (12%) |
| 2 | ADP | H | 502 | - | 25,29,29 | 1.22 | 3 (12%) | 25,45,45 | 2.31 | 4 (16%) |
| 2 | ADP | I | 502 | - | 25,29,29 | 1.21 | 2 (8%) | 25,45,45 | 2.33 | 4 (16%) |
| 2 | ADP | J | 502 | - | 25,29,29 | 1.19 | 3 (12%) | 25,45,45 | 2.32 | 4 (16%) |
| 2 | ADP | K | 502 | - | 25,29,29 | 1.33 | 3 (12%) | 25,45,45 | 2.30 | 4 (16%) |
| 2 | ADP | L | 502 | - | 25,29,29 | 1.47 | 3 (12%) | 25,45,45 | 2.27 | 3 (12%) |

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 | ADP | A | 1 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | B | 2 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | C | 3 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | D | 4 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | E | 5 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | F | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | G | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | H | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | I | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | J | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | K | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | L | 502 | - | - | 0/12/32/32 | 0/3/3/3 |

All (43) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | A | 1 | ADP | C8-N9 | -2.35 | 1.34 | 1.36 |
| 2 | J | 502 | ADP | C8-N9 | -2.29 | 1.34 | 1.36 |
| 2 | C | 3 | ADP | C5-N7 | -2.12 | 1.32 | 1.39 |
| 2 | A | 1 | ADP | C5-N7 | -2.06 | 1.32 | 1.39 |
| 2 | D | 4 | ADP | C5-N7 | -2.02 | 1.32 | 1.39 |
| 2 | F | 502 | ADP | PB-O2B | 2.01 | 1.62 | 1.54 |
| 2 | H | 502 | ADP | PB-O2B | 2.05 | 1.63 | 1.54 |
| 2 | L | 502 | ADP | PB-O2B | 2.07 | 1.63 | 1.54 |
| 2 | J | 502 | ADP | PB-O2B | 2.18 | 1.63 | 1.54 |
| 2 | I | 502 | ADP | PB-O3A | 2.19 | 1.63 | 1.60 |
| 2 | G | 502 | ADP | PA-O5' | 2.22 | 1.68 | 1.59 |
| 2 | G | 502 | ADP | C2-N3 | 2.23 | 1.35 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | C | 3 | ADP | PB-O2B | 2.37 | 1.64 | 1.54 |
| 2 | D | 4 | ADP | C5'-C4' | 2.38 | 1.59 | 1.51 |
| 2 | B | 2 | ADP | PB-O2B | 2.39 | 1.64 | 1.54 |
| 2 | K | 502 | ADP | PB-O2B | 2.42 | 1.64 | 1.54 |
| 2 | E | 5 | ADP | C2-N3 | 2.48 | 1.36 | 1.32 |
| 2 | A | 1 | ADP | O4'-C1' | 2.52 | 1.44 | 1.41 |
| 2 | H | 502 | ADP | PB-O3A | 2.56 | 1.64 | 1.60 |
| 2 | B | 2 | ADP | O4'-C1' | 2.66 | 1.44 | 1.41 |
| 2 | I | 502 | ADP | O4'-C1' | 2.70 | 1.45 | 1.41 |
| 2 | J | 502 | ADP | O4'-C1' | 2.76 | 1.45 | 1.41 |
| 2 | H | 502 | ADP | O4'-C1' | 2.77 | 1.45 | 1.41 |
| 2 | C | 3 | ADP | PB-O3A | 2.81 | 1.64 | 1.60 |
| 2 | F | 502 | ADP | O4'-C1' | 2.88 | 1.45 | 1.41 |
| 2 | K | 502 | ADP | O4'-C1' | 2.88 | 1.45 | 1.41 |
| 2 | F | 502 | ADP | PB-O3A | 3.01 | 1.64 | 1.60 |
| 2 | L | 502 | ADP | O4'-C1' | 3.13 | 1.45 | 1.41 |
| 2 | K | 502 | ADP | PB-O3A | 3.20 | 1.64 | 1.60 |
| 2 | G | 502 | ADP | O4'-C1' | 3.20 | 1.45 | 1.41 |
| 2 | B | 2 | ADP | PB-O3A | 3.26 | 1.65 | 1.60 |
| 2 | C | 3 | ADP | O4'-C1' | 3.66 | 1.46 | 1.41 |
| 2 | D | 4 | ADP | PB-O2B | 3.95 | 1.70 | 1.54 |
| 2 | E | 5 | ADP | PB-O2B | 3.95 | 1.70 | 1.54 |
| 2 | G | 502 | ADP | PB-O3A | 4.20 | 1.66 | 1.60 |
| 2 | A | 1 | ADP | PB-O2B | 4.29 | 1.72 | 1.54 |
| 2 | G | 502 | ADP | PB-O2B | 4.41 | 1.72 | 1.54 |
| 2 | A | 1 | ADP | PB-O3A | 4.42 | 1.66 | 1.60 |
| 2 | L | 502 | ADP | PB-O3A | 4.47 | 1.66 | 1.60 |
| 2 | D | 4 | ADP | O4'-C1' | 4.85 | 1.48 | 1.41 |
| 2 | E | 5 | ADP | PB-O3A | 5.03 | 1.67 | 1.60 |
| 2 | E | 5 | ADP | O4'-C1' | 5.40 | 1.48 | 1.41 |
| 2 | D | 4 | ADP | PB-O3A | 6.21 | 1.69 | 1.60 |

All (43) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | B | 2 | ADP | N3-C2-N1 | -9.53 | 120.71 | 128.86 |
| 2 | H | 502 | ADP | N3-C2-N1 | -9.38 | 120.84 | 128.86 |
| 2 | E | 5 | ADP | N3-C2-N1 | -9.32 | 120.89 | 128.86 |
| 2 | L | 502 | ADP | N3-C2-N1 | -9.25 | 120.95 | 128.86 |
| 2 | I | 502 | ADP | N3-C2-N1 | -9.24 | 120.96 | 128.86 |
| 2 | A | 1 | ADP | N3-C2-N1 | -9.17 | 121.02 | 128.86 |
| 2 | K | 502 | ADP | N3-C2-N1 | -9.13 | 121.05 | 128.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | J | 502 | ADP | N3-C2-N1 | -9.11 | 121.07 | 128.86 |
| 2 | C | 3 | ADP | N3-C2-N1 | -9.09 | 121.08 | 128.86 |
| 2 | F | 502 | ADP | N3-C2-N1 | -9.09 | 121.09 | 128.86 |
| 2 | G | 502 | ADP | N3-C2-N1 | -8.93 | 121.22 | 128.86 |
| 2 | D | 4 | ADP | N3-C2-N1 | -8.45 | 121.64 | 128.86 |
| 2 | E | 5 | ADP | C4'-O4'-C1' | -5.16 | 104.45 | 109.83 |
| 2 | D | 4 | ADP | C4'-O4'-C1' | -5.11 | 104.50 | 109.83 |
| 2 | A | 1 | ADP | C4'-O4'-C1' | -4.55 | 105.08 | 109.83 |
| 2 | I | 502 | ADP | C4'-O4'-C1' | -4.53 | 105.10 | 109.83 |
| 2 | F | 502 | ADP | C4'-O4'-C1' | -4.48 | 105.16 | 109.83 |
| 2 | K | 502 | ADP | C4'-O4'-C1' | -4.34 | 105.31 | 109.83 |
| 2 | J | 502 | ADP | C4'-O4'-C1' | -4.33 | 105.32 | 109.83 |
| 2 | B | 2 | ADP | C4'-O4'-C1' | -4.26 | 105.39 | 109.83 |
| 2 | G | 502 | ADP | C4'-O4'-C1' | -4.21 | 105.44 | 109.83 |
| 2 | H | 502 | ADP | C4'-O4'-C1' | -4.15 | 105.50 | 109.83 |
| 2 | L | 502 | ADP | C4'-O4'-C1' | -4.07 | 105.58 | 109.83 |
| 2 | C | 3 | ADP | C4'-O4'-C1' | -4.06 | 105.60 | 109.83 |
| 2 | G | 502 | ADP | PA-O3A-PB | -3.77 | 119.97 | 132.63 |
| 2 | A | 1 | ADP | PA-O3A-PB | -3.54 | 120.73 | 132.63 |
| 2 | D | 4 | ADP | PA-O3A-PB | -3.52 | 120.80 | 132.63 |
| 2 | J | 502 | ADP | PA-O3A-PB | -3.39 | 121.25 | 132.63 |
| 2 | E | 5 | ADP | PA-O3A-PB | -3.30 | 121.53 | 132.63 |
| 2 | I | 502 | ADP | PA-O3A-PB | -3.29 | 121.58 | 132.63 |
| 2 | F | 502 | ADP | PA-O3A-PB | -3.22 | 121.81 | 132.63 |
| 2 | C | 3 | ADP | PA-O3A-PB | -3.13 | 122.09 | 132.63 |
| 2 | K | 502 | ADP | PA-O3A-PB | -3.13 | 122.12 | 132.63 |
| 2 | B | 2 | ADP | PA-O3A-PB | -3.09 | 122.25 | 132.63 |
| 2 | H | 502 | ADP | PA-O3A-PB | -3.08 | 122.29 | 132.63 |
| 2 | L | 502 | ADP | PA-O3A-PB | -2.78 | 123.28 | 132.63 |
| 2 | J | 502 | ADP | C4-C5-N7 | -2.33 | 107.16 | 109.41 |
| 2 | F | 502 | ADP | C4-C5-N7 | -2.04 | 107.44 | 109.41 |
| 2 | I | 502 | ADP | O3B-PB-O1B | 2.01 | 118.42 | 110.60 |
| 2 | K | 502 | ADP | O3B-PB-O1B | 2.01 | 118.43 | 110.60 |
| 2 | H | 502 | ADP | O3B-PB-O1B | 2.02 | 118.49 | 110.60 |
| 2 | F | 502 | ADP | O3B-PB-O1B | 2.04 | 118.56 | 110.60 |
| 2 | E | 5 | ADP | O3B-PB-O1B | 2.08 | 118.73 | 110.60 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 51 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 1 | ADP | 6 | 0 |
| 2 | B | 2 | ADP | 5 | 0 |
| 2 | C | 3 | ADP | 6 | 0 |
| 2 | D | 4 | ADP | 5 | 0 |
| 2 | E | 5 | ADP | 6 | 0 |
| 2 | F | 502 | ADP | 3 | 0 |
| 2 | G | 502 | ADP | 4 | 0 |
| 2 | H | 502 | ADP | 2 | 0 |
| 2 | I | 502 | ADP | 5 | 0 |
| 2 | J | 502 | ADP | 3 | 0 |
| 2 | K | 502 | ADP | 2 | 0 |
| 2 | L | 502 | ADP | 4 | 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.