



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 12:27 PM JST

PDB ID : 5WQ9
EMDB ID : EMD-6677
Title : CryoEM structure of type II secretion system secretin GspD G453A mutant in *Vibrio cholerae*
Authors : Yan, Z.; Yin, M.; Li, X.
Deposited on : 2016-11-23
Resolution : 4.22 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

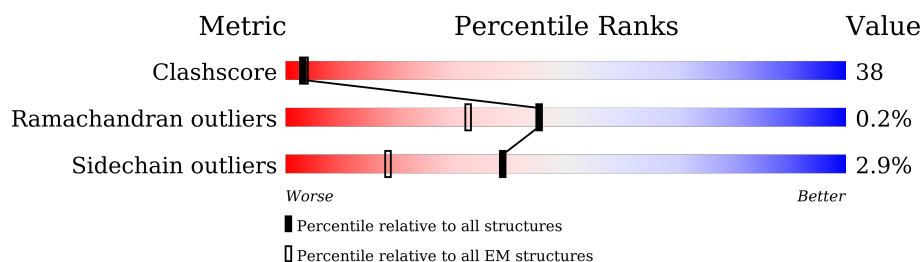
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.22 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 650 | <div> <div>12%</div> <div>41%</div> <div>33%</div> <div>•</div> <div>24%</div> </div> |
| 1 | B | 650 | <div> <div>12%</div> <div>40%</div> <div>33%</div> <div>•</div> <div>24%</div> </div> |
| 1 | C | 650 | <div> <div>12%</div> <div>40%</div> <div>33%</div> <div>•</div> <div>24%</div> </div> |
| 1 | D | 650 | <div> <div>12%</div> <div>41%</div> <div>33%</div> <div>•</div> <div>24%</div> </div> |
| 1 | E | 650 | <div> <div>12%</div> <div>41%</div> <div>33%</div> <div>•</div> <div>24%</div> </div> |
| 1 | F | 650 | <div> <div>12%</div> <div>41%</div> <div>33%</div> <div>•</div> <div>24%</div> </div> |
| 1 | G | 650 | <div> <div>12%</div> <div>40%</div> <div>33%</div> <div>•</div> <div>24%</div> </div> |
| 1 | H | 650 | <div> <div>12%</div> <div>40%</div> <div>33%</div> <div>•</div> <div>24%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | I | 650 | |
| 1 | J | 650 | |
| 1 | K | 650 | |
| 1 | L | 650 | |
| 1 | M | 650 | |
| 1 | N | 650 | |
| 1 | O | 650 | |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 56340 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Type II secretion system protein D.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | B | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | C | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | D | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | E | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | F | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | G | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | H | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | I | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | J | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | K | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | L | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | M | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | N | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |
| 1 | O | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2347 | 656 | 740 | 13 | | |

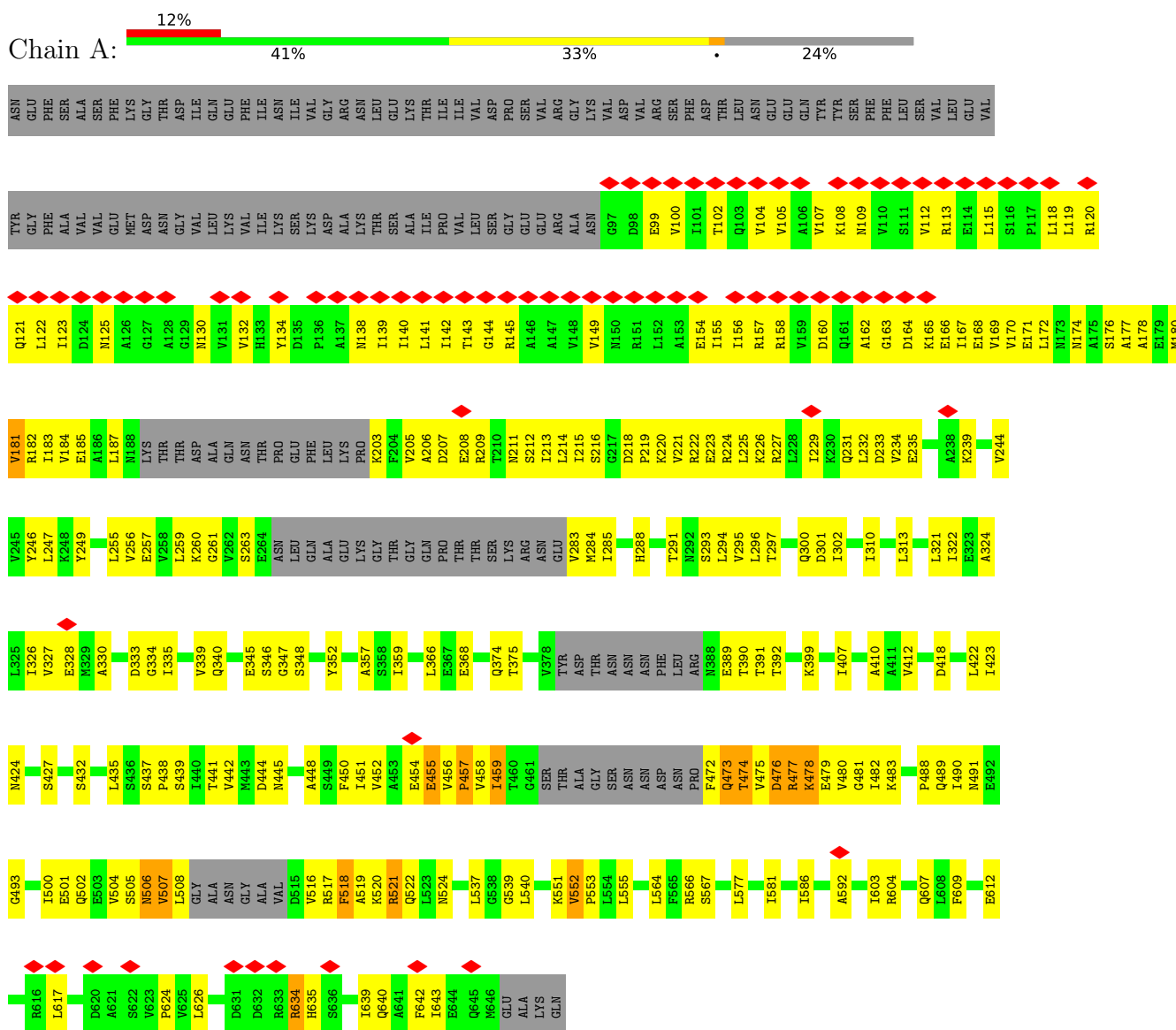
There are 15 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| B | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| C | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| D | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| E | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| F | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| G | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| H | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| I | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| J | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| K | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| L | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| M | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| N | 453 | ALA | GLY | engineered mutation | UNP P45779 |
| O | 453 | ALA | GLY | engineered mutation | UNP P45779 |

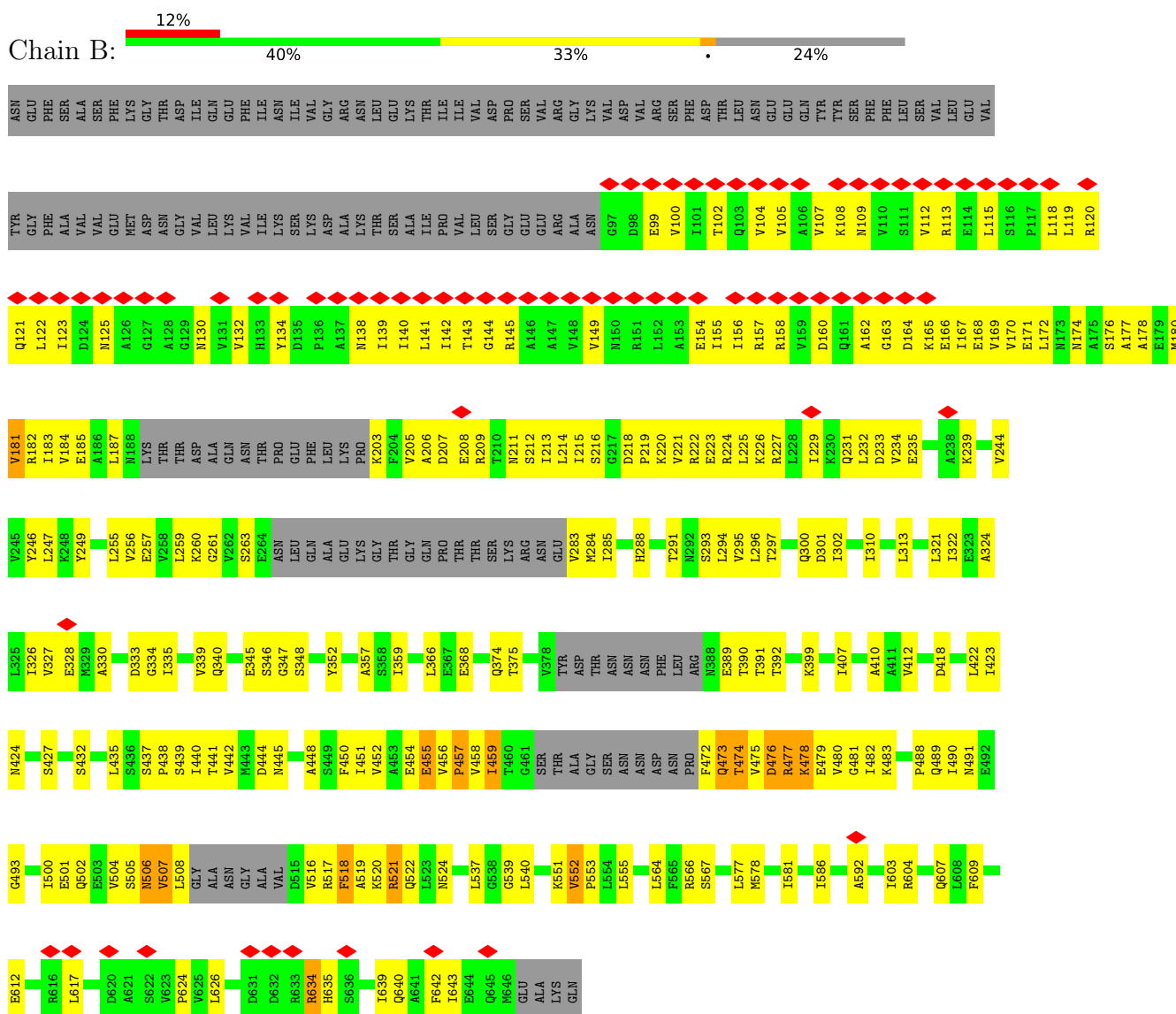
3 Residue-property plots

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

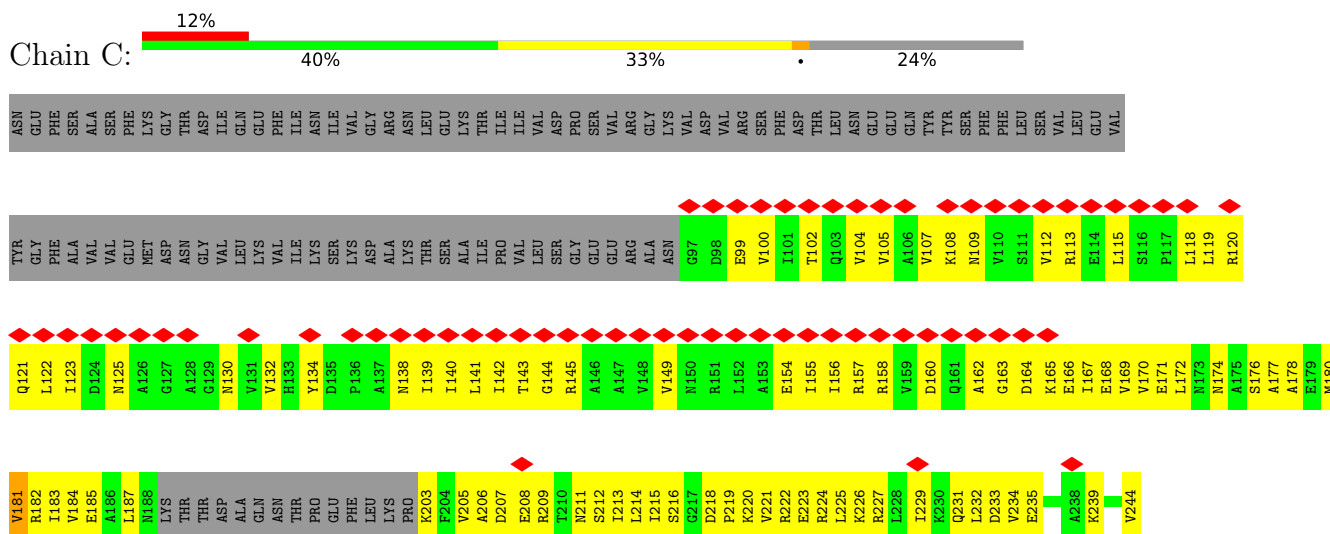
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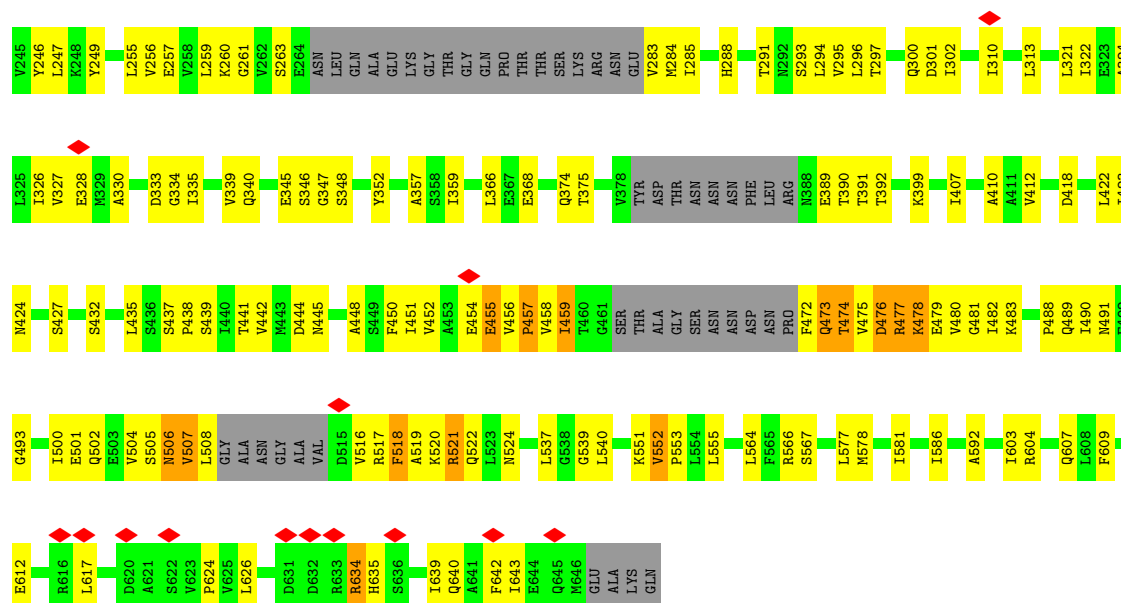


• Molecule 1: Type II secretion system protein D

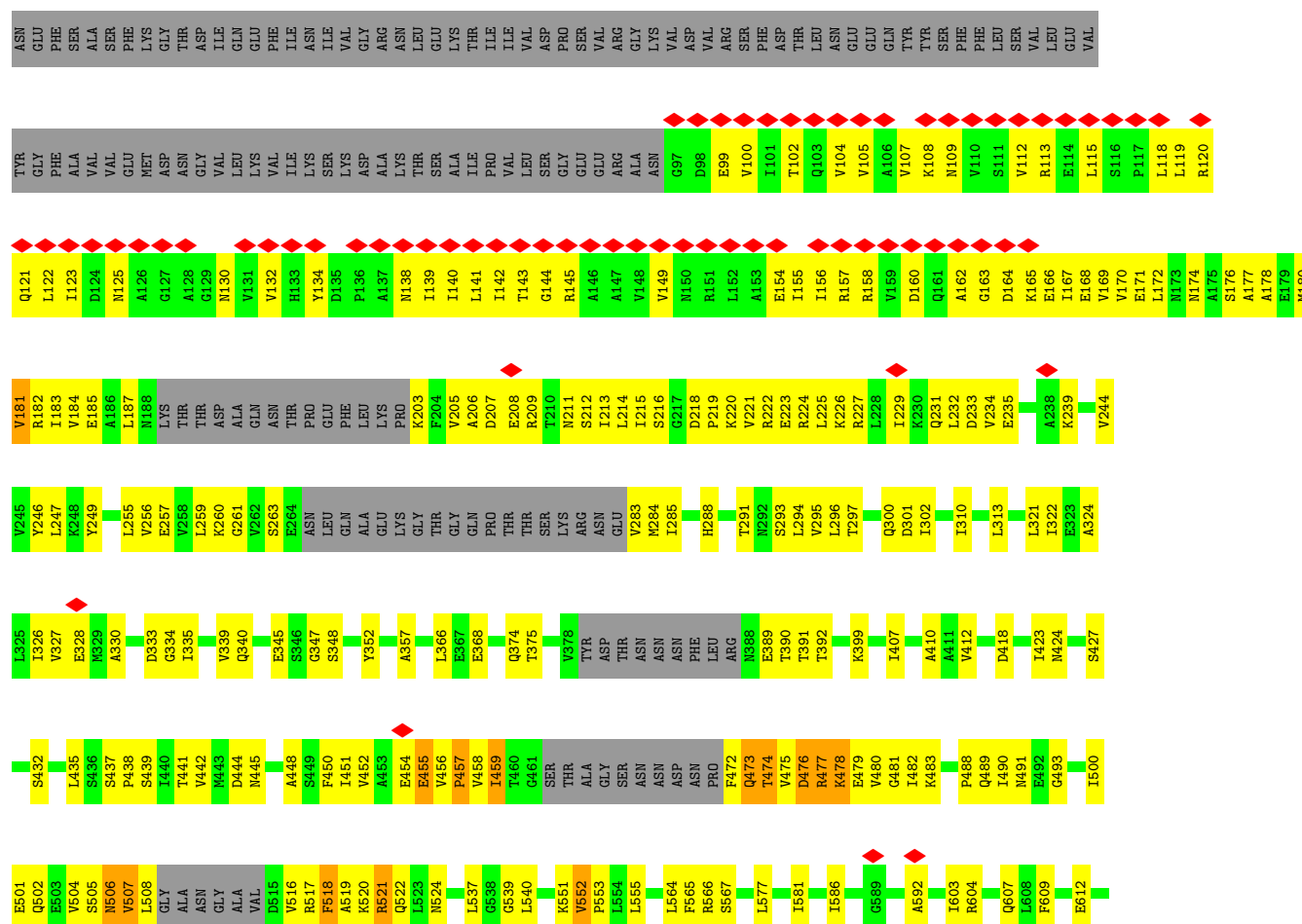


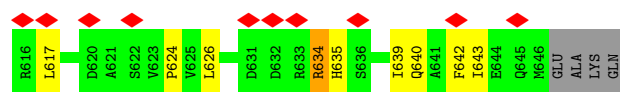
- Molecule 1: Type II secretion system protein D



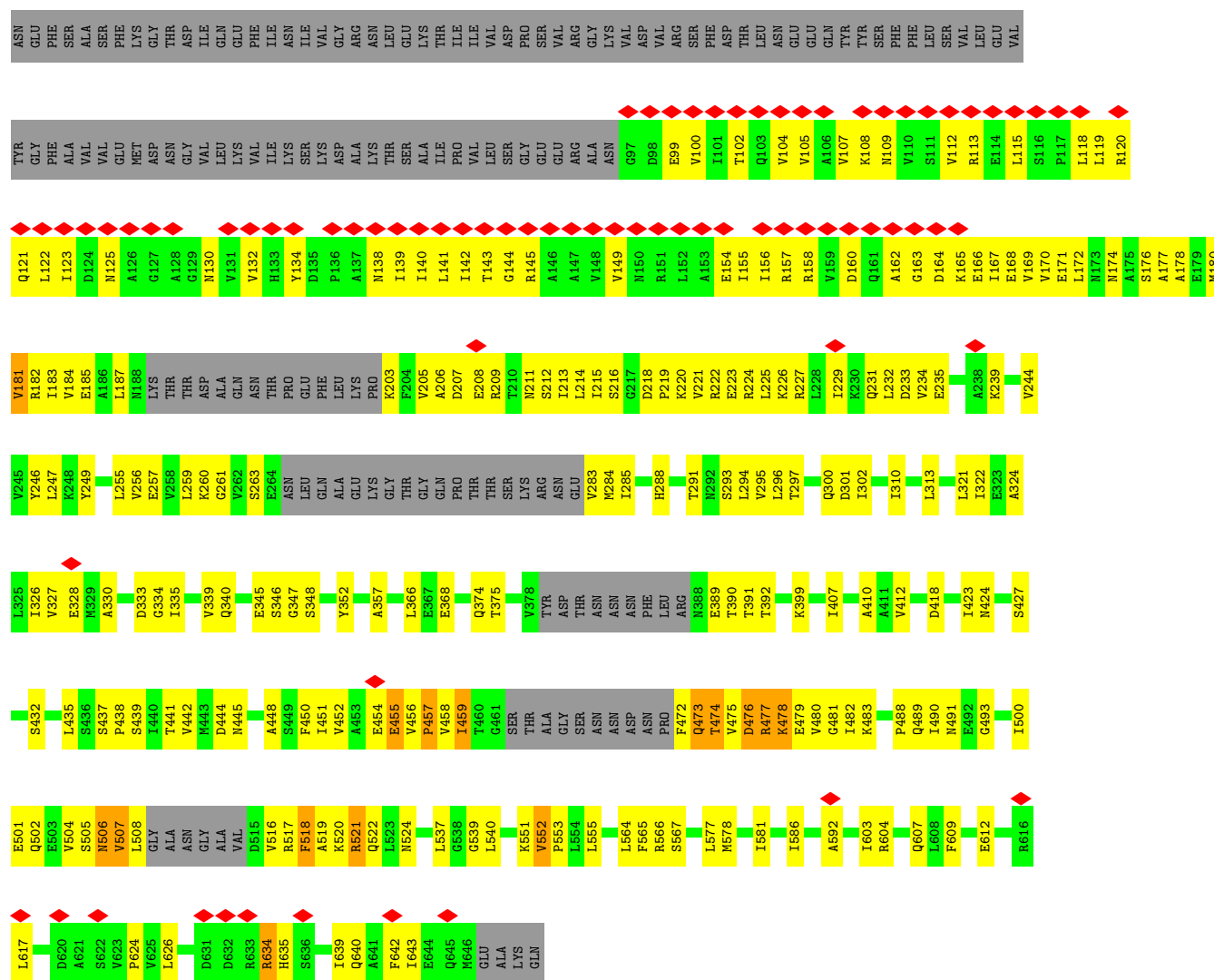
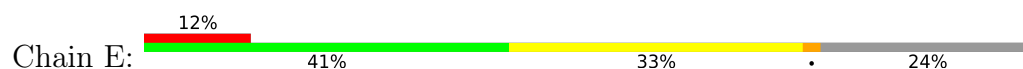


• Molecule 1: Type II secretion system protein D

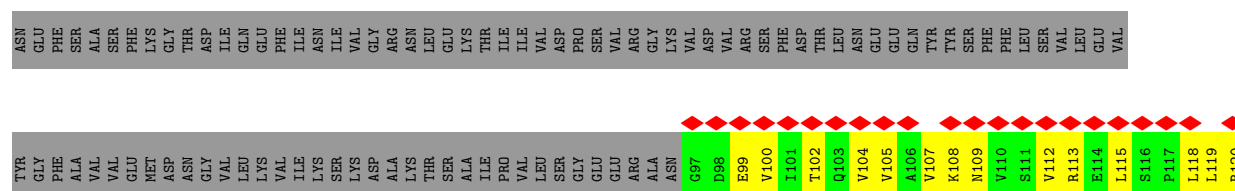
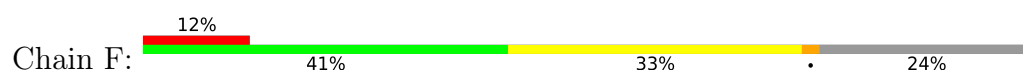


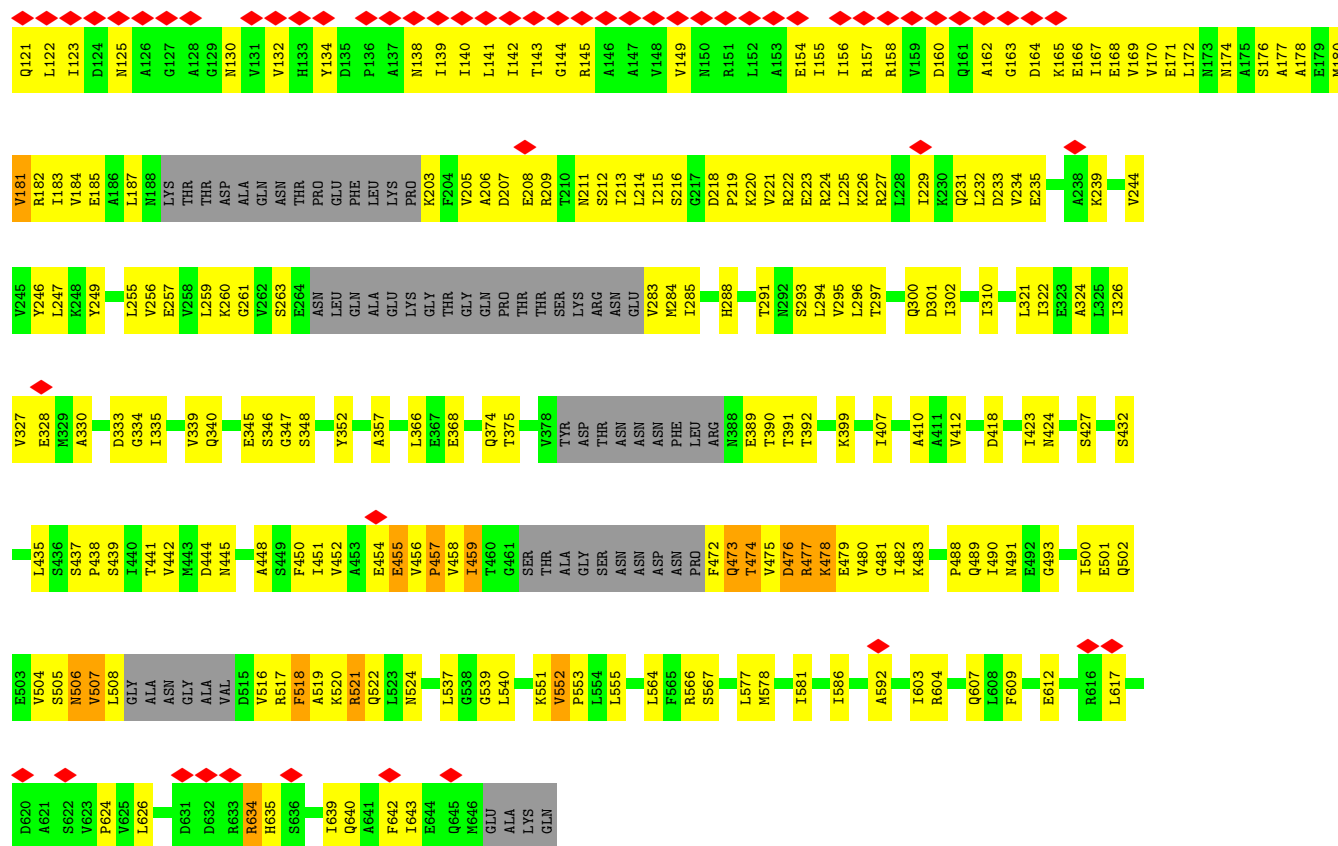


• Molecule 1: Type II secretion system protein D

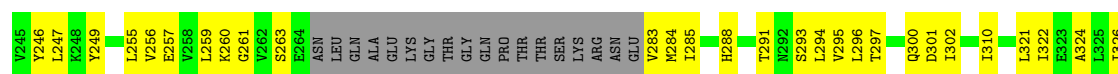
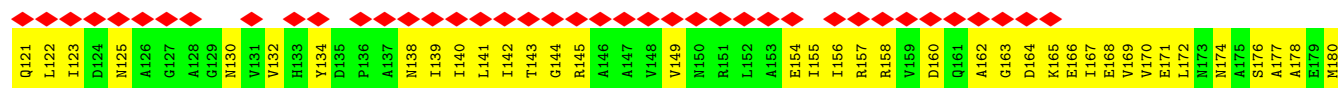
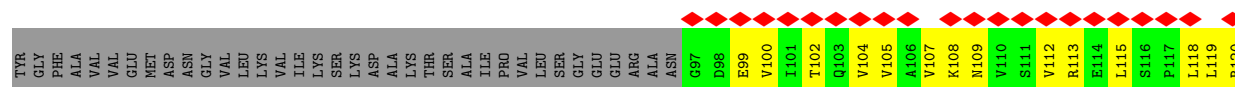
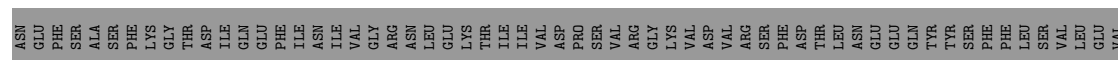
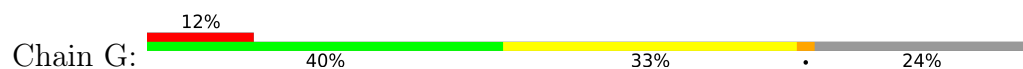


• Molecule 1: Type II secretion system protein D

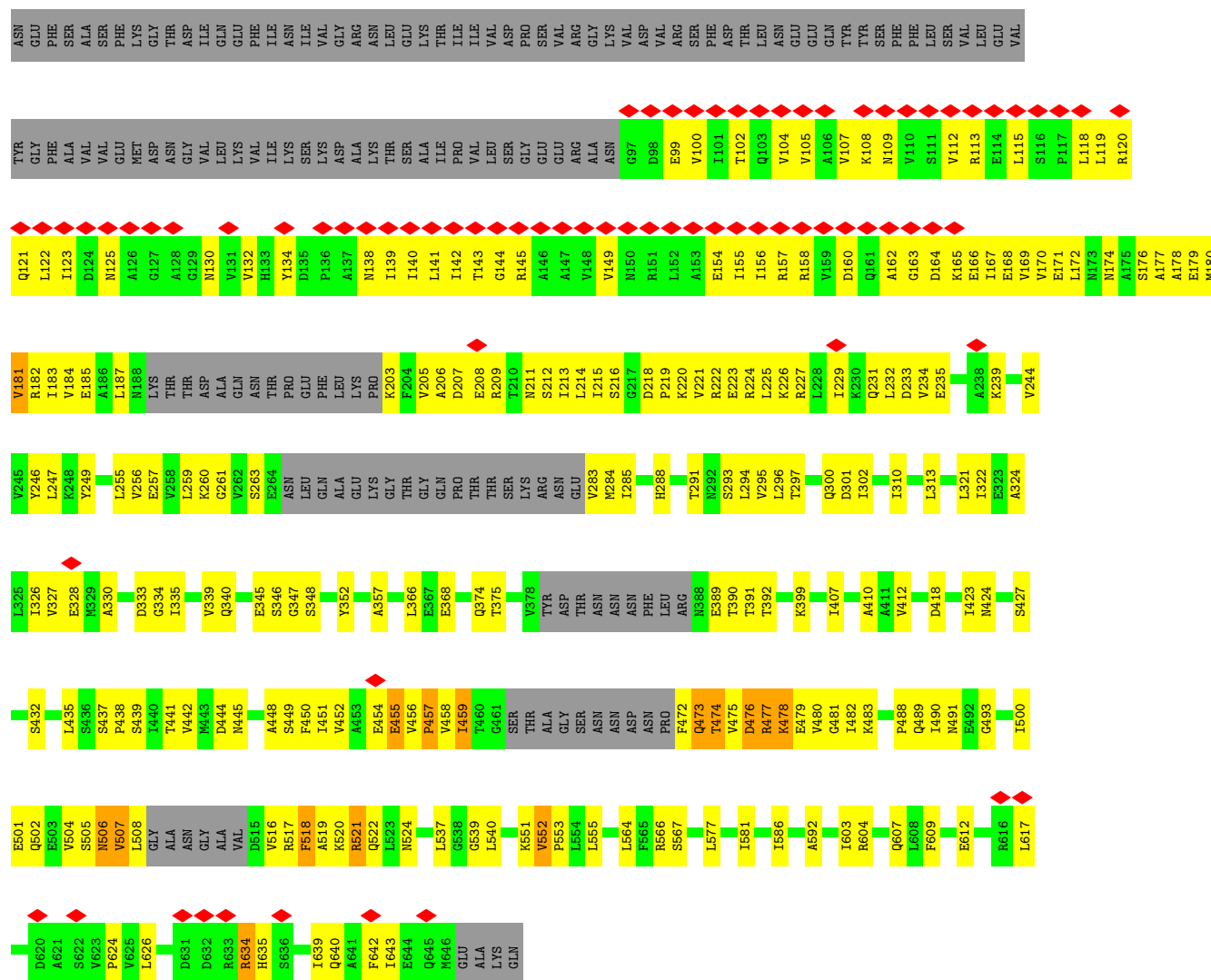




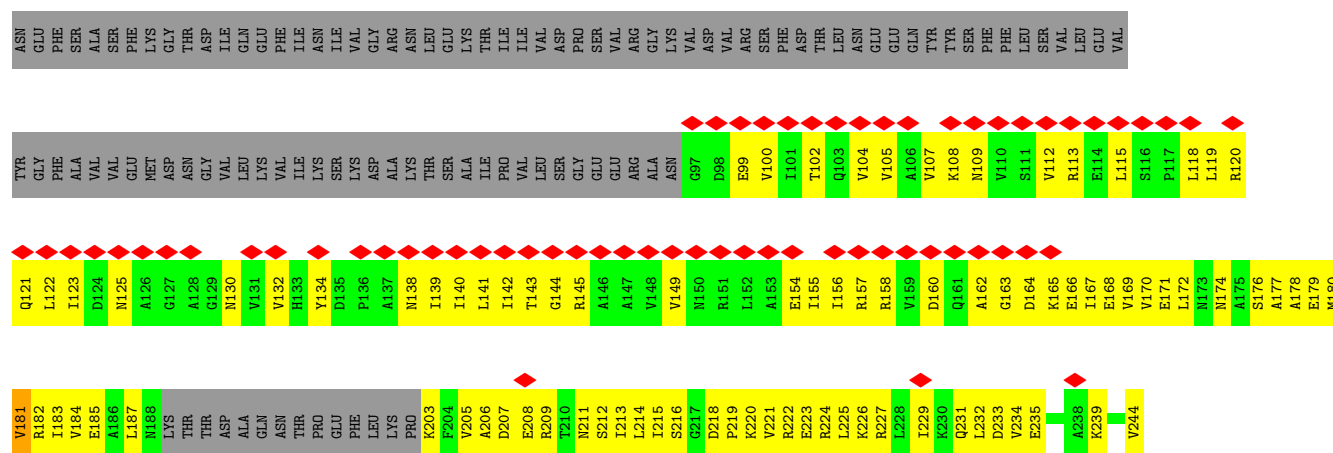
• Molecule 1: Type II secretion system protein D

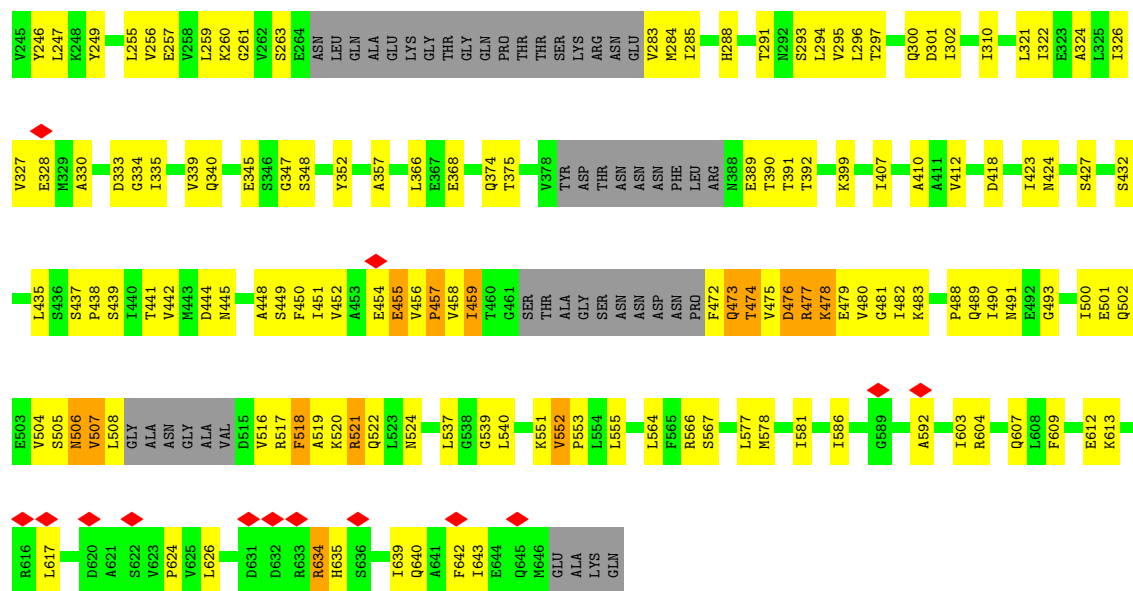




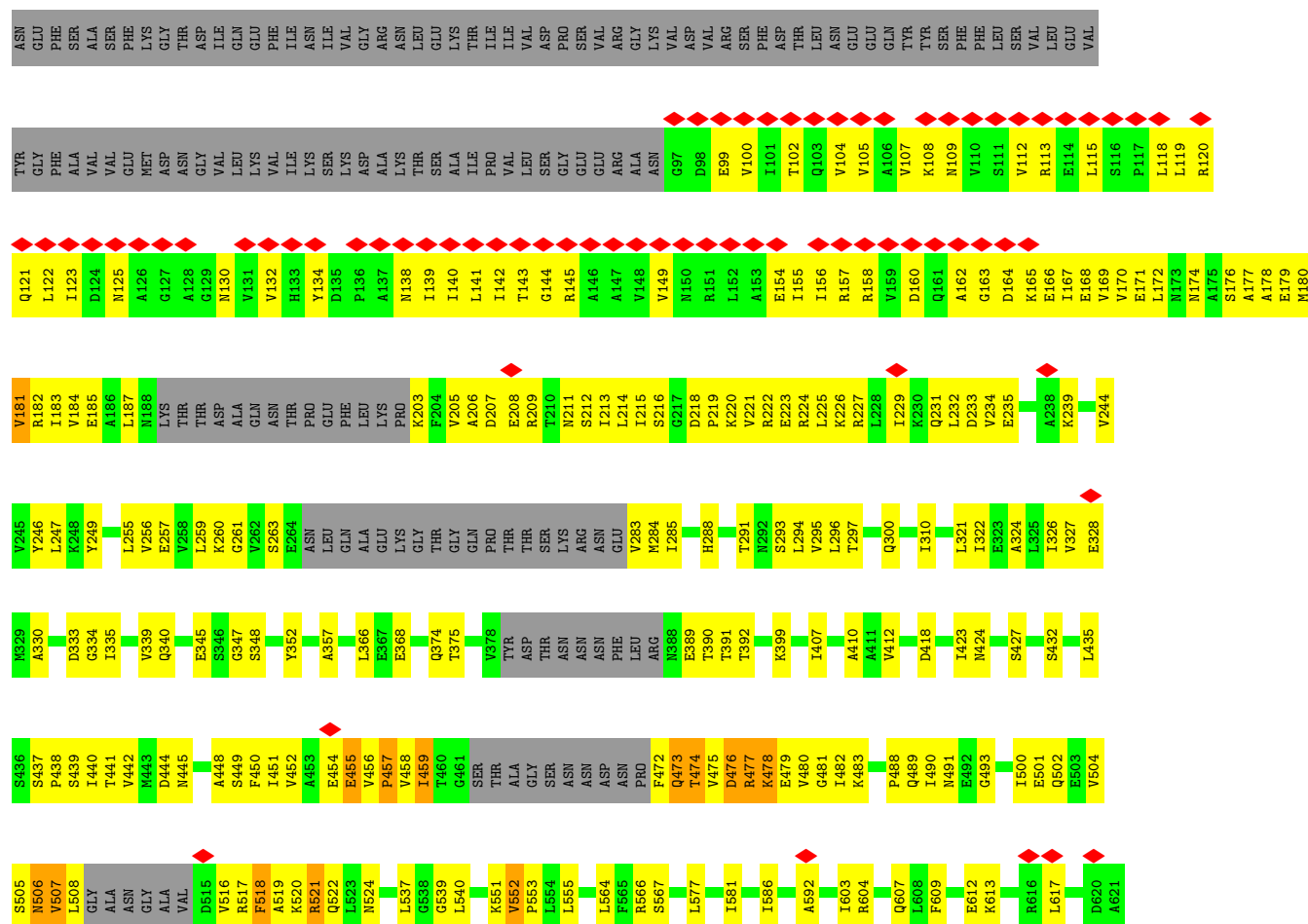
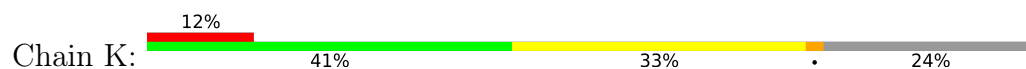


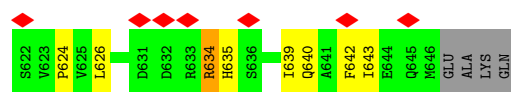
• Molecule 1: Type II secretion system protein D



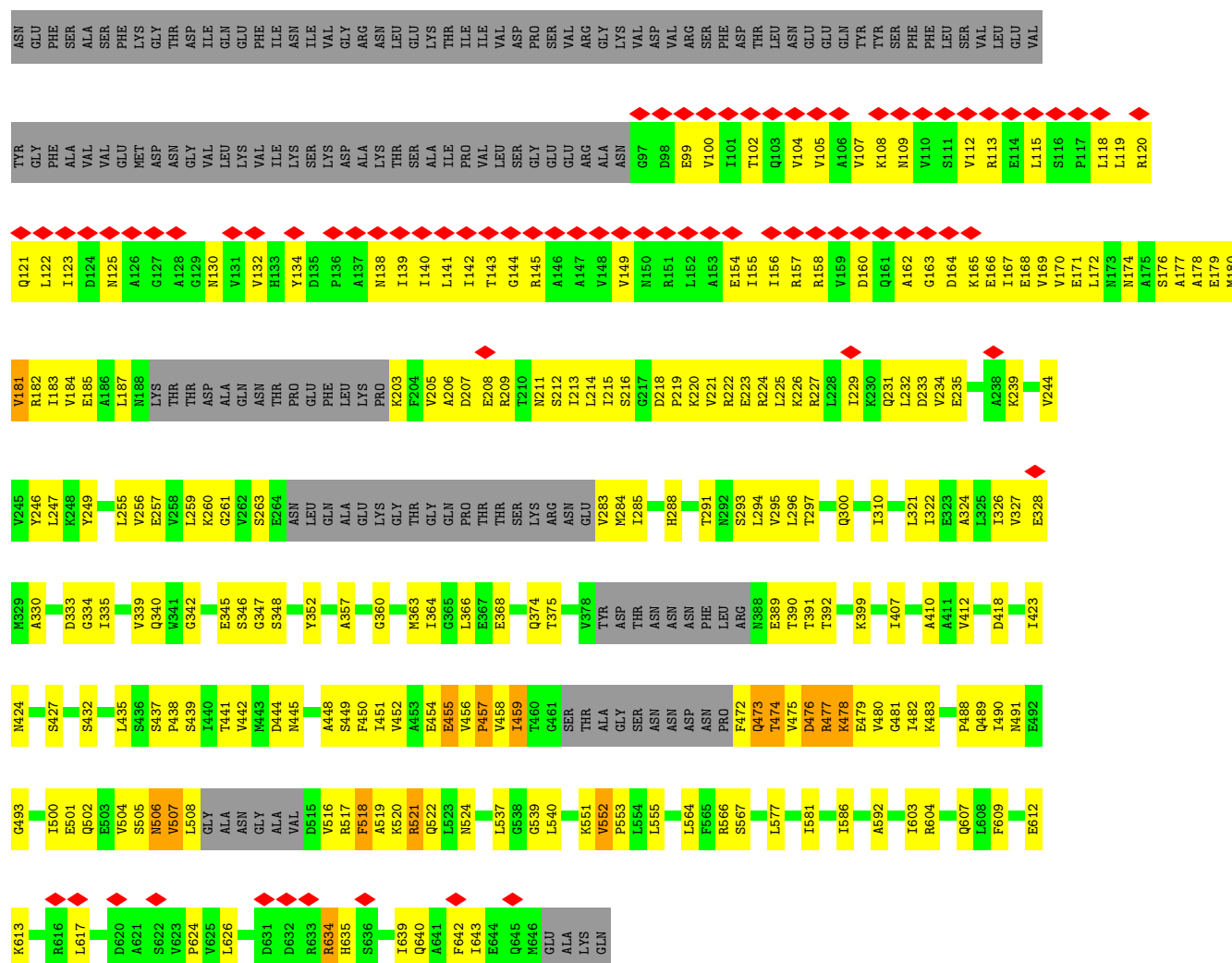
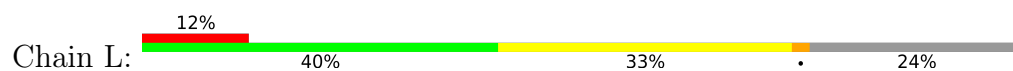


• Molecule 1: Type II secretion system protein D

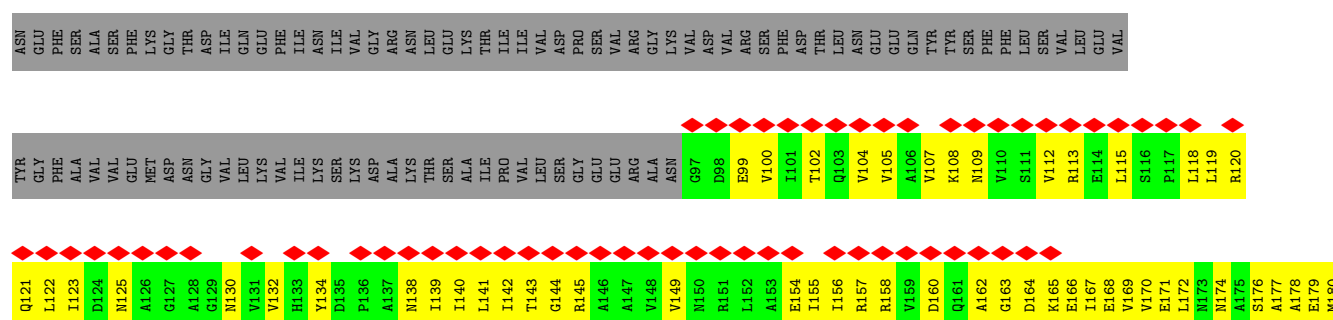


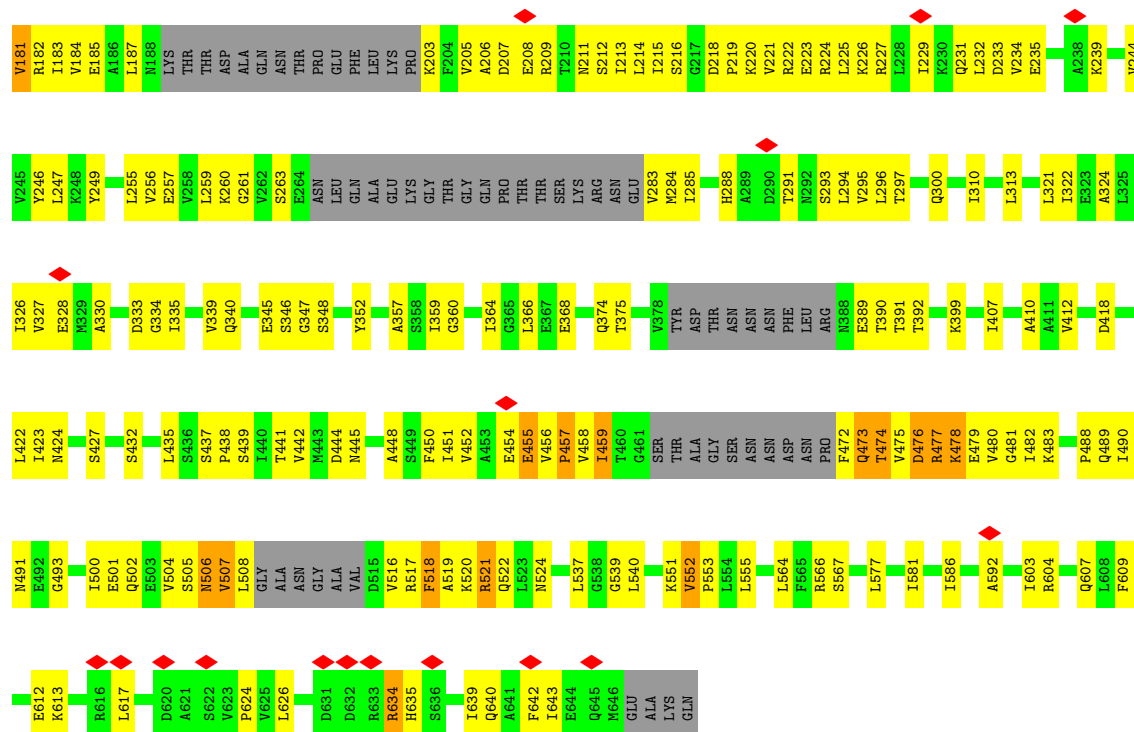


• Molecule 1: Type II secretion system protein D

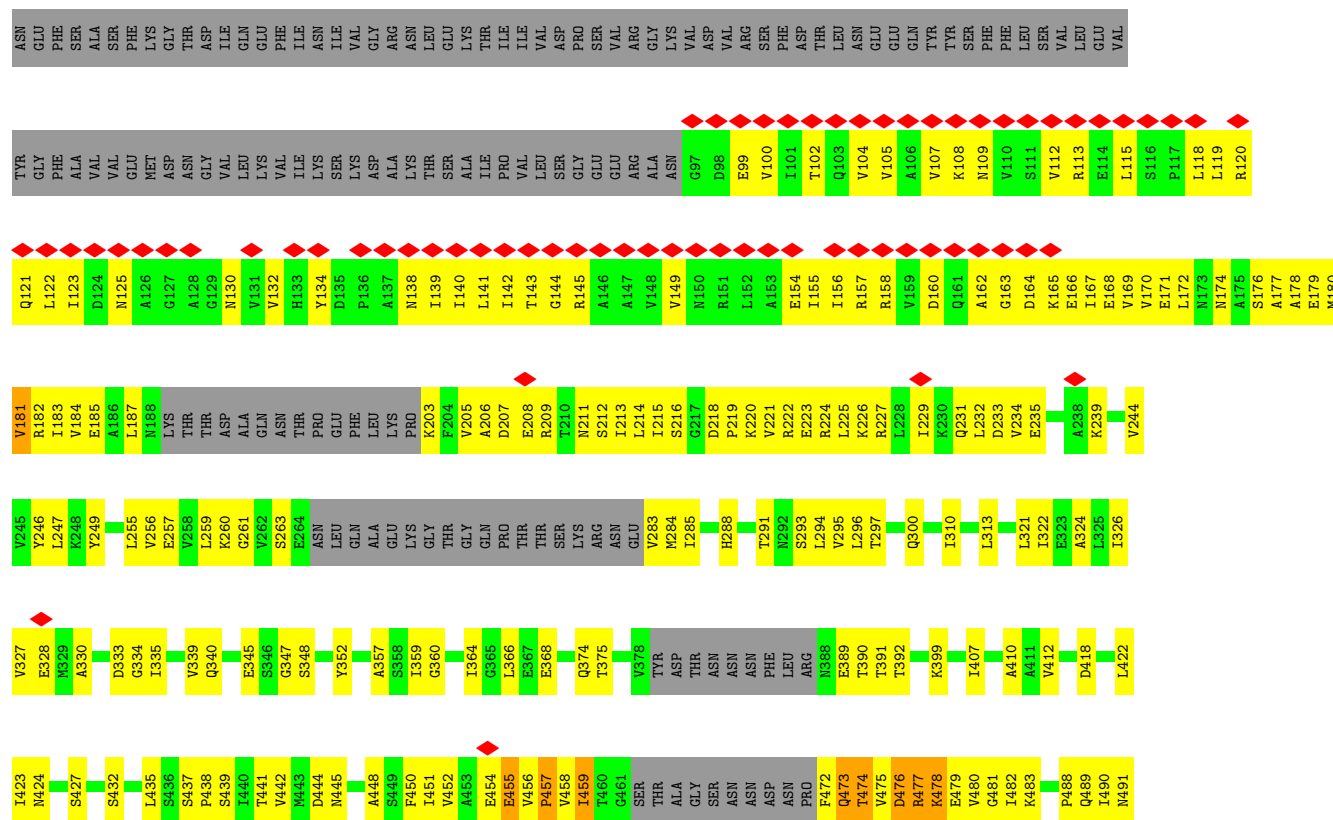


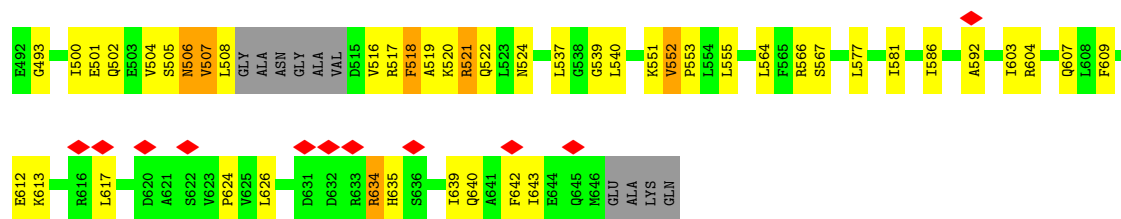
• Molecule 1: Type II secretion system protein D



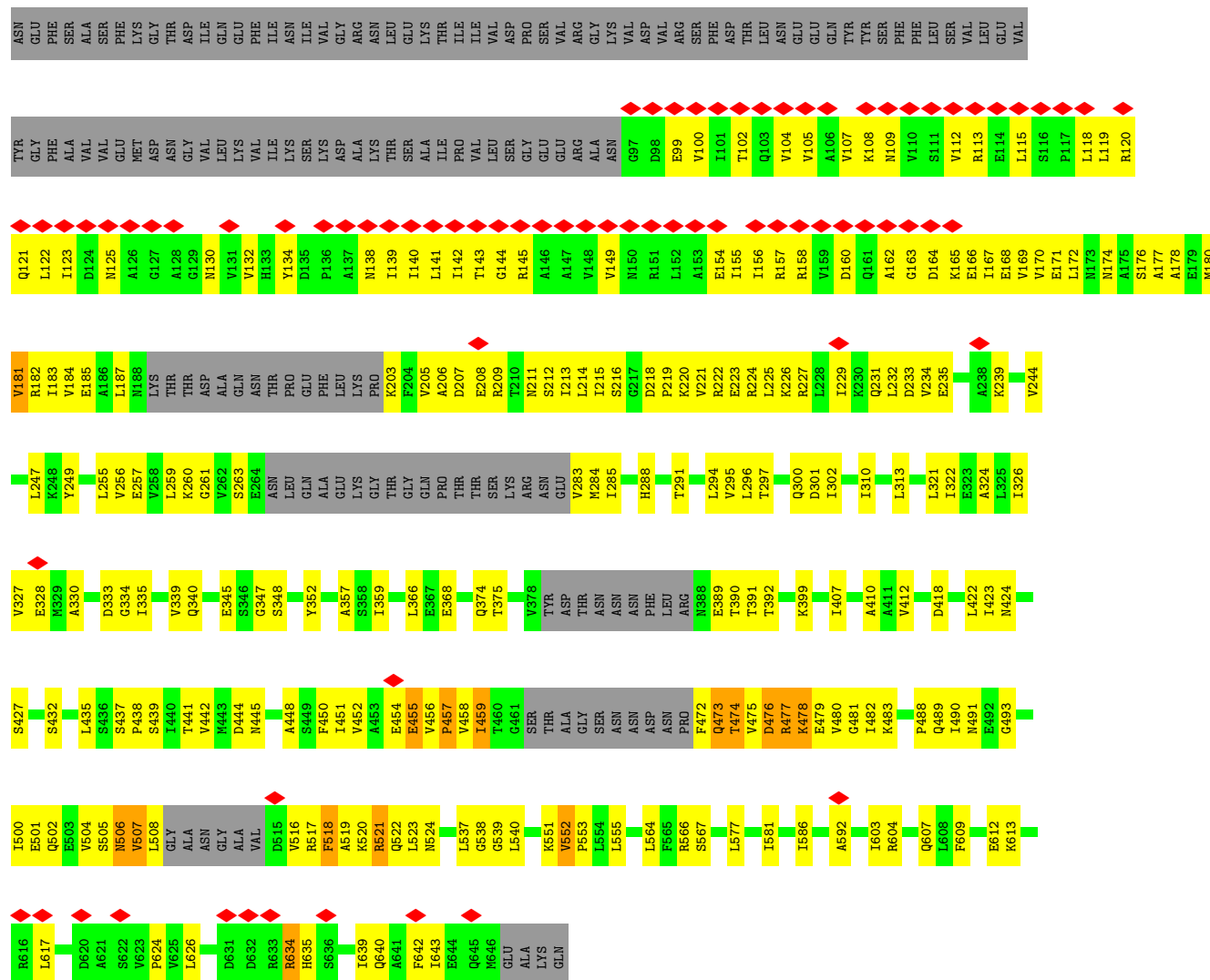
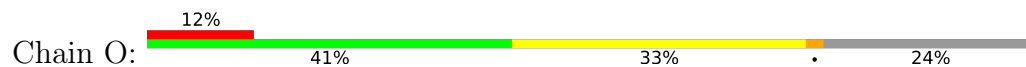


• Molecule 1: Type II secretion system protein D





• Molecule 1: Type II secretion system protein D



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C15 | Depositor |
| Number of particles used | 26955 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.6 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.109 | Depositor |
| Minimum map value | -0.046 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.02 | Depositor |
| Map size (Å) | 501.6, 501.6, 501.6 | wwPDB |
| Map dimensions | 380, 380, 380 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.32, 1.32, 1.32 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | B | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | C | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | D | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | E | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | F | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | G | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | H | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | I | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | J | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | K | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | L | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | M | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | N | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| 1 | O | 0.41 | 1/3786 (0.0%) | 0.64 | 4/5117 (0.1%) |
| All | All | 0.41 | 15/56790 (0.0%) | 0.64 | 60/76755 (0.1%) |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | M | 457 | PRO | N-CD | 5.24 | 1.55 | 1.47 |
| 1 | E | 457 | PRO | N-CD | 5.23 | 1.55 | 1.47 |
| 1 | J | 457 | PRO | N-CD | 5.23 | 1.55 | 1.47 |
| 1 | C | 457 | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 1 | B | 457 | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 1 | L | 457 | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 1 | A | 457 | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 1 | G | 457 | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 1 | H | 457 | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 1 | F | 457 | PRO | N-CD | 5.20 | 1.55 | 1.47 |
| 1 | O | 457 | PRO | N-CD | 5.20 | 1.55 | 1.47 |
| 1 | K | 457 | PRO | N-CD | 5.20 | 1.55 | 1.47 |
| 1 | D | 457 | PRO | N-CD | 5.19 | 1.55 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | N | 457 | PRO | N-CD | 5.19 | 1.55 | 1.47 |
| 1 | I | 457 | PRO | N-CD | 5.19 | 1.55 | 1.47 |

All (60) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | B | 507 | VAL | CB-CA-C | -10.70 | 91.07 | 111.40 |
| 1 | E | 507 | VAL | CB-CA-C | -10.70 | 91.07 | 111.40 |
| 1 | C | 507 | VAL | CB-CA-C | -10.70 | 91.07 | 111.40 |
| 1 | I | 507 | VAL | CB-CA-C | -10.70 | 91.08 | 111.40 |
| 1 | M | 507 | VAL | CB-CA-C | -10.70 | 91.08 | 111.40 |
| 1 | G | 507 | VAL | CB-CA-C | -10.69 | 91.08 | 111.40 |
| 1 | A | 507 | VAL | CB-CA-C | -10.69 | 91.09 | 111.40 |
| 1 | O | 507 | VAL | CB-CA-C | -10.69 | 91.09 | 111.40 |
| 1 | H | 507 | VAL | CB-CA-C | -10.69 | 91.09 | 111.40 |
| 1 | L | 507 | VAL | CB-CA-C | -10.69 | 91.09 | 111.40 |
| 1 | K | 507 | VAL | CB-CA-C | -10.69 | 91.09 | 111.40 |
| 1 | F | 507 | VAL | CB-CA-C | -10.68 | 91.10 | 111.40 |
| 1 | J | 507 | VAL | CB-CA-C | -10.68 | 91.10 | 111.40 |
| 1 | D | 507 | VAL | CB-CA-C | -10.68 | 91.11 | 111.40 |
| 1 | N | 507 | VAL | CB-CA-C | -10.68 | 91.11 | 111.40 |
| 1 | I | 552 | VAL | C-N-CD | -6.92 | 105.38 | 120.60 |
| 1 | D | 552 | VAL | C-N-CD | -6.92 | 105.39 | 120.60 |
| 1 | N | 552 | VAL | C-N-CD | -6.91 | 105.40 | 120.60 |
| 1 | C | 552 | VAL | C-N-CD | -6.90 | 105.41 | 120.60 |
| 1 | F | 552 | VAL | C-N-CD | -6.90 | 105.42 | 120.60 |
| 1 | J | 552 | VAL | C-N-CD | -6.90 | 105.41 | 120.60 |
| 1 | K | 552 | VAL | C-N-CD | -6.90 | 105.42 | 120.60 |
| 1 | A | 552 | VAL | C-N-CD | -6.90 | 105.42 | 120.60 |
| 1 | O | 552 | VAL | C-N-CD | -6.90 | 105.42 | 120.60 |
| 1 | M | 552 | VAL | C-N-CD | -6.90 | 105.43 | 120.60 |
| 1 | B | 552 | VAL | C-N-CD | -6.89 | 105.43 | 120.60 |
| 1 | G | 552 | VAL | C-N-CD | -6.89 | 105.43 | 120.60 |
| 1 | E | 552 | VAL | C-N-CD | -6.89 | 105.44 | 120.60 |
| 1 | H | 552 | VAL | C-N-CD | -6.88 | 105.46 | 120.60 |
| 1 | L | 552 | VAL | C-N-CD | -6.88 | 105.46 | 120.60 |
| 1 | D | 634 | ARG | N-CA-C | 5.34 | 125.43 | 111.00 |
| 1 | B | 634 | ARG | N-CA-C | 5.34 | 125.43 | 111.00 |
| 1 | C | 634 | ARG | N-CA-C | 5.33 | 125.40 | 111.00 |
| 1 | E | 634 | ARG | N-CA-C | 5.33 | 125.40 | 111.00 |
| 1 | F | 634 | ARG | N-CA-C | 5.33 | 125.40 | 111.00 |
| 1 | K | 634 | ARG | N-CA-C | 5.33 | 125.39 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | J | 634 | ARG | N-CA-C | 5.33 | 125.38 | 111.00 |
| 1 | M | 634 | ARG | N-CA-C | 5.33 | 125.38 | 111.00 |
| 1 | A | 634 | ARG | N-CA-C | 5.32 | 125.38 | 111.00 |
| 1 | H | 634 | ARG | N-CA-C | 5.32 | 125.37 | 111.00 |
| 1 | O | 634 | ARG | N-CA-C | 5.32 | 125.37 | 111.00 |
| 1 | G | 634 | ARG | N-CA-C | 5.32 | 125.37 | 111.00 |
| 1 | N | 634 | ARG | N-CA-C | 5.32 | 125.37 | 111.00 |
| 1 | L | 634 | ARG | N-CA-C | 5.32 | 125.36 | 111.00 |
| 1 | I | 634 | ARG | N-CA-C | 5.31 | 125.35 | 111.00 |
| 1 | D | 552 | VAL | C-N-CA | 5.25 | 144.05 | 122.00 |
| 1 | F | 552 | VAL | C-N-CA | 5.25 | 144.04 | 122.00 |
| 1 | E | 552 | VAL | C-N-CA | 5.25 | 144.04 | 122.00 |
| 1 | I | 552 | VAL | C-N-CA | 5.25 | 144.03 | 122.00 |
| 1 | J | 552 | VAL | C-N-CA | 5.25 | 144.03 | 122.00 |
| 1 | B | 552 | VAL | C-N-CA | 5.24 | 144.02 | 122.00 |
| 1 | K | 552 | VAL | C-N-CA | 5.24 | 144.03 | 122.00 |
| 1 | N | 552 | VAL | C-N-CA | 5.24 | 144.03 | 122.00 |
| 1 | A | 552 | VAL | C-N-CA | 5.24 | 144.02 | 122.00 |
| 1 | C | 552 | VAL | C-N-CA | 5.24 | 144.02 | 122.00 |
| 1 | G | 552 | VAL | C-N-CA | 5.24 | 144.01 | 122.00 |
| 1 | O | 552 | VAL | C-N-CA | 5.24 | 143.99 | 122.00 |
| 1 | H | 552 | VAL | C-N-CA | 5.23 | 143.98 | 122.00 |
| 1 | L | 552 | VAL | C-N-CA | 5.23 | 143.98 | 122.00 |
| 1 | M | 552 | VAL | C-N-CA | 5.23 | 143.98 | 122.00 |

There are no chirality outliers.

There are no planarity outliers.

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 | 3756 | 0 | 3858 | 323 | 0 |
| 1 | B | 3756 | 0 | 3858 | 327 | 0 |
| 1 | C | 3756 | 0 | 3858 | 320 | 0 |
| 1 | D | 3756 | 0 | 3858 | 317 | 0 |
| 1 | E | 3756 | 0 | 3858 | 319 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | F | 3756 | 0 | 3858 | 319 | 0 |
| 1 | G | 3756 | 0 | 3858 | 318 | 0 |
| 1 | H | 3756 | 0 | 3858 | 319 | 0 |
| 1 | I | 3756 | 0 | 3858 | 318 | 0 |
| 1 | J | 3756 | 0 | 3858 | 324 | 0 |
| 1 | K | 3756 | 0 | 3858 | 322 | 0 |
| 1 | L | 3756 | 0 | 3858 | 320 | 0 |
| 1 | M | 3756 | 0 | 3858 | 317 | 0 |
| 1 | N | 3756 | 0 | 3858 | 321 | 0 |
| 1 | O | 3756 | 0 | 3858 | 324 | 0 |
| All | All | 56340 | 0 | 57870 | 4309 | 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 38.

All (4309) 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:G:481:GLY:H | 1:G:505:SER:CB | 1.22 | 1.53 |
| 1:I:481:GLY:H | 1:I:505:SER:CB | 1.22 | 1.53 |
| 1:L:481:GLY:H | 1:L:505:SER:CB | 1.22 | 1.52 |
| 1:N:481:GLY:H | 1:N:505:SER:CB | 1.22 | 1.52 |
| 1:D:481:GLY:H | 1:D:505:SER:CB | 1.22 | 1.52 |
| 1:K:481:GLY:H | 1:K:505:SER:CB | 1.22 | 1.52 |
| 1:E:481:GLY:H | 1:E:505:SER:CB | 1.22 | 1.51 |
| 1:B:481:GLY:H | 1:B:505:SER:CB | 1.22 | 1.51 |
| 1:F:481:GLY:H | 1:F:505:SER:CB | 1.22 | 1.51 |
| 1:J:481:GLY:H | 1:J:505:SER:CB | 1.22 | 1.50 |
| 1:A:481:GLY:H | 1:A:505:SER:CB | 1.22 | 1.50 |
| 1:M:481:GLY:H | 1:M:505:SER:CB | 1.22 | 1.49 |
| 1:O:481:GLY:H | 1:O:505:SER:CB | 1.22 | 1.49 |
| 1:H:481:GLY:H | 1:H:505:SER:CB | 1.22 | 1.48 |
| 1:C:481:GLY:H | 1:C:505:SER:CB | 1.22 | 1.47 |
| 1:H:480:VAL:CB | 1:H:505:SER:OG | 1.65 | 1.45 |
| 1:D:480:VAL:CB | 1:D:505:SER:OG | 1.65 | 1.45 |
| 1:N:480:VAL:CB | 1:N:505:SER:OG | 1.65 | 1.45 |
| 1:I:480:VAL:CB | 1:I:505:SER:OG | 1.65 | 1.45 |
| 1:O:480:VAL:CB | 1:O:505:SER:OG | 1.65 | 1.45 |
| 1:C:480:VAL:CB | 1:C:505:SER:OG | 1.65 | 1.44 |
| 1:G:480:VAL:CB | 1:G:505:SER:OG | 1.65 | 1.44 |
| 1:M:480:VAL:CB | 1:M:505:SER:OG | 1.65 | 1.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:A:480:VAL:CB | 1:A:505:SER:OG | 1.65 | 1.43 |
| 1:L:480:VAL:CB | 1:L:505:SER:OG | 1.65 | 1.43 |
| 1:E:480:VAL:CB | 1:E:505:SER:OG | 1.65 | 1.43 |
| 1:K:481:GLY:N | 1:K:505:SER:HB3 | 1.12 | 1.43 |
| 1:J:481:GLY:N | 1:J:505:SER:HB3 | 1.12 | 1.43 |
| 1:B:480:VAL:CB | 1:B:505:SER:OG | 1.65 | 1.42 |
| 1:J:480:VAL:CB | 1:J:505:SER:OG | 1.65 | 1.42 |
| 1:K:480:VAL:CB | 1:K:505:SER:OG | 1.65 | 1.42 |
| 1:L:481:GLY:N | 1:L:505:SER:HB3 | 1.12 | 1.42 |
| 1:F:480:VAL:CB | 1:F:505:SER:OG | 1.65 | 1.42 |
| 1:I:481:GLY:N | 1:I:505:SER:HB3 | 1.12 | 1.42 |
| 1:M:481:GLY:N | 1:M:505:SER:HB3 | 1.12 | 1.40 |
| 1:H:481:GLY:N | 1:H:505:SER:HB3 | 1.12 | 1.40 |
| 1:D:481:GLY:N | 1:D:505:SER:HB3 | 1.12 | 1.39 |
| 1:C:481:GLY:N | 1:C:505:SER:HB3 | 1.12 | 1.39 |
| 1:E:481:GLY:N | 1:E:505:SER:HB3 | 1.12 | 1.39 |
| 1:F:481:GLY:N | 1:F:505:SER:HB3 | 1.12 | 1.38 |
| 1:B:481:GLY:N | 1:B:505:SER:HB3 | 1.12 | 1.38 |
| 1:N:481:GLY:N | 1:N:505:SER:HB3 | 1.12 | 1.37 |
| 1:G:481:GLY:N | 1:G:505:SER:HB3 | 1.12 | 1.37 |
| 1:O:481:GLY:N | 1:O:505:SER:HB3 | 1.12 | 1.37 |
| 1:A:481:GLY:N | 1:A:505:SER:HB3 | 1.12 | 1.37 |
| 1:C:480:VAL:CA | 1:C:505:SER:OG | 1.74 | 1.36 |
| 1:B:480:VAL:CA | 1:B:505:SER:OG | 1.74 | 1.35 |
| 1:D:480:VAL:CA | 1:D:505:SER:OG | 1.74 | 1.35 |
| 1:G:480:VAL:CA | 1:G:505:SER:OG | 1.74 | 1.35 |
| 1:M:480:VAL:CA | 1:M:505:SER:OG | 1.74 | 1.35 |
| 1:F:480:VAL:CA | 1:F:505:SER:OG | 1.74 | 1.34 |
| 1:J:480:VAL:CA | 1:J:505:SER:OG | 1.74 | 1.34 |
| 1:I:480:VAL:CA | 1:I:505:SER:OG | 1.74 | 1.34 |
| 1:L:480:VAL:CA | 1:L:505:SER:OG | 1.74 | 1.34 |
| 1:H:480:VAL:CA | 1:H:505:SER:OG | 1.74 | 1.34 |
| 1:N:480:VAL:CA | 1:N:505:SER:OG | 1.74 | 1.34 |
| 1:A:480:VAL:CA | 1:A:505:SER:OG | 1.74 | 1.33 |
| 1:E:480:VAL:CA | 1:E:505:SER:OG | 1.74 | 1.33 |
| 1:K:480:VAL:CA | 1:K:505:SER:OG | 1.74 | 1.33 |
| 1:O:480:VAL:CA | 1:O:505:SER:OG | 1.74 | 1.32 |
| 1:G:480:VAL:HB | 1:G:505:SER:OG | 1.15 | 1.31 |
| 1:H:480:VAL:HB | 1:H:505:SER:OG | 1.15 | 1.31 |
| 1:I:480:VAL:HB | 1:I:505:SER:OG | 1.15 | 1.31 |
| 1:F:480:VAL:HB | 1:F:505:SER:OG | 1.15 | 1.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:480:VAL:HB | 1:E:505:SER:OG | 1.15 | 1.29 |
| 1:J:459:ILE:HG23 | 1:J:474:THR:O | 1.31 | 1.28 |
| 1:D:459:ILE:HG23 | 1:D:474:THR:O | 1.31 | 1.27 |
| 1:D:480:VAL:HB | 1:D:505:SER:OG | 1.15 | 1.27 |
| 1:B:459:ILE:HG23 | 1:B:474:THR:O | 1.31 | 1.26 |
| 1:I:459:ILE:HG23 | 1:I:474:THR:O | 1.31 | 1.26 |
| 1:M:480:VAL:HB | 1:M:505:SER:OG | 1.15 | 1.26 |
| 1:B:481:GLY:N | 1:B:505:SER:CB | 1.88 | 1.25 |
| 1:M:459:ILE:HG23 | 1:M:474:THR:O | 1.31 | 1.25 |
| 1:A:459:ILE:HG23 | 1:A:474:THR:O | 1.31 | 1.25 |
| 1:K:459:ILE:HG23 | 1:K:474:THR:O | 1.31 | 1.25 |
| 1:N:480:VAL:HB | 1:N:505:SER:OG | 1.15 | 1.25 |
| 1:O:481:GLY:N | 1:O:505:SER:CB | 1.88 | 1.25 |
| 1:C:481:GLY:N | 1:C:505:SER:CB | 1.88 | 1.24 |
| 1:L:459:ILE:HG23 | 1:L:474:THR:O | 1.31 | 1.24 |
| 1:O:480:VAL:HB | 1:O:505:SER:OG | 1.15 | 1.24 |
| 1:F:459:ILE:HG23 | 1:F:474:THR:O | 1.31 | 1.24 |
| 1:C:480:VAL:HB | 1:C:505:SER:OG | 1.15 | 1.24 |
| 1:G:459:ILE:HG23 | 1:G:474:THR:O | 1.31 | 1.24 |
| 1:C:459:ILE:HG23 | 1:C:474:THR:O | 1.31 | 1.24 |
| 1:N:459:ILE:HG23 | 1:N:474:THR:O | 1.31 | 1.24 |
| 1:A:481:GLY:N | 1:A:505:SER:CB | 1.88 | 1.23 |
| 1:O:459:ILE:HG23 | 1:O:474:THR:O | 1.31 | 1.23 |
| 1:D:481:GLY:N | 1:D:505:SER:CB | 1.88 | 1.22 |
| 1:H:459:ILE:HG23 | 1:H:474:THR:O | 1.31 | 1.22 |
| 1:N:481:GLY:N | 1:N:505:SER:CB | 1.88 | 1.22 |
| 1:A:234:VAL:O | 1:B:209:ARG:NH1 | 1.72 | 1.22 |
| 1:B:234:VAL:O | 1:C:209:ARG:NH1 | 1.72 | 1.22 |
| 1:E:481:GLY:N | 1:E:505:SER:CB | 1.88 | 1.21 |
| 1:M:234:VAL:O | 1:N:209:ARG:NH1 | 1.72 | 1.21 |
| 1:E:459:ILE:HG23 | 1:E:474:THR:O | 1.31 | 1.21 |
| 1:I:234:VAL:O | 1:J:209:ARG:NH1 | 1.72 | 1.21 |
| 1:N:234:VAL:O | 1:O:209:ARG:NH1 | 1.72 | 1.21 |
| 1:B:480:VAL:HB | 1:B:505:SER:OG | 1.15 | 1.21 |
| 1:F:234:VAL:O | 1:G:209:ARG:NH1 | 1.72 | 1.20 |
| 1:H:234:VAL:O | 1:I:209:ARG:NH1 | 1.72 | 1.20 |
| 1:M:481:GLY:N | 1:M:505:SER:CB | 1.88 | 1.20 |
| 1:J:234:VAL:O | 1:K:209:ARG:NH1 | 1.72 | 1.20 |
| 1:L:480:VAL:HB | 1:L:505:SER:OG | 1.15 | 1.20 |
| 1:C:234:VAL:O | 1:D:209:ARG:NH1 | 1.72 | 1.20 |
| 1:E:234:VAL:O | 1:F:209:ARG:NH1 | 1.72 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:L:234:VAL:O | 1:M:209:ARG:NH1 | 1.72 | 1.20 |
| 1:A:209:ARG:NH1 | 1:O:234:VAL:O | 1.72 | 1.20 |
| 1:G:234:VAL:O | 1:H:209:ARG:NH1 | 1.72 | 1.19 |
| 1:A:480:VAL:HB | 1:A:505:SER:OG | 1.15 | 1.19 |
| 1:D:234:VAL:O | 1:E:209:ARG:NH1 | 1.72 | 1.19 |
| 1:L:481:GLY:N | 1:L:505:SER:CB | 1.88 | 1.18 |
| 1:K:480:VAL:HB | 1:K:505:SER:OG | 1.15 | 1.18 |
| 1:F:481:GLY:N | 1:F:505:SER:CB | 1.88 | 1.17 |
| 1:E:459:ILE:HG21 | 1:E:473:GLN:HB2 | 1.27 | 1.17 |
| 1:K:234:VAL:O | 1:L:209:ARG:NH1 | 1.72 | 1.17 |
| 1:G:481:GLY:N | 1:G:505:SER:CB | 1.88 | 1.17 |
| 1:G:459:ILE:HG21 | 1:G:473:GLN:HB2 | 1.27 | 1.17 |
| 1:J:480:VAL:HB | 1:J:505:SER:OG | 1.15 | 1.16 |
| 1:J:481:GLY:N | 1:J:505:SER:CB | 1.88 | 1.15 |
| 1:H:481:GLY:N | 1:H:505:SER:CB | 1.88 | 1.15 |
| 1:K:481:GLY:N | 1:K:505:SER:CB | 1.88 | 1.15 |
| 1:B:459:ILE:HG21 | 1:B:473:GLN:HB2 | 1.27 | 1.14 |
| 1:C:459:ILE:HG21 | 1:C:473:GLN:HB2 | 1.27 | 1.14 |
| 1:I:481:GLY:N | 1:I:505:SER:CB | 1.88 | 1.14 |
| 1:I:459:ILE:HG21 | 1:I:473:GLN:HB2 | 1.27 | 1.14 |
| 1:H:459:ILE:HG21 | 1:H:473:GLN:HB2 | 1.27 | 1.13 |
| 1:J:167:ILE:HA | 1:J:215:ILE:O | 1.49 | 1.12 |
| 1:J:459:ILE:HG21 | 1:J:473:GLN:HB2 | 1.27 | 1.12 |
| 1:O:459:ILE:HG21 | 1:O:473:GLN:HB2 | 1.27 | 1.12 |
| 1:D:459:ILE:HG21 | 1:D:473:GLN:HB2 | 1.27 | 1.12 |
| 1:I:167:ILE:HA | 1:I:215:ILE:O | 1.49 | 1.12 |
| 1:D:167:ILE:HA | 1:D:215:ILE:O | 1.49 | 1.12 |
| 1:K:167:ILE:HA | 1:K:215:ILE:O | 1.49 | 1.12 |
| 1:A:459:ILE:HG21 | 1:A:473:GLN:HB2 | 1.27 | 1.11 |
| 1:C:167:ILE:HA | 1:C:215:ILE:O | 1.49 | 1.11 |
| 1:E:167:ILE:HA | 1:E:215:ILE:O | 1.49 | 1.11 |
| 1:H:167:ILE:HA | 1:H:215:ILE:O | 1.49 | 1.10 |
| 1:K:459:ILE:HG21 | 1:K:473:GLN:HB2 | 1.27 | 1.10 |
| 1:B:167:ILE:HA | 1:B:215:ILE:O | 1.49 | 1.10 |
| 1:L:167:ILE:HA | 1:L:215:ILE:O | 1.49 | 1.10 |
| 1:M:459:ILE:HG21 | 1:M:473:GLN:HB2 | 1.27 | 1.10 |
| 1:L:459:ILE:HG21 | 1:L:473:GLN:HB2 | 1.27 | 1.10 |
| 1:A:167:ILE:HA | 1:A:215:ILE:O | 1.49 | 1.09 |
| 1:N:459:ILE:HG21 | 1:N:473:GLN:HB2 | 1.27 | 1.09 |
| 1:F:167:ILE:HA | 1:F:215:ILE:O | 1.49 | 1.09 |
| 1:F:459:ILE:HG21 | 1:F:473:GLN:HB2 | 1.27 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:612:GLU:HG3 | 1:I:642:PHE:CE2 | 1.88 | 1.09 |
| 1:K:612:GLU:HG3 | 1:L:642:PHE:CE2 | 1.88 | 1.09 |
| 1:M:612:GLU:HG3 | 1:N:642:PHE:CE2 | 1.88 | 1.09 |
| 1:G:507:VAL:HG13 | 1:G:507:VAL:O | 1.53 | 1.09 |
| 1:L:612:GLU:HG3 | 1:M:642:PHE:CE2 | 1.88 | 1.09 |
| 1:I:612:GLU:HG3 | 1:J:642:PHE:CE2 | 1.88 | 1.08 |
| 1:O:167:ILE:HA | 1:O:215:ILE:O | 1.49 | 1.08 |
| 1:G:167:ILE:HA | 1:G:215:ILE:O | 1.49 | 1.08 |
| 1:N:167:ILE:HA | 1:N:215:ILE:O | 1.49 | 1.08 |
| 1:A:642:PHE:CE2 | 1:O:612:GLU:HG3 | 1.88 | 1.08 |
| 1:J:612:GLU:HG3 | 1:K:642:PHE:CE2 | 1.88 | 1.08 |
| 1:M:167:ILE:HA | 1:M:215:ILE:O | 1.49 | 1.08 |
| 1:D:612:GLU:HG3 | 1:E:642:PHE:CE2 | 1.88 | 1.08 |
| 1:F:507:VAL:O | 1:F:507:VAL:HG13 | 1.53 | 1.08 |
| 1:M:507:VAL:HG13 | 1:M:507:VAL:O | 1.53 | 1.08 |
| 1:C:612:GLU:HG3 | 1:D:642:PHE:CE2 | 1.88 | 1.08 |
| 1:F:612:GLU:HG3 | 1:G:642:PHE:CE2 | 1.88 | 1.08 |
| 1:G:612:GLU:HG3 | 1:H:642:PHE:CE2 | 1.88 | 1.08 |
| 1:L:507:VAL:HG13 | 1:L:507:VAL:O | 1.53 | 1.08 |
| 1:N:612:GLU:HG3 | 1:O:642:PHE:CE2 | 1.88 | 1.08 |
| 1:A:612:GLU:HG3 | 1:B:642:PHE:CE2 | 1.88 | 1.07 |
| 1:A:458:VAL:O | 1:A:476:ASP:N | 1.87 | 1.07 |
| 1:B:507:VAL:HG13 | 1:B:507:VAL:O | 1.53 | 1.07 |
| 1:C:458:VAL:O | 1:C:476:ASP:N | 1.87 | 1.07 |
| 1:D:458:VAL:O | 1:D:476:ASP:N | 1.87 | 1.07 |
| 1:H:507:VAL:O | 1:H:507:VAL:HG13 | 1.53 | 1.07 |
| 1:D:479:GLU:OE1 | 1:D:479:GLU:N | 1.88 | 1.07 |
| 1:E:612:GLU:HG3 | 1:F:642:PHE:CE2 | 1.88 | 1.07 |
| 1:F:479:GLU:OE1 | 1:F:479:GLU:N | 1.88 | 1.07 |
| 1:J:458:VAL:O | 1:J:476:ASP:N | 1.87 | 1.07 |
| 1:B:612:GLU:HG3 | 1:C:642:PHE:CE2 | 1.88 | 1.07 |
| 1:I:458:VAL:O | 1:I:476:ASP:N | 1.87 | 1.07 |
| 1:B:479:GLU:OE1 | 1:B:479:GLU:N | 1.88 | 1.06 |
| 1:F:458:VAL:O | 1:F:476:ASP:N | 1.87 | 1.06 |
| 1:K:459:ILE:CG2 | 1:K:474:THR:O | 2.03 | 1.06 |
| 1:M:459:ILE:CG2 | 1:M:474:THR:O | 2.03 | 1.06 |
| 1:B:458:VAL:O | 1:B:476:ASP:N | 1.87 | 1.06 |
| 1:C:507:VAL:O | 1:C:507:VAL:HG13 | 1.53 | 1.06 |
| 1:H:459:ILE:CG2 | 1:H:474:THR:O | 2.03 | 1.06 |
| 1:K:507:VAL:O | 1:K:507:VAL:HG13 | 1.53 | 1.06 |
| 1:N:507:VAL:O | 1:N:507:VAL:HG13 | 1.53 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:507:VAL:O | 1:A:507:VAL:HG13 | 1.53 | 1.06 |
| 1:F:459:ILE:CG2 | 1:F:474:THR:O | 2.03 | 1.06 |
| 1:G:459:ILE:CG2 | 1:G:474:THR:O | 2.03 | 1.06 |
| 1:H:479:GLU:N | 1:H:479:GLU:OE1 | 1.88 | 1.06 |
| 1:I:459:ILE:CG2 | 1:I:474:THR:O | 2.03 | 1.06 |
| 1:J:459:ILE:CG2 | 1:J:474:THR:O | 2.03 | 1.06 |
| 1:N:458:VAL:O | 1:N:476:ASP:N | 1.87 | 1.06 |
| 1:A:235:GLU:OE1 | 1:A:235:GLU:N | 1.89 | 1.06 |
| 1:E:235:GLU:OE1 | 1:E:235:GLU:N | 1.89 | 1.06 |
| 1:E:459:ILE:CG2 | 1:E:474:THR:O | 2.03 | 1.06 |
| 1:L:459:ILE:CG2 | 1:L:474:THR:O | 2.03 | 1.06 |
| 1:M:458:VAL:O | 1:M:476:ASP:N | 1.87 | 1.06 |
| 1:O:459:ILE:CG2 | 1:O:474:THR:O | 2.03 | 1.06 |
| 1:A:459:ILE:CG2 | 1:A:474:THR:O | 2.03 | 1.06 |
| 1:B:235:GLU:OE1 | 1:B:235:GLU:N | 1.89 | 1.06 |
| 1:C:459:ILE:CG2 | 1:C:474:THR:O | 2.03 | 1.06 |
| 1:I:479:GLU:OE1 | 1:I:479:GLU:N | 1.88 | 1.06 |
| 1:N:459:ILE:CG2 | 1:N:474:THR:O | 2.03 | 1.06 |
| 1:E:458:VAL:O | 1:E:476:ASP:N | 1.87 | 1.05 |
| 1:E:479:GLU:N | 1:E:479:GLU:OE1 | 1.88 | 1.05 |
| 1:G:479:GLU:OE1 | 1:G:479:GLU:N | 1.88 | 1.05 |
| 1:K:458:VAL:O | 1:K:476:ASP:N | 1.87 | 1.05 |
| 1:L:458:VAL:O | 1:L:476:ASP:N | 1.87 | 1.05 |
| 1:M:235:GLU:OE1 | 1:M:235:GLU:N | 1.89 | 1.05 |
| 1:F:235:GLU:N | 1:F:235:GLU:OE1 | 1.89 | 1.05 |
| 1:L:235:GLU:OE1 | 1:L:235:GLU:N | 1.89 | 1.05 |
| 1:D:235:GLU:OE1 | 1:D:235:GLU:N | 1.89 | 1.05 |
| 1:D:459:ILE:CG2 | 1:D:474:THR:O | 2.03 | 1.05 |
| 1:H:458:VAL:O | 1:H:476:ASP:N | 1.87 | 1.05 |
| 1:O:235:GLU:OE1 | 1:O:235:GLU:N | 1.89 | 1.05 |
| 1:E:507:VAL:HG13 | 1:E:507:VAL:O | 1.53 | 1.05 |
| 1:K:479:GLU:N | 1:K:479:GLU:OE1 | 1.88 | 1.05 |
| 1:M:479:GLU:OE1 | 1:M:479:GLU:N | 1.88 | 1.05 |
| 1:N:479:GLU:OE1 | 1:N:479:GLU:N | 1.88 | 1.05 |
| 1:O:458:VAL:O | 1:O:476:ASP:N | 1.87 | 1.05 |
| 1:B:459:ILE:CG2 | 1:B:474:THR:O | 2.03 | 1.04 |
| 1:G:458:VAL:O | 1:G:476:ASP:N | 1.87 | 1.04 |
| 1:I:235:GLU:OE1 | 1:I:235:GLU:N | 1.89 | 1.04 |
| 1:N:235:GLU:N | 1:N:235:GLU:OE1 | 1.89 | 1.04 |
| 1:A:479:GLU:OE1 | 1:A:479:GLU:N | 1.88 | 1.04 |
| 1:C:235:GLU:N | 1:C:235:GLU:OE1 | 1.89 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:479:GLU:N | 1:C:479:GLU:OE1 | 1.88 | 1.04 |
| 1:H:235:GLU:OE1 | 1:H:235:GLU:N | 1.89 | 1.04 |
| 1:J:479:GLU:OE1 | 1:J:479:GLU:N | 1.88 | 1.04 |
| 1:O:479:GLU:OE1 | 1:O:479:GLU:N | 1.88 | 1.04 |
| 1:I:507:VAL:O | 1:I:507:VAL:HG13 | 1.53 | 1.04 |
| 1:J:507:VAL:HG13 | 1:J:507:VAL:O | 1.53 | 1.04 |
| 1:D:507:VAL:HG13 | 1:D:507:VAL:O | 1.53 | 1.04 |
| 1:J:235:GLU:OE1 | 1:J:235:GLU:N | 1.89 | 1.04 |
| 1:K:235:GLU:N | 1:K:235:GLU:OE1 | 1.89 | 1.03 |
| 1:L:479:GLU:OE1 | 1:L:479:GLU:N | 1.88 | 1.03 |
| 1:O:507:VAL:HG13 | 1:O:507:VAL:O | 1.53 | 1.03 |
| 1:G:235:GLU:OE1 | 1:G:235:GLU:N | 1.89 | 1.03 |
| 1:O:324:ALA:O | 1:O:437:SER:HB2 | 1.60 | 1.01 |
| 1:A:324:ALA:O | 1:A:437:SER:HB2 | 1.60 | 1.01 |
| 1:K:324:ALA:O | 1:K:437:SER:HB2 | 1.60 | 1.01 |
| 1:N:324:ALA:O | 1:N:437:SER:HB2 | 1.60 | 1.01 |
| 1:B:324:ALA:O | 1:B:437:SER:HB2 | 1.60 | 1.01 |
| 1:G:324:ALA:O | 1:G:437:SER:HB2 | 1.60 | 1.01 |
| 1:H:105:VAL:O | 1:H:140:ILE:HB | 1.61 | 1.01 |
| 1:J:324:ALA:O | 1:J:437:SER:HB2 | 1.60 | 1.01 |
| 1:L:105:VAL:O | 1:L:140:ILE:HB | 1.61 | 1.01 |
| 1:I:105:VAL:O | 1:I:140:ILE:HB | 1.61 | 1.01 |
| 1:M:324:ALA:O | 1:M:437:SER:HB2 | 1.60 | 1.01 |
| 1:C:324:ALA:O | 1:C:437:SER:HB2 | 1.60 | 1.00 |
| 1:E:105:VAL:O | 1:E:140:ILE:HB | 1.61 | 1.00 |
| 1:F:105:VAL:O | 1:F:140:ILE:HB | 1.61 | 1.00 |
| 1:F:324:ALA:O | 1:F:437:SER:HB2 | 1.60 | 1.00 |
| 1:M:105:VAL:O | 1:M:140:ILE:HB | 1.61 | 1.00 |
| 1:D:612:GLU:HG3 | 1:E:642:PHE:HE2 | 1.23 | 1.00 |
| 1:G:105:VAL:O | 1:G:140:ILE:HB | 1.61 | 1.00 |
| 1:L:324:ALA:O | 1:L:437:SER:HB2 | 1.60 | 1.00 |
| 1:N:105:VAL:O | 1:N:140:ILE:HB | 1.61 | 1.00 |
| 1:D:105:VAL:O | 1:D:140:ILE:HB | 1.61 | 1.00 |
| 1:F:612:GLU:HG3 | 1:G:642:PHE:HE2 | 1.22 | 1.00 |
| 1:K:105:VAL:O | 1:K:140:ILE:HB | 1.61 | 1.00 |
| 1:D:324:ALA:O | 1:D:437:SER:HB2 | 1.60 | 0.99 |
| 1:O:105:VAL:O | 1:O:140:ILE:HB | 1.61 | 0.99 |
| 1:E:612:GLU:HG3 | 1:F:642:PHE:HE2 | 1.22 | 0.99 |
| 1:C:105:VAL:O | 1:C:140:ILE:HB | 1.61 | 0.99 |
| 1:H:324:ALA:O | 1:H:437:SER:HB2 | 1.60 | 0.99 |
| 1:A:105:VAL:O | 1:A:140:ILE:HB | 1.61 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:105:VAL:O | 1:B:140:ILE:HB | 1.61 | 0.99 |
| 1:I:324:ALA:O | 1:I:437:SER:HB2 | 1.60 | 0.98 |
| 1:J:105:VAL:O | 1:J:140:ILE:HB | 1.61 | 0.98 |
| 1:I:612:GLU:HG3 | 1:J:642:PHE:HE2 | 1.22 | 0.98 |
| 1:I:456:VAL:HG23 | 1:I:457:PRO:HD2 | 1.46 | 0.98 |
| 1:J:456:VAL:HG23 | 1:J:457:PRO:HD2 | 1.46 | 0.98 |
| 1:E:324:ALA:O | 1:E:437:SER:HB2 | 1.60 | 0.98 |
| 1:K:456:VAL:HG23 | 1:K:457:PRO:HD2 | 1.46 | 0.98 |
| 1:H:456:VAL:HG23 | 1:H:457:PRO:HD2 | 1.46 | 0.98 |
| 1:L:456:VAL:HG23 | 1:L:457:PRO:HD2 | 1.46 | 0.98 |
| 1:O:456:VAL:HG23 | 1:O:457:PRO:HD2 | 1.46 | 0.98 |
| 1:B:612:GLU:HG3 | 1:C:642:PHE:HE2 | 1.22 | 0.97 |
| 1:M:456:VAL:HG23 | 1:M:457:PRO:HD2 | 1.46 | 0.97 |
| 1:N:456:VAL:HG23 | 1:N:457:PRO:HD2 | 1.46 | 0.97 |
| 1:A:456:VAL:HG23 | 1:A:457:PRO:HD2 | 1.46 | 0.97 |
| 1:G:456:VAL:HG23 | 1:G:457:PRO:HD2 | 1.46 | 0.97 |
| 1:G:612:GLU:HG3 | 1:H:642:PHE:HE2 | 1.23 | 0.97 |
| 1:B:456:VAL:HG23 | 1:B:457:PRO:HD2 | 1.46 | 0.97 |
| 1:L:612:GLU:HG3 | 1:M:642:PHE:HE2 | 1.22 | 0.96 |
| 1:C:456:VAL:HG23 | 1:C:457:PRO:HD2 | 1.46 | 0.96 |
| 1:F:456:VAL:HG23 | 1:F:457:PRO:HD2 | 1.46 | 0.96 |
| 1:D:456:VAL:HG23 | 1:D:457:PRO:HD2 | 1.46 | 0.96 |
| 1:N:612:GLU:HG3 | 1:O:642:PHE:HE2 | 1.22 | 0.96 |
| 1:A:480:VAL:C | 1:A:505:SER:OG | 2.05 | 0.96 |
| 1:E:456:VAL:HG23 | 1:E:457:PRO:HD2 | 1.46 | 0.95 |
| 1:O:480:VAL:C | 1:O:505:SER:OG | 2.05 | 0.95 |
| 1:B:480:VAL:C | 1:B:505:SER:OG | 2.05 | 0.95 |
| 1:E:480:VAL:C | 1:E:505:SER:OG | 2.05 | 0.95 |
| 1:D:480:VAL:C | 1:D:505:SER:OG | 2.05 | 0.95 |
| 1:F:480:VAL:C | 1:F:505:SER:OG | 2.05 | 0.95 |
| 1:K:612:GLU:HG3 | 1:L:642:PHE:HE2 | 1.22 | 0.94 |
| 1:N:480:VAL:C | 1:N:505:SER:OG | 2.05 | 0.94 |
| 1:C:480:VAL:C | 1:C:505:SER:OG | 2.05 | 0.94 |
| 1:L:480:VAL:C | 1:L:505:SER:OG | 2.05 | 0.94 |
| 1:G:480:VAL:C | 1:G:505:SER:OG | 2.05 | 0.94 |
| 1:H:480:VAL:C | 1:H:505:SER:OG | 2.05 | 0.94 |
| 1:K:480:VAL:C | 1:K:505:SER:OG | 2.05 | 0.94 |
| 1:J:612:GLU:HG3 | 1:K:642:PHE:HE2 | 1.22 | 0.94 |
| 1:M:480:VAL:C | 1:M:505:SER:OG | 2.05 | 0.94 |
| 1:J:480:VAL:C | 1:J:505:SER:OG | 2.05 | 0.93 |
| 1:M:612:GLU:HG3 | 1:N:642:PHE:HE2 | 1.23 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:480:VAL:C | 1:I:505:SER:OG | 2.05 | 0.93 |
| 1:J:609:PHE:CG | 1:K:639:ILE:CD1 | 2.52 | 0.93 |
| 1:A:612:GLU:HG3 | 1:B:642:PHE:HE2 | 1.23 | 0.93 |
| 1:H:609:PHE:CG | 1:I:639:ILE:CD1 | 2.52 | 0.93 |
| 1:L:609:PHE:CG | 1:M:639:ILE:CD1 | 2.52 | 0.93 |
| 1:N:218:ASP:HB2 | 1:N:221:VAL:H | 1.34 | 0.93 |
| 1:A:642:PHE:HE2 | 1:O:612:GLU:HG3 | 1.23 | 0.93 |
| 1:C:609:PHE:CD2 | 1:D:639:ILE:HD11 | 2.04 | 0.93 |
| 1:H:612:GLU:HG3 | 1:I:642:PHE:HE2 | 1.23 | 0.93 |
| 1:O:218:ASP:HB2 | 1:O:221:VAL:H | 1.34 | 0.93 |
| 1:M:218:ASP:HB2 | 1:M:221:VAL:H | 1.34 | 0.93 |
| 1:A:218:ASP:HB2 | 1:A:221:VAL:H | 1.34 | 0.93 |
| 1:C:609:PHE:CG | 1:D:639:ILE:CD1 | 2.52 | 0.93 |
| 1:K:609:PHE:CG | 1:L:639:ILE:CD1 | 2.52 | 0.93 |
| 1:A:609:PHE:CD2 | 1:B:639:ILE:HD11 | 2.04 | 0.92 |
| 1:A:609:PHE:CG | 1:B:639:ILE:CD1 | 2.52 | 0.92 |
| 1:F:609:PHE:CD2 | 1:G:639:ILE:HD11 | 2.04 | 0.92 |
| 1:K:609:PHE:CD2 | 1:L:639:ILE:HD11 | 2.04 | 0.92 |
| 1:L:218:ASP:HB2 | 1:L:221:VAL:H | 1.34 | 0.92 |
| 1:M:609:PHE:CG | 1:N:639:ILE:CD1 | 2.52 | 0.92 |
| 1:B:609:PHE:CG | 1:C:639:ILE:CD1 | 2.52 | 0.92 |
| 1:J:609:PHE:CD2 | 1:K:639:ILE:HD11 | 2.04 | 0.92 |
| 1:I:609:PHE:CG | 1:J:639:ILE:CD1 | 2.52 | 0.92 |
| 1:A:639:ILE:HD11 | 1:O:609:PHE:CD2 | 2.04 | 0.92 |
| 1:D:609:PHE:CD2 | 1:E:639:ILE:HD11 | 2.04 | 0.92 |
| 1:D:609:PHE:CG | 1:E:639:ILE:CD1 | 2.52 | 0.92 |
| 1:E:609:PHE:CG | 1:F:639:ILE:CD1 | 2.52 | 0.92 |
| 1:C:612:GLU:HG3 | 1:D:642:PHE:HE2 | 1.23 | 0.92 |
| 1:N:609:PHE:CG | 1:O:639:ILE:CD1 | 2.52 | 0.92 |
| 1:A:639:ILE:CD1 | 1:O:609:PHE:CG | 2.52 | 0.92 |
| 1:B:218:ASP:HB2 | 1:B:221:VAL:H | 1.34 | 0.92 |
| 1:B:609:PHE:CD2 | 1:C:639:ILE:HD11 | 2.04 | 0.92 |
| 1:E:609:PHE:CD2 | 1:F:639:ILE:HD11 | 2.04 | 0.92 |
| 1:F:609:PHE:CG | 1:G:639:ILE:CD1 | 2.52 | 0.92 |
| 1:N:506:ASN:HD22 | 1:N:507:VAL:N | 1.68 | 0.92 |
| 1:K:218:ASP:HB2 | 1:K:221:VAL:H | 1.34 | 0.92 |
| 1:K:506:ASN:HD22 | 1:K:507:VAL:N | 1.68 | 0.92 |
| 1:D:218:ASP:HB2 | 1:D:221:VAL:H | 1.34 | 0.92 |
| 1:I:609:PHE:CD2 | 1:J:639:ILE:HD11 | 2.04 | 0.92 |
| 1:G:218:ASP:HB2 | 1:G:221:VAL:H | 1.34 | 0.92 |
| 1:B:506:ASN:HD22 | 1:B:507:VAL:N | 1.68 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:218:ASP:HB2 | 1:F:221:VAL:H | 1.34 | 0.91 |
| 1:N:458:VAL:O | 1:N:475:VAL:HA | 1.70 | 0.91 |
| 1:O:458:VAL:O | 1:O:475:VAL:HA | 1.70 | 0.91 |
| 1:D:458:VAL:O | 1:D:475:VAL:HA | 1.70 | 0.91 |
| 1:H:506:ASN:HD22 | 1:H:507:VAL:N | 1.68 | 0.91 |
| 1:I:458:VAL:O | 1:I:475:VAL:HA | 1.70 | 0.91 |
| 1:I:506:ASN:HD22 | 1:I:507:VAL:N | 1.68 | 0.91 |
| 1:L:506:ASN:HD22 | 1:L:507:VAL:N | 1.68 | 0.91 |
| 1:I:218:ASP:HB2 | 1:I:221:VAL:H | 1.34 | 0.91 |
| 1:M:609:PHE:CD2 | 1:N:639:ILE:HD11 | 2.04 | 0.91 |
| 1:O:506:ASN:HD22 | 1:O:507:VAL:N | 1.68 | 0.91 |
| 1:G:609:PHE:CG | 1:H:639:ILE:CD1 | 2.52 | 0.91 |
| 1:H:218:ASP:HB2 | 1:H:221:VAL:H | 1.34 | 0.91 |
| 1:G:609:PHE:CD2 | 1:H:639:ILE:HD11 | 2.04 | 0.91 |
| 1:H:458:VAL:O | 1:H:475:VAL:HA | 1.70 | 0.91 |
| 1:H:609:PHE:CD2 | 1:I:639:ILE:HD11 | 2.04 | 0.91 |
| 1:J:458:VAL:O | 1:J:475:VAL:HA | 1.70 | 0.91 |
| 1:L:609:PHE:CD2 | 1:M:639:ILE:HD11 | 2.04 | 0.91 |
| 1:B:458:VAL:O | 1:B:475:VAL:HA | 1.70 | 0.91 |
| 1:E:218:ASP:HB2 | 1:E:221:VAL:H | 1.34 | 0.91 |
| 1:E:506:ASN:HD22 | 1:E:507:VAL:N | 1.68 | 0.91 |
| 1:G:458:VAL:O | 1:G:475:VAL:HA | 1.70 | 0.91 |
| 1:C:218:ASP:HB2 | 1:C:221:VAL:H | 1.34 | 0.91 |
| 1:C:506:ASN:HD22 | 1:C:507:VAL:N | 1.68 | 0.91 |
| 1:N:455:GLU:OE1 | 1:N:455:GLU:N | 2.04 | 0.91 |
| 1:E:455:GLU:N | 1:E:455:GLU:OE1 | 2.04 | 0.90 |
| 1:E:458:VAL:O | 1:E:475:VAL:HA | 1.70 | 0.90 |
| 1:F:506:ASN:HD22 | 1:F:507:VAL:N | 1.68 | 0.90 |
| 1:J:218:ASP:HB2 | 1:J:221:VAL:H | 1.34 | 0.90 |
| 1:M:458:VAL:O | 1:M:475:VAL:HA | 1.70 | 0.90 |
| 1:O:455:GLU:OE1 | 1:O:455:GLU:N | 2.04 | 0.90 |
| 1:A:506:ASN:HD22 | 1:A:507:VAL:N | 1.68 | 0.90 |
| 1:F:455:GLU:OE1 | 1:F:455:GLU:N | 2.04 | 0.90 |
| 1:M:506:ASN:HD22 | 1:M:507:VAL:N | 1.68 | 0.90 |
| 1:N:609:PHE:CD2 | 1:O:639:ILE:HD11 | 2.04 | 0.90 |
| 1:A:458:VAL:O | 1:A:475:VAL:HA | 1.70 | 0.90 |
| 1:D:455:GLU:OE1 | 1:D:455:GLU:N | 2.04 | 0.90 |
| 1:F:458:VAL:O | 1:F:475:VAL:HA | 1.70 | 0.90 |
| 1:I:455:GLU:OE1 | 1:I:455:GLU:N | 2.04 | 0.90 |
| 1:M:455:GLU:N | 1:M:455:GLU:OE1 | 2.04 | 0.90 |
| 1:J:455:GLU:OE1 | 1:J:455:GLU:N | 2.04 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:458:VAL:O | 1:K:475:VAL:HA | 1.70 | 0.90 |
| 1:J:506:ASN:HD22 | 1:J:507:VAL:N | 1.68 | 0.90 |
| 1:C:455:GLU:OE1 | 1:C:455:GLU:N | 2.04 | 0.90 |
| 1:H:455:GLU:N | 1:H:455:GLU:OE1 | 2.04 | 0.90 |
| 1:A:205:VAL:HB | 1:A:214:LEU:HB2 | 1.54 | 0.90 |
| 1:A:455:GLU:OE1 | 1:A:455:GLU:N | 2.04 | 0.90 |
| 1:B:205:VAL:HB | 1:B:214:LEU:HB2 | 1.54 | 0.90 |
| 1:D:506:ASN:HD22 | 1:D:507:VAL:N | 1.68 | 0.89 |
| 1:G:506:ASN:HD22 | 1:G:507:VAL:N | 1.68 | 0.89 |
| 1:K:455:GLU:OE1 | 1:K:455:GLU:N | 2.04 | 0.89 |
| 1:C:205:VAL:HB | 1:C:214:LEU:HB2 | 1.54 | 0.89 |
| 1:C:458:VAL:O | 1:C:475:VAL:HA | 1.70 | 0.89 |
| 1:O:205:VAL:HB | 1:O:214:LEU:HB2 | 1.54 | 0.89 |
| 1:G:455:GLU:OE1 | 1:G:455:GLU:N | 2.04 | 0.89 |
| 1:L:458:VAL:O | 1:L:475:VAL:HA | 1.70 | 0.89 |
| 1:L:455:GLU:OE1 | 1:L:455:GLU:N | 2.04 | 0.89 |
| 1:N:205:VAL:HB | 1:N:214:LEU:HB2 | 1.54 | 0.89 |
| 1:A:328:GLU:OE1 | 1:A:521:ARG:NH1 | 2.06 | 0.89 |
| 1:B:455:GLU:OE1 | 1:B:455:GLU:N | 2.04 | 0.89 |
| 1:L:328:GLU:OE1 | 1:L:521:ARG:NH1 | 2.06 | 0.89 |
| 1:D:205:VAL:HB | 1:D:214:LEU:HB2 | 1.54 | 0.88 |
| 1:D:328:GLU:OE1 | 1:D:521:ARG:NH1 | 2.06 | 0.88 |
| 1:O:328:GLU:OE1 | 1:O:521:ARG:NH1 | 2.06 | 0.88 |
| 1:B:169:VAL:HG22 | 1:B:214:LEU:HD22 | 1.56 | 0.88 |
| 1:I:205:VAL:HB | 1:I:214:LEU:HB2 | 1.54 | 0.88 |
| 1:M:328:GLU:OE1 | 1:M:521:ARG:NH1 | 2.06 | 0.88 |
| 1:H:205:VAL:HB | 1:H:214:LEU:HB2 | 1.54 | 0.88 |
| 1:J:480:VAL:HA | 1:J:505:SER:OG | 1.74 | 0.88 |
| 1:M:205:VAL:HB | 1:M:214:LEU:HB2 | 1.54 | 0.88 |
| 1:N:480:VAL:HA | 1:N:505:SER:OG | 1.73 | 0.88 |
| 1:E:328:GLU:OE1 | 1:E:521:ARG:NH1 | 2.06 | 0.88 |
| 1:K:328:GLU:OE1 | 1:K:521:ARG:NH1 | 2.06 | 0.88 |
| 1:D:169:VAL:HG22 | 1:D:214:LEU:HD22 | 1.56 | 0.88 |
| 1:O:480:VAL:HA | 1:O:505:SER:OG | 1.74 | 0.88 |
| 1:B:328:GLU:OE1 | 1:B:521:ARG:NH1 | 2.06 | 0.88 |
| 1:H:328:GLU:OE1 | 1:H:521:ARG:NH1 | 2.06 | 0.88 |
| 1:J:205:VAL:HB | 1:J:214:LEU:HB2 | 1.54 | 0.88 |
| 1:K:122:LEU:HD23 | 1:K:125:ASN:HD22 | 1.39 | 0.88 |
| 1:O:169:VAL:HG22 | 1:O:214:LEU:HD22 | 1.56 | 0.88 |
| 1:C:169:VAL:HG22 | 1:C:214:LEU:HD22 | 1.56 | 0.88 |
| 1:C:328:GLU:OE1 | 1:C:521:ARG:NH1 | 2.06 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:169:VAL:HG22 | 1:E:214:LEU:HD22 | 1.56 | 0.88 |
| 1:G:205:VAL:HB | 1:G:214:LEU:HB2 | 1.54 | 0.88 |
| 1:I:328:GLU:OE1 | 1:I:521:ARG:NH1 | 2.06 | 0.88 |
| 1:L:122:LEU:HD23 | 1:L:125:ASN:HD22 | 1.39 | 0.88 |
| 1:A:169:VAL:HG22 | 1:A:214:LEU:HD22 | 1.56 | 0.88 |
| 1:E:480:VAL:HA | 1:E:505:SER:OG | 1.74 | 0.88 |
| 1:K:480:VAL:HA | 1:K:505:SER:OG | 1.74 | 0.88 |
| 1:L:205:VAL:HB | 1:L:214:LEU:HB2 | 1.54 | 0.88 |
| 1:D:480:VAL:HA | 1:D:505:SER:OG | 1.74 | 0.87 |
| 1:E:205:VAL:HB | 1:E:214:LEU:HB2 | 1.54 | 0.87 |
| 1:C:480:VAL:HA | 1:C:505:SER:OG | 1.73 | 0.87 |
| 1:F:480:VAL:HA | 1:F:505:SER:OG | 1.74 | 0.87 |
| 1:I:480:VAL:HA | 1:I:505:SER:OG | 1.74 | 0.87 |
| 1:N:169:VAL:HG22 | 1:N:214:LEU:HD22 | 1.56 | 0.87 |
| 1:N:328:GLU:OE1 | 1:N:521:ARG:NH1 | 2.06 | 0.87 |
| 1:C:122:LEU:HD23 | 1:C:125:ASN:HD22 | 1.39 | 0.87 |
| 1:J:122:LEU:HD23 | 1:J:125:ASN:HD22 | 1.39 | 0.87 |
| 1:K:205:VAL:HB | 1:K:214:LEU:HB2 | 1.54 | 0.87 |
| 1:F:122:LEU:HD23 | 1:F:125:ASN:HD22 | 1.39 | 0.87 |
| 1:G:328:GLU:OE1 | 1:G:521:ARG:NH1 | 2.06 | 0.87 |
| 1:E:122:LEU:HD23 | 1:E:125:ASN:HD22 | 1.39 | 0.87 |
| 1:J:328:GLU:OE1 | 1:J:521:ARG:NH1 | 2.06 | 0.87 |
| 1:D:122:LEU:HD23 | 1:D:125:ASN:HD22 | 1.39 | 0.87 |
| 1:F:328:GLU:OE1 | 1:F:521:ARG:NH1 | 2.06 | 0.87 |
| 1:G:480:VAL:HA | 1:G:505:SER:OG | 1.74 | 0.87 |
| 1:M:480:VAL:HA | 1:M:505:SER:OG | 1.74 | 0.87 |
| 1:A:480:VAL:HA | 1:A:505:SER:OG | 1.74 | 0.87 |
| 1:F:169:VAL:HG22 | 1:F:214:LEU:HD22 | 1.56 | 0.87 |
| 1:F:205:VAL:HB | 1:F:214:LEU:HB2 | 1.54 | 0.87 |
| 1:G:122:LEU:HD23 | 1:G:125:ASN:HD22 | 1.39 | 0.87 |
| 1:G:169:VAL:HG22 | 1:G:214:LEU:HD22 | 1.56 | 0.87 |
| 1:M:122:LEU:HD23 | 1:M:125:ASN:HD22 | 1.39 | 0.86 |
| 1:B:122:LEU:HD23 | 1:B:125:ASN:HD22 | 1.39 | 0.86 |
| 1:B:480:VAL:HA | 1:B:505:SER:OG | 1.74 | 0.86 |
| 1:M:169:VAL:HG22 | 1:M:214:LEU:HD22 | 1.56 | 0.86 |
| 1:A:122:LEU:HD23 | 1:A:125:ASN:HD22 | 1.39 | 0.86 |
| 1:H:169:VAL:HG22 | 1:H:214:LEU:HD22 | 1.56 | 0.86 |
| 1:L:169:VAL:HG22 | 1:L:214:LEU:HD22 | 1.56 | 0.86 |
| 1:L:480:VAL:HA | 1:L:505:SER:OG | 1.74 | 0.86 |
| 1:B:473:GLN:OE1 | 1:B:473:GLN:N | 2.09 | 0.86 |
| 1:I:122:LEU:HD23 | 1:I:125:ASN:HD22 | 1.39 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:473:GLN:OE1 | 1:K:473:GLN:N | 2.09 | 0.86 |
| 1:A:473:GLN:OE1 | 1:A:473:GLN:N | 2.09 | 0.85 |
| 1:H:122:LEU:HD23 | 1:H:125:ASN:HD22 | 1.39 | 0.85 |
| 1:J:169:VAL:HG22 | 1:J:214:LEU:HD22 | 1.56 | 0.85 |
| 1:K:169:VAL:HG22 | 1:K:214:LEU:HD22 | 1.56 | 0.85 |
| 1:H:480:VAL:HA | 1:H:505:SER:OG | 1.74 | 0.85 |
| 1:L:473:GLN:OE1 | 1:L:473:GLN:N | 2.09 | 0.85 |
| 1:O:122:LEU:HD23 | 1:O:125:ASN:HD22 | 1.39 | 0.85 |
| 1:J:473:GLN:OE1 | 1:J:473:GLN:N | 2.09 | 0.85 |
| 1:C:473:GLN:OE1 | 1:C:473:GLN:N | 2.09 | 0.85 |
| 1:F:473:GLN:OE1 | 1:F:473:GLN:N | 2.09 | 0.85 |
| 1:N:122:LEU:HD23 | 1:N:125:ASN:HD22 | 1.39 | 0.85 |
| 1:O:473:GLN:OE1 | 1:O:473:GLN:N | 2.09 | 0.85 |
| 1:H:480:VAL:CA | 1:H:505:SER:CB | 2.55 | 0.85 |
| 1:N:480:VAL:CA | 1:N:505:SER:CB | 2.55 | 0.85 |
| 1:A:480:VAL:CA | 1:A:505:SER:CB | 2.55 | 0.85 |
| 1:I:169:VAL:HG22 | 1:I:214:LEU:HD22 | 1.56 | 0.85 |
| 1:K:480:VAL:CA | 1:K:505:SER:CB | 2.55 | 0.85 |
| 1:M:480:VAL:CA | 1:M:505:SER:CB | 2.55 | 0.85 |
| 1:G:473:GLN:OE1 | 1:G:473:GLN:N | 2.09 | 0.85 |
| 1:J:480:VAL:CA | 1:J:505:SER:CB | 2.55 | 0.85 |
| 1:M:473:GLN:OE1 | 1:M:473:GLN:N | 2.09 | 0.84 |
| 1:F:480:VAL:CA | 1:F:505:SER:CB | 2.55 | 0.84 |
| 1:I:480:VAL:CA | 1:I:505:SER:CB | 2.55 | 0.84 |
| 1:N:473:GLN:OE1 | 1:N:473:GLN:N | 2.09 | 0.84 |
| 1:C:480:VAL:CA | 1:C:505:SER:CB | 2.55 | 0.84 |
| 1:H:473:GLN:OE1 | 1:H:473:GLN:N | 2.09 | 0.84 |
| 1:O:480:VAL:CA | 1:O:505:SER:CB | 2.55 | 0.84 |
| 1:D:473:GLN:OE1 | 1:D:473:GLN:N | 2.09 | 0.84 |
| 1:L:480:VAL:CA | 1:L:505:SER:CB | 2.55 | 0.84 |
| 1:B:480:VAL:CA | 1:B:505:SER:CB | 2.55 | 0.84 |
| 1:D:480:VAL:CA | 1:D:505:SER:CB | 2.55 | 0.84 |
| 1:E:480:VAL:CA | 1:E:505:SER:CB | 2.55 | 0.84 |
| 1:G:480:VAL:CA | 1:G:505:SER:CB | 2.55 | 0.84 |
| 1:B:203:LYS:N | 1:B:216:SER:O | 2.11 | 0.83 |
| 1:H:203:LYS:N | 1:H:216:SER:O | 2.11 | 0.83 |
| 1:J:203:LYS:N | 1:J:216:SER:O | 2.11 | 0.83 |
| 1:K:203:LYS:N | 1:K:216:SER:O | 2.11 | 0.83 |
| 1:L:203:LYS:N | 1:L:216:SER:O | 2.11 | 0.83 |
| 1:O:203:LYS:N | 1:O:216:SER:O | 2.11 | 0.83 |
| 1:I:203:LYS:N | 1:I:216:SER:O | 2.11 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:473:GLN:N | 1:I:473:GLN:OE1 | 2.09 | 0.83 |
| 1:L:168:GLU:O | 1:L:214:LEU:HA | 1.79 | 0.83 |
| 1:C:203:LYS:N | 1:C:216:SER:O | 2.11 | 0.83 |
| 1:G:168:GLU:O | 1:G:214:LEU:HA | 1.79 | 0.83 |
| 1:G:203:LYS:N | 1:G:216:SER:O | 2.11 | 0.83 |
| 1:D:203:LYS:N | 1:D:216:SER:O | 2.11 | 0.82 |
| 1:I:168:GLU:O | 1:I:214:LEU:HA | 1.79 | 0.82 |
| 1:J:168:GLU:O | 1:J:214:LEU:HA | 1.79 | 0.82 |
| 1:E:203:LYS:N | 1:E:216:SER:O | 2.11 | 0.82 |
| 1:E:473:GLN:OE1 | 1:E:473:GLN:N | 2.09 | 0.82 |
| 1:O:168:GLU:O | 1:O:214:LEU:HA | 1.79 | 0.82 |
| 1:F:168:GLU:O | 1:F:214:LEU:HA | 1.79 | 0.82 |
| 1:M:168:GLU:O | 1:M:214:LEU:HA | 1.79 | 0.82 |
| 1:M:203:LYS:N | 1:M:216:SER:O | 2.11 | 0.82 |
| 1:N:203:LYS:N | 1:N:216:SER:O | 2.11 | 0.82 |
| 1:H:480:VAL:HA | 1:H:505:SER:CB | 2.10 | 0.82 |
| 1:A:504:VAL:CG1 | 1:A:521:ARG:HG2 | 2.10 | 0.82 |
| 1:D:168:GLU:O | 1:D:214:LEU:HA | 1.79 | 0.82 |
| 1:D:507:VAL:O | 1:D:507:VAL:CG1 | 2.28 | 0.82 |
| 1:F:203:LYS:N | 1:F:216:SER:O | 2.11 | 0.81 |
| 1:G:480:VAL:HA | 1:G:505:SER:CB | 2.10 | 0.81 |
| 1:M:504:VAL:CG1 | 1:M:521:ARG:HG2 | 2.10 | 0.81 |
| 1:O:480:VAL:HA | 1:O:505:SER:CB | 2.10 | 0.81 |
| 1:A:203:LYS:N | 1:A:216:SER:O | 2.11 | 0.81 |
| 1:A:480:VAL:HA | 1:A:505:SER:CB | 2.10 | 0.81 |
| 1:C:168:GLU:O | 1:C:214:LEU:HA | 1.79 | 0.81 |
| 1:E:168:GLU:O | 1:E:214:LEU:HA | 1.79 | 0.81 |
| 1:I:480:VAL:HA | 1:I:505:SER:CB | 2.10 | 0.81 |
| 1:J:480:VAL:HA | 1:J:505:SER:CB | 2.10 | 0.81 |
| 1:B:480:VAL:HA | 1:B:505:SER:CB | 2.10 | 0.81 |
| 1:C:480:VAL:HA | 1:C:505:SER:CB | 2.10 | 0.81 |
| 1:D:459:ILE:HA | 1:D:474:THR:O | 1.81 | 0.81 |
| 1:D:480:VAL:HA | 1:D:505:SER:CB | 2.10 | 0.81 |
| 1:D:504:VAL:CG1 | 1:D:521:ARG:HG2 | 2.10 | 0.81 |
| 1:E:480:VAL:HA | 1:E:505:SER:CB | 2.10 | 0.81 |
| 1:E:504:VAL:CG1 | 1:E:521:ARG:HG2 | 2.10 | 0.81 |
| 1:F:504:VAL:CG1 | 1:F:521:ARG:HG2 | 2.10 | 0.81 |
| 1:G:504:VAL:CG1 | 1:G:521:ARG:HG2 | 2.10 | 0.81 |
| 1:H:504:VAL:CG1 | 1:H:521:ARG:HG2 | 2.10 | 0.81 |
| 1:I:504:VAL:CG1 | 1:I:521:ARG:HG2 | 2.10 | 0.81 |
| 1:J:504:VAL:CG1 | 1:J:521:ARG:HG2 | 2.10 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:168:GLU:O | 1:K:214:LEU:HA | 1.79 | 0.81 |
| 1:K:504:VAL:CG1 | 1:K:521:ARG:HG2 | 2.10 | 0.81 |
| 1:L:504:VAL:CG1 | 1:L:521:ARG:HG2 | 2.10 | 0.81 |
| 1:N:168:GLU:O | 1:N:214:LEU:HA | 1.79 | 0.81 |
| 1:N:504:VAL:CG1 | 1:N:521:ARG:HG2 | 2.10 | 0.81 |
| 1:A:168:GLU:O | 1:A:214:LEU:HA | 1.79 | 0.81 |
| 1:E:507:VAL:O | 1:E:507:VAL:CG1 | 2.28 | 0.81 |
| 1:F:480:VAL:HA | 1:F:505:SER:CB | 2.10 | 0.81 |
| 1:K:172:LEU:HD11 | 1:K:213:ILE:HG13 | 1.63 | 0.81 |
| 1:B:504:VAL:CG1 | 1:B:521:ARG:HG2 | 2.10 | 0.81 |
| 1:M:172:LEU:HD11 | 1:M:213:ILE:HG13 | 1.63 | 0.81 |
| 1:C:459:ILE:HA | 1:C:474:THR:O | 1.81 | 0.81 |
| 1:H:168:GLU:O | 1:H:214:LEU:HA | 1.79 | 0.81 |
| 1:O:504:VAL:CG1 | 1:O:521:ARG:HG2 | 2.10 | 0.81 |
| 1:E:459:ILE:HA | 1:E:474:THR:O | 1.81 | 0.81 |
| 1:K:480:VAL:HA | 1:K:505:SER:CB | 2.10 | 0.81 |
| 1:L:480:VAL:HA | 1:L:505:SER:CB | 2.10 | 0.81 |
| 1:C:640:GLN:O | 1:C:643:ILE:HG22 | 1.81 | 0.81 |
| 1:D:640:GLN:O | 1:D:643:ILE:HG22 | 1.81 | 0.81 |
| 1:N:480:VAL:HA | 1:N:505:SER:CB | 2.10 | 0.81 |
| 1:M:480:VAL:HA | 1:M:505:SER:CB | 2.10 | 0.81 |
| 1:F:459:ILE:HA | 1:F:474:THR:O | 1.81 | 0.80 |
| 1:N:640:GLN:O | 1:N:643:ILE:HG22 | 1.81 | 0.80 |
| 1:I:172:LEU:HD11 | 1:I:213:ILE:HG13 | 1.63 | 0.80 |
| 1:L:640:GLN:O | 1:L:643:ILE:HG22 | 1.81 | 0.80 |
| 1:O:172:LEU:HD11 | 1:O:213:ILE:HG13 | 1.63 | 0.80 |
| 1:B:168:GLU:O | 1:B:214:LEU:HA | 1.79 | 0.80 |
| 1:B:459:ILE:HA | 1:B:474:THR:O | 1.81 | 0.80 |
| 1:M:481:GLY:CA | 1:M:505:SER:HB3 | 2.11 | 0.80 |
| 1:N:481:GLY:CA | 1:N:505:SER:HB3 | 2.11 | 0.80 |
| 1:N:507:VAL:O | 1:N:507:VAL:CG1 | 2.28 | 0.80 |
| 1:F:507:VAL:O | 1:F:507:VAL:CG1 | 2.28 | 0.80 |
| 1:J:459:ILE:HA | 1:J:474:THR:O | 1.81 | 0.80 |
| 1:L:481:GLY:CA | 1:L:505:SER:HB3 | 2.11 | 0.80 |
| 1:B:640:GLN:O | 1:B:643:ILE:HG22 | 1.81 | 0.80 |
| 1:C:504:VAL:CG1 | 1:C:521:ARG:HG2 | 2.10 | 0.80 |
| 1:G:459:ILE:HA | 1:G:474:THR:O | 1.81 | 0.80 |
| 1:H:481:GLY:CA | 1:H:505:SER:HB3 | 2.11 | 0.80 |
| 1:I:459:ILE:HA | 1:I:474:THR:O | 1.81 | 0.80 |
| 1:I:481:GLY:CA | 1:I:505:SER:HB3 | 2.11 | 0.80 |
| 1:K:640:GLN:O | 1:K:643:ILE:HG22 | 1.81 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:481:GLY:CA | 1:O:505:SER:HB3 | 2.11 | 0.80 |
| 1:D:481:GLY:CA | 1:D:505:SER:HB3 | 2.11 | 0.80 |
| 1:H:640:GLN:O | 1:H:643:ILE:HG22 | 1.81 | 0.80 |
| 1:J:640:GLN:O | 1:J:643:ILE:HG22 | 1.81 | 0.80 |
| 1:E:481:GLY:CA | 1:E:505:SER:HB3 | 2.11 | 0.80 |
| 1:E:640:GLN:O | 1:E:643:ILE:HG22 | 1.81 | 0.80 |
| 1:H:459:ILE:HA | 1:H:474:THR:O | 1.81 | 0.80 |
| 1:I:640:GLN:O | 1:I:643:ILE:HG22 | 1.81 | 0.80 |
| 1:J:480:VAL:C | 1:J:505:SER:CB | 2.50 | 0.80 |
| 1:K:368:GLU:HG3 | 1:K:399:LYS:HD2 | 1.64 | 0.80 |
| 1:K:459:ILE:HA | 1:K:474:THR:O | 1.81 | 0.80 |
| 1:K:481:GLY:CA | 1:K:505:SER:HB3 | 2.11 | 0.80 |
| 1:L:480:VAL:C | 1:L:505:SER:CB | 2.50 | 0.80 |
| 1:F:481:GLY:CA | 1:F:505:SER:HB3 | 2.11 | 0.80 |
| 1:I:480:VAL:C | 1:I:505:SER:CB | 2.50 | 0.80 |
| 1:J:481:GLY:CA | 1:J:505:SER:HB3 | 2.11 | 0.80 |
| 1:L:459:ILE:HA | 1:L:474:THR:O | 1.81 | 0.80 |
| 1:A:481:GLY:CA | 1:A:505:SER:HB3 | 2.11 | 0.80 |
| 1:A:640:GLN:O | 1:A:643:ILE:HG22 | 1.81 | 0.80 |
| 1:M:459:ILE:HA | 1:M:474:THR:O | 1.81 | 0.80 |
| 1:A:172:LEU:HD11 | 1:A:213:ILE:HG13 | 1.63 | 0.80 |
| 1:G:480:VAL:C | 1:G:505:SER:CB | 2.50 | 0.80 |
| 1:G:640:GLN:O | 1:G:643:ILE:HG22 | 1.81 | 0.80 |
| 1:M:640:GLN:O | 1:M:643:ILE:HG22 | 1.81 | 0.80 |
| 1:N:459:ILE:HA | 1:N:474:THR:O | 1.81 | 0.80 |
| 1:O:507:VAL:O | 1:O:507:VAL:CG1 | 2.28 | 0.80 |
| 1:A:459:ILE:HA | 1:A:474:THR:O | 1.81 | 0.79 |
| 1:G:481:GLY:CA | 1:G:505:SER:HB3 | 2.11 | 0.79 |
| 1:C:480:VAL:C | 1:C:505:SER:CB | 2.50 | 0.79 |
| 1:O:459:ILE:HA | 1:O:474:THR:O | 1.81 | 0.79 |
| 1:B:481:GLY:CA | 1:B:505:SER:HB3 | 2.11 | 0.79 |
| 1:H:172:LEU:HD11 | 1:H:213:ILE:HG13 | 1.63 | 0.79 |
| 1:J:507:VAL:O | 1:J:507:VAL:CG1 | 2.28 | 0.79 |
| 1:L:459:ILE:CG2 | 1:L:473:GLN:HB2 | 2.12 | 0.79 |
| 1:C:172:LEU:HD11 | 1:C:213:ILE:HG13 | 1.63 | 0.79 |
| 1:J:368:GLU:HG3 | 1:J:399:LYS:HD2 | 1.64 | 0.79 |
| 1:L:368:GLU:HG3 | 1:L:399:LYS:HD2 | 1.64 | 0.79 |
| 1:M:480:VAL:C | 1:M:505:SER:CB | 2.50 | 0.79 |
| 1:N:172:LEU:HD11 | 1:N:213:ILE:HG13 | 1.63 | 0.79 |
| 1:B:480:VAL:C | 1:B:505:SER:CB | 2.50 | 0.79 |
| 1:F:172:LEU:HD11 | 1:F:213:ILE:HG13 | 1.63 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:640:GLN:O | 1:O:643:ILE:HG22 | 1.81 | 0.79 |
| 1:H:368:GLU:HG3 | 1:H:399:LYS:HD2 | 1.64 | 0.79 |
| 1:L:172:LEU:HD11 | 1:L:213:ILE:HG13 | 1.63 | 0.79 |
| 1:N:368:GLU:HG3 | 1:N:399:LYS:HD2 | 1.64 | 0.79 |
| 1:B:368:GLU:HG3 | 1:B:399:LYS:HD2 | 1.64 | 0.79 |
| 1:C:481:GLY:CA | 1:C:505:SER:HB3 | 2.11 | 0.79 |
| 1:H:480:VAL:C | 1:H:505:SER:CB | 2.50 | 0.79 |
| 1:J:172:LEU:HD11 | 1:J:213:ILE:HG13 | 1.63 | 0.79 |
| 1:O:480:VAL:C | 1:O:505:SER:CB | 2.50 | 0.79 |
| 1:A:507:VAL:O | 1:A:507:VAL:CG1 | 2.28 | 0.79 |
| 1:E:368:GLU:HG3 | 1:E:399:LYS:HD2 | 1.64 | 0.79 |
| 1:E:480:VAL:C | 1:E:505:SER:CB | 2.50 | 0.79 |
| 1:F:640:GLN:O | 1:F:643:ILE:HG22 | 1.81 | 0.79 |
| 1:G:507:VAL:O | 1:G:507:VAL:CG1 | 2.28 | 0.78 |
| 1:K:459:ILE:CG2 | 1:K:473:GLN:HB2 | 2.12 | 0.78 |
| 1:A:480:VAL:C | 1:A:505:SER:CB | 2.50 | 0.78 |
| 1:A:624:PRO:HB2 | 1:O:435:LEU:HD13 | 1.65 | 0.78 |
| 1:C:368:GLU:HG3 | 1:C:399:LYS:HD2 | 1.64 | 0.78 |
| 1:D:368:GLU:HG3 | 1:D:399:LYS:HD2 | 1.64 | 0.78 |
| 1:G:368:GLU:HG3 | 1:G:399:LYS:HD2 | 1.64 | 0.78 |
| 1:O:368:GLU:HG3 | 1:O:399:LYS:HD2 | 1.64 | 0.78 |
| 1:O:459:ILE:CG2 | 1:O:473:GLN:HB2 | 2.12 | 0.78 |
| 1:K:480:VAL:C | 1:K:505:SER:CB | 2.50 | 0.78 |
| 1:D:480:VAL:C | 1:D:505:SER:CB | 2.50 | 0.78 |
| 1:E:172:LEU:HD11 | 1:E:213:ILE:HG13 | 1.63 | 0.78 |
| 1:F:480:VAL:C | 1:F:505:SER:CB | 2.50 | 0.78 |
| 1:F:552:VAL:HG21 | 1:F:555:LEU:HB2 | 1.66 | 0.78 |
| 1:H:435:LEU:HD13 | 1:I:624:PRO:HB2 | 1.65 | 0.78 |
| 1:M:368:GLU:HG3 | 1:M:399:LYS:HD2 | 1.64 | 0.78 |
| 1:B:435:LEU:HD13 | 1:C:624:PRO:HB2 | 1.65 | 0.78 |
| 1:I:368:GLU:HG3 | 1:I:399:LYS:HD2 | 1.64 | 0.78 |
| 1:D:172:LEU:HD11 | 1:D:213:ILE:HG13 | 1.63 | 0.78 |
| 1:G:172:LEU:HD11 | 1:G:213:ILE:HG13 | 1.63 | 0.78 |
| 1:I:435:LEU:HD13 | 1:J:624:PRO:HB2 | 1.65 | 0.78 |
| 1:D:552:VAL:HG21 | 1:D:555:LEU:HB2 | 1.66 | 0.78 |
| 1:G:552:VAL:HG21 | 1:G:555:LEU:HB2 | 1.66 | 0.78 |
| 1:M:435:LEU:HD13 | 1:N:624:PRO:HB2 | 1.65 | 0.78 |
| 1:B:172:LEU:HD11 | 1:B:213:ILE:HG13 | 1.63 | 0.78 |
| 1:C:552:VAL:HG21 | 1:C:555:LEU:HB2 | 1.66 | 0.78 |
| 1:F:435:LEU:HD13 | 1:G:624:PRO:HB2 | 1.65 | 0.78 |
| 1:K:507:VAL:O | 1:K:507:VAL:CG1 | 2.28 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:139:ILE:HG22 | 1:D:140:ILE:H | 1.50 | 0.77 |
| 1:G:435:LEU:HD13 | 1:H:624:PRO:HB2 | 1.65 | 0.77 |
| 1:I:139:ILE:HG22 | 1:I:140:ILE:H | 1.49 | 0.77 |
| 1:C:435:LEU:HD13 | 1:D:624:PRO:HB2 | 1.65 | 0.77 |
| 1:H:459:ILE:CG2 | 1:H:473:GLN:HB2 | 2.12 | 0.77 |
| 1:B:459:ILE:CG2 | 1:B:473:GLN:HB2 | 2.12 | 0.77 |
| 1:B:507:VAL:O | 1:B:507:VAL:CG1 | 2.28 | 0.77 |
| 1:C:459:ILE:CG2 | 1:C:473:GLN:HB2 | 2.12 | 0.77 |
| 1:E:504:VAL:HG13 | 1:E:521:ARG:HD3 | 1.67 | 0.77 |
| 1:E:552:VAL:HG21 | 1:E:555:LEU:HB2 | 1.66 | 0.77 |
| 1:C:504:VAL:HG13 | 1:C:521:ARG:HD3 | 1.67 | 0.77 |
| 1:H:139:ILE:HG22 | 1:H:140:ILE:H | 1.50 | 0.77 |
| 1:L:504:VAL:HG13 | 1:L:521:ARG:HD3 | 1.67 | 0.77 |
| 1:N:480:VAL:C | 1:N:505:SER:CB | 2.50 | 0.77 |
| 1:N:504:VAL:HG13 | 1:N:521:ARG:HD3 | 1.67 | 0.77 |
| 1:O:504:VAL:HG13 | 1:O:521:ARG:HD3 | 1.67 | 0.77 |
| 1:A:368:GLU:HG3 | 1:A:399:LYS:HD2 | 1.64 | 0.77 |
| 1:B:504:VAL:HG13 | 1:B:521:ARG:HD3 | 1.67 | 0.77 |
| 1:D:504:VAL:HG13 | 1:D:521:ARG:HD3 | 1.67 | 0.77 |
| 1:F:368:GLU:HG3 | 1:F:399:LYS:HD2 | 1.64 | 0.77 |
| 1:H:552:VAL:HG21 | 1:H:555:LEU:HB2 | 1.66 | 0.77 |
| 1:J:459:ILE:CG2 | 1:J:473:GLN:HB2 | 2.12 | 0.77 |
| 1:M:504:VAL:HG13 | 1:M:521:ARG:HD3 | 1.67 | 0.77 |
| 1:A:435:LEU:HD13 | 1:B:624:PRO:HB2 | 1.65 | 0.77 |
| 1:B:139:ILE:HG22 | 1:B:140:ILE:H | 1.49 | 0.77 |
| 1:I:459:ILE:CG2 | 1:I:473:GLN:HB2 | 2.12 | 0.77 |
| 1:N:139:ILE:HG22 | 1:N:140:ILE:H | 1.49 | 0.77 |
| 1:G:459:ILE:CG2 | 1:G:473:GLN:HB2 | 2.12 | 0.77 |
| 1:I:552:VAL:HG21 | 1:I:555:LEU:HB2 | 1.66 | 0.77 |
| 1:J:139:ILE:HG22 | 1:J:140:ILE:H | 1.49 | 0.77 |
| 1:M:139:ILE:HG22 | 1:M:140:ILE:H | 1.49 | 0.77 |
| 1:A:139:ILE:HG22 | 1:A:140:ILE:H | 1.49 | 0.77 |
| 1:A:459:ILE:CG2 | 1:A:473:GLN:HB2 | 2.12 | 0.77 |
| 1:D:459:ILE:CG2 | 1:D:473:GLN:HB2 | 2.12 | 0.77 |
| 1:F:139:ILE:HG22 | 1:F:140:ILE:H | 1.50 | 0.77 |
| 1:F:504:VAL:HG13 | 1:F:521:ARG:HD3 | 1.67 | 0.77 |
| 1:E:435:LEU:HD13 | 1:F:624:PRO:HB2 | 1.65 | 0.77 |
| 1:J:435:LEU:HD13 | 1:K:624:PRO:HB2 | 1.65 | 0.77 |
| 1:K:504:VAL:HG13 | 1:K:521:ARG:HD3 | 1.67 | 0.77 |
| 1:N:435:LEU:HD13 | 1:O:624:PRO:HB2 | 1.65 | 0.77 |
| 1:N:552:VAL:HG21 | 1:N:555:LEU:HB2 | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:504:VAL:HG13 | 1:A:521:ARG:HD3 | 1.67 | 0.77 |
| 1:H:504:VAL:HG13 | 1:H:521:ARG:HD3 | 1.67 | 0.77 |
| 1:K:435:LEU:HD13 | 1:L:624:PRO:HB2 | 1.65 | 0.77 |
| 1:L:435:LEU:HD13 | 1:M:624:PRO:HB2 | 1.65 | 0.77 |
| 1:M:130:ASN:HA | 1:M:143:THR:O | 1.85 | 0.77 |
| 1:O:139:ILE:HG22 | 1:O:140:ILE:H | 1.49 | 0.77 |
| 1:B:552:VAL:HG21 | 1:B:555:LEU:HB2 | 1.66 | 0.76 |
| 1:I:504:VAL:HG13 | 1:I:521:ARG:HD3 | 1.67 | 0.76 |
| 1:N:130:ASN:HA | 1:N:143:THR:O | 1.85 | 0.76 |
| 1:G:139:ILE:HG22 | 1:G:140:ILE:H | 1.50 | 0.76 |
| 1:G:504:VAL:HG13 | 1:G:521:ARG:HD3 | 1.67 | 0.76 |
| 1:D:130:ASN:HA | 1:D:143:THR:O | 1.85 | 0.76 |
| 1:L:552:VAL:HG21 | 1:L:555:LEU:HB2 | 1.66 | 0.76 |
| 1:E:130:ASN:HA | 1:E:143:THR:O | 1.85 | 0.76 |
| 1:K:130:ASN:HA | 1:K:143:THR:O | 1.85 | 0.76 |
| 1:K:552:VAL:HG21 | 1:K:555:LEU:HB2 | 1.66 | 0.76 |
| 1:A:552:VAL:HG21 | 1:A:555:LEU:HB2 | 1.66 | 0.76 |
| 1:D:435:LEU:HD13 | 1:E:624:PRO:HB2 | 1.65 | 0.76 |
| 1:J:130:ASN:HA | 1:J:143:THR:O | 1.85 | 0.76 |
| 1:J:552:VAL:HG21 | 1:J:555:LEU:HB2 | 1.66 | 0.76 |
| 1:M:552:VAL:HG21 | 1:M:555:LEU:HB2 | 1.65 | 0.76 |
| 1:H:507:VAL:O | 1:H:507:VAL:CG1 | 2.28 | 0.76 |
| 1:J:504:VAL:HG13 | 1:J:521:ARG:HD3 | 1.67 | 0.76 |
| 1:O:130:ASN:HA | 1:O:143:THR:O | 1.85 | 0.76 |
| 1:F:130:ASN:HA | 1:F:143:THR:O | 1.85 | 0.76 |
| 1:L:130:ASN:HA | 1:L:143:THR:O | 1.85 | 0.76 |
| 1:L:139:ILE:HG22 | 1:L:140:ILE:H | 1.50 | 0.76 |
| 1:C:130:ASN:HA | 1:C:143:THR:O | 1.85 | 0.76 |
| 1:O:507:VAL:HA | 1:O:518:PHE:HB3 | 1.67 | 0.76 |
| 1:A:507:VAL:HA | 1:A:518:PHE:HB3 | 1.67 | 0.76 |
| 1:C:507:VAL:O | 1:C:507:VAL:CG1 | 2.28 | 0.76 |
| 1:F:459:ILE:CG2 | 1:F:473:GLN:HB2 | 2.12 | 0.76 |
| 1:K:507:VAL:HA | 1:K:518:PHE:HB3 | 1.67 | 0.76 |
| 1:O:552:VAL:HG21 | 1:O:555:LEU:HB2 | 1.66 | 0.76 |
| 1:C:139:ILE:HG22 | 1:C:140:ILE:H | 1.49 | 0.75 |
| 1:E:459:ILE:CG2 | 1:E:473:GLN:HB2 | 2.12 | 0.75 |
| 1:I:130:ASN:HA | 1:I:143:THR:O | 1.85 | 0.75 |
| 1:K:139:ILE:HG22 | 1:K:140:ILE:H | 1.50 | 0.75 |
| 1:L:507:VAL:O | 1:L:507:VAL:CG1 | 2.28 | 0.75 |
| 1:A:130:ASN:HA | 1:A:143:THR:O | 1.85 | 0.75 |
| 1:G:130:ASN:HA | 1:G:143:THR:O | 1.85 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:507:VAL:HA | 1:J:518:PHE:HB3 | 1.67 | 0.75 |
| 1:E:507:VAL:HA | 1:E:518:PHE:HB3 | 1.67 | 0.75 |
| 1:L:507:VAL:HA | 1:L:518:PHE:HB3 | 1.67 | 0.75 |
| 1:B:130:ASN:HA | 1:B:143:THR:O | 1.85 | 0.75 |
| 1:F:507:VAL:HA | 1:F:518:PHE:HB3 | 1.67 | 0.75 |
| 1:N:507:VAL:HA | 1:N:518:PHE:HB3 | 1.67 | 0.75 |
| 1:B:507:VAL:HA | 1:B:518:PHE:HB3 | 1.67 | 0.75 |
| 1:G:507:VAL:HA | 1:G:518:PHE:HB3 | 1.67 | 0.75 |
| 1:E:221:VAL:O | 1:E:225:LEU:HB2 | 1.87 | 0.75 |
| 1:E:139:ILE:HG22 | 1:E:140:ILE:H | 1.49 | 0.75 |
| 1:H:507:VAL:HA | 1:H:518:PHE:HB3 | 1.67 | 0.75 |
| 1:L:221:VAL:O | 1:L:225:LEU:HB2 | 1.87 | 0.75 |
| 1:F:410:ALA:O | 1:F:424:ASN:HA | 1.87 | 0.74 |
| 1:I:507:VAL:HA | 1:I:518:PHE:HB3 | 1.67 | 0.74 |
| 1:J:221:VAL:O | 1:J:225:LEU:HB2 | 1.87 | 0.74 |
| 1:D:507:VAL:HA | 1:D:518:PHE:HB3 | 1.67 | 0.74 |
| 1:E:410:ALA:O | 1:E:424:ASN:HA | 1.87 | 0.74 |
| 1:H:130:ASN:HA | 1:H:143:THR:O | 1.85 | 0.74 |
| 1:I:221:VAL:O | 1:I:225:LEU:HB2 | 1.87 | 0.74 |
| 1:K:221:VAL:O | 1:K:225:LEU:HB2 | 1.87 | 0.74 |
| 1:K:410:ALA:O | 1:K:424:ASN:HA | 1.87 | 0.74 |
| 1:A:221:VAL:O | 1:A:225:LEU:HB2 | 1.87 | 0.74 |
| 1:C:507:VAL:HA | 1:C:518:PHE:HB3 | 1.67 | 0.74 |
| 1:D:221:VAL:O | 1:D:225:LEU:HB2 | 1.87 | 0.74 |
| 1:D:410:ALA:O | 1:D:424:ASN:HA | 1.87 | 0.74 |
| 1:F:221:VAL:O | 1:F:225:LEU:HB2 | 1.87 | 0.74 |
| 1:M:221:VAL:O | 1:M:225:LEU:HB2 | 1.87 | 0.74 |
| 1:G:410:ALA:O | 1:G:424:ASN:HA | 1.88 | 0.74 |
| 1:H:221:VAL:O | 1:H:225:LEU:HB2 | 1.87 | 0.74 |
| 1:M:507:VAL:HA | 1:M:518:PHE:HB3 | 1.67 | 0.74 |
| 1:N:459:ILE:CG2 | 1:N:473:GLN:HB2 | 2.12 | 0.74 |
| 1:I:221:VAL:HG13 | 1:I:225:LEU:HD12 | 1.69 | 0.74 |
| 1:H:410:ALA:O | 1:H:424:ASN:HA | 1.88 | 0.74 |
| 1:O:410:ALA:O | 1:O:424:ASN:HA | 1.87 | 0.74 |
| 1:C:410:ALA:O | 1:C:424:ASN:HA | 1.88 | 0.74 |
| 1:H:221:VAL:HG13 | 1:H:225:LEU:HD12 | 1.69 | 0.74 |
| 1:J:221:VAL:HG13 | 1:J:225:LEU:HD12 | 1.69 | 0.74 |
| 1:L:410:ALA:O | 1:L:424:ASN:HA | 1.87 | 0.74 |
| 1:N:410:ALA:O | 1:N:424:ASN:HA | 1.87 | 0.74 |
| 1:B:410:ALA:O | 1:B:424:ASN:HA | 1.87 | 0.74 |
| 1:K:221:VAL:HG13 | 1:K:225:LEU:HD12 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:221:VAL:HG13 | 1:L:225:LEU:HD12 | 1.69 | 0.74 |
| 1:F:456:VAL:CG2 | 1:F:457:PRO:HD2 | 2.18 | 0.74 |
| 1:G:221:VAL:O | 1:G:225:LEU:HB2 | 1.87 | 0.74 |
| 1:O:221:VAL:O | 1:O:225:LEU:HB2 | 1.87 | 0.74 |
| 1:B:221:VAL:O | 1:B:225:LEU:HB2 | 1.87 | 0.74 |
| 1:E:456:VAL:CG2 | 1:E:457:PRO:HD2 | 2.18 | 0.74 |
| 1:I:410:ALA:O | 1:I:424:ASN:HA | 1.88 | 0.74 |
| 1:N:456:VAL:CG2 | 1:N:457:PRO:HD2 | 2.18 | 0.74 |
| 1:O:456:VAL:CG2 | 1:O:457:PRO:HD2 | 2.18 | 0.74 |
| 1:A:410:ALA:O | 1:A:424:ASN:HA | 1.87 | 0.73 |
| 1:D:219:PRO:HA | 1:D:222:ARG:HB2 | 1.70 | 0.73 |
| 1:E:219:PRO:HA | 1:E:222:ARG:HB2 | 1.70 | 0.73 |
| 1:E:221:VAL:HG13 | 1:E:225:LEU:HD12 | 1.69 | 0.73 |
| 1:G:221:VAL:HG13 | 1:G:225:LEU:HD12 | 1.69 | 0.73 |
| 1:M:221:VAL:HG13 | 1:M:225:LEU:HD12 | 1.69 | 0.73 |
| 1:D:221:VAL:HG13 | 1:D:225:LEU:HD12 | 1.69 | 0.73 |
| 1:J:410:ALA:O | 1:J:424:ASN:HA | 1.87 | 0.73 |
| 1:O:221:VAL:HG13 | 1:O:225:LEU:HD12 | 1.69 | 0.73 |
| 1:D:456:VAL:CG2 | 1:D:457:PRO:HD2 | 2.18 | 0.73 |
| 1:G:456:VAL:CG2 | 1:G:457:PRO:HD2 | 2.18 | 0.73 |
| 1:F:219:PRO:HA | 1:F:222:ARG:HB2 | 1.70 | 0.73 |
| 1:A:456:VAL:CG2 | 1:A:457:PRO:HD2 | 2.18 | 0.73 |
| 1:A:221:VAL:HG13 | 1:A:225:LEU:HD12 | 1.69 | 0.73 |
| 1:K:219:PRO:HA | 1:K:222:ARG:HB2 | 1.70 | 0.73 |
| 1:M:410:ALA:O | 1:M:424:ASN:HA | 1.87 | 0.73 |
| 1:M:507:VAL:O | 1:M:507:VAL:CG1 | 2.28 | 0.73 |
| 1:F:221:VAL:HG13 | 1:F:225:LEU:HD12 | 1.69 | 0.73 |
| 1:J:219:PRO:HA | 1:J:222:ARG:HB2 | 1.70 | 0.73 |
| 1:N:221:VAL:O | 1:N:225:LEU:HB2 | 1.87 | 0.73 |
| 1:N:221:VAL:HG13 | 1:N:225:LEU:HD12 | 1.69 | 0.73 |
| 1:C:219:PRO:HA | 1:C:222:ARG:HB2 | 1.70 | 0.73 |
| 1:C:221:VAL:O | 1:C:225:LEU:HB2 | 1.87 | 0.73 |
| 1:C:456:VAL:CG2 | 1:C:457:PRO:HD2 | 2.18 | 0.73 |
| 1:G:219:PRO:HA | 1:G:222:ARG:HB2 | 1.70 | 0.73 |
| 1:H:456:VAL:CG2 | 1:H:457:PRO:HD2 | 2.18 | 0.73 |
| 1:C:221:VAL:HG13 | 1:C:225:LEU:HD12 | 1.69 | 0.73 |
| 1:I:507:VAL:O | 1:I:507:VAL:CG1 | 2.28 | 0.73 |
| 1:M:459:ILE:CG2 | 1:M:473:GLN:HB2 | 2.12 | 0.73 |
| 1:O:219:PRO:HA | 1:O:222:ARG:HB2 | 1.70 | 0.72 |
| 1:B:456:VAL:CG2 | 1:B:457:PRO:HD2 | 2.18 | 0.72 |
| 1:C:438:PRO:HG3 | 1:C:482:ILE:HG21 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:221:VAL:HG13 | 1:B:225:LEU:HD12 | 1.69 | 0.72 |
| 1:I:219:PRO:HA | 1:I:222:ARG:HB2 | 1.70 | 0.72 |
| 1:D:438:PRO:HG3 | 1:D:482:ILE:HG21 | 1.72 | 0.72 |
| 1:I:438:PRO:HG3 | 1:I:482:ILE:HG21 | 1.72 | 0.72 |
| 1:I:456:VAL:CG2 | 1:I:457:PRO:HD2 | 2.18 | 0.72 |
| 1:J:438:PRO:HG3 | 1:J:482:ILE:HG21 | 1.72 | 0.72 |
| 1:L:219:PRO:HA | 1:L:222:ARG:HB2 | 1.70 | 0.72 |
| 1:L:438:PRO:HG3 | 1:L:482:ILE:HG21 | 1.72 | 0.72 |
| 1:M:438:PRO:HG3 | 1:M:482:ILE:HG21 | 1.72 | 0.72 |
| 1:A:219:PRO:HA | 1:A:222:ARG:HB2 | 1.70 | 0.72 |
| 1:B:438:PRO:HG3 | 1:B:482:ILE:HG21 | 1.72 | 0.72 |
| 1:H:438:PRO:HG3 | 1:H:482:ILE:HG21 | 1.72 | 0.72 |
| 1:N:219:PRO:HA | 1:N:222:ARG:HB2 | 1.70 | 0.72 |
| 1:O:438:PRO:HG3 | 1:O:482:ILE:HG21 | 1.72 | 0.72 |
| 1:E:438:PRO:HG3 | 1:E:482:ILE:HG21 | 1.72 | 0.72 |
| 1:G:438:PRO:HG3 | 1:G:482:ILE:HG21 | 1.72 | 0.72 |
| 1:H:219:PRO:HA | 1:H:222:ARG:HB2 | 1.71 | 0.72 |
| 1:M:458:VAL:HG23 | 1:M:476:ASP:O | 1.90 | 0.72 |
| 1:N:458:VAL:HG23 | 1:N:476:ASP:O | 1.90 | 0.72 |
| 1:A:438:PRO:HG3 | 1:A:482:ILE:HG21 | 1.72 | 0.72 |
| 1:F:438:PRO:HG3 | 1:F:482:ILE:HG21 | 1.72 | 0.72 |
| 1:K:438:PRO:HG3 | 1:K:482:ILE:HG21 | 1.72 | 0.72 |
| 1:O:458:VAL:HG23 | 1:O:476:ASP:O | 1.90 | 0.71 |
| 1:E:609:PHE:CD1 | 1:F:639:ILE:HD13 | 2.25 | 0.71 |
| 1:H:458:VAL:HG23 | 1:H:476:ASP:O | 1.90 | 0.71 |
| 1:H:609:PHE:CD1 | 1:I:639:ILE:HD13 | 2.26 | 0.71 |
| 1:L:609:PHE:CD1 | 1:M:639:ILE:HD13 | 2.26 | 0.71 |
| 1:G:458:VAL:HG23 | 1:G:476:ASP:O | 1.90 | 0.71 |
| 1:J:458:VAL:HG23 | 1:J:476:ASP:O | 1.90 | 0.71 |
| 1:N:438:PRO:HG3 | 1:N:482:ILE:HG21 | 1.72 | 0.71 |
| 1:A:639:ILE:HD13 | 1:O:609:PHE:CD1 | 2.25 | 0.71 |
| 1:B:207:ASP:O | 1:B:211:ASN:N | 2.24 | 0.71 |
| 1:B:219:PRO:HA | 1:B:222:ARG:HB2 | 1.70 | 0.71 |
| 1:I:458:VAL:HG23 | 1:I:476:ASP:O | 1.90 | 0.71 |
| 1:I:609:PHE:CD1 | 1:J:639:ILE:HD13 | 2.26 | 0.71 |
| 1:K:609:PHE:CD1 | 1:L:639:ILE:HD13 | 2.26 | 0.71 |
| 1:M:207:ASP:O | 1:M:211:ASN:N | 2.24 | 0.71 |
| 1:M:609:PHE:CD1 | 1:N:639:ILE:HD13 | 2.26 | 0.71 |
| 1:F:609:PHE:CD1 | 1:G:639:ILE:HD13 | 2.26 | 0.71 |
| 1:G:609:PHE:CD1 | 1:H:639:ILE:HD13 | 2.26 | 0.71 |
| 1:I:207:ASP:O | 1:I:211:ASN:N | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:456:VAL:CG2 | 1:J:457:PRO:HD2 | 2.18 | 0.71 |
| 1:L:458:VAL:HG23 | 1:L:476:ASP:O | 1.90 | 0.71 |
| 1:A:458:VAL:HG23 | 1:A:476:ASP:O | 1.90 | 0.71 |
| 1:B:609:PHE:CD1 | 1:C:639:ILE:HD13 | 2.25 | 0.71 |
| 1:K:458:VAL:HG23 | 1:K:476:ASP:O | 1.90 | 0.71 |
| 1:N:609:PHE:CD1 | 1:O:639:ILE:HD13 | 2.26 | 0.71 |
| 1:F:458:VAL:HG23 | 1:F:476:ASP:O | 1.90 | 0.71 |
| 1:C:609:PHE:CD1 | 1:D:639:ILE:HD13 | 2.26 | 0.71 |
| 1:F:207:ASP:O | 1:F:211:ASN:N | 2.24 | 0.71 |
| 1:G:207:ASP:O | 1:G:211:ASN:N | 2.24 | 0.71 |
| 1:K:481:GLY:N | 1:K:505:SER:OG | 2.23 | 0.71 |
| 1:N:207:ASP:O | 1:N:211:ASN:N | 2.24 | 0.71 |
| 1:A:207:ASP:O | 1:A:211:ASN:N | 2.24 | 0.71 |
| 1:C:207:ASP:O | 1:C:211:ASN:N | 2.24 | 0.70 |
| 1:E:458:VAL:HG23 | 1:E:476:ASP:O | 1.90 | 0.70 |
| 1:K:207:ASP:O | 1:K:211:ASN:N | 2.24 | 0.70 |
| 1:L:207:ASP:O | 1:L:211:ASN:N | 2.24 | 0.70 |
| 1:L:456:VAL:CG2 | 1:L:457:PRO:HD2 | 2.18 | 0.70 |
| 1:D:207:ASP:O | 1:D:211:ASN:N | 2.24 | 0.70 |
| 1:C:609:PHE:CD2 | 1:D:639:ILE:CD1 | 2.75 | 0.70 |
| 1:J:609:PHE:CD1 | 1:K:639:ILE:HD13 | 2.25 | 0.70 |
| 1:K:456:VAL:CG2 | 1:K:457:PRO:HD2 | 2.18 | 0.70 |
| 1:L:481:GLY:N | 1:L:505:SER:OG | 2.23 | 0.70 |
| 1:E:458:VAL:O | 1:E:475:VAL:CA | 2.39 | 0.70 |
| 1:H:207:ASP:O | 1:H:211:ASN:N | 2.24 | 0.70 |
| 1:M:456:VAL:CG2 | 1:M:457:PRO:HD2 | 2.18 | 0.70 |
| 1:A:609:PHE:CD1 | 1:B:639:ILE:HD13 | 2.26 | 0.70 |
| 1:D:458:VAL:HG23 | 1:D:476:ASP:O | 1.90 | 0.70 |
| 1:M:219:PRO:HA | 1:M:222:ARG:HB2 | 1.71 | 0.70 |
| 1:B:458:VAL:HG23 | 1:B:476:ASP:O | 1.90 | 0.70 |
| 1:D:609:PHE:CD1 | 1:E:639:ILE:HD13 | 2.26 | 0.70 |
| 1:E:207:ASP:O | 1:E:211:ASN:N | 2.24 | 0.70 |
| 1:B:609:PHE:CD2 | 1:C:639:ILE:CD1 | 2.75 | 0.70 |
| 1:D:458:VAL:O | 1:D:475:VAL:CA | 2.39 | 0.70 |
| 1:F:458:VAL:O | 1:F:475:VAL:CA | 2.40 | 0.70 |
| 1:C:458:VAL:HG23 | 1:C:476:ASP:O | 1.90 | 0.70 |
| 1:M:328:GLU:CD | 1:M:521:ARG:NH1 | 2.45 | 0.70 |
| 1:N:328:GLU:CD | 1:N:521:ARG:NH1 | 2.45 | 0.70 |
| 1:O:207:ASP:O | 1:O:211:ASN:N | 2.24 | 0.70 |
| 1:L:328:GLU:CD | 1:L:521:ARG:NH1 | 2.45 | 0.70 |
| 1:J:207:ASP:O | 1:J:211:ASN:N | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:458:VAL:O | 1:A:475:VAL:CA | 2.39 | 0.69 |
| 1:I:609:PHE:CD2 | 1:J:639:ILE:CD1 | 2.75 | 0.69 |
| 1:K:328:GLU:CD | 1:K:521:ARG:NH1 | 2.45 | 0.69 |
| 1:L:458:VAL:O | 1:L:475:VAL:CA | 2.40 | 0.69 |
| 1:M:458:VAL:O | 1:M:475:VAL:CA | 2.40 | 0.69 |
| 1:O:328:GLU:CD | 1:O:521:ARG:NH1 | 2.45 | 0.69 |
| 1:M:481:GLY:N | 1:M:505:SER:OG | 2.23 | 0.69 |
| 1:N:458:VAL:O | 1:N:475:VAL:CA | 2.39 | 0.69 |
| 1:O:458:VAL:O | 1:O:475:VAL:CA | 2.39 | 0.69 |
| 1:F:328:GLU:CD | 1:F:521:ARG:NH1 | 2.45 | 0.69 |
| 1:G:328:GLU:CD | 1:G:521:ARG:NH1 | 2.45 | 0.69 |
| 1:M:609:PHE:CD2 | 1:N:639:ILE:CD1 | 2.75 | 0.69 |
| 1:A:328:GLU:CD | 1:A:521:ARG:NH1 | 2.45 | 0.69 |
| 1:B:458:VAL:O | 1:B:475:VAL:CA | 2.39 | 0.69 |
| 1:C:458:VAL:O | 1:C:475:VAL:CA | 2.40 | 0.69 |
| 1:G:458:VAL:O | 1:G:475:VAL:CA | 2.40 | 0.69 |
| 1:K:458:VAL:O | 1:K:475:VAL:CA | 2.40 | 0.69 |
| 1:J:328:GLU:CD | 1:J:521:ARG:NH1 | 2.45 | 0.69 |
| 1:B:328:GLU:CD | 1:B:521:ARG:NH1 | 2.45 | 0.69 |
| 1:J:458:VAL:O | 1:J:475:VAL:CA | 2.39 | 0.69 |
| 1:I:328:GLU:CD | 1:I:521:ARG:NH1 | 2.45 | 0.69 |
| 1:C:328:GLU:CD | 1:C:521:ARG:NH1 | 2.45 | 0.68 |
| 1:N:481:GLY:N | 1:N:505:SER:OG | 2.23 | 0.68 |
| 1:D:328:GLU:CD | 1:D:521:ARG:NH1 | 2.45 | 0.68 |
| 1:E:328:GLU:CD | 1:E:521:ARG:NH1 | 2.45 | 0.68 |
| 1:H:328:GLU:CD | 1:H:521:ARG:NH1 | 2.45 | 0.68 |
| 1:I:458:VAL:O | 1:I:475:VAL:CA | 2.40 | 0.68 |
| 1:H:458:VAL:O | 1:H:475:VAL:CA | 2.40 | 0.68 |
| 1:I:375:THR:HG23 | 1:I:390:THR:HG22 | 1.77 | 0.67 |
| 1:J:375:THR:HG23 | 1:J:390:THR:HG22 | 1.77 | 0.67 |
| 1:H:375:THR:HG23 | 1:H:390:THR:HG22 | 1.77 | 0.67 |
| 1:G:375:THR:HG23 | 1:G:390:THR:HG22 | 1.77 | 0.67 |
| 1:K:375:THR:HG23 | 1:K:390:THR:HG22 | 1.77 | 0.67 |
| 1:C:500:ILE:HD13 | 1:C:537:LEU:HD21 | 1.76 | 0.67 |
| 1:D:500:ILE:HD13 | 1:D:537:LEU:HD21 | 1.77 | 0.67 |
| 1:J:609:PHE:CD1 | 1:K:639:ILE:CD1 | 2.78 | 0.67 |
| 1:B:609:PHE:CD1 | 1:C:639:ILE:CD1 | 2.78 | 0.67 |
| 1:J:500:ILE:HD13 | 1:J:537:LEU:HD21 | 1.76 | 0.67 |
| 1:K:500:ILE:HD13 | 1:K:537:LEU:HD21 | 1.76 | 0.67 |
| 1:K:609:PHE:CD1 | 1:L:639:ILE:CD1 | 2.78 | 0.67 |
| 1:E:500:ILE:HD13 | 1:E:537:LEU:HD21 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:609:PHE:CD1 | 1:G:639:ILE:CD1 | 2.78 | 0.67 |
| 1:I:500:ILE:HD13 | 1:I:537:LEU:HD21 | 1.77 | 0.66 |
| 1:K:321:LEU:HD13 | 1:K:441:THR:OG1 | 1.96 | 0.66 |
| 1:G:609:PHE:CD1 | 1:H:639:ILE:CD1 | 2.78 | 0.66 |
| 1:I:609:PHE:CD1 | 1:J:639:ILE:CD1 | 2.78 | 0.66 |
| 1:A:639:ILE:CD1 | 1:O:609:PHE:CD1 | 2.78 | 0.66 |
| 1:B:375:THR:HG23 | 1:B:390:THR:HG22 | 1.77 | 0.66 |
| 1:B:481:GLY:N | 1:B:505:SER:OG | 2.23 | 0.66 |
| 1:J:321:LEU:HD13 | 1:J:441:THR:OG1 | 1.96 | 0.66 |
| 1:A:609:PHE:CD1 | 1:B:639:ILE:CD1 | 2.78 | 0.66 |
| 1:C:375:THR:HG23 | 1:C:390:THR:HG22 | 1.77 | 0.66 |
| 1:E:609:PHE:CD1 | 1:F:639:ILE:CD1 | 2.78 | 0.66 |
| 1:F:375:THR:HG23 | 1:F:390:THR:HG22 | 1.77 | 0.66 |
| 1:L:178:ALA:N | 1:L:208:GLU:OE2 | 2.28 | 0.66 |
| 1:L:321:LEU:HD13 | 1:L:441:THR:OG1 | 1.96 | 0.66 |
| 1:L:500:ILE:HD13 | 1:L:537:LEU:HD21 | 1.76 | 0.66 |
| 1:N:609:PHE:CD1 | 1:O:639:ILE:CD1 | 2.78 | 0.66 |
| 1:A:375:THR:HG23 | 1:A:390:THR:HG22 | 1.77 | 0.66 |
| 1:B:500:ILE:HD13 | 1:B:537:LEU:HD21 | 1.77 | 0.66 |
| 1:C:609:PHE:CD1 | 1:D:639:ILE:CD1 | 2.78 | 0.66 |
| 1:D:609:PHE:CD2 | 1:E:639:ILE:CD1 | 2.75 | 0.66 |
| 1:J:178:ALA:N | 1:J:208:GLU:OE2 | 2.28 | 0.66 |
| 1:L:375:THR:HG23 | 1:L:390:THR:HG22 | 1.77 | 0.66 |
| 1:L:609:PHE:CD1 | 1:M:639:ILE:CD1 | 2.78 | 0.66 |
| 1:N:609:PHE:CD2 | 1:O:639:ILE:CD1 | 2.75 | 0.66 |
| 1:O:140:ILE:HD13 | 1:O:156:ILE:HG23 | 1.78 | 0.66 |
| 1:H:500:ILE:HD13 | 1:H:537:LEU:HD21 | 1.76 | 0.66 |
| 1:L:140:ILE:HD13 | 1:L:156:ILE:HG23 | 1.78 | 0.66 |
| 1:M:140:ILE:HD13 | 1:M:156:ILE:HG23 | 1.78 | 0.66 |
| 1:M:327:VAL:HG11 | 1:N:603:ILE:HG21 | 1.78 | 0.66 |
| 1:M:500:ILE:HD13 | 1:M:537:LEU:HD21 | 1.77 | 0.66 |
| 1:N:327:VAL:HG11 | 1:O:603:ILE:HG21 | 1.78 | 0.66 |
| 1:A:172:LEU:O | 1:A:211:ASN:ND2 | 2.29 | 0.66 |
| 1:A:321:LEU:HD13 | 1:A:441:THR:OG1 | 1.96 | 0.66 |
| 1:B:442:VAL:HG21 | 1:B:488:PRO:HG3 | 1.78 | 0.66 |
| 1:D:375:THR:HG23 | 1:D:390:THR:HG22 | 1.77 | 0.66 |
| 1:F:500:ILE:HD13 | 1:F:537:LEU:HD21 | 1.77 | 0.66 |
| 1:G:458:VAL:HG21 | 1:G:478:LYS:HG2 | 1.78 | 0.66 |
| 1:H:609:PHE:CD2 | 1:I:639:ILE:CD1 | 2.75 | 0.66 |
| 1:M:321:LEU:HD13 | 1:M:441:THR:OG1 | 1.96 | 0.66 |
| 1:N:140:ILE:HD13 | 1:N:156:ILE:HG23 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:500:ILE:HD13 | 1:N:537:LEU:HD21 | 1.76 | 0.66 |
| 1:A:603:ILE:HG21 | 1:O:327:VAL:HG11 | 1.78 | 0.66 |
| 1:B:321:LEU:HD13 | 1:B:441:THR:OG1 | 1.96 | 0.66 |
| 1:C:172:LEU:O | 1:C:211:ASN:ND2 | 2.29 | 0.66 |
| 1:H:458:VAL:HG21 | 1:H:478:LYS:HG2 | 1.78 | 0.66 |
| 1:I:321:LEU:HD13 | 1:I:441:THR:OG1 | 1.96 | 0.66 |
| 1:O:172:LEU:O | 1:O:211:ASN:ND2 | 2.29 | 0.66 |
| 1:O:375:THR:HG23 | 1:O:390:THR:HG22 | 1.77 | 0.66 |
| 1:A:518:PHE:O | 1:B:455:GLU:OE1 | 2.14 | 0.66 |
| 1:D:172:LEU:O | 1:D:211:ASN:ND2 | 2.29 | 0.66 |
| 1:H:609:PHE:CD1 | 1:I:639:ILE:CD1 | 2.78 | 0.66 |
| 1:I:518:PHE:O | 1:J:455:GLU:OE1 | 2.14 | 0.66 |
| 1:L:172:LEU:O | 1:L:211:ASN:ND2 | 2.29 | 0.66 |
| 1:M:518:PHE:O | 1:N:455:GLU:OE1 | 2.14 | 0.66 |
| 1:N:172:LEU:O | 1:N:211:ASN:ND2 | 2.29 | 0.66 |
| 1:B:518:PHE:O | 1:C:455:GLU:OE1 | 2.14 | 0.66 |
| 1:C:321:LEU:HD13 | 1:C:441:THR:OG1 | 1.96 | 0.66 |
| 1:H:348:SER:HB2 | 1:I:412:VAL:HA | 1.78 | 0.66 |
| 1:J:348:SER:HB2 | 1:K:412:VAL:HA | 1.78 | 0.66 |
| 1:K:172:LEU:O | 1:K:211:ASN:ND2 | 2.29 | 0.66 |
| 1:L:327:VAL:HG11 | 1:M:603:ILE:HG21 | 1.78 | 0.66 |
| 1:L:518:PHE:O | 1:M:455:GLU:OE1 | 2.14 | 0.66 |
| 1:B:140:ILE:HD13 | 1:B:156:ILE:HG23 | 1.78 | 0.65 |
| 1:B:172:LEU:O | 1:B:211:ASN:ND2 | 2.29 | 0.65 |
| 1:D:458:VAL:HG21 | 1:D:478:LYS:HG2 | 1.78 | 0.65 |
| 1:D:609:PHE:CD1 | 1:E:639:ILE:CD1 | 2.78 | 0.65 |
| 1:E:458:VAL:HG21 | 1:E:478:LYS:HG2 | 1.78 | 0.65 |
| 1:E:518:PHE:O | 1:F:455:GLU:OE1 | 2.14 | 0.65 |
| 1:F:458:VAL:HG21 | 1:F:478:LYS:HG2 | 1.78 | 0.65 |
| 1:J:140:ILE:HD13 | 1:J:156:ILE:HG23 | 1.78 | 0.65 |
| 1:K:140:ILE:HD13 | 1:K:156:ILE:HG23 | 1.78 | 0.65 |
| 1:O:321:LEU:HD13 | 1:O:441:THR:OG1 | 1.96 | 0.65 |
| 1:C:178:ALA:N | 1:C:208:GLU:OE2 | 2.28 | 0.65 |
| 1:D:321:LEU:HD13 | 1:D:441:THR:OG1 | 1.96 | 0.65 |
| 1:D:442:VAL:HG21 | 1:D:488:PRO:HG3 | 1.78 | 0.65 |
| 1:D:518:PHE:O | 1:E:455:GLU:OE1 | 2.14 | 0.65 |
| 1:E:321:LEU:HD13 | 1:E:441:THR:OG1 | 1.96 | 0.65 |
| 1:G:172:LEU:O | 1:G:211:ASN:ND2 | 2.29 | 0.65 |
| 1:A:140:ILE:HD13 | 1:A:156:ILE:HG23 | 1.78 | 0.65 |
| 1:E:375:THR:HG23 | 1:E:390:THR:HG22 | 1.77 | 0.65 |
| 1:F:172:LEU:O | 1:F:211:ASN:ND2 | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:322:ILE:O | 1:G:439:SER:HA | 1.97 | 0.65 |
| 1:J:518:PHE:O | 1:K:455:GLU:OE1 | 2.14 | 0.65 |
| 1:L:348:SER:HB2 | 1:M:412:VAL:HA | 1.78 | 0.65 |
| 1:M:172:LEU:O | 1:M:211:ASN:ND2 | 2.29 | 0.65 |
| 1:N:375:THR:HG23 | 1:N:390:THR:HG22 | 1.77 | 0.65 |
| 1:O:442:VAL:HG21 | 1:O:488:PRO:HG3 | 1.78 | 0.65 |
| 1:C:458:VAL:HG21 | 1:C:478:LYS:HG2 | 1.78 | 0.65 |
| 1:D:322:ILE:O | 1:D:439:SER:HA | 1.97 | 0.65 |
| 1:G:609:PHE:CD2 | 1:H:639:ILE:CD1 | 2.75 | 0.65 |
| 1:H:327:VAL:HG11 | 1:I:603:ILE:HG21 | 1.78 | 0.65 |
| 1:M:609:PHE:CD1 | 1:N:639:ILE:CD1 | 2.78 | 0.65 |
| 1:O:500:ILE:HD13 | 1:O:537:LEU:HD21 | 1.76 | 0.65 |
| 1:A:327:VAL:HG11 | 1:B:603:ILE:HG21 | 1.78 | 0.65 |
| 1:A:328:GLU:CD | 1:A:521:ARG:HH11 | 2.00 | 0.65 |
| 1:A:481:GLY:N | 1:A:505:SER:OG | 2.23 | 0.65 |
| 1:A:500:ILE:HD13 | 1:A:537:LEU:HD21 | 1.77 | 0.65 |
| 1:C:140:ILE:HD13 | 1:C:156:ILE:HG23 | 1.78 | 0.65 |
| 1:F:321:LEU:HD13 | 1:F:441:THR:OG1 | 1.96 | 0.65 |
| 1:F:518:PHE:O | 1:G:455:GLU:OE1 | 2.14 | 0.65 |
| 1:G:500:ILE:HD13 | 1:G:537:LEU:HD21 | 1.77 | 0.65 |
| 1:H:518:PHE:O | 1:I:455:GLU:OE1 | 2.14 | 0.65 |
| 1:I:140:ILE:HD13 | 1:I:156:ILE:HG23 | 1.78 | 0.65 |
| 1:I:458:VAL:HG21 | 1:I:478:LYS:HG2 | 1.78 | 0.65 |
| 1:J:458:VAL:HG21 | 1:J:478:LYS:HG2 | 1.78 | 0.65 |
| 1:C:322:ILE:O | 1:C:439:SER:HA | 1.97 | 0.65 |
| 1:D:178:ALA:N | 1:D:208:GLU:OE2 | 2.28 | 0.65 |
| 1:E:442:VAL:HG21 | 1:E:488:PRO:HG3 | 1.78 | 0.65 |
| 1:G:327:VAL:HG11 | 1:H:603:ILE:HG21 | 1.78 | 0.65 |
| 1:H:321:LEU:HD13 | 1:H:441:THR:OG1 | 1.96 | 0.65 |
| 1:I:328:GLU:CD | 1:I:521:ARG:HH11 | 2.00 | 0.65 |
| 1:J:442:VAL:HG21 | 1:J:488:PRO:HG3 | 1.78 | 0.65 |
| 1:O:322:ILE:O | 1:O:439:SER:HA | 1.97 | 0.65 |
| 1:A:609:PHE:CD2 | 1:B:639:ILE:CD1 | 2.75 | 0.65 |
| 1:A:639:ILE:CD1 | 1:O:609:PHE:CD2 | 2.75 | 0.65 |
| 1:C:328:GLU:CD | 1:C:521:ARG:HH11 | 2.00 | 0.65 |
| 1:F:348:SER:HB2 | 1:G:412:VAL:HA | 1.78 | 0.65 |
| 1:H:172:LEU:O | 1:H:211:ASN:ND2 | 2.29 | 0.65 |
| 1:H:322:ILE:O | 1:H:439:SER:HA | 1.97 | 0.65 |
| 1:K:328:GLU:CD | 1:K:521:ARG:HH11 | 2.00 | 0.65 |
| 1:K:348:SER:HB2 | 1:L:412:VAL:HA | 1.78 | 0.65 |
| 1:A:455:GLU:OE1 | 1:O:518:PHE:O | 2.14 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:442:VAL:HG21 | 1:C:488:PRO:HG3 | 1.78 | 0.65 |
| 1:F:328:GLU:CD | 1:F:521:ARG:HH11 | 2.00 | 0.65 |
| 1:I:327:VAL:HG11 | 1:J:603:ILE:HG21 | 1.78 | 0.65 |
| 1:I:348:SER:HB2 | 1:J:412:VAL:HA | 1.78 | 0.65 |
| 1:K:327:VAL:HG11 | 1:L:603:ILE:HG21 | 1.78 | 0.65 |
| 1:K:442:VAL:HG21 | 1:K:488:PRO:HG3 | 1.78 | 0.65 |
| 1:N:321:LEU:HD13 | 1:N:441:THR:OG1 | 1.96 | 0.65 |
| 1:N:328:GLU:CD | 1:N:521:ARG:HH11 | 2.00 | 0.65 |
| 1:N:518:PHE:O | 1:O:455:GLU:OE1 | 2.14 | 0.65 |
| 1:F:609:PHE:CD2 | 1:G:639:ILE:CD1 | 2.75 | 0.65 |
| 1:M:375:THR:HG23 | 1:M:390:THR:HG22 | 1.77 | 0.65 |
| 1:N:348:SER:HB2 | 1:O:412:VAL:HA | 1.78 | 0.65 |
| 1:A:178:ALA:N | 1:A:208:GLU:OE2 | 2.28 | 0.65 |
| 1:B:178:ALA:N | 1:B:208:GLU:OE2 | 2.28 | 0.65 |
| 1:C:518:PHE:O | 1:D:455:GLU:OE1 | 2.14 | 0.65 |
| 1:D:328:GLU:CD | 1:D:521:ARG:HH11 | 2.00 | 0.65 |
| 1:F:327:VAL:HG11 | 1:G:603:ILE:HG21 | 1.78 | 0.65 |
| 1:H:442:VAL:HG21 | 1:H:488:PRO:HG3 | 1.78 | 0.65 |
| 1:I:442:VAL:HG21 | 1:I:488:PRO:HG3 | 1.78 | 0.65 |
| 1:J:172:LEU:O | 1:J:211:ASN:ND2 | 2.29 | 0.65 |
| 1:K:458:VAL:HG21 | 1:K:478:LYS:HG2 | 1.78 | 0.65 |
| 1:K:518:PHE:O | 1:L:455:GLU:OE1 | 2.14 | 0.65 |
| 1:N:322:ILE:O | 1:N:439:SER:HA | 1.97 | 0.65 |
| 1:A:322:ILE:O | 1:A:439:SER:HA | 1.97 | 0.64 |
| 1:F:322:ILE:O | 1:F:439:SER:HA | 1.97 | 0.64 |
| 1:I:172:LEU:O | 1:I:211:ASN:ND2 | 2.29 | 0.64 |
| 1:L:328:GLU:CD | 1:L:521:ARG:HH11 | 2.00 | 0.64 |
| 1:N:442:VAL:HG21 | 1:N:488:PRO:HG3 | 1.78 | 0.64 |
| 1:O:178:ALA:N | 1:O:208:GLU:OE2 | 2.28 | 0.64 |
| 1:A:442:VAL:HG21 | 1:A:488:PRO:HG3 | 1.78 | 0.64 |
| 1:G:328:GLU:CD | 1:G:521:ARG:HH11 | 2.00 | 0.64 |
| 1:G:348:SER:HB2 | 1:H:412:VAL:HA | 1.78 | 0.64 |
| 1:A:521:ARG:HD3 | 1:A:521:ARG:H | 1.63 | 0.64 |
| 1:E:172:LEU:O | 1:E:211:ASN:ND2 | 2.29 | 0.64 |
| 1:E:327:VAL:HG11 | 1:F:603:ILE:HG21 | 1.78 | 0.64 |
| 1:F:178:ALA:N | 1:F:208:GLU:OE2 | 2.28 | 0.64 |
| 1:G:321:LEU:HD13 | 1:G:441:THR:OG1 | 1.96 | 0.64 |
| 1:J:327:VAL:HG11 | 1:K:603:ILE:HG21 | 1.78 | 0.64 |
| 1:M:348:SER:HB2 | 1:N:412:VAL:HA | 1.78 | 0.64 |
| 1:O:458:VAL:HG21 | 1:O:478:LYS:HG2 | 1.78 | 0.64 |
| 1:O:521:ARG:HD3 | 1:O:521:ARG:H | 1.63 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:458:VAL:HG21 | 1:B:478:LYS:HG2 | 1.78 | 0.64 |
| 1:D:327:VAL:HG11 | 1:E:603:ILE:HG21 | 1.78 | 0.64 |
| 1:E:322:ILE:O | 1:E:439:SER:HA | 1.97 | 0.64 |
| 1:E:521:ARG:HD3 | 1:E:521:ARG:H | 1.63 | 0.64 |
| 1:G:442:VAL:HG21 | 1:G:488:PRO:HG3 | 1.78 | 0.64 |
| 1:H:140:ILE:HD13 | 1:H:156:ILE:HG23 | 1.78 | 0.64 |
| 1:N:521:ARG:HD3 | 1:N:521:ARG:H | 1.63 | 0.64 |
| 1:A:458:VAL:HG21 | 1:A:478:LYS:HG2 | 1.78 | 0.64 |
| 1:D:140:ILE:HD13 | 1:D:156:ILE:HG23 | 1.78 | 0.64 |
| 1:D:521:ARG:HD3 | 1:D:521:ARG:H | 1.63 | 0.64 |
| 1:F:140:ILE:HD13 | 1:F:156:ILE:HG23 | 1.78 | 0.64 |
| 1:F:442:VAL:HG21 | 1:F:488:PRO:HG3 | 1.78 | 0.64 |
| 1:G:140:ILE:HD13 | 1:G:156:ILE:HG23 | 1.78 | 0.64 |
| 1:L:540:LEU:HD22 | 1:M:452:VAL:HG21 | 1.80 | 0.64 |
| 1:M:458:VAL:HG21 | 1:M:478:LYS:HG2 | 1.78 | 0.64 |
| 1:E:140:ILE:HD13 | 1:E:156:ILE:HG23 | 1.78 | 0.64 |
| 1:E:178:ALA:N | 1:E:208:GLU:OE2 | 2.28 | 0.64 |
| 1:G:176:SER:OG | 1:G:208:GLU:OE2 | 2.16 | 0.64 |
| 1:I:322:ILE:O | 1:I:439:SER:HA | 1.97 | 0.64 |
| 1:M:322:ILE:O | 1:M:439:SER:HA | 1.97 | 0.64 |
| 1:M:442:VAL:HG21 | 1:M:488:PRO:HG3 | 1.78 | 0.64 |
| 1:M:521:ARG:HD3 | 1:M:521:ARG:H | 1.63 | 0.64 |
| 1:A:348:SER:HB2 | 1:B:412:VAL:HA | 1.78 | 0.64 |
| 1:B:327:VAL:HG11 | 1:C:603:ILE:HG21 | 1.78 | 0.64 |
| 1:B:328:GLU:CD | 1:B:521:ARG:HH11 | 2.00 | 0.64 |
| 1:B:521:ARG:HD3 | 1:B:521:ARG:H | 1.63 | 0.64 |
| 1:J:328:GLU:CD | 1:J:521:ARG:HH11 | 2.00 | 0.64 |
| 1:L:442:VAL:HG21 | 1:L:488:PRO:HG3 | 1.78 | 0.64 |
| 1:M:540:LEU:HD22 | 1:N:452:VAL:HG21 | 1.80 | 0.64 |
| 1:C:327:VAL:HG11 | 1:D:603:ILE:HG21 | 1.78 | 0.64 |
| 1:E:348:SER:HB2 | 1:F:412:VAL:HA | 1.78 | 0.64 |
| 1:K:322:ILE:O | 1:K:439:SER:HA | 1.97 | 0.64 |
| 1:A:176:SER:OG | 1:A:208:GLU:OE2 | 2.16 | 0.64 |
| 1:B:348:SER:HB2 | 1:C:412:VAL:HA | 1.78 | 0.64 |
| 1:G:518:PHE:O | 1:H:455:GLU:OE1 | 2.14 | 0.64 |
| 1:G:540:LEU:HD22 | 1:H:452:VAL:HG21 | 1.80 | 0.64 |
| 1:K:540:LEU:HD22 | 1:L:452:VAL:HG21 | 1.80 | 0.64 |
| 1:L:458:VAL:HG21 | 1:L:478:LYS:HG2 | 1.78 | 0.64 |
| 1:L:521:ARG:HD3 | 1:L:521:ARG:H | 1.63 | 0.64 |
| 1:B:322:ILE:O | 1:B:439:SER:HA | 1.97 | 0.64 |
| 1:C:348:SER:HB2 | 1:D:412:VAL:HA | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:348:SER:HB2 | 1:E:412:VAL:HA | 1.78 | 0.64 |
| 1:G:178:ALA:N | 1:G:208:GLU:OE2 | 2.28 | 0.64 |
| 1:M:504:VAL:HG11 | 1:M:521:ARG:HG2 | 1.80 | 0.64 |
| 1:N:178:ALA:N | 1:N:208:GLU:OE2 | 2.28 | 0.64 |
| 1:D:504:VAL:HG11 | 1:D:521:ARG:HG2 | 1.80 | 0.63 |
| 1:G:521:ARG:HD3 | 1:G:521:ARG:H | 1.63 | 0.63 |
| 1:I:521:ARG:HD3 | 1:I:521:ARG:H | 1.63 | 0.63 |
| 1:L:504:VAL:HG11 | 1:L:521:ARG:HG2 | 1.81 | 0.63 |
| 1:A:412:VAL:HA | 1:O:348:SER:HB2 | 1.78 | 0.63 |
| 1:A:639:ILE:HD12 | 1:O:609:PHE:CG | 2.34 | 0.63 |
| 1:B:176:SER:OG | 1:B:208:GLU:OE2 | 2.16 | 0.63 |
| 1:E:504:VAL:HG11 | 1:E:521:ARG:HG2 | 1.80 | 0.63 |
| 1:G:507:VAL:HA | 1:G:518:PHE:CB | 2.28 | 0.63 |
| 1:H:540:LEU:HD22 | 1:I:452:VAL:HG21 | 1.80 | 0.63 |
| 1:J:521:ARG:HD3 | 1:J:521:ARG:H | 1.63 | 0.63 |
| 1:K:504:VAL:HG11 | 1:K:521:ARG:HG2 | 1.81 | 0.63 |
| 1:N:458:VAL:HG21 | 1:N:478:LYS:HG2 | 1.78 | 0.63 |
| 1:C:521:ARG:HD3 | 1:C:521:ARG:H | 1.63 | 0.63 |
| 1:E:609:PHE:CG | 1:F:639:ILE:HD12 | 2.34 | 0.63 |
| 1:F:521:ARG:HD3 | 1:F:521:ARG:H | 1.63 | 0.63 |
| 1:F:609:PHE:CG | 1:G:639:ILE:HD12 | 2.34 | 0.63 |
| 1:H:176:SER:OG | 1:H:208:GLU:OE2 | 2.16 | 0.63 |
| 1:H:521:ARG:HD3 | 1:H:521:ARG:H | 1.63 | 0.63 |
| 1:I:257:GLU:OE1 | 1:I:257:GLU:HA | 1.99 | 0.63 |
| 1:J:322:ILE:O | 1:J:439:SER:HA | 1.97 | 0.63 |
| 1:L:322:ILE:O | 1:L:439:SER:HA | 1.97 | 0.63 |
| 1:O:176:SER:OG | 1:O:208:GLU:OE2 | 2.16 | 0.63 |
| 1:O:481:GLY:N | 1:O:505:SER:OG | 2.23 | 0.63 |
| 1:A:609:PHE:CG | 1:B:639:ILE:HD12 | 2.34 | 0.63 |
| 1:C:504:VAL:HG11 | 1:C:521:ARG:HG2 | 1.80 | 0.63 |
| 1:E:507:VAL:HA | 1:E:518:PHE:CB | 2.28 | 0.63 |
| 1:F:257:GLU:HA | 1:F:257:GLU:OE1 | 1.99 | 0.63 |
| 1:K:521:ARG:HD3 | 1:K:521:ARG:H | 1.63 | 0.63 |
| 1:M:507:VAL:HA | 1:M:518:PHE:CB | 2.28 | 0.63 |
| 1:N:540:LEU:HD22 | 1:O:452:VAL:HG21 | 1.80 | 0.63 |
| 1:N:609:PHE:CG | 1:O:639:ILE:HD12 | 2.34 | 0.63 |
| 1:A:519:ALA:HB2 | 1:B:454:GLU:HG3 | 1.81 | 0.63 |
| 1:F:540:LEU:HD22 | 1:G:452:VAL:HG21 | 1.80 | 0.63 |
| 1:B:519:ALA:HB2 | 1:C:454:GLU:HG3 | 1.81 | 0.63 |
| 1:E:257:GLU:OE1 | 1:E:257:GLU:HA | 1.99 | 0.63 |
| 1:H:244:VAL:HG22 | 1:H:295:VAL:HG22 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:504:VAL:HG11 | 1:J:521:ARG:HG2 | 1.80 | 0.63 |
| 1:J:540:LEU:HD22 | 1:K:452:VAL:HG21 | 1.80 | 0.63 |
| 1:M:178:ALA:N | 1:M:208:GLU:OE2 | 2.28 | 0.63 |
| 1:O:507:VAL:HA | 1:O:518:PHE:CB | 2.28 | 0.63 |
| 1:C:519:ALA:HB2 | 1:D:454:GLU:HG3 | 1.81 | 0.63 |
| 1:F:504:VAL:HG11 | 1:F:521:ARG:HG2 | 1.80 | 0.63 |
| 1:G:244:VAL:HG22 | 1:G:295:VAL:HG22 | 1.81 | 0.63 |
| 1:I:507:VAL:HA | 1:I:518:PHE:CB | 2.28 | 0.63 |
| 1:K:326:ILE:HD11 | 1:K:502:GLN:HE21 | 1.64 | 0.63 |
| 1:A:454:GLU:HG3 | 1:O:519:ALA:HB2 | 1.81 | 0.63 |
| 1:C:176:SER:OG | 1:C:208:GLU:OE2 | 2.16 | 0.63 |
| 1:D:609:PHE:CG | 1:E:639:ILE:HD12 | 2.34 | 0.63 |
| 1:E:164:ASP:O | 1:E:218:ASP:HA | 1.99 | 0.63 |
| 1:E:326:ILE:HD11 | 1:E:502:GLN:HE21 | 1.64 | 0.63 |
| 1:E:328:GLU:CD | 1:E:521:ARG:HH11 | 2.00 | 0.63 |
| 1:G:164:ASP:O | 1:G:218:ASP:HA | 1.99 | 0.63 |
| 1:J:257:GLU:OE1 | 1:J:257:GLU:HA | 1.99 | 0.63 |
| 1:K:178:ALA:N | 1:K:208:GLU:OE2 | 2.28 | 0.63 |
| 1:N:504:VAL:HG11 | 1:N:521:ARG:HG2 | 1.80 | 0.63 |
| 1:O:326:ILE:HD11 | 1:O:502:GLN:HE21 | 1.64 | 0.63 |
| 1:O:328:GLU:CD | 1:O:521:ARG:HH11 | 2.00 | 0.63 |
| 1:O:458:VAL:CG2 | 1:O:476:ASP:O | 2.47 | 0.63 |
| 1:A:326:ILE:HD11 | 1:A:502:GLN:HE21 | 1.64 | 0.63 |
| 1:A:458:VAL:CG2 | 1:A:476:ASP:O | 2.47 | 0.63 |
| 1:A:507:VAL:HA | 1:A:518:PHE:CB | 2.28 | 0.63 |
| 1:B:164:ASP:O | 1:B:218:ASP:HA | 1.99 | 0.63 |
| 1:B:260:LYS:O | 1:B:263:SER:OG | 2.17 | 0.63 |
| 1:E:540:LEU:HD22 | 1:F:452:VAL:HG21 | 1.80 | 0.63 |
| 1:I:540:LEU:HD22 | 1:J:452:VAL:HG21 | 1.80 | 0.63 |
| 1:J:458:VAL:CG2 | 1:J:476:ASP:O | 2.47 | 0.63 |
| 1:L:326:ILE:HD11 | 1:L:502:GLN:HE21 | 1.64 | 0.63 |
| 1:C:507:VAL:HA | 1:C:518:PHE:CB | 2.28 | 0.62 |
| 1:D:326:ILE:HD11 | 1:D:502:GLN:HE21 | 1.64 | 0.62 |
| 1:D:519:ALA:HB2 | 1:E:454:GLU:HG3 | 1.81 | 0.62 |
| 1:F:244:VAL:HG22 | 1:F:295:VAL:HG22 | 1.81 | 0.62 |
| 1:H:178:ALA:N | 1:H:208:GLU:OE2 | 2.28 | 0.62 |
| 1:I:244:VAL:HG22 | 1:I:295:VAL:HG22 | 1.81 | 0.62 |
| 1:I:458:VAL:CG2 | 1:I:476:ASP:O | 2.47 | 0.62 |
| 1:K:164:ASP:O | 1:K:218:ASP:HA | 1.99 | 0.62 |
| 1:O:164:ASP:O | 1:O:218:ASP:HA | 1.99 | 0.62 |
| 1:B:609:PHE:CG | 1:C:639:ILE:HD12 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:540:LEU:HD22 | 1:D:452:VAL:HG21 | 1.80 | 0.62 |
| 1:E:458:VAL:CG2 | 1:E:476:ASP:O | 2.47 | 0.62 |
| 1:I:164:ASP:O | 1:I:218:ASP:HA | 1.99 | 0.62 |
| 1:J:326:ILE:HD11 | 1:J:502:GLN:HE21 | 1.64 | 0.62 |
| 1:K:176:SER:OG | 1:K:208:GLU:OE2 | 2.16 | 0.62 |
| 1:N:489:GLN:NE2 | 1:O:249:TYR:O | 2.32 | 0.62 |
| 1:B:257:GLU:OE1 | 1:B:257:GLU:HA | 1.99 | 0.62 |
| 1:C:260:LYS:O | 1:C:263:SER:OG | 2.17 | 0.62 |
| 1:H:507:VAL:HA | 1:H:518:PHE:CB | 2.28 | 0.62 |
| 1:I:489:GLN:NE2 | 1:J:249:TYR:O | 2.32 | 0.62 |
| 1:L:507:VAL:HA | 1:L:518:PHE:CB | 2.28 | 0.62 |
| 1:N:164:ASP:O | 1:N:218:ASP:HA | 1.99 | 0.62 |
| 1:N:458:VAL:CG2 | 1:N:476:ASP:O | 2.47 | 0.62 |
| 1:B:504:VAL:HG11 | 1:B:521:ARG:HG2 | 1.81 | 0.62 |
| 1:C:164:ASP:O | 1:C:218:ASP:HA | 1.99 | 0.62 |
| 1:D:458:VAL:CG2 | 1:D:476:ASP:O | 2.47 | 0.62 |
| 1:E:244:VAL:HG22 | 1:E:295:VAL:HG22 | 1.81 | 0.62 |
| 1:F:458:VAL:CG2 | 1:F:476:ASP:O | 2.47 | 0.62 |
| 1:F:489:GLN:NE2 | 1:G:249:TYR:O | 2.32 | 0.62 |
| 1:F:507:VAL:HA | 1:F:518:PHE:CB | 2.28 | 0.62 |
| 1:G:489:GLN:NE2 | 1:H:249:TYR:O | 2.33 | 0.62 |
| 1:I:504:VAL:HG11 | 1:I:521:ARG:HG2 | 1.80 | 0.62 |
| 1:K:244:VAL:HG22 | 1:K:295:VAL:HG22 | 1.81 | 0.62 |
| 1:K:458:VAL:CG2 | 1:K:476:ASP:O | 2.47 | 0.62 |
| 1:K:489:GLN:NE2 | 1:L:249:TYR:O | 2.32 | 0.62 |
| 1:L:489:GLN:NE2 | 1:M:249:TYR:O | 2.32 | 0.62 |
| 1:M:519:ALA:HB2 | 1:N:454:GLU:HG3 | 1.81 | 0.62 |
| 1:N:519:ALA:HB2 | 1:O:454:GLU:HG3 | 1.81 | 0.62 |
| 1:A:489:GLN:NE2 | 1:B:249:TYR:O | 2.32 | 0.62 |
| 1:D:244:VAL:HG22 | 1:D:295:VAL:HG22 | 1.81 | 0.62 |
| 1:E:489:GLN:NE2 | 1:F:249:TYR:O | 2.32 | 0.62 |
| 1:G:504:VAL:HG11 | 1:G:521:ARG:HG2 | 1.80 | 0.62 |
| 1:H:257:GLU:OE1 | 1:H:257:GLU:HA | 1.99 | 0.62 |
| 1:H:328:GLU:CD | 1:H:521:ARG:HH11 | 2.00 | 0.62 |
| 1:H:458:VAL:CG2 | 1:H:476:ASP:O | 2.47 | 0.62 |
| 1:I:178:ALA:N | 1:I:208:GLU:OE2 | 2.28 | 0.62 |
| 1:J:244:VAL:HG22 | 1:J:295:VAL:HG22 | 1.81 | 0.62 |
| 1:K:507:VAL:HA | 1:K:518:PHE:CB | 2.28 | 0.62 |
| 1:L:176:SER:OG | 1:L:208:GLU:OE2 | 2.16 | 0.62 |
| 1:L:459:ILE:HG23 | 1:L:474:THR:C | 2.16 | 0.62 |
| 1:A:452:VAL:HG21 | 1:O:540:LEU:HD22 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:540:LEU:HD22 | 1:C:452:VAL:HG21 | 1.80 | 0.62 |
| 1:C:489:GLN:NE2 | 1:D:249:TYR:O | 2.32 | 0.62 |
| 1:E:539:GLY:HA2 | 1:E:577:LEU:O | 2.00 | 0.62 |
| 1:G:257:GLU:OE1 | 1:G:257:GLU:HA | 1.99 | 0.62 |
| 1:J:459:ILE:HG23 | 1:J:474:THR:C | 2.16 | 0.62 |
| 1:L:164:ASP:O | 1:L:218:ASP:HA | 1.99 | 0.62 |
| 1:M:176:SER:OG | 1:M:208:GLU:OE2 | 2.16 | 0.62 |
| 1:M:257:GLU:OE1 | 1:M:257:GLU:HA | 1.99 | 0.62 |
| 1:B:458:VAL:CG2 | 1:B:476:ASP:O | 2.47 | 0.62 |
| 1:C:257:GLU:HA | 1:C:257:GLU:OE1 | 1.99 | 0.62 |
| 1:D:260:LYS:O | 1:D:263:SER:OG | 2.17 | 0.62 |
| 1:D:489:GLN:NE2 | 1:E:249:TYR:O | 2.32 | 0.62 |
| 1:F:326:ILE:HD11 | 1:F:502:GLN:HE21 | 1.64 | 0.62 |
| 1:I:539:GLY:HA2 | 1:I:577:LEU:O | 2.00 | 0.62 |
| 1:J:507:VAL:HA | 1:J:518:PHE:CB | 2.28 | 0.62 |
| 1:L:458:VAL:CG2 | 1:L:476:ASP:O | 2.47 | 0.62 |
| 1:L:519:ALA:HB2 | 1:M:454:GLU:HG3 | 1.81 | 0.62 |
| 1:M:164:ASP:O | 1:M:218:ASP:HA | 1.99 | 0.62 |
| 1:M:489:GLN:NE2 | 1:N:249:TYR:O | 2.32 | 0.62 |
| 1:A:244:VAL:HG22 | 1:A:295:VAL:HG22 | 1.81 | 0.62 |
| 1:A:540:LEU:HD22 | 1:B:452:VAL:HG21 | 1.80 | 0.62 |
| 1:B:539:GLY:HA2 | 1:B:577:LEU:O | 2.00 | 0.62 |
| 1:C:326:ILE:HD11 | 1:C:502:GLN:HE21 | 1.64 | 0.62 |
| 1:C:458:VAL:CG2 | 1:C:476:ASP:O | 2.47 | 0.62 |
| 1:C:539:GLY:HA2 | 1:C:577:LEU:O | 2.00 | 0.62 |
| 1:C:609:PHE:CG | 1:D:639:ILE:HD12 | 2.34 | 0.62 |
| 1:D:164:ASP:O | 1:D:218:ASP:HA | 1.99 | 0.62 |
| 1:D:257:GLU:OE1 | 1:D:257:GLU:HA | 1.99 | 0.62 |
| 1:D:540:LEU:HD22 | 1:E:452:VAL:HG21 | 1.80 | 0.62 |
| 1:E:519:ALA:HB2 | 1:F:454:GLU:HG3 | 1.81 | 0.62 |
| 1:F:539:GLY:HA2 | 1:F:577:LEU:O | 2.00 | 0.62 |
| 1:I:176:SER:OG | 1:I:208:GLU:OE2 | 2.16 | 0.62 |
| 1:I:459:ILE:HG23 | 1:I:474:THR:C | 2.16 | 0.62 |
| 1:J:539:GLY:HA2 | 1:J:577:LEU:O | 2.00 | 0.62 |
| 1:N:244:VAL:HG22 | 1:N:295:VAL:HG22 | 1.81 | 0.62 |
| 1:C:226:LYS:HA | 1:C:229:ILE:HD12 | 1.82 | 0.62 |
| 1:D:507:VAL:HA | 1:D:518:PHE:CB | 2.28 | 0.62 |
| 1:H:489:GLN:NE2 | 1:I:249:TYR:O | 2.32 | 0.62 |
| 1:I:326:ILE:HD11 | 1:I:502:GLN:HE21 | 1.64 | 0.62 |
| 1:K:459:ILE:HG23 | 1:K:474:THR:C | 2.16 | 0.62 |
| 1:M:328:GLU:CD | 1:M:521:ARG:HH11 | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:507:VAL:HA | 1:N:518:PHE:CB | 2.28 | 0.62 |
| 1:A:164:ASP:O | 1:A:218:ASP:HA | 1.99 | 0.62 |
| 1:A:249:TYR:O | 1:O:489:GLN:NE2 | 2.32 | 0.62 |
| 1:A:257:GLU:OE1 | 1:A:257:GLU:HA | 1.99 | 0.62 |
| 1:B:489:GLN:NE2 | 1:C:249:TYR:O | 2.32 | 0.62 |
| 1:D:176:SER:OG | 1:D:208:GLU:OE2 | 2.16 | 0.62 |
| 1:D:539:GLY:HA2 | 1:D:577:LEU:O | 2.00 | 0.62 |
| 1:E:481:GLY:O | 1:E:505:SER:N | 2.33 | 0.62 |
| 1:F:481:GLY:O | 1:F:505:SER:N | 2.33 | 0.62 |
| 1:G:458:VAL:CG2 | 1:G:476:ASP:O | 2.47 | 0.62 |
| 1:G:481:GLY:O | 1:G:505:SER:N | 2.33 | 0.62 |
| 1:L:257:GLU:OE1 | 1:L:257:GLU:HA | 1.99 | 0.62 |
| 1:M:458:VAL:CG2 | 1:M:476:ASP:O | 2.47 | 0.62 |
| 1:O:504:VAL:HG11 | 1:O:521:ARG:HG2 | 1.80 | 0.62 |
| 1:B:506:ASN:O | 1:B:518:PHE:HB2 | 2.00 | 0.61 |
| 1:B:507:VAL:HA | 1:B:518:PHE:CB | 2.28 | 0.61 |
| 1:D:481:GLY:O | 1:D:505:SER:N | 2.33 | 0.61 |
| 1:E:260:LYS:O | 1:E:263:SER:OG | 2.17 | 0.61 |
| 1:G:519:ALA:HB2 | 1:H:454:GLU:HG3 | 1.81 | 0.61 |
| 1:G:522:GLN:HG2 | 1:H:451:ILE:CG2 | 2.30 | 0.61 |
| 1:H:519:ALA:HB2 | 1:I:454:GLU:HG3 | 1.81 | 0.61 |
| 1:J:176:SER:OG | 1:J:208:GLU:OE2 | 2.16 | 0.61 |
| 1:J:609:PHE:CG | 1:K:639:ILE:HD12 | 2.34 | 0.61 |
| 1:K:257:GLU:OE1 | 1:K:257:GLU:HA | 1.99 | 0.61 |
| 1:M:522:GLN:HG2 | 1:N:451:ILE:CG2 | 2.30 | 0.61 |
| 1:N:176:SER:OG | 1:N:208:GLU:OE2 | 2.16 | 0.61 |
| 1:N:326:ILE:HD11 | 1:N:502:GLN:HE21 | 1.64 | 0.61 |
| 1:A:504:VAL:HG11 | 1:A:521:ARG:HG2 | 1.80 | 0.61 |
| 1:A:506:ASN:O | 1:A:518:PHE:HB2 | 2.00 | 0.61 |
| 1:A:539:GLY:HA2 | 1:A:577:LEU:O | 2.00 | 0.61 |
| 1:D:226:LYS:HA | 1:D:229:ILE:HD12 | 1.82 | 0.61 |
| 1:H:164:ASP:O | 1:H:218:ASP:HA | 1.99 | 0.61 |
| 1:H:481:GLY:O | 1:H:505:SER:N | 2.33 | 0.61 |
| 1:H:539:GLY:HA2 | 1:H:577:LEU:O | 2.00 | 0.61 |
| 1:I:226:LYS:HA | 1:I:229:ILE:HD12 | 1.82 | 0.61 |
| 1:J:226:LYS:HA | 1:J:229:ILE:HD12 | 1.82 | 0.61 |
| 1:J:522:GLN:HG2 | 1:K:451:ILE:CG2 | 2.30 | 0.61 |
| 1:K:519:ALA:HB2 | 1:L:454:GLU:HG3 | 1.81 | 0.61 |
| 1:L:244:VAL:HG22 | 1:L:295:VAL:HG22 | 1.81 | 0.61 |
| 1:A:451:ILE:CG2 | 1:O:522:GLN:HG2 | 2.30 | 0.61 |
| 1:A:522:GLN:HG2 | 1:B:451:ILE:CG2 | 2.30 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:326:ILE:HD11 | 1:B:502:GLN:HE21 | 1.64 | 0.61 |
| 1:B:604:ARG:NH2 | 1:B:626:LEU:O | 2.34 | 0.61 |
| 1:C:244:VAL:HG22 | 1:C:295:VAL:HG22 | 1.81 | 0.61 |
| 1:C:481:GLY:O | 1:C:505:SER:N | 2.33 | 0.61 |
| 1:C:506:ASN:O | 1:C:518:PHE:HB2 | 2.01 | 0.61 |
| 1:D:604:ARG:NH2 | 1:D:626:LEU:O | 2.34 | 0.61 |
| 1:H:506:ASN:O | 1:H:518:PHE:HB2 | 2.01 | 0.61 |
| 1:I:519:ALA:HB2 | 1:J:454:GLU:HG3 | 1.81 | 0.61 |
| 1:I:609:PHE:CG | 1:J:639:ILE:HD12 | 2.34 | 0.61 |
| 1:K:539:GLY:HA2 | 1:K:577:LEU:O | 2.00 | 0.61 |
| 1:M:326:ILE:HD11 | 1:M:502:GLN:HE21 | 1.64 | 0.61 |
| 1:B:481:GLY:O | 1:B:505:SER:N | 2.33 | 0.61 |
| 1:B:522:GLN:HG2 | 1:C:451:ILE:CG2 | 2.30 | 0.61 |
| 1:D:506:ASN:O | 1:D:518:PHE:HB2 | 2.01 | 0.61 |
| 1:F:519:ALA:HB2 | 1:G:454:GLU:HG3 | 1.81 | 0.61 |
| 1:I:481:GLY:O | 1:I:505:SER:N | 2.33 | 0.61 |
| 1:I:604:ARG:NH2 | 1:I:626:LEU:O | 2.34 | 0.61 |
| 1:J:489:GLN:NE2 | 1:K:249:TYR:O | 2.32 | 0.61 |
| 1:J:604:ARG:NH2 | 1:J:626:LEU:O | 2.34 | 0.61 |
| 1:K:506:ASN:O | 1:K:518:PHE:HB2 | 2.00 | 0.61 |
| 1:O:506:ASN:O | 1:O:518:PHE:HB2 | 2.01 | 0.61 |
| 1:A:481:GLY:O | 1:A:505:SER:N | 2.33 | 0.61 |
| 1:B:477:ARG:HH11 | 1:B:477:ARG:CG | 2.14 | 0.61 |
| 1:E:226:LYS:HA | 1:E:229:ILE:HD12 | 1.82 | 0.61 |
| 1:F:452:VAL:O | 1:F:481:GLY:HA3 | 2.01 | 0.61 |
| 1:F:604:ARG:NH2 | 1:F:626:LEU:O | 2.34 | 0.61 |
| 1:H:504:VAL:HG11 | 1:H:521:ARG:HG2 | 1.80 | 0.61 |
| 1:J:477:ARG:HH11 | 1:J:477:ARG:CG | 2.14 | 0.61 |
| 1:J:481:GLY:O | 1:J:505:SER:N | 2.33 | 0.61 |
| 1:J:519:ALA:HB2 | 1:K:454:GLU:HG3 | 1.81 | 0.61 |
| 1:K:226:LYS:HA | 1:K:229:ILE:HD12 | 1.83 | 0.61 |
| 1:K:481:GLY:O | 1:K:505:SER:N | 2.33 | 0.61 |
| 1:N:184:VAL:HG13 | 1:N:187:LEU:HD12 | 1.82 | 0.61 |
| 1:N:257:GLU:HA | 1:N:257:GLU:OE1 | 1.99 | 0.61 |
| 1:N:522:GLN:HG2 | 1:O:451:ILE:CG2 | 2.30 | 0.61 |
| 1:O:184:VAL:HG13 | 1:O:187:LEU:HD12 | 1.82 | 0.61 |
| 1:B:226:LYS:HA | 1:B:229:ILE:HD12 | 1.83 | 0.61 |
| 1:C:452:VAL:O | 1:C:481:GLY:HA3 | 2.01 | 0.61 |
| 1:F:164:ASP:O | 1:F:218:ASP:HA | 1.99 | 0.61 |
| 1:F:260:LYS:O | 1:F:263:SER:OG | 2.17 | 0.61 |
| 1:H:477:ARG:HH11 | 1:H:477:ARG:CG | 2.14 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:481:GLY:O | 1:N:505:SER:N | 2.33 | 0.61 |
| 1:N:506:ASN:O | 1:N:518:PHE:HB2 | 2.01 | 0.61 |
| 1:O:481:GLY:O | 1:O:505:SER:N | 2.33 | 0.61 |
| 1:O:539:GLY:HA2 | 1:O:577:LEU:O | 2.00 | 0.61 |
| 1:E:604:ARG:NH2 | 1:E:626:LEU:O | 2.34 | 0.61 |
| 1:G:506:ASN:O | 1:G:518:PHE:HB2 | 2.01 | 0.61 |
| 1:H:452:VAL:O | 1:H:481:GLY:HA3 | 2.01 | 0.61 |
| 1:H:522:GLN:HG2 | 1:I:451:ILE:CG2 | 2.31 | 0.61 |
| 1:H:604:ARG:NH2 | 1:H:626:LEU:O | 2.34 | 0.61 |
| 1:I:452:VAL:O | 1:I:481:GLY:HA3 | 2.01 | 0.61 |
| 1:J:164:ASP:O | 1:J:218:ASP:HA | 1.99 | 0.61 |
| 1:K:452:VAL:O | 1:K:481:GLY:HA3 | 2.01 | 0.61 |
| 1:L:452:VAL:O | 1:L:481:GLY:HA3 | 2.01 | 0.61 |
| 1:L:477:ARG:HH11 | 1:L:477:ARG:CG | 2.14 | 0.61 |
| 1:L:481:GLY:O | 1:L:505:SER:N | 2.33 | 0.61 |
| 1:L:506:ASN:O | 1:L:518:PHE:HB2 | 2.01 | 0.61 |
| 1:L:539:GLY:HA2 | 1:L:577:LEU:O | 2.00 | 0.61 |
| 1:A:508:LEU:HD12 | 1:A:508:LEU:N | 2.16 | 0.61 |
| 1:C:604:ARG:NH2 | 1:C:626:LEU:O | 2.34 | 0.61 |
| 1:E:506:ASN:O | 1:E:518:PHE:HB2 | 2.00 | 0.61 |
| 1:E:522:GLN:HG2 | 1:F:451:ILE:CG2 | 2.30 | 0.61 |
| 1:G:452:VAL:O | 1:G:481:GLY:HA3 | 2.01 | 0.61 |
| 1:H:226:LYS:HA | 1:H:229:ILE:HD12 | 1.82 | 0.61 |
| 1:H:326:ILE:HD11 | 1:H:502:GLN:HE21 | 1.64 | 0.61 |
| 1:L:226:LYS:HA | 1:L:229:ILE:HD12 | 1.82 | 0.61 |
| 1:L:508:LEU:HD12 | 1:L:508:LEU:N | 2.16 | 0.61 |
| 1:L:522:GLN:HG2 | 1:M:451:ILE:CG2 | 2.30 | 0.61 |
| 1:M:184:VAL:HG13 | 1:M:187:LEU:HD12 | 1.82 | 0.61 |
| 1:M:506:ASN:O | 1:M:518:PHE:HB2 | 2.00 | 0.61 |
| 1:N:477:ARG:CG | 1:N:477:ARG:HH11 | 2.14 | 0.61 |
| 1:A:184:VAL:HG13 | 1:A:187:LEU:HD12 | 1.82 | 0.61 |
| 1:A:604:ARG:NH2 | 1:A:626:LEU:O | 2.34 | 0.61 |
| 1:B:477:ARG:HH11 | 1:B:477:ARG:HG2 | 1.66 | 0.61 |
| 1:C:477:ARG:HG2 | 1:C:477:ARG:HH11 | 1.66 | 0.61 |
| 1:C:522:GLN:HG2 | 1:D:451:ILE:CG2 | 2.31 | 0.61 |
| 1:E:184:VAL:HG13 | 1:E:187:LEU:HD12 | 1.82 | 0.61 |
| 1:E:477:ARG:HH11 | 1:E:477:ARG:CG | 2.14 | 0.61 |
| 1:G:326:ILE:HD11 | 1:G:502:GLN:HE21 | 1.64 | 0.61 |
| 1:G:539:GLY:HA2 | 1:G:577:LEU:O | 2.00 | 0.61 |
| 1:K:508:LEU:N | 1:K:508:LEU:HD12 | 2.16 | 0.61 |
| 1:K:522:GLN:HG2 | 1:L:451:ILE:CG2 | 2.30 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:609:PHE:CG | 1:M:639:ILE:HD12 | 2.34 | 0.61 |
| 1:M:481:GLY:O | 1:M:505:SER:N | 2.33 | 0.61 |
| 1:N:452:VAL:O | 1:N:481:GLY:HA3 | 2.01 | 0.61 |
| 1:O:452:VAL:O | 1:O:481:GLY:HA3 | 2.01 | 0.61 |
| 1:B:244:VAL:HG22 | 1:B:295:VAL:HG22 | 1.81 | 0.61 |
| 1:C:504:VAL:HG13 | 1:C:521:ARG:CD | 2.31 | 0.61 |
| 1:D:477:ARG:HG2 | 1:D:477:ARG:HH11 | 1.66 | 0.61 |
| 1:D:522:GLN:HG2 | 1:E:451:ILE:CG2 | 2.30 | 0.61 |
| 1:F:184:VAL:HG13 | 1:F:187:LEU:HD12 | 1.82 | 0.61 |
| 1:F:508:LEU:N | 1:F:508:LEU:HD12 | 2.16 | 0.61 |
| 1:G:604:ARG:NH2 | 1:G:626:LEU:O | 2.34 | 0.61 |
| 1:I:184:VAL:HG13 | 1:I:187:LEU:HD12 | 1.82 | 0.61 |
| 1:J:184:VAL:HG13 | 1:J:187:LEU:HD12 | 1.82 | 0.61 |
| 1:J:452:VAL:O | 1:J:481:GLY:HA3 | 2.01 | 0.61 |
| 1:K:480:VAL:HA | 1:K:505:SER:HB2 | 1.83 | 0.61 |
| 1:M:244:VAL:HG22 | 1:M:295:VAL:HG22 | 1.81 | 0.61 |
| 1:M:508:LEU:HD12 | 1:M:508:LEU:N | 2.16 | 0.61 |
| 1:M:604:ARG:NH2 | 1:M:626:LEU:O | 2.34 | 0.61 |
| 1:N:604:ARG:NH2 | 1:N:626:LEU:O | 2.34 | 0.61 |
| 1:O:458:VAL:HB | 1:O:476:ASP:O | 2.01 | 0.61 |
| 1:O:604:ARG:NH2 | 1:O:626:LEU:O | 2.34 | 0.61 |
| 1:A:477:ARG:HG2 | 1:A:477:ARG:HH11 | 1.66 | 0.60 |
| 1:D:458:VAL:HB | 1:D:476:ASP:O | 2.01 | 0.60 |
| 1:F:477:ARG:CG | 1:F:477:ARG:HH11 | 2.14 | 0.60 |
| 1:F:506:ASN:O | 1:F:518:PHE:HB2 | 2.01 | 0.60 |
| 1:I:508:LEU:HD12 | 1:I:508:LEU:N | 2.16 | 0.60 |
| 1:J:508:LEU:HD12 | 1:J:508:LEU:N | 2.16 | 0.60 |
| 1:K:604:ARG:NH2 | 1:K:626:LEU:O | 2.34 | 0.60 |
| 1:M:226:LYS:HA | 1:M:229:ILE:HD12 | 1.82 | 0.60 |
| 1:M:459:ILE:HG23 | 1:M:474:THR:C | 2.16 | 0.60 |
| 1:M:477:ARG:HH11 | 1:M:477:ARG:CG | 2.14 | 0.60 |
| 1:N:539:GLY:HA2 | 1:N:577:LEU:O | 2.00 | 0.60 |
| 1:O:477:ARG:HH11 | 1:O:477:ARG:CG | 2.14 | 0.60 |
| 1:A:226:LYS:HA | 1:A:229:ILE:HD12 | 1.82 | 0.60 |
| 1:D:184:VAL:HG13 | 1:D:187:LEU:HD12 | 1.82 | 0.60 |
| 1:D:452:VAL:O | 1:D:481:GLY:HA3 | 2.01 | 0.60 |
| 1:E:176:SER:OG | 1:E:208:GLU:OE2 | 2.16 | 0.60 |
| 1:G:260:LYS:O | 1:G:263:SER:OG | 2.17 | 0.60 |
| 1:G:459:ILE:HG23 | 1:G:474:THR:C | 2.16 | 0.60 |
| 1:H:184:VAL:HG13 | 1:H:187:LEU:HD12 | 1.82 | 0.60 |
| 1:H:480:VAL:HA | 1:H:505:SER:HB2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:506:ASN:O | 1:I:518:PHE:HB2 | 2.00 | 0.60 |
| 1:J:506:ASN:O | 1:J:518:PHE:HB2 | 2.01 | 0.60 |
| 1:L:480:VAL:HA | 1:L:505:SER:HB2 | 1.83 | 0.60 |
| 1:M:539:GLY:HA2 | 1:M:577:LEU:O | 2.00 | 0.60 |
| 1:N:459:ILE:HG23 | 1:N:474:THR:C | 2.16 | 0.60 |
| 1:N:480:VAL:HA | 1:N:505:SER:HB2 | 1.83 | 0.60 |
| 1:B:142:ILE:HD11 | 1:B:156:ILE:HD12 | 1.84 | 0.60 |
| 1:C:184:VAL:HG13 | 1:C:187:LEU:HD12 | 1.82 | 0.60 |
| 1:C:477:ARG:HH11 | 1:C:477:ARG:CG | 2.14 | 0.60 |
| 1:D:142:ILE:HD11 | 1:D:156:ILE:HD12 | 1.84 | 0.60 |
| 1:D:508:LEU:HD12 | 1:D:508:LEU:N | 2.16 | 0.60 |
| 1:E:452:VAL:O | 1:E:481:GLY:HA3 | 2.01 | 0.60 |
| 1:E:458:VAL:HB | 1:E:476:ASP:O | 2.01 | 0.60 |
| 1:F:438:PRO:HG3 | 1:F:482:ILE:CG2 | 2.32 | 0.60 |
| 1:F:522:GLN:HG2 | 1:G:451:ILE:CG2 | 2.31 | 0.60 |
| 1:G:184:VAL:HG13 | 1:G:187:LEU:HD12 | 1.82 | 0.60 |
| 1:G:477:ARG:HH11 | 1:G:477:ARG:CG | 2.14 | 0.60 |
| 1:G:508:LEU:HD12 | 1:G:508:LEU:N | 2.16 | 0.60 |
| 1:N:458:VAL:HB | 1:N:476:ASP:O | 2.01 | 0.60 |
| 1:N:508:LEU:N | 1:N:508:LEU:HD12 | 2.16 | 0.60 |
| 1:O:477:ARG:HH11 | 1:O:477:ARG:HG2 | 1.66 | 0.60 |
| 1:O:480:VAL:HA | 1:O:505:SER:HB2 | 1.83 | 0.60 |
| 1:O:504:VAL:HG13 | 1:O:521:ARG:CD | 2.31 | 0.60 |
| 1:A:458:VAL:HB | 1:A:476:ASP:O | 2.01 | 0.60 |
| 1:A:477:ARG:HH11 | 1:A:477:ARG:CG | 2.14 | 0.60 |
| 1:C:508:LEU:N | 1:C:508:LEU:HD12 | 2.16 | 0.60 |
| 1:D:477:ARG:HH11 | 1:D:477:ARG:CG | 2.14 | 0.60 |
| 1:F:226:LYS:HA | 1:F:229:ILE:HD12 | 1.83 | 0.60 |
| 1:F:504:VAL:HG13 | 1:F:521:ARG:CD | 2.31 | 0.60 |
| 1:H:459:ILE:HG23 | 1:H:474:THR:C | 2.16 | 0.60 |
| 1:I:522:GLN:HG2 | 1:J:451:ILE:CG2 | 2.31 | 0.60 |
| 1:K:184:VAL:HG13 | 1:K:187:LEU:HD12 | 1.82 | 0.60 |
| 1:A:142:ILE:HD11 | 1:A:156:ILE:HD12 | 1.84 | 0.60 |
| 1:B:452:VAL:O | 1:B:481:GLY:HA3 | 2.01 | 0.60 |
| 1:E:477:ARG:HH11 | 1:E:477:ARG:HG2 | 1.66 | 0.60 |
| 1:F:154:GLU:O | 1:F:158:ARG:HB2 | 2.02 | 0.60 |
| 1:I:260:LYS:O | 1:I:263:SER:OG | 2.17 | 0.60 |
| 1:I:438:PRO:HG3 | 1:I:482:ILE:CG2 | 2.32 | 0.60 |
| 1:I:477:ARG:HG2 | 1:I:477:ARG:HH11 | 1.66 | 0.60 |
| 1:J:477:ARG:HH11 | 1:J:477:ARG:HG2 | 1.66 | 0.60 |
| 1:L:166:GLU:HB2 | 1:L:222:ARG:HH21 | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:604:ARG:NH2 | 1:L:626:LEU:O | 2.34 | 0.60 |
| 1:O:166:GLU:HB2 | 1:O:222:ARG:HH21 | 1.67 | 0.60 |
| 1:O:257:GLU:OE1 | 1:O:257:GLU:HA | 1.99 | 0.60 |
| 1:B:504:VAL:HG13 | 1:B:521:ARG:CD | 2.31 | 0.60 |
| 1:E:154:GLU:O | 1:E:158:ARG:HB2 | 2.02 | 0.60 |
| 1:F:481:GLY:N | 1:F:505:SER:OG | 2.23 | 0.60 |
| 1:G:154:GLU:O | 1:G:158:ARG:HB2 | 2.02 | 0.60 |
| 1:H:438:PRO:HG3 | 1:H:482:ILE:CG2 | 2.32 | 0.60 |
| 1:L:184:VAL:HG13 | 1:L:187:LEU:HD12 | 1.82 | 0.60 |
| 1:M:506:ASN:HD22 | 1:M:506:ASN:C | 2.04 | 0.60 |
| 1:N:226:LYS:HA | 1:N:229:ILE:HD12 | 1.82 | 0.60 |
| 1:N:504:VAL:HG13 | 1:N:521:ARG:CD | 2.31 | 0.60 |
| 1:B:184:VAL:HG13 | 1:B:187:LEU:HD12 | 1.82 | 0.60 |
| 1:C:142:ILE:HD11 | 1:C:156:ILE:HD12 | 1.84 | 0.60 |
| 1:H:260:LYS:O | 1:H:263:SER:OG | 2.17 | 0.60 |
| 1:K:477:ARG:HH11 | 1:K:477:ARG:CG | 2.14 | 0.60 |
| 1:N:477:ARG:HH11 | 1:N:477:ARG:HG2 | 1.66 | 0.60 |
| 1:N:506:ASN:HD22 | 1:N:506:ASN:C | 2.04 | 0.60 |
| 1:O:244:VAL:HG22 | 1:O:295:VAL:HG22 | 1.81 | 0.60 |
| 1:C:154:GLU:O | 1:C:158:ARG:HB2 | 2.02 | 0.60 |
| 1:C:438:PRO:HG3 | 1:C:482:ILE:CG2 | 2.32 | 0.60 |
| 1:E:142:ILE:HD11 | 1:E:156:ILE:HD12 | 1.84 | 0.60 |
| 1:F:142:ILE:HD11 | 1:F:156:ILE:HD12 | 1.84 | 0.60 |
| 1:G:226:LYS:HA | 1:G:229:ILE:HD12 | 1.82 | 0.60 |
| 1:H:154:GLU:O | 1:H:158:ARG:HB2 | 2.02 | 0.60 |
| 1:I:477:ARG:HH11 | 1:I:477:ARG:CG | 2.14 | 0.60 |
| 1:I:480:VAL:HA | 1:I:505:SER:HB2 | 1.83 | 0.60 |
| 1:J:260:LYS:O | 1:J:263:SER:OG | 2.17 | 0.60 |
| 1:K:609:PHE:CG | 1:L:639:ILE:HD12 | 2.34 | 0.60 |
| 1:O:142:ILE:HD11 | 1:O:156:ILE:HD12 | 1.84 | 0.60 |
| 1:A:452:VAL:O | 1:A:481:GLY:HA3 | 2.01 | 0.60 |
| 1:A:506:ASN:HD22 | 1:A:506:ASN:C | 2.04 | 0.60 |
| 1:B:508:LEU:HD12 | 1:B:508:LEU:N | 2.16 | 0.60 |
| 1:C:458:VAL:HB | 1:C:476:ASP:O | 2.01 | 0.60 |
| 1:G:142:ILE:HD11 | 1:G:156:ILE:HD12 | 1.84 | 0.60 |
| 1:H:508:LEU:N | 1:H:508:LEU:HD12 | 2.16 | 0.60 |
| 1:I:104:VAL:HG22 | 1:I:141:LEU:HD23 | 1.84 | 0.60 |
| 1:M:458:VAL:HB | 1:M:476:ASP:O | 2.01 | 0.60 |
| 1:M:609:PHE:CG | 1:N:639:ILE:HD12 | 2.34 | 0.60 |
| 1:O:508:LEU:HD12 | 1:O:508:LEU:N | 2.16 | 0.60 |
| 1:B:480:VAL:HA | 1:B:505:SER:HB2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:154:GLU:O | 1:D:158:ARG:HB2 | 2.02 | 0.60 |
| 1:D:438:PRO:HG3 | 1:D:482:ILE:CG2 | 2.32 | 0.60 |
| 1:G:104:VAL:HG22 | 1:G:141:LEU:HD23 | 1.84 | 0.60 |
| 1:I:121:GLN:O | 1:I:125:ASN:N | 2.33 | 0.60 |
| 1:L:504:VAL:HG13 | 1:L:521:ARG:CD | 2.31 | 0.60 |
| 1:N:142:ILE:HD11 | 1:N:156:ILE:HD12 | 1.84 | 0.60 |
| 1:O:459:ILE:HG23 | 1:O:474:THR:C | 2.16 | 0.60 |
| 1:B:166:GLU:HB2 | 1:B:222:ARG:HH21 | 1.67 | 0.59 |
| 1:E:504:VAL:HG13 | 1:E:521:ARG:CD | 2.31 | 0.59 |
| 1:F:458:VAL:HB | 1:F:476:ASP:O | 2.01 | 0.59 |
| 1:G:438:PRO:HG3 | 1:G:482:ILE:CG2 | 2.32 | 0.59 |
| 1:G:609:PHE:CG | 1:H:639:ILE:HD12 | 2.34 | 0.59 |
| 1:H:477:ARG:HH11 | 1:H:477:ARG:HG2 | 1.66 | 0.59 |
| 1:H:490:ILE:HG22 | 1:H:491:ASN:O | 2.03 | 0.59 |
| 1:I:166:GLU:HB2 | 1:I:222:ARG:HH21 | 1.67 | 0.59 |
| 1:J:166:GLU:HB2 | 1:J:222:ARG:HH21 | 1.67 | 0.59 |
| 1:K:506:ASN:HD22 | 1:K:506:ASN:C | 2.04 | 0.59 |
| 1:O:226:LYS:HA | 1:O:229:ILE:HD12 | 1.82 | 0.59 |
| 1:C:166:GLU:HB2 | 1:C:222:ARG:HH21 | 1.67 | 0.59 |
| 1:E:438:PRO:HG3 | 1:E:482:ILE:CG2 | 2.32 | 0.59 |
| 1:E:480:VAL:HA | 1:E:505:SER:HB2 | 1.83 | 0.59 |
| 1:J:480:VAL:HA | 1:J:505:SER:HB2 | 1.83 | 0.59 |
| 1:K:477:ARG:HH11 | 1:K:477:ARG:HG2 | 1.66 | 0.59 |
| 1:L:490:ILE:HG22 | 1:L:491:ASN:O | 2.02 | 0.59 |
| 1:N:490:ILE:HG22 | 1:N:491:ASN:O | 2.03 | 0.59 |
| 1:A:490:ILE:HG22 | 1:A:491:ASN:O | 2.03 | 0.59 |
| 1:B:438:PRO:HG3 | 1:B:482:ILE:CG2 | 2.31 | 0.59 |
| 1:C:480:VAL:HA | 1:C:505:SER:HB2 | 1.83 | 0.59 |
| 1:F:490:ILE:HG22 | 1:F:491:ASN:O | 2.03 | 0.59 |
| 1:I:154:GLU:O | 1:I:158:ARG:HB2 | 2.02 | 0.59 |
| 1:I:504:VAL:HG13 | 1:I:521:ARG:CD | 2.31 | 0.59 |
| 1:J:490:ILE:HG22 | 1:J:491:ASN:O | 2.02 | 0.59 |
| 1:K:260:LYS:O | 1:K:263:SER:OG | 2.17 | 0.59 |
| 1:K:438:PRO:HG3 | 1:K:482:ILE:CG2 | 2.32 | 0.59 |
| 1:K:458:VAL:HB | 1:K:476:ASP:O | 2.01 | 0.59 |
| 1:M:452:VAL:O | 1:M:481:GLY:HA3 | 2.01 | 0.59 |
| 1:M:458:VAL:CB | 1:M:476:ASP:O | 2.51 | 0.59 |
| 1:N:166:GLU:HB2 | 1:N:222:ARG:HH21 | 1.67 | 0.59 |
| 1:N:438:PRO:HG3 | 1:N:482:ILE:CG2 | 2.32 | 0.59 |
| 1:N:458:VAL:CB | 1:N:476:ASP:O | 2.51 | 0.59 |
| 1:O:104:VAL:HG22 | 1:O:141:LEU:HD23 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:177:ALA:HB3 | 1:A:208:GLU:CG | 2.33 | 0.59 |
| 1:B:458:VAL:HB | 1:B:476:ASP:O | 2.01 | 0.59 |
| 1:E:166:GLU:HB2 | 1:E:222:ARG:HH21 | 1.67 | 0.59 |
| 1:F:166:GLU:HB2 | 1:F:222:ARG:HH21 | 1.67 | 0.59 |
| 1:F:459:ILE:HG23 | 1:F:474:THR:C | 2.16 | 0.59 |
| 1:H:459:ILE:HD12 | 1:H:459:ILE:H | 1.67 | 0.59 |
| 1:J:104:VAL:HG22 | 1:J:141:LEU:HD23 | 1.84 | 0.59 |
| 1:J:177:ALA:HB3 | 1:J:208:GLU:CG | 2.33 | 0.59 |
| 1:J:458:VAL:HB | 1:J:476:ASP:O | 2.01 | 0.59 |
| 1:K:104:VAL:HG22 | 1:K:141:LEU:HD23 | 1.84 | 0.59 |
| 1:L:438:PRO:HG3 | 1:L:482:ILE:CG2 | 2.32 | 0.59 |
| 1:O:177:ALA:HB3 | 1:O:208:GLU:CG | 2.33 | 0.59 |
| 1:O:458:VAL:CB | 1:O:476:ASP:O | 2.51 | 0.59 |
| 1:A:104:VAL:HG22 | 1:A:141:LEU:HD23 | 1.84 | 0.59 |
| 1:B:154:GLU:O | 1:B:158:ARG:HB2 | 2.02 | 0.59 |
| 1:B:458:VAL:CB | 1:B:476:ASP:O | 2.51 | 0.59 |
| 1:F:477:ARG:HH11 | 1:F:477:ARG:HG2 | 1.66 | 0.59 |
| 1:G:166:GLU:HB2 | 1:G:222:ARG:HH21 | 1.67 | 0.59 |
| 1:G:458:VAL:HB | 1:G:476:ASP:O | 2.01 | 0.59 |
| 1:H:104:VAL:HG22 | 1:H:141:LEU:HD23 | 1.84 | 0.59 |
| 1:K:177:ALA:HB3 | 1:K:208:GLU:CG | 2.33 | 0.59 |
| 1:L:260:LYS:O | 1:L:263:SER:OG | 2.17 | 0.59 |
| 1:L:458:VAL:CB | 1:L:476:ASP:O | 2.51 | 0.59 |
| 1:L:458:VAL:HB | 1:L:476:ASP:O | 2.01 | 0.59 |
| 1:M:166:GLU:HB2 | 1:M:222:ARG:HH21 | 1.67 | 0.59 |
| 1:M:177:ALA:HB3 | 1:M:208:GLU:CG | 2.33 | 0.59 |
| 1:A:458:VAL:CB | 1:A:476:ASP:O | 2.51 | 0.59 |
| 1:B:104:VAL:HG22 | 1:B:141:LEU:HD23 | 1.84 | 0.59 |
| 1:B:490:ILE:HG22 | 1:B:491:ASN:O | 2.02 | 0.59 |
| 1:C:104:VAL:HG22 | 1:C:141:LEU:HD23 | 1.84 | 0.59 |
| 1:C:490:ILE:HG22 | 1:C:491:ASN:O | 2.03 | 0.59 |
| 1:H:166:GLU:HB2 | 1:H:222:ARG:HH21 | 1.67 | 0.59 |
| 1:I:177:ALA:HB3 | 1:I:208:GLU:CG | 2.33 | 0.59 |
| 1:I:458:VAL:HB | 1:I:476:ASP:O | 2.01 | 0.59 |
| 1:J:459:ILE:H | 1:J:459:ILE:HD12 | 1.67 | 0.59 |
| 1:K:458:VAL:CB | 1:K:476:ASP:O | 2.51 | 0.59 |
| 1:K:504:VAL:HG13 | 1:K:521:ARG:CD | 2.31 | 0.59 |
| 1:K:609:PHE:CD2 | 1:L:639:ILE:CD1 | 2.75 | 0.59 |
| 1:M:142:ILE:HD11 | 1:M:156:ILE:HD12 | 1.84 | 0.59 |
| 1:M:477:ARG:HH11 | 1:M:477:ARG:HG2 | 1.66 | 0.59 |
| 1:A:438:PRO:HG3 | 1:A:482:ILE:CG2 | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:506:ASN:HD22 | 1:B:506:ASN:C | 2.04 | 0.59 |
| 1:E:459:ILE:H | 1:E:459:ILE:HD12 | 1.67 | 0.59 |
| 1:F:224:ARG:O | 1:F:227:ARG:HB2 | 2.03 | 0.59 |
| 1:F:459:ILE:H | 1:F:459:ILE:HD12 | 1.68 | 0.59 |
| 1:G:458:VAL:CB | 1:G:476:ASP:O | 2.51 | 0.59 |
| 1:G:480:VAL:HA | 1:G:505:SER:HB2 | 1.83 | 0.59 |
| 1:H:121:GLN:O | 1:H:125:ASN:N | 2.33 | 0.59 |
| 1:H:142:ILE:HD11 | 1:H:156:ILE:HD12 | 1.84 | 0.59 |
| 1:H:458:VAL:CB | 1:H:476:ASP:O | 2.51 | 0.59 |
| 1:H:609:PHE:CG | 1:I:639:ILE:HD12 | 2.34 | 0.59 |
| 1:I:458:VAL:CB | 1:I:476:ASP:O | 2.51 | 0.59 |
| 1:K:118:LEU:O | 1:K:121:GLN:HB3 | 2.03 | 0.59 |
| 1:M:260:LYS:O | 1:M:263:SER:OG | 2.17 | 0.59 |
| 1:N:104:VAL:HG22 | 1:N:141:LEU:HD23 | 1.84 | 0.59 |
| 1:O:154:GLU:O | 1:O:158:ARG:HB2 | 2.02 | 0.59 |
| 1:B:177:ALA:HB3 | 1:B:208:GLU:CG | 2.33 | 0.59 |
| 1:C:459:ILE:HD12 | 1:C:459:ILE:H | 1.68 | 0.59 |
| 1:C:506:ASN:HD22 | 1:C:507:VAL:H | 1.50 | 0.59 |
| 1:D:166:GLU:HB2 | 1:D:222:ARG:HH21 | 1.67 | 0.59 |
| 1:D:458:VAL:CB | 1:D:476:ASP:O | 2.51 | 0.59 |
| 1:D:490:ILE:HG22 | 1:D:491:ASN:O | 2.03 | 0.59 |
| 1:F:118:LEU:O | 1:F:121:GLN:HB3 | 2.03 | 0.59 |
| 1:F:176:SER:OG | 1:F:208:GLU:OE2 | 2.16 | 0.59 |
| 1:F:480:VAL:HA | 1:F:505:SER:HB2 | 1.83 | 0.59 |
| 1:J:154:GLU:O | 1:J:158:ARG:HB2 | 2.02 | 0.59 |
| 1:J:458:VAL:CB | 1:J:476:ASP:O | 2.51 | 0.59 |
| 1:K:166:GLU:HB2 | 1:K:222:ARG:HH21 | 1.67 | 0.59 |
| 1:N:177:ALA:HB3 | 1:N:208:GLU:CG | 2.33 | 0.59 |
| 1:C:458:VAL:CB | 1:C:476:ASP:O | 2.51 | 0.59 |
| 1:E:104:VAL:HG22 | 1:E:141:LEU:HD23 | 1.84 | 0.59 |
| 1:E:118:LEU:O | 1:E:121:GLN:HB3 | 2.03 | 0.59 |
| 1:E:224:ARG:O | 1:E:227:ARG:HB2 | 2.03 | 0.59 |
| 1:E:458:VAL:CB | 1:E:476:ASP:O | 2.51 | 0.59 |
| 1:F:458:VAL:CB | 1:F:476:ASP:O | 2.51 | 0.59 |
| 1:H:444:ASP:OD1 | 1:H:445:ASN:N | 2.36 | 0.59 |
| 1:H:504:VAL:HG13 | 1:H:521:ARG:CD | 2.31 | 0.59 |
| 1:J:118:LEU:O | 1:J:121:GLN:HB3 | 2.03 | 0.59 |
| 1:J:438:PRO:HG3 | 1:J:482:ILE:CG2 | 2.32 | 0.59 |
| 1:L:118:LEU:O | 1:L:121:GLN:HB3 | 2.03 | 0.59 |
| 1:M:480:VAL:HA | 1:M:505:SER:HB2 | 1.83 | 0.59 |
| 1:N:154:GLU:O | 1:N:158:ARG:HB2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:438:PRO:HG3 | 1:O:482:ILE:CG2 | 2.32 | 0.59 |
| 1:O:506:ASN:HD22 | 1:O:506:ASN:C | 2.04 | 0.59 |
| 1:A:166:GLU:HB2 | 1:A:222:ARG:HH21 | 1.67 | 0.59 |
| 1:A:504:VAL:HG13 | 1:A:521:ARG:CD | 2.31 | 0.59 |
| 1:E:508:LEU:N | 1:E:508:LEU:HD12 | 2.16 | 0.59 |
| 1:F:104:VAL:HG22 | 1:F:141:LEU:HD23 | 1.84 | 0.59 |
| 1:G:118:LEU:O | 1:G:121:GLN:HB3 | 2.03 | 0.59 |
| 1:G:444:ASP:OD1 | 1:G:445:ASN:N | 2.36 | 0.59 |
| 1:H:177:ALA:HB3 | 1:H:208:GLU:CG | 2.33 | 0.59 |
| 1:H:458:VAL:HB | 1:H:476:ASP:O | 2.01 | 0.59 |
| 1:I:142:ILE:HD11 | 1:I:156:ILE:HD12 | 1.84 | 0.59 |
| 1:I:444:ASP:OD1 | 1:I:445:ASN:N | 2.36 | 0.59 |
| 1:J:142:ILE:HD11 | 1:J:156:ILE:HD12 | 1.84 | 0.59 |
| 1:J:444:ASP:OD1 | 1:J:445:ASN:N | 2.36 | 0.59 |
| 1:J:506:ASN:HD22 | 1:J:506:ASN:C | 2.04 | 0.59 |
| 1:K:154:GLU:O | 1:K:158:ARG:HB2 | 2.02 | 0.59 |
| 1:L:177:ALA:HB3 | 1:L:208:GLU:CG | 2.33 | 0.59 |
| 1:L:506:ASN:HD22 | 1:L:506:ASN:C | 2.04 | 0.59 |
| 1:M:154:GLU:O | 1:M:158:ARG:HB2 | 2.02 | 0.59 |
| 1:D:104:VAL:HG22 | 1:D:141:LEU:HD23 | 1.83 | 0.58 |
| 1:G:459:ILE:H | 1:G:459:ILE:HD12 | 1.68 | 0.58 |
| 1:L:154:GLU:O | 1:L:158:ARG:HB2 | 2.02 | 0.58 |
| 1:N:459:ILE:HD12 | 1:N:459:ILE:H | 1.67 | 0.58 |
| 1:A:154:GLU:O | 1:A:158:ARG:HB2 | 2.02 | 0.58 |
| 1:C:444:ASP:OD1 | 1:C:445:ASN:N | 2.36 | 0.58 |
| 1:D:444:ASP:OD1 | 1:D:445:ASN:N | 2.36 | 0.58 |
| 1:F:177:ALA:HB3 | 1:F:208:GLU:CG | 2.33 | 0.58 |
| 1:F:444:ASP:OD1 | 1:F:445:ASN:N | 2.36 | 0.58 |
| 1:F:506:ASN:HD22 | 1:F:507:VAL:H | 1.50 | 0.58 |
| 1:G:177:ALA:HB3 | 1:G:208:GLU:CG | 2.33 | 0.58 |
| 1:J:504:VAL:HG13 | 1:J:521:ARG:CD | 2.31 | 0.58 |
| 1:K:142:ILE:HD11 | 1:K:156:ILE:HD12 | 1.84 | 0.58 |
| 1:L:142:ILE:HD11 | 1:L:156:ILE:HD12 | 1.84 | 0.58 |
| 1:N:206:ALA:HA | 1:N:212:SER:O | 2.04 | 0.58 |
| 1:A:480:VAL:HA | 1:A:505:SER:HB2 | 1.83 | 0.58 |
| 1:D:118:LEU:O | 1:D:121:GLN:HB3 | 2.03 | 0.58 |
| 1:E:444:ASP:OD1 | 1:E:445:ASN:N | 2.36 | 0.58 |
| 1:E:490:ILE:HG22 | 1:E:491:ASN:O | 2.02 | 0.58 |
| 1:G:206:ALA:HA | 1:G:212:SER:O | 2.04 | 0.58 |
| 1:G:504:VAL:HG13 | 1:G:521:ARG:CD | 2.31 | 0.58 |
| 1:J:224:ARG:O | 1:J:227:ARG:HB2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:444:ASP:OD1 | 1:K:445:ASN:N | 2.36 | 0.58 |
| 1:M:104:VAL:HG22 | 1:M:141:LEU:HD23 | 1.84 | 0.58 |
| 1:N:164:ASP:O | 1:N:219:PRO:HD2 | 2.04 | 0.58 |
| 1:A:206:ALA:HA | 1:A:212:SER:O | 2.04 | 0.58 |
| 1:D:506:ASN:HD22 | 1:D:506:ASN:C | 2.04 | 0.58 |
| 1:E:164:ASP:O | 1:E:219:PRO:HD2 | 2.04 | 0.58 |
| 1:G:224:ARG:O | 1:G:227:ARG:HB2 | 2.03 | 0.58 |
| 1:G:477:ARG:HH11 | 1:G:477:ARG:HG2 | 1.66 | 0.58 |
| 1:I:224:ARG:O | 1:I:227:ARG:HB2 | 2.03 | 0.58 |
| 1:I:490:ILE:HG22 | 1:I:491:ASN:O | 2.02 | 0.58 |
| 1:K:490:ILE:HG22 | 1:K:491:ASN:O | 2.03 | 0.58 |
| 1:L:104:VAL:HG22 | 1:L:141:LEU:HD23 | 1.84 | 0.58 |
| 1:M:118:LEU:O | 1:M:121:GLN:HB3 | 2.03 | 0.58 |
| 1:M:504:VAL:HG13 | 1:M:521:ARG:CD | 2.31 | 0.58 |
| 1:N:260:LYS:O | 1:N:263:SER:OG | 2.17 | 0.58 |
| 1:A:118:LEU:O | 1:A:121:GLN:HB3 | 2.03 | 0.58 |
| 1:B:206:ALA:HA | 1:B:212:SER:O | 2.04 | 0.58 |
| 1:C:177:ALA:HB3 | 1:C:208:GLU:CG | 2.33 | 0.58 |
| 1:D:206:ALA:HA | 1:D:212:SER:O | 2.03 | 0.58 |
| 1:E:107:VAL:HG22 | 1:E:160:ASP:HB2 | 1.86 | 0.58 |
| 1:G:490:ILE:HG22 | 1:G:491:ASN:O | 2.03 | 0.58 |
| 1:H:206:ALA:HA | 1:H:212:SER:O | 2.04 | 0.58 |
| 1:H:224:ARG:O | 1:H:227:ARG:HB2 | 2.03 | 0.58 |
| 1:L:477:ARG:HH11 | 1:L:477:ARG:HG2 | 1.66 | 0.58 |
| 1:N:224:ARG:O | 1:N:227:ARG:HB2 | 2.03 | 0.58 |
| 1:O:224:ARG:O | 1:O:227:ARG:HB2 | 2.03 | 0.58 |
| 1:B:444:ASP:OD1 | 1:B:445:ASN:N | 2.36 | 0.58 |
| 1:D:164:ASP:O | 1:D:219:PRO:HD2 | 2.04 | 0.58 |
| 1:F:164:ASP:O | 1:F:219:PRO:HD2 | 2.04 | 0.58 |
| 1:F:206:ALA:HA | 1:F:212:SER:O | 2.03 | 0.58 |
| 1:H:118:LEU:O | 1:H:121:GLN:HB3 | 2.03 | 0.58 |
| 1:H:506:ASN:HD22 | 1:H:506:ASN:C | 2.04 | 0.58 |
| 1:I:118:LEU:O | 1:I:121:GLN:HB3 | 2.03 | 0.58 |
| 1:I:506:ASN:HD22 | 1:I:506:ASN:C | 2.04 | 0.58 |
| 1:J:107:VAL:HG22 | 1:J:160:ASP:HB2 | 1.86 | 0.58 |
| 1:L:107:VAL:HG22 | 1:L:160:ASP:HB2 | 1.86 | 0.58 |
| 1:L:444:ASP:OD1 | 1:L:445:ASN:N | 2.36 | 0.58 |
| 1:M:164:ASP:O | 1:M:219:PRO:HD2 | 2.04 | 0.58 |
| 1:A:459:ILE:HG23 | 1:A:474:THR:C | 2.16 | 0.58 |
| 1:C:132:VAL:HG12 | 1:C:134:TYR:CE1 | 2.39 | 0.58 |
| 1:C:256:VAL:O | 1:C:260:LYS:HG2 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:459:ILE:H | 1:D:459:ILE:HD12 | 1.67 | 0.58 |
| 1:E:177:ALA:HB3 | 1:E:208:GLU:CG | 2.33 | 0.58 |
| 1:E:481:GLY:N | 1:E:505:SER:OG | 2.23 | 0.58 |
| 1:G:107:VAL:HG22 | 1:G:160:ASP:HB2 | 1.86 | 0.58 |
| 1:G:121:GLN:O | 1:G:125:ASN:N | 2.33 | 0.58 |
| 1:M:107:VAL:HG22 | 1:M:160:ASP:HB2 | 1.86 | 0.58 |
| 1:M:224:ARG:O | 1:M:227:ARG:HB2 | 2.03 | 0.58 |
| 1:M:438:PRO:HG3 | 1:M:482:ILE:CG2 | 2.32 | 0.58 |
| 1:M:444:ASP:OD1 | 1:M:445:ASN:N | 2.36 | 0.58 |
| 1:M:459:ILE:H | 1:M:459:ILE:HD12 | 1.68 | 0.58 |
| 1:M:490:ILE:HG22 | 1:M:491:ASN:O | 2.03 | 0.58 |
| 1:N:444:ASP:OD1 | 1:N:445:ASN:N | 2.36 | 0.58 |
| 1:O:105:VAL:HG11 | 1:O:157:ARG:HE | 1.69 | 0.58 |
| 1:O:164:ASP:O | 1:O:219:PRO:HD2 | 2.04 | 0.58 |
| 1:O:490:ILE:HG22 | 1:O:491:ASN:O | 2.02 | 0.58 |
| 1:B:118:LEU:O | 1:B:121:GLN:HB3 | 2.03 | 0.58 |
| 1:D:132:VAL:HG12 | 1:D:134:TYR:CE1 | 2.39 | 0.58 |
| 1:D:256:VAL:O | 1:D:260:LYS:HG2 | 2.04 | 0.58 |
| 1:E:256:VAL:O | 1:E:260:LYS:HG2 | 2.04 | 0.58 |
| 1:F:107:VAL:HG22 | 1:F:160:ASP:HB2 | 1.86 | 0.58 |
| 1:G:164:ASP:O | 1:G:219:PRO:HD2 | 2.04 | 0.58 |
| 1:H:256:VAL:O | 1:H:260:LYS:HG2 | 2.04 | 0.58 |
| 1:K:206:ALA:HA | 1:K:212:SER:O | 2.04 | 0.58 |
| 1:A:224:ARG:O | 1:A:227:ARG:HB2 | 2.03 | 0.58 |
| 1:A:459:ILE:H | 1:A:459:ILE:HD12 | 1.67 | 0.58 |
| 1:D:107:VAL:HG22 | 1:D:160:ASP:HB2 | 1.86 | 0.58 |
| 1:D:224:ARG:O | 1:D:227:ARG:HB2 | 2.03 | 0.58 |
| 1:D:504:VAL:HG13 | 1:D:521:ARG:CD | 2.31 | 0.58 |
| 1:H:107:VAL:HG22 | 1:H:160:ASP:HB2 | 1.86 | 0.58 |
| 1:I:107:VAL:HG22 | 1:I:160:ASP:HB2 | 1.86 | 0.58 |
| 1:I:132:VAL:HG12 | 1:I:134:TYR:CE1 | 2.39 | 0.58 |
| 1:K:107:VAL:HG22 | 1:K:160:ASP:HB2 | 1.86 | 0.58 |
| 1:K:224:ARG:O | 1:K:227:ARG:HB2 | 2.03 | 0.58 |
| 1:L:164:ASP:O | 1:L:219:PRO:HD2 | 2.04 | 0.58 |
| 1:M:105:VAL:HG11 | 1:M:157:ARG:HE | 1.69 | 0.58 |
| 1:O:118:LEU:O | 1:O:121:GLN:HB3 | 2.03 | 0.58 |
| 1:O:132:VAL:HG12 | 1:O:134:TYR:CE1 | 2.39 | 0.58 |
| 1:A:181:VAL:O | 1:A:185:GLU:HG3 | 2.04 | 0.58 |
| 1:A:444:ASP:OD1 | 1:A:445:ASN:N | 2.36 | 0.58 |
| 1:B:105:VAL:HG11 | 1:B:157:ARG:HE | 1.69 | 0.58 |
| 1:B:224:ARG:O | 1:B:227:ARG:HB2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:256:VAL:O | 1:B:260:LYS:HG2 | 2.04 | 0.58 |
| 1:C:224:ARG:O | 1:C:227:ARG:HB2 | 2.03 | 0.58 |
| 1:C:459:ILE:HG23 | 1:C:474:THR:C | 2.16 | 0.58 |
| 1:D:459:ILE:HG23 | 1:D:474:THR:C | 2.16 | 0.58 |
| 1:H:164:ASP:O | 1:H:219:PRO:HD2 | 2.04 | 0.58 |
| 1:I:459:ILE:H | 1:I:459:ILE:HD12 | 1.67 | 0.58 |
| 1:L:459:ILE:H | 1:L:459:ILE:HD12 | 1.67 | 0.58 |
| 1:M:206:ALA:HA | 1:M:212:SER:O | 2.04 | 0.58 |
| 1:O:444:ASP:OD1 | 1:O:445:ASN:N | 2.36 | 0.58 |
| 1:O:459:ILE:H | 1:O:459:ILE:HD12 | 1.67 | 0.58 |
| 1:A:107:VAL:HG22 | 1:A:160:ASP:HB2 | 1.86 | 0.57 |
| 1:B:107:VAL:HG22 | 1:B:160:ASP:HB2 | 1.86 | 0.57 |
| 1:B:459:ILE:H | 1:B:459:ILE:HD12 | 1.67 | 0.57 |
| 1:C:107:VAL:HG22 | 1:C:160:ASP:HB2 | 1.86 | 0.57 |
| 1:C:164:ASP:O | 1:C:219:PRO:HD2 | 2.04 | 0.57 |
| 1:D:177:ALA:HB3 | 1:D:208:GLU:CG | 2.33 | 0.57 |
| 1:D:480:VAL:HA | 1:D:505:SER:HB2 | 1.83 | 0.57 |
| 1:F:506:ASN:HD22 | 1:F:506:ASN:C | 2.04 | 0.57 |
| 1:I:206:ALA:HA | 1:I:212:SER:O | 2.04 | 0.57 |
| 1:I:256:VAL:O | 1:I:260:LYS:HG2 | 2.04 | 0.57 |
| 1:L:224:ARG:O | 1:L:227:ARG:HB2 | 2.03 | 0.57 |
| 1:O:181:VAL:O | 1:O:185:GLU:HG3 | 2.04 | 0.57 |
| 1:A:256:VAL:O | 1:A:260:LYS:HG2 | 2.04 | 0.57 |
| 1:B:132:VAL:HG12 | 1:B:134:TYR:CE1 | 2.39 | 0.57 |
| 1:B:181:VAL:O | 1:B:185:GLU:HG3 | 2.04 | 0.57 |
| 1:B:459:ILE:HG23 | 1:B:474:THR:C | 2.16 | 0.57 |
| 1:C:118:LEU:O | 1:C:121:GLN:HB3 | 2.03 | 0.57 |
| 1:K:132:VAL:HG12 | 1:K:134:TYR:CE1 | 2.39 | 0.57 |
| 1:L:132:VAL:HG12 | 1:L:134:TYR:CE1 | 2.39 | 0.57 |
| 1:L:256:VAL:O | 1:L:260:LYS:HG2 | 2.04 | 0.57 |
| 1:N:107:VAL:HG22 | 1:N:160:ASP:HB2 | 1.86 | 0.57 |
| 1:C:105:VAL:HG11 | 1:C:157:ARG:HE | 1.69 | 0.57 |
| 1:E:105:VAL:HG11 | 1:E:157:ARG:HE | 1.69 | 0.57 |
| 1:E:459:ILE:HG23 | 1:E:474:THR:C | 2.16 | 0.57 |
| 1:F:256:VAL:O | 1:F:260:LYS:HG2 | 2.04 | 0.57 |
| 1:H:507:VAL:CA | 1:H:518:PHE:HB3 | 2.35 | 0.57 |
| 1:I:164:ASP:O | 1:I:219:PRO:HD2 | 2.04 | 0.57 |
| 1:K:256:VAL:O | 1:K:260:LYS:HG2 | 2.04 | 0.57 |
| 1:L:506:ASN:HD22 | 1:L:507:VAL:H | 1.51 | 0.57 |
| 1:N:181:VAL:O | 1:N:185:GLU:HG3 | 2.04 | 0.57 |
| 1:O:107:VAL:HG22 | 1:O:160:ASP:HB2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:260:LYS:O | 1:O:263:SER:OG | 2.17 | 0.57 |
| 1:A:164:ASP:O | 1:A:219:PRO:HD2 | 2.04 | 0.57 |
| 1:E:206:ALA:HA | 1:E:212:SER:O | 2.04 | 0.57 |
| 1:E:507:VAL:CA | 1:E:518:PHE:HB3 | 2.35 | 0.57 |
| 1:I:181:VAL:O | 1:I:185:GLU:HG3 | 2.04 | 0.57 |
| 1:J:164:ASP:O | 1:J:219:PRO:HD2 | 2.04 | 0.57 |
| 1:M:256:VAL:O | 1:M:260:LYS:HG2 | 2.04 | 0.57 |
| 1:N:118:LEU:O | 1:N:121:GLN:HB3 | 2.03 | 0.57 |
| 1:N:132:VAL:HG12 | 1:N:134:TYR:CE1 | 2.39 | 0.57 |
| 1:N:256:VAL:O | 1:N:260:LYS:HG2 | 2.04 | 0.57 |
| 1:O:256:VAL:O | 1:O:260:LYS:HG2 | 2.04 | 0.57 |
| 1:A:105:VAL:HG11 | 1:A:157:ARG:HE | 1.69 | 0.57 |
| 1:A:132:VAL:HG12 | 1:A:134:TYR:CE1 | 2.39 | 0.57 |
| 1:B:112:VAL:HG21 | 1:B:140:ILE:HD11 | 1.87 | 0.57 |
| 1:C:206:ALA:HA | 1:C:212:SER:O | 2.03 | 0.57 |
| 1:G:181:VAL:O | 1:G:185:GLU:HG3 | 2.04 | 0.57 |
| 1:H:181:VAL:O | 1:H:185:GLU:HG3 | 2.04 | 0.57 |
| 1:J:105:VAL:HG11 | 1:J:157:ARG:HE | 1.69 | 0.57 |
| 1:K:164:ASP:O | 1:K:219:PRO:HD2 | 2.04 | 0.57 |
| 1:K:459:ILE:HD12 | 1:K:459:ILE:H | 1.68 | 0.57 |
| 1:L:206:ALA:HA | 1:L:212:SER:O | 2.04 | 0.57 |
| 1:C:112:VAL:HG21 | 1:C:140:ILE:HD11 | 1.87 | 0.57 |
| 1:F:181:VAL:O | 1:F:185:GLU:HG3 | 2.04 | 0.57 |
| 1:G:132:VAL:HG12 | 1:G:134:TYR:CE1 | 2.39 | 0.57 |
| 1:J:181:VAL:O | 1:J:185:GLU:HG3 | 2.04 | 0.57 |
| 1:K:181:VAL:O | 1:K:185:GLU:HG3 | 2.04 | 0.57 |
| 1:A:112:VAL:HG21 | 1:A:140:ILE:HD11 | 1.87 | 0.57 |
| 1:D:112:VAL:HG21 | 1:D:140:ILE:HD11 | 1.87 | 0.57 |
| 1:F:132:VAL:HG12 | 1:F:134:TYR:CE1 | 2.39 | 0.57 |
| 1:G:105:VAL:HG11 | 1:G:157:ARG:HE | 1.69 | 0.57 |
| 1:H:132:VAL:HG12 | 1:H:134:TYR:CE1 | 2.39 | 0.57 |
| 1:J:206:ALA:HA | 1:J:212:SER:O | 2.04 | 0.57 |
| 1:J:256:VAL:O | 1:J:260:LYS:HG2 | 2.04 | 0.57 |
| 1:L:105:VAL:HG11 | 1:L:157:ARG:HE | 1.69 | 0.57 |
| 1:O:206:ALA:HA | 1:O:212:SER:O | 2.04 | 0.57 |
| 1:D:507:VAL:CA | 1:D:518:PHE:HB3 | 2.35 | 0.57 |
| 1:E:181:VAL:O | 1:E:185:GLU:HG3 | 2.04 | 0.57 |
| 1:E:259:LEU:HD11 | 1:E:310:ILE:HG13 | 1.87 | 0.57 |
| 1:G:256:VAL:O | 1:G:260:LYS:HG2 | 2.04 | 0.57 |
| 1:H:259:LEU:HD11 | 1:H:310:ILE:HG13 | 1.86 | 0.57 |
| 1:J:132:VAL:HG12 | 1:J:134:TYR:CE1 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:105:VAL:HG11 | 1:K:157:ARG:HE | 1.69 | 0.57 |
| 1:M:181:VAL:O | 1:M:185:GLU:HG3 | 2.04 | 0.57 |
| 1:N:105:VAL:HG11 | 1:N:157:ARG:HE | 1.69 | 0.57 |
| 1:O:112:VAL:HG21 | 1:O:140:ILE:HD11 | 1.87 | 0.57 |
| 1:C:456:VAL:CG2 | 1:C:457:PRO:CD | 2.83 | 0.57 |
| 1:G:259:LEU:HD11 | 1:G:310:ILE:HG13 | 1.87 | 0.57 |
| 1:G:507:VAL:CA | 1:G:518:PHE:HB3 | 2.35 | 0.57 |
| 1:I:506:ASN:HD22 | 1:I:507:VAL:H | 1.50 | 0.57 |
| 1:L:181:VAL:O | 1:L:185:GLU:HG3 | 2.04 | 0.57 |
| 1:M:112:VAL:HG21 | 1:M:140:ILE:HD11 | 1.87 | 0.57 |
| 1:N:112:VAL:HG21 | 1:N:140:ILE:HD11 | 1.87 | 0.57 |
| 1:B:164:ASP:O | 1:B:219:PRO:HD2 | 2.04 | 0.57 |
| 1:C:181:VAL:O | 1:C:185:GLU:HG3 | 2.04 | 0.57 |
| 1:D:105:VAL:HG11 | 1:D:157:ARG:HE | 1.69 | 0.57 |
| 1:G:506:ASN:HD22 | 1:G:506:ASN:C | 2.04 | 0.57 |
| 1:H:105:VAL:HG11 | 1:H:157:ARG:HE | 1.69 | 0.57 |
| 1:I:172:LEU:HG | 1:I:212:SER:HA | 1.87 | 0.57 |
| 1:J:172:LEU:HG | 1:J:212:SER:HA | 1.87 | 0.57 |
| 1:K:507:VAL:CA | 1:K:518:PHE:HB3 | 2.35 | 0.57 |
| 1:L:112:VAL:HG21 | 1:L:140:ILE:HD11 | 1.87 | 0.57 |
| 1:A:121:GLN:O | 1:A:125:ASN:N | 2.33 | 0.56 |
| 1:B:507:VAL:CA | 1:B:518:PHE:HB3 | 2.35 | 0.56 |
| 1:D:259:LEU:HD11 | 1:D:310:ILE:HG13 | 1.87 | 0.56 |
| 1:D:456:VAL:CG2 | 1:D:457:PRO:CD | 2.83 | 0.56 |
| 1:E:112:VAL:HG21 | 1:E:140:ILE:HD11 | 1.87 | 0.56 |
| 1:E:132:VAL:HG12 | 1:E:134:TYR:CE1 | 2.39 | 0.56 |
| 1:F:259:LEU:HD11 | 1:F:310:ILE:HG13 | 1.87 | 0.56 |
| 1:G:456:VAL:CG2 | 1:G:457:PRO:CD | 2.83 | 0.56 |
| 1:I:259:LEU:HD11 | 1:I:310:ILE:HG13 | 1.87 | 0.56 |
| 1:J:180:MET:HE2 | 1:J:213:ILE:HD11 | 1.85 | 0.56 |
| 1:K:172:LEU:HG | 1:K:212:SER:HA | 1.87 | 0.56 |
| 1:L:172:LEU:HG | 1:L:212:SER:HA | 1.87 | 0.56 |
| 1:M:121:GLN:O | 1:M:125:ASN:N | 2.33 | 0.56 |
| 1:D:506:ASN:HD22 | 1:D:507:VAL:H | 1.51 | 0.56 |
| 1:F:121:GLN:O | 1:F:125:ASN:N | 2.33 | 0.56 |
| 1:O:456:VAL:CG2 | 1:O:457:PRO:CD | 2.83 | 0.56 |
| 1:A:504:VAL:CG1 | 1:A:521:ARG:CG | 2.83 | 0.56 |
| 1:B:121:GLN:O | 1:B:125:ASN:N | 2.33 | 0.56 |
| 1:C:259:LEU:HD11 | 1:C:310:ILE:HG13 | 1.87 | 0.56 |
| 1:C:506:ASN:HD22 | 1:C:506:ASN:C | 2.04 | 0.56 |
| 1:D:181:VAL:O | 1:D:185:GLU:HG3 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:506:ASN:HD22 | 1:E:506:ASN:C | 2.04 | 0.56 |
| 1:F:456:VAL:CG2 | 1:F:457:PRO:CD | 2.83 | 0.56 |
| 1:F:481:GLY:H | 1:F:505:SER:HB3 | 0.42 | 0.56 |
| 1:H:172:LEU:HG | 1:H:212:SER:HA | 1.87 | 0.56 |
| 1:K:112:VAL:HG21 | 1:K:140:ILE:HD11 | 1.87 | 0.56 |
| 1:K:330:ALA:HB3 | 1:K:432:SER:HB3 | 1.88 | 0.56 |
| 1:L:330:ALA:HB3 | 1:L:432:SER:HB3 | 1.88 | 0.56 |
| 1:M:172:LEU:HG | 1:M:212:SER:HA | 1.87 | 0.56 |
| 1:N:172:LEU:HG | 1:N:212:SER:HA | 1.87 | 0.56 |
| 1:A:260:LYS:O | 1:A:263:SER:OG | 2.17 | 0.56 |
| 1:D:504:VAL:CG1 | 1:D:521:ARG:CG | 2.83 | 0.56 |
| 1:F:112:VAL:HG21 | 1:F:140:ILE:HD11 | 1.87 | 0.56 |
| 1:J:259:LEU:HD11 | 1:J:310:ILE:HG13 | 1.87 | 0.56 |
| 1:J:507:VAL:CA | 1:J:518:PHE:HB3 | 2.35 | 0.56 |
| 1:M:132:VAL:HG12 | 1:M:134:TYR:CE1 | 2.39 | 0.56 |
| 1:M:259:LEU:HD11 | 1:M:310:ILE:HG13 | 1.87 | 0.56 |
| 1:O:172:LEU:HG | 1:O:212:SER:HA | 1.87 | 0.56 |
| 1:A:456:VAL:CG2 | 1:A:457:PRO:CD | 2.83 | 0.56 |
| 1:B:456:VAL:CG2 | 1:B:457:PRO:CD | 2.83 | 0.56 |
| 1:J:112:VAL:HG21 | 1:J:140:ILE:HD11 | 1.87 | 0.56 |
| 1:N:259:LEU:HD11 | 1:N:310:ILE:HG13 | 1.87 | 0.56 |
| 1:N:507:VAL:CA | 1:N:518:PHE:HB3 | 2.35 | 0.56 |
| 1:O:259:LEU:HD11 | 1:O:310:ILE:HG13 | 1.87 | 0.56 |
| 1:A:172:LEU:HG | 1:A:212:SER:HA | 1.87 | 0.56 |
| 1:A:259:LEU:HD11 | 1:A:310:ILE:HG13 | 1.87 | 0.56 |
| 1:A:507:VAL:CA | 1:A:518:PHE:HB3 | 2.35 | 0.56 |
| 1:C:330:ALA:HB3 | 1:C:432:SER:HB3 | 1.88 | 0.56 |
| 1:C:504:VAL:CG1 | 1:C:521:ARG:CG | 2.83 | 0.56 |
| 1:D:215:ILE:HD11 | 1:D:225:LEU:HD13 | 1.88 | 0.56 |
| 1:D:330:ALA:HB3 | 1:D:432:SER:HB3 | 1.88 | 0.56 |
| 1:E:215:ILE:HD11 | 1:E:225:LEU:HD13 | 1.88 | 0.56 |
| 1:F:105:VAL:HG11 | 1:F:157:ARG:HE | 1.69 | 0.56 |
| 1:H:456:VAL:CG2 | 1:H:457:PRO:CD | 2.83 | 0.56 |
| 1:I:207:ASP:OD1 | 1:I:209:ARG:N | 2.33 | 0.56 |
| 1:J:330:ALA:HB3 | 1:J:432:SER:HB3 | 1.88 | 0.56 |
| 1:O:121:GLN:O | 1:O:125:ASN:N | 2.33 | 0.56 |
| 1:A:506:ASN:HD22 | 1:A:507:VAL:H | 1.50 | 0.56 |
| 1:D:481:GLY:N | 1:D:505:SER:OG | 2.23 | 0.56 |
| 1:J:207:ASP:OD1 | 1:J:209:ARG:N | 2.33 | 0.56 |
| 1:L:259:LEU:HD11 | 1:L:310:ILE:HG13 | 1.87 | 0.56 |
| 1:M:330:ALA:HB3 | 1:M:432:SER:HB3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:456:VAL:CG2 | 1:N:457:PRO:CD | 2.83 | 0.56 |
| 1:C:215:ILE:HD11 | 1:C:225:LEU:HD13 | 1.88 | 0.56 |
| 1:D:521:ARG:HD3 | 1:D:521:ARG:N | 2.21 | 0.56 |
| 1:E:330:ALA:HB3 | 1:E:432:SER:HB3 | 1.88 | 0.56 |
| 1:E:456:VAL:CG2 | 1:E:457:PRO:CD | 2.83 | 0.56 |
| 1:F:215:ILE:HD11 | 1:F:225:LEU:HD13 | 1.88 | 0.56 |
| 1:F:521:ARG:HD3 | 1:F:521:ARG:N | 2.21 | 0.56 |
| 1:G:172:LEU:HG | 1:G:212:SER:HA | 1.87 | 0.56 |
| 1:G:506:ASN:HD22 | 1:G:507:VAL:H | 1.50 | 0.56 |
| 1:O:504:VAL:CG1 | 1:O:521:ARG:CG | 2.83 | 0.56 |
| 1:O:506:ASN:HD22 | 1:O:507:VAL:H | 1.50 | 0.56 |
| 1:H:521:ARG:HD3 | 1:H:521:ARG:N | 2.21 | 0.56 |
| 1:J:521:ARG:HD3 | 1:J:521:ARG:N | 2.21 | 0.56 |
| 1:L:521:ARG:HD3 | 1:L:521:ARG:N | 2.21 | 0.56 |
| 1:B:172:LEU:HG | 1:B:212:SER:HA | 1.87 | 0.56 |
| 1:B:259:LEU:HD11 | 1:B:310:ILE:HG13 | 1.87 | 0.56 |
| 1:B:330:ALA:HB3 | 1:B:432:SER:HB3 | 1.88 | 0.56 |
| 1:B:504:VAL:CG1 | 1:B:521:ARG:CG | 2.83 | 0.56 |
| 1:B:521:ARG:HD3 | 1:B:521:ARG:N | 2.21 | 0.56 |
| 1:C:207:ASP:O | 1:C:211:ASN:CA | 2.55 | 0.56 |
| 1:C:481:GLY:H | 1:C:505:SER:HB3 | 0.42 | 0.56 |
| 1:G:112:VAL:HG21 | 1:G:140:ILE:HD11 | 1.87 | 0.56 |
| 1:I:112:VAL:HG21 | 1:I:140:ILE:HD11 | 1.87 | 0.56 |
| 1:I:330:ALA:HB3 | 1:I:432:SER:HB3 | 1.88 | 0.56 |
| 1:C:121:GLN:O | 1:C:125:ASN:N | 2.33 | 0.55 |
| 1:G:215:ILE:HD11 | 1:G:225:LEU:HD13 | 1.88 | 0.55 |
| 1:J:207:ASP:O | 1:J:211:ASN:CA | 2.54 | 0.55 |
| 1:K:207:ASP:OD1 | 1:K:209:ARG:N | 2.33 | 0.55 |
| 1:K:259:LEU:HD11 | 1:K:310:ILE:HG13 | 1.87 | 0.55 |
| 1:L:207:ASP:O | 1:L:211:ASN:CA | 2.54 | 0.55 |
| 1:L:507:VAL:CA | 1:L:518:PHE:HB3 | 2.35 | 0.55 |
| 1:B:609:PHE:CE2 | 1:C:639:ILE:HD11 | 2.42 | 0.55 |
| 1:C:172:LEU:HG | 1:C:212:SER:HA | 1.87 | 0.55 |
| 1:E:177:ALA:HB3 | 1:E:208:GLU:HG2 | 1.89 | 0.55 |
| 1:E:207:ASP:O | 1:E:211:ASN:CA | 2.54 | 0.55 |
| 1:I:504:VAL:CG1 | 1:I:521:ARG:CG | 2.83 | 0.55 |
| 1:J:456:VAL:CG2 | 1:J:457:PRO:CD | 2.83 | 0.55 |
| 1:K:456:VAL:CG2 | 1:K:457:PRO:CD | 2.83 | 0.55 |
| 1:L:481:GLY:H | 1:L:505:SER:HB3 | 0.41 | 0.55 |
| 1:M:207:ASP:O | 1:M:211:ASN:CA | 2.54 | 0.55 |
| 1:M:507:VAL:CA | 1:M:518:PHE:HB3 | 2.35 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:207:ASP:O | 1:N:211:ASN:CA | 2.54 | 0.55 |
| 1:N:521:ARG:HD3 | 1:N:521:ARG:N | 2.21 | 0.55 |
| 1:B:215:ILE:HD11 | 1:B:225:LEU:HD13 | 1.88 | 0.55 |
| 1:E:521:ARG:HD3 | 1:E:521:ARG:N | 2.21 | 0.55 |
| 1:F:609:PHE:CE2 | 1:G:639:ILE:HD11 | 2.42 | 0.55 |
| 1:H:112:VAL:HG21 | 1:H:140:ILE:HD11 | 1.87 | 0.55 |
| 1:I:105:VAL:HG11 | 1:I:157:ARG:HE | 1.69 | 0.55 |
| 1:I:481:GLY:N | 1:I:505:SER:OG | 2.23 | 0.55 |
| 1:K:207:ASP:O | 1:K:211:ASN:CA | 2.55 | 0.55 |
| 1:K:521:ARG:HD3 | 1:K:521:ARG:N | 2.21 | 0.55 |
| 1:O:207:ASP:O | 1:O:211:ASN:CA | 2.55 | 0.55 |
| 1:A:207:ASP:O | 1:A:211:ASN:CA | 2.54 | 0.55 |
| 1:A:521:ARG:HD3 | 1:A:521:ARG:N | 2.21 | 0.55 |
| 1:C:507:VAL:CA | 1:C:518:PHE:HB3 | 2.35 | 0.55 |
| 1:C:609:PHE:CE2 | 1:D:639:ILE:HD11 | 2.42 | 0.55 |
| 1:D:121:GLN:O | 1:D:125:ASN:N | 2.33 | 0.55 |
| 1:F:172:LEU:HG | 1:F:212:SER:HA | 1.87 | 0.55 |
| 1:F:507:VAL:CA | 1:F:518:PHE:HB3 | 2.35 | 0.55 |
| 1:G:207:ASP:O | 1:G:211:ASN:CA | 2.54 | 0.55 |
| 1:H:207:ASP:O | 1:H:211:ASN:CA | 2.54 | 0.55 |
| 1:E:121:GLN:O | 1:E:125:ASN:N | 2.33 | 0.55 |
| 1:E:609:PHE:CE2 | 1:F:639:ILE:HD11 | 2.42 | 0.55 |
| 1:F:330:ALA:HB3 | 1:F:432:SER:HB3 | 1.88 | 0.55 |
| 1:H:330:ALA:HB3 | 1:H:432:SER:HB3 | 1.88 | 0.55 |
| 1:I:456:VAL:CG2 | 1:I:457:PRO:CD | 2.83 | 0.55 |
| 1:I:521:ARG:HD3 | 1:I:521:ARG:N | 2.21 | 0.55 |
| 1:L:456:VAL:CG2 | 1:L:457:PRO:CD | 2.83 | 0.55 |
| 1:N:330:ALA:HB3 | 1:N:432:SER:HB3 | 1.88 | 0.55 |
| 1:A:330:ALA:HB3 | 1:A:432:SER:HB3 | 1.88 | 0.55 |
| 1:B:207:ASP:O | 1:B:211:ASN:CA | 2.54 | 0.55 |
| 1:C:521:ARG:HD3 | 1:C:521:ARG:N | 2.21 | 0.55 |
| 1:D:172:LEU:HG | 1:D:212:SER:HA | 1.87 | 0.55 |
| 1:E:207:ASP:OD1 | 1:E:209:ARG:N | 2.33 | 0.55 |
| 1:E:504:VAL:CG1 | 1:E:521:ARG:CG | 2.83 | 0.55 |
| 1:G:521:ARG:HD3 | 1:G:521:ARG:N | 2.21 | 0.55 |
| 1:H:215:ILE:HD11 | 1:H:225:LEU:HD13 | 1.88 | 0.55 |
| 1:I:207:ASP:O | 1:I:211:ASN:CA | 2.55 | 0.55 |
| 1:I:215:ILE:HD11 | 1:I:225:LEU:HD13 | 1.88 | 0.55 |
| 1:I:481:GLY:H | 1:I:505:SER:HB3 | 0.42 | 0.55 |
| 1:A:215:ILE:HD11 | 1:A:225:LEU:HD13 | 1.88 | 0.55 |
| 1:D:177:ALA:HB3 | 1:D:208:GLU:HG2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:172:LEU:HG | 1:E:212:SER:HA | 1.87 | 0.55 |
| 1:M:504:VAL:CG1 | 1:M:521:ARG:CG | 2.83 | 0.55 |
| 1:A:609:PHE:CE2 | 1:B:639:ILE:HD11 | 2.42 | 0.55 |
| 1:H:177:ALA:HB3 | 1:H:208:GLU:HG2 | 1.89 | 0.55 |
| 1:M:456:VAL:CG2 | 1:M:457:PRO:CD | 2.83 | 0.55 |
| 1:O:481:GLY:H | 1:O:505:SER:HB3 | 0.42 | 0.55 |
| 1:O:521:ARG:HD3 | 1:O:521:ARG:N | 2.21 | 0.55 |
| 1:C:207:ASP:OD1 | 1:C:209:ARG:N | 2.33 | 0.55 |
| 1:F:207:ASP:O | 1:F:211:ASN:CA | 2.55 | 0.55 |
| 1:F:504:VAL:CG1 | 1:F:521:ARG:CG | 2.83 | 0.55 |
| 1:G:330:ALA:HB3 | 1:G:432:SER:HB3 | 1.88 | 0.55 |
| 1:J:506:ASN:HD22 | 1:J:507:VAL:H | 1.51 | 0.55 |
| 1:M:506:ASN:HD22 | 1:M:507:VAL:H | 1.50 | 0.55 |
| 1:F:177:ALA:HB3 | 1:F:208:GLU:HG2 | 1.89 | 0.55 |
| 1:J:215:ILE:HD11 | 1:J:225:LEU:HD13 | 1.88 | 0.55 |
| 1:M:215:ILE:HD11 | 1:M:225:LEU:HD13 | 1.88 | 0.55 |
| 1:N:504:VAL:CG1 | 1:N:521:ARG:CG | 2.83 | 0.55 |
| 1:O:215:ILE:HD11 | 1:O:225:LEU:HD13 | 1.88 | 0.55 |
| 1:O:507:VAL:CA | 1:O:518:PHE:HB3 | 2.35 | 0.55 |
| 1:A:177:ALA:HB3 | 1:A:208:GLU:HG2 | 1.89 | 0.54 |
| 1:B:177:ALA:HB3 | 1:B:208:GLU:HG2 | 1.89 | 0.54 |
| 1:D:207:ASP:O | 1:D:211:ASN:CA | 2.54 | 0.54 |
| 1:F:183:ILE:HD12 | 1:F:232:LEU:HD13 | 1.89 | 0.54 |
| 1:N:121:GLN:O | 1:N:125:ASN:N | 2.33 | 0.54 |
| 1:G:183:ILE:HD12 | 1:G:232:LEU:HD13 | 1.89 | 0.54 |
| 1:G:504:VAL:CG1 | 1:G:521:ARG:CG | 2.83 | 0.54 |
| 1:I:177:ALA:HB3 | 1:I:208:GLU:HG2 | 1.89 | 0.54 |
| 1:L:121:GLN:O | 1:L:125:ASN:N | 2.33 | 0.54 |
| 1:N:215:ILE:HD11 | 1:N:225:LEU:HD13 | 1.88 | 0.54 |
| 1:A:504:VAL:CG1 | 1:A:521:ARG:CD | 2.86 | 0.54 |
| 1:A:639:ILE:HD11 | 1:O:609:PHE:CE2 | 2.42 | 0.54 |
| 1:B:504:VAL:CG1 | 1:B:521:ARG:CD | 2.86 | 0.54 |
| 1:D:259:LEU:HD11 | 1:D:310:ILE:CG1 | 2.38 | 0.54 |
| 1:E:259:LEU:HD11 | 1:E:310:ILE:CG1 | 2.38 | 0.54 |
| 1:H:183:ILE:HD12 | 1:H:232:LEU:HD13 | 1.89 | 0.54 |
| 1:O:183:ILE:HD12 | 1:O:232:LEU:HD13 | 1.89 | 0.54 |
| 1:C:259:LEU:HD11 | 1:C:310:ILE:CG1 | 2.38 | 0.54 |
| 1:G:177:ALA:HB3 | 1:G:208:GLU:HG2 | 1.89 | 0.54 |
| 1:I:507:VAL:CA | 1:I:518:PHE:HB3 | 2.35 | 0.54 |
| 1:K:215:ILE:HD11 | 1:K:225:LEU:HD13 | 1.88 | 0.54 |
| 1:L:215:ILE:HD11 | 1:L:225:LEU:HD13 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:183:ILE:HD12 | 1:A:232:LEU:HD13 | 1.89 | 0.54 |
| 1:D:609:PHE:CE2 | 1:E:639:ILE:HD11 | 2.42 | 0.54 |
| 1:E:183:ILE:HD12 | 1:E:232:LEU:HD13 | 1.89 | 0.54 |
| 1:G:132:VAL:HA | 1:G:141:LEU:O | 2.08 | 0.54 |
| 1:H:132:VAL:HA | 1:H:141:LEU:O | 2.08 | 0.54 |
| 1:K:259:LEU:HD11 | 1:K:310:ILE:CG1 | 2.38 | 0.54 |
| 1:L:259:LEU:HD11 | 1:L:310:ILE:CG1 | 2.38 | 0.54 |
| 1:O:330:ALA:HB3 | 1:O:432:SER:HB3 | 1.88 | 0.54 |
| 1:C:504:VAL:CG1 | 1:C:521:ARG:CD | 2.86 | 0.54 |
| 1:I:504:VAL:CG1 | 1:I:521:ARG:CD | 2.86 | 0.54 |
| 1:K:481:GLY:H | 1:K:505:SER:HB3 | 0.42 | 0.54 |
| 1:N:132:VAL:HA | 1:N:141:LEU:O | 2.08 | 0.54 |
| 1:F:132:VAL:HA | 1:F:141:LEU:O | 2.08 | 0.54 |
| 1:F:259:LEU:HD11 | 1:F:310:ILE:CG1 | 2.38 | 0.54 |
| 1:H:259:LEU:HD11 | 1:H:310:ILE:CG1 | 2.38 | 0.54 |
| 1:I:132:VAL:HA | 1:I:141:LEU:O | 2.08 | 0.54 |
| 1:M:132:VAL:HA | 1:M:141:LEU:O | 2.08 | 0.54 |
| 1:M:259:LEU:HD11 | 1:M:310:ILE:CG1 | 2.38 | 0.54 |
| 1:M:521:ARG:HD3 | 1:M:521:ARG:N | 2.21 | 0.54 |
| 1:N:183:ILE:HD12 | 1:N:232:LEU:HD13 | 1.89 | 0.54 |
| 1:N:259:LEU:HD11 | 1:N:310:ILE:CG1 | 2.38 | 0.54 |
| 1:O:259:LEU:HD11 | 1:O:310:ILE:CG1 | 2.38 | 0.54 |
| 1:C:132:VAL:HA | 1:C:141:LEU:O | 2.08 | 0.54 |
| 1:J:259:LEU:HD11 | 1:J:310:ILE:CG1 | 2.38 | 0.54 |
| 1:J:459:ILE:CA | 1:J:474:THR:O | 2.55 | 0.54 |
| 1:L:504:VAL:CG1 | 1:L:521:ARG:CG | 2.83 | 0.54 |
| 1:L:609:PHE:CE2 | 1:M:639:ILE:HD11 | 2.42 | 0.54 |
| 1:N:481:GLY:H | 1:N:505:SER:HB3 | 0.42 | 0.54 |
| 1:O:504:VAL:CG1 | 1:O:521:ARG:CD | 2.86 | 0.54 |
| 1:B:183:ILE:HD12 | 1:B:232:LEU:HD13 | 1.89 | 0.54 |
| 1:B:259:LEU:HD11 | 1:B:310:ILE:CG1 | 2.38 | 0.54 |
| 1:D:183:ILE:HD12 | 1:D:232:LEU:HD13 | 1.89 | 0.54 |
| 1:J:609:PHE:CE2 | 1:K:639:ILE:HD11 | 2.42 | 0.54 |
| 1:O:177:ALA:HB3 | 1:O:208:GLU:HG2 | 1.89 | 0.54 |
| 1:F:207:ASP:OD1 | 1:F:209:ARG:N | 2.33 | 0.54 |
| 1:G:259:LEU:HD11 | 1:G:310:ILE:CG1 | 2.38 | 0.54 |
| 1:J:177:ALA:HB3 | 1:J:208:GLU:HG2 | 1.89 | 0.54 |
| 1:L:177:ALA:HB3 | 1:L:208:GLU:HG2 | 1.89 | 0.54 |
| 1:B:132:VAL:HA | 1:B:141:LEU:O | 2.08 | 0.53 |
| 1:C:177:ALA:HB3 | 1:C:208:GLU:HG2 | 1.89 | 0.53 |
| 1:I:183:ILE:HD12 | 1:I:232:LEU:HD13 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:504:VAL:CG1 | 1:J:521:ARG:CD | 2.86 | 0.53 |
| 1:J:504:VAL:CG1 | 1:J:521:ARG:CG | 2.83 | 0.53 |
| 1:M:183:ILE:HD12 | 1:M:232:LEU:HD13 | 1.89 | 0.53 |
| 1:N:177:ALA:HB3 | 1:N:208:GLU:HG2 | 1.89 | 0.53 |
| 1:C:481:GLY:N | 1:C:505:SER:OG | 2.23 | 0.53 |
| 1:G:504:VAL:CG1 | 1:G:521:ARG:CD | 2.86 | 0.53 |
| 1:H:481:GLY:H | 1:H:505:SER:HB3 | 0.42 | 0.53 |
| 1:H:609:PHE:CE2 | 1:I:639:ILE:HD11 | 2.42 | 0.53 |
| 1:K:177:ALA:HB3 | 1:K:208:GLU:HG2 | 1.89 | 0.53 |
| 1:B:508:LEU:N | 1:B:508:LEU:CD1 | 2.72 | 0.53 |
| 1:E:508:LEU:N | 1:E:508:LEU:CD1 | 2.72 | 0.53 |
| 1:H:504:VAL:CG1 | 1:H:521:ARG:CD | 2.86 | 0.53 |
| 1:I:259:LEU:HD11 | 1:I:310:ILE:CG1 | 2.38 | 0.53 |
| 1:J:132:VAL:HA | 1:J:141:LEU:O | 2.08 | 0.53 |
| 1:M:504:VAL:CG1 | 1:M:521:ARG:CD | 2.86 | 0.53 |
| 1:N:180:MET:HE2 | 1:N:213:ILE:HD11 | 1.89 | 0.53 |
| 1:O:132:VAL:HA | 1:O:141:LEU:O | 2.08 | 0.53 |
| 1:C:183:ILE:HD12 | 1:C:232:LEU:HD13 | 1.89 | 0.53 |
| 1:D:504:VAL:CG1 | 1:D:521:ARG:CD | 2.86 | 0.53 |
| 1:F:504:VAL:CG1 | 1:F:521:ARG:CD | 2.86 | 0.53 |
| 1:L:132:VAL:HA | 1:L:141:LEU:O | 2.08 | 0.53 |
| 1:L:504:VAL:CG1 | 1:L:521:ARG:CD | 2.86 | 0.53 |
| 1:C:508:LEU:N | 1:C:508:LEU:CD1 | 2.72 | 0.53 |
| 1:D:132:VAL:HA | 1:D:141:LEU:O | 2.08 | 0.53 |
| 1:K:504:VAL:CG1 | 1:K:521:ARG:CD | 2.86 | 0.53 |
| 1:M:177:ALA:HB3 | 1:M:208:GLU:HG2 | 1.89 | 0.53 |
| 1:M:459:ILE:CA | 1:M:474:THR:O | 2.55 | 0.53 |
| 1:B:481:GLY:H | 1:B:505:SER:HB3 | 0.42 | 0.53 |
| 1:C:155:ILE:HG12 | 1:C:158:ARG:NH2 | 2.24 | 0.53 |
| 1:D:142:ILE:HG22 | 1:D:149:VAL:HG22 | 1.91 | 0.53 |
| 1:E:504:VAL:CG1 | 1:E:521:ARG:CD | 2.86 | 0.53 |
| 1:G:508:LEU:N | 1:G:508:LEU:CD1 | 2.72 | 0.53 |
| 1:J:155:ILE:HG12 | 1:J:158:ARG:NH2 | 2.24 | 0.53 |
| 1:L:142:ILE:HG22 | 1:L:149:VAL:HG22 | 1.91 | 0.53 |
| 1:N:504:VAL:CG1 | 1:N:521:ARG:CD | 2.86 | 0.53 |
| 1:O:508:LEU:N | 1:O:508:LEU:CD1 | 2.72 | 0.53 |
| 1:A:259:LEU:HD11 | 1:A:310:ILE:CG1 | 2.38 | 0.53 |
| 1:A:508:LEU:N | 1:A:508:LEU:CD1 | 2.72 | 0.53 |
| 1:C:174:ASN:HB2 | 1:C:233:ASP:O | 2.09 | 0.53 |
| 1:E:132:VAL:HA | 1:E:141:LEU:O | 2.08 | 0.53 |
| 1:E:142:ILE:HG22 | 1:E:149:VAL:HG22 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:504:VAL:CG1 | 1:H:521:ARG:CG | 2.83 | 0.53 |
| 1:I:609:PHE:CE2 | 1:J:639:ILE:HD11 | 2.42 | 0.53 |
| 1:B:142:ILE:HG22 | 1:B:149:VAL:HG22 | 1.91 | 0.53 |
| 1:F:155:ILE:HG12 | 1:F:158:ARG:NH2 | 2.24 | 0.53 |
| 1:G:174:ASN:HB2 | 1:G:233:ASP:O | 2.09 | 0.53 |
| 1:H:142:ILE:HG22 | 1:H:149:VAL:HG22 | 1.91 | 0.53 |
| 1:I:142:ILE:HG22 | 1:I:149:VAL:HG22 | 1.91 | 0.53 |
| 1:I:155:ILE:HG12 | 1:I:158:ARG:NH2 | 2.24 | 0.53 |
| 1:J:183:ILE:HD12 | 1:J:232:LEU:HD13 | 1.89 | 0.53 |
| 1:K:142:ILE:HG22 | 1:K:149:VAL:HG22 | 1.91 | 0.53 |
| 1:K:155:ILE:HG12 | 1:K:158:ARG:NH2 | 2.24 | 0.53 |
| 1:L:609:PHE:CD2 | 1:M:639:ILE:CD1 | 2.75 | 0.53 |
| 1:D:174:ASN:HB2 | 1:D:233:ASP:O | 2.09 | 0.53 |
| 1:G:345:GLU:OE2 | 1:G:418:ASP:OD2 | 2.27 | 0.53 |
| 1:H:174:ASN:HB2 | 1:H:233:ASP:O | 2.09 | 0.53 |
| 1:I:459:ILE:CA | 1:I:474:THR:O | 2.55 | 0.53 |
| 1:K:183:ILE:HD12 | 1:K:232:LEU:HD13 | 1.89 | 0.53 |
| 1:K:609:PHE:CE2 | 1:L:639:ILE:HD11 | 2.42 | 0.53 |
| 1:N:609:PHE:CE2 | 1:O:639:ILE:HD11 | 2.42 | 0.53 |
| 1:D:508:LEU:N | 1:D:508:LEU:CD1 | 2.72 | 0.53 |
| 1:E:155:ILE:HG12 | 1:E:158:ARG:NH2 | 2.24 | 0.53 |
| 1:F:142:ILE:HG22 | 1:F:149:VAL:HG22 | 1.91 | 0.53 |
| 1:F:345:GLU:OE2 | 1:F:418:ASP:OD2 | 2.27 | 0.53 |
| 1:H:155:ILE:HG12 | 1:H:158:ARG:NH2 | 2.24 | 0.53 |
| 1:H:345:GLU:OE2 | 1:H:418:ASP:OD2 | 2.27 | 0.53 |
| 1:K:132:VAL:HA | 1:K:141:LEU:O | 2.08 | 0.53 |
| 1:K:504:VAL:CG1 | 1:K:521:ARG:CG | 2.83 | 0.53 |
| 1:L:155:ILE:HG12 | 1:L:158:ARG:NH2 | 2.24 | 0.53 |
| 1:M:142:ILE:HG22 | 1:M:149:VAL:HG22 | 1.91 | 0.53 |
| 1:N:142:ILE:HG22 | 1:N:149:VAL:HG22 | 1.91 | 0.53 |
| 1:E:481:GLY:H | 1:E:505:SER:HB3 | 0.42 | 0.52 |
| 1:G:142:ILE:HG22 | 1:G:149:VAL:HG22 | 1.91 | 0.52 |
| 1:G:609:PHE:CE2 | 1:H:639:ILE:HD11 | 2.42 | 0.52 |
| 1:H:223:GLU:O | 1:H:227:ARG:HG3 | 2.10 | 0.52 |
| 1:J:142:ILE:HG22 | 1:J:149:VAL:HG22 | 1.91 | 0.52 |
| 1:N:174:ASN:HB2 | 1:N:233:ASP:O | 2.09 | 0.52 |
| 1:O:142:ILE:HG22 | 1:O:149:VAL:HG22 | 1.91 | 0.52 |
| 1:A:132:VAL:HA | 1:A:141:LEU:O | 2.08 | 0.52 |
| 1:A:142:ILE:HG22 | 1:A:149:VAL:HG22 | 1.91 | 0.52 |
| 1:A:626:LEU:HD23 | 1:O:435:LEU:HD21 | 1.91 | 0.52 |
| 1:C:142:ILE:HG22 | 1:C:149:VAL:HG22 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:345:GLU:OE2 | 1:E:418:ASP:OD2 | 2.27 | 0.52 |
| 1:G:108:LYS:HA | 1:G:138:ASN:HD21 | 1.75 | 0.52 |
| 1:I:223:GLU:O | 1:I:227:ARG:HG3 | 2.09 | 0.52 |
| 1:K:174:ASN:HB2 | 1:K:233:ASP:O | 2.09 | 0.52 |
| 1:L:183:ILE:HD12 | 1:L:232:LEU:HD13 | 1.89 | 0.52 |
| 1:M:174:ASN:HB2 | 1:M:233:ASP:O | 2.09 | 0.52 |
| 1:A:223:GLU:O | 1:A:227:ARG:HG3 | 2.10 | 0.52 |
| 1:B:174:ASN:HB2 | 1:B:233:ASP:O | 2.09 | 0.52 |
| 1:D:155:ILE:HG12 | 1:D:158:ARG:NH2 | 2.24 | 0.52 |
| 1:G:155:ILE:HG12 | 1:G:158:ARG:NH2 | 2.24 | 0.52 |
| 1:H:163:GLY:O | 1:H:165:LYS:HG3 | 2.10 | 0.52 |
| 1:I:345:GLU:OE2 | 1:I:418:ASP:OD2 | 2.27 | 0.52 |
| 1:L:180:MET:HE2 | 1:L:213:ILE:HD11 | 1.90 | 0.52 |
| 1:M:508:LEU:N | 1:M:508:LEU:CD1 | 2.72 | 0.52 |
| 1:N:223:GLU:O | 1:N:227:ARG:HG3 | 2.10 | 0.52 |
| 1:O:174:ASN:HB2 | 1:O:233:ASP:O | 2.09 | 0.52 |
| 1:A:104:VAL:HA | 1:A:140:ILE:O | 2.10 | 0.52 |
| 1:A:109:ASN:ND2 | 1:A:160:ASP:O | 2.43 | 0.52 |
| 1:A:155:ILE:HG12 | 1:A:158:ARG:NH2 | 2.24 | 0.52 |
| 1:A:163:GLY:O | 1:A:165:LYS:HG3 | 2.10 | 0.52 |
| 1:A:174:ASN:HB2 | 1:A:233:ASP:O | 2.09 | 0.52 |
| 1:A:435:LEU:HD21 | 1:B:626:LEU:HD23 | 1.91 | 0.52 |
| 1:A:459:ILE:CA | 1:A:474:THR:O | 2.55 | 0.52 |
| 1:B:109:ASN:ND2 | 1:B:160:ASP:O | 2.43 | 0.52 |
| 1:C:104:VAL:HA | 1:C:140:ILE:O | 2.10 | 0.52 |
| 1:D:108:LYS:HA | 1:D:138:ASN:HD21 | 1.75 | 0.52 |
| 1:D:207:ASP:OD1 | 1:D:209:ARG:N | 2.33 | 0.52 |
| 1:F:508:LEU:N | 1:F:508:LEU:CD1 | 2.72 | 0.52 |
| 1:H:105:VAL:O | 1:H:140:ILE:CB | 2.49 | 0.52 |
| 1:I:435:LEU:HD21 | 1:J:626:LEU:HD23 | 1.91 | 0.52 |
| 1:I:508:LEU:N | 1:I:508:LEU:CD1 | 2.72 | 0.52 |
| 1:J:345:GLU:OE2 | 1:J:418:ASP:OD2 | 2.27 | 0.52 |
| 1:J:521:ARG:CD | 1:J:521:ARG:N | 2.73 | 0.52 |
| 1:L:174:ASN:HB2 | 1:L:233:ASP:O | 2.09 | 0.52 |
| 1:M:140:ILE:HD13 | 1:M:156:ILE:CG2 | 2.40 | 0.52 |
| 1:M:155:ILE:HG12 | 1:M:158:ARG:NH2 | 2.24 | 0.52 |
| 1:M:481:GLY:H | 1:M:505:SER:HB3 | 0.41 | 0.52 |
| 1:N:435:LEU:HD21 | 1:O:626:LEU:HD23 | 1.91 | 0.52 |
| 1:O:207:ASP:OD1 | 1:O:209:ARG:N | 2.33 | 0.52 |
| 1:A:140:ILE:HD13 | 1:A:156:ILE:CG2 | 2.40 | 0.52 |
| 1:B:104:VAL:HA | 1:B:140:ILE:O | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:223:GLU:O | 1:B:227:ARG:HG3 | 2.10 | 0.52 |
| 1:C:109:ASN:ND2 | 1:C:160:ASP:O | 2.43 | 0.52 |
| 1:D:104:VAL:HA | 1:D:140:ILE:O | 2.10 | 0.52 |
| 1:E:506:ASN:HD22 | 1:E:507:VAL:H | 1.51 | 0.52 |
| 1:G:223:GLU:O | 1:G:227:ARG:HG3 | 2.10 | 0.52 |
| 1:G:640:GLN:NE2 | 1:G:643:ILE:CG2 | 2.73 | 0.52 |
| 1:H:109:ASN:ND2 | 1:H:160:ASP:O | 2.43 | 0.52 |
| 1:I:109:ASN:ND2 | 1:I:160:ASP:O | 2.43 | 0.52 |
| 1:J:109:ASN:ND2 | 1:J:160:ASP:O | 2.43 | 0.52 |
| 1:J:163:GLY:O | 1:J:165:LYS:HG3 | 2.10 | 0.52 |
| 1:J:435:LEU:HD21 | 1:K:626:LEU:HD23 | 1.91 | 0.52 |
| 1:K:108:LYS:HA | 1:K:138:ASN:HD21 | 1.75 | 0.52 |
| 1:K:109:ASN:ND2 | 1:K:160:ASP:O | 2.43 | 0.52 |
| 1:K:121:GLN:O | 1:K:125:ASN:N | 2.33 | 0.52 |
| 1:M:223:GLU:O | 1:M:227:ARG:HG3 | 2.10 | 0.52 |
| 1:N:104:VAL:HA | 1:N:140:ILE:O | 2.10 | 0.52 |
| 1:N:122:LEU:HD23 | 1:N:125:ASN:ND2 | 2.19 | 0.52 |
| 1:N:508:LEU:N | 1:N:508:LEU:CD1 | 2.72 | 0.52 |
| 1:O:163:GLY:O | 1:O:165:LYS:HG3 | 2.10 | 0.52 |
| 1:O:223:GLU:O | 1:O:227:ARG:HG3 | 2.10 | 0.52 |
| 1:B:163:GLY:O | 1:B:165:LYS:HG3 | 2.10 | 0.52 |
| 1:C:221:VAL:HG22 | 1:C:224:ARG:HH21 | 1.75 | 0.52 |
| 1:C:223:GLU:O | 1:C:227:ARG:HG3 | 2.10 | 0.52 |
| 1:D:223:GLU:O | 1:D:227:ARG:HG3 | 2.10 | 0.52 |
| 1:D:521:ARG:CD | 1:D:521:ARG:N | 2.73 | 0.52 |
| 1:E:163:GLY:O | 1:E:165:LYS:HG3 | 2.10 | 0.52 |
| 1:E:521:ARG:CD | 1:E:521:ARG:N | 2.73 | 0.52 |
| 1:F:174:ASN:HB2 | 1:F:233:ASP:O | 2.09 | 0.52 |
| 1:G:109:ASN:ND2 | 1:G:160:ASP:O | 2.43 | 0.52 |
| 1:G:207:ASP:OD1 | 1:G:209:ARG:N | 2.33 | 0.52 |
| 1:H:108:LYS:HA | 1:H:138:ASN:HD21 | 1.75 | 0.52 |
| 1:I:521:ARG:CD | 1:I:521:ARG:N | 2.73 | 0.52 |
| 1:I:640:GLN:NE2 | 1:I:643:ILE:CG2 | 2.73 | 0.52 |
| 1:J:108:LYS:HA | 1:J:138:ASN:HD21 | 1.75 | 0.52 |
| 1:J:174:ASN:HB2 | 1:J:233:ASP:O | 2.09 | 0.52 |
| 1:J:481:GLY:H | 1:J:505:SER:HB3 | 0.42 | 0.52 |
| 1:K:345:GLU:OE2 | 1:K:418:ASP:OD2 | 2.27 | 0.52 |
| 1:K:521:ARG:CD | 1:K:521:ARG:N | 2.73 | 0.52 |
| 1:L:508:LEU:N | 1:L:508:LEU:CD1 | 2.72 | 0.52 |
| 1:N:155:ILE:HG12 | 1:N:158:ARG:NH2 | 2.24 | 0.52 |
| 1:O:104:VAL:HA | 1:O:140:ILE:O | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:477:ARG:CG | 1:A:477:ARG:NH1 | 2.73 | 0.52 |
| 1:A:640:GLN:NE2 | 1:A:643:ILE:CG2 | 2.73 | 0.52 |
| 1:B:506:ASN:HD22 | 1:B:507:VAL:H | 1.51 | 0.52 |
| 1:B:640:GLN:NE2 | 1:B:643:ILE:CG2 | 2.73 | 0.52 |
| 1:D:345:GLU:OE2 | 1:D:418:ASP:OD2 | 2.27 | 0.52 |
| 1:F:163:GLY:O | 1:F:165:LYS:HG3 | 2.10 | 0.52 |
| 1:G:122:LEU:HD23 | 1:G:125:ASN:ND2 | 2.19 | 0.52 |
| 1:K:508:LEU:N | 1:K:508:LEU:CD1 | 2.72 | 0.52 |
| 1:K:640:GLN:NE2 | 1:K:643:ILE:CG2 | 2.73 | 0.52 |
| 1:M:224:ARG:HA | 1:M:227:ARG:HD2 | 1.92 | 0.52 |
| 1:N:640:GLN:NE2 | 1:N:643:ILE:CG2 | 2.73 | 0.52 |
| 1:O:109:ASN:ND2 | 1:O:160:ASP:O | 2.43 | 0.52 |
| 1:D:109:ASN:ND2 | 1:D:160:ASP:O | 2.43 | 0.52 |
| 1:D:640:GLN:NE2 | 1:D:643:ILE:CG2 | 2.73 | 0.52 |
| 1:F:223:GLU:O | 1:F:227:ARG:HG3 | 2.10 | 0.52 |
| 1:F:640:GLN:NE2 | 1:F:643:ILE:CG2 | 2.73 | 0.52 |
| 1:G:163:GLY:O | 1:G:165:LYS:HG3 | 2.10 | 0.52 |
| 1:J:508:LEU:N | 1:J:508:LEU:CD1 | 2.72 | 0.52 |
| 1:K:163:GLY:O | 1:K:165:LYS:HG3 | 2.10 | 0.52 |
| 1:L:109:ASN:ND2 | 1:L:160:ASP:O | 2.43 | 0.52 |
| 1:L:163:GLY:O | 1:L:165:LYS:HG3 | 2.10 | 0.52 |
| 1:N:224:ARG:HA | 1:N:227:ARG:HD2 | 1.92 | 0.52 |
| 1:O:221:VAL:HG22 | 1:O:224:ARG:HH21 | 1.75 | 0.52 |
| 1:A:481:GLY:H | 1:A:505:SER:HB3 | 0.42 | 0.52 |
| 1:B:140:ILE:HD13 | 1:B:156:ILE:CG2 | 2.40 | 0.52 |
| 1:C:345:GLU:OE2 | 1:C:418:ASP:OD2 | 2.27 | 0.52 |
| 1:C:521:ARG:CD | 1:C:521:ARG:N | 2.73 | 0.52 |
| 1:E:104:VAL:HA | 1:E:140:ILE:O | 2.10 | 0.52 |
| 1:E:640:GLN:NE2 | 1:E:643:ILE:CG2 | 2.73 | 0.52 |
| 1:F:104:VAL:HA | 1:F:140:ILE:O | 2.10 | 0.52 |
| 1:F:109:ASN:ND2 | 1:F:160:ASP:O | 2.43 | 0.52 |
| 1:H:508:LEU:N | 1:H:508:LEU:CD1 | 2.72 | 0.52 |
| 1:H:640:GLN:NE2 | 1:H:643:ILE:CG2 | 2.73 | 0.52 |
| 1:I:174:ASN:HB2 | 1:I:233:ASP:O | 2.09 | 0.52 |
| 1:J:140:ILE:HD13 | 1:J:156:ILE:CG2 | 2.40 | 0.52 |
| 1:J:223:GLU:O | 1:J:227:ARG:HG3 | 2.10 | 0.52 |
| 1:K:435:LEU:HD21 | 1:L:626:LEU:HD23 | 1.91 | 0.52 |
| 1:L:140:ILE:HD13 | 1:L:156:ILE:CG2 | 2.40 | 0.52 |
| 1:L:224:ARG:HA | 1:L:227:ARG:HD2 | 1.92 | 0.52 |
| 1:L:345:GLU:OE2 | 1:L:418:ASP:OD2 | 2.27 | 0.52 |
| 1:M:435:LEU:HD21 | 1:N:626:LEU:HD23 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:640:GLN:NE2 | 1:M:643:ILE:CG2 | 2.73 | 0.52 |
| 1:D:140:ILE:HD13 | 1:D:156:ILE:CG2 | 2.40 | 0.52 |
| 1:D:163:GLY:O | 1:D:165:LYS:HG3 | 2.10 | 0.52 |
| 1:E:122:LEU:HD23 | 1:E:125:ASN:ND2 | 2.19 | 0.52 |
| 1:E:174:ASN:HB2 | 1:E:233:ASP:O | 2.09 | 0.52 |
| 1:E:456:VAL:HG22 | 1:E:457:PRO:N | 2.25 | 0.52 |
| 1:F:221:VAL:HG22 | 1:F:224:ARG:HH21 | 1.75 | 0.52 |
| 1:F:521:ARG:CD | 1:F:521:ARG:N | 2.73 | 0.52 |
| 1:H:521:ARG:CD | 1:H:521:ARG:N | 2.73 | 0.52 |
| 1:L:521:ARG:CD | 1:L:521:ARG:N | 2.73 | 0.52 |
| 1:O:224:ARG:HA | 1:O:227:ARG:HD2 | 1.92 | 0.52 |
| 1:B:155:ILE:HG12 | 1:B:158:ARG:NH2 | 2.24 | 0.51 |
| 1:E:223:GLU:O | 1:E:227:ARG:HG3 | 2.09 | 0.51 |
| 1:J:640:GLN:NE2 | 1:J:643:ILE:CG2 | 2.73 | 0.51 |
| 1:L:223:GLU:O | 1:L:227:ARG:HG3 | 2.10 | 0.51 |
| 1:O:155:ILE:HG12 | 1:O:158:ARG:NH2 | 2.24 | 0.51 |
| 1:B:221:VAL:HG22 | 1:B:224:ARG:HH21 | 1.75 | 0.51 |
| 1:B:345:GLU:OE2 | 1:B:418:ASP:OD2 | 2.27 | 0.51 |
| 1:B:456:VAL:HG22 | 1:B:457:PRO:N | 2.26 | 0.51 |
| 1:C:163:GLY:O | 1:C:165:LYS:HG3 | 2.10 | 0.51 |
| 1:D:224:ARG:HA | 1:D:227:ARG:HD2 | 1.92 | 0.51 |
| 1:E:108:LYS:HA | 1:E:138:ASN:HD21 | 1.75 | 0.51 |
| 1:G:521:ARG:CD | 1:G:521:ARG:N | 2.73 | 0.51 |
| 1:H:435:LEU:HD21 | 1:I:626:LEU:HD23 | 1.91 | 0.51 |
| 1:K:456:VAL:HG22 | 1:K:457:PRO:N | 2.26 | 0.51 |
| 1:M:104:VAL:HA | 1:M:140:ILE:O | 2.10 | 0.51 |
| 1:M:109:ASN:ND2 | 1:M:160:ASP:O | 2.43 | 0.51 |
| 1:M:521:ARG:CD | 1:M:521:ARG:N | 2.73 | 0.51 |
| 1:N:109:ASN:ND2 | 1:N:160:ASP:O | 2.43 | 0.51 |
| 1:N:345:GLU:OE2 | 1:N:418:ASP:OD2 | 2.27 | 0.51 |
| 1:C:640:GLN:NE2 | 1:C:643:ILE:CG2 | 2.73 | 0.51 |
| 1:D:459:ILE:CA | 1:D:474:THR:O | 2.55 | 0.51 |
| 1:E:221:VAL:HG22 | 1:E:224:ARG:HH21 | 1.75 | 0.51 |
| 1:E:224:ARG:HA | 1:E:227:ARG:HD2 | 1.92 | 0.51 |
| 1:G:104:VAL:HA | 1:G:140:ILE:O | 2.10 | 0.51 |
| 1:I:163:GLY:O | 1:I:165:LYS:HG3 | 2.10 | 0.51 |
| 1:J:224:ARG:HA | 1:J:227:ARG:HD2 | 1.92 | 0.51 |
| 1:K:224:ARG:HA | 1:K:227:ARG:HD2 | 1.92 | 0.51 |
| 1:L:640:GLN:NE2 | 1:L:643:ILE:CG2 | 2.73 | 0.51 |
| 1:N:521:ARG:CD | 1:N:521:ARG:N | 2.73 | 0.51 |
| 1:O:108:LYS:HA | 1:O:138:ASN:HD21 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:140:ILE:HD13 | 1:O:156:ILE:CG2 | 2.40 | 0.51 |
| 1:O:345:GLU:OE2 | 1:O:418:ASP:OD2 | 2.27 | 0.51 |
| 1:A:456:VAL:HG22 | 1:A:457:PRO:N | 2.26 | 0.51 |
| 1:B:108:LYS:HA | 1:B:138:ASN:HD21 | 1.75 | 0.51 |
| 1:B:435:LEU:HD21 | 1:C:626:LEU:HD23 | 1.91 | 0.51 |
| 1:D:477:ARG:CG | 1:D:477:ARG:NH1 | 2.73 | 0.51 |
| 1:E:109:ASN:ND2 | 1:E:160:ASP:O | 2.43 | 0.51 |
| 1:G:140:ILE:HD13 | 1:G:156:ILE:CG2 | 2.40 | 0.51 |
| 1:G:481:GLY:H | 1:G:505:SER:HB3 | 0.42 | 0.51 |
| 1:I:105:VAL:O | 1:I:140:ILE:CB | 2.49 | 0.51 |
| 1:J:456:VAL:HG22 | 1:J:457:PRO:N | 2.26 | 0.51 |
| 1:K:223:GLU:O | 1:K:227:ARG:HG3 | 2.10 | 0.51 |
| 1:M:609:PHE:CE2 | 1:N:639:ILE:HD11 | 2.42 | 0.51 |
| 1:N:108:LYS:HA | 1:N:138:ASN:HD21 | 1.75 | 0.51 |
| 1:N:163:GLY:O | 1:N:165:LYS:HG3 | 2.10 | 0.51 |
| 1:O:521:ARG:CD | 1:O:521:ARG:N | 2.73 | 0.51 |
| 1:O:640:GLN:NE2 | 1:O:643:ILE:CG2 | 2.73 | 0.51 |
| 1:A:108:LYS:HA | 1:A:138:ASN:HD21 | 1.75 | 0.51 |
| 1:A:224:ARG:HA | 1:A:227:ARG:HD2 | 1.92 | 0.51 |
| 1:A:345:GLU:OE2 | 1:A:418:ASP:OD2 | 2.27 | 0.51 |
| 1:B:521:ARG:CD | 1:B:521:ARG:N | 2.73 | 0.51 |
| 1:D:456:VAL:HG22 | 1:D:457:PRO:N | 2.26 | 0.51 |
| 1:E:140:ILE:HD13 | 1:E:156:ILE:CG2 | 2.40 | 0.51 |
| 1:H:506:ASN:HD22 | 1:H:507:VAL:H | 1.50 | 0.51 |
| 1:I:140:ILE:HD13 | 1:I:156:ILE:CG2 | 2.40 | 0.51 |
| 1:I:224:ARG:HA | 1:I:227:ARG:HD2 | 1.92 | 0.51 |
| 1:J:121:GLN:O | 1:J:125:ASN:N | 2.33 | 0.51 |
| 1:L:459:ILE:CA | 1:L:474:THR:O | 2.55 | 0.51 |
| 1:M:108:LYS:HA | 1:M:138:ASN:HD21 | 1.75 | 0.51 |
| 1:M:163:GLY:O | 1:M:165:LYS:HG3 | 2.10 | 0.51 |
| 1:M:345:GLU:OE2 | 1:M:418:ASP:OD2 | 2.27 | 0.51 |
| 1:A:221:VAL:HG22 | 1:A:224:ARG:HH21 | 1.75 | 0.51 |
| 1:A:521:ARG:CD | 1:A:521:ARG:N | 2.73 | 0.51 |
| 1:H:481:GLY:N | 1:H:505:SER:OG | 2.23 | 0.51 |
| 1:L:108:LYS:HA | 1:L:138:ASN:HD21 | 1.74 | 0.51 |
| 1:N:333:ASP:OD1 | 1:N:334:GLY:N | 2.44 | 0.51 |
| 1:O:477:ARG:CG | 1:O:477:ARG:NH1 | 2.73 | 0.51 |
| 1:C:224:ARG:HA | 1:C:227:ARG:HD2 | 1.92 | 0.51 |
| 1:D:481:GLY:H | 1:D:505:SER:HB3 | 0.42 | 0.51 |
| 1:E:435:LEU:HD21 | 1:F:626:LEU:HD23 | 1.91 | 0.51 |
| 1:F:108:LYS:HA | 1:F:138:ASN:HD21 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:224:ARG:HA | 1:F:227:ARG:HD2 | 1.92 | 0.51 |
| 1:J:104:VAL:HA | 1:J:140:ILE:O | 2.10 | 0.51 |
| 1:K:104:VAL:HA | 1:K:140:ILE:O | 2.10 | 0.51 |
| 1:L:221:VAL:HG22 | 1:L:224:ARG:HH21 | 1.75 | 0.51 |
| 1:L:435:LEU:HD21 | 1:M:626:LEU:HD23 | 1.91 | 0.51 |
| 1:N:221:VAL:HG22 | 1:N:224:ARG:HH21 | 1.75 | 0.51 |
| 1:C:140:ILE:HD13 | 1:C:156:ILE:CG2 | 2.40 | 0.51 |
| 1:C:459:ILE:CA | 1:C:474:THR:O | 2.55 | 0.51 |
| 1:K:478:LYS:HD2 | 1:K:518:PHE:CZ | 2.46 | 0.51 |
| 1:M:478:LYS:HD2 | 1:M:518:PHE:CZ | 2.46 | 0.51 |
| 1:D:221:VAL:HG22 | 1:D:224:ARG:HH21 | 1.75 | 0.51 |
| 1:D:435:LEU:HD21 | 1:E:626:LEU:HD23 | 1.91 | 0.51 |
| 1:H:456:VAL:HG22 | 1:H:457:PRO:N | 2.26 | 0.51 |
| 1:H:459:ILE:CA | 1:H:474:THR:O | 2.55 | 0.51 |
| 1:I:221:VAL:HG22 | 1:I:224:ARG:HH21 | 1.75 | 0.51 |
| 1:K:506:ASN:HD22 | 1:K:507:VAL:H | 1.50 | 0.51 |
| 1:L:104:VAL:HA | 1:L:140:ILE:O | 2.10 | 0.51 |
| 1:A:207:ASP:OD1 | 1:A:209:ARG:N | 2.33 | 0.51 |
| 1:B:477:ARG:CG | 1:B:477:ARG:NH1 | 2.73 | 0.51 |
| 1:C:108:LYS:HA | 1:C:138:ASN:HD21 | 1.75 | 0.51 |
| 1:E:459:ILE:CA | 1:E:474:THR:O | 2.56 | 0.51 |
| 1:F:456:VAL:HG22 | 1:F:457:PRO:N | 2.26 | 0.51 |
| 1:H:224:ARG:HA | 1:H:227:ARG:HD2 | 1.92 | 0.51 |
| 1:L:333:ASP:OD1 | 1:L:334:GLY:N | 2.44 | 0.51 |
| 1:M:333:ASP:OD1 | 1:M:334:GLY:N | 2.44 | 0.51 |
| 1:N:506:ASN:HD22 | 1:N:507:VAL:H | 1.50 | 0.51 |
| 1:O:333:ASP:OD1 | 1:O:334:GLY:N | 2.44 | 0.51 |
| 1:C:477:ARG:CG | 1:C:477:ARG:NH1 | 2.73 | 0.50 |
| 1:D:478:LYS:HD2 | 1:D:518:PHE:CZ | 2.46 | 0.50 |
| 1:E:333:ASP:OD1 | 1:E:334:GLY:N | 2.44 | 0.50 |
| 1:F:140:ILE:HD13 | 1:F:156:ILE:CG2 | 2.40 | 0.50 |
| 1:H:221:VAL:HG22 | 1:H:224:ARG:HH21 | 1.75 | 0.50 |
| 1:I:235:GLU:H | 1:I:235:GLU:CD | 2.11 | 0.50 |
| 1:I:456:VAL:HG22 | 1:I:457:PRO:N | 2.26 | 0.50 |
| 1:J:105:VAL:O | 1:J:140:ILE:CB | 2.49 | 0.50 |
| 1:O:122:LEU:HD23 | 1:O:125:ASN:ND2 | 2.19 | 0.50 |
| 1:B:224:ARG:HA | 1:B:227:ARG:HD2 | 1.92 | 0.50 |
| 1:C:435:LEU:HD21 | 1:D:626:LEU:HD23 | 1.91 | 0.50 |
| 1:C:478:LYS:HD2 | 1:C:518:PHE:CZ | 2.46 | 0.50 |
| 1:F:177:ALA:HB1 | 1:F:206:ALA:HB1 | 1.94 | 0.50 |
| 1:F:321:LEU:CD1 | 1:F:441:THR:OG1 | 2.60 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:435:LEU:HD21 | 1:G:626:LEU:HD23 | 1.91 | 0.50 |
| 1:J:122:LEU:HD23 | 1:J:125:ASN:ND2 | 2.19 | 0.50 |
| 1:J:221:VAL:HG22 | 1:J:224:ARG:HH21 | 1.75 | 0.50 |
| 1:J:478:LYS:HD2 | 1:J:518:PHE:CZ | 2.46 | 0.50 |
| 1:K:333:ASP:OD1 | 1:K:334:GLY:N | 2.44 | 0.50 |
| 1:M:456:VAL:HG22 | 1:M:457:PRO:N | 2.26 | 0.50 |
| 1:A:177:ALA:HB1 | 1:A:206:ALA:HB1 | 1.94 | 0.50 |
| 1:C:456:VAL:HG22 | 1:C:457:PRO:N | 2.26 | 0.50 |
| 1:F:519:ALA:CB | 1:G:454:GLU:HG3 | 2.41 | 0.50 |
| 1:G:177:ALA:HB1 | 1:G:206:ALA:HB1 | 1.94 | 0.50 |
| 1:G:519:ALA:CB | 1:H:454:GLU:HG3 | 2.41 | 0.50 |
| 1:H:333:ASP:OD1 | 1:H:334:GLY:N | 2.44 | 0.50 |
| 1:I:108:LYS:HA | 1:I:138:ASN:HD21 | 1.75 | 0.50 |
| 1:I:180:MET:SD | 1:I:183:ILE:HD11 | 2.51 | 0.50 |
| 1:J:333:ASP:OD1 | 1:J:334:GLY:N | 2.44 | 0.50 |
| 1:L:177:ALA:HB1 | 1:L:206:ALA:HB1 | 1.94 | 0.50 |
| 1:L:478:LYS:HD2 | 1:L:518:PHE:CZ | 2.46 | 0.50 |
| 1:M:177:ALA:HB1 | 1:M:206:ALA:HB1 | 1.94 | 0.50 |
| 1:M:221:VAL:HG22 | 1:M:224:ARG:HH21 | 1.75 | 0.50 |
| 1:E:321:LEU:CD1 | 1:E:441:THR:OG1 | 2.60 | 0.50 |
| 1:E:459:ILE:HD12 | 1:E:459:ILE:N | 2.27 | 0.50 |
| 1:E:519:ALA:CB | 1:F:454:GLU:HG3 | 2.41 | 0.50 |
| 1:F:333:ASP:OD1 | 1:F:334:GLY:N | 2.44 | 0.50 |
| 1:G:224:ARG:HA | 1:G:227:ARG:HD2 | 1.92 | 0.50 |
| 1:G:321:LEU:CD1 | 1:G:441:THR:OG1 | 2.60 | 0.50 |
| 1:G:456:VAL:HG22 | 1:G:457:PRO:N | 2.26 | 0.50 |
| 1:H:478:LYS:HD2 | 1:H:518:PHE:CZ | 2.46 | 0.50 |
| 1:I:104:VAL:HA | 1:I:140:ILE:O | 2.10 | 0.50 |
| 1:J:180:MET:SD | 1:J:183:ILE:HD11 | 2.51 | 0.50 |
| 1:N:177:ALA:HB1 | 1:N:206:ALA:HB1 | 1.94 | 0.50 |
| 1:N:456:VAL:HG22 | 1:N:457:PRO:N | 2.26 | 0.50 |
| 1:O:177:ALA:HB1 | 1:O:206:ALA:HB1 | 1.94 | 0.50 |
| 1:A:454:GLU:HG3 | 1:O:519:ALA:CB | 2.41 | 0.50 |
| 1:A:519:ALA:CB | 1:B:454:GLU:HG3 | 2.41 | 0.50 |
| 1:B:333:ASP:OD1 | 1:B:334:GLY:N | 2.44 | 0.50 |
| 1:C:122:LEU:HD23 | 1:C:125:ASN:ND2 | 2.19 | 0.50 |
| 1:C:205:VAL:HG12 | 1:C:206:ALA:N | 2.27 | 0.50 |
| 1:D:459:ILE:HD12 | 1:D:459:ILE:N | 2.27 | 0.50 |
| 1:F:459:ILE:HD12 | 1:F:459:ILE:N | 2.27 | 0.50 |
| 1:G:333:ASP:OD1 | 1:G:334:GLY:N | 2.44 | 0.50 |
| 1:G:435:LEU:HD21 | 1:H:626:LEU:HD23 | 1.91 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:552:VAL:HG23 | 1:G:553:PRO:C | 2.32 | 0.50 |
| 1:H:104:VAL:HA | 1:H:140:ILE:O | 2.10 | 0.50 |
| 1:H:180:MET:SD | 1:H:183:ILE:HD11 | 2.51 | 0.50 |
| 1:H:207:ASP:OD1 | 1:H:209:ARG:N | 2.33 | 0.50 |
| 1:H:552:VAL:HG23 | 1:H:553:PRO:C | 2.32 | 0.50 |
| 1:I:177:ALA:HB1 | 1:I:206:ALA:HB1 | 1.94 | 0.50 |
| 1:K:177:ALA:HB1 | 1:K:206:ALA:HB1 | 1.94 | 0.50 |
| 1:K:221:VAL:HG22 | 1:K:224:ARG:HH21 | 1.75 | 0.50 |
| 1:M:552:VAL:HG23 | 1:M:553:PRO:C | 2.32 | 0.50 |
| 1:N:180:MET:SD | 1:N:183:ILE:HD11 | 2.51 | 0.50 |
| 1:N:478:LYS:HD2 | 1:N:518:PHE:CZ | 2.46 | 0.50 |
| 1:C:333:ASP:OD1 | 1:C:334:GLY:N | 2.44 | 0.50 |
| 1:C:458:VAL:O | 1:C:475:VAL:C | 2.49 | 0.50 |
| 1:D:177:ALA:HB1 | 1:D:206:ALA:HB1 | 1.94 | 0.50 |
| 1:D:321:LEU:CD1 | 1:D:441:THR:OG1 | 2.60 | 0.50 |
| 1:E:180:MET:SD | 1:E:183:ILE:HD11 | 2.51 | 0.50 |
| 1:F:102:THR:OG1 | 1:F:142:ILE:O | 2.25 | 0.50 |
| 1:F:180:MET:SD | 1:F:183:ILE:HD11 | 2.51 | 0.50 |
| 1:G:478:LYS:HD2 | 1:G:518:PHE:CZ | 2.46 | 0.50 |
| 1:H:177:ALA:HB1 | 1:H:206:ALA:HB1 | 1.94 | 0.50 |
| 1:H:519:ALA:CB | 1:I:454:GLU:HG3 | 2.41 | 0.50 |
| 1:J:177:ALA:HB1 | 1:J:206:ALA:HB1 | 1.94 | 0.50 |
| 1:K:140:ILE:HD13 | 1:K:156:ILE:CG2 | 2.40 | 0.50 |
| 1:K:180:MET:SD | 1:K:183:ILE:HD11 | 2.51 | 0.50 |
| 1:K:552:VAL:HG23 | 1:K:553:PRO:C | 2.32 | 0.50 |
| 1:L:552:VAL:HG23 | 1:L:553:PRO:C | 2.32 | 0.50 |
| 1:O:180:MET:SD | 1:O:183:ILE:HD11 | 2.51 | 0.50 |
| 1:O:459:ILE:CA | 1:O:474:THR:O | 2.55 | 0.50 |
| 1:A:333:ASP:OD1 | 1:A:334:GLY:N | 2.44 | 0.50 |
| 1:B:177:ALA:HB1 | 1:B:206:ALA:HB1 | 1.94 | 0.50 |
| 1:B:205:VAL:HG12 | 1:B:206:ALA:N | 2.27 | 0.50 |
| 1:C:180:MET:SD | 1:C:183:ILE:HD11 | 2.51 | 0.50 |
| 1:D:180:MET:SD | 1:D:183:ILE:HD11 | 2.51 | 0.50 |
| 1:D:205:VAL:HG12 | 1:D:206:ALA:N | 2.27 | 0.50 |
| 1:E:177:ALA:HB1 | 1:E:206:ALA:HB1 | 1.94 | 0.50 |
| 1:F:478:LYS:HD2 | 1:F:518:PHE:CZ | 2.46 | 0.50 |
| 1:F:552:VAL:HG23 | 1:F:553:PRO:C | 2.32 | 0.50 |
| 1:G:180:MET:SD | 1:G:183:ILE:HD11 | 2.51 | 0.50 |
| 1:G:221:VAL:HG22 | 1:G:224:ARG:HH21 | 1.75 | 0.50 |
| 1:H:140:ILE:HD13 | 1:H:156:ILE:CG2 | 2.40 | 0.50 |
| 1:H:321:LEU:CD1 | 1:H:441:THR:OG1 | 2.60 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:105:VAL:O | 1:K:140:ILE:CB | 2.49 | 0.50 |
| 1:K:519:ALA:CB | 1:L:454:GLU:HG3 | 2.41 | 0.50 |
| 1:M:180:MET:SD | 1:M:183:ILE:HD11 | 2.51 | 0.50 |
| 1:M:205:VAL:HG12 | 1:M:206:ALA:N | 2.27 | 0.50 |
| 1:N:519:ALA:CB | 1:O:454:GLU:HG3 | 2.41 | 0.50 |
| 1:A:180:MET:SD | 1:A:183:ILE:HD11 | 2.51 | 0.50 |
| 1:A:205:VAL:HG12 | 1:A:206:ALA:N | 2.27 | 0.50 |
| 1:B:519:ALA:CB | 1:C:454:GLU:HG3 | 2.41 | 0.50 |
| 1:C:177:ALA:HB1 | 1:C:206:ALA:HB1 | 1.94 | 0.50 |
| 1:E:478:LYS:HD2 | 1:E:518:PHE:CZ | 2.46 | 0.50 |
| 1:F:477:ARG:N | 1:F:477:ARG:HD2 | 2.27 | 0.50 |
| 1:G:459:ILE:CA | 1:G:474:THR:O | 2.55 | 0.50 |
| 1:K:435:LEU:HD11 | 1:L:607:GLN:HE22 | 1.77 | 0.50 |
| 1:K:477:ARG:N | 1:K:477:ARG:HD2 | 2.27 | 0.50 |
| 1:L:459:ILE:HD12 | 1:L:459:ILE:N | 2.27 | 0.50 |
| 1:L:519:ALA:CB | 1:M:454:GLU:HG3 | 2.41 | 0.50 |
| 1:N:552:VAL:HG23 | 1:N:553:PRO:C | 2.32 | 0.50 |
| 1:A:478:LYS:HD2 | 1:A:518:PHE:CZ | 2.46 | 0.50 |
| 1:B:180:MET:SD | 1:B:183:ILE:HD11 | 2.51 | 0.50 |
| 1:B:218:ASP:N | 1:B:221:VAL:HB | 2.27 | 0.50 |
| 1:C:218:ASP:N | 1:C:221:VAL:HB | 2.27 | 0.50 |
| 1:D:333:ASP:OD1 | 1:D:334:GLY:N | 2.44 | 0.50 |
| 1:E:205:VAL:HG12 | 1:E:206:ALA:N | 2.27 | 0.50 |
| 1:F:459:ILE:CA | 1:F:474:THR:O | 2.55 | 0.50 |
| 1:I:478:LYS:HD2 | 1:I:518:PHE:CZ | 2.46 | 0.50 |
| 1:I:519:ALA:CB | 1:J:454:GLU:HG3 | 2.41 | 0.50 |
| 1:J:205:VAL:HG12 | 1:J:206:ALA:N | 2.27 | 0.50 |
| 1:J:519:ALA:CB | 1:K:454:GLU:HG3 | 2.41 | 0.50 |
| 1:J:552:VAL:HG23 | 1:J:553:PRO:C | 2.32 | 0.50 |
| 1:K:205:VAL:HG12 | 1:K:206:ALA:N | 2.27 | 0.50 |
| 1:K:458:VAL:O | 1:K:475:VAL:C | 2.49 | 0.50 |
| 1:L:180:MET:SD | 1:L:183:ILE:HD11 | 2.51 | 0.50 |
| 1:M:459:ILE:HD12 | 1:M:459:ILE:N | 2.27 | 0.50 |
| 1:O:456:VAL:HG22 | 1:O:457:PRO:N | 2.26 | 0.50 |
| 1:O:552:VAL:HG23 | 1:O:553:PRO:C | 2.32 | 0.50 |
| 1:F:442:VAL:HG12 | 1:F:448:ALA:HB2 | 1.94 | 0.49 |
| 1:G:218:ASP:N | 1:G:221:VAL:HB | 2.27 | 0.49 |
| 1:H:205:VAL:HG12 | 1:H:206:ALA:N | 2.27 | 0.49 |
| 1:H:218:ASP:N | 1:H:221:VAL:HB | 2.27 | 0.49 |
| 1:I:552:VAL:HG23 | 1:I:553:PRO:C | 2.32 | 0.49 |
| 1:L:435:LEU:HD11 | 1:M:607:GLN:HE22 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:456:VAL:HG22 | 1:L:457:PRO:N | 2.26 | 0.49 |
| 1:N:459:ILE:HD12 | 1:N:459:ILE:N | 2.27 | 0.49 |
| 1:O:321:LEU:CD1 | 1:O:441:THR:OG1 | 2.60 | 0.49 |
| 1:A:218:ASP:N | 1:A:221:VAL:HB | 2.27 | 0.49 |
| 1:A:506:ASN:O | 1:A:519:ALA:N | 2.46 | 0.49 |
| 1:C:321:LEU:CD1 | 1:C:441:THR:OG1 | 2.60 | 0.49 |
| 1:C:506:ASN:O | 1:C:519:ALA:N | 2.46 | 0.49 |
| 1:D:477:ARG:HD2 | 1:D:477:ARG:N | 2.27 | 0.49 |
| 1:G:442:VAL:HG12 | 1:G:448:ALA:HB2 | 1.94 | 0.49 |
| 1:G:459:ILE:HD12 | 1:G:459:ILE:N | 2.27 | 0.49 |
| 1:H:235:GLU:H | 1:H:235:GLU:CD | 2.12 | 0.49 |
| 1:I:218:ASP:N | 1:I:221:VAL:HB | 2.27 | 0.49 |
| 1:J:435:LEU:HD11 | 1:K:607:GLN:HE22 | 1.77 | 0.49 |
| 1:K:459:ILE:HD12 | 1:K:459:ILE:N | 2.27 | 0.49 |
| 1:M:477:ARG:N | 1:M:477:ARG:HD2 | 2.27 | 0.49 |
| 1:N:140:ILE:HD13 | 1:N:156:ILE:CG2 | 2.40 | 0.49 |
| 1:N:442:VAL:HG12 | 1:N:448:ALA:HB2 | 1.94 | 0.49 |
| 1:N:477:ARG:CG | 1:N:477:ARG:NH1 | 2.73 | 0.49 |
| 1:O:478:LYS:HD2 | 1:O:518:PHE:CZ | 2.46 | 0.49 |
| 1:O:506:ASN:O | 1:O:519:ALA:N | 2.46 | 0.49 |
| 1:C:459:ILE:HD12 | 1:C:459:ILE:N | 2.27 | 0.49 |
| 1:D:218:ASP:N | 1:D:221:VAL:HB | 2.27 | 0.49 |
| 1:D:506:ASN:O | 1:D:519:ALA:N | 2.45 | 0.49 |
| 1:E:105:VAL:O | 1:E:140:ILE:CB | 2.49 | 0.49 |
| 1:E:218:ASP:N | 1:E:221:VAL:HB | 2.27 | 0.49 |
| 1:E:442:VAL:HG12 | 1:E:448:ALA:HB2 | 1.94 | 0.49 |
| 1:E:552:VAL:HG23 | 1:E:553:PRO:C | 2.32 | 0.49 |
| 1:H:477:ARG:N | 1:H:477:ARG:HD2 | 2.27 | 0.49 |
| 1:I:205:VAL:HG12 | 1:I:206:ALA:N | 2.27 | 0.49 |
| 1:I:321:LEU:CD1 | 1:I:441:THR:OG1 | 2.60 | 0.49 |
| 1:I:435:LEU:HD11 | 1:J:607:GLN:HE22 | 1.77 | 0.49 |
| 1:I:477:ARG:N | 1:I:477:ARG:HD2 | 2.27 | 0.49 |
| 1:N:506:ASN:O | 1:N:519:ALA:N | 2.45 | 0.49 |
| 1:O:442:VAL:HG12 | 1:O:448:ALA:HB2 | 1.94 | 0.49 |
| 1:O:459:ILE:HD12 | 1:O:459:ILE:N | 2.27 | 0.49 |
| 1:A:442:VAL:HG12 | 1:A:448:ALA:HB2 | 1.94 | 0.49 |
| 1:B:459:ILE:CA | 1:B:474:THR:O | 2.55 | 0.49 |
| 1:D:552:VAL:HG23 | 1:D:553:PRO:C | 2.32 | 0.49 |
| 1:F:205:VAL:HG12 | 1:F:206:ALA:N | 2.27 | 0.49 |
| 1:F:472:PHE:CD1 | 1:F:472:PHE:C | 2.86 | 0.49 |
| 1:I:167:ILE:CA | 1:I:215:ILE:O | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:333:ASP:OD1 | 1:I:334:GLY:N | 2.44 | 0.49 |
| 1:J:218:ASP:N | 1:J:221:VAL:HB | 2.27 | 0.49 |
| 1:J:459:ILE:HD12 | 1:J:459:ILE:N | 2.27 | 0.49 |
| 1:K:122:LEU:HD23 | 1:K:125:ASN:ND2 | 2.19 | 0.49 |
| 1:L:218:ASP:N | 1:L:221:VAL:HB | 2.27 | 0.49 |
| 1:L:458:VAL:O | 1:L:475:VAL:C | 2.49 | 0.49 |
| 1:N:205:VAL:HG12 | 1:N:206:ALA:N | 2.27 | 0.49 |
| 1:N:218:ASP:N | 1:N:221:VAL:HB | 2.27 | 0.49 |
| 1:O:205:VAL:HG12 | 1:O:206:ALA:N | 2.27 | 0.49 |
| 1:B:552:VAL:HG23 | 1:B:553:PRO:C | 2.32 | 0.49 |
| 1:F:218:ASP:N | 1:F:221:VAL:HB | 2.27 | 0.49 |
| 1:L:205:VAL:HG12 | 1:L:206:ALA:N | 2.27 | 0.49 |
| 1:L:321:LEU:CD1 | 1:L:441:THR:OG1 | 2.60 | 0.49 |
| 1:M:519:ALA:CB | 1:N:454:GLU:HG3 | 2.41 | 0.49 |
| 1:N:321:LEU:CD1 | 1:N:441:THR:OG1 | 2.60 | 0.49 |
| 1:B:478:LYS:HD2 | 1:B:518:PHE:CZ | 2.46 | 0.49 |
| 1:B:586:ILE:HG21 | 1:B:592:ALA:HB2 | 1.95 | 0.49 |
| 1:C:472:PHE:CD1 | 1:C:472:PHE:C | 2.86 | 0.49 |
| 1:C:519:ALA:CB | 1:D:454:GLU:HG3 | 2.41 | 0.49 |
| 1:G:177:ALA:N | 1:G:211:ASN:OD1 | 2.41 | 0.49 |
| 1:H:122:LEU:HD23 | 1:H:125:ASN:ND2 | 2.19 | 0.49 |
| 1:H:442:VAL:HG12 | 1:H:448:ALA:HB2 | 1.94 | 0.49 |
| 1:J:321:LEU:CD1 | 1:J:441:THR:OG1 | 2.60 | 0.49 |
| 1:J:458:VAL:O | 1:J:475:VAL:C | 2.49 | 0.49 |
| 1:L:177:ALA:N | 1:L:211:ASN:OD1 | 2.41 | 0.49 |
| 1:L:442:VAL:HG12 | 1:L:448:ALA:HB2 | 1.94 | 0.49 |
| 1:M:177:ALA:N | 1:M:211:ASN:OD1 | 2.41 | 0.49 |
| 1:M:321:LEU:CD1 | 1:M:441:THR:OG1 | 2.60 | 0.49 |
| 1:M:442:VAL:HG12 | 1:M:448:ALA:HB2 | 1.95 | 0.49 |
| 1:B:477:ARG:HD2 | 1:B:477:ARG:N | 2.27 | 0.49 |
| 1:H:435:LEU:HD11 | 1:I:607:GLN:HE22 | 1.77 | 0.49 |
| 1:L:105:VAL:O | 1:L:140:ILE:CB | 2.49 | 0.49 |
| 1:O:218:ASP:N | 1:O:221:VAL:HB | 2.27 | 0.49 |
| 1:B:321:LEU:CD1 | 1:B:441:THR:OG1 | 2.60 | 0.49 |
| 1:C:586:ILE:HG21 | 1:C:592:ALA:HB2 | 1.95 | 0.49 |
| 1:I:459:ILE:HD12 | 1:I:459:ILE:N | 2.27 | 0.49 |
| 1:K:177:ALA:O | 1:K:180:MET:N | 2.46 | 0.49 |
| 1:K:321:LEU:CD1 | 1:K:441:THR:OG1 | 2.60 | 0.49 |
| 1:M:177:ALA:O | 1:M:180:MET:N | 2.46 | 0.49 |
| 1:M:435:LEU:HD11 | 1:N:607:GLN:HE22 | 1.77 | 0.49 |
| 1:O:472:PHE:CD1 | 1:O:472:PHE:C | 2.86 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:477:ARG:HD2 | 1:O:477:ARG:N | 2.27 | 0.49 |
| 1:A:586:ILE:HG21 | 1:A:592:ALA:HB2 | 1.95 | 0.49 |
| 1:B:442:VAL:HG12 | 1:B:448:ALA:HB2 | 1.94 | 0.49 |
| 1:B:506:ASN:O | 1:B:519:ALA:N | 2.45 | 0.49 |
| 1:D:442:VAL:HG12 | 1:D:448:ALA:HB2 | 1.94 | 0.49 |
| 1:E:506:ASN:O | 1:E:519:ALA:N | 2.45 | 0.49 |
| 1:K:374:GLN:HG3 | 1:L:392:THR:O | 2.13 | 0.49 |
| 1:K:442:VAL:HG12 | 1:K:448:ALA:HB2 | 1.94 | 0.49 |
| 1:A:459:ILE:HD12 | 1:A:459:ILE:N | 2.27 | 0.49 |
| 1:G:205:VAL:HG12 | 1:G:206:ALA:N | 2.27 | 0.49 |
| 1:G:374:GLN:HG3 | 1:H:392:THR:O | 2.13 | 0.49 |
| 1:G:477:ARG:HD2 | 1:G:477:ARG:N | 2.27 | 0.49 |
| 1:H:374:GLN:HG3 | 1:I:392:THR:O | 2.13 | 0.49 |
| 1:H:477:ARG:CG | 1:H:477:ARG:NH1 | 2.73 | 0.49 |
| 1:I:177:ALA:O | 1:I:180:MET:N | 2.46 | 0.49 |
| 1:I:506:ASN:O | 1:I:519:ALA:N | 2.46 | 0.49 |
| 1:K:218:ASP:N | 1:K:221:VAL:HB | 2.27 | 0.49 |
| 1:L:374:GLN:HG3 | 1:M:392:THR:O | 2.13 | 0.49 |
| 1:L:477:ARG:HD2 | 1:L:477:ARG:N | 2.27 | 0.49 |
| 1:O:177:ALA:O | 1:O:180:MET:N | 2.46 | 0.49 |
| 1:A:552:VAL:HG23 | 1:A:553:PRO:C | 2.32 | 0.48 |
| 1:C:552:VAL:HG23 | 1:C:553:PRO:C | 2.32 | 0.48 |
| 1:E:472:PHE:C | 1:E:472:PHE:CD1 | 2.86 | 0.48 |
| 1:G:506:ASN:O | 1:G:519:ALA:N | 2.46 | 0.48 |
| 1:K:177:ALA:N | 1:K:211:ASN:OD1 | 2.41 | 0.48 |
| 1:K:459:ILE:CA | 1:K:474:THR:O | 2.55 | 0.48 |
| 1:K:506:ASN:O | 1:K:519:ALA:N | 2.46 | 0.48 |
| 1:L:177:ALA:O | 1:L:180:MET:N | 2.46 | 0.48 |
| 1:M:218:ASP:N | 1:M:221:VAL:HB | 2.27 | 0.48 |
| 1:M:374:GLN:HG3 | 1:N:392:THR:O | 2.13 | 0.48 |
| 1:N:374:GLN:HG3 | 1:O:392:THR:O | 2.13 | 0.48 |
| 1:N:374:GLN:O | 1:N:391:THR:HG22 | 2.13 | 0.48 |
| 1:B:472:PHE:C | 1:B:472:PHE:CD1 | 2.86 | 0.48 |
| 1:D:458:VAL:O | 1:D:475:VAL:C | 2.49 | 0.48 |
| 1:F:113:ARG:HD2 | 1:F:134:TYR:HD2 | 1.79 | 0.48 |
| 1:F:374:GLN:O | 1:F:391:THR:HG22 | 2.14 | 0.48 |
| 1:G:479:GLU:H | 1:G:479:GLU:CD | 2.07 | 0.48 |
| 1:H:458:VAL:O | 1:H:475:VAL:C | 2.49 | 0.48 |
| 1:I:442:VAL:HG12 | 1:I:448:ALA:HB2 | 1.94 | 0.48 |
| 1:L:506:ASN:O | 1:L:519:ALA:N | 2.45 | 0.48 |
| 1:M:113:ARG:HD2 | 1:M:134:TYR:HD2 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:177:ALA:O | 1:N:180:MET:N | 2.46 | 0.48 |
| 1:N:177:ALA:N | 1:N:211:ASN:OD1 | 2.41 | 0.48 |
| 1:B:207:ASP:OD1 | 1:B:209:ARG:N | 2.33 | 0.48 |
| 1:C:374:GLN:O | 1:C:391:THR:HG22 | 2.13 | 0.48 |
| 1:D:435:LEU:HD11 | 1:E:607:GLN:HE22 | 1.77 | 0.48 |
| 1:F:506:ASN:O | 1:F:519:ALA:N | 2.45 | 0.48 |
| 1:H:459:ILE:HD12 | 1:H:459:ILE:N | 2.27 | 0.48 |
| 1:J:374:GLN:HG3 | 1:K:392:THR:O | 2.13 | 0.48 |
| 1:M:472:PHE:C | 1:M:472:PHE:CD1 | 2.86 | 0.48 |
| 1:A:321:LEU:CD1 | 1:A:441:THR:OG1 | 2.60 | 0.48 |
| 1:C:113:ARG:HD2 | 1:C:134:TYR:HD2 | 1.79 | 0.48 |
| 1:D:586:ILE:HG21 | 1:D:592:ALA:HB2 | 1.95 | 0.48 |
| 1:G:113:ARG:HD2 | 1:G:134:TYR:HD2 | 1.79 | 0.48 |
| 1:H:113:ARG:HD2 | 1:H:134:TYR:HD2 | 1.79 | 0.48 |
| 1:I:458:VAL:O | 1:I:475:VAL:C | 2.49 | 0.48 |
| 1:J:177:ALA:O | 1:J:180:MET:N | 2.46 | 0.48 |
| 1:J:442:VAL:HG12 | 1:J:448:ALA:HB2 | 1.94 | 0.48 |
| 1:J:477:ARG:HD2 | 1:J:477:ARG:N | 2.27 | 0.48 |
| 1:L:113:ARG:HD2 | 1:L:134:TYR:HD2 | 1.79 | 0.48 |
| 1:M:506:ASN:O | 1:M:519:ALA:N | 2.46 | 0.48 |
| 1:N:477:ARG:N | 1:N:477:ARG:HD2 | 2.27 | 0.48 |
| 1:O:586:ILE:HG21 | 1:O:592:ALA:HB2 | 1.95 | 0.48 |
| 1:A:392:THR:O | 1:O:374:GLN:HG3 | 2.13 | 0.48 |
| 1:A:435:LEU:HD11 | 1:B:607:GLN:HE22 | 1.77 | 0.48 |
| 1:A:472:PHE:CD1 | 1:A:472:PHE:C | 2.86 | 0.48 |
| 1:D:519:ALA:CB | 1:E:454:GLU:HG3 | 2.41 | 0.48 |
| 1:H:177:ALA:O | 1:H:180:MET:N | 2.46 | 0.48 |
| 1:I:374:GLN:HG3 | 1:J:392:THR:O | 2.13 | 0.48 |
| 1:K:504:VAL:HG12 | 1:K:521:ARG:HG2 | 1.94 | 0.48 |
| 1:O:113:ARG:HD2 | 1:O:134:TYR:HD2 | 1.79 | 0.48 |
| 1:O:180:MET:HE2 | 1:O:213:ILE:HD11 | 1.94 | 0.48 |
| 1:O:374:GLN:O | 1:O:391:THR:HG22 | 2.14 | 0.48 |
| 1:B:374:GLN:O | 1:B:391:THR:HG22 | 2.14 | 0.48 |
| 1:C:435:LEU:HD11 | 1:D:607:GLN:HE22 | 1.77 | 0.48 |
| 1:E:374:GLN:O | 1:E:391:THR:HG22 | 2.13 | 0.48 |
| 1:E:477:ARG:N | 1:E:477:ARG:HD2 | 2.27 | 0.48 |
| 1:G:119:LEU:HD12 | 1:G:134:TYR:OH | 2.14 | 0.48 |
| 1:G:235:GLU:H | 1:G:235:GLU:CD | 2.11 | 0.48 |
| 1:G:477:ARG:CG | 1:G:477:ARG:NH1 | 2.73 | 0.48 |
| 1:H:119:LEU:HD12 | 1:H:134:TYR:OH | 2.14 | 0.48 |
| 1:H:506:ASN:O | 1:H:519:ALA:N | 2.45 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:374:GLN:O | 1:I:391:THR:HG22 | 2.14 | 0.48 |
| 1:K:374:GLN:O | 1:K:391:THR:HG22 | 2.14 | 0.48 |
| 1:M:458:VAL:O | 1:M:475:VAL:C | 2.49 | 0.48 |
| 1:M:477:ARG:CG | 1:M:477:ARG:NH1 | 2.73 | 0.48 |
| 1:A:113:ARG:HD2 | 1:A:134:TYR:HD2 | 1.79 | 0.48 |
| 1:A:177:ALA:O | 1:A:180:MET:N | 2.46 | 0.48 |
| 1:F:235:GLU:H | 1:F:235:GLU:CD | 2.11 | 0.48 |
| 1:F:479:GLU:H | 1:F:479:GLU:CD | 2.07 | 0.48 |
| 1:G:177:ALA:O | 1:G:180:MET:N | 2.46 | 0.48 |
| 1:H:374:GLN:O | 1:H:391:THR:HG22 | 2.13 | 0.48 |
| 1:J:113:ARG:HD2 | 1:J:134:TYR:HD2 | 1.79 | 0.48 |
| 1:J:506:ASN:O | 1:J:519:ALA:N | 2.46 | 0.48 |
| 1:K:113:ARG:HD2 | 1:K:134:TYR:HD2 | 1.79 | 0.48 |
| 1:L:374:GLN:O | 1:L:391:THR:HG22 | 2.14 | 0.48 |
| 1:A:225:LEU:HD23 | 1:A:225:LEU:HA | 1.74 | 0.48 |
| 1:A:247:LEU:HD11 | 1:A:294:LEU:HD23 | 1.96 | 0.48 |
| 1:B:177:ALA:O | 1:B:180:MET:N | 2.46 | 0.48 |
| 1:C:442:VAL:HG12 | 1:C:448:ALA:HB2 | 1.94 | 0.48 |
| 1:E:113:ARG:HD2 | 1:E:134:TYR:HD2 | 1.79 | 0.48 |
| 1:F:119:LEU:HD12 | 1:F:134:TYR:OH | 2.14 | 0.48 |
| 1:G:458:VAL:O | 1:G:475:VAL:C | 2.49 | 0.48 |
| 1:J:335:ILE:HG22 | 1:L:617:LEU:HD13 | 1.96 | 0.48 |
| 1:K:335:ILE:HG22 | 1:M:617:LEU:HD13 | 1.96 | 0.48 |
| 1:L:122:LEU:HD23 | 1:L:125:ASN:ND2 | 2.19 | 0.48 |
| 1:M:586:ILE:HG21 | 1:M:592:ALA:HB2 | 1.95 | 0.48 |
| 1:N:108:LYS:HA | 1:N:138:ASN:ND2 | 2.29 | 0.48 |
| 1:N:435:LEU:HD11 | 1:O:607:GLN:HE22 | 1.77 | 0.48 |
| 1:N:458:VAL:O | 1:N:475:VAL:C | 2.49 | 0.48 |
| 1:A:108:LYS:HA | 1:A:138:ASN:ND2 | 2.29 | 0.48 |
| 1:A:261:GLY:HA3 | 1:B:284:MET:HG2 | 1.96 | 0.48 |
| 1:A:374:GLN:HG3 | 1:B:392:THR:O | 2.13 | 0.48 |
| 1:B:435:LEU:HD11 | 1:C:607:GLN:HE22 | 1.77 | 0.48 |
| 1:B:459:ILE:HD12 | 1:B:459:ILE:N | 2.27 | 0.48 |
| 1:C:247:LEU:HD11 | 1:C:294:LEU:HD23 | 1.96 | 0.48 |
| 1:E:435:LEU:HD11 | 1:F:607:GLN:HE22 | 1.77 | 0.48 |
| 1:H:108:LYS:HA | 1:H:138:ASN:ND2 | 2.29 | 0.48 |
| 1:I:108:LYS:HA | 1:I:138:ASN:ND2 | 2.29 | 0.48 |
| 1:I:119:LEU:HD12 | 1:I:134:TYR:OH | 2.14 | 0.48 |
| 1:I:247:LEU:HD11 | 1:I:294:LEU:HD23 | 1.96 | 0.48 |
| 1:I:335:ILE:HG22 | 1:K:617:LEU:HD13 | 1.96 | 0.48 |
| 1:J:108:LYS:HA | 1:J:138:ASN:ND2 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:472:PHE:C | 1:J:472:PHE:CD1 | 2.86 | 0.48 |
| 1:K:247:LEU:HD11 | 1:K:294:LEU:HD23 | 1.96 | 0.48 |
| 1:L:586:ILE:HG21 | 1:L:592:ALA:HB2 | 1.95 | 0.48 |
| 1:M:180:MET:HE2 | 1:M:213:ILE:HD11 | 1.95 | 0.48 |
| 1:N:247:LEU:HD11 | 1:N:294:LEU:HD23 | 1.96 | 0.48 |
| 1:O:108:LYS:HA | 1:O:138:ASN:ND2 | 2.29 | 0.48 |
| 1:A:284:MET:HG2 | 1:O:261:GLY:HA3 | 1.96 | 0.48 |
| 1:B:108:LYS:HA | 1:B:138:ASN:ND2 | 2.29 | 0.48 |
| 1:B:226:LYS:HA | 1:B:229:ILE:HB | 1.96 | 0.48 |
| 1:B:374:GLN:HG3 | 1:C:392:THR:O | 2.13 | 0.48 |
| 1:D:113:ARG:HD2 | 1:D:134:TYR:HD2 | 1.78 | 0.48 |
| 1:D:374:GLN:HG3 | 1:E:392:THR:O | 2.13 | 0.48 |
| 1:E:255:LEU:HA | 1:E:255:LEU:HD23 | 1.73 | 0.48 |
| 1:F:283:VAL:HA | 1:F:297:THR:O | 2.14 | 0.48 |
| 1:F:435:LEU:HD11 | 1:G:607:GLN:HE22 | 1.77 | 0.48 |
| 1:G:108:LYS:HA | 1:G:138:ASN:ND2 | 2.29 | 0.48 |
| 1:G:261:GLY:HA3 | 1:H:284:MET:HG2 | 1.96 | 0.48 |
| 1:G:335:ILE:HG22 | 1:I:617:LEU:HD13 | 1.96 | 0.48 |
| 1:H:335:ILE:HG22 | 1:J:617:LEU:HD13 | 1.96 | 0.48 |
| 1:I:472:PHE:CD1 | 1:I:472:PHE:C | 2.86 | 0.48 |
| 1:J:478:LYS:HD2 | 1:J:518:PHE:HZ | 1.79 | 0.48 |
| 1:K:586:ILE:HG21 | 1:K:592:ALA:HB2 | 1.95 | 0.48 |
| 1:L:119:LEU:HD12 | 1:L:134:TYR:OH | 2.14 | 0.48 |
| 1:L:335:ILE:HG22 | 1:N:617:LEU:HD13 | 1.96 | 0.48 |
| 1:L:478:LYS:HD2 | 1:L:518:PHE:HZ | 1.79 | 0.48 |
| 1:N:235:GLU:H | 1:N:235:GLU:CD | 2.11 | 0.48 |
| 1:C:177:ALA:O | 1:C:180:MET:N | 2.46 | 0.47 |
| 1:C:374:GLN:HG3 | 1:D:392:THR:O | 2.13 | 0.47 |
| 1:D:226:LYS:HA | 1:D:229:ILE:HB | 1.96 | 0.47 |
| 1:D:472:PHE:CD1 | 1:D:472:PHE:C | 2.86 | 0.47 |
| 1:E:235:GLU:H | 1:E:235:GLU:CD | 2.11 | 0.47 |
| 1:E:374:GLN:HG3 | 1:F:392:THR:O | 2.13 | 0.47 |
| 1:G:283:VAL:HA | 1:G:297:THR:O | 2.14 | 0.47 |
| 1:H:261:GLY:HA3 | 1:I:284:MET:HG2 | 1.96 | 0.47 |
| 1:M:119:LEU:HD12 | 1:M:134:TYR:OH | 2.14 | 0.47 |
| 1:M:235:GLU:H | 1:M:235:GLU:CD | 2.11 | 0.47 |
| 1:M:374:GLN:O | 1:M:391:THR:HG22 | 2.13 | 0.47 |
| 1:O:328:GLU:HG2 | 1:O:577:LEU:HG | 1.96 | 0.47 |
| 1:O:458:VAL:O | 1:O:475:VAL:C | 2.49 | 0.47 |
| 1:A:607:GLN:HE22 | 1:O:435:LEU:HD11 | 1.77 | 0.47 |
| 1:B:261:GLY:HA3 | 1:C:284:MET:HG2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:335:ILE:HG22 | 1:E:617:LEU:HD13 | 1.95 | 0.47 |
| 1:C:477:ARG:N | 1:C:477:ARG:HD2 | 2.27 | 0.47 |
| 1:D:177:ALA:O | 1:D:180:MET:N | 2.46 | 0.47 |
| 1:E:283:VAL:HA | 1:E:297:THR:O | 2.14 | 0.47 |
| 1:F:122:LEU:HD23 | 1:F:125:ASN:ND2 | 2.19 | 0.47 |
| 1:F:261:GLY:HA3 | 1:G:284:MET:HG2 | 1.96 | 0.47 |
| 1:F:374:GLN:HG3 | 1:G:392:THR:O | 2.13 | 0.47 |
| 1:G:374:GLN:O | 1:G:391:THR:HG22 | 2.14 | 0.47 |
| 1:H:586:ILE:HG21 | 1:H:592:ALA:HB2 | 1.95 | 0.47 |
| 1:I:239:LYS:HE3 | 1:I:300:GLN:HB2 | 1.97 | 0.47 |
| 1:I:261:GLY:HA3 | 1:J:284:MET:HG2 | 1.96 | 0.47 |
| 1:I:586:ILE:HG21 | 1:I:592:ALA:HB2 | 1.95 | 0.47 |
| 1:J:177:ALA:N | 1:J:211:ASN:OD1 | 2.41 | 0.47 |
| 1:M:207:ASP:OD1 | 1:M:209:ARG:N | 2.33 | 0.47 |
| 1:M:457:PRO:HA | 1:M:477:ARG:HE | 1.79 | 0.47 |
| 1:N:113:ARG:HD2 | 1:N:134:TYR:HD2 | 1.79 | 0.47 |
| 1:N:283:VAL:HA | 1:N:297:THR:O | 2.14 | 0.47 |
| 1:N:457:PRO:HA | 1:N:477:ARG:HE | 1.80 | 0.47 |
| 1:A:328:GLU:HG2 | 1:A:577:LEU:HG | 1.96 | 0.47 |
| 1:A:477:ARG:N | 1:A:477:ARG:HD2 | 2.27 | 0.47 |
| 1:D:374:GLN:O | 1:D:391:THR:HG22 | 2.13 | 0.47 |
| 1:E:119:LEU:HD12 | 1:E:134:TYR:OH | 2.14 | 0.47 |
| 1:E:247:LEU:HD11 | 1:E:294:LEU:HD23 | 1.96 | 0.47 |
| 1:F:335:ILE:HG22 | 1:H:617:LEU:HD13 | 1.96 | 0.47 |
| 1:G:435:LEU:HD11 | 1:H:607:GLN:HE22 | 1.77 | 0.47 |
| 1:J:119:LEU:HD12 | 1:J:134:TYR:OH | 2.14 | 0.47 |
| 1:J:239:LYS:HE3 | 1:J:300:GLN:HB2 | 1.97 | 0.47 |
| 1:J:374:GLN:O | 1:J:391:THR:HG22 | 2.14 | 0.47 |
| 1:J:586:ILE:HG21 | 1:J:592:ALA:HB2 | 1.95 | 0.47 |
| 1:K:108:LYS:HA | 1:K:138:ASN:ND2 | 2.29 | 0.47 |
| 1:K:477:ARG:CG | 1:K:477:ARG:NH1 | 2.73 | 0.47 |
| 1:K:634:ARG:HG3 | 1:K:635:HIS:O | 2.15 | 0.47 |
| 1:M:167:ILE:CA | 1:M:215:ILE:O | 2.42 | 0.47 |
| 1:M:247:LEU:HD11 | 1:M:294:LEU:HD23 | 1.96 | 0.47 |
| 1:M:283:VAL:HA | 1:M:297:THR:O | 2.14 | 0.47 |
| 1:B:335:ILE:HG22 | 1:D:617:LEU:HD13 | 1.96 | 0.47 |
| 1:C:283:VAL:HA | 1:C:297:THR:O | 2.14 | 0.47 |
| 1:C:457:PRO:HA | 1:C:477:ARG:HE | 1.80 | 0.47 |
| 1:D:457:PRO:HA | 1:D:477:ARG:HE | 1.80 | 0.47 |
| 1:D:507:VAL:HG22 | 1:D:508:LEU:N | 2.29 | 0.47 |
| 1:E:177:ALA:O | 1:E:180:MET:N | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:586:ILE:HG21 | 1:E:592:ALA:HB2 | 1.95 | 0.47 |
| 1:F:108:LYS:HA | 1:F:138:ASN:ND2 | 2.29 | 0.47 |
| 1:F:226:LYS:HA | 1:F:229:ILE:HB | 1.96 | 0.47 |
| 1:F:239:LYS:HE3 | 1:F:300:GLN:HB2 | 1.97 | 0.47 |
| 1:F:457:PRO:HA | 1:F:477:ARG:HE | 1.80 | 0.47 |
| 1:F:507:VAL:HG22 | 1:F:508:LEU:N | 2.29 | 0.47 |
| 1:G:239:LYS:HE3 | 1:G:300:GLN:HB2 | 1.97 | 0.47 |
| 1:G:247:LEU:HD11 | 1:G:294:LEU:HD23 | 1.96 | 0.47 |
| 1:G:457:PRO:HA | 1:G:477:ARG:HE | 1.79 | 0.47 |
| 1:I:113:ARG:HD2 | 1:I:134:TYR:HD2 | 1.78 | 0.47 |
| 1:J:167:ILE:CA | 1:J:215:ILE:O | 2.42 | 0.47 |
| 1:L:108:LYS:HA | 1:L:138:ASN:ND2 | 2.29 | 0.47 |
| 1:L:457:PRO:HA | 1:L:477:ARG:HE | 1.80 | 0.47 |
| 1:N:261:GLY:HA3 | 1:O:284:MET:HG2 | 1.96 | 0.47 |
| 1:O:235:GLU:H | 1:O:235:GLU:CD | 2.11 | 0.47 |
| 1:A:120:ARG:HG2 | 1:A:123:ILE:HD12 | 1.96 | 0.47 |
| 1:A:122:LEU:HD23 | 1:A:125:ASN:ND2 | 2.19 | 0.47 |
| 1:A:226:LYS:HA | 1:A:229:ILE:HB | 1.96 | 0.47 |
| 1:A:457:PRO:HA | 1:A:477:ARG:HE | 1.79 | 0.47 |
| 1:B:119:LEU:HD12 | 1:B:134:TYR:OH | 2.14 | 0.47 |
| 1:C:108:LYS:HA | 1:C:138:ASN:ND2 | 2.29 | 0.47 |
| 1:D:235:GLU:H | 1:D:235:GLU:CD | 2.12 | 0.47 |
| 1:D:283:VAL:HA | 1:D:297:THR:O | 2.14 | 0.47 |
| 1:D:335:ILE:HG22 | 1:F:617:LEU:HD13 | 1.95 | 0.47 |
| 1:D:634:ARG:HG3 | 1:D:635:HIS:O | 2.15 | 0.47 |
| 1:F:177:ALA:N | 1:F:211:ASN:OD1 | 2.41 | 0.47 |
| 1:G:158:ARG:O | 1:G:162:ALA:HB2 | 2.15 | 0.47 |
| 1:G:586:ILE:HG21 | 1:G:592:ALA:HB2 | 1.95 | 0.47 |
| 1:H:283:VAL:HA | 1:H:297:THR:O | 2.14 | 0.47 |
| 1:I:328:GLU:HG2 | 1:I:577:LEU:HG | 1.96 | 0.47 |
| 1:J:261:GLY:HA3 | 1:K:284:MET:HG2 | 1.96 | 0.47 |
| 1:L:235:GLU:H | 1:L:235:GLU:CD | 2.11 | 0.47 |
| 1:L:239:LYS:HE3 | 1:L:300:GLN:HB2 | 1.97 | 0.47 |
| 1:L:472:PHE:CD1 | 1:L:472:PHE:C | 2.86 | 0.47 |
| 1:L:634:ARG:HG3 | 1:L:635:HIS:O | 2.15 | 0.47 |
| 1:M:239:LYS:HE3 | 1:M:300:GLN:HB2 | 1.97 | 0.47 |
| 1:M:335:ILE:HG22 | 1:O:617:LEU:HD13 | 1.96 | 0.47 |
| 1:N:119:LEU:HD12 | 1:N:134:TYR:OH | 2.14 | 0.47 |
| 1:N:158:ARG:O | 1:N:162:ALA:HB2 | 2.15 | 0.47 |
| 1:N:459:ILE:CA | 1:N:474:THR:O | 2.55 | 0.47 |
| 1:N:586:ILE:HG21 | 1:N:592:ALA:HB2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:283:VAL:HA | 1:O:297:THR:O | 2.14 | 0.47 |
| 1:O:457:PRO:HA | 1:O:477:ARG:HE | 1.80 | 0.47 |
| 1:A:235:GLU:H | 1:A:235:GLU:CD | 2.11 | 0.47 |
| 1:A:374:GLN:O | 1:A:391:THR:HG22 | 2.14 | 0.47 |
| 1:B:120:ARG:HG2 | 1:B:123:ILE:HD12 | 1.96 | 0.47 |
| 1:B:507:VAL:HG22 | 1:B:508:LEU:N | 2.29 | 0.47 |
| 1:C:226:LYS:HA | 1:C:229:ILE:HB | 1.96 | 0.47 |
| 1:C:235:GLU:H | 1:C:235:GLU:CD | 2.11 | 0.47 |
| 1:C:261:GLY:HA3 | 1:D:284:MET:HG2 | 1.96 | 0.47 |
| 1:E:479:GLU:H | 1:E:479:GLU:CD | 2.07 | 0.47 |
| 1:F:477:ARG:CG | 1:F:477:ARG:NH1 | 2.73 | 0.47 |
| 1:F:634:ARG:HG3 | 1:F:635:HIS:O | 2.15 | 0.47 |
| 1:H:158:ARG:O | 1:H:162:ALA:HB2 | 2.15 | 0.47 |
| 1:H:239:LYS:HE3 | 1:H:300:GLN:HB2 | 1.97 | 0.47 |
| 1:J:504:VAL:HG12 | 1:J:521:ARG:HG2 | 1.94 | 0.47 |
| 1:J:634:ARG:HG3 | 1:J:635:HIS:O | 2.15 | 0.47 |
| 1:K:119:LEU:HD12 | 1:K:134:TYR:OH | 2.14 | 0.47 |
| 1:K:239:LYS:HE3 | 1:K:300:GLN:HB2 | 1.97 | 0.47 |
| 1:L:247:LEU:HD11 | 1:L:294:LEU:HD23 | 1.96 | 0.47 |
| 1:N:226:LYS:HA | 1:N:229:ILE:HB | 1.96 | 0.47 |
| 1:N:328:GLU:HG2 | 1:N:577:LEU:HG | 1.96 | 0.47 |
| 1:O:158:ARG:O | 1:O:162:ALA:HB2 | 2.15 | 0.47 |
| 1:A:105:VAL:O | 1:A:140:ILE:CB | 2.49 | 0.47 |
| 1:A:119:LEU:HD12 | 1:A:134:TYR:OH | 2.14 | 0.47 |
| 1:A:335:ILE:HG22 | 1:C:617:LEU:HD13 | 1.96 | 0.47 |
| 1:A:617:LEU:HD13 | 1:N:335:ILE:HG22 | 1.95 | 0.47 |
| 1:B:105:VAL:O | 1:B:140:ILE:CB | 2.49 | 0.47 |
| 1:B:113:ARG:HD2 | 1:B:134:TYR:HD2 | 1.79 | 0.47 |
| 1:B:235:GLU:H | 1:B:235:GLU:CD | 2.11 | 0.47 |
| 1:B:283:VAL:HA | 1:B:297:THR:O | 2.14 | 0.47 |
| 1:B:478:LYS:HD2 | 1:B:518:PHE:HZ | 1.79 | 0.47 |
| 1:B:617:LEU:HD13 | 1:O:335:ILE:HG22 | 1.96 | 0.47 |
| 1:B:634:ARG:HG3 | 1:B:635:HIS:O | 2.15 | 0.47 |
| 1:C:119:LEU:HD12 | 1:C:134:TYR:OH | 2.14 | 0.47 |
| 1:D:478:LYS:HD2 | 1:D:518:PHE:HZ | 1.79 | 0.47 |
| 1:E:108:LYS:HA | 1:E:138:ASN:ND2 | 2.29 | 0.47 |
| 1:E:335:ILE:HG22 | 1:G:617:LEU:HD13 | 1.95 | 0.47 |
| 1:E:478:LYS:HD2 | 1:E:518:PHE:HZ | 1.79 | 0.47 |
| 1:F:177:ALA:O | 1:F:180:MET:N | 2.46 | 0.47 |
| 1:G:478:LYS:HD2 | 1:G:518:PHE:HZ | 1.79 | 0.47 |
| 1:I:283:VAL:HA | 1:I:297:THR:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:457:PRO:HA | 1:I:477:ARG:HE | 1.80 | 0.47 |
| 1:J:120:ARG:HG2 | 1:J:123:ILE:HD12 | 1.96 | 0.47 |
| 1:J:226:LYS:HA | 1:J:229:ILE:HB | 1.96 | 0.47 |
| 1:J:457:PRO:HA | 1:J:477:ARG:HE | 1.79 | 0.47 |
| 1:K:120:ARG:HG2 | 1:K:123:ILE:HD12 | 1.96 | 0.47 |
| 1:K:261:GLY:HA3 | 1:L:284:MET:HG2 | 1.96 | 0.47 |
| 1:K:457:PRO:HA | 1:K:477:ARG:HE | 1.80 | 0.47 |
| 1:L:207:ASP:OD1 | 1:L:209:ARG:N | 2.33 | 0.47 |
| 1:L:283:VAL:HA | 1:L:297:THR:O | 2.14 | 0.47 |
| 1:M:108:LYS:HA | 1:M:138:ASN:ND2 | 2.29 | 0.47 |
| 1:N:207:ASP:OD1 | 1:N:209:ARG:N | 2.33 | 0.47 |
| 1:O:120:ARG:HG2 | 1:O:123:ILE:HD12 | 1.96 | 0.47 |
| 1:O:167:ILE:CA | 1:O:215:ILE:O | 2.42 | 0.47 |
| 1:O:478:LYS:HD2 | 1:O:518:PHE:HZ | 1.79 | 0.47 |
| 1:A:634:ARG:HG3 | 1:A:635:HIS:O | 2.15 | 0.47 |
| 1:B:328:GLU:HG2 | 1:B:577:LEU:HG | 1.96 | 0.47 |
| 1:B:457:PRO:HA | 1:B:477:ARG:HE | 1.79 | 0.47 |
| 1:C:120:ARG:HG2 | 1:C:123:ILE:HD12 | 1.96 | 0.47 |
| 1:C:180:MET:HE2 | 1:C:213:ILE:HD11 | 1.97 | 0.47 |
| 1:D:180:MET:HE2 | 1:D:213:ILE:HD11 | 1.97 | 0.47 |
| 1:E:239:LYS:HE3 | 1:E:300:GLN:HB2 | 1.97 | 0.47 |
| 1:E:261:GLY:HA3 | 1:F:284:MET:HG2 | 1.96 | 0.47 |
| 1:F:586:ILE:HG21 | 1:F:592:ALA:HB2 | 1.95 | 0.47 |
| 1:H:328:GLU:HG2 | 1:H:577:LEU:HG | 1.96 | 0.47 |
| 1:H:472:PHE:C | 1:H:472:PHE:CD1 | 2.86 | 0.47 |
| 1:I:120:ARG:HG2 | 1:I:123:ILE:HD12 | 1.96 | 0.47 |
| 1:I:478:LYS:HD2 | 1:I:518:PHE:HZ | 1.79 | 0.47 |
| 1:K:328:GLU:HG2 | 1:K:577:LEU:HG | 1.96 | 0.47 |
| 1:M:158:ARG:O | 1:M:162:ALA:HB2 | 2.15 | 0.47 |
| 1:N:478:LYS:HD2 | 1:N:518:PHE:HZ | 1.79 | 0.47 |
| 1:A:478:LYS:HD2 | 1:A:518:PHE:HZ | 1.79 | 0.47 |
| 1:B:182:ARG:HA | 1:B:185:GLU:CD | 2.36 | 0.47 |
| 1:B:450:PHE:O | 1:B:483:LYS:HA | 2.15 | 0.47 |
| 1:B:504:VAL:HG12 | 1:B:521:ARG:HG2 | 1.94 | 0.47 |
| 1:C:158:ARG:O | 1:C:162:ALA:HB2 | 2.15 | 0.47 |
| 1:D:119:LEU:HD12 | 1:D:134:TYR:OH | 2.14 | 0.47 |
| 1:E:328:GLU:HG2 | 1:E:577:LEU:HG | 1.96 | 0.47 |
| 1:G:481:GLY:N | 1:G:505:SER:OG | 2.23 | 0.47 |
| 1:I:438:PRO:HB3 | 1:I:450:PHE:CE2 | 2.50 | 0.47 |
| 1:J:328:GLU:HG2 | 1:J:577:LEU:HG | 1.96 | 0.47 |
| 1:J:438:PRO:HB3 | 1:J:450:PHE:CE2 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:283:VAL:HA | 1:K:297:THR:O | 2.14 | 0.47 |
| 1:K:438:PRO:HB3 | 1:K:450:PHE:CE2 | 2.50 | 0.47 |
| 1:K:476:ASP:N | 1:K:476:ASP:OD1 | 2.48 | 0.47 |
| 1:L:158:ARG:O | 1:L:162:ALA:HB2 | 2.15 | 0.47 |
| 1:M:122:LEU:HD23 | 1:M:125:ASN:ND2 | 2.19 | 0.47 |
| 1:N:239:LYS:HE3 | 1:N:300:GLN:HB2 | 1.97 | 0.47 |
| 1:O:119:LEU:HD12 | 1:O:134:TYR:OH | 2.14 | 0.47 |
| 1:A:102:THR:OG1 | 1:A:142:ILE:O | 2.25 | 0.47 |
| 1:A:182:ARG:HA | 1:A:185:GLU:CD | 2.36 | 0.47 |
| 1:B:247:LEU:HD11 | 1:B:294:LEU:HD23 | 1.96 | 0.47 |
| 1:C:634:ARG:HG3 | 1:C:635:HIS:O | 2.15 | 0.47 |
| 1:D:108:LYS:HA | 1:D:138:ASN:ND2 | 2.29 | 0.47 |
| 1:D:158:ARG:O | 1:D:162:ALA:HB2 | 2.15 | 0.47 |
| 1:D:247:LEU:HD11 | 1:D:294:LEU:HD23 | 1.96 | 0.47 |
| 1:D:328:GLU:HG2 | 1:D:577:LEU:HG | 1.96 | 0.47 |
| 1:E:458:VAL:O | 1:E:475:VAL:C | 2.49 | 0.47 |
| 1:F:450:PHE:O | 1:F:483:LYS:HA | 2.15 | 0.47 |
| 1:G:328:GLU:HG2 | 1:G:577:LEU:HG | 1.96 | 0.47 |
| 1:H:207:ASP:O | 1:H:211:ASN:HA | 2.16 | 0.47 |
| 1:I:226:LYS:HA | 1:I:229:ILE:HB | 1.96 | 0.47 |
| 1:J:283:VAL:HA | 1:J:297:THR:O | 2.14 | 0.47 |
| 1:J:450:PHE:O | 1:J:483:LYS:HA | 2.15 | 0.47 |
| 1:K:158:ARG:O | 1:K:162:ALA:HB2 | 2.15 | 0.47 |
| 1:K:450:PHE:O | 1:K:483:LYS:HA | 2.15 | 0.47 |
| 1:L:261:GLY:HA3 | 1:M:284:MET:HG2 | 1.96 | 0.47 |
| 1:M:261:GLY:HA3 | 1:N:284:MET:HG2 | 1.96 | 0.47 |
| 1:M:506:ASN:O | 1:M:518:PHE:CB | 2.63 | 0.47 |
| 1:O:105:VAL:O | 1:O:140:ILE:CB | 2.49 | 0.47 |
| 1:O:226:LYS:HA | 1:O:229:ILE:HB | 1.96 | 0.47 |
| 1:O:247:LEU:HD11 | 1:O:294:LEU:HD23 | 1.96 | 0.47 |
| 1:O:450:PHE:O | 1:O:483:LYS:HA | 2.15 | 0.47 |
| 1:O:634:ARG:HG3 | 1:O:635:HIS:O | 2.15 | 0.47 |
| 1:A:458:VAL:O | 1:A:475:VAL:C | 2.49 | 0.46 |
| 1:C:182:ARG:HA | 1:C:185:GLU:CD | 2.36 | 0.46 |
| 1:D:177:ALA:N | 1:D:211:ASN:OD1 | 2.41 | 0.46 |
| 1:D:450:PHE:O | 1:D:483:LYS:HA | 2.15 | 0.46 |
| 1:D:476:ASP:N | 1:D:476:ASP:OD1 | 2.48 | 0.46 |
| 1:F:105:VAL:O | 1:F:140:ILE:CB | 2.49 | 0.46 |
| 1:F:158:ARG:O | 1:F:162:ALA:HB2 | 2.15 | 0.46 |
| 1:G:450:PHE:O | 1:G:483:LYS:HA | 2.15 | 0.46 |
| 1:H:120:ARG:HG2 | 1:H:123:ILE:HD12 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:438:PRO:HB3 | 1:H:450:PHE:CE2 | 2.50 | 0.46 |
| 1:I:158:ARG:O | 1:I:162:ALA:HB2 | 2.15 | 0.46 |
| 1:J:247:LEU:HD11 | 1:J:294:LEU:HD23 | 1.96 | 0.46 |
| 1:L:438:PRO:HB3 | 1:L:450:PHE:CE2 | 2.50 | 0.46 |
| 1:L:506:ASN:O | 1:L:518:PHE:CB | 2.63 | 0.46 |
| 1:N:102:THR:OG1 | 1:N:142:ILE:O | 2.25 | 0.46 |
| 1:A:283:VAL:HA | 1:A:297:THR:O | 2.14 | 0.46 |
| 1:C:239:LYS:HE3 | 1:C:300:GLN:HB2 | 1.97 | 0.46 |
| 1:D:239:LYS:HE3 | 1:D:300:GLN:HB2 | 1.97 | 0.46 |
| 1:F:458:VAL:O | 1:F:475:VAL:C | 2.49 | 0.46 |
| 1:G:207:ASP:O | 1:G:211:ASN:HA | 2.16 | 0.46 |
| 1:H:182:ARG:HA | 1:H:185:GLU:CD | 2.36 | 0.46 |
| 1:J:476:ASP:N | 1:J:476:ASP:OD1 | 2.48 | 0.46 |
| 1:L:120:ARG:HG2 | 1:L:123:ILE:HD12 | 1.96 | 0.46 |
| 1:L:328:GLU:HG2 | 1:L:577:LEU:HG | 1.96 | 0.46 |
| 1:L:477:ARG:CG | 1:L:477:ARG:NH1 | 2.73 | 0.46 |
| 1:M:634:ARG:HG3 | 1:M:635:HIS:O | 2.15 | 0.46 |
| 1:N:120:ARG:HG2 | 1:N:123:ILE:HD12 | 1.96 | 0.46 |
| 1:O:507:VAL:HG22 | 1:O:508:LEU:N | 2.29 | 0.46 |
| 1:A:158:ARG:O | 1:A:162:ALA:HB2 | 2.15 | 0.46 |
| 1:A:227:ARG:O | 1:A:231:GLN:HG3 | 2.16 | 0.46 |
| 1:A:239:LYS:HE3 | 1:A:300:GLN:HB2 | 1.97 | 0.46 |
| 1:D:120:ARG:HG2 | 1:D:123:ILE:HD12 | 1.96 | 0.46 |
| 1:D:261:GLY:HA3 | 1:E:284:MET:HG2 | 1.96 | 0.46 |
| 1:D:438:PRO:HB3 | 1:D:450:PHE:CE2 | 2.50 | 0.46 |
| 1:F:328:GLU:HG2 | 1:F:577:LEU:HG | 1.96 | 0.46 |
| 1:G:438:PRO:HB3 | 1:G:450:PHE:CE2 | 2.50 | 0.46 |
| 1:H:634:ARG:HG3 | 1:H:635:HIS:O | 2.15 | 0.46 |
| 1:I:207:ASP:O | 1:I:211:ASN:HA | 2.16 | 0.46 |
| 1:I:634:ARG:HG3 | 1:I:635:HIS:O | 2.15 | 0.46 |
| 1:J:158:ARG:O | 1:J:162:ALA:HB2 | 2.15 | 0.46 |
| 1:N:450:PHE:O | 1:N:483:LYS:HA | 2.15 | 0.46 |
| 1:O:239:LYS:HE3 | 1:O:300:GLN:HB2 | 1.97 | 0.46 |
| 1:B:180:MET:HE2 | 1:B:213:ILE:HD11 | 1.97 | 0.46 |
| 1:C:340:GLN:HE21 | 1:C:352:TYR:HB2 | 1.81 | 0.46 |
| 1:C:476:ASP:N | 1:C:476:ASP:OD1 | 2.48 | 0.46 |
| 1:D:340:GLN:HE21 | 1:D:352:TYR:HB2 | 1.81 | 0.46 |
| 1:E:227:ARG:O | 1:E:231:GLN:HG3 | 2.16 | 0.46 |
| 1:G:182:ARG:HA | 1:G:185:GLU:CD | 2.36 | 0.46 |
| 1:H:457:PRO:HA | 1:H:477:ARG:HE | 1.80 | 0.46 |
| 1:I:182:ARG:HA | 1:I:185:GLU:CD | 2.36 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:203:LYS:N | 1:I:216:SER:HG | 2.14 | 0.46 |
| 1:I:476:ASP:N | 1:I:476:ASP:OD1 | 2.48 | 0.46 |
| 1:K:225:LEU:HD23 | 1:K:225:LEU:HA | 1.74 | 0.46 |
| 1:M:328:GLU:HG2 | 1:M:577:LEU:HG | 1.96 | 0.46 |
| 1:M:438:PRO:HB3 | 1:M:450:PHE:CE2 | 2.50 | 0.46 |
| 1:N:203:LYS:N | 1:N:216:SER:HG | 2.14 | 0.46 |
| 1:O:182:ARG:HA | 1:O:185:GLU:CD | 2.36 | 0.46 |
| 1:A:506:ASN:O | 1:A:518:PHE:CB | 2.63 | 0.46 |
| 1:B:340:GLN:HE21 | 1:B:352:TYR:HB2 | 1.81 | 0.46 |
| 1:B:476:ASP:N | 1:B:476:ASP:OD1 | 2.48 | 0.46 |
| 1:B:506:ASN:O | 1:B:518:PHE:CB | 2.63 | 0.46 |
| 1:C:105:VAL:O | 1:C:140:ILE:CB | 2.49 | 0.46 |
| 1:C:438:PRO:HB3 | 1:C:450:PHE:CE2 | 2.50 | 0.46 |
| 1:C:504:VAL:HG12 | 1:C:521:ARG:HG2 | 1.94 | 0.46 |
| 1:D:207:ASP:O | 1:D:211:ASN:HA | 2.16 | 0.46 |
| 1:E:205:VAL:HG12 | 1:E:206:ALA:H | 1.81 | 0.46 |
| 1:E:340:GLN:HE21 | 1:E:352:TYR:HB2 | 1.81 | 0.46 |
| 1:E:457:PRO:HA | 1:E:477:ARG:HE | 1.79 | 0.46 |
| 1:E:476:ASP:N | 1:E:476:ASP:OD1 | 2.48 | 0.46 |
| 1:E:634:ARG:HG3 | 1:E:635:HIS:O | 2.15 | 0.46 |
| 1:F:227:ARG:O | 1:F:231:GLN:HG3 | 2.16 | 0.46 |
| 1:F:247:LEU:HD11 | 1:F:294:LEU:HD23 | 1.96 | 0.46 |
| 1:H:247:LEU:HD11 | 1:H:294:LEU:HD23 | 1.96 | 0.46 |
| 1:H:476:ASP:N | 1:H:476:ASP:OD1 | 2.48 | 0.46 |
| 1:H:478:LYS:HD2 | 1:H:518:PHE:HZ | 1.79 | 0.46 |
| 1:J:207:ASP:O | 1:J:211:ASN:HA | 2.16 | 0.46 |
| 1:J:340:GLN:HE21 | 1:J:352:TYR:HB2 | 1.81 | 0.46 |
| 1:K:226:LYS:HA | 1:K:229:ILE:HB | 1.96 | 0.46 |
| 1:K:501:GLU:HG2 | 1:K:524:ASN:HB2 | 1.98 | 0.46 |
| 1:L:203:LYS:N | 1:L:216:SER:HG | 2.14 | 0.46 |
| 1:L:501:GLU:HG2 | 1:L:524:ASN:HB2 | 1.98 | 0.46 |
| 1:L:507:VAL:HG22 | 1:L:508:LEU:N | 2.29 | 0.46 |
| 1:M:205:VAL:HG12 | 1:M:206:ALA:H | 1.81 | 0.46 |
| 1:O:177:ALA:N | 1:O:211:ASN:OD1 | 2.41 | 0.46 |
| 1:A:340:GLN:HE21 | 1:A:352:TYR:HB2 | 1.81 | 0.46 |
| 1:C:177:ALA:N | 1:C:211:ASN:OD1 | 2.41 | 0.46 |
| 1:C:328:GLU:HG2 | 1:C:577:LEU:HG | 1.96 | 0.46 |
| 1:D:140:ILE:HG21 | 1:D:156:ILE:HD13 | 1.98 | 0.46 |
| 1:D:203:LYS:N | 1:D:216:SER:HG | 2.14 | 0.46 |
| 1:D:255:LEU:HD23 | 1:D:255:LEU:HA | 1.73 | 0.46 |
| 1:E:140:ILE:HG21 | 1:E:156:ILE:HD13 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:226:LYS:HA | 1:E:229:ILE:HB | 1.96 | 0.46 |
| 1:F:207:ASP:O | 1:F:211:ASN:HA | 2.16 | 0.46 |
| 1:F:504:VAL:HG12 | 1:F:521:ARG:O | 2.16 | 0.46 |
| 1:G:227:ARG:O | 1:G:231:GLN:HG3 | 2.16 | 0.46 |
| 1:G:634:ARG:HG3 | 1:G:635:HIS:O | 2.15 | 0.46 |
| 1:H:227:ARG:O | 1:H:231:GLN:HG3 | 2.16 | 0.46 |
| 1:J:140:ILE:HG21 | 1:J:156:ILE:HD13 | 1.98 | 0.46 |
| 1:J:205:VAL:HG12 | 1:J:206:ALA:H | 1.81 | 0.46 |
| 1:J:501:GLU:HG2 | 1:J:524:ASN:HB2 | 1.98 | 0.46 |
| 1:K:203:LYS:N | 1:K:216:SER:HG | 2.14 | 0.46 |
| 1:K:235:GLU:H | 1:K:235:GLU:CD | 2.11 | 0.46 |
| 1:K:340:GLN:HE21 | 1:K:352:TYR:HB2 | 1.81 | 0.46 |
| 1:K:478:LYS:HD2 | 1:K:518:PHE:HZ | 1.79 | 0.46 |
| 1:L:182:ARG:HA | 1:L:185:GLU:CD | 2.36 | 0.46 |
| 1:L:476:ASP:N | 1:L:476:ASP:OD1 | 2.48 | 0.46 |
| 1:M:226:LYS:HA | 1:M:229:ILE:HB | 1.96 | 0.46 |
| 1:M:450:PHE:O | 1:M:483:LYS:HA | 2.15 | 0.46 |
| 1:N:438:PRO:HB3 | 1:N:450:PHE:CE2 | 2.50 | 0.46 |
| 1:N:506:ASN:O | 1:N:518:PHE:CB | 2.63 | 0.46 |
| 1:N:634:ARG:HG3 | 1:N:635:HIS:O | 2.15 | 0.46 |
| 1:B:227:ARG:O | 1:B:231:GLN:HG3 | 2.16 | 0.46 |
| 1:C:140:ILE:HG21 | 1:C:156:ILE:HD13 | 1.98 | 0.46 |
| 1:D:182:ARG:HA | 1:D:185:GLU:CD | 2.36 | 0.46 |
| 1:E:182:ARG:HA | 1:E:185:GLU:CD | 2.36 | 0.46 |
| 1:E:450:PHE:O | 1:E:483:LYS:HA | 2.15 | 0.46 |
| 1:F:182:ARG:HA | 1:F:185:GLU:CD | 2.36 | 0.46 |
| 1:F:438:PRO:HB3 | 1:F:450:PHE:CE2 | 2.50 | 0.46 |
| 1:G:476:ASP:N | 1:G:476:ASP:OD1 | 2.48 | 0.46 |
| 1:I:122:LEU:HD23 | 1:I:125:ASN:ND2 | 2.19 | 0.46 |
| 1:J:182:ARG:HA | 1:J:185:GLU:CD | 2.36 | 0.46 |
| 1:J:339:VAL:HG22 | 1:J:423:ILE:HG12 | 1.98 | 0.46 |
| 1:J:507:VAL:HG22 | 1:J:508:LEU:N | 2.30 | 0.46 |
| 1:K:506:ASN:O | 1:K:518:PHE:CB | 2.63 | 0.46 |
| 1:L:226:LYS:HA | 1:L:229:ILE:HB | 1.96 | 0.46 |
| 1:L:504:VAL:HG12 | 1:L:521:ARG:O | 2.16 | 0.46 |
| 1:M:120:ARG:HG2 | 1:M:123:ILE:HD12 | 1.96 | 0.46 |
| 1:M:203:LYS:N | 1:M:216:SER:HG | 2.14 | 0.46 |
| 1:M:501:GLU:HG2 | 1:M:524:ASN:HB2 | 1.98 | 0.46 |
| 1:N:322:ILE:HG23 | 1:N:581:ILE:HD11 | 1.98 | 0.46 |
| 1:N:472:PHE:CD1 | 1:N:472:PHE:C | 2.86 | 0.46 |
| 1:N:476:ASP:N | 1:N:476:ASP:OD1 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:450:PHE:O | 1:A:483:LYS:HA | 2.15 | 0.46 |
| 1:A:476:ASP:N | 1:A:476:ASP:OD1 | 2.48 | 0.46 |
| 1:A:504:VAL:HG12 | 1:A:521:ARG:O | 2.16 | 0.46 |
| 1:B:158:ARG:O | 1:B:162:ALA:HB2 | 2.15 | 0.46 |
| 1:D:227:ARG:O | 1:D:231:GLN:HG3 | 2.16 | 0.46 |
| 1:E:120:ARG:HG2 | 1:E:123:ILE:HD12 | 1.96 | 0.46 |
| 1:E:207:ASP:O | 1:E:211:ASN:HA | 2.16 | 0.46 |
| 1:F:140:ILE:HG21 | 1:F:156:ILE:HD13 | 1.98 | 0.46 |
| 1:F:171:GLU:HA | 1:F:212:SER:OG | 2.16 | 0.46 |
| 1:F:203:LYS:N | 1:F:216:SER:HG | 2.14 | 0.46 |
| 1:G:339:VAL:HG22 | 1:G:423:ILE:HG12 | 1.98 | 0.46 |
| 1:H:205:VAL:HG12 | 1:H:206:ALA:H | 1.81 | 0.46 |
| 1:H:450:PHE:O | 1:H:483:LYS:HA | 2.15 | 0.46 |
| 1:H:501:GLU:HG2 | 1:H:524:ASN:HB2 | 1.98 | 0.46 |
| 1:H:504:VAL:HG12 | 1:H:521:ARG:O | 2.16 | 0.46 |
| 1:I:140:ILE:HG21 | 1:I:156:ILE:HD13 | 1.98 | 0.46 |
| 1:I:450:PHE:O | 1:I:483:LYS:HA | 2.15 | 0.46 |
| 1:I:501:GLU:HG2 | 1:I:524:ASN:HB2 | 1.98 | 0.46 |
| 1:J:504:VAL:HG12 | 1:J:521:ARG:O | 2.16 | 0.46 |
| 1:L:339:VAL:HG22 | 1:L:423:ILE:HG12 | 1.98 | 0.46 |
| 1:M:227:ARG:O | 1:M:231:GLN:HG3 | 2.16 | 0.46 |
| 1:M:476:ASP:N | 1:M:476:ASP:OD1 | 2.48 | 0.46 |
| 1:N:182:ARG:HA | 1:N:185:GLU:CD | 2.36 | 0.46 |
| 1:N:504:VAL:HG12 | 1:N:521:ARG:O | 2.16 | 0.46 |
| 1:O:205:VAL:HG12 | 1:O:206:ALA:H | 1.81 | 0.46 |
| 1:O:215:ILE:HD12 | 1:O:215:ILE:HA | 1.82 | 0.46 |
| 1:O:340:GLN:HE21 | 1:O:352:TYR:HB2 | 1.81 | 0.46 |
| 1:A:322:ILE:HG23 | 1:A:581:ILE:HD11 | 1.98 | 0.46 |
| 1:B:239:LYS:HE3 | 1:B:300:GLN:HB2 | 1.97 | 0.46 |
| 1:D:157:ARG:HA | 1:D:160:ASP:HB3 | 1.98 | 0.46 |
| 1:D:171:GLU:HA | 1:D:212:SER:OG | 2.16 | 0.46 |
| 1:D:479:GLU:H | 1:D:479:GLU:CD | 2.07 | 0.46 |
| 1:E:158:ARG:O | 1:E:162:ALA:HB2 | 2.15 | 0.46 |
| 1:E:171:GLU:HA | 1:E:212:SER:OG | 2.16 | 0.46 |
| 1:E:322:ILE:HG23 | 1:E:581:ILE:HD11 | 1.98 | 0.46 |
| 1:E:504:VAL:HG12 | 1:E:521:ARG:HG2 | 1.94 | 0.46 |
| 1:F:340:GLN:HE21 | 1:F:352:TYR:HB2 | 1.81 | 0.46 |
| 1:F:476:ASP:N | 1:F:476:ASP:OD1 | 2.48 | 0.46 |
| 1:G:140:ILE:HG21 | 1:G:156:ILE:HD13 | 1.98 | 0.46 |
| 1:G:203:LYS:N | 1:G:216:SER:HG | 2.14 | 0.46 |
| 1:G:226:LYS:HA | 1:G:229:ILE:HB | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:501:GLU:HG2 | 1:G:524:ASN:HB2 | 1.98 | 0.46 |
| 1:H:339:VAL:HG22 | 1:H:423:ILE:HG12 | 1.98 | 0.46 |
| 1:I:227:ARG:O | 1:I:231:GLN:HG3 | 2.16 | 0.46 |
| 1:I:339:VAL:HG22 | 1:I:423:ILE:HG12 | 1.98 | 0.46 |
| 1:I:340:GLN:HE21 | 1:I:352:TYR:HB2 | 1.81 | 0.46 |
| 1:K:205:VAL:HG12 | 1:K:206:ALA:H | 1.81 | 0.46 |
| 1:L:450:PHE:O | 1:L:483:LYS:HA | 2.15 | 0.46 |
| 1:M:322:ILE:HG23 | 1:M:581:ILE:HD11 | 1.98 | 0.46 |
| 1:O:227:ARG:O | 1:O:231:GLN:HG3 | 2.16 | 0.46 |
| 1:O:322:ILE:HG23 | 1:O:581:ILE:HD11 | 1.98 | 0.46 |
| 1:B:157:ARG:HA | 1:B:160:ASP:HB3 | 1.99 | 0.46 |
| 1:B:322:ILE:HG23 | 1:B:581:ILE:HD11 | 1.98 | 0.46 |
| 1:C:450:PHE:O | 1:C:483:LYS:HA | 2.15 | 0.46 |
| 1:C:478:LYS:HD2 | 1:C:518:PHE:HZ | 1.79 | 0.46 |
| 1:C:506:ASN:O | 1:C:518:PHE:CB | 2.63 | 0.46 |
| 1:D:504:VAL:HG12 | 1:D:521:ARG:O | 2.16 | 0.46 |
| 1:E:438:PRO:HB3 | 1:E:450:PHE:CE2 | 2.50 | 0.46 |
| 1:F:120:ARG:HG2 | 1:F:123:ILE:HD12 | 1.96 | 0.46 |
| 1:G:171:GLU:HA | 1:G:212:SER:OG | 2.16 | 0.46 |
| 1:H:140:ILE:HG21 | 1:H:156:ILE:HD13 | 1.98 | 0.46 |
| 1:I:177:ALA:N | 1:I:211:ASN:OD1 | 2.41 | 0.46 |
| 1:I:504:VAL:HG12 | 1:I:521:ARG:HG2 | 1.94 | 0.46 |
| 1:L:205:VAL:HG12 | 1:L:206:ALA:H | 1.81 | 0.46 |
| 1:L:340:GLN:HE21 | 1:L:352:TYR:HB2 | 1.81 | 0.46 |
| 1:M:182:ARG:HA | 1:M:185:GLU:CD | 2.36 | 0.46 |
| 1:M:339:VAL:HG22 | 1:M:423:ILE:HG12 | 1.98 | 0.46 |
| 1:M:478:LYS:HD2 | 1:M:518:PHE:HZ | 1.79 | 0.46 |
| 1:O:476:ASP:N | 1:O:476:ASP:OD1 | 2.48 | 0.46 |
| 1:A:140:ILE:HG21 | 1:A:156:ILE:HD13 | 1.98 | 0.45 |
| 1:A:504:VAL:HG12 | 1:A:521:ARG:HG2 | 1.94 | 0.45 |
| 1:B:140:ILE:HG21 | 1:B:156:ILE:HD13 | 1.98 | 0.45 |
| 1:B:167:ILE:CA | 1:B:215:ILE:O | 2.42 | 0.45 |
| 1:B:203:LYS:N | 1:B:216:SER:HG | 2.14 | 0.45 |
| 1:B:205:VAL:HG12 | 1:B:206:ALA:H | 1.81 | 0.45 |
| 1:C:171:GLU:HA | 1:C:212:SER:OG | 2.16 | 0.45 |
| 1:F:322:ILE:HG23 | 1:F:581:ILE:HD11 | 1.98 | 0.45 |
| 1:G:120:ARG:HG2 | 1:G:123:ILE:HD12 | 1.96 | 0.45 |
| 1:H:171:GLU:HA | 1:H:212:SER:OG | 2.16 | 0.45 |
| 1:H:226:LYS:HA | 1:H:229:ILE:HB | 1.96 | 0.45 |
| 1:I:171:GLU:HA | 1:I:212:SER:OG | 2.16 | 0.45 |
| 1:I:506:ASN:O | 1:I:518:PHE:CB | 2.63 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:203:LYS:N | 1:J:216:SER:HG | 2.14 | 0.45 |
| 1:J:227:ARG:O | 1:J:231:GLN:HG3 | 2.16 | 0.45 |
| 1:K:140:ILE:HG21 | 1:K:156:ILE:HD13 | 1.98 | 0.45 |
| 1:K:207:ASP:O | 1:K:211:ASN:HA | 2.16 | 0.45 |
| 1:K:339:VAL:HG22 | 1:K:423:ILE:HG12 | 1.98 | 0.45 |
| 1:L:227:ARG:O | 1:L:231:GLN:HG3 | 2.16 | 0.45 |
| 1:N:105:VAL:O | 1:N:140:ILE:CB | 2.49 | 0.45 |
| 1:O:157:ARG:HA | 1:O:160:ASP:HB3 | 1.98 | 0.45 |
| 1:O:203:LYS:N | 1:O:216:SER:HG | 2.14 | 0.45 |
| 1:O:438:PRO:HB3 | 1:O:450:PHE:CE2 | 2.50 | 0.45 |
| 1:O:506:ASN:O | 1:O:518:PHE:CB | 2.63 | 0.45 |
| 1:A:177:ALA:N | 1:A:211:ASN:OD1 | 2.41 | 0.45 |
| 1:A:180:MET:HE2 | 1:A:213:ILE:HD11 | 1.97 | 0.45 |
| 1:A:207:ASP:O | 1:A:211:ASN:HA | 2.16 | 0.45 |
| 1:B:225:LEU:HD23 | 1:B:225:LEU:HA | 1.74 | 0.45 |
| 1:B:504:VAL:HG12 | 1:B:521:ARG:O | 2.16 | 0.45 |
| 1:C:227:ARG:O | 1:C:231:GLN:HG3 | 2.16 | 0.45 |
| 1:C:322:ILE:HG23 | 1:C:581:ILE:HD11 | 1.98 | 0.45 |
| 1:C:522:GLN:H | 1:D:451:ILE:HG23 | 1.82 | 0.45 |
| 1:D:322:ILE:HG23 | 1:D:581:ILE:HD11 | 1.98 | 0.45 |
| 1:F:339:VAL:HG22 | 1:F:423:ILE:HG12 | 1.98 | 0.45 |
| 1:H:340:GLN:HE21 | 1:H:352:TYR:HB2 | 1.81 | 0.45 |
| 1:H:506:ASN:O | 1:H:518:PHE:CB | 2.63 | 0.45 |
| 1:K:227:ARG:O | 1:K:231:GLN:HG3 | 2.16 | 0.45 |
| 1:K:472:PHE:CD1 | 1:K:472:PHE:C | 2.86 | 0.45 |
| 1:L:207:ASP:O | 1:L:211:ASN:HA | 2.16 | 0.45 |
| 1:N:501:GLU:HG2 | 1:N:524:ASN:HB2 | 1.98 | 0.45 |
| 1:O:140:ILE:HG21 | 1:O:156:ILE:HD13 | 1.98 | 0.45 |
| 1:O:207:ASP:O | 1:O:211:ASN:HA | 2.16 | 0.45 |
| 1:A:203:LYS:N | 1:A:216:SER:HG | 2.14 | 0.45 |
| 1:A:218:ASP:O | 1:A:222:ARG:N | 2.50 | 0.45 |
| 1:A:451:ILE:HG23 | 1:O:522:GLN:H | 1.82 | 0.45 |
| 1:B:207:ASP:O | 1:B:211:ASN:HA | 2.16 | 0.45 |
| 1:B:218:ASP:O | 1:B:222:ARG:N | 2.50 | 0.45 |
| 1:C:491:ASN:ND2 | 1:D:249:TYR:OH | 2.50 | 0.45 |
| 1:D:122:LEU:HD23 | 1:D:125:ASN:ND2 | 2.19 | 0.45 |
| 1:D:504:VAL:HG12 | 1:D:521:ARG:HG2 | 1.94 | 0.45 |
| 1:E:477:ARG:CG | 1:E:477:ARG:NH1 | 2.73 | 0.45 |
| 1:G:322:ILE:HG23 | 1:G:581:ILE:HD11 | 1.98 | 0.45 |
| 1:H:203:LYS:N | 1:H:216:SER:HG | 2.14 | 0.45 |
| 1:I:218:ASP:O | 1:I:222:ARG:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:504:VAL:HG12 | 1:K:521:ARG:O | 2.16 | 0.45 |
| 1:L:218:ASP:O | 1:L:222:ARG:N | 2.50 | 0.45 |
| 1:L:322:ILE:HG23 | 1:L:581:ILE:HD11 | 1.98 | 0.45 |
| 1:M:218:ASP:O | 1:M:222:ARG:N | 2.50 | 0.45 |
| 1:M:340:GLN:HE21 | 1:M:352:TYR:HB2 | 1.81 | 0.45 |
| 1:M:507:VAL:HG22 | 1:M:508:LEU:N | 2.29 | 0.45 |
| 1:N:207:ASP:O | 1:N:211:ASN:HA | 2.16 | 0.45 |
| 1:N:227:ARG:O | 1:N:231:GLN:HG3 | 2.16 | 0.45 |
| 1:N:340:GLN:HE21 | 1:N:352:TYR:HB2 | 1.81 | 0.45 |
| 1:B:171:GLU:HA | 1:B:212:SER:OG | 2.16 | 0.45 |
| 1:B:438:PRO:HB3 | 1:B:450:PHE:CE2 | 2.50 | 0.45 |
| 1:C:504:VAL:HG12 | 1:C:521:ARG:O | 2.16 | 0.45 |
| 1:D:205:VAL:HG12 | 1:D:206:ALA:H | 1.81 | 0.45 |
| 1:D:219:PRO:HA | 1:D:222:ARG:CB | 2.45 | 0.45 |
| 1:E:339:VAL:HG22 | 1:E:423:ILE:HG12 | 1.98 | 0.45 |
| 1:F:157:ARG:HA | 1:F:160:ASP:HB3 | 1.98 | 0.45 |
| 1:F:501:GLU:HG2 | 1:F:524:ASN:HB2 | 1.98 | 0.45 |
| 1:H:218:ASP:O | 1:H:222:ARG:N | 2.50 | 0.45 |
| 1:I:491:ASN:ND2 | 1:J:249:TYR:OH | 2.50 | 0.45 |
| 1:K:182:ARG:HA | 1:K:185:GLU:CD | 2.36 | 0.45 |
| 1:L:140:ILE:HG21 | 1:L:156:ILE:HD13 | 1.98 | 0.45 |
| 1:M:140:ILE:HG21 | 1:M:156:ILE:HD13 | 1.98 | 0.45 |
| 1:M:207:ASP:O | 1:M:211:ASN:HA | 2.16 | 0.45 |
| 1:O:504:VAL:HG12 | 1:O:521:ARG:O | 2.16 | 0.45 |
| 1:A:438:PRO:HB3 | 1:A:450:PHE:CE2 | 2.50 | 0.45 |
| 1:A:504:VAL:HG11 | 1:A:521:ARG:CG | 2.47 | 0.45 |
| 1:B:177:ALA:N | 1:B:211:ASN:OD1 | 2.41 | 0.45 |
| 1:F:478:LYS:HD2 | 1:F:518:PHE:HZ | 1.79 | 0.45 |
| 1:G:220:LYS:O | 1:G:224:ARG:HG2 | 2.17 | 0.45 |
| 1:G:340:GLN:HE21 | 1:G:352:TYR:HB2 | 1.81 | 0.45 |
| 1:H:322:ILE:HG23 | 1:H:581:ILE:HD11 | 1.98 | 0.45 |
| 1:J:491:ASN:ND2 | 1:K:249:TYR:OH | 2.50 | 0.45 |
| 1:J:506:ASN:O | 1:J:518:PHE:CB | 2.63 | 0.45 |
| 1:L:522:GLN:H | 1:M:451:ILE:HG23 | 1.82 | 0.45 |
| 1:A:220:LYS:O | 1:A:224:ARG:HG2 | 2.17 | 0.45 |
| 1:A:522:GLN:H | 1:B:451:ILE:HG23 | 1.82 | 0.45 |
| 1:B:491:ASN:ND2 | 1:C:249:TYR:OH | 2.50 | 0.45 |
| 1:B:504:VAL:HG11 | 1:B:521:ARG:CG | 2.47 | 0.45 |
| 1:C:167:ILE:CA | 1:C:215:ILE:O | 2.42 | 0.45 |
| 1:C:504:VAL:HG11 | 1:C:521:ARG:CG | 2.47 | 0.45 |
| 1:D:220:LYS:O | 1:D:224:ARG:HG2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:339:VAL:HG22 | 1:D:423:ILE:HG12 | 1.98 | 0.45 |
| 1:D:491:ASN:ND2 | 1:E:249:TYR:OH | 2.50 | 0.45 |
| 1:E:504:VAL:HG12 | 1:E:521:ARG:O | 2.16 | 0.45 |
| 1:F:220:LYS:O | 1:F:224:ARG:HG2 | 2.17 | 0.45 |
| 1:G:157:ARG:HA | 1:G:160:ASP:HB3 | 1.98 | 0.45 |
| 1:G:472:PHE:CD1 | 1:G:472:PHE:C | 2.86 | 0.45 |
| 1:G:506:ASN:O | 1:G:518:PHE:CB | 2.63 | 0.45 |
| 1:I:504:VAL:HG12 | 1:I:521:ARG:O | 2.16 | 0.45 |
| 1:J:171:GLU:HA | 1:J:212:SER:OG | 2.16 | 0.45 |
| 1:K:322:ILE:HG23 | 1:K:581:ILE:HD11 | 1.98 | 0.45 |
| 1:M:504:VAL:HG12 | 1:M:521:ARG:O | 2.16 | 0.45 |
| 1:M:522:GLN:H | 1:N:451:ILE:HG23 | 1.82 | 0.45 |
| 1:N:339:VAL:HG22 | 1:N:423:ILE:HG12 | 1.98 | 0.45 |
| 1:N:507:VAL:HG22 | 1:N:508:LEU:N | 2.29 | 0.45 |
| 1:O:504:VAL:HG11 | 1:O:521:ARG:CG | 2.47 | 0.45 |
| 1:A:347:GLY:H | 1:B:366:LEU:HD21 | 1.82 | 0.45 |
| 1:A:456:VAL:CG2 | 1:A:457:PRO:N | 2.80 | 0.45 |
| 1:C:218:ASP:O | 1:C:222:ARG:N | 2.50 | 0.45 |
| 1:C:347:GLY:H | 1:D:366:LEU:HD21 | 1.82 | 0.45 |
| 1:D:522:GLN:H | 1:E:451:ILE:HG23 | 1.82 | 0.45 |
| 1:E:609:PHE:CB | 1:F:639:ILE:HD12 | 2.47 | 0.45 |
| 1:F:180:MET:HE2 | 1:F:213:ILE:HD11 | 1.98 | 0.45 |
| 1:F:205:VAL:HG12 | 1:F:206:ALA:H | 1.81 | 0.45 |
| 1:F:347:GLY:H | 1:G:366:LEU:HD21 | 1.82 | 0.45 |
| 1:G:504:VAL:HG12 | 1:G:521:ARG:O | 2.16 | 0.45 |
| 1:H:220:LYS:O | 1:H:224:ARG:HG2 | 2.17 | 0.45 |
| 1:H:347:GLY:H | 1:I:366:LEU:HD21 | 1.82 | 0.45 |
| 1:H:456:VAL:CG2 | 1:H:457:PRO:N | 2.80 | 0.45 |
| 1:H:507:VAL:HG22 | 1:H:508:LEU:N | 2.29 | 0.45 |
| 1:I:347:GLY:H | 1:J:366:LEU:HD21 | 1.82 | 0.45 |
| 1:L:102:THR:OG1 | 1:L:142:ILE:O | 2.25 | 0.45 |
| 1:N:609:PHE:CB | 1:O:639:ILE:HD12 | 2.47 | 0.45 |
| 1:O:481:GLY:O | 1:O:505:SER:HB3 | 2.17 | 0.45 |
| 1:A:205:VAL:HG12 | 1:A:206:ALA:H | 1.81 | 0.45 |
| 1:A:366:LEU:HD21 | 1:O:347:GLY:H | 1.82 | 0.45 |
| 1:B:458:VAL:O | 1:B:475:VAL:C | 2.49 | 0.45 |
| 1:C:203:LYS:N | 1:C:216:SER:HG | 2.14 | 0.45 |
| 1:C:205:VAL:HG12 | 1:C:206:ALA:H | 1.81 | 0.45 |
| 1:C:207:ASP:O | 1:C:211:ASN:HA | 2.16 | 0.45 |
| 1:D:105:VAL:O | 1:D:140:ILE:CB | 2.49 | 0.45 |
| 1:E:220:LYS:O | 1:E:224:ARG:HG2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:218:ASP:O | 1:G:222:ARG:N | 2.50 | 0.45 |
| 1:H:255:LEU:HA | 1:H:255:LEU:HD23 | 1.73 | 0.45 |
| 1:I:220:LYS:O | 1:I:224:ARG:HG2 | 2.17 | 0.45 |
| 1:I:255:LEU:HD23 | 1:I:255:LEU:HA | 1.73 | 0.45 |
| 1:I:322:ILE:HG23 | 1:I:581:ILE:HD11 | 1.98 | 0.45 |
| 1:J:218:ASP:O | 1:J:222:ARG:N | 2.50 | 0.45 |
| 1:J:322:ILE:HG23 | 1:J:581:ILE:HD11 | 1.98 | 0.45 |
| 1:L:220:LYS:O | 1:L:224:ARG:HG2 | 2.17 | 0.45 |
| 1:M:220:LYS:O | 1:M:224:ARG:HG2 | 2.17 | 0.45 |
| 1:N:140:ILE:HG21 | 1:N:156:ILE:HD13 | 1.98 | 0.45 |
| 1:B:347:GLY:H | 1:C:366:LEU:HD21 | 1.82 | 0.45 |
| 1:B:609:PHE:CB | 1:C:639:ILE:HD12 | 2.47 | 0.45 |
| 1:C:219:PRO:HA | 1:C:222:ARG:CB | 2.45 | 0.45 |
| 1:C:339:VAL:HG22 | 1:C:423:ILE:HG12 | 1.98 | 0.45 |
| 1:D:501:GLU:HG2 | 1:D:524:ASN:HB2 | 1.98 | 0.45 |
| 1:E:157:ARG:HA | 1:E:160:ASP:HB3 | 1.98 | 0.45 |
| 1:E:456:VAL:CG2 | 1:E:457:PRO:N | 2.80 | 0.45 |
| 1:E:501:GLU:HG2 | 1:E:524:ASN:HB2 | 1.98 | 0.45 |
| 1:F:491:ASN:ND2 | 1:G:249:TYR:OH | 2.50 | 0.45 |
| 1:F:522:GLN:H | 1:G:451:ILE:HG23 | 1.82 | 0.45 |
| 1:G:491:ASN:ND2 | 1:H:249:TYR:OH | 2.50 | 0.45 |
| 1:G:507:VAL:HG22 | 1:G:508:LEU:N | 2.29 | 0.45 |
| 1:J:220:LYS:O | 1:J:224:ARG:HG2 | 2.17 | 0.45 |
| 1:J:255:LEU:HD23 | 1:J:255:LEU:HA | 1.73 | 0.45 |
| 1:K:220:LYS:O | 1:K:224:ARG:HG2 | 2.17 | 0.45 |
| 1:L:157:ARG:HA | 1:L:160:ASP:HB3 | 1.98 | 0.45 |
| 1:M:491:ASN:ND2 | 1:N:249:TYR:OH | 2.50 | 0.45 |
| 1:N:218:ASP:O | 1:N:222:ARG:N | 2.50 | 0.45 |
| 1:N:220:LYS:O | 1:N:224:ARG:HG2 | 2.17 | 0.45 |
| 1:N:491:ASN:ND2 | 1:O:249:TYR:OH | 2.50 | 0.45 |
| 1:N:504:VAL:HG11 | 1:N:521:ARG:CG | 2.47 | 0.45 |
| 1:A:639:ILE:HD12 | 1:O:609:PHE:CB | 2.47 | 0.45 |
| 1:B:339:VAL:HG22 | 1:B:423:ILE:HG12 | 1.98 | 0.45 |
| 1:B:456:VAL:CG2 | 1:B:457:PRO:N | 2.80 | 0.45 |
| 1:D:456:VAL:CG2 | 1:D:457:PRO:N | 2.80 | 0.45 |
| 1:D:506:ASN:O | 1:D:518:PHE:CB | 2.63 | 0.45 |
| 1:E:177:ALA:N | 1:E:211:ASN:OD1 | 2.41 | 0.45 |
| 1:E:203:LYS:N | 1:E:216:SER:HG | 2.14 | 0.45 |
| 1:F:506:ASN:O | 1:F:518:PHE:CB | 2.63 | 0.45 |
| 1:J:522:GLN:H | 1:K:451:ILE:HG23 | 1.82 | 0.45 |
| 1:K:218:ASP:O | 1:K:222:ARG:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:491:ASN:ND2 | 1:M:249:TYR:OH | 2.50 | 0.45 |
| 1:M:171:GLU:HA | 1:M:212:SER:OG | 2.16 | 0.45 |
| 1:N:205:VAL:HG12 | 1:N:206:ALA:H | 1.81 | 0.45 |
| 1:N:481:GLY:O | 1:N:505:SER:HB3 | 2.17 | 0.45 |
| 1:O:218:ASP:O | 1:O:222:ARG:N | 2.50 | 0.45 |
| 1:O:352:TYR:CD2 | 1:O:567:SER:HB2 | 2.52 | 0.45 |
| 1:A:339:VAL:HG22 | 1:A:423:ILE:HG12 | 1.98 | 0.44 |
| 1:A:352:TYR:CD2 | 1:A:567:SER:HB2 | 2.52 | 0.44 |
| 1:A:481:GLY:O | 1:A:505:SER:HB3 | 2.17 | 0.44 |
| 1:A:491:ASN:ND2 | 1:B:249:TYR:OH | 2.50 | 0.44 |
| 1:C:157:ARG:HA | 1:C:160:ASP:HB3 | 1.98 | 0.44 |
| 1:C:501:GLU:HG2 | 1:C:524:ASN:HB2 | 1.98 | 0.44 |
| 1:D:167:ILE:CA | 1:D:215:ILE:O | 2.42 | 0.44 |
| 1:E:347:GLY:H | 1:F:366:LEU:HD21 | 1.82 | 0.44 |
| 1:F:504:VAL:HG12 | 1:F:521:ARG:HG2 | 1.94 | 0.44 |
| 1:G:347:GLY:H | 1:H:366:LEU:HD21 | 1.82 | 0.44 |
| 1:G:456:VAL:CG2 | 1:G:457:PRO:N | 2.80 | 0.44 |
| 1:I:157:ARG:HA | 1:I:160:ASP:HB3 | 1.99 | 0.44 |
| 1:I:507:VAL:HG22 | 1:I:508:LEU:N | 2.29 | 0.44 |
| 1:I:522:GLN:H | 1:J:451:ILE:HG23 | 1.82 | 0.44 |
| 1:J:347:GLY:H | 1:K:366:LEU:HD21 | 1.82 | 0.44 |
| 1:M:389:GLU:OE2 | 1:M:391:THR:HB | 2.18 | 0.44 |
| 1:M:504:VAL:HG11 | 1:M:521:ARG:CG | 2.47 | 0.44 |
| 1:N:504:VAL:HG12 | 1:N:521:ARG:HG2 | 1.94 | 0.44 |
| 1:O:501:GLU:HG2 | 1:O:524:ASN:HB2 | 1.98 | 0.44 |
| 1:O:504:VAL:HG12 | 1:O:521:ARG:HG2 | 1.94 | 0.44 |
| 1:A:171:GLU:HA | 1:A:212:SER:OG | 2.16 | 0.44 |
| 1:A:249:TYR:OH | 1:O:491:ASN:ND2 | 2.50 | 0.44 |
| 1:B:220:LYS:O | 1:B:224:ARG:HG2 | 2.17 | 0.44 |
| 1:E:522:GLN:H | 1:F:451:ILE:HG23 | 1.82 | 0.44 |
| 1:F:215:ILE:HD12 | 1:F:215:ILE:HA | 1.82 | 0.44 |
| 1:I:219:PRO:HA | 1:I:222:ARG:CB | 2.45 | 0.44 |
| 1:I:456:VAL:CG2 | 1:I:457:PRO:N | 2.80 | 0.44 |
| 1:J:481:GLY:O | 1:J:505:SER:HB3 | 2.17 | 0.44 |
| 1:K:481:GLY:O | 1:K:505:SER:HB3 | 2.17 | 0.44 |
| 1:K:507:VAL:HG22 | 1:K:508:LEU:N | 2.30 | 0.44 |
| 1:K:522:GLN:H | 1:L:451:ILE:HG23 | 1.82 | 0.44 |
| 1:L:352:TYR:CD2 | 1:L:567:SER:HB2 | 2.53 | 0.44 |
| 1:N:215:ILE:HD12 | 1:N:215:ILE:HA | 1.82 | 0.44 |
| 1:N:347:GLY:H | 1:O:366:LEU:HD21 | 1.82 | 0.44 |
| 1:O:220:LYS:O | 1:O:224:ARG:HG2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:339:VAL:HG22 | 1:O:423:ILE:HG12 | 1.98 | 0.44 |
| 1:A:427:SER:HB2 | 1:O:553:PRO:HB3 | 2.00 | 0.44 |
| 1:C:389:GLU:OE2 | 1:C:391:THR:HB | 2.18 | 0.44 |
| 1:E:491:ASN:ND2 | 1:F:249:TYR:OH | 2.50 | 0.44 |
| 1:E:507:VAL:HG22 | 1:E:508:LEU:N | 2.30 | 0.44 |
| 1:F:218:ASP:O | 1:F:222:ARG:N | 2.50 | 0.44 |
| 1:F:389:GLU:OE2 | 1:F:391:THR:HB | 2.17 | 0.44 |
| 1:G:205:VAL:HG12 | 1:G:206:ALA:H | 1.81 | 0.44 |
| 1:G:522:GLN:H | 1:H:451:ILE:HG23 | 1.82 | 0.44 |
| 1:H:609:PHE:CB | 1:I:639:ILE:HD12 | 2.47 | 0.44 |
| 1:I:205:VAL:HG12 | 1:I:206:ALA:H | 1.81 | 0.44 |
| 1:I:609:PHE:CE1 | 1:J:639:ILE:HD13 | 2.52 | 0.44 |
| 1:J:225:LEU:HD23 | 1:J:225:LEU:HA | 1.74 | 0.44 |
| 1:J:235:GLU:H | 1:J:235:GLU:CD | 2.11 | 0.44 |
| 1:K:167:ILE:CA | 1:K:215:ILE:O | 2.42 | 0.44 |
| 1:K:352:TYR:CD2 | 1:K:567:SER:HB2 | 2.52 | 0.44 |
| 1:K:491:ASN:ND2 | 1:L:249:TYR:OH | 2.50 | 0.44 |
| 1:L:389:GLU:OE2 | 1:L:391:THR:HB | 2.17 | 0.44 |
| 1:L:456:VAL:CG2 | 1:L:457:PRO:N | 2.80 | 0.44 |
| 1:L:491:ASN:O | 1:L:493:GLY:N | 2.51 | 0.44 |
| 1:M:456:VAL:CG2 | 1:M:457:PRO:N | 2.80 | 0.44 |
| 1:N:157:ARG:HA | 1:N:160:ASP:HB3 | 1.98 | 0.44 |
| 1:N:352:TYR:CD2 | 1:N:567:SER:HB2 | 2.52 | 0.44 |
| 1:N:389:GLU:OE2 | 1:N:391:THR:HB | 2.18 | 0.44 |
| 1:O:456:VAL:CG2 | 1:O:457:PRO:N | 2.80 | 0.44 |
| 1:A:501:GLU:HG2 | 1:A:524:ASN:HB2 | 1.98 | 0.44 |
| 1:B:522:GLN:H | 1:C:451:ILE:HG23 | 1.82 | 0.44 |
| 1:C:255:LEU:HA | 1:C:255:LEU:HD23 | 1.73 | 0.44 |
| 1:D:218:ASP:O | 1:D:222:ARG:N | 2.50 | 0.44 |
| 1:F:553:PRO:HB3 | 1:G:427:SER:HB2 | 2.00 | 0.44 |
| 1:F:609:PHE:CB | 1:G:639:ILE:HD12 | 2.47 | 0.44 |
| 1:G:255:LEU:HA | 1:G:255:LEU:HD23 | 1.73 | 0.44 |
| 1:H:491:ASN:ND2 | 1:I:249:TYR:OH | 2.50 | 0.44 |
| 1:H:553:PRO:HB3 | 1:I:427:SER:HB2 | 2.00 | 0.44 |
| 1:H:609:PHE:CE1 | 1:I:639:ILE:HD13 | 2.52 | 0.44 |
| 1:I:218:ASP:O | 1:I:222:ARG:HG3 | 2.18 | 0.44 |
| 1:I:481:GLY:O | 1:I:505:SER:HB3 | 2.17 | 0.44 |
| 1:J:609:PHE:CE1 | 1:K:639:ILE:HD13 | 2.52 | 0.44 |
| 1:M:609:PHE:CB | 1:N:639:ILE:HD12 | 2.47 | 0.44 |
| 1:N:171:GLU:HA | 1:N:212:SER:OG | 2.16 | 0.44 |
| 1:N:218:ASP:O | 1:N:222:ARG:HG3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:219:PRO:HA | 1:B:222:ARG:CB | 2.45 | 0.44 |
| 1:B:389:GLU:OE2 | 1:B:391:THR:HB | 2.18 | 0.44 |
| 1:C:220:LYS:O | 1:C:224:ARG:HG2 | 2.17 | 0.44 |
| 1:D:389:GLU:OE2 | 1:D:391:THR:HB | 2.18 | 0.44 |
| 1:F:218:ASP:O | 1:F:222:ARG:HG3 | 2.18 | 0.44 |
| 1:F:352:TYR:CD2 | 1:F:567:SER:HB2 | 2.52 | 0.44 |
| 1:G:218:ASP:O | 1:G:222:ARG:HG3 | 2.18 | 0.44 |
| 1:G:609:PHE:CB | 1:H:639:ILE:HD12 | 2.47 | 0.44 |
| 1:I:389:GLU:OE2 | 1:I:391:THR:HB | 2.17 | 0.44 |
| 1:I:609:PHE:CB | 1:J:639:ILE:HD12 | 2.47 | 0.44 |
| 1:J:139:ILE:HG22 | 1:J:140:ILE:N | 2.27 | 0.44 |
| 1:K:180:MET:HB3 | 1:K:180:MET:HE3 | 1.88 | 0.44 |
| 1:K:491:ASN:O | 1:K:493:GLY:N | 2.51 | 0.44 |
| 1:L:219:PRO:HA | 1:L:222:ARG:CB | 2.45 | 0.44 |
| 1:L:609:PHE:CB | 1:M:639:ILE:HD12 | 2.47 | 0.44 |
| 1:M:157:ARG:HA | 1:M:160:ASP:HB3 | 1.98 | 0.44 |
| 1:M:553:PRO:HB3 | 1:N:427:SER:HB2 | 2.00 | 0.44 |
| 1:A:167:ILE:CA | 1:A:215:ILE:O | 2.42 | 0.44 |
| 1:A:177:ALA:HB3 | 1:A:208:GLU:HG3 | 2.00 | 0.44 |
| 1:B:218:ASP:O | 1:B:222:ARG:HG3 | 2.18 | 0.44 |
| 1:B:553:PRO:HB3 | 1:C:427:SER:HB2 | 2.00 | 0.44 |
| 1:C:479:GLU:H | 1:C:479:GLU:CD | 2.07 | 0.44 |
| 1:C:609:PHE:CB | 1:D:639:ILE:HD12 | 2.47 | 0.44 |
| 1:D:347:GLY:H | 1:E:366:LEU:HD21 | 1.82 | 0.44 |
| 1:E:506:ASN:O | 1:E:518:PHE:CB | 2.63 | 0.44 |
| 1:G:389:GLU:OE2 | 1:G:391:THR:HB | 2.18 | 0.44 |
| 1:H:389:GLU:OE2 | 1:H:391:THR:HB | 2.18 | 0.44 |
| 1:I:491:ASN:O | 1:I:493:GLY:N | 2.51 | 0.44 |
| 1:I:518:PHE:O | 1:I:518:PHE:HD1 | 2.01 | 0.44 |
| 1:J:491:ASN:O | 1:J:493:GLY:N | 2.51 | 0.44 |
| 1:J:553:PRO:HB3 | 1:K:427:SER:HB2 | 2.00 | 0.44 |
| 1:K:218:ASP:O | 1:K:222:ARG:HG3 | 2.18 | 0.44 |
| 1:K:456:VAL:CG2 | 1:K:457:PRO:N | 2.80 | 0.44 |
| 1:L:218:ASP:O | 1:L:222:ARG:HG3 | 2.18 | 0.44 |
| 1:M:352:TYR:CD2 | 1:M:567:SER:HB2 | 2.52 | 0.44 |
| 1:M:491:ASN:O | 1:M:493:GLY:N | 2.51 | 0.44 |
| 1:M:518:PHE:O | 1:M:518:PHE:HD1 | 2.01 | 0.44 |
| 1:N:225:LEU:HD23 | 1:N:225:LEU:HA | 1.74 | 0.44 |
| 1:O:518:PHE:O | 1:O:518:PHE:HD1 | 2.01 | 0.44 |
| 1:A:157:ARG:HA | 1:A:160:ASP:HB3 | 1.98 | 0.44 |
| 1:A:218:ASP:O | 1:A:222:ARG:HG3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:609:PHE:CB | 1:B:639:ILE:HD12 | 2.47 | 0.44 |
| 1:B:285:ILE:HD12 | 1:B:296:LEU:CD2 | 2.48 | 0.44 |
| 1:B:501:GLU:HG2 | 1:B:524:ASN:HB2 | 1.98 | 0.44 |
| 1:B:609:PHE:CE1 | 1:C:639:ILE:HD13 | 2.52 | 0.44 |
| 1:C:507:VAL:HG22 | 1:C:508:LEU:N | 2.29 | 0.44 |
| 1:C:609:PHE:CE1 | 1:D:639:ILE:HD13 | 2.52 | 0.44 |
| 1:D:218:ASP:O | 1:D:222:ARG:HG3 | 2.18 | 0.44 |
| 1:D:553:PRO:HB3 | 1:E:427:SER:HB2 | 2.00 | 0.44 |
| 1:D:609:PHE:CB | 1:E:639:ILE:HD12 | 2.47 | 0.44 |
| 1:E:167:ILE:CA | 1:E:215:ILE:O | 2.42 | 0.44 |
| 1:G:105:VAL:O | 1:G:140:ILE:CB | 2.49 | 0.44 |
| 1:G:518:PHE:O | 1:G:518:PHE:HD1 | 2.01 | 0.44 |
| 1:K:553:PRO:HB3 | 1:L:427:SER:HB2 | 2.00 | 0.44 |
| 1:L:177:ALA:HB3 | 1:L:208:GLU:HG3 | 2.00 | 0.44 |
| 1:M:105:VAL:O | 1:M:140:ILE:CB | 2.49 | 0.44 |
| 1:N:522:GLN:H | 1:O:451:ILE:HG23 | 1.82 | 0.44 |
| 1:O:171:GLU:HA | 1:O:212:SER:OG | 2.16 | 0.44 |
| 1:O:479:GLU:H | 1:O:479:GLU:CD | 2.07 | 0.44 |
| 1:A:100:VAL:HG13 | 1:A:144:GLY:HA2 | 2.00 | 0.44 |
| 1:A:609:PHE:CE1 | 1:B:639:ILE:HD13 | 2.52 | 0.44 |
| 1:B:481:GLY:O | 1:B:505:SER:HB3 | 2.17 | 0.44 |
| 1:B:491:ASN:O | 1:B:493:GLY:N | 2.51 | 0.44 |
| 1:C:518:PHE:O | 1:C:518:PHE:HD1 | 2.01 | 0.44 |
| 1:E:218:ASP:O | 1:E:222:ARG:HG3 | 2.18 | 0.44 |
| 1:E:285:ILE:HD12 | 1:E:296:LEU:CD2 | 2.48 | 0.44 |
| 1:F:456:VAL:CG2 | 1:F:457:PRO:N | 2.80 | 0.44 |
| 1:G:139:ILE:HG22 | 1:G:140:ILE:N | 2.27 | 0.44 |
| 1:H:352:TYR:CD2 | 1:H:567:SER:HB2 | 2.53 | 0.44 |
| 1:H:491:ASN:O | 1:H:493:GLY:N | 2.51 | 0.44 |
| 1:J:157:ARG:HA | 1:J:160:ASP:HB3 | 1.99 | 0.44 |
| 1:L:171:GLU:HA | 1:L:212:SER:OG | 2.16 | 0.44 |
| 1:L:285:ILE:HD12 | 1:L:296:LEU:CD2 | 2.48 | 0.44 |
| 1:L:504:VAL:HG11 | 1:L:521:ARG:CG | 2.47 | 0.44 |
| 1:M:347:GLY:H | 1:N:366:LEU:HD21 | 1.82 | 0.44 |
| 1:M:481:GLY:O | 1:M:505:SER:HB3 | 2.17 | 0.44 |
| 1:O:285:ILE:HD12 | 1:O:296:LEU:CD2 | 2.48 | 0.44 |
| 1:A:518:PHE:O | 1:A:518:PHE:HD1 | 2.01 | 0.44 |
| 1:B:100:VAL:HG13 | 1:B:144:GLY:HA2 | 2.00 | 0.44 |
| 1:B:352:TYR:CD2 | 1:B:567:SER:HB2 | 2.52 | 0.44 |
| 1:C:218:ASP:O | 1:C:222:ARG:HG3 | 2.18 | 0.44 |
| 1:D:285:ILE:HD12 | 1:D:296:LEU:CD2 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:491:ASN:O | 1:D:493:GLY:N | 2.51 | 0.44 |
| 1:D:518:PHE:O | 1:D:518:PHE:HD1 | 2.01 | 0.44 |
| 1:E:105:VAL:CG1 | 1:E:157:ARG:HE | 2.31 | 0.44 |
| 1:E:218:ASP:O | 1:E:222:ARG:N | 2.50 | 0.44 |
| 1:E:389:GLU:OE2 | 1:E:391:THR:HB | 2.18 | 0.44 |
| 1:E:491:ASN:O | 1:E:493:GLY:N | 2.51 | 0.44 |
| 1:F:285:ILE:HD12 | 1:F:296:LEU:CD2 | 2.48 | 0.44 |
| 1:F:491:ASN:O | 1:F:493:GLY:N | 2.51 | 0.44 |
| 1:F:518:PHE:O | 1:F:518:PHE:HD1 | 2.01 | 0.44 |
| 1:G:491:ASN:O | 1:G:493:GLY:N | 2.51 | 0.44 |
| 1:H:481:GLY:O | 1:H:505:SER:HB3 | 2.17 | 0.44 |
| 1:I:352:TYR:CD2 | 1:I:567:SER:HB2 | 2.52 | 0.44 |
| 1:J:518:PHE:O | 1:J:518:PHE:HD1 | 2.01 | 0.44 |
| 1:K:609:PHE:CB | 1:L:639:ILE:HD12 | 2.47 | 0.44 |
| 1:L:481:GLY:O | 1:L:505:SER:HB3 | 2.17 | 0.44 |
| 1:M:177:ALA:HB3 | 1:M:208:GLU:HG3 | 2.00 | 0.44 |
| 1:M:218:ASP:O | 1:M:222:ARG:HG3 | 2.18 | 0.44 |
| 1:O:100:VAL:HG13 | 1:O:144:GLY:HA2 | 2.00 | 0.44 |
| 1:O:177:ALA:HB3 | 1:O:208:GLU:HG3 | 2.00 | 0.44 |
| 1:O:389:GLU:OE2 | 1:O:391:THR:HB | 2.17 | 0.44 |
| 1:A:553:PRO:HB3 | 1:B:427:SER:HB2 | 2.00 | 0.43 |
| 1:A:639:ILE:HD13 | 1:O:609:PHE:CE1 | 2.52 | 0.43 |
| 1:C:100:VAL:HG13 | 1:C:144:GLY:HA2 | 2.00 | 0.43 |
| 1:C:285:ILE:HD12 | 1:C:296:LEU:CD2 | 2.48 | 0.43 |
| 1:C:456:VAL:CG2 | 1:C:457:PRO:N | 2.80 | 0.43 |
| 1:C:491:ASN:O | 1:C:493:GLY:N | 2.51 | 0.43 |
| 1:E:100:VAL:HG13 | 1:E:144:GLY:HA2 | 2.00 | 0.43 |
| 1:G:609:PHE:CE1 | 1:H:639:ILE:HD13 | 2.52 | 0.43 |
| 1:H:105:VAL:CG1 | 1:H:157:ARG:HE | 2.32 | 0.43 |
| 1:H:522:GLN:H | 1:I:451:ILE:HG23 | 1.82 | 0.43 |
| 1:H:643:ILE:HD12 | 1:H:643:ILE:HA | 1.86 | 0.43 |
| 1:J:389:GLU:OE2 | 1:J:391:THR:HB | 2.17 | 0.43 |
| 1:J:609:PHE:CB | 1:K:639:ILE:HD12 | 2.47 | 0.43 |
| 1:K:347:GLY:H | 1:L:366:LEU:HD21 | 1.82 | 0.43 |
| 1:K:389:GLU:OE2 | 1:K:391:THR:HB | 2.17 | 0.43 |
| 1:K:609:PHE:CE1 | 1:L:639:ILE:HD13 | 2.52 | 0.43 |
| 1:L:225:LEU:HD23 | 1:L:225:LEU:HA | 1.74 | 0.43 |
| 1:L:518:PHE:O | 1:L:518:PHE:HD1 | 2.01 | 0.43 |
| 1:N:285:ILE:HD12 | 1:N:296:LEU:CD2 | 2.48 | 0.43 |
| 1:N:456:VAL:CG2 | 1:N:457:PRO:N | 2.80 | 0.43 |
| 1:N:491:ASN:O | 1:N:493:GLY:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:491:ASN:O | 1:A:493:GLY:N | 2.51 | 0.43 |
| 1:C:553:PRO:HB3 | 1:D:427:SER:HB2 | 2.00 | 0.43 |
| 1:D:177:ALA:HB3 | 1:D:208:GLU:HG3 | 2.00 | 0.43 |
| 1:E:481:GLY:O | 1:E:505:SER:HB3 | 2.17 | 0.43 |
| 1:F:100:VAL:HG13 | 1:F:144:GLY:HA2 | 2.00 | 0.43 |
| 1:G:100:VAL:HG13 | 1:G:144:GLY:HA2 | 2.00 | 0.43 |
| 1:H:218:ASP:O | 1:H:222:ARG:HG3 | 2.18 | 0.43 |
| 1:I:553:PRO:HB3 | 1:J:427:SER:HB2 | 2.00 | 0.43 |
| 1:J:477:ARG:CG | 1:J:477:ARG:NH1 | 2.73 | 0.43 |
| 1:K:171:GLU:HA | 1:K:212:SER:OG | 2.16 | 0.43 |
| 1:A:219:PRO:HA | 1:A:222:ARG:CB | 2.45 | 0.43 |
| 1:A:255:LEU:HD23 | 1:A:255:LEU:HA | 1.73 | 0.43 |
| 1:A:389:GLU:OE2 | 1:A:391:THR:HB | 2.18 | 0.43 |
| 1:B:255:LEU:HA | 1:B:255:LEU:HD23 | 1.73 | 0.43 |
| 1:B:518:PHE:O | 1:B:518:PHE:HD1 | 2.01 | 0.43 |
| 1:C:352:TYR:CD2 | 1:C:567:SER:HB2 | 2.52 | 0.43 |
| 1:G:285:ILE:HD12 | 1:G:296:LEU:CD2 | 2.48 | 0.43 |
| 1:G:481:GLY:O | 1:G:505:SER:HB3 | 2.17 | 0.43 |
| 1:I:177:ALA:HB3 | 1:I:208:GLU:HG3 | 2.00 | 0.43 |
| 1:J:177:ALA:HB3 | 1:J:208:GLU:HG3 | 2.00 | 0.43 |
| 1:J:456:VAL:CG2 | 1:J:457:PRO:N | 2.80 | 0.43 |
| 1:K:105:VAL:CG1 | 1:K:157:ARG:HE | 2.32 | 0.43 |
| 1:K:285:ILE:HD12 | 1:K:296:LEU:CD2 | 2.48 | 0.43 |
| 1:N:167:ILE:CA | 1:N:215:ILE:O | 2.42 | 0.43 |
| 1:N:518:PHE:O | 1:N:518:PHE:HD1 | 2.01 | 0.43 |
| 1:O:218:ASP:O | 1:O:222:ARG:HG3 | 2.18 | 0.43 |
| 1:D:100:VAL:HG13 | 1:D:144:GLY:HA2 | 2.00 | 0.43 |
| 1:D:352:TYR:CD2 | 1:D:567:SER:HB2 | 2.52 | 0.43 |
| 1:E:352:TYR:CD2 | 1:E:567:SER:HB2 | 2.52 | 0.43 |
| 1:H:518:PHE:O | 1:H:518:PHE:HD1 | 2.01 | 0.43 |
| 1:N:139:ILE:HG22 | 1:N:140:ILE:N | 2.27 | 0.43 |
| 1:B:516:VAL:O | 1:B:516:VAL:HG23 | 2.19 | 0.43 |
| 1:F:255:LEU:HD23 | 1:F:255:LEU:HA | 1.73 | 0.43 |
| 1:G:352:TYR:CD2 | 1:G:567:SER:HB2 | 2.52 | 0.43 |
| 1:G:553:PRO:HB3 | 1:H:427:SER:HB2 | 2.00 | 0.43 |
| 1:H:177:ALA:N | 1:H:211:ASN:OD1 | 2.41 | 0.43 |
| 1:J:219:PRO:HA | 1:J:222:ARG:CB | 2.45 | 0.43 |
| 1:J:285:ILE:HD12 | 1:J:296:LEU:CD2 | 2.48 | 0.43 |
| 1:K:157:ARG:HA | 1:K:160:ASP:HB3 | 1.98 | 0.43 |
| 1:K:504:VAL:HG11 | 1:K:521:ARG:CG | 2.47 | 0.43 |
| 1:N:100:VAL:HG13 | 1:N:144:GLY:HA2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:507:VAL:HG22 | 1:A:508:LEU:N | 2.30 | 0.43 |
| 1:B:435:LEU:CD2 | 1:C:626:LEU:HD23 | 2.49 | 0.43 |
| 1:C:177:ALA:HB3 | 1:C:208:GLU:HG3 | 2.00 | 0.43 |
| 1:C:225:LEU:HD23 | 1:C:225:LEU:HA | 1.74 | 0.43 |
| 1:D:435:LEU:CD2 | 1:E:626:LEU:HD23 | 2.49 | 0.43 |
| 1:E:102:THR:HA | 1:E:143:THR:HA | 2.01 | 0.43 |
| 1:E:518:PHE:O | 1:E:518:PHE:HD1 | 2.01 | 0.43 |
| 1:E:553:PRO:HB3 | 1:F:427:SER:HB2 | 2.00 | 0.43 |
| 1:F:167:ILE:CA | 1:F:215:ILE:O | 2.42 | 0.43 |
| 1:G:105:VAL:CG1 | 1:G:157:ARG:HE | 2.32 | 0.43 |
| 1:H:102:THR:HA | 1:H:143:THR:HA | 2.01 | 0.43 |
| 1:H:157:ARG:HA | 1:H:160:ASP:HB3 | 1.99 | 0.43 |
| 1:I:225:LEU:HA | 1:I:225:LEU:HD23 | 1.74 | 0.43 |
| 1:J:102:THR:HA | 1:J:143:THR:HA | 2.01 | 0.43 |
| 1:J:218:ASP:O | 1:J:222:ARG:HG3 | 2.18 | 0.43 |
| 1:J:352:TYR:CD2 | 1:J:567:SER:HB2 | 2.53 | 0.43 |
| 1:N:609:PHE:CE1 | 1:O:639:ILE:HD13 | 2.52 | 0.43 |
| 1:H:100:VAL:HG13 | 1:H:144:GLY:HA2 | 2.00 | 0.43 |
| 1:H:504:VAL:HG12 | 1:H:521:ARG:HG2 | 1.94 | 0.43 |
| 1:I:285:ILE:HD12 | 1:I:296:LEU:CD2 | 2.48 | 0.43 |
| 1:I:357:ALA:HB3 | 1:I:407:ILE:HD11 | 2.01 | 0.43 |
| 1:K:102:THR:HA | 1:K:143:THR:HA | 2.01 | 0.43 |
| 1:K:458:VAL:CG2 | 1:K:478:LYS:HG2 | 2.48 | 0.43 |
| 1:L:553:PRO:HB3 | 1:M:427:SER:HB2 | 2.00 | 0.43 |
| 1:M:100:VAL:HG13 | 1:M:144:GLY:HA2 | 2.00 | 0.43 |
| 1:M:102:THR:HA | 1:M:143:THR:HA | 2.01 | 0.43 |
| 1:M:435:LEU:CD2 | 1:N:626:LEU:HD23 | 2.49 | 0.43 |
| 1:M:504:VAL:HG12 | 1:M:521:ARG:HG2 | 1.94 | 0.43 |
| 1:B:177:ALA:HB3 | 1:B:208:GLU:HG3 | 2.00 | 0.43 |
| 1:D:102:THR:HA | 1:D:143:THR:HA | 2.01 | 0.43 |
| 1:D:609:PHE:CE1 | 1:E:639:ILE:HD13 | 2.52 | 0.43 |
| 1:G:102:THR:HA | 1:G:143:THR:HA | 2.01 | 0.43 |
| 1:G:435:LEU:CD2 | 1:H:626:LEU:HD23 | 2.49 | 0.43 |
| 1:H:285:ILE:HD12 | 1:H:296:LEU:CD2 | 2.48 | 0.43 |
| 1:H:357:ALA:HB3 | 1:H:407:ILE:HD11 | 2.01 | 0.43 |
| 1:I:102:THR:HA | 1:I:143:THR:HA | 2.01 | 0.43 |
| 1:I:105:VAL:CG1 | 1:I:157:ARG:HE | 2.31 | 0.43 |
| 1:I:180:MET:HB3 | 1:I:180:MET:HE3 | 1.87 | 0.43 |
| 1:N:435:LEU:CD2 | 1:O:626:LEU:HD23 | 2.49 | 0.43 |
| 1:N:521:ARG:HA | 1:O:451:ILE:O | 2.19 | 0.43 |
| 1:N:553:PRO:HB3 | 1:O:427:SER:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:491:ASN:O | 1:O:493:GLY:N | 2.51 | 0.43 |
| 1:A:458:VAL:CG2 | 1:A:478:LYS:HG2 | 2.48 | 0.43 |
| 1:B:458:VAL:CG2 | 1:B:478:LYS:HG2 | 2.48 | 0.43 |
| 1:C:481:GLY:O | 1:C:505:SER:HB3 | 2.17 | 0.43 |
| 1:C:516:VAL:O | 1:C:516:VAL:HG23 | 2.19 | 0.43 |
| 1:D:521:ARG:HA | 1:E:451:ILE:O | 2.19 | 0.43 |
| 1:E:215:ILE:HD12 | 1:E:215:ILE:HA | 1.82 | 0.43 |
| 1:F:102:THR:HA | 1:F:143:THR:HA | 2.01 | 0.43 |
| 1:F:435:LEU:CD2 | 1:G:626:LEU:HD23 | 2.49 | 0.43 |
| 1:F:481:GLY:O | 1:F:505:SER:HB3 | 2.17 | 0.43 |
| 1:G:357:ALA:HB3 | 1:G:407:ILE:HD11 | 2.01 | 0.43 |
| 1:H:166:GLU:HB3 | 1:H:167:ILE:H | 1.67 | 0.43 |
| 1:I:100:VAL:HG13 | 1:I:144:GLY:HA2 | 2.00 | 0.43 |
| 1:I:435:LEU:CD2 | 1:J:626:LEU:HD23 | 2.49 | 0.43 |
| 1:J:225:LEU:O | 1:J:229:ILE:HG13 | 2.19 | 0.43 |
| 1:J:521:ARG:HA | 1:K:451:ILE:O | 2.19 | 0.43 |
| 1:K:166:GLU:HB3 | 1:K:167:ILE:H | 1.67 | 0.43 |
| 1:K:225:LEU:O | 1:K:229:ILE:HG13 | 2.19 | 0.43 |
| 1:L:435:LEU:CD2 | 1:M:626:LEU:HD23 | 2.49 | 0.43 |
| 1:M:285:ILE:HD12 | 1:M:296:LEU:CD2 | 2.48 | 0.43 |
| 1:N:102:THR:HA | 1:N:143:THR:HA | 2.01 | 0.43 |
| 1:N:479:GLU:H | 1:N:479:GLU:CD | 2.07 | 0.43 |
| 1:N:516:VAL:O | 1:N:516:VAL:HG23 | 2.19 | 0.43 |
| 1:O:219:PRO:HA | 1:O:222:ARG:CB | 2.45 | 0.43 |
| 1:A:451:ILE:O | 1:O:521:ARG:HA | 2.19 | 0.43 |
| 1:A:516:VAL:O | 1:A:516:VAL:HG23 | 2.19 | 0.43 |
| 1:A:626:LEU:HD23 | 1:O:435:LEU:CD2 | 2.49 | 0.43 |
| 1:C:521:ARG:HA | 1:D:451:ILE:O | 2.19 | 0.43 |
| 1:E:609:PHE:CE1 | 1:F:639:ILE:HD13 | 2.52 | 0.43 |
| 1:F:105:VAL:CG1 | 1:F:157:ARG:HE | 2.32 | 0.43 |
| 1:G:115:LEU:HB3 | 1:G:119:LEU:HG | 2.01 | 0.43 |
| 1:H:521:ARG:HA | 1:I:451:ILE:O | 2.19 | 0.43 |
| 1:J:301:ASP:OD1 | 1:J:302:ILE:N | 2.52 | 0.43 |
| 1:J:504:VAL:HG11 | 1:J:521:ARG:CG | 2.47 | 0.43 |
| 1:K:435:LEU:CD2 | 1:L:626:LEU:HD23 | 2.49 | 0.43 |
| 1:L:102:THR:HA | 1:L:143:THR:HA | 2.01 | 0.43 |
| 1:L:115:LEU:HB3 | 1:L:119:LEU:HG | 2.01 | 0.43 |
| 1:M:115:LEU:HB3 | 1:M:119:LEU:HG | 2.01 | 0.43 |
| 1:M:166:GLU:HB3 | 1:M:167:ILE:H | 1.67 | 0.43 |
| 1:O:102:THR:HA | 1:O:143:THR:HA | 2.01 | 0.43 |
| 1:C:105:VAL:CG1 | 1:C:157:ARG:HE | 2.32 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:516:VAL:HG23 | 1:E:516:VAL:O | 2.19 | 0.42 |
| 1:G:504:VAL:HG12 | 1:G:521:ARG:HG2 | 1.94 | 0.42 |
| 1:H:115:LEU:HB3 | 1:H:119:LEU:HG | 2.01 | 0.42 |
| 1:K:99:GLU:O | 1:K:145:ARG:HA | 2.19 | 0.42 |
| 1:K:115:LEU:HB3 | 1:K:119:LEU:HG | 2.01 | 0.42 |
| 1:K:219:PRO:HA | 1:K:222:ARG:CB | 2.45 | 0.42 |
| 1:L:225:LEU:O | 1:L:229:ILE:HG13 | 2.19 | 0.42 |
| 1:L:521:ARG:HA | 1:M:451:ILE:O | 2.19 | 0.42 |
| 1:L:551:LYS:HB3 | 1:L:566:ARG:HG2 | 2.01 | 0.42 |
| 1:M:215:ILE:HD12 | 1:M:215:ILE:HA | 1.82 | 0.42 |
| 1:M:551:LYS:HB3 | 1:M:566:ARG:HG2 | 2.01 | 0.42 |
| 1:O:301:ASP:OD1 | 1:O:302:ILE:N | 2.52 | 0.42 |
| 1:A:435:LEU:CD2 | 1:B:626:LEU:HD23 | 2.49 | 0.42 |
| 1:C:102:THR:HA | 1:C:143:THR:HA | 2.01 | 0.42 |
| 1:C:458:VAL:CG2 | 1:C:478:LYS:HG2 | 2.48 | 0.42 |
| 1:D:357:ALA:HB3 | 1:D:407:ILE:HD11 | 2.01 | 0.42 |
| 1:D:481:GLY:O | 1:D:505:SER:HB3 | 2.17 | 0.42 |
| 1:E:180:MET:HE2 | 1:E:213:ILE:HD11 | 2.01 | 0.42 |
| 1:E:225:LEU:HD23 | 1:E:225:LEU:HA | 1.74 | 0.42 |
| 1:E:357:ALA:HB3 | 1:E:407:ILE:HD11 | 2.01 | 0.42 |
| 1:F:115:LEU:HB3 | 1:F:119:LEU:HG | 2.01 | 0.42 |
| 1:F:177:ALA:HB3 | 1:F:208:GLU:HG3 | 2.00 | 0.42 |
| 1:F:219:PRO:HA | 1:F:222:ARG:CB | 2.45 | 0.42 |
| 1:F:225:LEU:HD23 | 1:F:225:LEU:HA | 1.74 | 0.42 |
| 1:F:357:ALA:HB3 | 1:F:407:ILE:HD11 | 2.01 | 0.42 |
| 1:F:609:PHE:CE1 | 1:G:639:ILE:HD13 | 2.52 | 0.42 |
| 1:H:539:GLY:CA | 1:H:577:LEU:O | 2.68 | 0.42 |
| 1:I:170:VAL:HG11 | 1:I:229:ILE:HG21 | 2.01 | 0.42 |
| 1:J:357:ALA:HB3 | 1:J:407:ILE:HD11 | 2.01 | 0.42 |
| 1:J:609:PHE:CD2 | 1:K:639:ILE:CD1 | 2.75 | 0.42 |
| 1:K:177:ALA:HB3 | 1:K:208:GLU:HG3 | 2.00 | 0.42 |
| 1:L:99:GLU:O | 1:L:145:ARG:HA | 2.19 | 0.42 |
| 1:L:105:VAL:CG1 | 1:L:157:ARG:HE | 2.31 | 0.42 |
| 1:L:347:GLY:H | 1:M:366:LEU:HD21 | 1.82 | 0.42 |
| 1:L:609:PHE:CE1 | 1:M:639:ILE:HD13 | 2.52 | 0.42 |
| 1:M:170:VAL:HG11 | 1:M:229:ILE:HG21 | 2.01 | 0.42 |
| 1:M:609:PHE:CE1 | 1:N:639:ILE:HD13 | 2.53 | 0.42 |
| 1:N:170:VAL:HG11 | 1:N:229:ILE:HG21 | 2.01 | 0.42 |
| 1:N:551:LYS:HB3 | 1:N:566:ARG:HG2 | 2.01 | 0.42 |
| 1:O:170:VAL:HG11 | 1:O:229:ILE:HG21 | 2.01 | 0.42 |
| 1:O:643:ILE:HD12 | 1:O:643:ILE:HA | 1.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:THR:HA | 1:A:143:THR:HA | 2.01 | 0.42 |
| 1:A:285:ILE:HD12 | 1:A:296:LEU:CD2 | 2.48 | 0.42 |
| 1:A:551:LYS:HB3 | 1:A:566:ARG:HG2 | 2.01 | 0.42 |
| 1:B:225:LEU:O | 1:B:229:ILE:HG13 | 2.19 | 0.42 |
| 1:B:551:LYS:HB3 | 1:B:566:ARG:HG2 | 2.01 | 0.42 |
| 1:C:181:VAL:HG12 | 1:C:185:GLU:OE2 | 2.20 | 0.42 |
| 1:E:170:VAL:HG11 | 1:E:229:ILE:HG21 | 2.01 | 0.42 |
| 1:E:435:LEU:CD2 | 1:F:626:LEU:HD23 | 2.49 | 0.42 |
| 1:G:99:GLU:O | 1:G:145:ARG:HA | 2.19 | 0.42 |
| 1:G:521:ARG:HA | 1:H:451:ILE:O | 2.19 | 0.42 |
| 1:I:115:LEU:HB3 | 1:I:119:LEU:HG | 2.01 | 0.42 |
| 1:J:115:LEU:HB3 | 1:J:119:LEU:HG | 2.01 | 0.42 |
| 1:L:100:VAL:HG13 | 1:L:144:GLY:HA2 | 2.00 | 0.42 |
| 1:M:516:VAL:O | 1:M:516:VAL:HG23 | 2.19 | 0.42 |
| 1:N:115:LEU:HB3 | 1:N:119:LEU:HG | 2.01 | 0.42 |
| 1:N:177:ALA:HB3 | 1:N:208:GLU:HG3 | 2.00 | 0.42 |
| 1:O:181:VAL:HG12 | 1:O:185:GLU:OE2 | 2.20 | 0.42 |
| 1:A:181:VAL:HG12 | 1:A:185:GLU:OE2 | 2.20 | 0.42 |
| 1:A:225:LEU:O | 1:A:229:ILE:HG13 | 2.19 | 0.42 |
| 1:C:551:LYS:HB3 | 1:C:566:ARG:HG2 | 2.01 | 0.42 |
| 1:D:170:VAL:HG11 | 1:D:229:ILE:HG21 | 2.01 | 0.42 |
| 1:F:170:VAL:HG11 | 1:F:229:ILE:HG21 | 2.01 | 0.42 |
| 1:F:516:VAL:HG23 | 1:F:516:VAL:O | 2.19 | 0.42 |
| 1:G:454:GLU:CD | 1:G:454:GLU:N | 2.73 | 0.42 |
| 1:H:435:LEU:CD2 | 1:I:626:LEU:HD23 | 2.49 | 0.42 |
| 1:J:100:VAL:HG13 | 1:J:144:GLY:HA2 | 2.00 | 0.42 |
| 1:J:170:VAL:HG11 | 1:J:229:ILE:HG21 | 2.01 | 0.42 |
| 1:J:435:LEU:CD2 | 1:K:626:LEU:HD23 | 2.49 | 0.42 |
| 1:J:458:VAL:CG2 | 1:J:478:LYS:HG2 | 2.48 | 0.42 |
| 1:K:247:LEU:CD1 | 1:K:255:LEU:HD12 | 2.50 | 0.42 |
| 1:K:551:LYS:HB3 | 1:K:566:ARG:HG2 | 2.01 | 0.42 |
| 1:M:225:LEU:O | 1:M:229:ILE:HG13 | 2.19 | 0.42 |
| 1:N:181:VAL:HG12 | 1:N:185:GLU:OE2 | 2.20 | 0.42 |
| 1:N:219:PRO:HA | 1:N:222:ARG:CB | 2.45 | 0.42 |
| 1:O:458:VAL:CG2 | 1:O:478:LYS:HG2 | 2.48 | 0.42 |
| 1:O:551:LYS:HB3 | 1:O:566:ARG:HG2 | 2.01 | 0.42 |
| 1:B:102:THR:HA | 1:B:143:THR:HA | 2.01 | 0.42 |
| 1:B:122:LEU:HD23 | 1:B:125:ASN:ND2 | 2.19 | 0.42 |
| 1:B:181:VAL:HG12 | 1:B:185:GLU:OE2 | 2.20 | 0.42 |
| 1:B:454:GLU:CD | 1:B:454:GLU:N | 2.73 | 0.42 |
| 1:C:170:VAL:HG11 | 1:C:229:ILE:HG21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:357:ALA:HB3 | 1:C:407:ILE:HD11 | 2.01 | 0.42 |
| 1:E:539:GLY:CA | 1:E:577:LEU:O | 2.68 | 0.42 |
| 1:F:454:GLU:N | 1:F:454:GLU:CD | 2.73 | 0.42 |
| 1:H:99:GLU:O | 1:H:145:ARG:HA | 2.19 | 0.42 |
| 1:H:170:VAL:HG11 | 1:H:229:ILE:HG21 | 2.01 | 0.42 |
| 1:I:225:LEU:O | 1:I:229:ILE:HG13 | 2.19 | 0.42 |
| 1:I:504:VAL:HG11 | 1:I:521:ARG:CG | 2.47 | 0.42 |
| 1:I:521:ARG:HA | 1:J:451:ILE:O | 2.19 | 0.42 |
| 1:K:100:VAL:HG13 | 1:K:144:GLY:HA2 | 2.00 | 0.42 |
| 1:M:181:VAL:HG12 | 1:M:185:GLU:OE2 | 2.20 | 0.42 |
| 1:M:521:ARG:HA | 1:N:451:ILE:O | 2.19 | 0.42 |
| 1:O:105:VAL:CG1 | 1:O:157:ARG:HE | 2.31 | 0.42 |
| 1:A:454:GLU:CD | 1:A:454:GLU:N | 2.73 | 0.42 |
| 1:B:170:VAL:HG11 | 1:B:229:ILE:HG21 | 2.01 | 0.42 |
| 1:C:207:ASP:OD2 | 1:C:209:ARG:HB3 | 2.20 | 0.42 |
| 1:C:435:LEU:CD2 | 1:D:626:LEU:HD23 | 2.49 | 0.42 |
| 1:D:352:TYR:OH | 1:D:565:PHE:O | 2.33 | 0.42 |
| 1:E:225:LEU:O | 1:E:229:ILE:HG13 | 2.19 | 0.42 |
| 1:E:521:ARG:HA | 1:F:451:ILE:O | 2.19 | 0.42 |
| 1:F:521:ARG:HA | 1:G:451:ILE:O | 2.19 | 0.42 |
| 1:H:247:LEU:CD1 | 1:H:255:LEU:HD12 | 2.50 | 0.42 |
| 1:H:454:GLU:CD | 1:H:454:GLU:N | 2.73 | 0.42 |
| 1:K:518:PHE:O | 1:K:518:PHE:HD1 | 2.01 | 0.42 |
| 1:M:219:PRO:HA | 1:M:222:ARG:CB | 2.45 | 0.42 |
| 1:N:207:ASP:OD2 | 1:N:209:ARG:HB3 | 2.20 | 0.42 |
| 1:N:357:ALA:HB3 | 1:N:407:ILE:HD11 | 2.01 | 0.42 |
| 1:O:225:LEU:HD23 | 1:O:225:LEU:HA | 1.74 | 0.42 |
| 1:A:170:VAL:HG11 | 1:A:229:ILE:HG21 | 2.01 | 0.42 |
| 1:A:521:ARG:HA | 1:B:451:ILE:O | 2.19 | 0.42 |
| 1:C:247:LEU:CD1 | 1:C:255:LEU:HD12 | 2.50 | 0.42 |
| 1:E:339:VAL:HB | 1:E:564:LEU:O | 2.20 | 0.42 |
| 1:F:225:LEU:O | 1:F:229:ILE:HG13 | 2.19 | 0.42 |
| 1:J:99:GLU:O | 1:J:145:ARG:HA | 2.19 | 0.42 |
| 1:K:357:ALA:HB3 | 1:K:407:ILE:HD11 | 2.01 | 0.42 |
| 1:L:170:VAL:HG11 | 1:L:229:ILE:HG21 | 2.01 | 0.42 |
| 1:O:115:LEU:HB3 | 1:O:119:LEU:HG | 2.01 | 0.42 |
| 1:A:115:LEU:HB3 | 1:A:119:LEU:HG | 2.01 | 0.42 |
| 1:A:642:PHE:CE2 | 1:O:612:GLU:CG | 2.81 | 0.42 |
| 1:B:207:ASP:OD2 | 1:B:209:ARG:HB3 | 2.20 | 0.42 |
| 1:C:454:GLU:CD | 1:C:454:GLU:N | 2.73 | 0.42 |
| 1:D:115:LEU:HB3 | 1:D:119:LEU:HG | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:225:LEU:O | 1:D:229:ILE:HG13 | 2.19 | 0.42 |
| 1:D:458:VAL:CG2 | 1:D:478:LYS:HG2 | 2.48 | 0.42 |
| 1:E:115:LEU:HB3 | 1:E:119:LEU:HG | 2.01 | 0.42 |
| 1:E:247:LEU:CD1 | 1:E:255:LEU:HD12 | 2.50 | 0.42 |
| 1:F:99:GLU:O | 1:F:145:ARG:HA | 2.19 | 0.42 |
| 1:G:170:VAL:HG11 | 1:G:229:ILE:HG21 | 2.01 | 0.42 |
| 1:H:225:LEU:HA | 1:H:225:LEU:HD23 | 1.74 | 0.42 |
| 1:H:504:VAL:HG11 | 1:H:521:ARG:CG | 2.47 | 0.42 |
| 1:I:539:GLY:CA | 1:I:577:LEU:O | 2.68 | 0.42 |
| 1:J:247:LEU:CD1 | 1:J:255:LEU:HD12 | 2.50 | 0.42 |
| 1:J:481:GLY:N | 1:J:505:SER:OG | 2.23 | 0.42 |
| 1:J:516:VAL:O | 1:J:516:VAL:HG23 | 2.19 | 0.42 |
| 1:J:551:LYS:HB3 | 1:J:566:ARG:HG2 | 2.01 | 0.42 |
| 1:L:181:VAL:HG12 | 1:L:185:GLU:OE2 | 2.20 | 0.42 |
| 1:M:479:GLU:H | 1:M:479:GLU:CD | 2.07 | 0.42 |
| 1:O:207:ASP:OD2 | 1:O:209:ARG:HB3 | 2.20 | 0.42 |
| 1:O:357:ALA:HB3 | 1:O:407:ILE:HD11 | 2.01 | 0.42 |
| 1:O:454:GLU:CD | 1:O:454:GLU:N | 2.73 | 0.42 |
| 1:B:247:LEU:CD1 | 1:B:255:LEU:HD12 | 2.50 | 0.42 |
| 1:B:301:ASP:OD1 | 1:B:302:ILE:N | 2.52 | 0.42 |
| 1:B:479:GLU:H | 1:B:479:GLU:CD | 2.07 | 0.42 |
| 1:C:301:ASP:OD1 | 1:C:302:ILE:N | 2.52 | 0.42 |
| 1:D:551:LYS:HB3 | 1:D:566:ARG:HG2 | 2.01 | 0.42 |
| 1:E:454:GLU:CD | 1:E:454:GLU:N | 2.73 | 0.42 |
| 1:G:225:LEU:O | 1:G:229:ILE:HG13 | 2.19 | 0.42 |
| 1:G:301:ASP:OD1 | 1:G:302:ILE:N | 2.52 | 0.42 |
| 1:G:504:VAL:HG11 | 1:G:521:ARG:CG | 2.47 | 0.42 |
| 1:H:219:PRO:HA | 1:H:222:ARG:CB | 2.45 | 0.42 |
| 1:H:301:ASP:OD1 | 1:H:302:ILE:N | 2.52 | 0.42 |
| 1:I:247:LEU:CD1 | 1:I:255:LEU:HD12 | 2.50 | 0.42 |
| 1:I:516:VAL:HG23 | 1:I:516:VAL:O | 2.19 | 0.42 |
| 1:K:170:VAL:HG11 | 1:K:229:ILE:HG21 | 2.01 | 0.42 |
| 1:L:247:LEU:CD1 | 1:L:255:LEU:HD12 | 2.50 | 0.42 |
| 1:L:339:VAL:HB | 1:L:564:LEU:O | 2.20 | 0.42 |
| 1:M:339:VAL:HB | 1:M:564:LEU:O | 2.20 | 0.42 |
| 1:M:539:GLY:CA | 1:M:577:LEU:O | 2.68 | 0.42 |
| 1:N:247:LEU:CD1 | 1:N:255:LEU:HD12 | 2.50 | 0.42 |
| 1:O:516:VAL:O | 1:O:516:VAL:HG23 | 2.19 | 0.42 |
| 1:A:142:ILE:CG2 | 1:A:149:VAL:HG22 | 2.50 | 0.42 |
| 1:A:301:ASP:OD1 | 1:A:302:ILE:N | 2.52 | 0.42 |
| 1:B:123:ILE:HG23 | 1:B:130:ASN:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:521:ARG:HA | 1:C:451:ILE:O | 2.19 | 0.42 |
| 1:C:115:LEU:HB3 | 1:C:119:LEU:HG | 2.01 | 0.42 |
| 1:D:181:VAL:HG12 | 1:D:185:GLU:OE2 | 2.20 | 0.42 |
| 1:D:454:GLU:CD | 1:D:454:GLU:N | 2.73 | 0.42 |
| 1:F:181:VAL:HG12 | 1:F:185:GLU:OE2 | 2.20 | 0.42 |
| 1:F:301:ASP:OD1 | 1:F:302:ILE:N | 2.52 | 0.42 |
| 1:F:339:VAL:HB | 1:F:564:LEU:O | 2.20 | 0.42 |
| 1:F:506:ASN:C | 1:F:506:ASN:ND2 | 2.73 | 0.42 |
| 1:G:167:ILE:CA | 1:G:215:ILE:O | 2.42 | 0.42 |
| 1:G:247:LEU:CD1 | 1:G:255:LEU:HD12 | 2.50 | 0.42 |
| 1:G:339:VAL:HB | 1:G:564:LEU:O | 2.20 | 0.42 |
| 1:H:207:ASP:OD2 | 1:H:209:ARG:HB3 | 2.20 | 0.42 |
| 1:I:207:ASP:OD2 | 1:I:209:ARG:HB3 | 2.20 | 0.42 |
| 1:I:301:ASP:OD1 | 1:I:302:ILE:N | 2.52 | 0.42 |
| 1:L:504:VAL:HG12 | 1:L:521:ARG:HG2 | 1.94 | 0.42 |
| 1:M:99:GLU:O | 1:M:145:ARG:HA | 2.20 | 0.42 |
| 1:M:357:ALA:HB3 | 1:M:407:ILE:HD11 | 2.01 | 0.42 |
| 1:M:454:GLU:CD | 1:M:454:GLU:N | 2.73 | 0.42 |
| 1:N:225:LEU:O | 1:N:229:ILE:HG13 | 2.19 | 0.42 |
| 1:N:454:GLU:N | 1:N:454:GLU:CD | 2.73 | 0.42 |
| 1:O:225:LEU:O | 1:O:229:ILE:HG13 | 2.19 | 0.42 |
| 1:A:339:VAL:HB | 1:A:564:LEU:O | 2.20 | 0.41 |
| 1:B:139:ILE:HG22 | 1:B:140:ILE:N | 2.27 | 0.41 |
| 1:B:357:ALA:HB3 | 1:B:407:ILE:HD11 | 2.01 | 0.41 |
| 1:C:123:ILE:HG23 | 1:C:130:ASN:HB2 | 2.02 | 0.41 |
| 1:C:225:LEU:O | 1:C:229:ILE:HG13 | 2.19 | 0.41 |
| 1:D:215:ILE:HD12 | 1:D:215:ILE:HA | 1.82 | 0.41 |
| 1:D:301:ASP:OD1 | 1:D:302:ILE:N | 2.52 | 0.41 |
| 1:H:339:VAL:HB | 1:H:564:LEU:O | 2.20 | 0.41 |
| 1:J:643:ILE:HD12 | 1:J:643:ILE:HA | 1.86 | 0.41 |
| 1:K:181:VAL:HG12 | 1:K:185:GLU:OE2 | 2.20 | 0.41 |
| 1:K:246:TYR:HD1 | 1:K:293:SER:HB3 | 1.85 | 0.41 |
| 1:K:454:GLU:CD | 1:K:454:GLU:N | 2.73 | 0.41 |
| 1:K:521:ARG:HA | 1:L:451:ILE:O | 2.19 | 0.41 |
| 1:L:454:GLU:CD | 1:L:454:GLU:N | 2.73 | 0.41 |
| 1:A:247:LEU:CD1 | 1:A:255:LEU:HD12 | 2.50 | 0.41 |
| 1:C:139:ILE:HG22 | 1:C:140:ILE:N | 2.27 | 0.41 |
| 1:C:288:HIS:HD2 | 1:C:291:THR:HB | 1.86 | 0.41 |
| 1:D:166:GLU:HB3 | 1:D:167:ILE:H | 1.67 | 0.41 |
| 1:D:339:VAL:HB | 1:D:564:LEU:O | 2.20 | 0.41 |
| 1:D:516:VAL:O | 1:D:516:VAL:HG23 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:640:GLN:NE2 | 1:D:643:ILE:HG21 | 2.35 | 0.41 |
| 1:E:181:VAL:HG12 | 1:E:185:GLU:OE2 | 2.20 | 0.41 |
| 1:E:246:TYR:HD1 | 1:E:293:SER:HB3 | 1.85 | 0.41 |
| 1:E:301:ASP:OD1 | 1:E:302:ILE:N | 2.52 | 0.41 |
| 1:F:504:VAL:HG11 | 1:F:521:ARG:CG | 2.47 | 0.41 |
| 1:G:207:ASP:OD2 | 1:G:209:ARG:HB3 | 2.20 | 0.41 |
| 1:H:516:VAL:HG23 | 1:H:516:VAL:O | 2.19 | 0.41 |
| 1:I:339:VAL:HB | 1:I:564:LEU:O | 2.20 | 0.41 |
| 1:I:454:GLU:N | 1:I:454:GLU:CD | 2.73 | 0.41 |
| 1:L:139:ILE:C | 1:L:140:ILE:HG13 | 2.41 | 0.41 |
| 1:M:140:ILE:HG21 | 1:M:156:ILE:HG21 | 2.02 | 0.41 |
| 1:M:288:HIS:HD2 | 1:M:291:THR:HB | 1.86 | 0.41 |
| 1:N:113:ARG:HD2 | 1:N:134:TYR:CD2 | 2.55 | 0.41 |
| 1:N:140:ILE:HG21 | 1:N:156:ILE:HG21 | 2.02 | 0.41 |
| 1:N:288:HIS:HD2 | 1:N:291:THR:HB | 1.85 | 0.41 |
| 1:O:247:LEU:CD1 | 1:O:255:LEU:HD12 | 2.50 | 0.41 |
| 1:A:99:GLU:O | 1:A:145:ARG:HA | 2.19 | 0.41 |
| 1:A:246:TYR:HD1 | 1:A:293:SER:HB3 | 1.86 | 0.41 |
| 1:A:256:VAL:HG23 | 1:A:285:ILE:HG22 | 2.03 | 0.41 |
| 1:A:357:ALA:HB3 | 1:A:407:ILE:HD11 | 2.01 | 0.41 |
| 1:B:115:LEU:HB3 | 1:B:119:LEU:HG | 2.01 | 0.41 |
| 1:B:440:ILE:HD12 | 1:B:440:ILE:HA | 1.91 | 0.41 |
| 1:C:142:ILE:CG2 | 1:C:149:VAL:HG22 | 2.50 | 0.41 |
| 1:D:246:TYR:HD1 | 1:D:293:SER:HB3 | 1.86 | 0.41 |
| 1:D:247:LEU:CD1 | 1:D:255:LEU:HD12 | 2.50 | 0.41 |
| 1:E:140:ILE:HG21 | 1:E:156:ILE:HG21 | 2.02 | 0.41 |
| 1:E:352:TYR:OH | 1:E:565:PHE:O | 2.33 | 0.41 |
| 1:E:458:VAL:CG2 | 1:E:478:LYS:HG2 | 2.48 | 0.41 |
| 1:E:551:LYS:HB3 | 1:E:566:ARG:HG2 | 2.01 | 0.41 |
| 1:F:246:TYR:HD1 | 1:F:293:SER:HB3 | 1.85 | 0.41 |
| 1:G:516:VAL:HG23 | 1:G:516:VAL:O | 2.19 | 0.41 |
| 1:H:288:HIS:HD2 | 1:H:291:THR:HB | 1.86 | 0.41 |
| 1:I:99:GLU:O | 1:I:145:ARG:HA | 2.19 | 0.41 |
| 1:I:551:LYS:HB3 | 1:I:566:ARG:HG2 | 2.01 | 0.41 |
| 1:I:643:ILE:HD12 | 1:I:643:ILE:HA | 1.86 | 0.41 |
| 1:J:207:ASP:OD2 | 1:J:209:ARG:HB3 | 2.20 | 0.41 |
| 1:J:339:VAL:HB | 1:J:564:LEU:O | 2.20 | 0.41 |
| 1:K:139:ILE:HG22 | 1:K:140:ILE:N | 2.27 | 0.41 |
| 1:L:357:ALA:HB3 | 1:L:407:ILE:HD11 | 2.01 | 0.41 |
| 1:M:113:ARG:HD2 | 1:M:134:TYR:CD2 | 2.55 | 0.41 |
| 1:M:139:ILE:C | 1:M:140:ILE:HG13 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:178:ALA:O | 1:M:181:VAL:HB | 2.21 | 0.41 |
| 1:N:142:ILE:CG2 | 1:N:149:VAL:HG22 | 2.50 | 0.41 |
| 1:O:99:GLU:O | 1:O:145:ARG:HA | 2.19 | 0.41 |
| 1:O:140:ILE:HG21 | 1:O:156:ILE:HG21 | 2.02 | 0.41 |
| 1:A:123:ILE:HG23 | 1:A:130:ASN:HB2 | 2.02 | 0.41 |
| 1:B:178:ALA:O | 1:B:181:VAL:HB | 2.21 | 0.41 |
| 1:B:313:LEU:HD11 | 1:C:295:VAL:HG21 | 2.03 | 0.41 |
| 1:B:643:ILE:HD12 | 1:B:643:ILE:HA | 1.86 | 0.41 |
| 1:E:178:ALA:O | 1:E:181:VAL:HB | 2.21 | 0.41 |
| 1:F:640:GLN:NE2 | 1:F:643:ILE:HG21 | 2.35 | 0.41 |
| 1:G:181:VAL:HG12 | 1:G:185:GLU:OE2 | 2.20 | 0.41 |
| 1:G:577:LEU:O | 1:G:578:MET:HE2 | 2.21 | 0.41 |
| 1:I:123:ILE:HG23 | 1:I:130:ASN:HB2 | 2.02 | 0.41 |
| 1:I:458:VAL:CG2 | 1:I:478:LYS:HG2 | 2.48 | 0.41 |
| 1:J:139:ILE:C | 1:J:140:ILE:HG13 | 2.41 | 0.41 |
| 1:J:246:TYR:HD1 | 1:J:293:SER:HB3 | 1.86 | 0.41 |
| 1:J:454:GLU:CD | 1:J:454:GLU:N | 2.73 | 0.41 |
| 1:K:123:ILE:HG23 | 1:K:130:ASN:HB2 | 2.02 | 0.41 |
| 1:K:139:ILE:C | 1:K:140:ILE:HG13 | 2.41 | 0.41 |
| 1:K:339:VAL:HB | 1:K:564:LEU:O | 2.20 | 0.41 |
| 1:L:178:ALA:O | 1:L:181:VAL:HB | 2.21 | 0.41 |
| 1:L:479:GLU:H | 1:L:479:GLU:CD | 2.07 | 0.41 |
| 1:M:142:ILE:CG2 | 1:M:149:VAL:HG22 | 2.50 | 0.41 |
| 1:M:247:LEU:CD1 | 1:M:255:LEU:HD12 | 2.50 | 0.41 |
| 1:N:256:VAL:HG23 | 1:N:285:ILE:HG22 | 2.03 | 0.41 |
| 1:N:458:VAL:CG2 | 1:N:478:LYS:HG2 | 2.48 | 0.41 |
| 1:N:539:GLY:CA | 1:N:577:LEU:O | 2.68 | 0.41 |
| 1:O:113:ARG:HD2 | 1:O:134:TYR:CD2 | 2.55 | 0.41 |
| 1:A:178:ALA:O | 1:A:181:VAL:HB | 2.21 | 0.41 |
| 1:A:215:ILE:HD12 | 1:A:215:ILE:HA | 1.82 | 0.41 |
| 1:B:99:GLU:O | 1:B:145:ARG:HA | 2.19 | 0.41 |
| 1:B:339:VAL:HB | 1:B:564:LEU:O | 2.20 | 0.41 |
| 1:B:640:GLN:NE2 | 1:B:643:ILE:HG21 | 2.35 | 0.41 |
| 1:C:313:LEU:HD11 | 1:D:295:VAL:HG21 | 2.03 | 0.41 |
| 1:C:577:LEU:O | 1:C:578:MET:HE2 | 2.20 | 0.41 |
| 1:D:140:ILE:HG21 | 1:D:156:ILE:HG21 | 2.02 | 0.41 |
| 1:E:207:ASP:OD2 | 1:E:209:ARG:HB3 | 2.20 | 0.41 |
| 1:E:504:VAL:HG11 | 1:E:521:ARG:CG | 2.47 | 0.41 |
| 1:F:140:ILE:HG21 | 1:F:156:ILE:HG21 | 2.02 | 0.41 |
| 1:F:178:ALA:O | 1:F:181:VAL:HB | 2.21 | 0.41 |
| 1:F:539:GLY:CA | 1:F:577:LEU:O | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:345:GLU:HG3 | 1:G:346:SER:H | 1.86 | 0.41 |
| 1:H:345:GLU:HG3 | 1:H:346:SER:H | 1.86 | 0.41 |
| 1:J:577:LEU:O | 1:J:578:MET:HE2 | 2.20 | 0.41 |
| 1:K:178:ALA:O | 1:K:181:VAL:HB | 2.21 | 0.41 |
| 1:K:288:HIS:HD2 | 1:K:291:THR:HB | 1.86 | 0.41 |
| 1:L:123:ILE:HG23 | 1:L:130:ASN:HB2 | 2.02 | 0.41 |
| 1:L:140:ILE:HG21 | 1:L:156:ILE:HG21 | 2.02 | 0.41 |
| 1:L:207:ASP:OD2 | 1:L:209:ARG:HB3 | 2.20 | 0.41 |
| 1:L:256:VAL:HG23 | 1:L:285:ILE:HG22 | 2.03 | 0.41 |
| 1:L:288:HIS:HD2 | 1:L:291:THR:HB | 1.86 | 0.41 |
| 1:M:246:TYR:HD1 | 1:M:293:SER:HB3 | 1.86 | 0.41 |
| 1:N:99:GLU:O | 1:N:145:ARG:HA | 2.19 | 0.41 |
| 1:N:178:ALA:O | 1:N:181:VAL:HB | 2.21 | 0.41 |
| 1:N:246:TYR:HD1 | 1:N:293:SER:HB3 | 1.85 | 0.41 |
| 1:O:288:HIS:HD2 | 1:O:291:THR:HB | 1.86 | 0.41 |
| 1:O:339:VAL:HB | 1:O:564:LEU:O | 2.20 | 0.41 |
| 1:A:166:GLU:HB3 | 1:A:167:ILE:H | 1.67 | 0.41 |
| 1:A:313:LEU:HD11 | 1:B:295:VAL:HG21 | 2.03 | 0.41 |
| 1:B:132:VAL:HG22 | 1:B:142:ILE:HG23 | 2.03 | 0.41 |
| 1:C:99:GLU:O | 1:C:145:ARG:HA | 2.20 | 0.41 |
| 1:C:339:VAL:HB | 1:C:564:LEU:O | 2.20 | 0.41 |
| 1:D:207:ASP:OD2 | 1:D:209:ARG:HB3 | 2.20 | 0.41 |
| 1:D:225:LEU:HD23 | 1:D:225:LEU:HA | 1.74 | 0.41 |
| 1:E:99:GLU:O | 1:E:145:ARG:HA | 2.19 | 0.41 |
| 1:E:288:HIS:HD2 | 1:E:291:THR:HB | 1.86 | 0.41 |
| 1:F:288:HIS:HD2 | 1:F:291:THR:HB | 1.86 | 0.41 |
| 1:F:458:VAL:CG2 | 1:F:478:LYS:HG2 | 2.48 | 0.41 |
| 1:F:577:LEU:O | 1:F:578:MET:HE2 | 2.21 | 0.41 |
| 1:G:256:VAL:HG13 | 1:G:257:GLU:N | 2.36 | 0.41 |
| 1:H:246:TYR:HD1 | 1:H:293:SER:HB3 | 1.85 | 0.41 |
| 1:I:246:TYR:HD1 | 1:I:293:SER:HB3 | 1.86 | 0.41 |
| 1:J:123:ILE:HG23 | 1:J:130:ASN:HB2 | 2.02 | 0.41 |
| 1:J:178:ALA:O | 1:J:181:VAL:HB | 2.21 | 0.41 |
| 1:J:181:VAL:HG12 | 1:J:185:GLU:OE2 | 2.20 | 0.41 |
| 1:L:516:VAL:O | 1:L:516:VAL:HG23 | 2.19 | 0.41 |
| 1:M:207:ASP:OD2 | 1:M:209:ARG:HB3 | 2.20 | 0.41 |
| 1:O:139:ILE:C | 1:O:140:ILE:HG13 | 2.41 | 0.41 |
| 1:A:113:ARG:HD2 | 1:A:134:TYR:CD2 | 2.55 | 0.41 |
| 1:A:132:VAL:HG22 | 1:A:142:ILE:HG23 | 2.03 | 0.41 |
| 1:A:207:ASP:OD2 | 1:A:209:ARG:HB3 | 2.20 | 0.41 |
| 1:A:288:HIS:HD2 | 1:A:291:THR:HB | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:256:VAL:HG13 | 1:B:257:GLU:N | 2.36 | 0.41 |
| 1:B:345:GLU:HG3 | 1:B:346:SER:H | 1.86 | 0.41 |
| 1:C:215:ILE:HD12 | 1:C:215:ILE:HA | 1.82 | 0.41 |
| 1:C:256:VAL:HG23 | 1:C:285:ILE:HG22 | 2.03 | 0.41 |
| 1:C:640:GLN:NE2 | 1:C:643:ILE:HG21 | 2.35 | 0.41 |
| 1:D:123:ILE:HG23 | 1:D:130:ASN:HB2 | 2.02 | 0.41 |
| 1:D:256:VAL:HG13 | 1:D:257:GLU:N | 2.36 | 0.41 |
| 1:E:142:ILE:CG2 | 1:E:149:VAL:HG22 | 2.50 | 0.41 |
| 1:F:207:ASP:OD2 | 1:F:209:ARG:HB3 | 2.20 | 0.41 |
| 1:F:551:LYS:HB3 | 1:F:566:ARG:HG2 | 2.01 | 0.41 |
| 1:H:225:LEU:O | 1:H:229:ILE:HG13 | 2.19 | 0.41 |
| 1:H:577:LEU:O | 1:H:578:MET:HE2 | 2.21 | 0.41 |
| 1:K:207:ASP:OD2 | 1:K:209:ARG:HB3 | 2.20 | 0.41 |
| 1:K:516:VAL:HG23 | 1:K:516:VAL:O | 2.19 | 0.41 |
| 1:K:613:LYS:HG3 | 1:K:613:LYS:O | 2.21 | 0.41 |
| 1:L:215:ILE:HD12 | 1:L:215:ILE:HA | 1.82 | 0.41 |
| 1:N:139:ILE:C | 1:N:140:ILE:HG13 | 2.41 | 0.41 |
| 1:N:313:LEU:HD11 | 1:O:295:VAL:HG21 | 2.03 | 0.41 |
| 1:A:139:ILE:HG22 | 1:A:140:ILE:N | 2.27 | 0.41 |
| 1:A:295:VAL:HG21 | 1:O:313:LEU:HD11 | 2.03 | 0.41 |
| 1:A:345:GLU:HG3 | 1:A:346:SER:H | 1.86 | 0.41 |
| 1:B:246:TYR:HD1 | 1:B:293:SER:HB3 | 1.85 | 0.41 |
| 1:B:577:LEU:O | 1:B:578:MET:HE2 | 2.21 | 0.41 |
| 1:C:132:VAL:HG22 | 1:C:142:ILE:HG23 | 2.03 | 0.41 |
| 1:C:140:ILE:HG21 | 1:C:156:ILE:HG21 | 2.02 | 0.41 |
| 1:C:155:ILE:O | 1:C:158:ARG:HB3 | 2.21 | 0.41 |
| 1:C:246:TYR:HD1 | 1:C:293:SER:HB3 | 1.86 | 0.41 |
| 1:D:504:VAL:HG11 | 1:D:521:ARG:CG | 2.47 | 0.41 |
| 1:E:177:ALA:HB3 | 1:E:208:GLU:HG3 | 2.00 | 0.41 |
| 1:E:506:ASN:C | 1:E:506:ASN:ND2 | 2.73 | 0.41 |
| 1:F:113:ARG:HD2 | 1:F:134:TYR:CD2 | 2.55 | 0.41 |
| 1:F:345:GLU:HG3 | 1:F:346:SER:H | 1.86 | 0.41 |
| 1:G:215:ILE:HA | 1:G:215:ILE:HD12 | 1.82 | 0.41 |
| 1:G:225:LEU:HD23 | 1:G:225:LEU:HA | 1.74 | 0.41 |
| 1:G:551:LYS:HB3 | 1:G:566:ARG:HG2 | 2.01 | 0.41 |
| 1:H:142:ILE:CG2 | 1:H:149:VAL:HG22 | 2.50 | 0.41 |
| 1:H:256:VAL:HG13 | 1:H:257:GLU:N | 2.36 | 0.41 |
| 1:I:345:GLU:HG3 | 1:I:346:SER:H | 1.86 | 0.41 |
| 1:J:613:LYS:HG3 | 1:J:613:LYS:O | 2.21 | 0.41 |
| 1:K:215:ILE:HA | 1:K:215:ILE:HD12 | 1.82 | 0.41 |
| 1:K:459:ILE:HG13 | 1:K:475:VAL:HG12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:643:ILE:HD12 | 1:K:643:ILE:HA | 1.86 | 0.41 |
| 1:L:179:GLU:O | 1:L:183:ILE:HG23 | 2.21 | 0.41 |
| 1:L:342:GLY:HA3 | 1:L:363:MET:HE1 | 2.03 | 0.41 |
| 1:N:105:VAL:CG1 | 1:N:157:ARG:HE | 2.32 | 0.41 |
| 1:O:166:GLU:HB3 | 1:O:167:ILE:H | 1.67 | 0.41 |
| 1:O:178:ALA:O | 1:O:181:VAL:HB | 2.21 | 0.41 |
| 1:A:140:ILE:HG21 | 1:A:156:ILE:HG21 | 2.02 | 0.41 |
| 1:C:178:ALA:O | 1:C:181:VAL:HB | 2.21 | 0.41 |
| 1:E:139:ILE:HG22 | 1:E:140:ILE:N | 2.27 | 0.41 |
| 1:E:640:GLN:NE2 | 1:E:643:ILE:HG21 | 2.35 | 0.41 |
| 1:F:247:LEU:CD1 | 1:F:255:LEU:HD12 | 2.50 | 0.41 |
| 1:F:256:VAL:HG13 | 1:F:257:GLU:N | 2.36 | 0.41 |
| 1:F:552:VAL:H | 1:F:552:VAL:HG22 | 1.59 | 0.41 |
| 1:G:140:ILE:HG21 | 1:G:156:ILE:HG21 | 2.02 | 0.41 |
| 1:G:155:ILE:O | 1:G:158:ARG:HB3 | 2.21 | 0.41 |
| 1:G:180:MET:HE2 | 1:G:213:ILE:HD11 | 2.01 | 0.41 |
| 1:H:113:ARG:HD2 | 1:H:134:TYR:CD2 | 2.55 | 0.41 |
| 1:H:123:ILE:HG23 | 1:H:130:ASN:HB2 | 2.02 | 0.41 |
| 1:H:524:ASN:OD1 | 1:I:449:SER:HB2 | 2.21 | 0.41 |
| 1:H:551:LYS:HB3 | 1:H:566:ARG:HG2 | 2.02 | 0.41 |
| 1:I:178:ALA:O | 1:I:181:VAL:HB | 2.21 | 0.41 |
| 1:I:181:VAL:HG12 | 1:I:185:GLU:OE2 | 2.20 | 0.41 |
| 1:I:256:VAL:HG13 | 1:I:257:GLU:N | 2.36 | 0.41 |
| 1:I:288:HIS:HD2 | 1:I:291:THR:HB | 1.86 | 0.41 |
| 1:I:524:ASN:OD1 | 1:J:449:SER:HB2 | 2.21 | 0.41 |
| 1:J:102:THR:OG1 | 1:J:142:ILE:O | 2.25 | 0.41 |
| 1:J:105:VAL:CG1 | 1:J:157:ARG:HE | 2.32 | 0.41 |
| 1:J:142:ILE:CG2 | 1:J:149:VAL:HG22 | 2.50 | 0.41 |
| 1:J:288:HIS:HD2 | 1:J:291:THR:HB | 1.86 | 0.41 |
| 1:J:459:ILE:HG13 | 1:J:475:VAL:HG12 | 2.03 | 0.41 |
| 1:J:524:ASN:OD1 | 1:K:449:SER:HB2 | 2.21 | 0.41 |
| 1:J:539:GLY:CA | 1:J:577:LEU:O | 2.68 | 0.41 |
| 1:K:140:ILE:HG21 | 1:K:156:ILE:HG21 | 2.02 | 0.41 |
| 1:K:179:GLU:O | 1:K:183:ILE:HG23 | 2.21 | 0.41 |
| 1:K:440:ILE:HD12 | 1:K:440:ILE:HA | 1.91 | 0.41 |
| 1:K:479:GLU:H | 1:K:479:GLU:CD | 2.07 | 0.41 |
| 1:K:640:GLN:NE2 | 1:K:643:ILE:HG21 | 2.35 | 0.41 |
| 1:L:142:ILE:CG2 | 1:L:149:VAL:HG22 | 2.50 | 0.41 |
| 1:L:246:TYR:HD1 | 1:L:293:SER:HB3 | 1.86 | 0.41 |
| 1:L:459:ILE:HG13 | 1:L:475:VAL:HG12 | 2.03 | 0.41 |
| 1:L:506:ASN:C | 1:L:506:ASN:ND2 | 2.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:613:LYS:HG3 | 1:L:613:LYS:O | 2.21 | 0.41 |
| 1:L:640:GLN:NE2 | 1:L:643:ILE:HG21 | 2.36 | 0.41 |
| 1:M:123:ILE:HG23 | 1:M:130:ASN:HB2 | 2.02 | 0.41 |
| 1:M:179:GLU:O | 1:M:183:ILE:HG23 | 2.21 | 0.41 |
| 1:M:313:LEU:HD11 | 1:N:295:VAL:HG21 | 2.03 | 0.41 |
| 1:M:613:LYS:HG3 | 1:M:613:LYS:O | 2.21 | 0.41 |
| 1:M:640:GLN:NE2 | 1:M:643:ILE:HG21 | 2.36 | 0.41 |
| 1:N:339:VAL:HB | 1:N:564:LEU:O | 2.20 | 0.41 |
| 1:N:643:ILE:HD12 | 1:N:643:ILE:HA | 1.86 | 0.41 |
| 1:O:123:ILE:HG23 | 1:O:130:ASN:HB2 | 2.02 | 0.41 |
| 1:O:359:ILE:HD13 | 1:O:422:LEU:HB2 | 2.03 | 0.41 |
| 1:O:539:GLY:CA | 1:O:577:LEU:O | 2.68 | 0.41 |
| 1:A:359:ILE:HD13 | 1:A:422:LEU:HB2 | 2.04 | 0.41 |
| 1:B:139:ILE:C | 1:B:140:ILE:HG13 | 2.41 | 0.41 |
| 1:B:215:ILE:HD12 | 1:B:215:ILE:HA | 1.82 | 0.41 |
| 1:B:359:ILE:HD13 | 1:B:422:LEU:HB2 | 2.03 | 0.41 |
| 1:D:105:VAL:CG1 | 1:D:157:ARG:HE | 2.31 | 0.41 |
| 1:D:139:ILE:HG22 | 1:D:140:ILE:N | 2.27 | 0.41 |
| 1:D:139:ILE:C | 1:D:140:ILE:HG13 | 2.41 | 0.41 |
| 1:D:313:LEU:HD11 | 1:E:295:VAL:HG21 | 2.03 | 0.41 |
| 1:F:123:ILE:HG23 | 1:F:130:ASN:HB2 | 2.02 | 0.41 |
| 1:G:524:ASN:OD1 | 1:H:449:SER:HB2 | 2.21 | 0.41 |
| 1:G:640:GLN:NE2 | 1:G:643:ILE:HG21 | 2.35 | 0.41 |
| 1:H:139:ILE:C | 1:H:140:ILE:HG13 | 2.41 | 0.41 |
| 1:H:181:VAL:HG12 | 1:H:185:GLU:OE2 | 2.20 | 0.41 |
| 1:I:139:ILE:C | 1:I:140:ILE:HG13 | 2.41 | 0.41 |
| 1:J:155:ILE:O | 1:J:158:ARG:HB3 | 2.21 | 0.41 |
| 1:L:345:GLU:HG3 | 1:L:346:SER:H | 1.86 | 0.41 |
| 1:N:640:GLN:NE2 | 1:N:643:ILE:HG21 | 2.35 | 0.41 |
| 1:B:113:ARG:HD2 | 1:B:134:TYR:CD2 | 2.55 | 0.40 |
| 1:B:288:HIS:HD2 | 1:B:291:THR:HB | 1.86 | 0.40 |
| 1:C:139:ILE:C | 1:C:140:ILE:HG13 | 2.41 | 0.40 |
| 1:C:345:GLU:HG3 | 1:C:346:SER:H | 1.86 | 0.40 |
| 1:D:99:GLU:O | 1:D:145:ARG:HA | 2.19 | 0.40 |
| 1:D:132:VAL:HG22 | 1:D:142:ILE:HG23 | 2.03 | 0.40 |
| 1:D:155:ILE:O | 1:D:158:ARG:HB3 | 2.21 | 0.40 |
| 1:D:178:ALA:O | 1:D:181:VAL:HB | 2.21 | 0.40 |
| 1:E:139:ILE:C | 1:E:140:ILE:HG13 | 2.41 | 0.40 |
| 1:E:313:LEU:HD11 | 1:F:295:VAL:HG21 | 2.03 | 0.40 |
| 1:E:577:LEU:O | 1:E:578:MET:HE2 | 2.21 | 0.40 |
| 1:E:643:ILE:HD12 | 1:E:643:ILE:HA | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:113:ARG:HD2 | 1:G:134:TYR:CD2 | 2.55 | 0.40 |
| 1:G:123:ILE:HG23 | 1:G:130:ASN:HB2 | 2.02 | 0.40 |
| 1:G:285:ILE:HD12 | 1:G:296:LEU:HD23 | 2.03 | 0.40 |
| 1:G:613:LYS:O | 1:G:613:LYS:HG3 | 2.21 | 0.40 |
| 1:H:132:VAL:HG22 | 1:H:142:ILE:HG23 | 2.03 | 0.40 |
| 1:I:459:ILE:HG13 | 1:I:475:VAL:HG12 | 2.03 | 0.40 |
| 1:J:479:GLU:H | 1:J:479:GLU:CD | 2.07 | 0.40 |
| 1:K:155:ILE:O | 1:K:158:ARG:HB3 | 2.21 | 0.40 |
| 1:N:613:LYS:HG3 | 1:N:613:LYS:O | 2.21 | 0.40 |
| 1:O:506:ASN:C | 1:O:506:ASN:ND2 | 2.73 | 0.40 |
| 1:A:139:ILE:C | 1:A:140:ILE:HG13 | 2.41 | 0.40 |
| 1:A:451:ILE:HG21 | 1:O:522:GLN:HG2 | 2.04 | 0.40 |
| 1:A:522:GLN:HG2 | 1:B:451:ILE:HG21 | 2.04 | 0.40 |
| 1:B:140:ILE:HG21 | 1:B:156:ILE:HG21 | 2.02 | 0.40 |
| 1:E:552:VAL:H | 1:E:552:VAL:HG22 | 1.59 | 0.40 |
| 1:F:155:ILE:O | 1:F:158:ARG:HB3 | 2.21 | 0.40 |
| 1:G:177:ALA:HB3 | 1:G:208:GLU:HG3 | 2.00 | 0.40 |
| 1:G:178:ALA:O | 1:G:181:VAL:HB | 2.21 | 0.40 |
| 1:G:246:TYR:HD1 | 1:G:293:SER:HB3 | 1.86 | 0.40 |
| 1:H:640:GLN:NE2 | 1:H:643:ILE:HG21 | 2.35 | 0.40 |
| 1:I:132:VAL:HG22 | 1:I:142:ILE:HG23 | 2.03 | 0.40 |
| 1:I:155:ILE:O | 1:I:158:ARG:HB3 | 2.21 | 0.40 |
| 1:I:285:ILE:HD12 | 1:I:296:LEU:HD23 | 2.04 | 0.40 |
| 1:J:113:ARG:HD2 | 1:J:134:TYR:CD2 | 2.55 | 0.40 |
| 1:J:179:GLU:O | 1:J:183:ILE:HG23 | 2.21 | 0.40 |
| 1:K:142:ILE:CG2 | 1:K:149:VAL:HG22 | 2.50 | 0.40 |
| 1:M:345:GLU:HG3 | 1:M:346:SER:H | 1.86 | 0.40 |
| 1:M:359:ILE:HD13 | 1:M:422:LEU:HB2 | 2.03 | 0.40 |
| 1:N:179:GLU:O | 1:N:183:ILE:HG23 | 2.21 | 0.40 |
| 1:N:359:ILE:HD13 | 1:N:422:LEU:HB2 | 2.04 | 0.40 |
| 1:O:132:VAL:HG22 | 1:O:142:ILE:HG23 | 2.03 | 0.40 |
| 1:O:142:ILE:CG2 | 1:O:149:VAL:HG22 | 2.50 | 0.40 |
| 1:A:105:VAL:CG1 | 1:A:157:ARG:HE | 2.32 | 0.40 |
| 1:A:155:ILE:O | 1:A:158:ARG:HB3 | 2.21 | 0.40 |
| 1:A:612:GLU:CG | 1:B:642:PHE:CE2 | 2.81 | 0.40 |
| 1:B:105:VAL:CG1 | 1:B:157:ARG:HE | 2.31 | 0.40 |
| 1:B:142:ILE:CG2 | 1:B:149:VAL:HG22 | 2.50 | 0.40 |
| 1:B:256:VAL:HG23 | 1:B:285:ILE:HG22 | 2.03 | 0.40 |
| 1:C:359:ILE:HD13 | 1:C:422:LEU:HB2 | 2.03 | 0.40 |
| 1:E:166:GLU:HB3 | 1:E:167:ILE:H | 1.67 | 0.40 |
| 1:E:256:VAL:HG23 | 1:E:285:ILE:HG22 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:345:GLU:HG3 | 1:E:346:SER:H | 1.86 | 0.40 |
| 1:F:524:ASN:OD1 | 1:G:449:SER:HB2 | 2.21 | 0.40 |
| 1:G:132:VAL:HG22 | 1:G:142:ILE:HG23 | 2.03 | 0.40 |
| 1:G:142:ILE:CG2 | 1:G:149:VAL:HG22 | 2.50 | 0.40 |
| 1:G:288:HIS:HD2 | 1:G:291:THR:HB | 1.86 | 0.40 |
| 1:H:155:ILE:O | 1:H:158:ARG:HB3 | 2.21 | 0.40 |
| 1:H:179:GLU:O | 1:H:183:ILE:HG23 | 2.21 | 0.40 |
| 1:H:458:VAL:CG2 | 1:H:478:LYS:HG2 | 2.48 | 0.40 |
| 1:I:113:ARG:HD2 | 1:I:134:TYR:CD2 | 2.55 | 0.40 |
| 1:I:313:LEU:HD11 | 1:J:295:VAL:HG21 | 2.03 | 0.40 |
| 1:I:479:GLU:H | 1:I:479:GLU:CD | 2.07 | 0.40 |
| 1:J:256:VAL:HG23 | 1:J:285:ILE:HG22 | 2.03 | 0.40 |
| 1:J:256:VAL:HG13 | 1:J:257:GLU:N | 2.36 | 0.40 |
| 1:K:113:ARG:HD2 | 1:K:134:TYR:CD2 | 2.55 | 0.40 |
| 1:K:524:ASN:OD1 | 1:L:449:SER:HB2 | 2.21 | 0.40 |
| 1:L:360:GLY:O | 1:L:364:ILE:HG12 | 2.22 | 0.40 |
| 1:L:524:ASN:N | 1:L:524:ASN:OD1 | 2.55 | 0.40 |
| 1:M:360:GLY:O | 1:M:364:ILE:HG12 | 2.22 | 0.40 |
| 1:M:459:ILE:HG13 | 1:M:475:VAL:HG12 | 2.03 | 0.40 |
| 1:M:552:VAL:H | 1:M:552:VAL:HG22 | 1.59 | 0.40 |
| 1:O:155:ILE:O | 1:O:158:ARG:HB3 | 2.21 | 0.40 |
| 1:O:256:VAL:HG13 | 1:O:257:GLU:N | 2.36 | 0.40 |
| 1:O:524:ASN:N | 1:O:524:ASN:OD1 | 2.55 | 0.40 |
| 1:B:155:ILE:O | 1:B:158:ARG:HB3 | 2.21 | 0.40 |
| 1:B:539:GLY:CA | 1:B:577:LEU:O | 2.68 | 0.40 |
| 1:D:288:HIS:HD2 | 1:D:291:THR:HB | 1.86 | 0.40 |
| 1:E:256:VAL:HG13 | 1:E:257:GLU:N | 2.36 | 0.40 |
| 1:F:139:ILE:C | 1:F:140:ILE:HG13 | 2.41 | 0.40 |
| 1:H:459:ILE:HG13 | 1:H:475:VAL:HG12 | 2.03 | 0.40 |
| 1:H:613:LYS:O | 1:H:613:LYS:HG3 | 2.21 | 0.40 |
| 1:J:285:ILE:HD12 | 1:J:296:LEU:HD23 | 2.03 | 0.40 |
| 1:K:256:VAL:HG13 | 1:K:257:GLU:N | 2.36 | 0.40 |
| 1:L:155:ILE:O | 1:L:158:ARG:HB3 | 2.21 | 0.40 |
| 1:L:167:ILE:CA | 1:L:215:ILE:O | 2.42 | 0.40 |
| 1:M:105:VAL:CG1 | 1:M:157:ARG:HE | 2.32 | 0.40 |
| 1:N:123:ILE:HG23 | 1:N:130:ASN:HB2 | 2.02 | 0.40 |
| 1:N:155:ILE:O | 1:N:158:ARG:HB3 | 2.21 | 0.40 |
| 1:N:506:ASN:C | 1:N:506:ASN:ND2 | 2.73 | 0.40 |
| 1:O:256:VAL:HG23 | 1:O:285:ILE:HG22 | 2.03 | 0.40 |
| 1:O:613:LYS:HG3 | 1:O:613:LYS:O | 2.21 | 0.40 |
| 1:O:640:GLN:NE2 | 1:O:643:ILE:HG21 | 2.35 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:539:GLY:CA | 1:A:577:LEU:O | 2.68 | 0.40 |
| 1:B:459:ILE:HG13 | 1:B:475:VAL:HG12 | 2.03 | 0.40 |
| 1:B:522:GLN:HG2 | 1:C:451:ILE:HG21 | 2.04 | 0.40 |
| 1:C:459:ILE:HG13 | 1:C:475:VAL:HG12 | 2.03 | 0.40 |
| 1:D:459:ILE:HG13 | 1:D:475:VAL:HG12 | 2.03 | 0.40 |
| 1:F:285:ILE:HD12 | 1:F:296:LEU:HD23 | 2.04 | 0.40 |
| 1:G:360:GLY:O | 1:G:364:ILE:HG12 | 2.22 | 0.40 |
| 1:H:178:ALA:O | 1:H:181:VAL:HB | 2.21 | 0.40 |
| 1:H:285:ILE:HD12 | 1:H:296:LEU:HD23 | 2.04 | 0.40 |
| 1:H:479:GLU:H | 1:H:479:GLU:CD | 2.07 | 0.40 |
| 1:I:140:ILE:HG21 | 1:I:156:ILE:HG21 | 2.02 | 0.40 |
| 1:I:179:GLU:O | 1:I:183:ILE:HG23 | 2.21 | 0.40 |
| 1:J:140:ILE:HG21 | 1:J:156:ILE:HG21 | 2.02 | 0.40 |
| 1:J:640:GLN:NE2 | 1:J:643:ILE:HG21 | 2.35 | 0.40 |
| 1:K:119:LEU:HD13 | 1:K:132:VAL:HG11 | 2.04 | 0.40 |
| 1:K:132:VAL:HG22 | 1:K:142:ILE:HG23 | 2.03 | 0.40 |
| 1:K:506:ASN:C | 1:K:506:ASN:ND2 | 2.73 | 0.40 |
| 1:L:119:LEU:HD13 | 1:L:132:VAL:HG11 | 2.04 | 0.40 |
| 1:L:256:VAL:HG13 | 1:L:257:GLU:N | 2.36 | 0.40 |
| 1:M:155:ILE:O | 1:M:158:ARG:HB3 | 2.21 | 0.40 |
| 1:N:360:GLY:O | 1:N:364:ILE:HG12 | 2.22 | 0.40 |
| 1:O:523:LEU:HD22 | 1:O:538:GLY:HA3 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1 | A | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | B | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | C | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | D | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | E | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | F | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | G | 481/650 (74%) | 458 (95%) | 22 (5%) | 1 (0%) | 44 | 77 |
| 1 | H | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | I | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | J | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | K | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | L | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | M | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | N | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| 1 | O | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%) | 44 | 77 |
| All | All | 7215/9750 (74%) | 6884 (95%) | 316 (4%) | 15 (0%) | 45 | 77 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 181 | VAL |
| 1 | B | 181 | VAL |
| 1 | C | 181 | VAL |
| 1 | E | 181 | VAL |
| 1 | F | 181 | VAL |
| 1 | G | 181 | VAL |
| 1 | H | 181 | VAL |
| 1 | I | 181 | VAL |
| 1 | J | 181 | VAL |
| 1 | K | 181 | VAL |
| 1 | L | 181 | VAL |
| 1 | M | 181 | VAL |
| 1 | N | 181 | VAL |
| 1 | O | 181 | VAL |
| 1 | D | 181 | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | B | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | C | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | D | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | E | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | F | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | G | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | H | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | I | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | J | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | K | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | L | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | M | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | N | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| 1 | O | 415/550 (76%) | 403 (97%) | 12 (3%) | 37 | 58 |
| All | All | 6225/8250 (76%) | 6045 (97%) | 180 (3%) | 39 | 58 |

All (180) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 455 | GLU |
| 1 | A | 459 | ILE |
| 1 | A | 473 | GLN |
| 1 | A | 474 | THR |
| 1 | A | 476 | ASP |
| 1 | A | 477 | ARG |
| 1 | A | 478 | LYS |
| 1 | A | 506 | ASN |
| 1 | A | 517 | ARG |
| 1 | A | 518 | PHE |
| 1 | A | 520 | LYS |
| 1 | A | 521 | ARG |
| 1 | B | 455 | GLU |
| 1 | B | 459 | ILE |
| 1 | B | 473 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 474 | THR |
| 1 | B | 476 | ASP |
| 1 | B | 477 | ARG |
| 1 | B | 478 | LYS |
| 1 | B | 506 | ASN |
| 1 | B | 517 | ARG |
| 1 | B | 518 | PHE |
| 1 | B | 520 | LYS |
| 1 | B | 521 | ARG |
| 1 | C | 455 | GLU |
| 1 | C | 459 | ILE |
| 1 | C | 473 | GLN |
| 1 | C | 474 | THR |
| 1 | C | 476 | ASP |
| 1 | C | 477 | ARG |
| 1 | C | 478 | LYS |
| 1 | C | 506 | ASN |
| 1 | C | 517 | ARG |
| 1 | C | 518 | PHE |
| 1 | C | 520 | LYS |
| 1 | C | 521 | ARG |
| 1 | D | 455 | GLU |
| 1 | D | 459 | ILE |
| 1 | D | 473 | GLN |
| 1 | D | 474 | THR |
| 1 | D | 476 | ASP |
| 1 | D | 477 | ARG |
| 1 | D | 478 | LYS |
| 1 | D | 506 | ASN |
| 1 | D | 517 | ARG |
| 1 | D | 518 | PHE |
| 1 | D | 520 | LYS |
| 1 | D | 521 | ARG |
| 1 | E | 455 | GLU |
| 1 | E | 459 | ILE |
| 1 | E | 473 | GLN |
| 1 | E | 474 | THR |
| 1 | E | 476 | ASP |
| 1 | E | 477 | ARG |
| 1 | E | 478 | LYS |
| 1 | E | 506 | ASN |
| 1 | E | 517 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 518 | PHE |
| 1 | E | 520 | LYS |
| 1 | E | 521 | ARG |
| 1 | F | 455 | GLU |
| 1 | F | 459 | ILE |
| 1 | F | 473 | GLN |
| 1 | F | 474 | THR |
| 1 | F | 476 | ASP |
| 1 | F | 477 | ARG |
| 1 | F | 478 | LYS |
| 1 | F | 506 | ASN |
| 1 | F | 517 | ARG |
| 1 | F | 518 | PHE |
| 1 | F | 520 | LYS |
| 1 | F | 521 | ARG |
| 1 | G | 455 | GLU |
| 1 | G | 459 | ILE |
| 1 | G | 473 | GLN |
| 1 | G | 474 | THR |
| 1 | G | 476 | ASP |
| 1 | G | 477 | ARG |
| 1 | G | 478 | LYS |
| 1 | G | 506 | ASN |
| 1 | G | 517 | ARG |
| 1 | G | 518 | PHE |
| 1 | G | 520 | LYS |
| 1 | G | 521 | ARG |
| 1 | H | 455 | GLU |
| 1 | H | 459 | ILE |
| 1 | H | 473 | GLN |
| 1 | H | 474 | THR |
| 1 | H | 476 | ASP |
| 1 | H | 477 | ARG |
| 1 | H | 478 | LYS |
| 1 | H | 506 | ASN |
| 1 | H | 517 | ARG |
| 1 | H | 518 | PHE |
| 1 | H | 520 | LYS |
| 1 | H | 521 | ARG |
| 1 | I | 455 | GLU |
| 1 | I | 459 | ILE |
| 1 | I | 473 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 474 | THR |
| 1 | I | 476 | ASP |
| 1 | I | 477 | ARG |
| 1 | I | 478 | LYS |
| 1 | I | 506 | ASN |
| 1 | I | 517 | ARG |
| 1 | I | 518 | PHE |
| 1 | I | 520 | LYS |
| 1 | I | 521 | ARG |
| 1 | J | 455 | GLU |
| 1 | J | 459 | ILE |
| 1 | J | 473 | GLN |
| 1 | J | 474 | THR |
| 1 | J | 476 | ASP |
| 1 | J | 477 | ARG |
| 1 | J | 478 | LYS |
| 1 | J | 506 | ASN |
| 1 | J | 517 | ARG |
| 1 | J | 518 | PHE |
| 1 | J | 520 | LYS |
| 1 | J | 521 | ARG |
| 1 | K | 455 | GLU |
| 1 | K | 459 | ILE |
| 1 | K | 473 | GLN |
| 1 | K | 474 | THR |
| 1 | K | 476 | ASP |
| 1 | K | 477 | ARG |
| 1 | K | 478 | LYS |
| 1 | K | 506 | ASN |
| 1 | K | 517 | ARG |
| 1 | K | 518 | PHE |
| 1 | K | 520 | LYS |
| 1 | K | 521 | ARG |
| 1 | L | 455 | GLU |
| 1 | L | 459 | ILE |
| 1 | L | 473 | GLN |
| 1 | L | 474 | THR |
| 1 | L | 476 | ASP |
| 1 | L | 477 | ARG |
| 1 | L | 478 | LYS |
| 1 | L | 506 | ASN |
| 1 | L | 517 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 518 | PHE |
| 1 | L | 520 | LYS |
| 1 | L | 521 | ARG |
| 1 | M | 455 | GLU |
| 1 | M | 459 | ILE |
| 1 | M | 473 | GLN |
| 1 | M | 474 | THR |
| 1 | M | 476 | ASP |
| 1 | M | 477 | ARG |
| 1 | M | 478 | LYS |
| 1 | M | 506 | ASN |
| 1 | M | 517 | ARG |
| 1 | M | 518 | PHE |
| 1 | M | 520 | LYS |
| 1 | M | 521 | ARG |
| 1 | N | 455 | GLU |
| 1 | N | 459 | ILE |
| 1 | N | 473 | GLN |
| 1 | N | 474 | THR |
| 1 | N | 476 | ASP |
| 1 | N | 477 | ARG |
| 1 | N | 478 | LYS |
| 1 | N | 506 | ASN |
| 1 | N | 517 | ARG |
| 1 | N | 518 | PHE |
| 1 | N | 520 | LYS |
| 1 | N | 521 | ARG |
| 1 | O | 455 | GLU |
| 1 | O | 459 | ILE |
| 1 | O | 473 | GLN |
| 1 | O | 474 | THR |
| 1 | O | 476 | ASP |
| 1 | O | 477 | ARG |
| 1 | O | 478 | LYS |
| 1 | O | 506 | ASN |
| 1 | O | 517 | ARG |
| 1 | O | 518 | PHE |
| 1 | O | 520 | LYS |
| 1 | O | 521 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 125 | ASN |
| 1 | A | 138 | ASN |
| 1 | A | 288 | HIS |
| 1 | A | 300 | GLN |
| 1 | A | 340 | GLN |
| 1 | A | 354 | ASN |
| 1 | A | 424 | ASN |
| 1 | A | 428 | ASN |
| 1 | A | 502 | GLN |
| 1 | A | 506 | ASN |
| 1 | A | 640 | GLN |
| 1 | B | 125 | ASN |
| 1 | B | 138 | ASN |
| 1 | B | 288 | HIS |
| 1 | B | 300 | GLN |
| 1 | B | 340 | GLN |
| 1 | B | 354 | ASN |
| 1 | B | 424 | ASN |
| 1 | B | 428 | ASN |
| 1 | B | 502 | GLN |
| 1 | B | 506 | ASN |
| 1 | B | 640 | GLN |
| 1 | C | 125 | ASN |
| 1 | C | 138 | ASN |
| 1 | C | 288 | HIS |
| 1 | C | 300 | GLN |
| 1 | C | 340 | GLN |
| 1 | C | 354 | ASN |
| 1 | C | 424 | ASN |
| 1 | C | 428 | ASN |
| 1 | C | 502 | GLN |
| 1 | C | 506 | ASN |
| 1 | C | 640 | GLN |
| 1 | D | 125 | ASN |
| 1 | D | 138 | ASN |
| 1 | D | 288 | HIS |
| 1 | D | 300 | GLN |
| 1 | D | 340 | GLN |
| 1 | D | 354 | ASN |
| 1 | D | 424 | ASN |
| 1 | D | 428 | ASN |
| 1 | D | 502 | GLN |
| 1 | D | 506 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 640 | GLN |
| 1 | E | 125 | ASN |
| 1 | E | 138 | ASN |
| 1 | E | 288 | HIS |
| 1 | E | 300 | GLN |
| 1 | E | 340 | GLN |
| 1 | E | 354 | ASN |
| 1 | E | 424 | ASN |
| 1 | E | 428 | ASN |
| 1 | E | 502 | GLN |
| 1 | E | 506 | ASN |
| 1 | E | 640 | GLN |
| 1 | F | 125 | ASN |
| 1 | F | 138 | ASN |
| 1 | F | 288 | HIS |
| 1 | F | 300 | GLN |
| 1 | F | 340 | GLN |
| 1 | F | 354 | ASN |
| 1 | F | 424 | ASN |
| 1 | F | 428 | ASN |
| 1 | F | 502 | GLN |
| 1 | F | 506 | ASN |
| 1 | F | 640 | GLN |
| 1 | G | 125 | ASN |
| 1 | G | 138 | ASN |
| 1 | G | 288 | HIS |
| 1 | G | 300 | GLN |
| 1 | G | 340 | GLN |
| 1 | G | 354 | ASN |
| 1 | G | 424 | ASN |
| 1 | G | 428 | ASN |
| 1 | G | 502 | GLN |
| 1 | G | 506 | ASN |
| 1 | G | 640 | GLN |
| 1 | H | 125 | ASN |
| 1 | H | 138 | ASN |
| 1 | H | 288 | HIS |
| 1 | H | 300 | GLN |
| 1 | H | 340 | GLN |
| 1 | H | 354 | ASN |
| 1 | H | 424 | ASN |
| 1 | H | 428 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 502 | GLN |
| 1 | H | 506 | ASN |
| 1 | H | 640 | GLN |
| 1 | I | 125 | ASN |
| 1 | I | 138 | ASN |
| 1 | I | 288 | HIS |
| 1 | I | 300 | GLN |
| 1 | I | 340 | GLN |
| 1 | I | 354 | ASN |
| 1 | I | 424 | ASN |
| 1 | I | 428 | ASN |
| 1 | I | 502 | GLN |
| 1 | I | 506 | ASN |
| 1 | I | 640 | GLN |
| 1 | J | 125 | ASN |
| 1 | J | 138 | ASN |
| 1 | J | 288 | HIS |
| 1 | J | 300 | GLN |
| 1 | J | 340 | GLN |
| 1 | J | 354 | ASN |
| 1 | J | 424 | ASN |
| 1 | J | 428 | ASN |
| 1 | J | 502 | GLN |
| 1 | J | 506 | ASN |
| 1 | J | 640 | GLN |
| 1 | K | 125 | ASN |
| 1 | K | 138 | ASN |
| 1 | K | 288 | HIS |
| 1 | K | 300 | GLN |
| 1 | K | 340 | GLN |
| 1 | K | 354 | ASN |
| 1 | K | 424 | ASN |
| 1 | K | 428 | ASN |
| 1 | K | 502 | GLN |
| 1 | K | 506 | ASN |
| 1 | K | 640 | GLN |
| 1 | L | 125 | ASN |
| 1 | L | 138 | ASN |
| 1 | L | 288 | HIS |
| 1 | L | 300 | GLN |
| 1 | L | 340 | GLN |
| 1 | L | 354 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 424 | ASN |
| 1 | L | 428 | ASN |
| 1 | L | 502 | GLN |
| 1 | L | 506 | ASN |
| 1 | L | 640 | GLN |
| 1 | M | 125 | ASN |
| 1 | M | 138 | ASN |
| 1 | M | 288 | HIS |
| 1 | M | 300 | GLN |
| 1 | M | 340 | GLN |
| 1 | M | 354 | ASN |
| 1 | M | 424 | ASN |
| 1 | M | 428 | ASN |
| 1 | M | 502 | GLN |
| 1 | M | 506 | ASN |
| 1 | M | 640 | GLN |
| 1 | N | 125 | ASN |
| 1 | N | 138 | ASN |
| 1 | N | 288 | HIS |
| 1 | N | 300 | GLN |
| 1 | N | 340 | GLN |
| 1 | N | 354 | ASN |
| 1 | N | 424 | ASN |
| 1 | N | 428 | ASN |
| 1 | N | 502 | GLN |
| 1 | N | 506 | ASN |
| 1 | N | 640 | GLN |
| 1 | O | 125 | ASN |
| 1 | O | 138 | ASN |
| 1 | O | 288 | HIS |
| 1 | O | 300 | GLN |
| 1 | O | 340 | GLN |
| 1 | O | 354 | ASN |
| 1 | O | 424 | ASN |
| 1 | O | 428 | ASN |
| 1 | O | 502 | GLN |
| 1 | O | 506 | ASN |
| 1 | O | 640 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

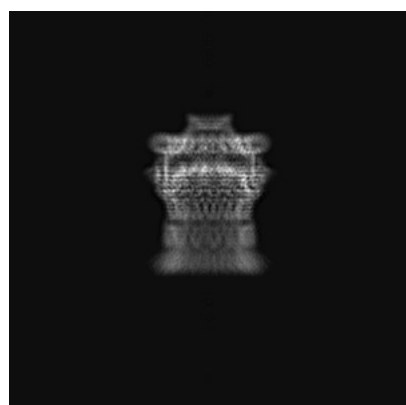
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6677. These allow visual inspection of the internal detail of the map and identification of artifacts.

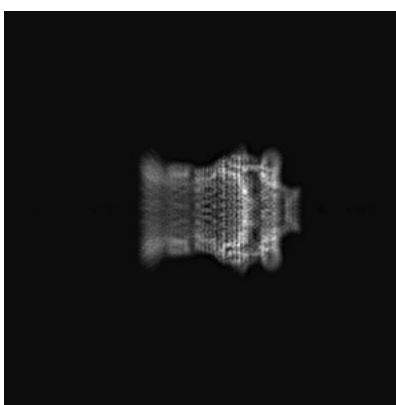
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

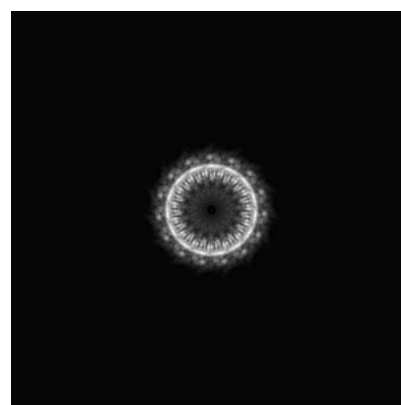
6.1.1 Primary map



X



Y

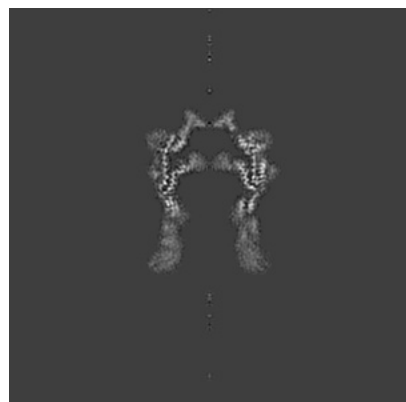


Z

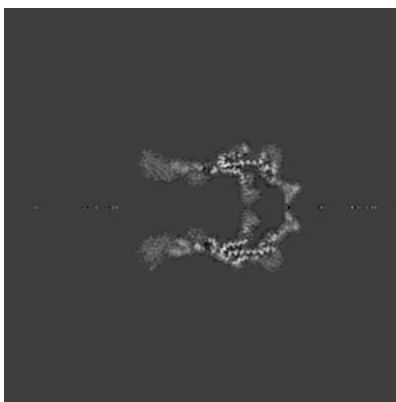
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

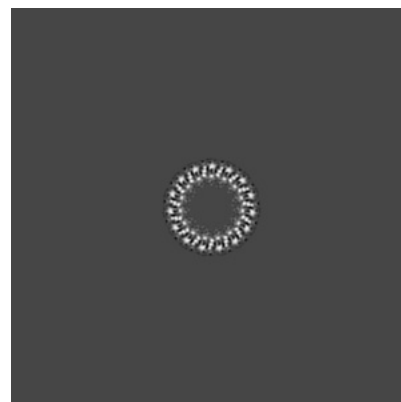
6.2.1 Primary map



X Index: 190



Y Index: 190



Z Index: 190

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

6.3 Largest variance slices [i](#)

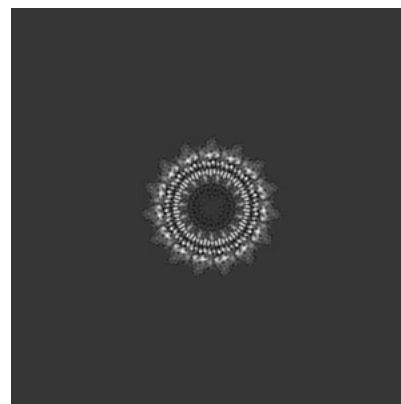
6.3.1 Primary map



X Index: 224



Y Index: 224

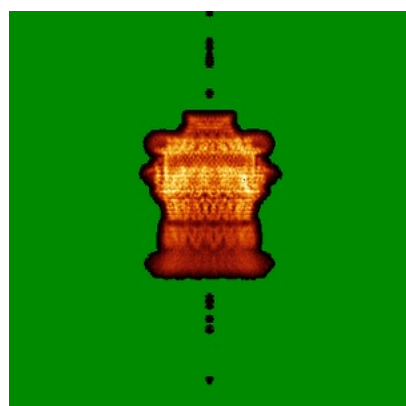


Z Index: 223

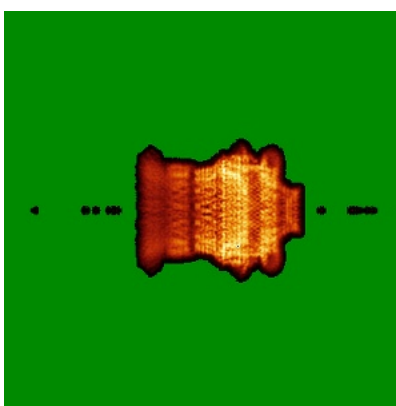
The images above show the largest variance slices of the map in three orthogonal directions.

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

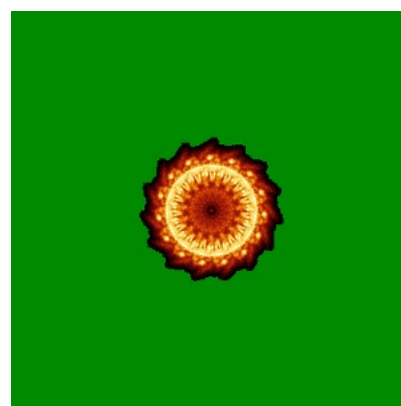
6.4.1 Primary map



X



Y

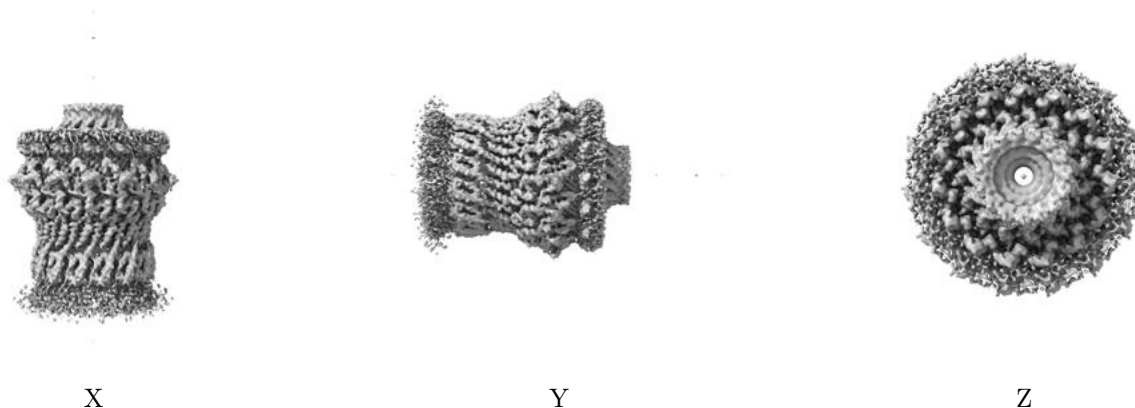


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

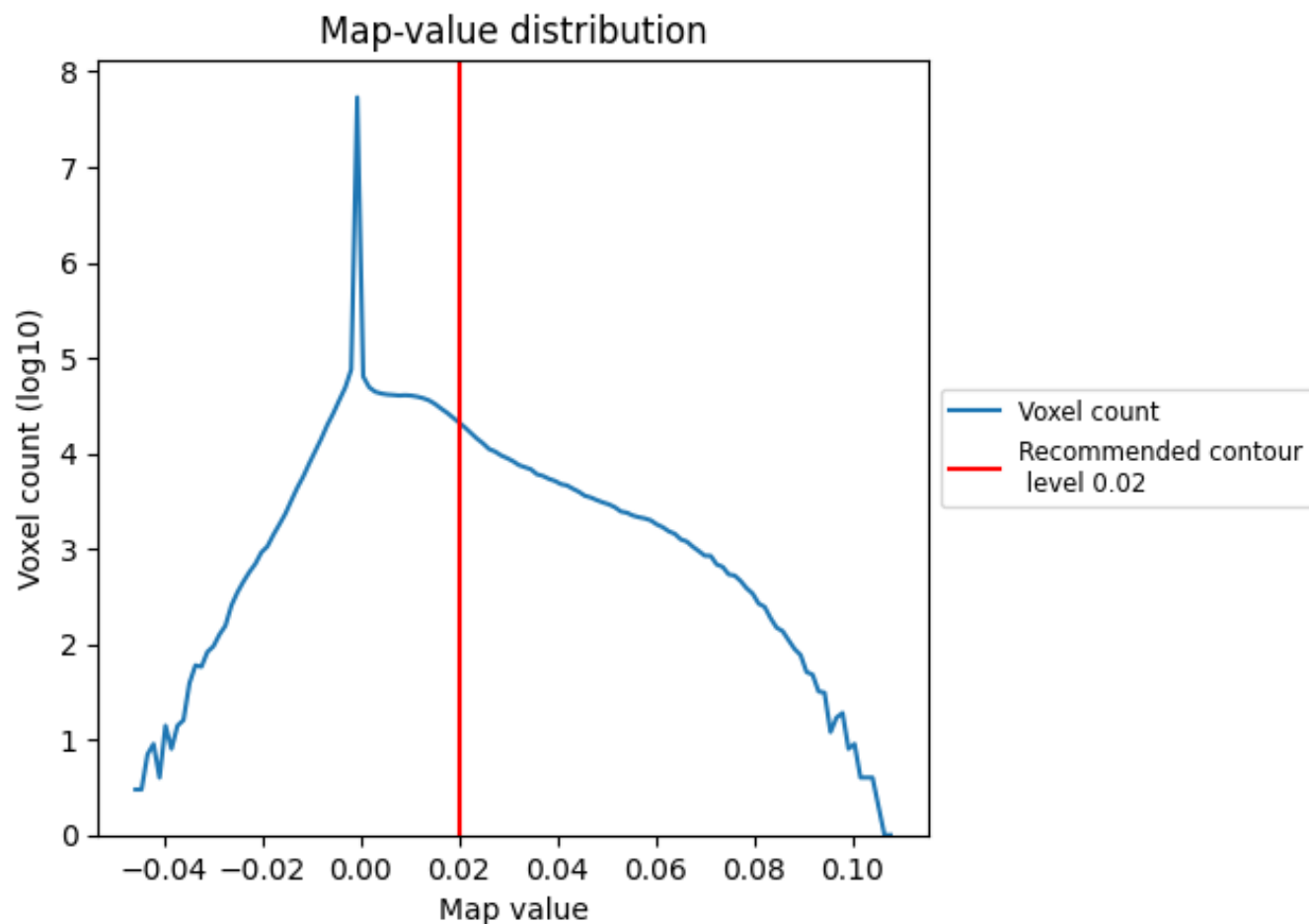
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

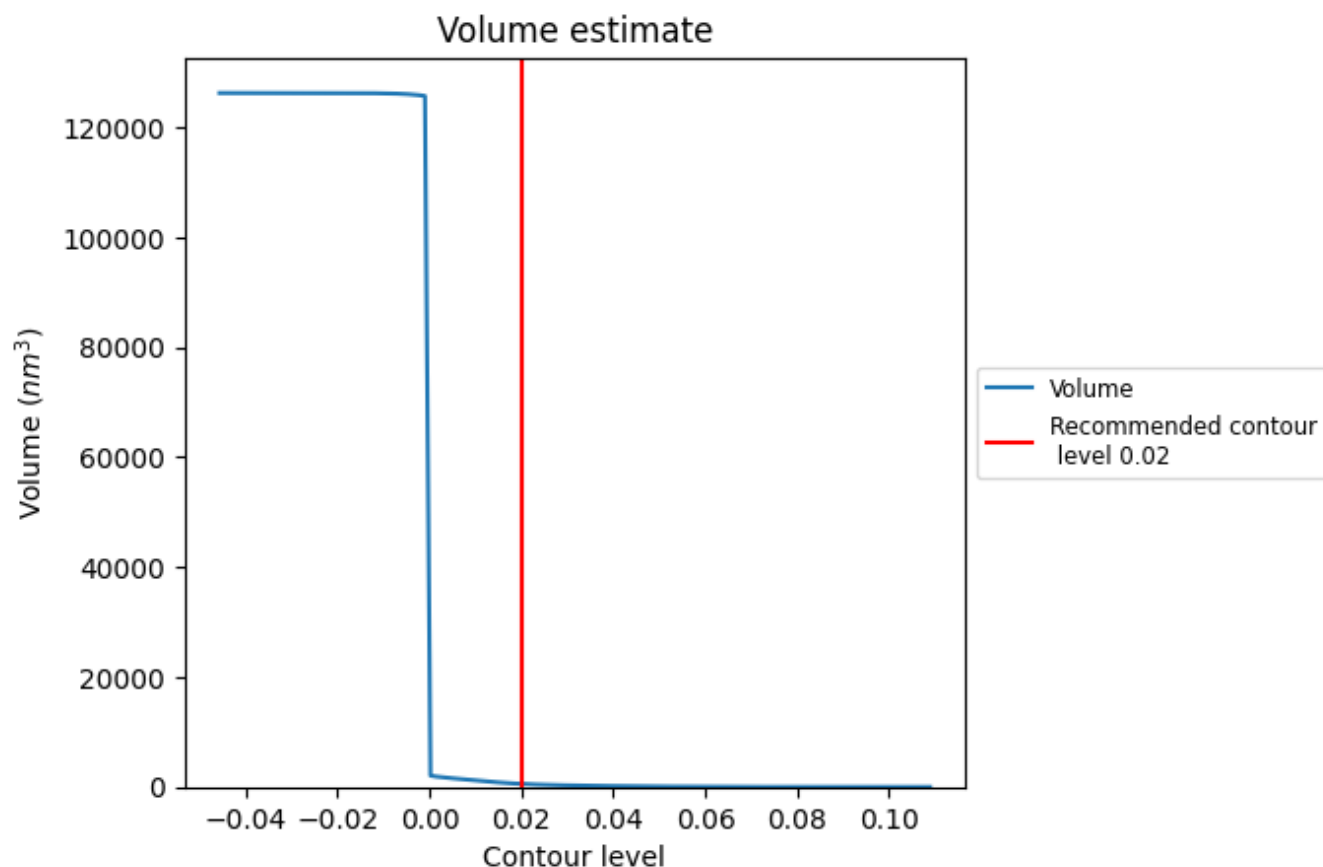
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

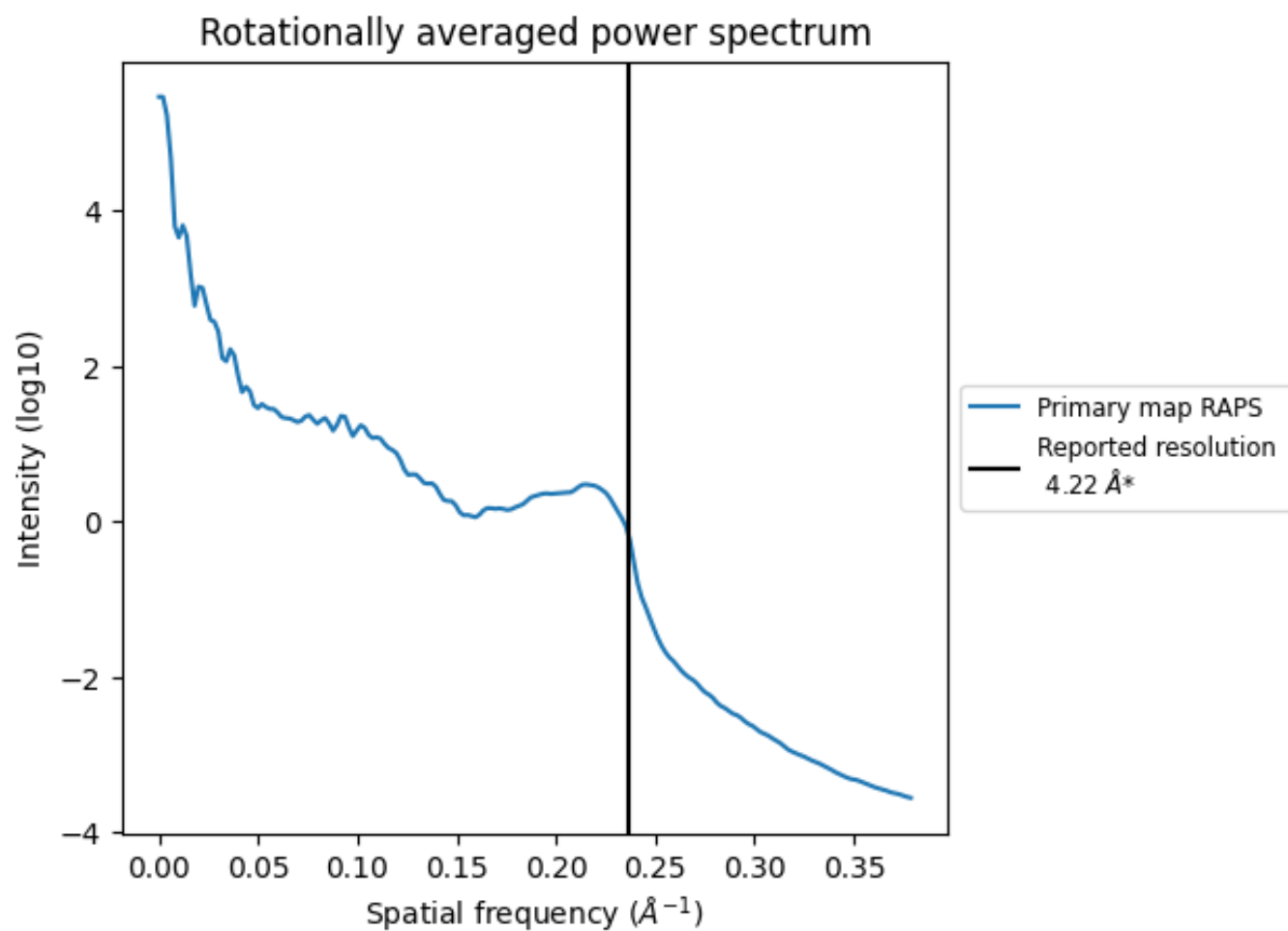
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 559 nm^3 ; this corresponds to an approximate mass of 505 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.237 Å⁻¹

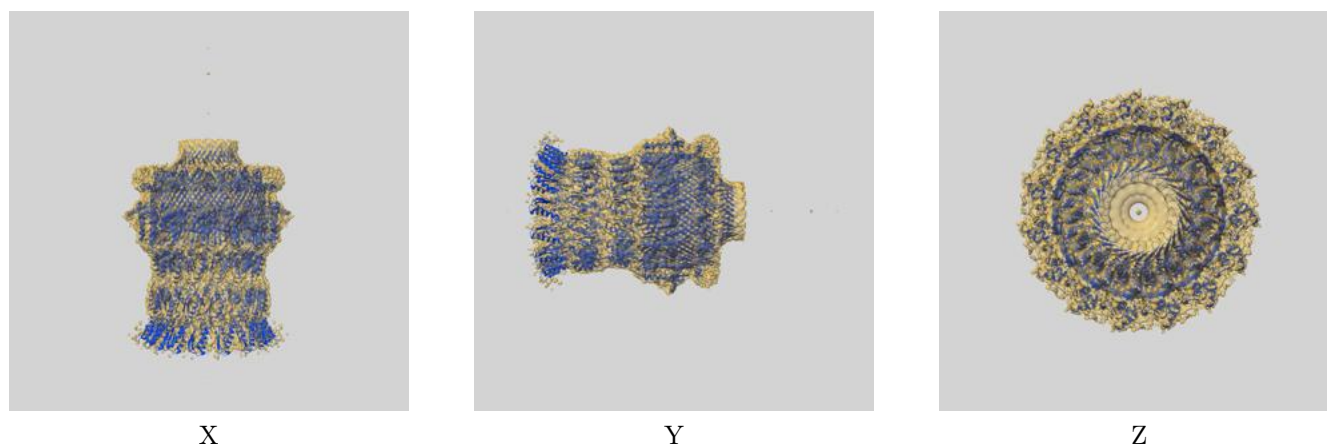
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

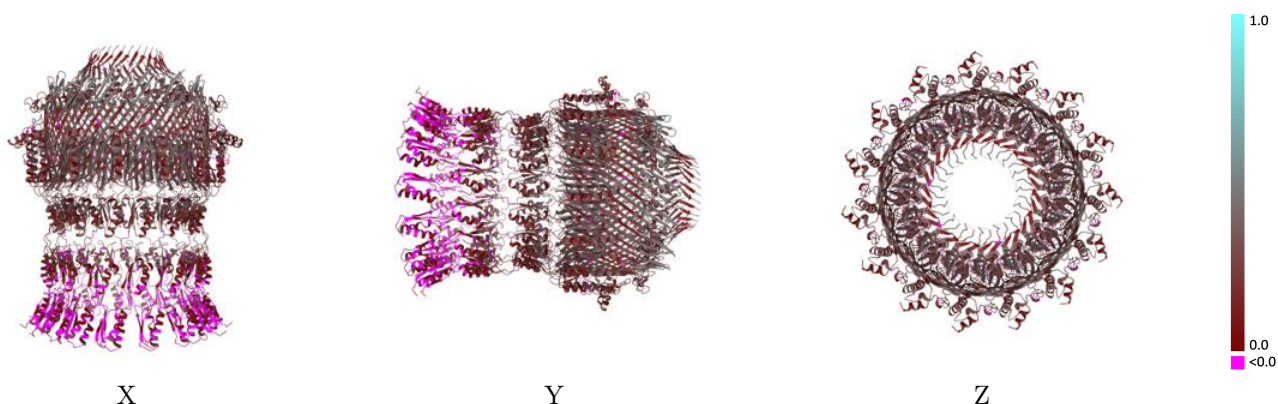
This section contains information regarding the fit between EMDB map EMD-6677 and PDB model 5WQ9. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



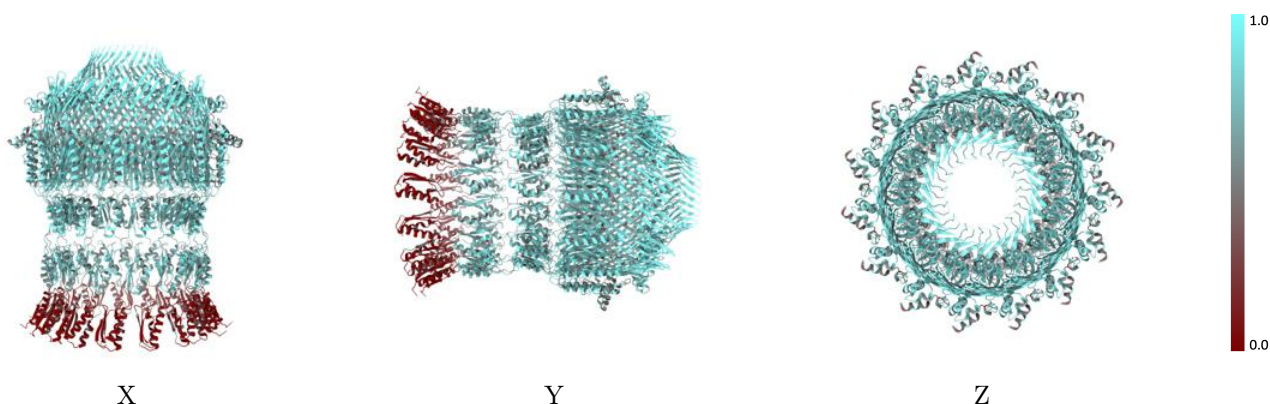
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



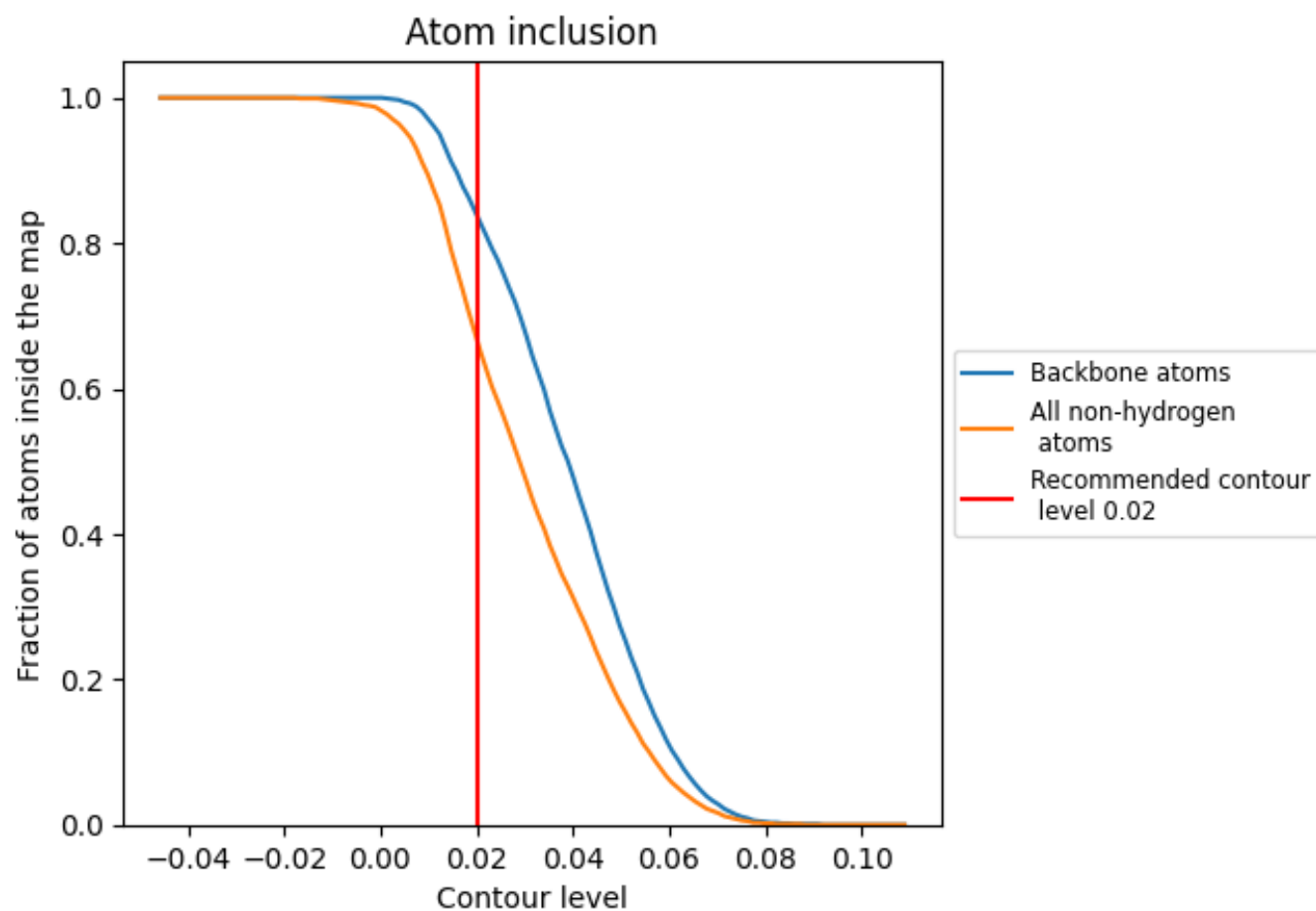
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|--------------------|
| All | <div></div> 0.6680 | <div></div> 0.2360 |
| A | <div></div> 0.6690 | <div></div> 0.2340 |
| B | <div></div> 0.6700 | <div></div> 0.2350 |
| C | <div></div> 0.6680 | <div></div> 0.2340 |
| D | <div></div> 0.6700 | <div></div> 0.2350 |
| E | <div></div> 0.6680 | <div></div> 0.2360 |
| F | <div></div> 0.6670 | <div></div> 0.2370 |
| G | <div></div> 0.6680 | <div></div> 0.2360 |
| H | <div></div> 0.6700 | <div></div> 0.2390 |
| I | <div></div> 0.6690 | <div></div> 0.2390 |
| J | <div></div> 0.6680 | <div></div> 0.2390 |
| K | <div></div> 0.6680 | <div></div> 0.2370 |
| L | <div></div> 0.6700 | <div></div> 0.2360 |
| M | <div></div> 0.6660 | <div></div> 0.2360 |
| N | <div></div> 0.6680 | <div></div> 0.2340 |
| O | <div></div> 0.6680 | <div></div> 0.2350 |

1.0

0.0

<0.0