



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:44 am GMT

PDB ID : 1O19
EMDB ID: : EMD-1001
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM
TOMOGRAMS OF INSECT FLIGHT MUSCLE
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.
Deposited on : 2002-11-15
Resolution : 70.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

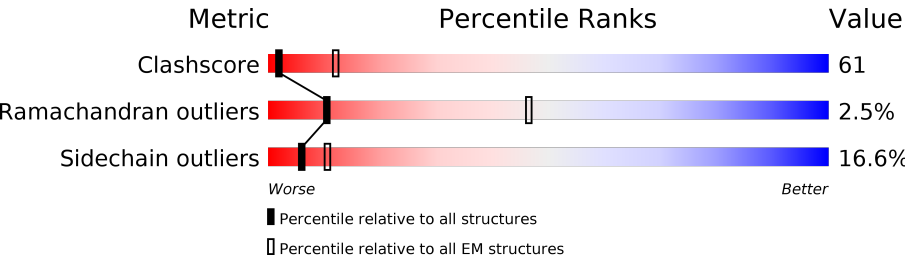
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 70.00 Å.

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















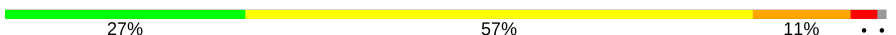



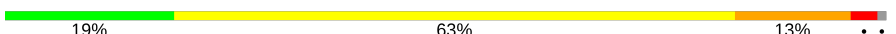
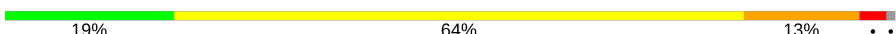





| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 840 | 25% 52% 19% . |
| 1 | D | 840 | 26% 51% 19% . |
| 1 | G | 840 | 25% 52% 19% . |
| 1 | J | 840 | 26% 51% 19% . |
| 1 | M | 840 | 26% 50% 20% . |
| 1 | S | 840 | 25% 52% 19% . |
| 2 | B | 145 | 66% 26% 6% . |
| 2 | E | 145 | 64% 27% 6% . |
| 2 | H | 145 | 64% 27% 6% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | K | 145 |  64% 26% 6% . |
| 2 | N | 145 |  64% 27% 6% . |
| 2 | T | 145 |  65% 26% 6% . |
| 3 | C | 147 |  60% 37% . |
| 3 | F | 147 |  60% 38% . |
| 3 | I | 147 |  61% 37% . |
| 3 | L | 147 |  61% 37% . |
| 3 | O | 147 |  61% 37% . |
| 3 | U | 147 |  57% 40% . |
| 4 | 1 | 375 |  62% 29% 6% .. |
| 4 | 2 | 375 |  53% 35% 9% .. |
| 4 | 3 | 375 |  54% 35% 8% .. |
| 4 | 4 | 375 |  27% 57% 11% .. |
| 4 | 5 | 375 |  24% 60% 12% .. |
| 4 | 6 | 375 |  24% 60% 12% .. |
| 4 | 7 | 375 |  27% 58% 11% .. |
| 4 | 8 | 375 |  19% 63% 13% .. |
| 4 | 9 | 375 |  19% 64% 13% .. |
| 4 | V | 375 |  50% 39% 8% .. |
| 4 | W | 375 |  54% 35% 9% .. |
| 4 | X | 375 |  61% 30% 7% .. |
| 4 | Y | 375 |  61% 30% 7% .. |
| 4 | Z | 375 |  57% 32% 8% .. |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | MLY | A | 505 | - | - | X | - |
| 1 | MLY | A | 553 | - | - | X | - |
| 1 | MLY | A | 764 | - | - | X | - |
| 1 | MLY | A | 768 | - | - | X | - |
| 1 | MLY | A | 782 | - | - | X | - |
| 1 | MLY | A | 839 | - | - | X | - |
| 1 | MLY | D | 553 | - | - | X | - |
| 1 | MLY | D | 782 | - | - | X | - |
| 1 | MLY | D | 839 | - | - | X | - |
| 1 | MLY | G | 295 | - | - | X | - |
| 1 | MLY | G | 553 | - | - | X | - |
| 1 | MLY | G | 764 | - | - | X | - |
| 1 | MLY | G | 768 | - | - | X | - |
| 1 | MLY | G | 84 | - | - | X | - |
| 1 | MLY | J | 295 | - | - | X | - |
| 1 | MLY | J | 505 | - | - | X | - |
| 1 | MLY | J | 553 | - | - | X | - |
| 1 | MLY | J | 764 | - | - | X | - |
| 1 | MLY | J | 768 | - | - | X | - |
| 1 | MLY | J | 839 | - | - | X | - |
| 1 | MLY | J | 84 | - | - | X | - |
| 1 | MLY | M | 35 | - | - | X | - |
| 1 | MLY | M | 553 | - | - | X | - |
| 1 | MLY | M | 839 | - | - | X | - |
| 1 | MLY | M | 84 | - | - | X | - |
| 1 | MLY | S | 505 | - | - | X | - |
| 1 | MLY | S | 764 | - | - | X | - |
| 1 | MLY | S | 839 | - | - | X | - |
| 1 | MLY | S | 84 | - | - | X | - |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 94966 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 SKELETAL MUSCLE MYOSIN II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | D | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | G | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | J | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | M | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | S | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | B | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | E | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | H | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | K | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | N | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | T | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | C | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | F | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | I | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | L | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | O | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | U | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |

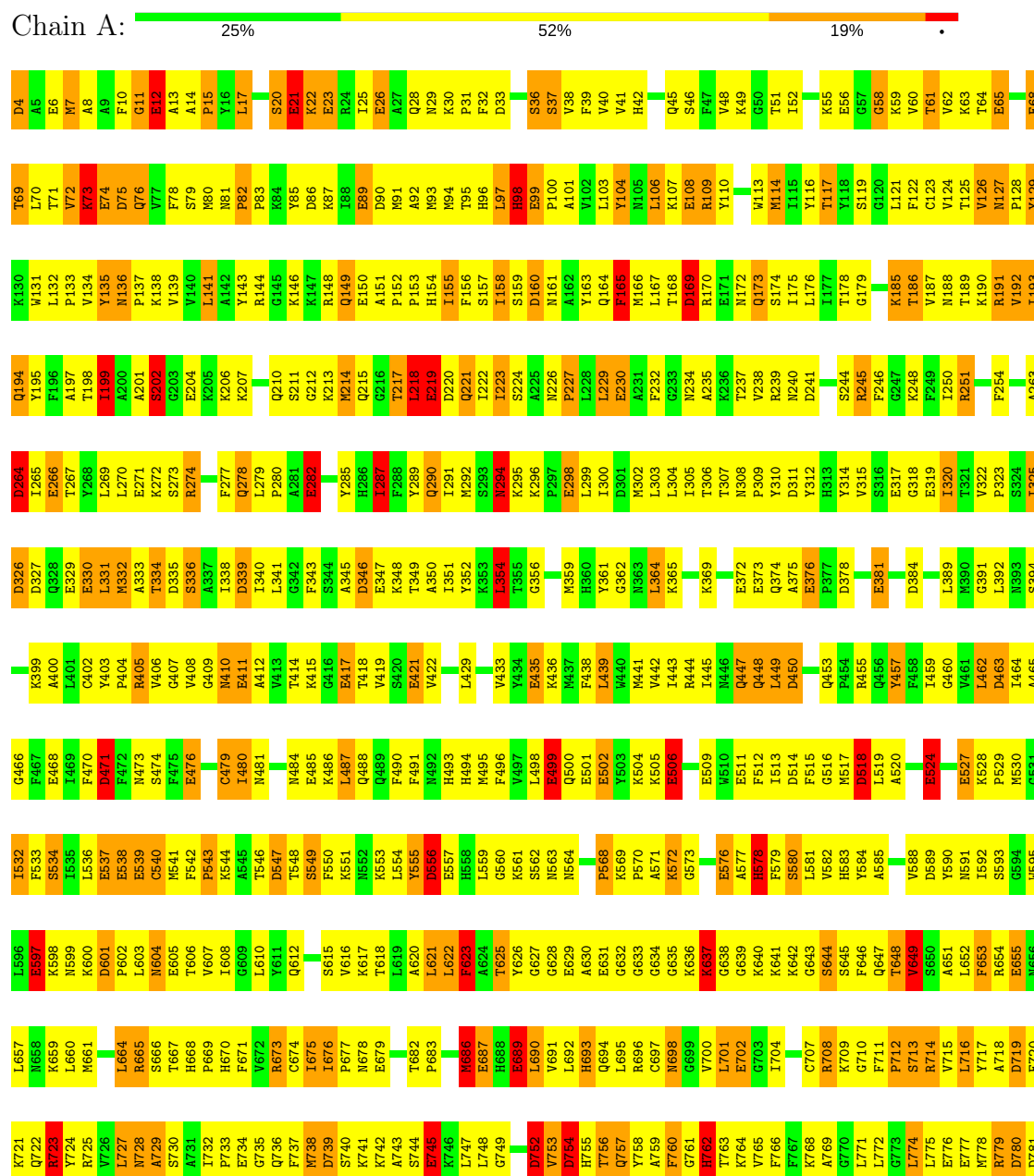
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | 1 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 2 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 3 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 4 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 5 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 6 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 7 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 8 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 9 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | V | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | W | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | X | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | Y | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | Z | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

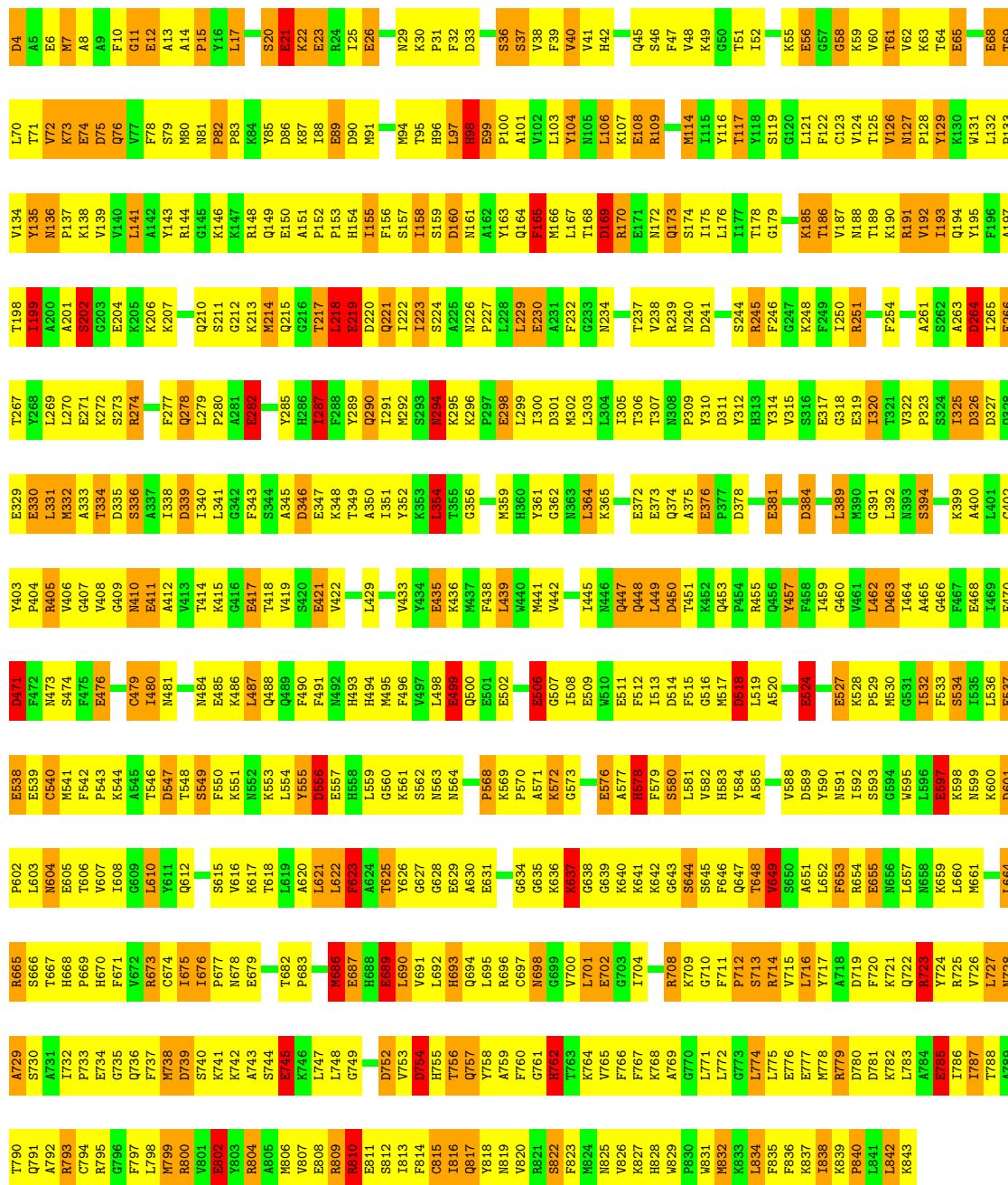
• Molecule 1: SKELETAL MUSCLE MYOSIN II





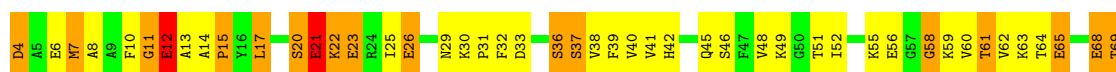
• Molecule 1: SKELETAL MUSCLE MYOSIN II

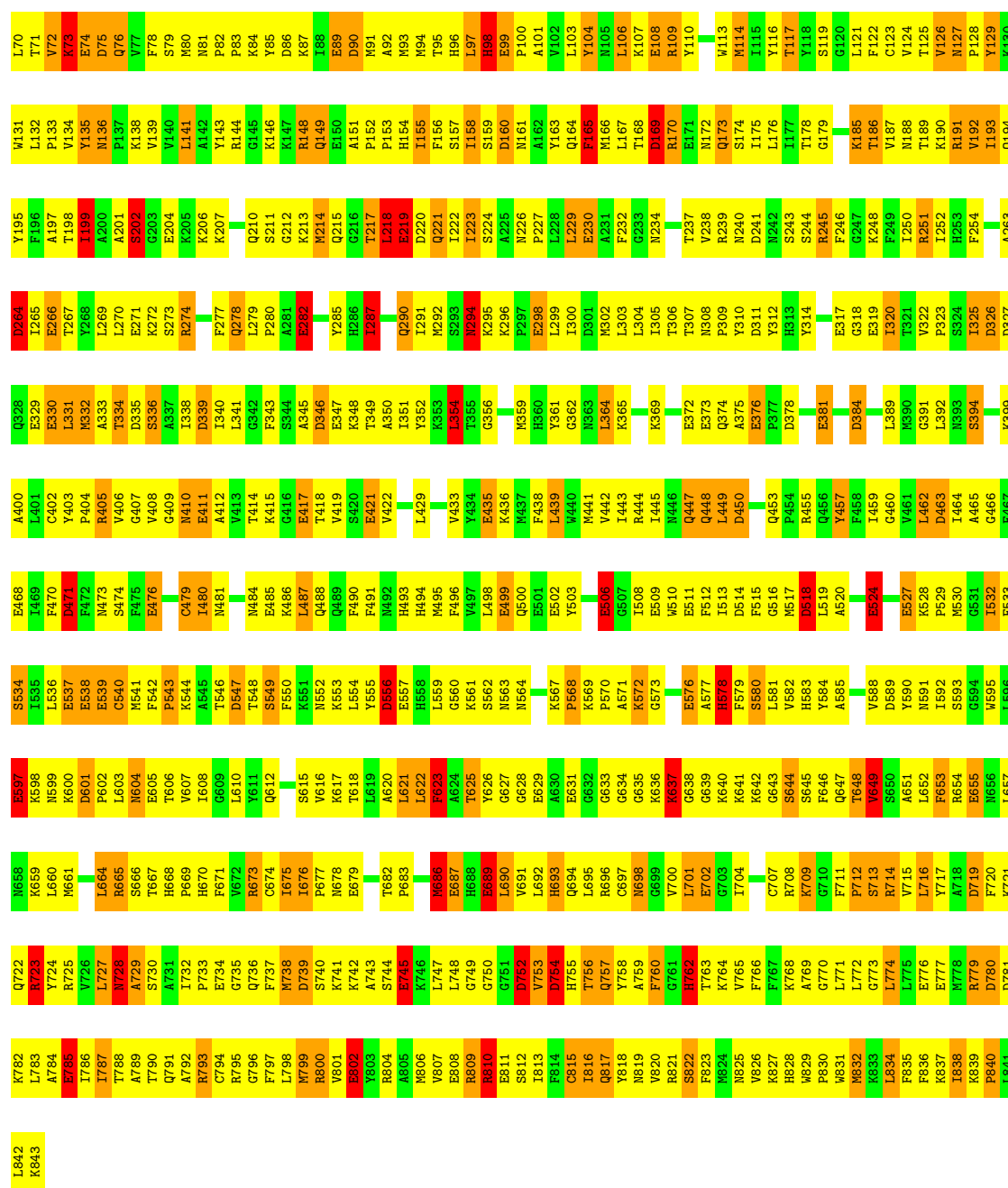
Chain D: 26% 51% 19%



• Molecule 1: SKELETAL MUSCLE MYOSIN II

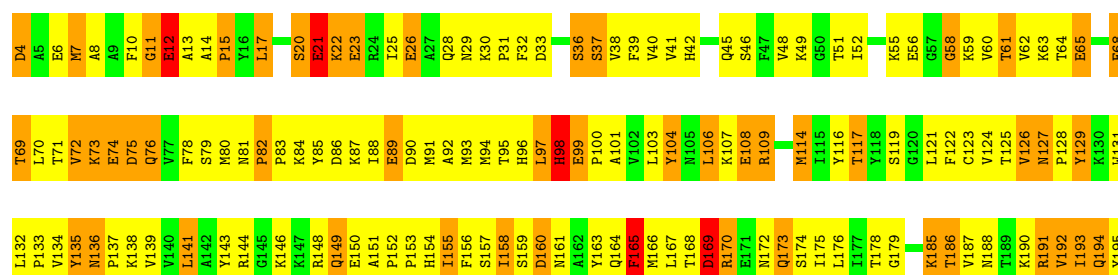
Chain G: 25% 52% 19%

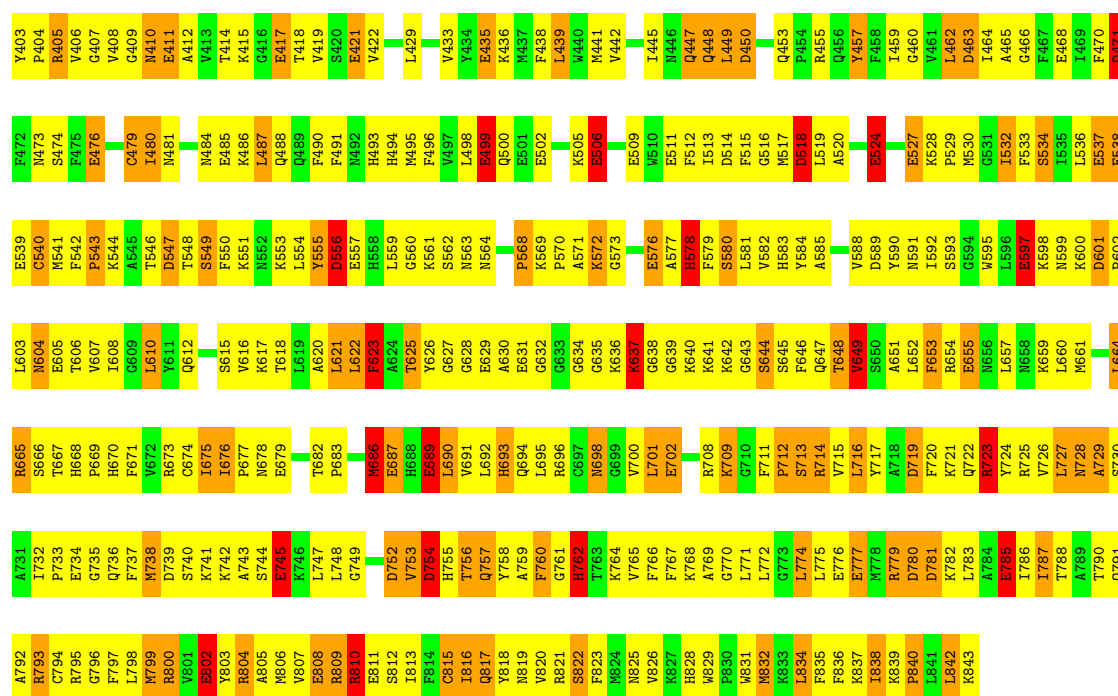




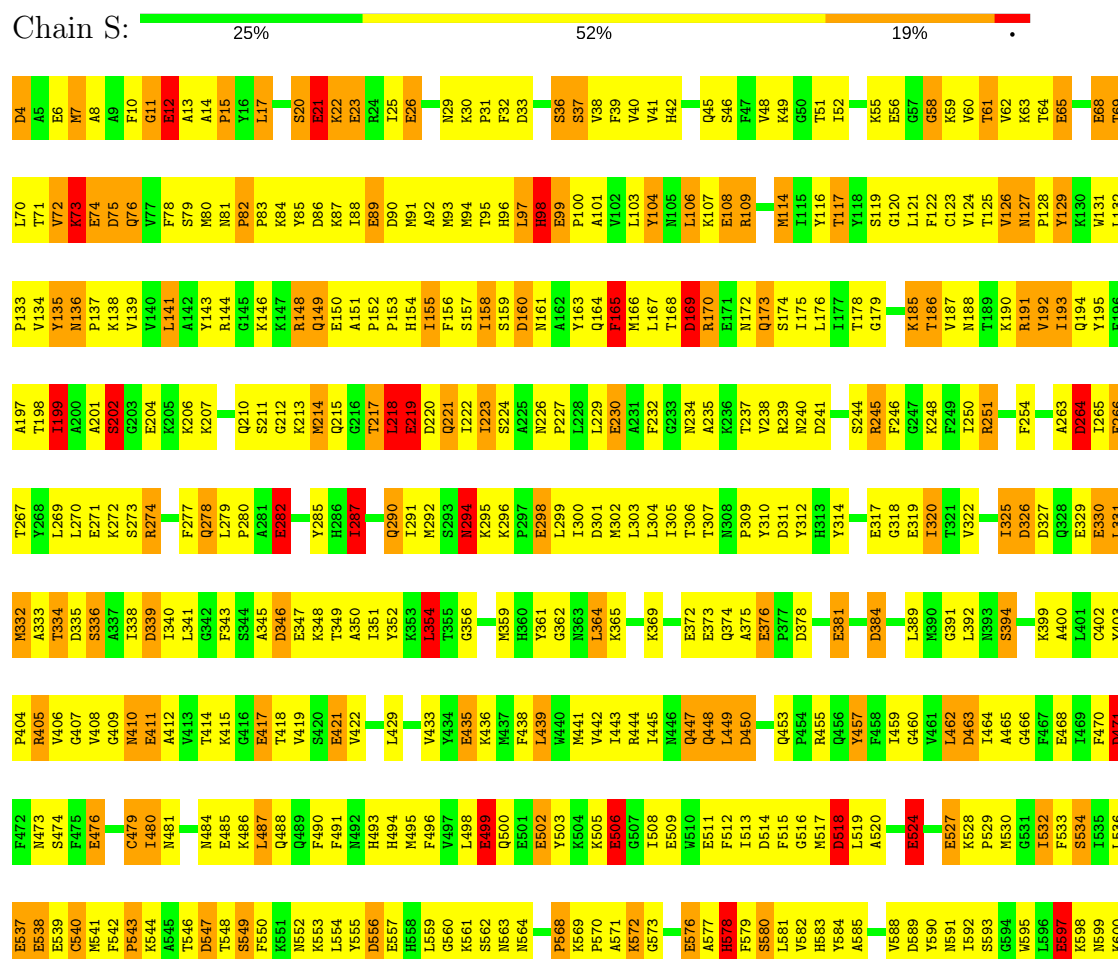
Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain J: 26% 51% 19%

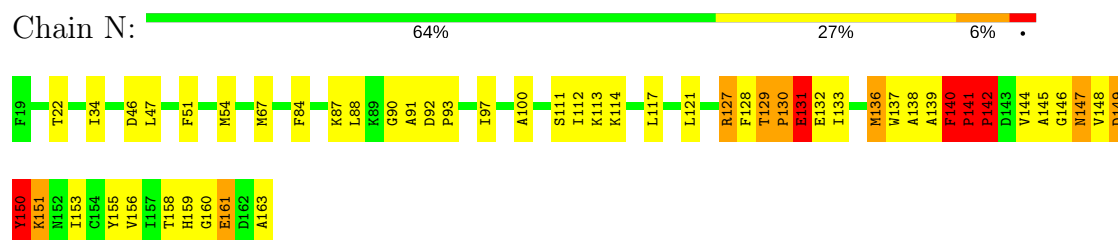




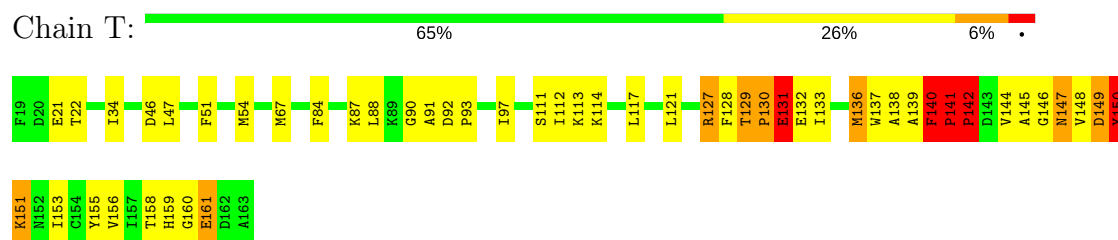
• Molecule 1: SKELETAL MUSCLE MYOSIN II



- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



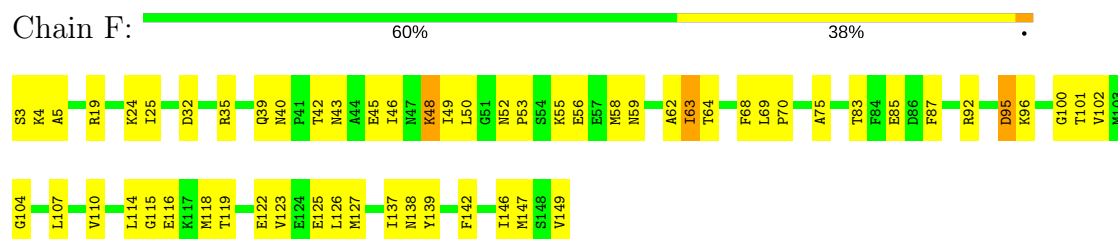
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



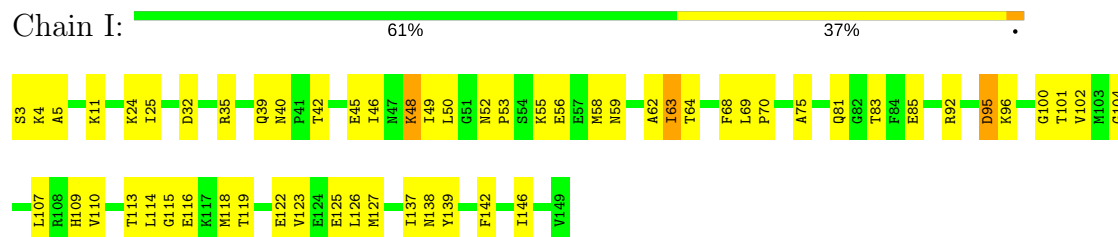
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



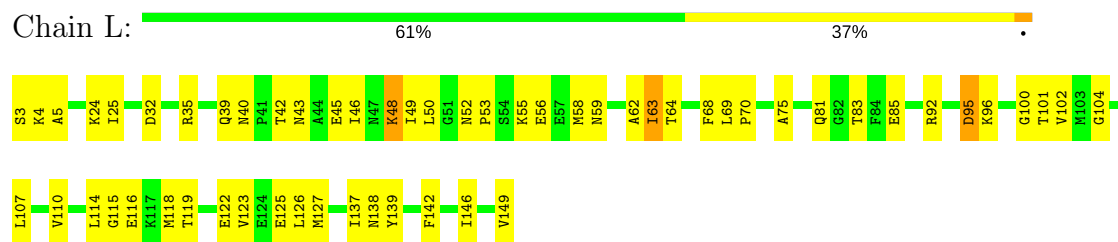
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



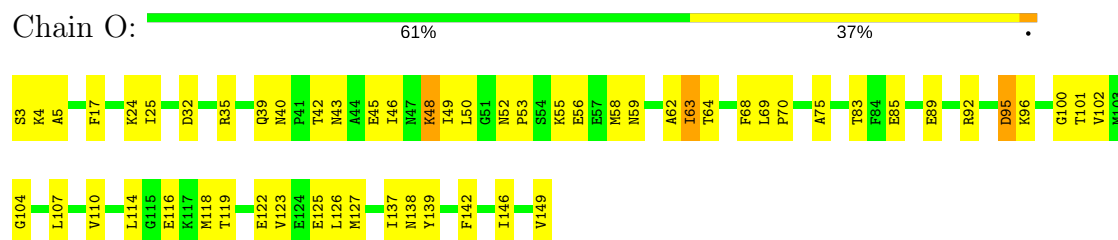
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



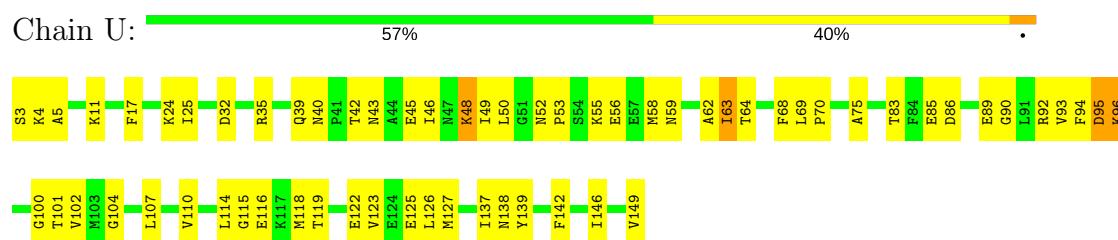
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



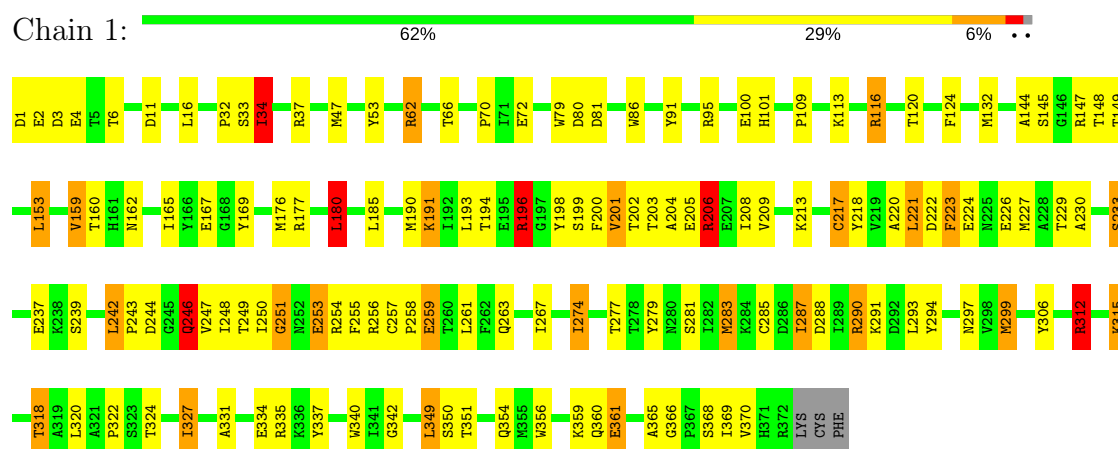
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



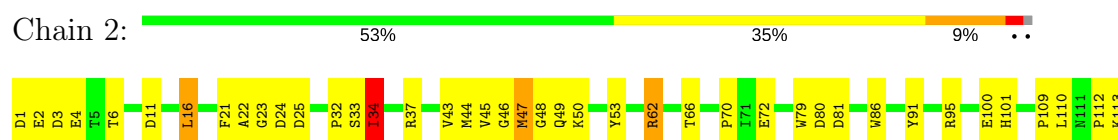
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

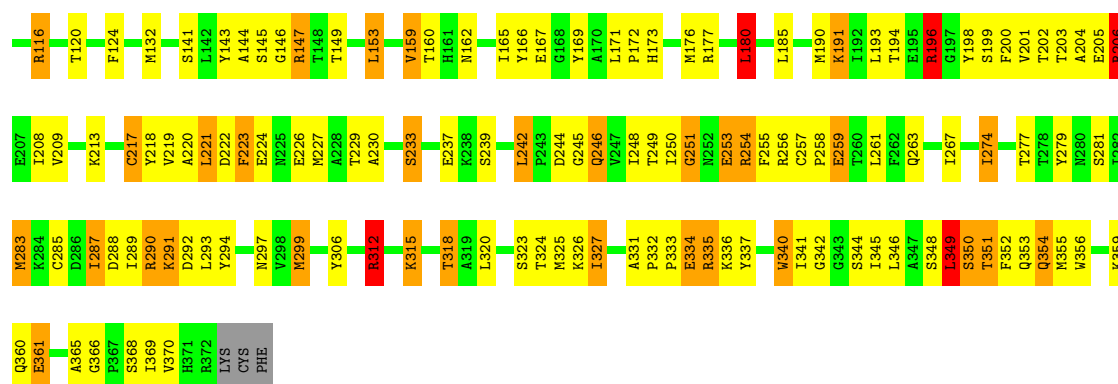


• Molecule 4: SKELETAL MUSCLE ACTIN



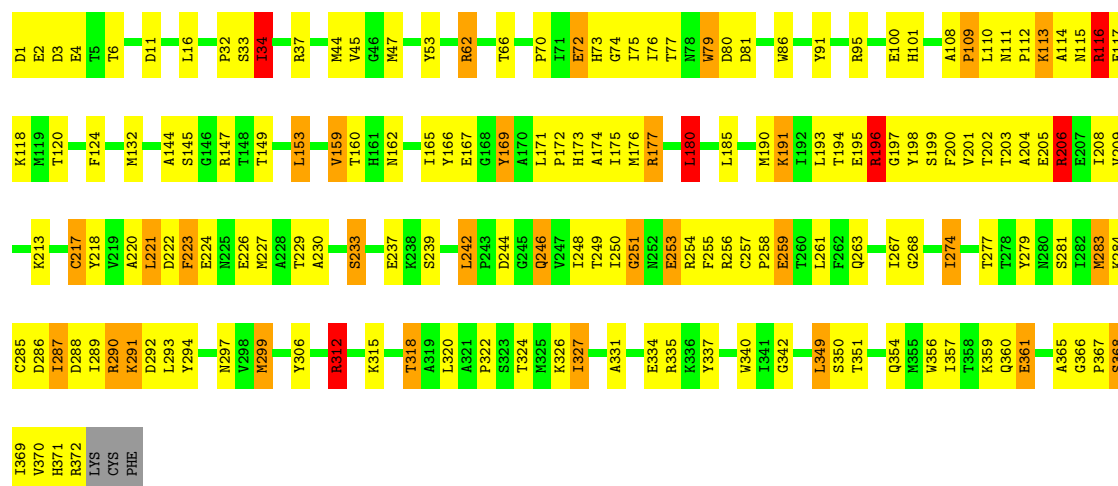
• Molecule 4: SKELETAL MUSCLE ACTIN





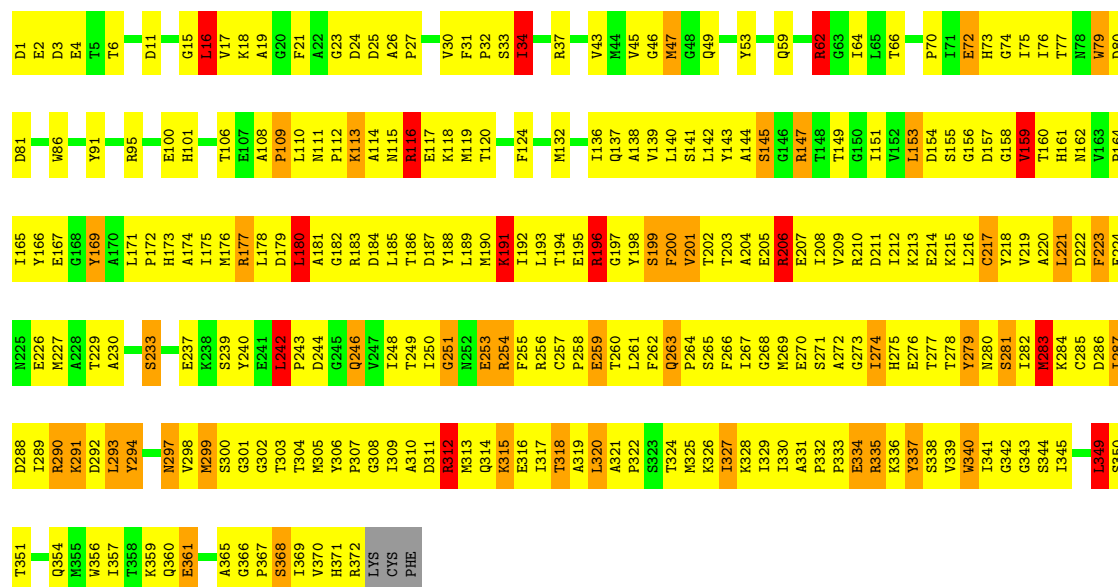
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 3: 54% 35% 8% ..

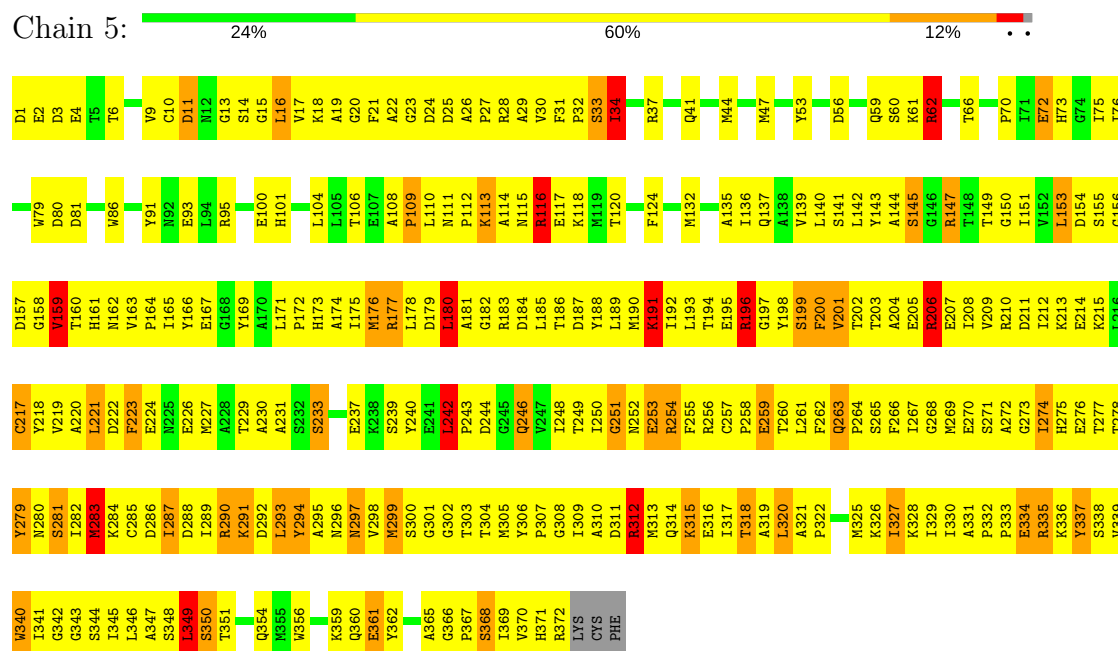


• Molecule 4: SKELETAL MUSCLE ACTIN

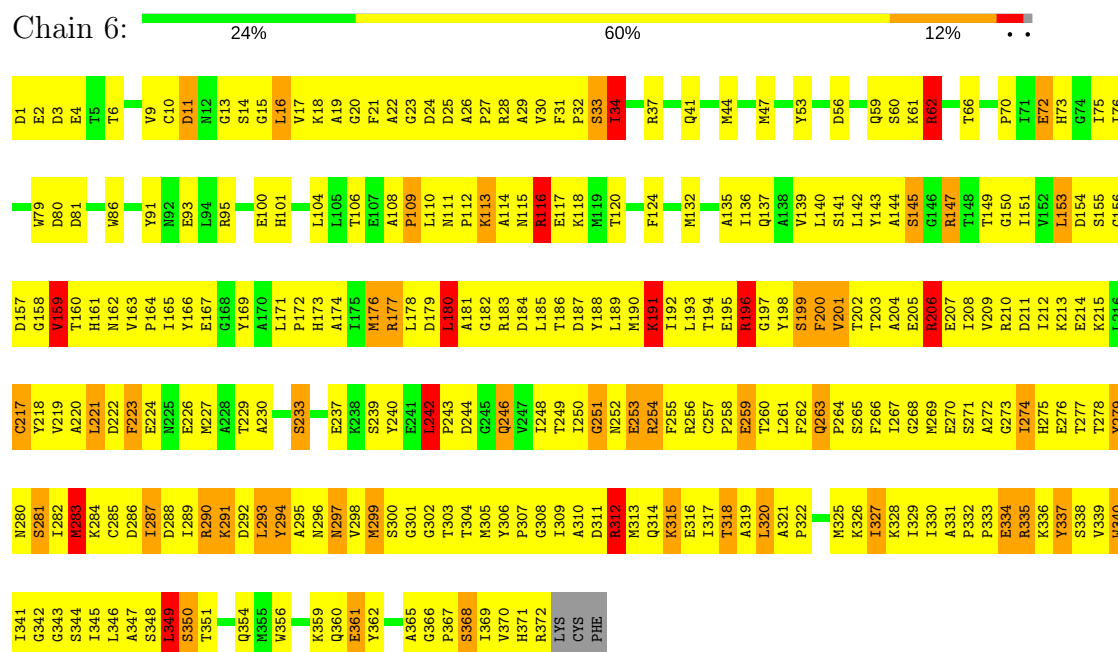
Chain 4: 27% 57% 11% ..



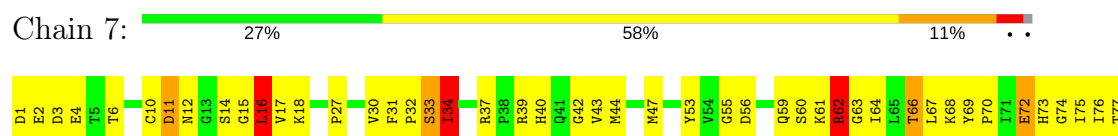
• Molecule 4: SKELETAL MUSCLE ACTIN

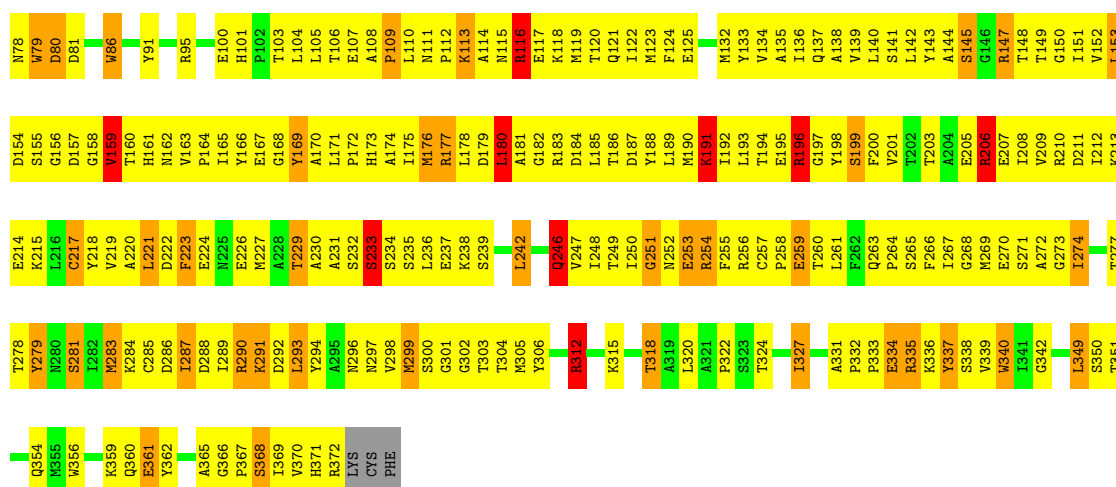


• Molecule 4: SKELETAL MUSCLE ACTIN



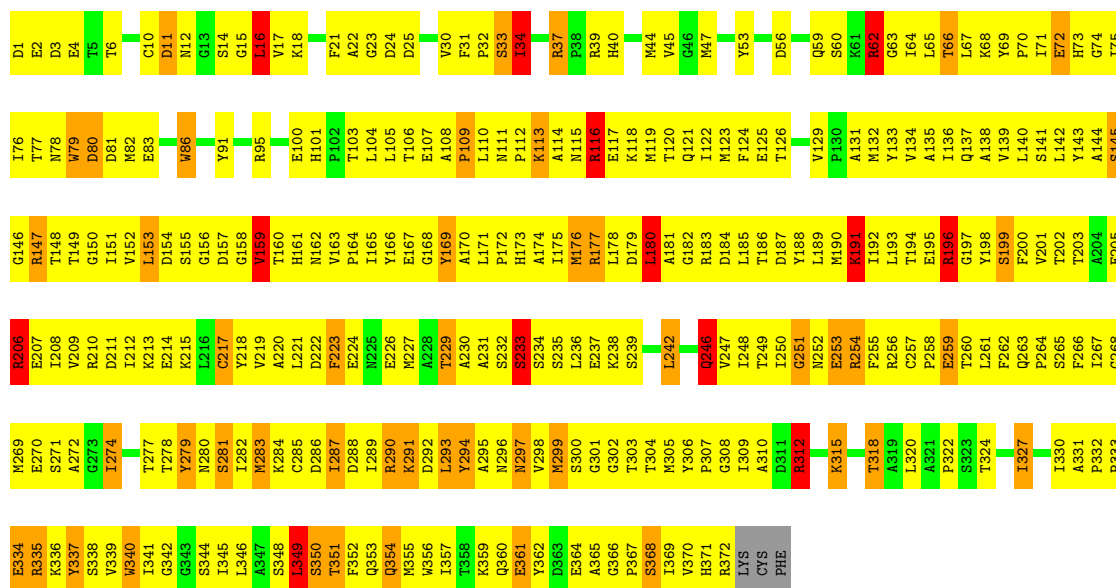
• Molecule 4: SKELETAL MUSCLE ACTIN





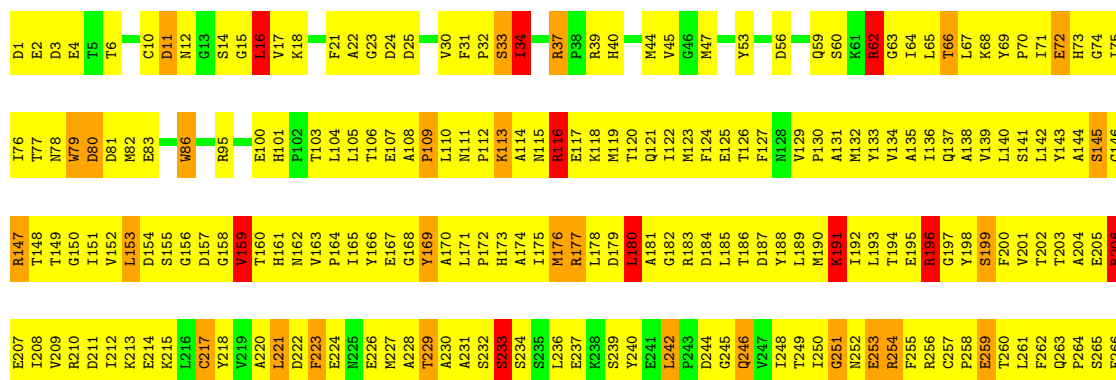
• Molecule 4: SKELETAL MUSCLE ACTIN

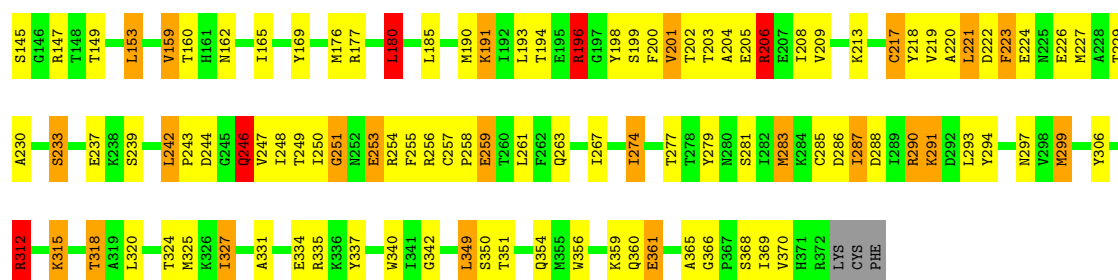
Chain 8: 19% 63% 13% . .



• Molecule 4: SKELETAL MUSCLE ACTIN

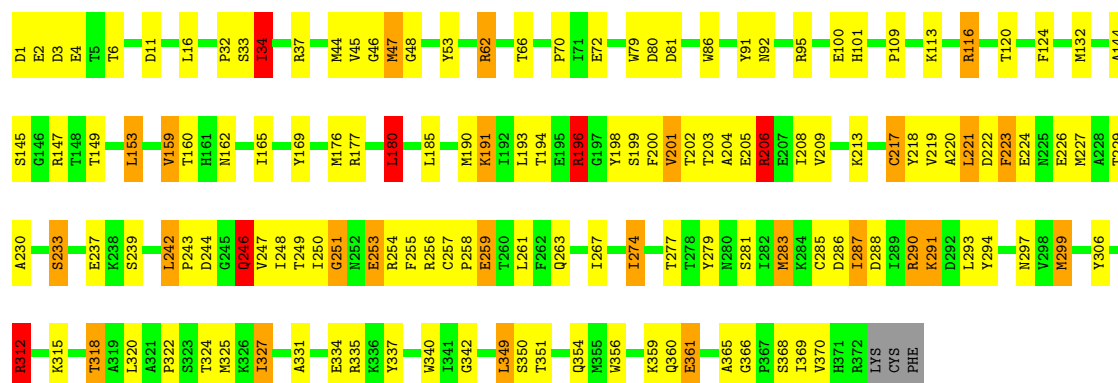
Chain 9: 19% 64% 13% . .





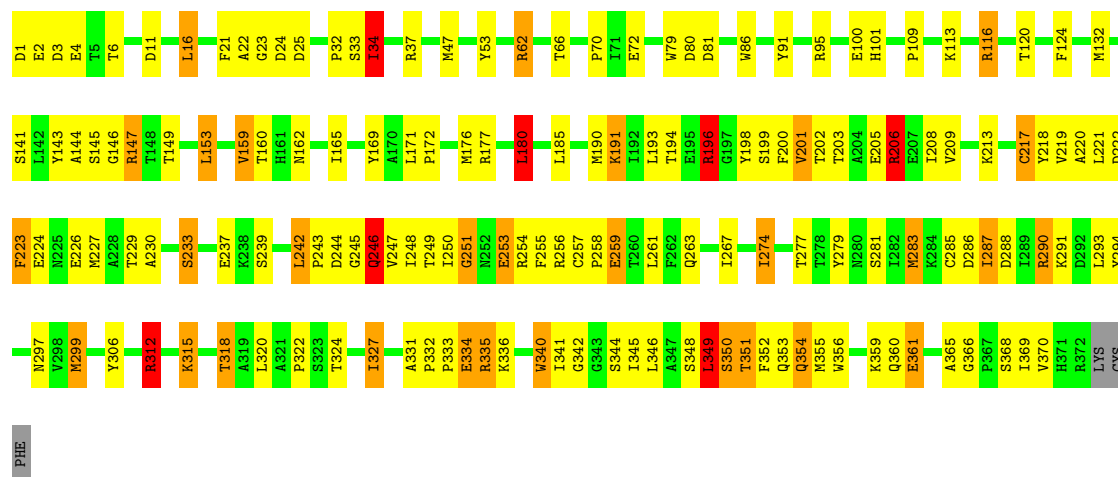
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain Y: 61% 30% 7% ..



• Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z: 57% 32% 8% ..



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | TOMOGRAPHY | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of tilted images used | Not provided | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | Not provided | Depositor |
| Voltage (kV) | Not provided | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | KODAK S0163 FILM | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 >2 | RMSZ | # Z >2 |
| 1 | A | 1.77 | 68/6448 (1.1%) | 1.82 | 116/8729 (1.3%) |
| 1 | D | 1.77 | 66/6448 (1.0%) | 1.82 | 115/8729 (1.3%) |
| 1 | G | 1.77 | 67/6449 (1.0%) | 1.82 | 118/8732 (1.4%) |
| 1 | J | 1.79 | 68/6449 (1.1%) | 1.87 | 118/8732 (1.4%) |
| 1 | M | 1.77 | 66/6447 (1.0%) | 1.83 | 119/8726 (1.4%) |
| 1 | S | 1.78 | 69/6446 (1.1%) | 1.85 | 119/8723 (1.4%) |
| 2 | B | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 2 | E | 1.21 | 10/1148 (0.9%) | 1.62 | 16/1548 (1.0%) |
| 2 | H | 1.22 | 10/1148 (0.9%) | 1.62 | 16/1548 (1.0%) |
| 2 | K | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 2 | N | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 2 | T | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 3 | C | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | F | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | I | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | L | 0.79 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | O | 0.79 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | U | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 4 | 1 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | 2 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 3 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 4 | 0.89 | 2/2968 (0.1%) | 1.64 | 50/4023 (1.2%) |
| 4 | 5 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | 6 | 0.89 | 1/2968 (0.0%) | 1.64 | 52/4023 (1.3%) |
| 4 | 7 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | 8 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 9 | 0.89 | 2/2968 (0.1%) | 1.64 | 50/4023 (1.2%) |
| 4 | V | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | W | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | X | 0.89 | 1/2968 (0.0%) | 1.64 | 52/4023 (1.3%) |
| 4 | Y | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | Z | 0.89 | 2/2968 (0.1%) | 1.64 | 50/4023 (1.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| All | All | 1.34 | 490/93943 (0.5%) | 1.68 | 1542/127131 (1.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 1 | 4 |
| 1 | D | 1 | 4 |
| 1 | G | 1 | 5 |
| 1 | J | 1 | 6 |
| 1 | M | 1 | 7 |
| 1 | S | 1 | 7 |
| 2 | B | 0 | 3 |
| 2 | E | 0 | 3 |
| 2 | H | 0 | 3 |
| 2 | K | 0 | 3 |
| 2 | N | 0 | 3 |
| 2 | T | 0 | 3 |
| 3 | C | 0 | 2 |
| 3 | F | 0 | 2 |
| 3 | I | 0 | 2 |
| 3 | L | 0 | 2 |
| 3 | O | 0 | 2 |
| 3 | U | 0 | 2 |
| 4 | 1 | 0 | 1 |
| 4 | 2 | 0 | 1 |
| 4 | 3 | 0 | 1 |
| 4 | 4 | 0 | 1 |
| 4 | 5 | 0 | 1 |
| 4 | 6 | 0 | 1 |
| 4 | 7 | 0 | 1 |
| 4 | 8 | 0 | 1 |
| 4 | 9 | 0 | 1 |
| 4 | V | 0 | 1 |
| 4 | W | 0 | 1 |
| 4 | X | 0 | 1 |
| 4 | Y | 0 | 1 |
| 4 | Z | 0 | 1 |
| All | All | 6 | 77 |

All (490) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | J | 649 | VAL | CB-CG1 | 53.33 | 2.64 | 1.52 |
| 1 | S | 649 | VAL | CB-CG1 | 53.30 | 2.64 | 1.52 |
| 1 | M | 649 | VAL | CB-CG1 | 53.28 | 2.64 | 1.52 |
| 1 | G | 649 | VAL | CB-CG1 | 53.26 | 2.64 | 1.52 |
| 1 | D | 649 | VAL | CB-CG1 | 53.22 | 2.64 | 1.52 |
| 1 | A | 649 | VAL | CB-CG1 | 53.21 | 2.64 | 1.52 |
| 1 | G | 623 | PHE | CB-CG | 48.14 | 2.33 | 1.51 |
| 1 | D | 623 | PHE | CB-CG | 48.14 | 2.33 | 1.51 |
| 1 | J | 623 | PHE | CB-CG | 48.13 | 2.33 | 1.51 |
| 1 | S | 623 | PHE | CB-CG | 48.11 | 2.33 | 1.51 |
| 1 | M | 623 | PHE | CB-CG | 48.10 | 2.33 | 1.51 |
| 1 | A | 623 | PHE | CB-CG | 48.09 | 2.33 | 1.51 |
| 1 | A | 649 | VAL | CB-CG2 | 46.26 | 2.50 | 1.52 |
| 1 | G | 649 | VAL | CB-CG2 | 46.23 | 2.50 | 1.52 |
| 1 | J | 649 | VAL | CB-CG2 | 46.21 | 2.49 | 1.52 |
| 1 | S | 649 | VAL | CB-CG2 | 46.18 | 2.49 | 1.52 |
| 1 | M | 649 | VAL | CB-CG2 | 46.15 | 2.49 | 1.52 |
| 1 | D | 649 | VAL | CB-CG2 | 46.11 | 2.49 | 1.52 |
| 1 | G | 648 | THR | CB-OG1 | 34.41 | 2.12 | 1.43 |
| 1 | J | 648 | THR | CB-OG1 | 34.40 | 2.12 | 1.43 |
| 1 | M | 648 | THR | CB-OG1 | 34.38 | 2.12 | 1.43 |
| 1 | S | 648 | THR | CB-OG1 | 34.36 | 2.12 | 1.43 |
| 1 | A | 648 | THR | CB-OG1 | 34.33 | 2.12 | 1.43 |
| 1 | D | 648 | THR | CB-OG1 | 34.33 | 2.12 | 1.43 |
| 1 | S | 648 | THR | CB-CG2 | -30.71 | 0.51 | 1.52 |
| 1 | M | 648 | THR | CB-CG2 | -30.70 | 0.51 | 1.52 |
| 1 | J | 648 | THR | CB-CG2 | -30.70 | 0.51 | 1.52 |
| 1 | A | 648 | THR | CB-CG2 | -30.69 | 0.51 | 1.52 |
| 1 | G | 648 | THR | CB-CG2 | -30.65 | 0.51 | 1.52 |
| 1 | D | 648 | THR | CB-CG2 | -30.64 | 0.51 | 1.52 |
| 1 | J | 709 | LYS | C-N | 17.56 | 1.64 | 1.33 |
| 1 | S | 769 | ALA | C-N | 16.37 | 1.62 | 1.33 |
| 1 | S | 637 | LYS | C-N | -15.05 | 1.05 | 1.33 |
| 1 | M | 637 | LYS | C-N | -15.03 | 1.05 | 1.33 |
| 1 | J | 637 | LYS | C-N | -14.99 | 1.06 | 1.33 |
| 1 | D | 637 | LYS | C-N | -14.97 | 1.06 | 1.33 |
| 1 | A | 637 | LYS | C-N | -14.81 | 1.06 | 1.33 |
| 1 | G | 637 | LYS | C-N | -14.74 | 1.06 | 1.33 |
| 1 | G | 649 | VAL | C-N | -13.50 | 1.02 | 1.34 |
| 1 | A | 649 | VAL | C-N | -13.48 | 1.03 | 1.34 |
| 1 | D | 649 | VAL | C-N | -13.45 | 1.03 | 1.34 |
| 1 | M | 649 | VAL | C-N | -13.39 | 1.03 | 1.34 |
| 2 | H | 150 | TYR | CB-CG | -13.37 | 1.31 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | S | 649 | VAL | C-N | -13.37 | 1.03 | 1.34 |
| 1 | J | 649 | VAL | C-N | -13.32 | 1.03 | 1.34 |
| 2 | T | 150 | TYR | CB-CG | -13.32 | 1.31 | 1.51 |
| 2 | K | 150 | TYR | CB-CG | -13.31 | 1.31 | 1.51 |
| 2 | E | 150 | TYR | CB-CG | -13.31 | 1.31 | 1.51 |
| 2 | N | 150 | TYR | CB-CG | -13.29 | 1.31 | 1.51 |
| 2 | B | 150 | TYR | CB-CG | -13.25 | 1.31 | 1.51 |
| 2 | E | 140 | PHE | C-N | -12.98 | 1.09 | 1.34 |
| 2 | B | 140 | PHE | C-N | -12.96 | 1.09 | 1.34 |
| 2 | K | 140 | PHE | C-N | -12.90 | 1.09 | 1.34 |
| 2 | N | 140 | PHE | C-N | -12.90 | 1.09 | 1.34 |
| 2 | T | 140 | PHE | C-N | -12.87 | 1.09 | 1.34 |
| 2 | H | 140 | PHE | C-N | -12.78 | 1.09 | 1.34 |
| 2 | B | 150 | TYR | CG-CD2 | -11.32 | 1.24 | 1.39 |
| 2 | K | 150 | TYR | CG-CD2 | -11.23 | 1.24 | 1.39 |
| 2 | H | 150 | TYR | CG-CD2 | -11.20 | 1.24 | 1.39 |
| 2 | T | 150 | TYR | CG-CD2 | -11.20 | 1.24 | 1.39 |
| 2 | N | 150 | TYR | CG-CD2 | -11.17 | 1.24 | 1.39 |
| 2 | E | 150 | TYR | CG-CD2 | -11.12 | 1.24 | 1.39 |
| 2 | K | 141 | PRO | N-CD | -10.57 | 1.33 | 1.47 |
| 2 | N | 141 | PRO | N-CD | -10.55 | 1.33 | 1.47 |
| 2 | T | 141 | PRO | N-CD | -10.54 | 1.33 | 1.47 |
| 2 | B | 141 | PRO | N-CD | -10.48 | 1.33 | 1.47 |
| 2 | E | 141 | PRO | N-CD | -10.43 | 1.33 | 1.47 |
| 2 | H | 141 | PRO | N-CD | -10.37 | 1.33 | 1.47 |
| 1 | M | 709 | LYS | C-N | 9.26 | 1.49 | 1.33 |
| 1 | J | 476 | GLU | CD-OE1 | 8.92 | 1.35 | 1.25 |
| 1 | M | 476 | GLU | CD-OE1 | 8.89 | 1.35 | 1.25 |
| 1 | S | 476 | GLU | CD-OE1 | 8.86 | 1.35 | 1.25 |
| 1 | J | 785 | GLU | C-N | 8.77 | 1.54 | 1.34 |
| 1 | D | 476 | GLU | CD-OE1 | 8.77 | 1.35 | 1.25 |
| 1 | G | 476 | GLU | CD-OE1 | 8.73 | 1.35 | 1.25 |
| 1 | A | 622 | LEU | C-N | 8.72 | 1.54 | 1.34 |
| 1 | M | 622 | LEU | C-N | 8.72 | 1.54 | 1.34 |
| 1 | J | 622 | LEU | C-N | 8.71 | 1.54 | 1.34 |
| 1 | A | 476 | GLU | CD-OE1 | 8.69 | 1.35 | 1.25 |
| 1 | S | 622 | LEU | C-N | 8.69 | 1.54 | 1.34 |
| 1 | D | 622 | LEU | C-N | 8.63 | 1.53 | 1.34 |
| 1 | G | 622 | LEU | C-N | 8.59 | 1.53 | 1.34 |
| 1 | G | 411 | GLU | CD-OE1 | 8.32 | 1.34 | 1.25 |
| 1 | M | 745 | GLU | CD-OE2 | 8.30 | 1.34 | 1.25 |
| 1 | J | 745 | GLU | CD-OE2 | 8.27 | 1.34 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 150 | TYR | CA-CB | -8.25 | 1.35 | 1.53 |
| 1 | D | 745 | GLU | CD-OE2 | 8.25 | 1.34 | 1.25 |
| 1 | J | 411 | GLU | CD-OE1 | 8.24 | 1.34 | 1.25 |
| 1 | M | 411 | GLU | CD-OE1 | 8.24 | 1.34 | 1.25 |
| 2 | N | 150 | TYR | CA-CB | -8.24 | 1.35 | 1.53 |
| 2 | K | 150 | TYR | CA-CB | -8.24 | 1.35 | 1.53 |
| 1 | S | 745 | GLU | CD-OE2 | 8.23 | 1.34 | 1.25 |
| 1 | G | 745 | GLU | CD-OE2 | 8.22 | 1.34 | 1.25 |
| 2 | H | 150 | TYR | CA-CB | -8.21 | 1.35 | 1.53 |
| 2 | T | 150 | TYR | CA-CB | -8.20 | 1.35 | 1.53 |
| 1 | S | 411 | GLU | CD-OE1 | 8.19 | 1.34 | 1.25 |
| 1 | A | 411 | GLU | CD-OE1 | 8.18 | 1.34 | 1.25 |
| 1 | D | 411 | GLU | CD-OE1 | 8.12 | 1.34 | 1.25 |
| 1 | S | 108 | GLU | CD-OE1 | 8.09 | 1.34 | 1.25 |
| 2 | E | 150 | TYR | CA-CB | -8.08 | 1.36 | 1.53 |
| 1 | A | 745 | GLU | CD-OE2 | 8.08 | 1.34 | 1.25 |
| 1 | A | 381 | GLU | CD-OE1 | 8.03 | 1.34 | 1.25 |
| 1 | G | 108 | GLU | CD-OE1 | 7.98 | 1.34 | 1.25 |
| 1 | M | 108 | GLU | CD-OE1 | 7.93 | 1.34 | 1.25 |
| 1 | A | 108 | GLU | CD-OE1 | 7.91 | 1.34 | 1.25 |
| 1 | G | 381 | GLU | CD-OE1 | 7.91 | 1.34 | 1.25 |
| 1 | J | 108 | GLU | CD-OE1 | 7.84 | 1.34 | 1.25 |
| 1 | M | 381 | GLU | CD-OE1 | 7.82 | 1.34 | 1.25 |
| 1 | S | 202 | SER | CB-OG | 7.81 | 1.52 | 1.42 |
| 1 | S | 381 | GLU | CD-OE1 | 7.81 | 1.34 | 1.25 |
| 1 | D | 381 | GLU | CD-OE1 | 7.78 | 1.34 | 1.25 |
| 1 | J | 381 | GLU | CD-OE1 | 7.77 | 1.34 | 1.25 |
| 1 | J | 202 | SER | CB-OG | 7.76 | 1.52 | 1.42 |
| 1 | A | 202 | SER | CB-OG | 7.76 | 1.52 | 1.42 |
| 1 | D | 202 | SER | CB-OG | 7.73 | 1.52 | 1.42 |
| 1 | G | 202 | SER | CB-OG | 7.71 | 1.52 | 1.42 |
| 1 | M | 202 | SER | CB-OG | 7.68 | 1.52 | 1.42 |
| 1 | D | 108 | GLU | CD-OE1 | 7.64 | 1.34 | 1.25 |
| 1 | A | 689 | GLU | CD-OE2 | 7.55 | 1.33 | 1.25 |
| 1 | G | 689 | GLU | CD-OE2 | 7.55 | 1.33 | 1.25 |
| 1 | S | 689 | GLU | CD-OE2 | 7.54 | 1.33 | 1.25 |
| 1 | D | 689 | GLU | CD-OE2 | 7.49 | 1.33 | 1.25 |
| 1 | S | 347 | GLU | CD-OE1 | 7.46 | 1.33 | 1.25 |
| 1 | A | 347 | GLU | CD-OE1 | 7.43 | 1.33 | 1.25 |
| 1 | M | 689 | GLU | CD-OE2 | 7.43 | 1.33 | 1.25 |
| 1 | J | 689 | GLU | CD-OE2 | 7.38 | 1.33 | 1.25 |
| 1 | J | 347 | GLU | CD-OE1 | 7.37 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 23 | GLU | CD-OE1 | 7.36 | 1.33 | 1.25 |
| 1 | M | 347 | GLU | CD-OE1 | 7.33 | 1.33 | 1.25 |
| 1 | D | 23 | GLU | CD-OE1 | 7.33 | 1.33 | 1.25 |
| 1 | S | 23 | GLU | CD-OE1 | 7.30 | 1.33 | 1.25 |
| 1 | J | 23 | GLU | CD-OE1 | 7.28 | 1.33 | 1.25 |
| 1 | D | 347 | GLU | CD-OE1 | 7.27 | 1.33 | 1.25 |
| 1 | G | 347 | GLU | CD-OE1 | 7.25 | 1.33 | 1.25 |
| 1 | M | 23 | GLU | CD-OE1 | 7.24 | 1.33 | 1.25 |
| 1 | G | 23 | GLU | CD-OE1 | 7.22 | 1.33 | 1.25 |
| 1 | M | 511 | GLU | CD-OE1 | 7.19 | 1.33 | 1.25 |
| 1 | J | 511 | GLU | CD-OE1 | 7.17 | 1.33 | 1.25 |
| 1 | A | 511 | GLU | CD-OE1 | 7.16 | 1.33 | 1.25 |
| 1 | S | 511 | GLU | CD-OE1 | 7.16 | 1.33 | 1.25 |
| 1 | M | 524 | GLU | CD-OE1 | 7.09 | 1.33 | 1.25 |
| 1 | S | 785 | GLU | C-N | -7.09 | 1.17 | 1.34 |
| 1 | S | 330 | GLU | CD-OE1 | 7.08 | 1.33 | 1.25 |
| 1 | J | 330 | GLU | CD-OE1 | 7.08 | 1.33 | 1.25 |
| 1 | D | 68 | GLU | CD-OE2 | 7.07 | 1.33 | 1.25 |
| 1 | J | 524 | GLU | CD-OE1 | 7.07 | 1.33 | 1.25 |
| 1 | G | 26 | GLU | CD-OE1 | 7.06 | 1.33 | 1.25 |
| 1 | S | 524 | GLU | CD-OE1 | 7.06 | 1.33 | 1.25 |
| 1 | S | 811 | GLU | CD-OE1 | 7.04 | 1.33 | 1.25 |
| 1 | G | 68 | GLU | CD-OE2 | 7.02 | 1.33 | 1.25 |
| 1 | D | 511 | GLU | CD-OE1 | 6.99 | 1.33 | 1.25 |
| 1 | M | 330 | GLU | CD-OE1 | 6.99 | 1.33 | 1.25 |
| 1 | M | 811 | GLU | CD-OE1 | 6.98 | 1.33 | 1.25 |
| 1 | D | 524 | GLU | CD-OE1 | 6.95 | 1.33 | 1.25 |
| 1 | D | 376 | GLU | CD-OE1 | 6.95 | 1.33 | 1.25 |
| 1 | G | 376 | GLU | CD-OE1 | 6.94 | 1.33 | 1.25 |
| 1 | A | 376 | GLU | CD-OE1 | 6.93 | 1.33 | 1.25 |
| 1 | G | 330 | GLU | CD-OE1 | 6.93 | 1.33 | 1.25 |
| 1 | S | 68 | GLU | CD-OE2 | 6.93 | 1.33 | 1.25 |
| 1 | D | 26 | GLU | CD-OE1 | 6.92 | 1.33 | 1.25 |
| 1 | J | 26 | GLU | CD-OE1 | 6.92 | 1.33 | 1.25 |
| 1 | S | 26 | GLU | CD-OE1 | 6.91 | 1.33 | 1.25 |
| 1 | A | 68 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | A | 655 | GLU | CD-OE1 | 6.89 | 1.33 | 1.25 |
| 1 | S | 655 | GLU | CD-OE1 | 6.89 | 1.33 | 1.25 |
| 1 | A | 524 | GLU | CD-OE1 | 6.89 | 1.33 | 1.25 |
| 1 | J | 811 | GLU | CD-OE1 | 6.88 | 1.33 | 1.25 |
| 1 | J | 68 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | A | 330 | GLU | CD-OE1 | 6.86 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | M | 376 | GLU | CD-OE1 | 6.86 | 1.33 | 1.25 |
| 1 | S | 376 | GLU | CD-OE1 | 6.86 | 1.33 | 1.25 |
| 1 | D | 811 | GLU | CD-OE1 | 6.86 | 1.33 | 1.25 |
| 1 | J | 376 | GLU | CD-OE1 | 6.85 | 1.33 | 1.25 |
| 1 | G | 524 | GLU | CD-OE1 | 6.85 | 1.33 | 1.25 |
| 1 | M | 68 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | A | 26 | GLU | CD-OE1 | 6.82 | 1.33 | 1.25 |
| 1 | S | 319 | GLU | CD-OE1 | 6.81 | 1.33 | 1.25 |
| 1 | M | 26 | GLU | CD-OE1 | 6.81 | 1.33 | 1.25 |
| 1 | J | 538 | GLU | CD-OE1 | 6.80 | 1.33 | 1.25 |
| 1 | G | 511 | GLU | CD-OE1 | 6.78 | 1.33 | 1.25 |
| 1 | J | 319 | GLU | CD-OE1 | 6.78 | 1.33 | 1.25 |
| 1 | M | 319 | GLU | CD-OE1 | 6.75 | 1.33 | 1.25 |
| 1 | D | 330 | GLU | CD-OE1 | 6.72 | 1.33 | 1.25 |
| 1 | A | 811 | GLU | CD-OE1 | 6.71 | 1.33 | 1.25 |
| 1 | M | 538 | GLU | CD-OE1 | 6.70 | 1.33 | 1.25 |
| 1 | J | 655 | GLU | CD-OE1 | 6.69 | 1.33 | 1.25 |
| 1 | S | 538 | GLU | CD-OE1 | 6.69 | 1.33 | 1.25 |
| 1 | G | 655 | GLU | CD-OE1 | 6.67 | 1.32 | 1.25 |
| 1 | M | 655 | GLU | CD-OE1 | 6.66 | 1.32 | 1.25 |
| 1 | G | 811 | GLU | CD-OE1 | 6.62 | 1.32 | 1.25 |
| 1 | G | 785 | GLU | C-N | 6.60 | 1.49 | 1.34 |
| 1 | G | 319 | GLU | CD-OE1 | 6.59 | 1.32 | 1.25 |
| 1 | A | 538 | GLU | CD-OE1 | 6.59 | 1.32 | 1.25 |
| 2 | E | 150 | TYR | CD2-CE2 | -6.59 | 1.29 | 1.39 |
| 1 | D | 655 | GLU | CD-OE1 | 6.58 | 1.32 | 1.25 |
| 1 | G | 502 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | G | 538 | GLU | CD-OE1 | 6.58 | 1.32 | 1.25 |
| 1 | A | 266 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | D | 319 | GLU | CD-OE1 | 6.54 | 1.32 | 1.25 |
| 1 | S | 266 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | D | 538 | GLU | CD-OE2 | -6.53 | 1.18 | 1.25 |
| 1 | G | 99 | GLU | CD-OE2 | 6.53 | 1.32 | 1.25 |
| 1 | D | 266 | GLU | CD-OE2 | 6.52 | 1.32 | 1.25 |
| 1 | D | 538 | GLU | CD-OE1 | 6.51 | 1.32 | 1.25 |
| 1 | J | 266 | GLU | CD-OE2 | 6.51 | 1.32 | 1.25 |
| 1 | M | 266 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 2 | B | 150 | TYR | CD2-CE2 | -6.49 | 1.29 | 1.39 |
| 1 | G | 89 | GLU | CD-OE1 | 6.49 | 1.32 | 1.25 |
| 1 | S | 538 | GLU | CD-OE2 | -6.49 | 1.18 | 1.25 |
| 2 | N | 150 | TYR | CD2-CE2 | -6.48 | 1.29 | 1.39 |
| 1 | D | 99 | GLU | CD-OE2 | 6.46 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 319 | GLU | CD-OE1 | 6.45 | 1.32 | 1.25 |
| 1 | S | 89 | GLU | CD-OE1 | 6.43 | 1.32 | 1.25 |
| 1 | J | 89 | GLU | CD-OE1 | 6.41 | 1.32 | 1.25 |
| 1 | M | 538 | GLU | CD-OE2 | -6.41 | 1.18 | 1.25 |
| 1 | A | 502 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 1 | M | 808 | GLU | CD-OE1 | 6.40 | 1.32 | 1.25 |
| 1 | A | 605 | GLU | CD-OE1 | 6.40 | 1.32 | 1.25 |
| 1 | J | 808 | GLU | CD-OE1 | 6.40 | 1.32 | 1.25 |
| 1 | A | 89 | GLU | CD-OE1 | 6.39 | 1.32 | 1.25 |
| 1 | A | 538 | GLU | CD-OE2 | -6.39 | 1.18 | 1.25 |
| 1 | M | 6 | GLU | CD-OE1 | 6.38 | 1.32 | 1.25 |
| 1 | S | 6 | GLU | CD-OE1 | 6.38 | 1.32 | 1.25 |
| 1 | S | 808 | GLU | CD-OE1 | 6.38 | 1.32 | 1.25 |
| 1 | M | 89 | GLU | CD-OE1 | 6.38 | 1.32 | 1.25 |
| 1 | J | 6 | GLU | CD-OE1 | 6.37 | 1.32 | 1.25 |
| 1 | G | 266 | GLU | CD-OE2 | 6.37 | 1.32 | 1.25 |
| 1 | G | 605 | GLU | CD-OE1 | 6.36 | 1.32 | 1.25 |
| 1 | A | 808 | GLU | CD-OE1 | 6.36 | 1.32 | 1.25 |
| 1 | J | 538 | GLU | CD-OE2 | -6.36 | 1.18 | 1.25 |
| 1 | G | 808 | GLU | CD-OE1 | 6.35 | 1.32 | 1.25 |
| 2 | T | 150 | TYR | CD2-CE2 | -6.35 | 1.29 | 1.39 |
| 2 | K | 150 | TYR | CD2-CE2 | -6.34 | 1.29 | 1.39 |
| 1 | D | 6 | GLU | CD-OE1 | 6.34 | 1.32 | 1.25 |
| 1 | D | 808 | GLU | CD-OE1 | 6.33 | 1.32 | 1.25 |
| 1 | G | 802 | GLU | CD-OE1 | 6.33 | 1.32 | 1.25 |
| 1 | M | 502 | GLU | CD-OE2 | 6.33 | 1.32 | 1.25 |
| 2 | B | 150 | TYR | N-CA | -6.32 | 1.33 | 1.46 |
| 1 | S | 99 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | J | 99 | GLU | CD-OE2 | 6.31 | 1.32 | 1.25 |
| 4 | Y | 259 | GLU | CG-CD | 6.31 | 1.61 | 1.51 |
| 4 | 4 | 259 | GLU | CG-CD | 6.30 | 1.61 | 1.51 |
| 1 | S | 802 | GLU | CD-OE1 | 6.30 | 1.32 | 1.25 |
| 1 | G | 538 | GLU | CD-OE2 | -6.30 | 1.18 | 1.25 |
| 4 | 6 | 259 | GLU | CG-CD | 6.30 | 1.61 | 1.51 |
| 2 | H | 150 | TYR | CD2-CE2 | -6.29 | 1.29 | 1.39 |
| 1 | D | 89 | GLU | CD-OE1 | 6.29 | 1.32 | 1.25 |
| 1 | M | 99 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 1 | M | 605 | GLU | CD-OE1 | 6.27 | 1.32 | 1.25 |
| 1 | A | 6 | GLU | CD-OE1 | 6.27 | 1.32 | 1.25 |
| 1 | J | 502 | GLU | CD-OE2 | 6.27 | 1.32 | 1.25 |
| 1 | J | 802 | GLU | CD-OE1 | 6.26 | 1.32 | 1.25 |
| 4 | 9 | 259 | GLU | CG-CD | 6.26 | 1.61 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | G | 6 | GLU | CD-OE1 | 6.26 | 1.32 | 1.25 |
| 4 | X | 259 | GLU | CG-CD | 6.26 | 1.61 | 1.51 |
| 1 | S | 502 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | D | 502 | GLU | CD-OE2 | 6.25 | 1.32 | 1.25 |
| 4 | 3 | 259 | GLU | CG-CD | 6.25 | 1.61 | 1.51 |
| 4 | 5 | 259 | GLU | CG-CD | 6.24 | 1.61 | 1.51 |
| 4 | W | 259 | GLU | CG-CD | 6.24 | 1.61 | 1.51 |
| 2 | T | 150 | TYR | N-CA | -6.24 | 1.33 | 1.46 |
| 1 | S | 605 | GLU | CD-OE1 | 6.23 | 1.32 | 1.25 |
| 2 | H | 150 | TYR | N-CA | -6.23 | 1.33 | 1.46 |
| 1 | D | 802 | GLU | CD-OE1 | 6.23 | 1.32 | 1.25 |
| 4 | V | 259 | GLU | CG-CD | 6.22 | 1.61 | 1.51 |
| 4 | 2 | 259 | GLU | CG-CD | 6.21 | 1.61 | 1.51 |
| 1 | D | 605 | GLU | CD-OE1 | 6.21 | 1.32 | 1.25 |
| 4 | 7 | 259 | GLU | CG-CD | 6.21 | 1.61 | 1.51 |
| 4 | 1 | 259 | GLU | CG-CD | 6.20 | 1.61 | 1.51 |
| 2 | N | 150 | TYR | N-CA | -6.20 | 1.33 | 1.46 |
| 4 | Z | 259 | GLU | CG-CD | 6.19 | 1.61 | 1.51 |
| 1 | D | 509 | GLU | CD-OE1 | 6.18 | 1.32 | 1.25 |
| 1 | A | 99 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | J | 605 | GLU | CD-OE1 | 6.18 | 1.32 | 1.25 |
| 2 | K | 150 | TYR | N-CA | -6.17 | 1.34 | 1.46 |
| 1 | G | 509 | GLU | CD-OE1 | 6.16 | 1.32 | 1.25 |
| 4 | 8 | 259 | GLU | CG-CD | 6.16 | 1.61 | 1.51 |
| 1 | M | 329 | GLU | CD-OE1 | 6.14 | 1.32 | 1.25 |
| 2 | E | 150 | TYR | N-CA | -6.14 | 1.34 | 1.46 |
| 1 | A | 509 | GLU | CD-OE1 | 6.14 | 1.32 | 1.25 |
| 1 | A | 329 | GLU | CD-OE1 | 6.13 | 1.32 | 1.25 |
| 1 | M | 509 | GLU | CD-OE1 | 6.13 | 1.32 | 1.25 |
| 1 | S | 329 | GLU | CD-OE1 | 6.12 | 1.32 | 1.25 |
| 1 | J | 329 | GLU | CD-OE1 | 6.07 | 1.32 | 1.25 |
| 1 | A | 417 | GLU | CD-OE1 | 6.06 | 1.32 | 1.25 |
| 1 | J | 509 | GLU | CD-OE1 | 6.06 | 1.32 | 1.25 |
| 1 | M | 230 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | S | 230 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | M | 802 | GLU | CD-OE1 | 6.02 | 1.32 | 1.25 |
| 1 | G | 476 | GLU | CD-OE2 | -6.00 | 1.19 | 1.25 |
| 1 | D | 417 | GLU | CD-OE1 | 5.96 | 1.32 | 1.25 |
| 1 | J | 527 | GLU | CD-OE1 | 5.94 | 1.32 | 1.25 |
| 1 | M | 417 | GLU | CD-OE1 | 5.93 | 1.32 | 1.25 |
| 1 | G | 417 | GLU | CD-OE1 | 5.93 | 1.32 | 1.25 |
| 1 | G | 329 | GLU | CD-OE1 | 5.93 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | D | 329 | GLU | CD-OE1 | 5.93 | 1.32 | 1.25 |
| 1 | S | 509 | GLU | CD-OE1 | 5.92 | 1.32 | 1.25 |
| 1 | J | 540 | CYS | CB-SG | -5.90 | 1.72 | 1.81 |
| 1 | J | 230 | GLU | CD-OE2 | 5.89 | 1.32 | 1.25 |
| 1 | A | 476 | GLU | CD-OE2 | -5.88 | 1.19 | 1.25 |
| 1 | G | 540 | CYS | CB-SG | -5.87 | 1.72 | 1.81 |
| 1 | J | 417 | GLU | CD-OE1 | 5.87 | 1.32 | 1.25 |
| 1 | J | 476 | GLU | CD-OE2 | -5.85 | 1.19 | 1.25 |
| 1 | A | 802 | GLU | CD-OE1 | 5.85 | 1.32 | 1.25 |
| 1 | D | 785 | GLU | CD-OE2 | 5.85 | 1.32 | 1.25 |
| 1 | M | 540 | CYS | CB-SG | -5.85 | 1.72 | 1.81 |
| 1 | D | 468 | GLU | CD-OE1 | 5.83 | 1.32 | 1.25 |
| 1 | A | 74 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 1 | G | 230 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 1 | G | 218 | LEU | CB-CG | 5.82 | 1.69 | 1.52 |
| 1 | M | 527 | GLU | CD-OE1 | 5.81 | 1.32 | 1.25 |
| 1 | S | 540 | CYS | CB-SG | -5.81 | 1.72 | 1.81 |
| 1 | D | 230 | GLU | CD-OE2 | 5.81 | 1.32 | 1.25 |
| 1 | M | 74 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | A | 468 | GLU | CD-OE1 | 5.79 | 1.32 | 1.25 |
| 1 | S | 417 | GLU | CD-OE1 | 5.79 | 1.32 | 1.25 |
| 1 | S | 74 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | M | 499 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | M | 468 | GLU | CD-OE1 | 5.78 | 1.32 | 1.25 |
| 1 | J | 499 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | J | 74 | GLU | CD-OE2 | 5.77 | 1.32 | 1.25 |
| 1 | S | 476 | GLU | CD-OE2 | -5.77 | 1.19 | 1.25 |
| 1 | S | 499 | GLU | CD-OE2 | 5.77 | 1.31 | 1.25 |
| 1 | J | 468 | GLU | CD-OE1 | 5.77 | 1.31 | 1.25 |
| 1 | A | 230 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | M | 421 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | M | 476 | GLU | CD-OE2 | -5.75 | 1.19 | 1.25 |
| 1 | D | 540 | CYS | CB-SG | -5.75 | 1.72 | 1.81 |
| 1 | S | 468 | GLU | CD-OE1 | 5.75 | 1.31 | 1.25 |
| 1 | J | 421 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | J | 597 | GLU | CD-OE1 | 5.75 | 1.31 | 1.25 |
| 1 | S | 785 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | A | 785 | GLU | CD-OE2 | 5.73 | 1.31 | 1.25 |
| 1 | S | 527 | GLU | CD-OE1 | 5.73 | 1.31 | 1.25 |
| 1 | A | 597 | GLU | CD-OE1 | 5.73 | 1.31 | 1.25 |
| 1 | D | 476 | GLU | CD-OE2 | -5.72 | 1.19 | 1.25 |
| 1 | G | 597 | GLU | CD-OE1 | 5.72 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | D | 218 | LEU | CB-CG | 5.71 | 1.69 | 1.52 |
| 1 | A | 625 | THR | CB-CG2 | 5.71 | 1.71 | 1.52 |
| 1 | J | 625 | THR | CB-CG2 | 5.71 | 1.71 | 1.52 |
| 1 | A | 540 | CYS | CB-SG | -5.70 | 1.72 | 1.81 |
| 1 | G | 74 | GLU | CD-OE2 | 5.70 | 1.31 | 1.25 |
| 1 | M | 625 | THR | CB-CG2 | 5.70 | 1.71 | 1.52 |
| 1 | S | 625 | THR | CB-CG2 | 5.70 | 1.71 | 1.52 |
| 1 | S | 421 | GLU | CD-OE2 | 5.69 | 1.31 | 1.25 |
| 1 | J | 218 | LEU | CB-CG | 5.68 | 1.69 | 1.52 |
| 1 | D | 625 | THR | CB-CG2 | 5.67 | 1.71 | 1.52 |
| 1 | A | 527 | GLU | CD-OE1 | 5.67 | 1.31 | 1.25 |
| 1 | G | 785 | GLU | CD-OE2 | 5.67 | 1.31 | 1.25 |
| 1 | G | 625 | THR | CB-CG2 | 5.65 | 1.71 | 1.52 |
| 1 | S | 218 | LEU | CB-CG | 5.65 | 1.69 | 1.52 |
| 1 | A | 218 | LEU | CB-CG | 5.64 | 1.69 | 1.52 |
| 1 | M | 218 | LEU | CB-CG | 5.64 | 1.69 | 1.52 |
| 1 | D | 597 | GLU | CD-OE1 | 5.63 | 1.31 | 1.25 |
| 1 | D | 499 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | G | 527 | GLU | CD-OE1 | 5.63 | 1.31 | 1.25 |
| 1 | J | 785 | GLU | CD-OE2 | 5.61 | 1.31 | 1.25 |
| 1 | M | 785 | GLU | CD-OE2 | 5.61 | 1.31 | 1.25 |
| 1 | D | 74 | GLU | CD-OE2 | 5.60 | 1.31 | 1.25 |
| 1 | D | 687 | GLU | CD-OE1 | 5.60 | 1.31 | 1.25 |
| 1 | G | 687 | GLU | CD-OE1 | 5.59 | 1.31 | 1.25 |
| 1 | A | 687 | GLU | CD-OE1 | 5.59 | 1.31 | 1.25 |
| 1 | J | 373 | GLU | CD-OE1 | 5.59 | 1.31 | 1.25 |
| 1 | M | 687 | GLU | CD-OE1 | 5.58 | 1.31 | 1.25 |
| 1 | A | 421 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 2 | H | 150 | TYR | CE1-CZ | 5.58 | 1.45 | 1.38 |
| 1 | G | 468 | GLU | CD-OE1 | 5.56 | 1.31 | 1.25 |
| 1 | G | 373 | GLU | CD-OE1 | 5.55 | 1.31 | 1.25 |
| 1 | S | 687 | GLU | CD-OE1 | 5.54 | 1.31 | 1.25 |
| 1 | J | 687 | GLU | CD-OE1 | 5.53 | 1.31 | 1.25 |
| 1 | S | 373 | GLU | CD-OE1 | 5.53 | 1.31 | 1.25 |
| 1 | S | 597 | GLU | CD-OE1 | 5.53 | 1.31 | 1.25 |
| 1 | D | 373 | GLU | CD-OE1 | 5.52 | 1.31 | 1.25 |
| 1 | D | 527 | GLU | CD-OE1 | 5.52 | 1.31 | 1.25 |
| 1 | M | 597 | GLU | CD-OE1 | 5.52 | 1.31 | 1.25 |
| 1 | G | 298 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 1 | G | 499 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 2 | K | 131 | GLU | N-CA | 5.51 | 1.57 | 1.46 |
| 2 | E | 150 | TYR | CE1-CZ | 5.51 | 1.45 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | M | 373 | GLU | CD-OE1 | 5.49 | 1.31 | 1.25 |
| 1 | M | 777 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | G | 506 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | G | 421 | GLU | CD-OE2 | 5.47 | 1.31 | 1.25 |
| 1 | A | 373 | GLU | CD-OE1 | 5.47 | 1.31 | 1.25 |
| 1 | J | 777 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | A | 777 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 2 | T | 131 | GLU | N-CA | 5.45 | 1.57 | 1.46 |
| 2 | B | 150 | TYR | CE1-CZ | 5.44 | 1.45 | 1.38 |
| 1 | D | 777 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | S | 298 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | A | 479 | CYS | CB-SG | -5.43 | 1.73 | 1.81 |
| 1 | A | 499 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 2 | N | 131 | GLU | N-CA | 5.42 | 1.57 | 1.46 |
| 1 | A | 65 | GLU | CD-OE1 | 5.41 | 1.31 | 1.25 |
| 1 | G | 777 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 2 | H | 131 | GLU | N-CA | 5.40 | 1.57 | 1.46 |
| 1 | G | 479 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |
| 1 | S | 777 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | A | 506 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | S | 479 | CYS | CB-SG | -5.39 | 1.73 | 1.81 |
| 1 | D | 218 | LEU | C-N | -5.37 | 1.21 | 1.34 |
| 1 | D | 421 | GLU | CD-OE2 | 5.37 | 1.31 | 1.25 |
| 1 | D | 298 | GLU | CD-OE2 | 5.36 | 1.31 | 1.25 |
| 2 | E | 131 | GLU | N-CA | 5.36 | 1.57 | 1.46 |
| 1 | A | 218 | LEU | C-N | -5.36 | 1.21 | 1.34 |
| 2 | B | 131 | GLU | N-CA | 5.35 | 1.57 | 1.46 |
| 2 | N | 150 | TYR | CE1-CZ | 5.35 | 1.45 | 1.38 |
| 1 | J | 218 | LEU | C-N | -5.35 | 1.21 | 1.34 |
| 2 | T | 150 | TYR | CE1-CZ | 5.35 | 1.45 | 1.38 |
| 1 | M | 479 | CYS | CB-SG | -5.35 | 1.73 | 1.81 |
| 2 | K | 150 | TYR | CE1-CZ | 5.34 | 1.45 | 1.38 |
| 1 | M | 218 | LEU | C-N | -5.34 | 1.21 | 1.34 |
| 1 | D | 65 | GLU | CD-OE1 | 5.34 | 1.31 | 1.25 |
| 1 | J | 479 | CYS | CB-SG | -5.31 | 1.73 | 1.81 |
| 1 | J | 679 | GLU | CD-OE2 | 5.31 | 1.31 | 1.25 |
| 1 | S | 218 | LEU | C-N | -5.31 | 1.21 | 1.34 |
| 1 | G | 218 | LEU | C-N | -5.31 | 1.21 | 1.34 |
| 1 | S | 679 | GLU | CD-OE2 | 5.29 | 1.31 | 1.25 |
| 1 | J | 65 | GLU | CD-OE1 | 5.29 | 1.31 | 1.25 |
| 1 | M | 679 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | G | 679 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 298 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |
| 1 | J | 298 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |
| 1 | S | 527 | GLU | CD-OE2 | -5.26 | 1.19 | 1.25 |
| 1 | D | 679 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 1 | M | 298 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 2 | K | 149 | ASP | CB-CG | 5.25 | 1.62 | 1.51 |
| 1 | D | 479 | CYS | CB-SG | -5.25 | 1.73 | 1.81 |
| 1 | M | 65 | GLU | CD-OE1 | 5.23 | 1.31 | 1.25 |
| 1 | S | 21 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | S | 702 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | G | 65 | GLU | CD-OE1 | 5.21 | 1.31 | 1.25 |
| 2 | N | 149 | ASP | CB-CG | 5.21 | 1.62 | 1.51 |
| 1 | D | 282 | GLU | CD-OE1 | 5.21 | 1.31 | 1.25 |
| 1 | D | 702 | GLU | CD-OE2 | 5.21 | 1.31 | 1.25 |
| 1 | J | 702 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | S | 506 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | J | 506 | GLU | CD-OE2 | 5.19 | 1.31 | 1.25 |
| 1 | S | 65 | GLU | CD-OE1 | 5.18 | 1.31 | 1.25 |
| 1 | M | 527 | GLU | CD-OE2 | -5.18 | 1.20 | 1.25 |
| 2 | T | 149 | ASP | CB-CG | 5.18 | 1.62 | 1.51 |
| 1 | A | 679 | GLU | CD-OE2 | 5.18 | 1.31 | 1.25 |
| 1 | J | 527 | GLU | CD-OE2 | -5.17 | 1.20 | 1.25 |
| 1 | A | 21 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | A | 702 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | G | 21 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | S | 282 | GLU | CD-OE1 | 5.15 | 1.31 | 1.25 |
| 1 | M | 506 | GLU | CD-OE2 | 5.15 | 1.31 | 1.25 |
| 1 | D | 506 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 2 | B | 149 | ASP | CB-CG | 5.14 | 1.62 | 1.51 |
| 1 | S | 12 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 2 | E | 149 | ASP | CB-CG | 5.12 | 1.62 | 1.51 |
| 1 | J | 282 | GLU | CD-OE1 | 5.12 | 1.31 | 1.25 |
| 4 | V | 259 | GLU | CB-CG | 5.12 | 1.61 | 1.52 |
| 1 | M | 702 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | G | 702 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | G | 697 | CYS | CB-SG | 5.10 | 1.91 | 1.82 |
| 1 | J | 150 | GLU | CD-OE1 | 5.10 | 1.31 | 1.25 |
| 1 | M | 12 | GLU | CD-OE2 | 5.10 | 1.31 | 1.25 |
| 1 | M | 21 | GLU | CD-OE2 | 5.10 | 1.31 | 1.25 |
| 1 | A | 527 | GLU | CD-OE2 | -5.09 | 1.20 | 1.25 |
| 4 | 1 | 259 | GLU | CB-CG | 5.08 | 1.61 | 1.52 |
| 1 | A | 697 | CYS | CB-SG | 5.08 | 1.90 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | A | 539 | GLU | CD-OE1 | 5.08 | 1.31 | 1.25 |
| 4 | 8 | 259 | GLU | CB-CG | 5.07 | 1.61 | 1.52 |
| 1 | G | 12 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 2 | H | 149 | ASP | CB-CG | 5.06 | 1.62 | 1.51 |
| 1 | M | 150 | GLU | CD-OE1 | 5.06 | 1.31 | 1.25 |
| 1 | A | 150 | GLU | CD-OE1 | 5.06 | 1.31 | 1.25 |
| 4 | 4 | 259 | GLU | CB-CG | 5.06 | 1.61 | 1.52 |
| 4 | 9 | 259 | GLU | CB-CG | 5.05 | 1.61 | 1.52 |
| 1 | A | 282 | GLU | CD-OE1 | 5.05 | 1.31 | 1.25 |
| 1 | J | 21 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | S | 150 | GLU | CD-OE1 | 5.04 | 1.31 | 1.25 |
| 4 | 3 | 259 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 4 | W | 259 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 4 | Z | 259 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 4 | 7 | 259 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 1 | J | 12 | GLU | CD-OE2 | 5.03 | 1.31 | 1.25 |
| 4 | 5 | 259 | GLU | CB-CG | 5.03 | 1.61 | 1.52 |
| 1 | G | 539 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 1 | D | 21 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 4 | 2 | 259 | GLU | CB-CG | 5.02 | 1.61 | 1.52 |
| 1 | D | 56 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 1 | D | 697 | CYS | CB-SG | 5.02 | 1.90 | 1.82 |
| 1 | S | 697 | CYS | CB-SG | 5.02 | 1.90 | 1.82 |
| 1 | G | 282 | GLU | CD-OE1 | 5.01 | 1.31 | 1.25 |
| 1 | A | 12 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |
| 4 | Y | 259 | GLU | CB-CG | 5.00 | 1.61 | 1.52 |
| 1 | D | 150 | GLU | CD-OE1 | 5.00 | 1.31 | 1.25 |

All (1542) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | G | 637 | LYS | O-C-N | -58.53 | 23.70 | 123.20 |
| 1 | D | 637 | LYS | O-C-N | -58.47 | 23.79 | 123.20 |
| 1 | M | 637 | LYS | O-C-N | -58.47 | 23.80 | 123.20 |
| 1 | S | 637 | LYS | O-C-N | -58.47 | 23.80 | 123.20 |
| 1 | J | 637 | LYS | O-C-N | -58.47 | 23.81 | 123.20 |
| 1 | A | 637 | LYS | O-C-N | -58.44 | 23.86 | 123.20 |
| 1 | J | 709 | LYS | O-C-N | -39.10 | 56.73 | 123.20 |
| 1 | J | 649 | VAL | CG1-CB-CG2 | -34.02 | 56.48 | 110.90 |
| 1 | D | 649 | VAL | CG1-CB-CG2 | -34.00 | 56.49 | 110.90 |
| 1 | M | 649 | VAL | CG1-CB-CG2 | -34.00 | 56.50 | 110.90 |
| 1 | A | 649 | VAL | CG1-CB-CG2 | -33.99 | 56.51 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | G | 649 | VAL | CG1-CB-CG2 | -33.99 | 56.52 | 110.90 |
| 1 | S | 649 | VAL | CG1-CB-CG2 | -33.99 | 56.52 | 110.90 |
| 1 | J | 648 | THR | CA-CB-OG1 | -31.72 | 42.39 | 109.00 |
| 1 | S | 648 | THR | CA-CB-OG1 | -31.71 | 42.41 | 109.00 |
| 1 | M | 648 | THR | CA-CB-OG1 | -31.71 | 42.41 | 109.00 |
| 1 | G | 648 | THR | CA-CB-OG1 | -31.70 | 42.44 | 109.00 |
| 1 | A | 648 | THR | CA-CB-OG1 | -31.69 | 42.45 | 109.00 |
| 1 | D | 648 | THR | CA-CB-OG1 | -31.69 | 42.45 | 109.00 |
| 2 | E | 150 | TYR | CB-CG-CD2 | -28.67 | 103.80 | 121.00 |
| 2 | H | 150 | TYR | CB-CG-CD2 | -28.64 | 103.81 | 121.00 |
| 2 | T | 150 | TYR | CB-CG-CD2 | -28.64 | 103.82 | 121.00 |
| 2 | K | 150 | TYR | CB-CG-CD2 | -28.59 | 103.84 | 121.00 |
| 2 | B | 150 | TYR | CB-CG-CD2 | -28.55 | 103.87 | 121.00 |
| 2 | N | 150 | TYR | CB-CG-CD2 | -28.53 | 103.88 | 121.00 |
| 1 | G | 649 | VAL | CA-CB-CG1 | -28.52 | 68.12 | 110.90 |
| 1 | D | 649 | VAL | CA-CB-CG1 | -28.49 | 68.16 | 110.90 |
| 1 | J | 649 | VAL | CA-CB-CG1 | -28.48 | 68.17 | 110.90 |
| 1 | M | 649 | VAL | CA-CB-CG1 | -28.46 | 68.20 | 110.90 |
| 1 | S | 649 | VAL | CA-CB-CG1 | -28.45 | 68.22 | 110.90 |
| 1 | A | 649 | VAL | CA-CB-CG1 | -28.44 | 68.24 | 110.90 |
| 1 | G | 649 | VAL | CA-CB-CG2 | -28.18 | 68.63 | 110.90 |
| 1 | D | 649 | VAL | CA-CB-CG2 | -28.16 | 68.67 | 110.90 |
| 1 | J | 649 | VAL | CA-CB-CG2 | -28.16 | 68.67 | 110.90 |
| 1 | M | 649 | VAL | CA-CB-CG2 | -28.15 | 68.67 | 110.90 |
| 1 | A | 649 | VAL | CA-CB-CG2 | -28.15 | 68.67 | 110.90 |
| 1 | S | 649 | VAL | CA-CB-CG2 | -28.11 | 68.73 | 110.90 |
| 1 | S | 648 | THR | CA-CB-CG2 | -25.62 | 76.53 | 112.40 |
| 1 | M | 648 | THR | CA-CB-CG2 | -25.60 | 76.56 | 112.40 |
| 1 | J | 648 | THR | CA-CB-CG2 | -25.57 | 76.59 | 112.40 |
| 1 | D | 648 | THR | CA-CB-CG2 | -25.54 | 76.64 | 112.40 |
| 1 | A | 648 | THR | CA-CB-CG2 | -25.44 | 76.79 | 112.40 |
| 1 | G | 648 | THR | CA-CB-CG2 | -25.36 | 76.90 | 112.40 |
| 1 | S | 785 | GLU | O-C-N | -23.89 | 84.48 | 122.70 |
| 2 | H | 150 | TYR | CG-CD2-CE2 | -20.88 | 104.60 | 121.30 |
| 2 | T | 150 | TYR | CG-CD2-CE2 | -20.64 | 104.79 | 121.30 |
| 2 | E | 150 | TYR | CG-CD2-CE2 | -20.61 | 104.81 | 121.30 |
| 2 | N | 150 | TYR | CG-CD2-CE2 | -20.59 | 104.82 | 121.30 |
| 2 | K | 150 | TYR | CG-CD2-CE2 | -20.57 | 104.85 | 121.30 |
| 2 | B | 150 | TYR | CG-CD2-CE2 | -20.54 | 104.87 | 121.30 |
| 1 | M | 709 | LYS | O-C-N | -19.71 | 89.70 | 123.20 |
| 2 | K | 150 | TYR | CD1-CG-CD2 | 19.50 | 139.35 | 117.90 |
| 2 | T | 150 | TYR | CD1-CG-CD2 | 19.49 | 139.34 | 117.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2 | H | 150 | TYR | CD1-CG-CD2 | 19.49 | 139.34 | 117.90 |
| 2 | N | 150 | TYR | CD1-CG-CD2 | 19.47 | 139.32 | 117.90 |
| 2 | E | 150 | TYR | CD1-CG-CD2 | 19.45 | 139.30 | 117.90 |
| 2 | B | 150 | TYR | CD1-CG-CD2 | 19.41 | 139.25 | 117.90 |
| 2 | E | 150 | TYR | CG-CD1-CE1 | -18.55 | 106.46 | 121.30 |
| 2 | H | 150 | TYR | CG-CD1-CE1 | -18.50 | 106.50 | 121.30 |
| 2 | T | 150 | TYR | CG-CD1-CE1 | -18.48 | 106.52 | 121.30 |
| 2 | K | 150 | TYR | CG-CD1-CE1 | -18.45 | 106.54 | 121.30 |
| 2 | N | 150 | TYR | CG-CD1-CE1 | -18.39 | 106.59 | 121.30 |
| 2 | B | 150 | TYR | CG-CD1-CE1 | -18.31 | 106.66 | 121.30 |
| 1 | M | 800 | ARG | NE-CZ-NH2 | -16.63 | 111.98 | 120.30 |
| 1 | D | 800 | ARG | NE-CZ-NH2 | -16.56 | 112.02 | 120.30 |
| 1 | J | 800 | ARG | NE-CZ-NH2 | -16.53 | 112.03 | 120.30 |
| 1 | S | 800 | ARG | NE-CZ-NH2 | -16.37 | 112.12 | 120.30 |
| 1 | G | 800 | ARG | NE-CZ-NH2 | -16.28 | 112.16 | 120.30 |
| 1 | A | 800 | ARG | NE-CZ-NH2 | -16.10 | 112.25 | 120.30 |
| 1 | G | 623 | PHE | CB-CG-CD2 | -13.78 | 111.16 | 120.80 |
| 1 | S | 623 | PHE | CB-CG-CD2 | -13.67 | 111.23 | 120.80 |
| 1 | A | 623 | PHE | CB-CG-CD2 | -13.66 | 111.24 | 120.80 |
| 1 | D | 623 | PHE | CB-CG-CD2 | -13.64 | 111.25 | 120.80 |
| 1 | M | 623 | PHE | CB-CG-CD2 | -13.63 | 111.26 | 120.80 |
| 1 | J | 623 | PHE | CB-CG-CD2 | -13.63 | 111.26 | 120.80 |
| 1 | S | 769 | ALA | CA-C-N | -13.05 | 90.10 | 116.20 |
| 1 | S | 623 | PHE | CB-CG-CD1 | 12.39 | 129.47 | 120.80 |
| 1 | A | 623 | PHE | CB-CG-CD1 | 12.37 | 129.46 | 120.80 |
| 1 | S | 785 | GLU | CA-C-N | 12.35 | 144.36 | 117.20 |
| 1 | M | 623 | PHE | CB-CG-CD1 | 12.32 | 129.43 | 120.80 |
| 1 | J | 623 | PHE | CB-CG-CD1 | 12.31 | 129.42 | 120.80 |
| 1 | G | 623 | PHE | CB-CG-CD1 | 12.29 | 129.40 | 120.80 |
| 1 | J | 623 | PHE | CA-CB-CG | -12.27 | 84.46 | 113.90 |
| 1 | M | 623 | PHE | CA-CB-CG | -12.27 | 84.46 | 113.90 |
| 1 | S | 623 | PHE | CA-CB-CG | -12.26 | 84.48 | 113.90 |
| 1 | A | 623 | PHE | CA-CB-CG | -12.25 | 84.50 | 113.90 |
| 1 | D | 623 | PHE | CA-CB-CG | -12.23 | 84.53 | 113.90 |
| 1 | G | 623 | PHE | CA-CB-CG | -12.20 | 84.61 | 113.90 |
| 1 | D | 623 | PHE | CB-CG-CD1 | 12.08 | 129.26 | 120.80 |
| 1 | J | 98 | HIS | CB-CA-C | -11.60 | 87.21 | 110.40 |
| 1 | M | 98 | HIS | CB-CA-C | -11.60 | 87.21 | 110.40 |
| 1 | S | 98 | HIS | CB-CA-C | -11.57 | 87.27 | 110.40 |
| 1 | G | 98 | HIS | CB-CA-C | -11.55 | 87.29 | 110.40 |
| 1 | D | 98 | HIS | CB-CA-C | -11.55 | 87.31 | 110.40 |
| 1 | A | 98 | HIS | CB-CA-C | -11.54 | 87.32 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | D | 568 | PRO | O-C-N | 10.70 | 139.81 | 122.70 |
| 1 | G | 568 | PRO | O-C-N | 10.69 | 139.80 | 122.70 |
| 1 | A | 568 | PRO | O-C-N | 10.68 | 139.78 | 122.70 |
| 1 | J | 568 | PRO | O-C-N | 10.64 | 139.73 | 122.70 |
| 1 | M | 568 | PRO | O-C-N | 10.62 | 139.69 | 122.70 |
| 1 | S | 568 | PRO | O-C-N | 10.57 | 139.61 | 122.70 |
| 2 | E | 141 | PRO | CA-N-CD | 10.28 | 126.09 | 111.70 |
| 2 | H | 141 | PRO | CA-N-CD | 10.26 | 126.06 | 111.70 |
| 2 | T | 141 | PRO | CA-N-CD | 10.23 | 126.03 | 111.70 |
| 2 | K | 141 | PRO | CA-N-CD | 10.22 | 126.02 | 111.70 |
| 2 | N | 141 | PRO | CA-N-CD | 10.18 | 125.96 | 111.70 |
| 2 | B | 141 | PRO | CA-N-CD | 10.12 | 125.87 | 111.70 |
| 1 | G | 327 | ASP | CB-CG-OD1 | -10.07 | 109.23 | 118.30 |
| 1 | M | 625 | THR | CA-CB-CG2 | -10.07 | 98.30 | 112.40 |
| 1 | G | 625 | THR | CA-CB-CG2 | -10.06 | 98.31 | 112.40 |
| 1 | S | 625 | THR | CA-CB-CG2 | -10.06 | 98.32 | 112.40 |
| 1 | J | 625 | THR | CA-CB-CG2 | -10.06 | 98.32 | 112.40 |
| 1 | S | 327 | ASP | CB-CG-OD1 | -10.05 | 109.25 | 118.30 |
| 1 | A | 625 | THR | CA-CB-CG2 | -10.03 | 98.36 | 112.40 |
| 1 | J | 327 | ASP | CB-CG-OD1 | -10.01 | 109.30 | 118.30 |
| 1 | A | 327 | ASP | CB-CG-OD1 | -9.99 | 109.31 | 118.30 |
| 1 | D | 625 | THR | CA-CB-CG2 | -9.99 | 98.41 | 112.40 |
| 1 | M | 327 | ASP | CB-CG-OD1 | -9.98 | 109.32 | 118.30 |
| 1 | D | 327 | ASP | CB-CG-OD1 | -9.94 | 109.36 | 118.30 |
| 1 | A | 241 | ASP | CB-CG-OD1 | -9.88 | 109.41 | 118.30 |
| 1 | G | 241 | ASP | CB-CG-OD1 | -9.85 | 109.44 | 118.30 |
| 1 | S | 241 | ASP | CB-CG-OD1 | -9.80 | 109.48 | 118.30 |
| 1 | M | 241 | ASP | CB-CG-OD1 | -9.80 | 109.48 | 118.30 |
| 3 | C | 63 | ILE | O-C-N | 9.76 | 138.32 | 122.70 |
| 1 | D | 241 | ASP | CB-CG-OD1 | -9.76 | 109.52 | 118.30 |
| 3 | O | 63 | ILE | O-C-N | 9.75 | 138.29 | 122.70 |
| 3 | I | 63 | ILE | O-C-N | 9.72 | 138.25 | 122.70 |
| 3 | L | 63 | ILE | O-C-N | 9.72 | 138.25 | 122.70 |
| 3 | U | 63 | ILE | O-C-N | 9.72 | 138.25 | 122.70 |
| 1 | D | 728 | ASN | O-C-N | 9.71 | 138.24 | 122.70 |
| 3 | F | 63 | ILE | O-C-N | 9.71 | 138.24 | 122.70 |
| 1 | J | 241 | ASP | CB-CG-OD1 | -9.71 | 109.56 | 118.30 |
| 1 | J | 728 | ASN | O-C-N | 9.70 | 138.21 | 122.70 |
| 1 | M | 728 | ASN | O-C-N | 9.68 | 138.19 | 122.70 |
| 1 | A | 728 | ASN | O-C-N | 9.63 | 138.11 | 122.70 |
| 1 | G | 728 | ASN | O-C-N | 9.60 | 138.06 | 122.70 |
| 1 | S | 728 | ASN | O-C-N | 9.59 | 138.05 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | G | 264 | ASP | CB-CG-OD2 | -9.50 | 109.75 | 118.30 |
| 1 | J | 264 | ASP | CB-CG-OD2 | -9.47 | 109.78 | 118.30 |
| 1 | D | 264 | ASP | CB-CG-OD2 | -9.44 | 109.80 | 118.30 |
| 1 | M | 264 | ASP | CB-CG-OD2 | -9.40 | 109.84 | 118.30 |
| 2 | E | 150 | TYR | N-CA-CB | -9.40 | 93.68 | 110.60 |
| 1 | A | 264 | ASP | CB-CG-OD2 | -9.38 | 109.86 | 118.30 |
| 2 | N | 150 | TYR | N-CA-CB | -9.38 | 93.72 | 110.60 |
| 1 | S | 264 | ASP | CB-CG-OD2 | -9.37 | 109.87 | 118.30 |
| 2 | T | 150 | TYR | N-CA-CB | -9.37 | 93.74 | 110.60 |
| 2 | K | 150 | TYR | N-CA-CB | -9.35 | 93.78 | 110.60 |
| 2 | H | 150 | TYR | N-CA-CB | -9.33 | 93.80 | 110.60 |
| 2 | B | 150 | TYR | N-CA-CB | -9.33 | 93.81 | 110.60 |
| 4 | 7 | 356 | TRP | CD1-CG-CD2 | 9.19 | 113.65 | 106.30 |
| 4 | W | 356 | TRP | CD1-CG-CD2 | 9.16 | 113.63 | 106.30 |
| 4 | 9 | 356 | TRP | CD1-CG-CD2 | 9.15 | 113.62 | 106.30 |
| 4 | 2 | 356 | TRP | CD1-CG-CD2 | 9.15 | 113.62 | 106.30 |
| 4 | 5 | 356 | TRP | CD1-CG-CD2 | 9.14 | 113.61 | 106.30 |
| 4 | 8 | 356 | TRP | CD1-CG-CD2 | 9.14 | 113.61 | 106.30 |
| 4 | 4 | 356 | TRP | CD1-CG-CD2 | 9.13 | 113.61 | 106.30 |
| 4 | 3 | 356 | TRP | CD1-CG-CD2 | 9.11 | 113.59 | 106.30 |
| 4 | 1 | 356 | TRP | CD1-CG-CD2 | 9.10 | 113.58 | 106.30 |
| 4 | X | 356 | TRP | CD1-CG-CD2 | 9.08 | 113.57 | 106.30 |
| 4 | 6 | 356 | TRP | CD1-CG-CD2 | 9.05 | 113.54 | 106.30 |
| 1 | S | 378 | ASP | CB-CG-OD2 | 9.04 | 126.43 | 118.30 |
| 4 | Y | 356 | TRP | CD1-CG-CD2 | 9.04 | 113.53 | 106.30 |
| 4 | V | 356 | TRP | CD1-CG-CD2 | 9.03 | 113.53 | 106.30 |
| 4 | Z | 356 | TRP | CD1-CG-CD2 | 9.00 | 113.50 | 106.30 |
| 1 | J | 378 | ASP | CB-CG-OD2 | 8.98 | 126.38 | 118.30 |
| 1 | M | 378 | ASP | CB-CG-OD2 | 8.94 | 126.34 | 118.30 |
| 1 | J | 352 | TYR | CB-CG-CD1 | 8.93 | 126.36 | 121.00 |
| 1 | J | 709 | LYS | C-N-CA | -8.91 | 103.58 | 122.30 |
| 1 | D | 378 | ASP | CB-CG-OD2 | 8.90 | 126.31 | 118.30 |
| 1 | S | 352 | TYR | CB-CG-CD1 | 8.86 | 126.32 | 121.00 |
| 1 | M | 352 | TYR | CB-CG-CD1 | 8.85 | 126.31 | 121.00 |
| 1 | G | 352 | TYR | CB-CG-CD1 | 8.83 | 126.30 | 121.00 |
| 1 | A | 378 | ASP | CB-CG-OD2 | 8.83 | 126.24 | 118.30 |
| 1 | G | 378 | ASP | CB-CG-OD2 | 8.81 | 126.23 | 118.30 |
| 1 | D | 352 | TYR | CB-CG-CD1 | 8.80 | 126.28 | 121.00 |
| 2 | E | 138 | ALA | O-C-N | -8.76 | 108.69 | 122.70 |
| 1 | A | 352 | TYR | CB-CG-CD1 | 8.75 | 126.25 | 121.00 |
| 2 | T | 138 | ALA | O-C-N | -8.73 | 108.74 | 122.70 |
| 4 | 1 | 177 | ARG | NE-CZ-NH2 | -8.70 | 115.95 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | H | 138 | ALA | O-C-N | -8.70 | 108.79 | 122.70 |
| 2 | K | 138 | ALA | O-C-N | -8.69 | 108.79 | 122.70 |
| 2 | N | 138 | ALA | O-C-N | -8.68 | 108.81 | 122.70 |
| 2 | B | 138 | ALA | O-C-N | -8.68 | 108.82 | 122.70 |
| 4 | 8 | 177 | ARG | NE-CZ-NH2 | -8.65 | 115.97 | 120.30 |
| 4 | 4 | 177 | ARG | NE-CZ-NH2 | -8.64 | 115.98 | 120.30 |
| 4 | W | 177 | ARG | NE-CZ-NH2 | -8.62 | 115.99 | 120.30 |
| 4 | 6 | 177 | ARG | NE-CZ-NH2 | -8.62 | 115.99 | 120.30 |
| 4 | 2 | 86 | TRP | CD1-CG-CD2 | 8.58 | 113.17 | 106.30 |
| 4 | Z | 177 | ARG | NE-CZ-NH2 | -8.56 | 116.02 | 120.30 |
| 4 | X | 177 | ARG | NE-CZ-NH2 | -8.55 | 116.02 | 120.30 |
| 4 | 2 | 177 | ARG | NE-CZ-NH2 | -8.55 | 116.03 | 120.30 |
| 4 | X | 86 | TRP | CD1-CG-CD2 | 8.54 | 113.13 | 106.30 |
| 4 | 9 | 177 | ARG | NE-CZ-NH2 | -8.54 | 116.03 | 120.30 |
| 4 | V | 177 | ARG | NE-CZ-NH2 | -8.53 | 116.04 | 120.30 |
| 1 | D | 601 | ASP | CB-CG-OD1 | -8.52 | 110.63 | 118.30 |
| 4 | 5 | 177 | ARG | NE-CZ-NH2 | -8.52 | 116.04 | 120.30 |
| 4 | V | 86 | TRP | CD1-CG-CD2 | 8.52 | 113.11 | 106.30 |
| 4 | W | 86 | TRP | CD1-CG-CD2 | 8.52 | 113.11 | 106.30 |
| 1 | M | 601 | ASP | CB-CG-OD1 | -8.51 | 110.64 | 118.30 |
| 4 | Y | 86 | TRP | CD1-CG-CD2 | 8.51 | 113.11 | 106.30 |
| 4 | 9 | 86 | TRP | CD1-CG-CD2 | 8.51 | 113.11 | 106.30 |
| 1 | J | 601 | ASP | CB-CG-OD1 | -8.50 | 110.65 | 118.30 |
| 4 | 1 | 86 | TRP | CD1-CG-CD2 | 8.49 | 113.09 | 106.30 |
| 4 | 4 | 86 | TRP | CD1-CG-CD2 | 8.49 | 113.09 | 106.30 |
| 4 | 3 | 86 | TRP | CD1-CG-CD2 | 8.48 | 113.09 | 106.30 |
| 4 | 3 | 177 | ARG | NE-CZ-NH2 | -8.47 | 116.06 | 120.30 |
| 1 | G | 601 | ASP | CB-CG-OD1 | -8.47 | 110.67 | 118.30 |
| 4 | 6 | 86 | TRP | CD1-CG-CD2 | 8.46 | 113.07 | 106.30 |
| 4 | 8 | 86 | TRP | CD1-CG-CD2 | 8.45 | 113.06 | 106.30 |
| 4 | Y | 177 | ARG | NE-CZ-NH2 | -8.45 | 116.07 | 120.30 |
| 1 | A | 601 | ASP | CB-CG-OD1 | -8.43 | 110.71 | 118.30 |
| 1 | S | 601 | ASP | CB-CG-OD1 | -8.43 | 110.71 | 118.30 |
| 1 | S | 33 | ASP | CB-CG-OD1 | -8.43 | 110.72 | 118.30 |
| 4 | 7 | 177 | ARG | NE-CZ-NH2 | -8.40 | 116.10 | 120.30 |
| 4 | 5 | 86 | TRP | CD1-CG-CD2 | 8.39 | 113.01 | 106.30 |
| 1 | M | 352 | TYR | CB-CG-CD2 | -8.38 | 115.97 | 121.00 |
| 4 | Z | 86 | TRP | CD1-CG-CD2 | 8.38 | 113.00 | 106.30 |
| 1 | M | 33 | ASP | CB-CG-OD1 | -8.38 | 110.76 | 118.30 |
| 4 | 7 | 86 | TRP | CD1-CG-CD2 | 8.37 | 113.00 | 106.30 |
| 1 | J | 33 | ASP | CB-CG-OD1 | -8.36 | 110.78 | 118.30 |
| 1 | S | 352 | TYR | CB-CG-CD2 | -8.31 | 116.01 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | D | 33 | ASP | CB-CG-OD1 | -8.29 | 110.84 | 118.30 |
| 1 | A | 352 | TYR | CB-CG-CD2 | -8.26 | 116.04 | 121.00 |
| 1 | J | 352 | TYR | CB-CG-CD2 | -8.26 | 116.05 | 121.00 |
| 1 | A | 33 | ASP | CB-CG-OD1 | -8.26 | 110.87 | 118.30 |
| 1 | G | 33 | ASP | CB-CG-OD1 | -8.19 | 110.93 | 118.30 |
| 1 | G | 352 | TYR | CB-CG-CD2 | -8.19 | 116.09 | 121.00 |
| 1 | D | 352 | TYR | CB-CG-CD2 | -8.17 | 116.09 | 121.00 |
| 4 | W | 356 | TRP | CE2-CD2-CG | -8.04 | 100.86 | 107.30 |
| 4 | 7 | 356 | TRP | CE2-CD2-CG | -8.01 | 100.89 | 107.30 |
| 4 | 2 | 356 | TRP | CE2-CD2-CG | -7.99 | 100.91 | 107.30 |
| 1 | A | 637 | LYS | CA-C-N | 7.99 | 132.17 | 116.20 |
| 4 | 5 | 356 | TRP | CE2-CD2-CG | -7.97 | 100.93 | 107.30 |
| 4 | 1 | 356 | TRP | CE2-CD2-CG | -7.96 | 100.94 | 107.30 |
| 1 | A | 339 | ASP | CB-CG-OD1 | -7.94 | 111.15 | 118.30 |
| 4 | 8 | 356 | TRP | CE2-CD2-CG | -7.94 | 100.95 | 107.30 |
| 1 | D | 637 | LYS | CA-C-N | 7.93 | 132.07 | 116.20 |
| 1 | G | 339 | ASP | CB-CG-OD1 | -7.93 | 111.16 | 118.30 |
| 4 | 3 | 356 | TRP | CE2-CD2-CG | -7.93 | 100.96 | 107.30 |
| 1 | D | 339 | ASP | CB-CG-OD1 | -7.93 | 111.17 | 118.30 |
| 4 | 4 | 356 | TRP | CE2-CD2-CG | -7.93 | 100.96 | 107.30 |
| 4 | V | 356 | TRP | CE2-CD2-CG | -7.93 | 100.96 | 107.30 |
| 4 | 6 | 356 | TRP | CE2-CD2-CG | -7.92 | 100.96 | 107.30 |
| 1 | S | 637 | LYS | CA-C-N | 7.92 | 132.04 | 116.20 |
| 1 | J | 637 | LYS | CA-C-N | 7.91 | 132.01 | 116.20 |
| 4 | 9 | 356 | TRP | CE2-CD2-CG | -7.91 | 100.97 | 107.30 |
| 1 | M | 637 | LYS | CA-C-N | 7.89 | 131.99 | 116.20 |
| 4 | Z | 356 | TRP | CE2-CD2-CG | -7.89 | 100.99 | 107.30 |
| 1 | M | 339 | ASP | CB-CG-OD1 | -7.88 | 111.20 | 118.30 |
| 1 | G | 637 | LYS | CA-C-N | 7.88 | 131.96 | 116.20 |
| 4 | Y | 356 | TRP | CE2-CD2-CG | -7.87 | 101.00 | 107.30 |
| 1 | J | 339 | ASP | CB-CG-OD1 | -7.87 | 111.22 | 118.30 |
| 1 | S | 339 | ASP | CB-CG-OD1 | -7.87 | 111.22 | 118.30 |
| 4 | X | 356 | TRP | CE2-CD2-CG | -7.86 | 101.01 | 107.30 |
| 2 | B | 150 | TYR | CD1-CE1-CZ | -7.85 | 112.73 | 119.80 |
| 2 | K | 150 | TYR | CD1-CE1-CZ | -7.80 | 112.78 | 119.80 |
| 1 | D | 202 | SER | CB-CA-C | -7.79 | 95.30 | 110.10 |
| 1 | A | 202 | SER | CB-CA-C | -7.78 | 95.32 | 110.10 |
| 2 | N | 150 | TYR | CD1-CE1-CZ | -7.77 | 112.81 | 119.80 |
| 1 | M | 202 | SER | CB-CA-C | -7.76 | 95.35 | 110.10 |
| 1 | S | 653 | PHE | CB-CG-CD1 | -7.76 | 115.36 | 120.80 |
| 2 | E | 150 | TYR | CD1-CE1-CZ | -7.75 | 112.82 | 119.80 |
| 1 | J | 202 | SER | CB-CA-C | -7.75 | 95.36 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | G | 202 | SER | CB-CA-C | -7.75 | 95.37 | 110.10 |
| 4 | X | 312 | ARG | NE-CZ-NH2 | 7.74 | 124.17 | 120.30 |
| 4 | 8 | 312 | ARG | NE-CZ-NH2 | 7.72 | 124.16 | 120.30 |
| 1 | S | 202 | SER | CB-CA-C | -7.71 | 95.45 | 110.10 |
| 2 | H | 150 | TYR | CD1-CE1-CZ | -7.71 | 112.86 | 119.80 |
| 4 | 1 | 312 | ARG | NE-CZ-NH2 | 7.70 | 124.15 | 120.30 |
| 4 | W | 312 | ARG | NE-CZ-NH2 | 7.68 | 124.14 | 120.30 |
| 4 | 7 | 312 | ARG | NE-CZ-NH2 | 7.66 | 124.13 | 120.30 |
| 1 | M | 653 | PHE | CB-CG-CD1 | -7.66 | 115.44 | 120.80 |
| 2 | T | 150 | TYR | CD1-CE1-CZ | -7.65 | 112.91 | 119.80 |
| 4 | V | 312 | ARG | NE-CZ-NH2 | 7.65 | 124.12 | 120.30 |
| 4 | V | 86 | TRP | CE2-CD2-CG | -7.63 | 101.19 | 107.30 |
| 1 | J | 653 | PHE | CB-CG-CD1 | -7.63 | 115.46 | 120.80 |
| 4 | 3 | 312 | ARG | NE-CZ-NH2 | 7.63 | 124.11 | 120.30 |
| 4 | 9 | 312 | ARG | NE-CZ-NH2 | 7.62 | 124.11 | 120.30 |
| 1 | G | 654 | ARG | NE-CZ-NH1 | 7.62 | 124.11 | 120.30 |
| 4 | 5 | 312 | ARG | NE-CZ-NH2 | 7.62 | 124.11 | 120.30 |
| 4 | 2 | 312 | ARG | NE-CZ-NH2 | 7.60 | 124.10 | 120.30 |
| 4 | 6 | 86 | TRP | CE2-CD2-CG | -7.60 | 101.22 | 107.30 |
| 1 | G | 653 | PHE | CB-CG-CD1 | -7.59 | 115.48 | 120.80 |
| 4 | 6 | 312 | ARG | NE-CZ-NH2 | 7.59 | 124.09 | 120.30 |
| 4 | 5 | 86 | TRP | CE2-CD2-CG | -7.58 | 101.23 | 107.30 |
| 1 | A | 654 | ARG | NE-CZ-NH1 | 7.58 | 124.09 | 120.30 |
| 4 | 2 | 86 | TRP | CE2-CD2-CG | -7.58 | 101.24 | 107.30 |
| 4 | Z | 312 | ARG | NE-CZ-NH2 | 7.56 | 124.08 | 120.30 |
| 1 | D | 653 | PHE | CB-CG-CD1 | -7.56 | 115.51 | 120.80 |
| 4 | 3 | 86 | TRP | CE2-CD2-CG | -7.56 | 101.25 | 107.30 |
| 4 | 1 | 86 | TRP | CE2-CD2-CG | -7.56 | 101.25 | 107.30 |
| 4 | 4 | 86 | TRP | CE2-CD2-CG | -7.56 | 101.25 | 107.30 |
| 4 | W | 86 | TRP | CE2-CD2-CG | -7.55 | 101.26 | 107.30 |
| 4 | X | 86 | TRP | CE2-CD2-CG | -7.54 | 101.27 | 107.30 |
| 4 | 8 | 86 | TRP | CE2-CD2-CG | -7.54 | 101.27 | 107.30 |
| 4 | Y | 86 | TRP | CE2-CD2-CG | -7.53 | 101.28 | 107.30 |
| 4 | Y | 312 | ARG | NE-CZ-NH2 | 7.52 | 124.06 | 120.30 |
| 4 | 9 | 86 | TRP | CE2-CD2-CG | -7.51 | 101.29 | 107.30 |
| 3 | U | 63 | ILE | CG1-CB-CG2 | -7.50 | 94.90 | 111.40 |
| 4 | 7 | 86 | TRP | CE2-CD2-CG | -7.49 | 101.31 | 107.30 |
| 3 | C | 63 | ILE | CG1-CB-CG2 | -7.49 | 94.92 | 111.40 |
| 3 | I | 63 | ILE | CG1-CB-CG2 | -7.49 | 94.92 | 111.40 |
| 4 | 4 | 312 | ARG | NE-CZ-NH2 | 7.48 | 124.04 | 120.30 |
| 3 | L | 63 | ILE | CG1-CB-CG2 | -7.48 | 94.95 | 111.40 |
| 3 | O | 63 | ILE | CG1-CB-CG2 | -7.47 | 94.96 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3 | F | 63 | ILE | CG1-CB-CG2 | -7.46 | 94.98 | 111.40 |
| 2 | B | 127 | ARG | NE-CZ-NH2 | 7.45 | 124.03 | 120.30 |
| 1 | A | 653 | PHE | CB-CG-CD1 | -7.45 | 115.58 | 120.80 |
| 4 | Z | 86 | TRP | CE2-CD2-CG | -7.45 | 101.34 | 107.30 |
| 1 | G | 346 | ASP | CB-CG-OD2 | -7.44 | 111.60 | 118.30 |
| 1 | M | 518 | ASP | CB-CG-OD1 | -7.44 | 111.61 | 118.30 |
| 4 | Z | 254 | ARG | NE-CZ-NH2 | -7.43 | 116.58 | 120.30 |
| 1 | J | 518 | ASP | CB-CG-OD1 | -7.42 | 111.62 | 118.30 |
| 1 | J | 654 | ARG | NE-CZ-NH1 | 7.41 | 124.01 | 120.30 |
| 3 | I | 63 | ILE | CA-C-N | -7.41 | 100.91 | 117.20 |
| 4 | 7 | 233 | SER | CA-C-N | -7.40 | 100.93 | 117.20 |
| 4 | X | 233 | SER | CA-C-N | -7.38 | 100.97 | 117.20 |
| 4 | X | 254 | ARG | NE-CZ-NH2 | -7.38 | 116.61 | 120.30 |
| 4 | 1 | 180 | LEU | CA-CB-CG | 7.37 | 132.25 | 115.30 |
| 1 | A | 346 | ASP | CB-CG-OD2 | -7.37 | 111.67 | 118.30 |
| 3 | L | 63 | ILE | CA-C-N | -7.37 | 100.99 | 117.20 |
| 1 | M | 654 | ARG | NE-CZ-NH1 | 7.37 | 123.98 | 120.30 |
| 4 | Z | 233 | SER | CA-C-N | -7.37 | 101.00 | 117.20 |
| 4 | 7 | 180 | LEU | CA-CB-CG | 7.36 | 132.23 | 115.30 |
| 1 | S | 654 | ARG | NE-CZ-NH1 | 7.36 | 123.98 | 120.30 |
| 4 | 9 | 233 | SER | CA-C-N | -7.36 | 101.01 | 117.20 |
| 1 | S | 518 | ASP | CB-CG-OD1 | -7.36 | 111.68 | 118.30 |
| 3 | U | 63 | ILE | CA-C-N | -7.36 | 101.02 | 117.20 |
| 4 | 1 | 233 | SER | CA-C-N | -7.36 | 101.02 | 117.20 |
| 4 | W | 180 | LEU | CA-CB-CG | 7.36 | 132.22 | 115.30 |
| 4 | 3 | 180 | LEU | CA-CB-CG | 7.35 | 132.21 | 115.30 |
| 3 | C | 63 | ILE | CA-C-N | -7.35 | 101.03 | 117.20 |
| 4 | 6 | 233 | SER | CA-C-N | -7.35 | 101.02 | 117.20 |
| 4 | 2 | 233 | SER | CA-C-N | -7.35 | 101.03 | 117.20 |
| 4 | W | 233 | SER | CA-C-N | -7.35 | 101.03 | 117.20 |
| 1 | D | 346 | ASP | CB-CG-OD2 | -7.35 | 111.69 | 118.30 |
| 1 | D | 518 | ASP | CB-CG-OD1 | -7.35 | 111.69 | 118.30 |
| 4 | V | 233 | SER | CA-C-N | -7.35 | 101.03 | 117.20 |
| 4 | 8 | 233 | SER | CA-C-N | -7.35 | 101.04 | 117.20 |
| 4 | X | 180 | LEU | CA-CB-CG | 7.35 | 132.20 | 115.30 |
| 4 | Z | 180 | LEU | CA-CB-CG | 7.34 | 132.19 | 115.30 |
| 3 | O | 63 | ILE | CA-C-N | -7.34 | 101.05 | 117.20 |
| 4 | 2 | 180 | LEU | CA-CB-CG | 7.34 | 132.18 | 115.30 |
| 4 | Y | 233 | SER | CA-C-N | -7.34 | 101.06 | 117.20 |
| 1 | G | 709 | LYS | C-N-CA | 7.33 | 137.70 | 122.30 |
| 4 | 4 | 233 | SER | CA-C-N | -7.33 | 101.07 | 117.20 |
| 3 | F | 63 | ILE | CA-C-N | -7.33 | 101.07 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | D | 654 | ARG | NE-CZ-NH1 | 7.33 | 123.96 | 120.30 |
| 4 | 6 | 180 | LEU | CA-CB-CG | 7.33 | 132.15 | 115.30 |
| 4 | 8 | 180 | LEU | CA-CB-CG | 7.33 | 132.15 | 115.30 |
| 4 | Y | 180 | LEU | CA-CB-CG | 7.32 | 132.15 | 115.30 |
| 1 | G | 709 | LYS | CA-C-N | -7.32 | 101.56 | 116.20 |
| 4 | 3 | 233 | SER | CA-C-N | -7.32 | 101.09 | 117.20 |
| 4 | 5 | 180 | LEU | CA-CB-CG | 7.32 | 132.13 | 115.30 |
| 4 | 5 | 233 | SER | CA-C-N | -7.32 | 101.10 | 117.20 |
| 4 | 4 | 180 | LEU | CA-CB-CG | 7.32 | 132.13 | 115.30 |
| 4 | 9 | 180 | LEU | CA-CB-CG | 7.31 | 132.11 | 115.30 |
| 1 | A | 518 | ASP | CB-CG-OD1 | -7.31 | 111.72 | 118.30 |
| 4 | V | 180 | LEU | CA-CB-CG | 7.31 | 132.11 | 115.30 |
| 1 | S | 104 | TYR | CB-CG-CD2 | 7.30 | 125.38 | 121.00 |
| 1 | G | 518 | ASP | CB-CG-OD1 | -7.28 | 111.75 | 118.30 |
| 2 | E | 127 | ARG | NE-CZ-NH2 | 7.28 | 123.94 | 120.30 |
| 4 | 8 | 79 | TRP | CD1-CG-CD2 | 7.27 | 112.12 | 106.30 |
| 4 | 5 | 254 | ARG | NE-CZ-NH2 | -7.26 | 116.67 | 120.30 |
| 1 | M | 346 | ASP | CB-CG-OD2 | -7.26 | 111.77 | 118.30 |
| 4 | 1 | 254 | ARG | NE-CZ-NH2 | -7.26 | 116.67 | 120.30 |
| 1 | J | 346 | ASP | CB-CG-OD2 | -7.25 | 111.77 | 118.30 |
| 1 | S | 346 | ASP | CB-CG-OD2 | -7.25 | 111.77 | 118.30 |
| 4 | 2 | 79 | TRP | CD1-CG-CD2 | 7.25 | 112.10 | 106.30 |
| 4 | X | 79 | TRP | CD1-CG-CD2 | 7.25 | 112.10 | 106.30 |
| 4 | 7 | 340 | TRP | CE2-CD2-CG | -7.25 | 101.50 | 107.30 |
| 4 | 7 | 254 | ARG | NE-CZ-NH2 | -7.22 | 116.69 | 120.30 |
| 4 | V | 340 | TRP | CE2-CD2-CG | -7.21 | 101.53 | 107.30 |
| 1 | A | 148 | ARG | NE-CZ-NH2 | -7.21 | 116.69 | 120.30 |
| 1 | G | 104 | TYR | CB-CG-CD2 | 7.21 | 125.32 | 121.00 |
| 1 | M | 104 | TYR | CB-CG-CD2 | 7.21 | 125.32 | 121.00 |
| 4 | Z | 79 | TRP | CD1-CG-CD2 | 7.21 | 112.06 | 106.30 |
| 4 | X | 206 | ARG | NE-CZ-NH1 | 7.20 | 123.90 | 120.30 |
| 4 | 6 | 254 | ARG | NE-CZ-NH2 | -7.20 | 116.70 | 120.30 |
| 4 | Z | 340 | TRP | CE2-CD2-CG | -7.19 | 101.55 | 107.30 |
| 1 | J | 104 | TYR | CB-CG-CD2 | 7.19 | 125.31 | 121.00 |
| 1 | A | 104 | TYR | CB-CG-CD2 | 7.19 | 125.31 | 121.00 |
| 4 | 1 | 79 | TRP | CD1-CG-CD2 | 7.19 | 112.05 | 106.30 |
| 4 | 6 | 79 | TRP | CD1-CG-CD2 | 7.18 | 112.04 | 106.30 |
| 4 | 6 | 206 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 4 | Y | 254 | ARG | NE-CZ-NH2 | -7.18 | 116.71 | 120.30 |
| 4 | 1 | 340 | TRP | CE2-CD2-CG | -7.17 | 101.56 | 107.30 |
| 4 | Y | 79 | TRP | CD1-CG-CD2 | 7.17 | 112.04 | 106.30 |
| 4 | Z | 206 | ARG | NE-CZ-NH1 | 7.17 | 123.89 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 3 | 340 | TRP | CE2-CD2-CG | -7.17 | 101.56 | 107.30 |
| 4 | 9 | 79 | TRP | CD1-CG-CD2 | 7.17 | 112.04 | 106.30 |
| 4 | W | 79 | TRP | CD1-CG-CD2 | 7.17 | 112.04 | 106.30 |
| 4 | 4 | 79 | TRP | CD1-CG-CD2 | 7.17 | 112.03 | 106.30 |
| 4 | 8 | 340 | TRP | CE2-CD2-CG | -7.17 | 101.57 | 107.30 |
| 4 | 8 | 254 | ARG | NE-CZ-NH2 | -7.16 | 116.72 | 120.30 |
| 2 | K | 150 | TYR | CB-CG-CD1 | -7.16 | 116.71 | 121.00 |
| 4 | 3 | 254 | ARG | NE-CZ-NH2 | -7.16 | 116.72 | 120.30 |
| 4 | 1 | 206 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 1 | A | 568 | PRO | CA-C-N | -7.14 | 101.49 | 117.20 |
| 4 | 4 | 206 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 2 | N | 150 | TYR | CB-CG-CD1 | -7.13 | 116.72 | 121.00 |
| 4 | 7 | 79 | TRP | CD1-CG-CD2 | 7.13 | 112.01 | 106.30 |
| 4 | 3 | 206 | ARG | NE-CZ-NH1 | 7.13 | 123.86 | 120.30 |
| 4 | 9 | 340 | TRP | CE2-CD2-CG | -7.12 | 101.60 | 107.30 |
| 2 | H | 127 | ARG | NE-CZ-NH2 | 7.12 | 123.86 | 120.30 |
| 1 | M | 568 | PRO | CA-C-N | -7.12 | 101.53 | 117.20 |
| 1 | G | 568 | PRO | CA-C-N | -7.12 | 101.53 | 117.20 |
| 4 | 2 | 254 | ARG | NE-CZ-NH2 | -7.12 | 116.74 | 120.30 |
| 1 | J | 148 | ARG | NE-CZ-NH2 | -7.12 | 116.74 | 120.30 |
| 4 | 4 | 340 | TRP | CE2-CD2-CG | -7.11 | 101.61 | 107.30 |
| 4 | 3 | 79 | TRP | CD1-CG-CD2 | 7.10 | 111.98 | 106.30 |
| 2 | H | 150 | TYR | CB-CG-CD1 | -7.10 | 116.74 | 121.00 |
| 4 | W | 340 | TRP | CE2-CD2-CG | -7.10 | 101.62 | 107.30 |
| 4 | 4 | 254 | ARG | NE-CZ-NH2 | -7.10 | 116.75 | 120.30 |
| 2 | N | 127 | ARG | NE-CZ-NH2 | 7.09 | 123.85 | 120.30 |
| 4 | 6 | 340 | TRP | CE2-CD2-CG | -7.09 | 101.63 | 107.30 |
| 1 | D | 148 | ARG | NE-CZ-NH2 | -7.09 | 116.76 | 120.30 |
| 1 | S | 568 | PRO | CA-C-N | -7.09 | 101.60 | 117.20 |
| 2 | T | 127 | ARG | NE-CZ-NH2 | 7.09 | 123.84 | 120.30 |
| 2 | T | 150 | TYR | CB-CG-CD1 | -7.09 | 116.75 | 121.00 |
| 4 | W | 254 | ARG | NE-CZ-NH2 | -7.09 | 116.76 | 120.30 |
| 4 | X | 340 | TRP | CE2-CD2-CG | -7.08 | 101.63 | 107.30 |
| 1 | J | 568 | PRO | CA-C-N | -7.08 | 101.62 | 117.20 |
| 4 | 5 | 79 | TRP | CD1-CG-CD2 | 7.08 | 111.97 | 106.30 |
| 4 | 9 | 254 | ARG | NE-CZ-NH2 | -7.08 | 116.76 | 120.30 |
| 4 | V | 79 | TRP | CD1-CG-CD2 | 7.08 | 111.97 | 106.30 |
| 4 | V | 206 | ARG | NE-CZ-NH1 | 7.08 | 123.84 | 120.30 |
| 4 | 2 | 340 | TRP | CE2-CD2-CG | -7.08 | 101.64 | 107.30 |
| 2 | K | 127 | ARG | NE-CZ-NH2 | 7.08 | 123.84 | 120.30 |
| 1 | D | 568 | PRO | CA-C-N | -7.08 | 101.63 | 117.20 |
| 4 | 2 | 206 | ARG | NE-CZ-NH1 | 7.07 | 123.84 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | V | 47 | MET | CA-CB-CG | -7.07 | 101.28 | 113.30 |
| 4 | 9 | 206 | ARG | NE-CZ-NH1 | 7.06 | 123.83 | 120.30 |
| 4 | Y | 340 | TRP | CE2-CD2-CG | -7.06 | 101.65 | 107.30 |
| 4 | 1 | 47 | MET | CA-CB-CG | -7.06 | 101.30 | 113.30 |
| 1 | M | 709 | LYS | C-N-CA | -7.06 | 107.48 | 122.30 |
| 4 | 5 | 340 | TRP | CE2-CD2-CG | -7.06 | 101.65 | 107.30 |
| 4 | 8 | 47 | MET | CA-CB-CG | -7.06 | 101.30 | 113.30 |
| 4 | V | 254 | ARG | NE-CZ-NH2 | -7.06 | 116.77 | 120.30 |
| 4 | W | 206 | ARG | NE-CZ-NH1 | 7.06 | 123.83 | 120.30 |
| 4 | 7 | 47 | MET | CA-CB-CG | -7.05 | 101.31 | 113.30 |
| 1 | J | 264 | ASP | N-CA-CB | -7.04 | 97.92 | 110.60 |
| 4 | 7 | 206 | ARG | NE-CZ-NH1 | 7.04 | 123.82 | 120.30 |
| 4 | 1 | 340 | TRP | CD1-CG-CD2 | 7.04 | 111.93 | 106.30 |
| 2 | B | 150 | TYR | CB-CG-CD1 | -7.03 | 116.78 | 121.00 |
| 4 | 4 | 47 | MET | CA-CB-CG | -7.03 | 101.35 | 113.30 |
| 1 | M | 264 | ASP | N-CA-CB | -7.03 | 97.95 | 110.60 |
| 4 | 1 | 79 | TRP | CE2-CD2-CG | -7.03 | 101.68 | 107.30 |
| 4 | 5 | 47 | MET | CA-CB-CG | -7.03 | 101.36 | 113.30 |
| 4 | Y | 47 | MET | CA-CB-CG | -7.03 | 101.36 | 113.30 |
| 4 | 2 | 79 | TRP | CE2-CD2-CG | -7.02 | 101.68 | 107.30 |
| 4 | 9 | 47 | MET | CA-CB-CG | -7.02 | 101.36 | 113.30 |
| 4 | 8 | 79 | TRP | CE2-CD2-CG | -7.02 | 101.69 | 107.30 |
| 4 | W | 47 | MET | CA-CB-CG | -7.02 | 101.37 | 113.30 |
| 4 | X | 47 | MET | CA-CB-CG | -7.02 | 101.37 | 113.30 |
| 4 | X | 79 | TRP | CE2-CD2-CG | -7.02 | 101.69 | 107.30 |
| 4 | 3 | 47 | MET | CA-CB-CG | -7.01 | 101.38 | 113.30 |
| 4 | 6 | 47 | MET | CA-CB-CG | -7.01 | 101.38 | 113.30 |
| 4 | Y | 206 | ARG | NE-CZ-NH1 | 7.01 | 123.81 | 120.30 |
| 1 | S | 264 | ASP | N-CA-CB | -7.01 | 97.99 | 110.60 |
| 4 | Y | 79 | TRP | CE2-CD2-CG | -7.00 | 101.70 | 107.30 |
| 4 | Z | 79 | TRP | CE2-CD2-CG | -7.00 | 101.70 | 107.30 |
| 1 | A | 218 | LEU | CB-CG-CD1 | 7.00 | 122.90 | 111.00 |
| 2 | E | 150 | TYR | CB-CG-CD1 | -7.00 | 116.80 | 121.00 |
| 1 | D | 218 | LEU | CB-CG-CD1 | 6.99 | 122.89 | 111.00 |
| 1 | M | 217 | THR | N-CA-CB | 6.99 | 123.59 | 110.30 |
| 1 | D | 264 | ASP | N-CA-CB | -6.99 | 98.02 | 110.60 |
| 1 | S | 218 | LEU | CB-CG-CD1 | 6.99 | 122.88 | 111.00 |
| 1 | D | 217 | THR | N-CA-CB | 6.99 | 123.57 | 110.30 |
| 1 | M | 218 | LEU | CB-CG-CD1 | 6.99 | 122.88 | 111.00 |
| 4 | 2 | 47 | MET | CA-CB-CG | -6.99 | 101.42 | 113.30 |
| 4 | 7 | 340 | TRP | CD1-CG-CD2 | 6.99 | 111.89 | 106.30 |
| 1 | G | 217 | THR | N-CA-CB | 6.98 | 123.56 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | V | 340 | TRP | CD1-CG-CD2 | 6.98 | 111.89 | 106.30 |
| 1 | A | 264 | ASP | N-CA-CB | -6.98 | 98.04 | 110.60 |
| 1 | A | 217 | THR | N-CA-CB | 6.97 | 123.55 | 110.30 |
| 4 | 8 | 340 | TRP | CD1-CG-CD2 | 6.97 | 111.88 | 106.30 |
| 4 | 9 | 79 | TRP | CE2-CD2-CG | -6.97 | 101.72 | 107.30 |
| 4 | Z | 47 | MET | CA-CB-CG | -6.97 | 101.45 | 113.30 |
| 1 | G | 218 | LEU | CB-CG-CD1 | 6.97 | 122.84 | 111.00 |
| 4 | Y | 340 | TRP | CD1-CG-CD2 | 6.96 | 111.87 | 106.30 |
| 1 | G | 148 | ARG | NE-CZ-NH2 | -6.96 | 116.82 | 120.30 |
| 1 | J | 217 | THR | N-CA-CB | 6.96 | 123.53 | 110.30 |
| 1 | J | 218 | LEU | CB-CG-CD1 | 6.96 | 122.83 | 111.00 |
| 4 | Z | 340 | TRP | CD1-CG-CD2 | 6.96 | 111.87 | 106.30 |
| 1 | G | 264 | ASP | N-CA-CB | -6.95 | 98.08 | 110.60 |
| 4 | 8 | 206 | ARG | NE-CZ-NH1 | 6.95 | 123.77 | 120.30 |
| 1 | S | 217 | THR | N-CA-CB | 6.95 | 123.50 | 110.30 |
| 1 | M | 148 | ARG | NE-CZ-NH2 | -6.95 | 116.83 | 120.30 |
| 4 | 6 | 79 | TRP | CE2-CD2-CG | -6.94 | 101.75 | 107.30 |
| 1 | D | 104 | TYR | CB-CG-CD2 | 6.94 | 125.16 | 121.00 |
| 4 | 3 | 79 | TRP | CE2-CD2-CG | -6.94 | 101.75 | 107.30 |
| 4 | 5 | 206 | ARG | NE-CZ-NH1 | 6.94 | 123.77 | 120.30 |
| 4 | 9 | 340 | TRP | CD1-CG-CD2 | 6.93 | 111.85 | 106.30 |
| 1 | S | 148 | ARG | NE-CZ-NH2 | -6.93 | 116.83 | 120.30 |
| 4 | 7 | 79 | TRP | CE2-CD2-CG | -6.93 | 101.76 | 107.30 |
| 4 | W | 79 | TRP | CE2-CD2-CG | -6.93 | 101.76 | 107.30 |
| 4 | V | 79 | TRP | CE2-CD2-CG | -6.92 | 101.76 | 107.30 |
| 4 | 4 | 340 | TRP | CD1-CG-CD2 | 6.92 | 111.84 | 106.30 |
| 4 | 4 | 79 | TRP | CE2-CD2-CG | -6.92 | 101.77 | 107.30 |
| 4 | X | 340 | TRP | CD1-CG-CD2 | 6.91 | 111.83 | 106.30 |
| 4 | W | 340 | TRP | CD1-CG-CD2 | 6.90 | 111.82 | 106.30 |
| 4 | 2 | 340 | TRP | CD1-CG-CD2 | 6.89 | 111.81 | 106.30 |
| 1 | M | 728 | ASN | CA-C-N | -6.88 | 102.05 | 117.20 |
| 4 | 5 | 340 | TRP | CD1-CG-CD2 | 6.88 | 111.81 | 106.30 |
| 4 | 3 | 340 | TRP | CD1-CG-CD2 | 6.88 | 111.80 | 106.30 |
| 4 | 5 | 79 | TRP | CE2-CD2-CG | -6.88 | 101.80 | 107.30 |
| 1 | G | 728 | ASN | CA-C-N | -6.88 | 102.07 | 117.20 |
| 1 | S | 75 | ASP | N-CA-CB | 6.87 | 122.97 | 110.60 |
| 1 | G | 450 | ASP | CB-CG-OD2 | 6.87 | 124.48 | 118.30 |
| 1 | A | 75 | ASP | N-CA-CB | 6.87 | 122.96 | 110.60 |
| 1 | D | 728 | ASN | CA-C-N | -6.87 | 102.10 | 117.20 |
| 1 | J | 728 | ASN | CA-C-N | -6.87 | 102.09 | 117.20 |
| 1 | G | 75 | ASP | N-CA-CB | 6.86 | 122.95 | 110.60 |
| 1 | J | 75 | ASP | N-CA-CB | 6.86 | 122.95 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 6 | 340 | TRP | CD1-CG-CD2 | 6.86 | 111.79 | 106.30 |
| 1 | S | 728 | ASN | CA-C-N | -6.85 | 102.13 | 117.20 |
| 1 | A | 728 | ASN | CA-C-N | -6.84 | 102.15 | 117.20 |
| 1 | S | 555 | TYR | CB-CG-CD2 | -6.82 | 116.91 | 121.00 |
| 1 | M | 75 | ASP | N-CA-CB | 6.80 | 122.84 | 110.60 |
| 1 | M | 450 | ASP | CB-CG-OD2 | 6.79 | 124.41 | 118.30 |
| 1 | M | 555 | TYR | CB-CG-CD2 | -6.79 | 116.93 | 121.00 |
| 1 | D | 450 | ASP | CB-CG-OD2 | 6.78 | 124.40 | 118.30 |
| 1 | S | 450 | ASP | CB-CG-OD2 | 6.77 | 124.39 | 118.30 |
| 1 | D | 75 | ASP | N-CA-CB | 6.76 | 122.78 | 110.60 |
| 1 | G | 781 | ASP | CB-CG-OD1 | -6.73 | 112.24 | 118.30 |
| 1 | J | 555 | TYR | CB-CG-CD2 | -6.73 | 116.96 | 121.00 |
| 1 | M | 709 | LYS | CA-C-N | -6.73 | 102.75 | 116.20 |
| 1 | A | 450 | ASP | CB-CG-OD2 | 6.71 | 124.34 | 118.30 |
| 1 | J | 450 | ASP | CB-CG-OD2 | 6.71 | 124.34 | 118.30 |
| 4 | 5 | 196 | ARG | NE-CZ-NH1 | 6.71 | 123.66 | 120.30 |
| 1 | S | 75 | ASP | CB-CG-OD2 | 6.70 | 124.33 | 118.30 |
| 1 | G | 555 | TYR | CB-CG-CD2 | -6.68 | 116.99 | 121.00 |
| 1 | M | 219 | GLU | N-CA-C | -6.68 | 92.98 | 111.00 |
| 1 | G | 756 | THR | N-CA-CB | -6.67 | 97.62 | 110.30 |
| 1 | S | 756 | THR | N-CA-CB | -6.67 | 97.63 | 110.30 |
| 1 | S | 219 | GLU | N-CA-C | -6.65 | 93.04 | 111.00 |
| 1 | J | 219 | GLU | N-CA-C | -6.65 | 93.06 | 111.00 |
| 1 | D | 756 | THR | N-CA-CB | -6.64 | 97.67 | 110.30 |
| 1 | J | 75 | ASP | CB-CG-OD2 | 6.64 | 124.28 | 118.30 |
| 1 | G | 219 | GLU | N-CA-C | -6.64 | 93.06 | 111.00 |
| 1 | M | 756 | THR | N-CA-CB | -6.64 | 97.69 | 110.30 |
| 4 | 5 | 169 | TYR | CB-CG-CD2 | -6.64 | 117.02 | 121.00 |
| 1 | A | 781 | ASP | CB-CG-OD1 | -6.62 | 112.34 | 118.30 |
| 1 | J | 756 | THR | N-CA-CB | -6.62 | 97.72 | 110.30 |
| 1 | M | 75 | ASP | CB-CG-OD2 | 6.62 | 124.25 | 118.30 |
| 1 | A | 219 | GLU | N-CA-C | -6.61 | 93.15 | 111.00 |
| 4 | 7 | 196 | ARG | NE-CZ-NH1 | 6.61 | 123.61 | 120.30 |
| 1 | D | 781 | ASP | CB-CG-OD1 | -6.61 | 112.35 | 118.30 |
| 1 | J | 781 | ASP | CB-CG-OD1 | -6.61 | 112.35 | 118.30 |
| 4 | V | 169 | TYR | CB-CG-CD2 | -6.61 | 117.04 | 121.00 |
| 1 | M | 781 | ASP | CB-CG-OD1 | -6.60 | 112.36 | 118.30 |
| 1 | D | 219 | GLU | N-CA-C | -6.59 | 93.20 | 111.00 |
| 1 | A | 756 | THR | N-CA-CB | -6.59 | 97.78 | 110.30 |
| 4 | Y | 169 | TYR | CB-CG-CD2 | -6.59 | 117.05 | 121.00 |
| 1 | A | 75 | ASP | CB-CG-OD2 | 6.58 | 124.22 | 118.30 |
| 1 | D | 555 | TYR | CB-CG-CD2 | -6.57 | 117.06 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 75 | ASP | CB-CG-OD2 | 6.57 | 124.21 | 118.30 |
| 1 | S | 781 | ASP | CB-CG-OD1 | -6.57 | 112.39 | 118.30 |
| 1 | D | 332 | MET | CG-SD-CE | -6.56 | 89.71 | 100.20 |
| 4 | Y | 283 | MET | CG-SD-CE | 6.55 | 110.69 | 100.20 |
| 1 | M | 332 | MET | CG-SD-CE | -6.55 | 89.72 | 100.20 |
| 1 | G | 332 | MET | CG-SD-CE | -6.55 | 89.72 | 100.20 |
| 4 | 3 | 283 | MET | CG-SD-CE | 6.55 | 110.68 | 100.20 |
| 1 | J | 141 | LEU | CB-CA-C | -6.54 | 97.77 | 110.20 |
| 4 | 7 | 283 | MET | CG-SD-CE | 6.54 | 110.67 | 100.20 |
| 1 | A | 169 | ASP | CB-CG-OD1 | -6.54 | 112.41 | 118.30 |
| 4 | 8 | 169 | TYR | CB-CG-CD2 | -6.54 | 117.07 | 121.00 |
| 4 | X | 196 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |
| 4 | 2 | 283 | MET | CG-SD-CE | 6.54 | 110.67 | 100.20 |
| 4 | X | 283 | MET | CG-SD-CE | 6.54 | 110.67 | 100.20 |
| 1 | A | 332 | MET | CG-SD-CE | -6.54 | 89.74 | 100.20 |
| 4 | 4 | 283 | MET | CG-SD-CE | 6.54 | 110.66 | 100.20 |
| 4 | W | 283 | MET | CG-SD-CE | 6.54 | 110.66 | 100.20 |
| 4 | 2 | 169 | TYR | CB-CG-CD2 | -6.54 | 117.08 | 121.00 |
| 4 | 6 | 196 | ARG | NE-CZ-NH1 | 6.53 | 123.57 | 120.30 |
| 1 | S | 141 | LEU | CB-CA-C | -6.53 | 97.79 | 110.20 |
| 4 | 5 | 283 | MET | CG-SD-CE | 6.53 | 110.65 | 100.20 |
| 4 | Z | 283 | MET | CG-SD-CE | 6.53 | 110.65 | 100.20 |
| 4 | 6 | 283 | MET | CG-SD-CE | 6.53 | 110.64 | 100.20 |
| 4 | 1 | 196 | ARG | NE-CZ-NH1 | 6.53 | 123.56 | 120.30 |
| 1 | A | 555 | TYR | CB-CG-CD2 | -6.52 | 117.09 | 121.00 |
| 1 | M | 141 | LEU | CB-CA-C | -6.52 | 97.81 | 110.20 |
| 4 | 1 | 283 | MET | CG-SD-CE | 6.52 | 110.64 | 100.20 |
| 4 | 8 | 283 | MET | CG-SD-CE | 6.52 | 110.63 | 100.20 |
| 1 | G | 141 | LEU | CB-CA-C | -6.52 | 97.81 | 110.20 |
| 1 | J | 332 | MET | CG-SD-CE | -6.52 | 89.77 | 100.20 |
| 1 | S | 332 | MET | CG-SD-CE | -6.52 | 89.77 | 100.20 |
| 1 | A | 343 | PHE | CB-CG-CD1 | 6.52 | 125.36 | 120.80 |
| 1 | G | 343 | PHE | CB-CG-CD1 | 6.51 | 125.36 | 120.80 |
| 4 | 9 | 283 | MET | CG-SD-CE | 6.51 | 110.62 | 100.20 |
| 4 | W | 169 | TYR | CB-CG-CD2 | -6.51 | 117.09 | 121.00 |
| 1 | D | 141 | LEU | CB-CA-C | -6.51 | 97.84 | 110.20 |
| 1 | J | 169 | ASP | CB-CG-OD1 | -6.50 | 112.45 | 118.30 |
| 4 | V | 283 | MET | CG-SD-CE | 6.50 | 110.61 | 100.20 |
| 1 | D | 343 | PHE | CB-CG-CD1 | 6.50 | 125.35 | 120.80 |
| 1 | M | 169 | ASP | CB-CG-OD1 | -6.50 | 112.45 | 118.30 |
| 1 | G | 75 | ASP | CB-CG-OD2 | 6.50 | 124.15 | 118.30 |
| 1 | G | 334 | THR | CA-CB-CG2 | -6.49 | 103.31 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4 | 3 | 159 | VAL | CB-CA-C | -6.49 | 99.06 | 111.40 |
| 1 | D | 334 | THR | CA-CB-CG2 | -6.49 | 103.31 | 112.40 |
| 4 | 4 | 169 | TYR | CB-CG-CD2 | -6.49 | 117.11 | 121.00 |
| 4 | X | 159 | VAL | CB-CA-C | -6.49 | 99.07 | 111.40 |
| 4 | Y | 159 | VAL | CB-CA-C | -6.48 | 99.08 | 111.40 |
| 4 | 4 | 159 | VAL | CB-CA-C | -6.48 | 99.09 | 111.40 |
| 4 | 6 | 159 | VAL | CB-CA-C | -6.48 | 99.09 | 111.40 |
| 4 | 7 | 159 | VAL | CB-CA-C | -6.48 | 99.09 | 111.40 |
| 4 | 9 | 196 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |
| 4 | 8 | 196 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |
| 1 | A | 334 | THR | CA-CB-CG2 | -6.47 | 103.34 | 112.40 |
| 4 | 6 | 169 | TYR | CB-CG-CD2 | -6.47 | 117.12 | 121.00 |
| 4 | V | 159 | VAL | CB-CA-C | -6.47 | 99.11 | 111.40 |
| 4 | Z | 169 | TYR | CB-CG-CD2 | -6.47 | 117.12 | 121.00 |
| 4 | 9 | 159 | VAL | CB-CA-C | -6.46 | 99.12 | 111.40 |
| 4 | 8 | 159 | VAL | CB-CA-C | -6.46 | 99.12 | 111.40 |
| 1 | G | 169 | ASP | CB-CG-OD1 | -6.46 | 112.48 | 118.30 |
| 4 | W | 196 | ARG | NE-CZ-NH1 | 6.46 | 123.53 | 120.30 |
| 4 | 3 | 169 | TYR | CB-CG-CD2 | -6.46 | 117.12 | 121.00 |
| 1 | S | 334 | THR | CA-CB-CG2 | -6.45 | 103.37 | 112.40 |
| 4 | W | 159 | VAL | CB-CA-C | -6.45 | 99.14 | 111.40 |
| 4 | X | 169 | TYR | CB-CG-CD2 | -6.45 | 117.13 | 121.00 |
| 4 | 5 | 159 | VAL | CB-CA-C | -6.45 | 99.14 | 111.40 |
| 4 | Z | 159 | VAL | CB-CA-C | -6.45 | 99.14 | 111.40 |
| 4 | 1 | 159 | VAL | CB-CA-C | -6.45 | 99.15 | 111.40 |
| 2 | E | 141 | PRO | N-CD-CG | -6.45 | 93.53 | 103.20 |
| 1 | M | 810 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | M | 334 | THR | CA-CB-CG2 | -6.44 | 103.38 | 112.40 |
| 4 | 2 | 159 | VAL | CB-CA-C | -6.44 | 99.16 | 111.40 |
| 2 | H | 141 | PRO | N-CD-CG | -6.44 | 93.54 | 103.20 |
| 4 | 7 | 169 | TYR | CB-CG-CD2 | -6.43 | 117.14 | 121.00 |
| 1 | D | 169 | ASP | CB-CG-OD1 | -6.43 | 112.51 | 118.30 |
| 1 | S | 169 | ASP | CB-CG-OD1 | -6.43 | 112.51 | 118.30 |
| 1 | A | 141 | LEU | CB-CA-C | -6.43 | 97.98 | 110.20 |
| 4 | Y | 34 | ILE | CA-CB-CG2 | -6.43 | 98.05 | 110.90 |
| 1 | J | 129 | TYR | CB-CG-CD2 | -6.42 | 117.14 | 121.00 |
| 4 | 8 | 34 | ILE | CA-CB-CG2 | -6.42 | 98.05 | 110.90 |
| 4 | V | 196 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 |
| 1 | J | 334 | THR | CA-CB-CG2 | -6.42 | 103.41 | 112.40 |
| 4 | 3 | 34 | ILE | CA-CB-CG2 | -6.42 | 98.06 | 110.90 |
| 4 | 9 | 34 | ILE | CA-CB-CG2 | -6.42 | 98.06 | 110.90 |
| 4 | W | 34 | ILE | CA-CB-CG2 | -6.42 | 98.06 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4 | 3 | 196 | ARG | NE-CZ-NH1 | 6.41 | 123.51 | 120.30 |
| 4 | 4 | 196 | ARG | NE-CZ-NH1 | 6.41 | 123.51 | 120.30 |
| 4 | 7 | 34 | ILE | CA-CB-CG2 | -6.41 | 98.07 | 110.90 |
| 2 | N | 141 | PRO | N-CD-CG | -6.41 | 93.58 | 103.20 |
| 1 | J | 779 | ARG | NE-CZ-NH1 | 6.41 | 123.50 | 120.30 |
| 4 | 9 | 169 | TYR | CB-CG-CD2 | -6.41 | 117.16 | 121.00 |
| 1 | G | 589 | ASP | CB-CG-OD1 | -6.40 | 112.54 | 118.30 |
| 1 | A | 589 | ASP | CB-CG-OD1 | -6.40 | 112.54 | 118.30 |
| 1 | M | 589 | ASP | CB-CG-OD1 | -6.40 | 112.54 | 118.30 |
| 1 | S | 129 | TYR | CB-CG-CD2 | -6.40 | 117.16 | 121.00 |
| 4 | 5 | 34 | ILE | CA-CB-CG2 | -6.40 | 98.10 | 110.90 |
| 4 | Z | 34 | ILE | CA-CB-CG2 | -6.40 | 98.11 | 110.90 |
| 1 | S | 327 | ASP | CB-CG-OD2 | 6.40 | 124.06 | 118.30 |
| 2 | K | 141 | PRO | N-CD-CG | -6.39 | 93.61 | 103.20 |
| 4 | 6 | 34 | ILE | CA-CB-CG2 | -6.39 | 98.11 | 110.90 |
| 1 | J | 589 | ASP | CB-CG-OD1 | -6.39 | 112.55 | 118.30 |
| 4 | V | 34 | ILE | CA-CB-CG2 | -6.39 | 98.12 | 110.90 |
| 4 | X | 34 | ILE | CA-CB-CG2 | -6.38 | 98.13 | 110.90 |
| 1 | M | 343 | PHE | CB-CG-CD1 | 6.38 | 125.27 | 120.80 |
| 1 | S | 589 | ASP | CB-CG-OD1 | -6.38 | 112.56 | 118.30 |
| 4 | 1 | 34 | ILE | CA-CB-CG2 | -6.38 | 98.13 | 110.90 |
| 4 | 2 | 34 | ILE | CA-CB-CG2 | -6.38 | 98.14 | 110.90 |
| 4 | 4 | 34 | ILE | CA-CB-CG2 | -6.38 | 98.15 | 110.90 |
| 1 | A | 341 | LEU | CB-CA-C | 6.37 | 122.30 | 110.20 |
| 2 | T | 141 | PRO | N-CD-CG | -6.37 | 93.65 | 103.20 |
| 4 | Y | 196 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 4 | 1 | 169 | TYR | CB-CG-CD2 | -6.36 | 117.19 | 121.00 |
| 1 | G | 341 | LEU | CB-CA-C | 6.34 | 122.25 | 110.20 |
| 1 | M | 129 | TYR | CB-CG-CD2 | -6.34 | 117.20 | 121.00 |
| 2 | B | 141 | PRO | N-CD-CG | -6.33 | 93.70 | 103.20 |
| 1 | D | 589 | ASP | CB-CG-OD1 | -6.33 | 112.60 | 118.30 |
| 1 | M | 578 | HIS | N-CA-CB | 6.33 | 121.99 | 110.60 |
| 1 | J | 810 | ARG | NE-CZ-NH1 | 6.32 | 123.46 | 120.30 |
| 1 | S | 343 | PHE | CB-CG-CD1 | 6.32 | 125.23 | 120.80 |
| 1 | S | 578 | HIS | N-CA-CB | 6.32 | 121.98 | 110.60 |
| 4 | X | 217 | CYS | CA-CB-SG | -6.32 | 102.62 | 114.00 |
| 1 | M | 341 | LEU | CB-CA-C | 6.32 | 122.21 | 110.20 |
| 1 | D | 129 | TYR | CB-CG-CD2 | -6.32 | 117.21 | 121.00 |
| 1 | G | 590 | TYR | CB-CG-CD2 | 6.32 | 124.79 | 121.00 |
| 1 | G | 578 | HIS | N-CA-CB | 6.32 | 121.97 | 110.60 |
| 4 | Z | 196 | ARG | NE-CZ-NH1 | 6.32 | 123.46 | 120.30 |
| 1 | J | 343 | PHE | CB-CG-CD1 | 6.31 | 125.22 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | S | 779 | ARG | NE-CZ-NH1 | 6.30 | 123.45 | 120.30 |
| 1 | S | 341 | LEU | CB-CA-C | 6.30 | 122.17 | 110.20 |
| 4 | 1 | 217 | CYS | CA-CB-SG | -6.30 | 102.67 | 114.00 |
| 4 | 5 | 217 | CYS | CA-CB-SG | -6.30 | 102.67 | 114.00 |
| 4 | 2 | 196 | ARG | NE-CZ-NH1 | 6.29 | 123.45 | 120.30 |
| 4 | 8 | 217 | CYS | CA-CB-SG | -6.29 | 102.67 | 114.00 |
| 1 | J | 341 | LEU | CB-CA-C | 6.29 | 122.15 | 110.20 |
| 4 | 7 | 217 | CYS | CA-CB-SG | -6.29 | 102.68 | 114.00 |
| 4 | 4 | 217 | CYS | CA-CB-SG | -6.29 | 102.68 | 114.00 |
| 4 | V | 217 | CYS | CA-CB-SG | -6.29 | 102.68 | 114.00 |
| 4 | 6 | 217 | CYS | CA-CB-SG | -6.29 | 102.69 | 114.00 |
| 1 | A | 578 | HIS | N-CA-CB | 6.28 | 121.91 | 110.60 |
| 4 | 2 | 217 | CYS | CA-CB-SG | -6.28 | 102.69 | 114.00 |
| 1 | J | 327 | ASP | CB-CG-OD2 | 6.28 | 123.95 | 118.30 |
| 4 | Z | 217 | CYS | CA-CB-SG | -6.28 | 102.70 | 114.00 |
| 4 | 9 | 217 | CYS | CA-CB-SG | -6.28 | 102.70 | 114.00 |
| 1 | A | 463 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 4 | Y | 217 | CYS | CA-CB-SG | -6.28 | 102.70 | 114.00 |
| 1 | J | 760 | PHE | CB-CG-CD2 | -6.27 | 116.41 | 120.80 |
| 4 | 3 | 217 | CYS | CA-CB-SG | -6.27 | 102.72 | 114.00 |
| 2 | N | 129 | THR | CB-CA-C | -6.27 | 94.68 | 111.60 |
| 1 | D | 341 | LEU | CB-CA-C | 6.26 | 122.10 | 110.20 |
| 1 | J | 578 | HIS | N-CA-CB | 6.26 | 121.88 | 110.60 |
| 4 | W | 217 | CYS | CA-CB-SG | -6.26 | 102.73 | 114.00 |
| 1 | D | 760 | PHE | CB-CG-CD2 | -6.25 | 116.43 | 120.80 |
| 2 | K | 129 | THR | CB-CA-C | -6.24 | 94.76 | 111.60 |
| 1 | M | 327 | ASP | CB-CG-OD2 | 6.24 | 123.91 | 118.30 |
| 2 | T | 129 | THR | CB-CA-C | -6.24 | 94.76 | 111.60 |
| 2 | H | 129 | THR | CB-CA-C | -6.21 | 94.82 | 111.60 |
| 1 | D | 578 | HIS | N-CA-CB | 6.21 | 121.78 | 110.60 |
| 1 | A | 129 | TYR | CB-CG-CD2 | -6.20 | 117.28 | 121.00 |
| 1 | A | 780 | ASP | CB-CG-OD2 | 6.20 | 123.88 | 118.30 |
| 1 | G | 129 | TYR | CB-CG-CD2 | -6.20 | 117.28 | 121.00 |
| 1 | G | 104 | TYR | CB-CG-CD1 | -6.19 | 117.28 | 121.00 |
| 1 | J | 214 | MET | CG-SD-CE | 6.18 | 110.09 | 100.20 |
| 1 | M | 698 | ASN | CB-CA-C | -6.18 | 98.04 | 110.40 |
| 1 | S | 214 | MET | CG-SD-CE | 6.18 | 110.09 | 100.20 |
| 1 | M | 779 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 1 | G | 327 | ASP | CB-CG-OD2 | 6.17 | 123.86 | 118.30 |
| 1 | S | 698 | ASN | CB-CA-C | -6.17 | 98.06 | 110.40 |
| 1 | D | 327 | ASP | CB-CG-OD2 | 6.17 | 123.85 | 118.30 |
| 1 | D | 590 | TYR | CB-CG-CD2 | 6.17 | 124.70 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 129 | THR | CB-CA-C | -6.17 | 94.95 | 111.60 |
| 2 | E | 129 | THR | CB-CA-C | -6.17 | 94.95 | 111.60 |
| 1 | A | 698 | ASN | CB-CA-C | -6.16 | 98.08 | 110.40 |
| 1 | D | 214 | MET | CG-SD-CE | 6.16 | 110.06 | 100.20 |
| 1 | A | 214 | MET | CG-SD-CE | 6.16 | 110.06 | 100.20 |
| 1 | G | 810 | ARG | NE-CZ-NH1 | 6.16 | 123.38 | 120.30 |
| 1 | A | 327 | ASP | CB-CG-OD2 | 6.16 | 123.84 | 118.30 |
| 4 | 3 | 259 | GLU | CA-CB-CG | 6.16 | 126.94 | 113.40 |
| 1 | S | 752 | ASP | CB-CG-OD2 | 6.15 | 123.84 | 118.30 |
| 1 | G | 214 | MET | CG-SD-CE | 6.15 | 110.04 | 100.20 |
| 2 | K | 141 | PRO | N-CA-CB | -6.15 | 95.83 | 102.60 |
| 4 | 2 | 259 | GLU | CA-CB-CG | 6.15 | 126.93 | 113.40 |
| 4 | W | 259 | GLU | CA-CB-CG | 6.15 | 126.93 | 113.40 |
| 3 | F | 58 | MET | CG-SD-CE | 6.15 | 110.04 | 100.20 |
| 1 | M | 463 | ASP | CB-CG-OD2 | -6.15 | 112.77 | 118.30 |
| 1 | M | 214 | MET | CG-SD-CE | 6.14 | 110.03 | 100.20 |
| 2 | N | 141 | PRO | N-CA-CB | -6.14 | 95.84 | 102.60 |
| 2 | E | 129 | THR | CA-CB-CG2 | 6.14 | 120.99 | 112.40 |
| 2 | T | 141 | PRO | N-CA-CB | -6.14 | 95.85 | 102.60 |
| 4 | 1 | 259 | GLU | CA-CB-CG | 6.14 | 126.90 | 113.40 |
| 4 | V | 259 | GLU | CA-CB-CG | 6.14 | 126.90 | 113.40 |
| 1 | S | 104 | TYR | CB-CG-CD1 | -6.14 | 117.32 | 121.00 |
| 1 | D | 779 | ARG | NE-CZ-NH1 | 6.13 | 123.37 | 120.30 |
| 1 | J | 698 | ASN | CB-CA-C | -6.13 | 98.14 | 110.40 |
| 4 | 9 | 259 | GLU | CA-CB-CG | 6.13 | 126.89 | 113.40 |
| 2 | H | 141 | PRO | N-CA-CB | -6.13 | 95.86 | 102.60 |
| 1 | S | 682 | THR | CA-CB-CG2 | -6.13 | 103.82 | 112.40 |
| 4 | 8 | 259 | GLU | CA-CB-CG | 6.13 | 126.88 | 113.40 |
| 2 | E | 141 | PRO | N-CA-CB | -6.13 | 95.86 | 102.60 |
| 4 | X | 259 | GLU | CA-CB-CG | 6.13 | 126.88 | 113.40 |
| 3 | O | 58 | MET | CG-SD-CE | 6.12 | 110.00 | 100.20 |
| 1 | J | 752 | ASP | CB-CG-OD2 | 6.12 | 123.81 | 118.30 |
| 1 | S | 810 | ARG | NE-CZ-NH1 | 6.12 | 123.36 | 120.30 |
| 4 | 5 | 259 | GLU | CA-CB-CG | 6.12 | 126.86 | 113.40 |
| 4 | Z | 259 | GLU | CA-CB-CG | 6.12 | 126.86 | 113.40 |
| 1 | G | 463 | ASP | CB-CG-OD2 | -6.12 | 112.80 | 118.30 |
| 4 | 4 | 259 | GLU | CA-CB-CG | 6.12 | 126.86 | 113.40 |
| 4 | 7 | 259 | GLU | CA-CB-CG | 6.12 | 126.86 | 113.40 |
| 4 | Y | 259 | GLU | CA-CB-CG | 6.12 | 126.85 | 113.40 |
| 4 | 6 | 259 | GLU | CA-CB-CG | 6.11 | 126.85 | 113.40 |
| 1 | J | 590 | TYR | CB-CG-CD2 | 6.11 | 124.67 | 121.00 |
| 1 | G | 698 | ASN | CB-CA-C | -6.11 | 98.18 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 760 | PHE | CB-CG-CD2 | -6.11 | 116.53 | 120.80 |
| 1 | D | 698 | ASN | CB-CA-C | -6.10 | 98.19 | 110.40 |
| 1 | S | 760 | PHE | CB-CG-CD2 | -6.10 | 116.53 | 120.80 |
| 1 | A | 810 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 3 | L | 58 | MET | CG-SD-CE | 6.10 | 109.96 | 100.20 |
| 1 | S | 463 | ASP | CB-CG-OD2 | -6.10 | 112.81 | 118.30 |
| 1 | J | 104 | TYR | CB-CG-CD1 | -6.09 | 117.34 | 121.00 |
| 1 | M | 760 | PHE | CB-CG-CD2 | -6.09 | 116.54 | 120.80 |
| 4 | 2 | 349 | LEU | CA-C-N | -6.09 | 103.81 | 117.20 |
| 1 | M | 104 | TYR | CB-CG-CD1 | -6.08 | 117.35 | 121.00 |
| 1 | A | 682 | THR | CA-CB-CG2 | -6.08 | 103.88 | 112.40 |
| 1 | J | 682 | THR | CA-CB-CG2 | -6.08 | 103.89 | 112.40 |
| 4 | 7 | 349 | LEU | CA-C-N | -6.08 | 103.82 | 117.20 |
| 1 | J | 463 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |
| 4 | 3 | 349 | LEU | CA-C-N | -6.08 | 103.83 | 117.20 |
| 4 | 4 | 349 | LEU | CA-C-N | -6.08 | 103.83 | 117.20 |
| 1 | M | 682 | THR | CA-CB-CG2 | -6.07 | 103.90 | 112.40 |
| 1 | G | 625 | THR | CA-CB-OG1 | 6.07 | 121.75 | 109.00 |
| 4 | 9 | 349 | LEU | CA-C-N | -6.07 | 103.85 | 117.20 |
| 4 | 9 | 16 | LEU | CA-CB-CG | 6.07 | 129.25 | 115.30 |
| 1 | D | 104 | TYR | CB-CG-CD1 | -6.06 | 117.36 | 121.00 |
| 1 | J | 450 | ASP | CB-CG-OD1 | -6.06 | 112.84 | 118.30 |
| 1 | J | 625 | THR | CA-CB-OG1 | 6.06 | 121.72 | 109.00 |
| 3 | U | 58 | MET | CG-SD-CE | 6.06 | 109.90 | 100.20 |
| 4 | Z | 16 | LEU | CA-CB-CG | 6.06 | 129.24 | 115.30 |
| 2 | B | 129 | THR | CA-CB-CG2 | 6.06 | 120.88 | 112.40 |
| 1 | D | 810 | ARG | NE-CZ-NH1 | 6.06 | 123.33 | 120.30 |
| 4 | V | 16 | LEU | CA-CB-CG | 6.05 | 129.23 | 115.30 |
| 4 | V | 349 | LEU | CA-C-N | -6.05 | 103.88 | 117.20 |
| 4 | 3 | 16 | LEU | CA-CB-CG | 6.05 | 129.22 | 115.30 |
| 4 | V | 335 | ARG | NE-CZ-NH2 | -6.05 | 117.28 | 120.30 |
| 1 | M | 450 | ASP | CB-CG-OD1 | -6.05 | 112.86 | 118.30 |
| 4 | 6 | 16 | LEU | CA-CB-CG | 6.05 | 129.21 | 115.30 |
| 4 | X | 16 | LEU | CA-CB-CG | 6.05 | 129.21 | 115.30 |
| 4 | 6 | 349 | LEU | CA-C-N | -6.04 | 103.90 | 117.20 |
| 4 | Z | 349 | LEU | CA-C-N | -6.04 | 103.90 | 117.20 |
| 1 | S | 590 | TYR | CB-CG-CD2 | 6.04 | 124.63 | 121.00 |
| 1 | S | 665 | ARG | NE-CZ-NH2 | -6.04 | 117.28 | 120.30 |
| 4 | 2 | 16 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 4 | 8 | 16 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 2 | B | 141 | PRO | N-CA-CB | -6.04 | 95.95 | 102.60 |
| 1 | M | 752 | ASP | CB-CG-OD2 | 6.04 | 123.74 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 1 | 16 | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 3 | C | 58 | MET | CG-SD-CE | 6.04 | 109.86 | 100.20 |
| 2 | H | 129 | THR | CA-CB-CG2 | 6.04 | 120.86 | 112.40 |
| 3 | I | 58 | MET | CG-SD-CE | 6.04 | 109.86 | 100.20 |
| 4 | 5 | 349 | LEU | CA-C-N | -6.04 | 103.92 | 117.20 |
| 4 | X | 349 | LEU | CA-C-N | -6.04 | 103.92 | 117.20 |
| 4 | Y | 16 | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 1 | A | 779 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 1 | D | 682 | THR | CA-CB-CG2 | -6.03 | 103.95 | 112.40 |
| 1 | G | 682 | THR | CA-CB-CG2 | -6.03 | 103.95 | 112.40 |
| 1 | M | 192 | VAL | CA-CB-CG1 | -6.03 | 101.85 | 110.90 |
| 1 | S | 625 | THR | CA-CB-OG1 | 6.03 | 121.67 | 109.00 |
| 4 | 7 | 16 | LEU | CA-CB-CG | 6.03 | 129.17 | 115.30 |
| 4 | W | 16 | LEU | CA-CB-CG | 6.03 | 129.17 | 115.30 |
| 1 | D | 378 | ASP | CB-CG-OD1 | -6.03 | 112.87 | 118.30 |
| 1 | S | 192 | VAL | CA-CB-CG1 | -6.03 | 101.85 | 110.90 |
| 1 | M | 625 | THR | CA-CB-OG1 | 6.03 | 121.66 | 109.00 |
| 4 | 5 | 16 | LEU | CA-CB-CG | 6.03 | 129.17 | 115.30 |
| 4 | W | 349 | LEU | CA-C-N | -6.03 | 103.94 | 117.20 |
| 4 | 1 | 349 | LEU | CA-C-N | -6.03 | 103.95 | 117.20 |
| 4 | 8 | 79 | TRP | CG-CD2-CE3 | 6.03 | 139.32 | 133.90 |
| 1 | D | 625 | THR | CA-CB-OG1 | 6.02 | 121.64 | 109.00 |
| 1 | G | 346 | ASP | CB-CG-OD1 | 6.02 | 123.72 | 118.30 |
| 4 | 4 | 16 | LEU | CA-CB-CG | 6.02 | 129.15 | 115.30 |
| 1 | J | 192 | VAL | CA-CB-CG1 | -6.02 | 101.88 | 110.90 |
| 4 | 8 | 349 | LEU | CA-C-N | -6.02 | 103.97 | 117.20 |
| 4 | Y | 349 | LEU | CA-C-N | -6.01 | 103.97 | 117.20 |
| 1 | A | 590 | TYR | CB-CG-CD2 | 6.01 | 124.61 | 121.00 |
| 1 | A | 625 | THR | CA-CB-OG1 | 6.01 | 121.62 | 109.00 |
| 2 | T | 129 | THR | CA-CB-CG2 | 6.00 | 120.80 | 112.40 |
| 1 | G | 760 | PHE | CB-CG-CD2 | -6.00 | 116.60 | 120.80 |
| 1 | J | 447 | GLN | N-CA-CB | 6.00 | 121.40 | 110.60 |
| 1 | J | 665 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 |
| 1 | A | 447 | GLN | N-CA-CB | 6.00 | 121.39 | 110.60 |
| 1 | D | 346 | ASP | CB-CG-OD1 | 6.00 | 123.70 | 118.30 |
| 1 | S | 447 | GLN | N-CA-CB | 6.00 | 121.39 | 110.60 |
| 1 | M | 447 | GLN | N-CA-CB | 5.99 | 121.38 | 110.60 |
| 1 | G | 192 | VAL | CA-CB-CG1 | -5.99 | 101.92 | 110.90 |
| 1 | S | 450 | ASP | CB-CG-OD1 | -5.99 | 112.91 | 118.30 |
| 1 | D | 192 | VAL | CA-CB-CG1 | -5.99 | 101.92 | 110.90 |
| 1 | S | 785 | GLU | C-N-CA | 5.99 | 136.66 | 121.70 |
| 1 | G | 780 | ASP | CB-CG-OD2 | 5.98 | 123.68 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | K | 129 | THR | CA-CB-CG2 | 5.98 | 120.78 | 112.40 |
| 4 | W | 335 | ARG | NE-CZ-NH2 | -5.98 | 117.31 | 120.30 |
| 1 | G | 779 | ARG | NE-CZ-NH1 | 5.98 | 123.29 | 120.30 |
| 4 | 7 | 116 | ARG | NE-CZ-NH1 | 5.98 | 123.29 | 120.30 |
| 1 | D | 471 | ASP | CB-CG-OD1 | -5.98 | 112.92 | 118.30 |
| 1 | A | 665 | ARG | NE-CZ-NH2 | -5.97 | 117.31 | 120.30 |
| 1 | G | 447 | GLN | N-CA-CB | 5.96 | 121.34 | 110.60 |
| 1 | D | 447 | GLN | N-CA-CB | 5.96 | 121.33 | 110.60 |
| 1 | S | 780 | ASP | CB-CG-OD2 | 5.96 | 123.66 | 118.30 |
| 1 | M | 665 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 4 | 1 | 79 | TRP | CG-CD2-CE3 | 5.96 | 139.26 | 133.90 |
| 4 | Z | 79 | TRP | CG-CD2-CE3 | 5.96 | 139.26 | 133.90 |
| 1 | G | 754 | ASP | CB-CG-OD2 | -5.96 | 112.94 | 118.30 |
| 2 | N | 129 | THR | CA-CB-CG2 | 5.95 | 120.73 | 112.40 |
| 1 | D | 339 | ASP | CB-CG-OD2 | 5.95 | 123.65 | 118.30 |
| 4 | 1 | 335 | ARG | NE-CZ-NH2 | -5.95 | 117.33 | 120.30 |
| 1 | M | 590 | TYR | CB-CG-CD2 | 5.94 | 124.57 | 121.00 |
| 4 | X | 79 | TRP | CG-CD2-CE3 | 5.94 | 139.25 | 133.90 |
| 1 | D | 450 | ASP | CB-CG-OD1 | -5.94 | 112.96 | 118.30 |
| 1 | D | 463 | ASP | CB-CG-OD2 | -5.93 | 112.96 | 118.30 |
| 1 | D | 780 | ASP | CB-CG-OD2 | 5.93 | 123.64 | 118.30 |
| 4 | 2 | 79 | TRP | CG-CD2-CE3 | 5.93 | 139.24 | 133.90 |
| 4 | 3 | 335 | ARG | NE-CZ-NH2 | -5.93 | 117.33 | 120.30 |
| 1 | J | 378 | ASP | CB-CG-OD1 | -5.93 | 112.97 | 118.30 |
| 1 | M | 346 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | S | 378 | ASP | CB-CG-OD1 | -5.93 | 112.97 | 118.30 |
| 1 | A | 754 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 1 | G | 339 | ASP | CB-CG-OD2 | 5.92 | 123.63 | 118.30 |
| 1 | S | 346 | ASP | CB-CG-OD1 | 5.92 | 123.63 | 118.30 |
| 1 | M | 780 | ASP | CB-CG-OD2 | 5.92 | 123.63 | 118.30 |
| 1 | S | 754 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 4 | X | 254 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | A | 104 | TYR | CB-CG-CD1 | -5.92 | 117.45 | 121.00 |
| 4 | Z | 116 | ARG | NE-CZ-NH1 | 5.91 | 123.26 | 120.30 |
| 1 | A | 192 | VAL | CA-CB-CG1 | -5.91 | 102.03 | 110.90 |
| 1 | M | 378 | ASP | CB-CG-OD1 | -5.91 | 112.98 | 118.30 |
| 1 | D | 754 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | G | 378 | ASP | CB-CG-OD1 | -5.91 | 112.98 | 118.30 |
| 1 | J | 780 | ASP | CB-CG-OD2 | 5.91 | 123.62 | 118.30 |
| 1 | D | 738 | MET | CG-SD-CE | 5.90 | 109.65 | 100.20 |
| 4 | 7 | 200 | PHE | CA-C-N | -5.90 | 104.21 | 117.20 |
| 1 | A | 809 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 815 | CYS | CA-CB-SG | -5.90 | 103.38 | 114.00 |
| 1 | D | 556 | ASP | CB-CG-OD1 | -5.90 | 112.99 | 118.30 |
| 1 | G | 665 | ARG | NE-CZ-NH2 | -5.89 | 117.35 | 120.30 |
| 1 | J | 754 | ASP | CB-CG-OD2 | -5.89 | 112.99 | 118.30 |
| 1 | G | 450 | ASP | CB-CG-OD1 | -5.89 | 113.00 | 118.30 |
| 1 | G | 752 | ASP | CB-CG-OD2 | 5.89 | 123.60 | 118.30 |
| 4 | 3 | 79 | TRP | CG-CD2-CE3 | 5.89 | 139.20 | 133.90 |
| 4 | 8 | 335 | ARG | NE-CZ-NH2 | -5.89 | 117.36 | 120.30 |
| 4 | 1 | 200 | PHE | CA-C-N | -5.89 | 104.25 | 117.20 |
| 1 | J | 346 | ASP | CB-CG-OD1 | 5.89 | 123.60 | 118.30 |
| 4 | 3 | 200 | PHE | CA-C-N | -5.89 | 104.25 | 117.20 |
| 4 | 6 | 200 | PHE | CA-C-N | -5.88 | 104.27 | 117.20 |
| 4 | W | 200 | PHE | CA-C-N | -5.88 | 104.27 | 117.20 |
| 4 | Y | 79 | TRP | CG-CD2-CE3 | 5.88 | 139.19 | 133.90 |
| 4 | 6 | 79 | TRP | CG-CD2-CE3 | 5.88 | 139.19 | 133.90 |
| 1 | G | 738 | MET | CG-SD-CE | 5.87 | 109.60 | 100.20 |
| 4 | 9 | 116 | ARG | NE-CZ-NH1 | 5.87 | 123.24 | 120.30 |
| 4 | V | 200 | PHE | CA-C-N | -5.87 | 104.28 | 117.20 |
| 4 | X | 200 | PHE | CA-C-N | -5.87 | 104.28 | 117.20 |
| 4 | X | 335 | ARG | NE-CZ-NH2 | -5.87 | 117.36 | 120.30 |
| 4 | 6 | 335 | ARG | NE-CZ-NH2 | -5.87 | 117.37 | 120.30 |
| 1 | S | 339 | ASP | CB-CG-OD2 | 5.87 | 123.58 | 118.30 |
| 1 | A | 450 | ASP | CB-CG-OD1 | -5.86 | 113.02 | 118.30 |
| 1 | A | 378 | ASP | CB-CG-OD1 | -5.86 | 113.03 | 118.30 |
| 4 | 4 | 116 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 4 | 5 | 200 | PHE | CA-C-N | -5.86 | 104.31 | 117.20 |
| 4 | 8 | 200 | PHE | CA-C-N | -5.86 | 104.31 | 117.20 |
| 4 | X | 116 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | G | 780 | ASP | CB-CG-OD1 | -5.86 | 113.03 | 118.30 |
| 4 | 3 | 116 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 4 | 7 | 335 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | S | 809 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 4 | Y | 200 | PHE | CA-C-N | -5.85 | 104.32 | 117.20 |
| 4 | 9 | 200 | PHE | CA-C-N | -5.85 | 104.33 | 117.20 |
| 1 | M | 815 | CYS | CA-CB-SG | -5.85 | 103.47 | 114.00 |
| 1 | A | 738 | MET | CG-SD-CE | 5.85 | 109.56 | 100.20 |
| 1 | J | 738 | MET | CG-SD-CE | 5.85 | 109.56 | 100.20 |
| 1 | S | 738 | MET | CG-SD-CE | 5.85 | 109.55 | 100.20 |
| 4 | V | 116 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 4 | 2 | 200 | PHE | CA-C-N | -5.84 | 104.35 | 117.20 |
| 4 | 9 | 79 | TRP | CG-CD2-CE3 | 5.84 | 139.16 | 133.90 |
| 1 | M | 339 | ASP | CB-CG-OD2 | 5.84 | 123.56 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | M | 738 | MET | CG-SD-CE | 5.84 | 109.54 | 100.20 |
| 1 | A | 780 | ASP | CB-CG-OD1 | -5.83 | 113.05 | 118.30 |
| 1 | G | 556 | ASP | CB-CG-OD1 | -5.83 | 113.05 | 118.30 |
| 4 | 4 | 79 | TRP | CG-CD2-CE3 | 5.83 | 139.15 | 133.90 |
| 4 | 5 | 79 | TRP | CG-CD2-CE3 | 5.83 | 139.15 | 133.90 |
| 1 | S | 815 | CYS | CA-CB-SG | -5.83 | 103.51 | 114.00 |
| 1 | J | 815 | CYS | CA-CB-SG | -5.83 | 103.51 | 114.00 |
| 4 | W | 116 | ARG | NE-CZ-NH1 | 5.83 | 123.21 | 120.30 |
| 4 | 4 | 200 | PHE | CA-C-N | -5.83 | 104.39 | 117.20 |
| 1 | M | 556 | ASP | CB-CG-OD1 | -5.82 | 113.06 | 118.30 |
| 1 | J | 556 | ASP | CB-CG-OD1 | -5.82 | 113.06 | 118.30 |
| 1 | M | 754 | ASP | CB-CG-OD2 | -5.82 | 113.06 | 118.30 |
| 4 | 3 | 95 | ARG | CA-CB-CG | 5.82 | 126.19 | 113.40 |
| 4 | 9 | 254 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 1 | G | 809 | ARG | NE-CZ-NH2 | -5.81 | 117.39 | 120.30 |
| 4 | 4 | 95 | ARG | CA-CB-CG | 5.81 | 126.19 | 113.40 |
| 1 | A | 471 | ASP | CB-CG-OD1 | -5.81 | 113.07 | 118.30 |
| 4 | W | 79 | TRP | CG-CD2-CE3 | 5.81 | 139.13 | 133.90 |
| 1 | D | 815 | CYS | CA-CB-SG | -5.81 | 103.55 | 114.00 |
| 1 | A | 752 | ASP | CB-CG-OD2 | 5.80 | 123.52 | 118.30 |
| 4 | Z | 200 | PHE | CA-C-N | -5.80 | 104.43 | 117.20 |
| 4 | 7 | 79 | TRP | CG-CD2-CE3 | 5.80 | 139.12 | 133.90 |
| 4 | 7 | 254 | ARG | NE-CZ-NH1 | 5.80 | 123.20 | 120.30 |
| 1 | M | 471 | ASP | CB-CG-OD1 | -5.80 | 113.08 | 118.30 |
| 4 | W | 95 | ARG | CA-CB-CG | 5.80 | 126.15 | 113.40 |
| 1 | S | 471 | ASP | CB-CG-OD1 | -5.79 | 113.08 | 118.30 |
| 4 | 2 | 95 | ARG | CA-CB-CG | 5.79 | 126.14 | 113.40 |
| 4 | Z | 335 | ARG | NE-CZ-NH2 | -5.79 | 117.40 | 120.30 |
| 1 | J | 339 | ASP | CB-CG-OD2 | 5.79 | 123.51 | 118.30 |
| 1 | S | 556 | ASP | CB-CG-OD1 | -5.79 | 113.09 | 118.30 |
| 1 | A | 556 | ASP | CB-CG-OD1 | -5.79 | 113.09 | 118.30 |
| 1 | D | 665 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 4 | 1 | 95 | ARG | CA-CB-CG | 5.79 | 126.13 | 113.40 |
| 4 | 9 | 95 | ARG | CA-CB-CG | 5.79 | 126.13 | 113.40 |
| 4 | X | 95 | ARG | CA-CB-CG | 5.79 | 126.13 | 113.40 |
| 1 | A | 339 | ASP | CB-CG-OD2 | 5.78 | 123.50 | 118.30 |
| 1 | J | 471 | ASP | CB-CG-OD1 | -5.78 | 113.09 | 118.30 |
| 4 | 1 | 254 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 4 | 5 | 335 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 4 | V | 79 | TRP | CG-CD2-CE3 | 5.78 | 139.11 | 133.90 |
| 4 | 2 | 335 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 1 | D | 809 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | J | 809 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 1 | M | 809 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 4 | 8 | 95 | ARG | CA-CB-CG | 5.78 | 126.11 | 113.40 |
| 4 | 4 | 335 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 1 | D | 752 | ASP | CB-CG-OD2 | 5.77 | 123.50 | 118.30 |
| 4 | 7 | 95 | ARG | CA-CB-CG | 5.77 | 126.10 | 113.40 |
| 4 | 6 | 95 | ARG | CA-CB-CG | 5.77 | 126.09 | 113.40 |
| 4 | Z | 95 | ARG | CA-CB-CG | 5.77 | 126.09 | 113.40 |
| 4 | Y | 95 | ARG | CA-CB-CG | 5.77 | 126.09 | 113.40 |
| 4 | V | 95 | ARG | CA-CB-CG | 5.76 | 126.08 | 113.40 |
| 4 | 9 | 335 | ARG | NE-CZ-NH2 | -5.76 | 117.42 | 120.30 |
| 4 | Z | 254 | ARG | NE-CZ-NH1 | 5.76 | 123.18 | 120.30 |
| 1 | D | 352 | TYR | N-CA-CB | 5.76 | 120.96 | 110.60 |
| 4 | 4 | 254 | ARG | NE-CZ-NH1 | 5.76 | 123.18 | 120.30 |
| 2 | B | 149 | ASP | N-CA-CB | 5.75 | 120.96 | 110.60 |
| 4 | 5 | 254 | ARG | NE-CZ-NH1 | 5.75 | 123.18 | 120.30 |
| 4 | Y | 254 | ARG | NE-CZ-NH1 | 5.75 | 123.18 | 120.30 |
| 1 | S | 4 | ASP | CB-CG-OD2 | 5.75 | 123.47 | 118.30 |
| 4 | 5 | 116 | ARG | NE-CZ-NH1 | 5.75 | 123.17 | 120.30 |
| 4 | 8 | 254 | ARG | NE-CZ-NH1 | 5.75 | 123.17 | 120.30 |
| 1 | A | 346 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | M | 165 | PHE | N-CA-CB | -5.75 | 100.26 | 110.60 |
| 4 | 5 | 95 | ARG | CA-CB-CG | 5.75 | 126.04 | 113.40 |
| 1 | G | 471 | ASP | CB-CG-OD1 | -5.74 | 113.13 | 118.30 |
| 4 | 2 | 116 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 1 | S | 780 | ASP | CB-CG-OD1 | -5.73 | 113.14 | 118.30 |
| 1 | A | 165 | PHE | N-CA-CB | -5.73 | 100.29 | 110.60 |
| 4 | Y | 335 | ARG | CA-CB-CG | 5.72 | 125.99 | 113.40 |
| 2 | H | 149 | ASP | N-CA-CB | 5.72 | 120.90 | 110.60 |
| 1 | J | 4 | ASP | CB-CG-OD2 | 5.72 | 123.45 | 118.30 |
| 2 | T | 149 | ASP | N-CA-CB | 5.72 | 120.89 | 110.60 |
| 4 | Z | 335 | ARG | CA-CB-CG | 5.71 | 125.97 | 113.40 |
| 4 | 1 | 116 | ARG | NE-CZ-NH1 | 5.71 | 123.16 | 120.30 |
| 4 | 5 | 335 | ARG | CA-CB-CG | 5.71 | 125.97 | 113.40 |
| 4 | 9 | 335 | ARG | CA-CB-CG | 5.71 | 125.97 | 113.40 |
| 1 | S | 165 | PHE | N-CA-CB | -5.71 | 100.32 | 110.60 |
| 1 | G | 4 | ASP | CB-CG-OD2 | 5.71 | 123.43 | 118.30 |
| 1 | D | 4 | ASP | CB-CG-OD2 | 5.70 | 123.43 | 118.30 |
| 1 | G | 165 | PHE | N-CA-CB | -5.70 | 100.33 | 110.60 |
| 1 | J | 165 | PHE | N-CA-CB | -5.70 | 100.33 | 110.60 |
| 1 | G | 815 | CYS | CA-CB-SG | -5.70 | 103.74 | 114.00 |
| 4 | 8 | 335 | ARG | CA-CB-CG | 5.70 | 125.94 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4 | 7 | 335 | ARG | CA-CB-CG | 5.70 | 125.94 | 113.40 |
| 1 | A | 4 | ASP | CB-CG-OD2 | 5.70 | 123.43 | 118.30 |
| 4 | 3 | 335 | ARG | CA-CB-CG | 5.70 | 125.93 | 113.40 |
| 1 | M | 780 | ASP | CB-CG-OD1 | -5.69 | 113.17 | 118.30 |
| 4 | 8 | 116 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 4 | 1 | 335 | ARG | CA-CB-CG | 5.69 | 125.92 | 113.40 |
| 4 | 6 | 335 | ARG | CA-CB-CG | 5.69 | 125.92 | 113.40 |
| 4 | X | 335 | ARG | CA-CB-CG | 5.69 | 125.92 | 113.40 |
| 1 | D | 165 | PHE | N-CA-CB | -5.69 | 100.36 | 110.60 |
| 4 | 2 | 254 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 4 | W | 335 | ARG | CA-CB-CG | 5.69 | 125.92 | 113.40 |
| 4 | 2 | 335 | ARG | CA-CB-CG | 5.69 | 125.92 | 113.40 |
| 4 | V | 335 | ARG | CA-CB-CG | 5.69 | 125.91 | 113.40 |
| 2 | E | 149 | ASP | N-CA-CB | 5.68 | 120.83 | 110.60 |
| 4 | 4 | 335 | ARG | CA-CB-CG | 5.68 | 125.91 | 113.40 |
| 4 | V | 254 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 4 | W | 254 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 1 | D | 780 | ASP | CB-CG-OD1 | -5.68 | 113.19 | 118.30 |
| 4 | 3 | 254 | ARG | NE-CZ-NH1 | 5.67 | 123.14 | 120.30 |
| 2 | N | 149 | ASP | N-CA-CB | 5.67 | 120.80 | 110.60 |
| 1 | M | 4 | ASP | CB-CG-OD2 | 5.66 | 123.40 | 118.30 |
| 4 | 5 | 279 | TYR | CB-CG-CD2 | -5.66 | 117.60 | 121.00 |
| 1 | G | 352 | TYR | N-CA-CB | 5.66 | 120.78 | 110.60 |
| 4 | Y | 335 | ARG | NE-CZ-NH2 | -5.65 | 117.47 | 120.30 |
| 4 | 6 | 254 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 |
| 1 | G | 693 | HIS | CA-CB-CG | -5.64 | 104.01 | 113.60 |
| 4 | Y | 116 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | G | 781 | ASP | CB-CG-OD2 | 5.63 | 123.37 | 118.30 |
| 1 | D | 781 | ASP | CB-CG-OD2 | 5.63 | 123.37 | 118.30 |
| 1 | G | 785 | GLU | O-C-N | 5.63 | 131.71 | 122.70 |
| 4 | 1 | 294 | TYR | CB-CG-CD2 | -5.63 | 117.62 | 121.00 |
| 1 | J | 352 | TYR | N-CA-CB | 5.62 | 120.72 | 110.60 |
| 1 | M | 352 | TYR | N-CA-CB | 5.62 | 120.72 | 110.60 |
| 1 | S | 693 | HIS | CA-CB-CG | -5.62 | 104.04 | 113.60 |
| 4 | 6 | 116 | ARG | NE-CZ-NH1 | 5.62 | 123.11 | 120.30 |
| 2 | K | 149 | ASP | N-CA-CB | 5.62 | 120.71 | 110.60 |
| 4 | 1 | 113 | LYS | CA-CB-CG | 5.61 | 125.74 | 113.40 |
| 4 | 9 | 113 | LYS | CA-CB-CG | 5.61 | 125.73 | 113.40 |
| 1 | A | 352 | TYR | N-CA-CB | 5.61 | 120.69 | 110.60 |
| 1 | S | 352 | TYR | N-CA-CB | 5.60 | 120.68 | 110.60 |
| 1 | J | 693 | HIS | CA-CB-CG | -5.60 | 104.08 | 113.60 |
| 1 | M | 686 | MET | N-CA-CB | -5.60 | 100.53 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 4 | 113 | LYS | CA-CB-CG | 5.59 | 125.71 | 113.40 |
| 4 | 8 | 356 | TRP | CG-CD2-CE3 | 5.59 | 138.94 | 133.90 |
| 4 | 8 | 294 | TYR | CB-CG-CD2 | -5.59 | 117.64 | 121.00 |
| 4 | W | 356 | TRP | CG-CD2-CE3 | 5.59 | 138.93 | 133.90 |
| 4 | 7 | 356 | TRP | CG-CD2-CE3 | 5.59 | 138.93 | 133.90 |
| 1 | M | 693 | HIS | CA-CB-CG | -5.59 | 104.10 | 113.60 |
| 4 | 7 | 11 | ASP | CB-CG-OD1 | 5.59 | 123.33 | 118.30 |
| 4 | Y | 113 | LYS | CA-CB-CG | 5.59 | 125.69 | 113.40 |
| 1 | D | 693 | HIS | CA-CB-CG | -5.58 | 104.11 | 113.60 |
| 4 | W | 113 | LYS | CA-CB-CG | 5.58 | 125.68 | 113.40 |
| 4 | 3 | 356 | TRP | CG-CD2-CE3 | 5.58 | 138.92 | 133.90 |
| 4 | Z | 113 | LYS | CA-CB-CG | 5.58 | 125.68 | 113.40 |
| 4 | 2 | 113 | LYS | CA-CB-CG | 5.58 | 125.67 | 113.40 |
| 4 | 6 | 113 | LYS | CA-CB-CG | 5.57 | 125.66 | 113.40 |
| 1 | A | 241 | ASP | CB-CG-OD2 | 5.57 | 123.31 | 118.30 |
| 4 | 5 | 294 | TYR | CB-CG-CD2 | -5.57 | 117.66 | 121.00 |
| 1 | J | 780 | ASP | CB-CG-OD1 | -5.57 | 113.29 | 118.30 |
| 4 | 3 | 113 | LYS | CA-CB-CG | 5.57 | 125.65 | 113.40 |
| 4 | 8 | 279 | TYR | CB-CG-CD2 | -5.57 | 117.66 | 121.00 |
| 4 | Y | 279 | TYR | CB-CG-CD2 | -5.57 | 117.66 | 121.00 |
| 1 | A | 752 | ASP | CB-CA-C | 5.57 | 121.53 | 110.40 |
| 4 | 3 | 254 | ARG | N-CA-CB | -5.57 | 100.58 | 110.60 |
| 4 | V | 113 | LYS | CA-CB-CG | 5.57 | 125.64 | 113.40 |
| 4 | 5 | 113 | LYS | CA-CB-CG | 5.56 | 125.64 | 113.40 |
| 4 | 7 | 113 | LYS | CA-CB-CG | 5.56 | 125.64 | 113.40 |
| 4 | 7 | 294 | TYR | CB-CG-CD2 | -5.56 | 117.66 | 121.00 |
| 1 | D | 384 | ASP | CB-CG-OD1 | -5.55 | 113.30 | 118.30 |
| 4 | 7 | 279 | TYR | CB-CG-CD2 | -5.55 | 117.67 | 121.00 |
| 1 | G | 320 | ILE | CB-CA-C | -5.55 | 100.50 | 111.60 |
| 4 | X | 113 | LYS | CA-CB-CG | 5.55 | 125.61 | 113.40 |
| 1 | M | 33 | ASP | CB-CG-OD2 | 5.55 | 123.29 | 118.30 |
| 1 | G | 686 | MET | N-CA-CB | -5.55 | 100.62 | 110.60 |
| 1 | J | 686 | MET | N-CA-CB | -5.55 | 100.62 | 110.60 |
| 4 | 5 | 254 | ARG | N-CA-CB | -5.55 | 100.62 | 110.60 |
| 1 | S | 686 | MET | N-CA-CB | -5.54 | 100.62 | 110.60 |
| 4 | V | 254 | ARG | N-CA-CB | -5.54 | 100.62 | 110.60 |
| 1 | D | 306 | THR | CA-CB-CG2 | -5.54 | 104.64 | 112.40 |
| 4 | 8 | 113 | LYS | CA-CB-CG | 5.54 | 125.59 | 113.40 |
| 4 | 6 | 254 | ARG | N-CA-CB | -5.54 | 100.63 | 110.60 |
| 4 | 2 | 356 | TRP | CG-CD2-CE3 | 5.54 | 138.88 | 133.90 |
| 4 | 1 | 356 | TRP | CG-CD2-CE3 | 5.54 | 138.88 | 133.90 |
| 4 | 6 | 279 | TYR | CB-CG-CD2 | -5.54 | 117.68 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 2 | 279 | TYR | CB-CG-CD2 | -5.53 | 117.68 | 121.00 |
| 4 | 8 | 254 | ARG | N-CA-CB | -5.53 | 100.64 | 110.60 |
| 4 | 4 | 279 | TYR | CB-CG-CD2 | -5.53 | 117.68 | 121.00 |
| 4 | 2 | 254 | ARG | N-CA-CB | -5.53 | 100.65 | 110.60 |
| 4 | 4 | 356 | TRP | CG-CD2-CE3 | 5.53 | 138.88 | 133.90 |
| 1 | D | 752 | ASP | CB-CA-C | 5.53 | 121.45 | 110.40 |
| 1 | A | 781 | ASP | CB-CG-OD2 | 5.53 | 123.27 | 118.30 |
| 4 | W | 279 | TYR | CB-CG-CD2 | -5.53 | 117.68 | 121.00 |
| 4 | 3 | 294 | TYR | CB-CG-CD2 | -5.52 | 117.69 | 121.00 |
| 4 | 9 | 254 | ARG | N-CA-CB | -5.52 | 100.66 | 110.60 |
| 4 | V | 294 | TYR | CB-CG-CD2 | -5.52 | 117.69 | 121.00 |
| 1 | J | 781 | ASP | CB-CG-OD2 | 5.52 | 123.27 | 118.30 |
| 1 | D | 686 | MET | N-CA-CB | -5.52 | 100.67 | 110.60 |
| 1 | A | 693 | HIS | CA-CB-CG | -5.52 | 104.22 | 113.60 |
| 4 | 5 | 356 | TRP | CG-CD2-CE3 | 5.52 | 138.86 | 133.90 |
| 4 | 9 | 294 | TYR | CB-CG-CD2 | -5.52 | 117.69 | 121.00 |
| 4 | Z | 254 | ARG | N-CA-CB | -5.52 | 100.67 | 110.60 |
| 1 | A | 686 | MET | N-CA-CB | -5.51 | 100.67 | 110.60 |
| 4 | 3 | 11 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 4 | 6 | 294 | TYR | CB-CG-CD2 | -5.51 | 117.69 | 121.00 |
| 4 | 8 | 11 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 1 | J | 752 | ASP | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 1 | M | 752 | ASP | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 4 | 7 | 254 | ARG | N-CA-CB | -5.51 | 100.68 | 110.60 |
| 4 | X | 254 | ARG | N-CA-CB | -5.51 | 100.68 | 110.60 |
| 4 | Z | 11 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 4 | 1 | 254 | ARG | N-CA-CB | -5.51 | 100.68 | 110.60 |
| 4 | 1 | 279 | TYR | CB-CG-CD2 | -5.51 | 117.69 | 121.00 |
| 1 | J | 547 | ASP | CB-CG-OD2 | 5.51 | 123.26 | 118.30 |
| 1 | S | 752 | ASP | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 4 | 9 | 356 | TRP | CG-CD2-CE3 | 5.51 | 138.86 | 133.90 |
| 1 | J | 33 | ASP | CB-CG-OD2 | 5.50 | 123.25 | 118.30 |
| 4 | 5 | 11 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 4 | W | 11 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 4 | 4 | 254 | ARG | N-CA-CB | -5.50 | 100.70 | 110.60 |
| 1 | D | 723 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | J | 320 | ILE | CB-CA-C | -5.50 | 100.60 | 111.60 |
| 4 | 6 | 356 | TRP | CG-CD2-CE3 | 5.50 | 138.85 | 133.90 |
| 1 | D | 33 | ASP | CB-CG-OD2 | 5.50 | 123.25 | 118.30 |
| 1 | G | 306 | THR | CA-CB-CG2 | -5.50 | 104.70 | 112.40 |
| 1 | M | 781 | ASP | CB-CG-OD2 | 5.50 | 123.25 | 118.30 |
| 4 | V | 279 | TYR | CB-CG-CD2 | -5.50 | 117.70 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | W | 254 | ARG | N-CA-CB | -5.49 | 100.71 | 110.60 |
| 1 | G | 752 | ASP | CB-CA-C | 5.49 | 121.38 | 110.40 |
| 4 | X | 356 | TRP | CG-CD2-CE3 | 5.49 | 138.84 | 133.90 |
| 1 | M | 320 | ILE | CB-CA-C | -5.49 | 100.62 | 111.60 |
| 4 | Z | 294 | TYR | CB-CG-CD2 | -5.49 | 117.71 | 121.00 |
| 1 | S | 320 | ILE | CB-CA-C | -5.49 | 100.63 | 111.60 |
| 1 | S | 781 | ASP | CB-CG-OD2 | 5.49 | 123.24 | 118.30 |
| 4 | 4 | 294 | TYR | CB-CG-CD2 | -5.49 | 117.71 | 121.00 |
| 4 | 4 | 11 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | D | 320 | ILE | CB-CA-C | -5.48 | 100.64 | 111.60 |
| 1 | M | 326 | ASP | CB-CG-OD2 | 5.48 | 123.23 | 118.30 |
| 1 | M | 723 | ARG | NE-CZ-NH1 | 5.48 | 123.04 | 120.30 |
| 4 | V | 356 | TRP | CG-CD2-CE3 | 5.48 | 138.83 | 133.90 |
| 4 | X | 11 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 4 | Y | 254 | ARG | N-CA-CB | -5.48 | 100.74 | 110.60 |
| 4 | X | 294 | TYR | CB-CG-CD2 | -5.47 | 117.72 | 121.00 |
| 4 | 4 | 79 | TRP | CB-CG-CD1 | -5.47 | 119.89 | 127.00 |
| 4 | Z | 356 | TRP | CG-CD2-CE3 | 5.47 | 138.82 | 133.90 |
| 4 | 3 | 279 | TYR | CB-CG-CD2 | -5.47 | 117.72 | 121.00 |
| 1 | J | 343 | PHE | CB-CG-CD2 | -5.47 | 116.97 | 120.80 |
| 1 | A | 306 | THR | CA-CB-CG2 | -5.47 | 104.75 | 112.40 |
| 4 | V | 147 | ARG | NE-CZ-NH2 | -5.47 | 117.57 | 120.30 |
| 4 | 9 | 11 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 4 | W | 294 | TYR | CB-CG-CD2 | -5.46 | 117.72 | 121.00 |
| 1 | S | 547 | ASP | CB-CG-OD2 | 5.46 | 123.21 | 118.30 |
| 4 | 2 | 294 | TYR | CB-CG-CD2 | -5.46 | 117.73 | 121.00 |
| 4 | V | 11 | ASP | CB-CG-OD1 | 5.46 | 123.21 | 118.30 |
| 4 | 8 | 356 | TRP | CB-CG-CD1 | -5.45 | 119.91 | 127.00 |
| 1 | J | 326 | ASP | CB-CG-OD2 | 5.45 | 123.21 | 118.30 |
| 1 | M | 343 | PHE | CB-CG-CD2 | -5.45 | 116.98 | 120.80 |
| 1 | G | 326 | ASP | CB-CG-OD2 | 5.45 | 123.20 | 118.30 |
| 4 | 6 | 79 | TRP | CB-CG-CD1 | -5.45 | 119.92 | 127.00 |
| 4 | Y | 294 | TYR | CB-CG-CD2 | -5.45 | 117.73 | 121.00 |
| 4 | 2 | 79 | TRP | CB-CG-CD1 | -5.45 | 119.92 | 127.00 |
| 4 | 1 | 11 | ASP | CB-CG-OD1 | 5.44 | 123.20 | 118.30 |
| 4 | Y | 11 | ASP | CB-CG-OD1 | 5.44 | 123.20 | 118.30 |
| 4 | 9 | 79 | TRP | CB-CG-CD1 | -5.44 | 119.93 | 127.00 |
| 4 | X | 356 | TRP | CB-CG-CD1 | -5.44 | 119.93 | 127.00 |
| 1 | A | 33 | ASP | CB-CG-OD2 | 5.44 | 123.19 | 118.30 |
| 1 | S | 33 | ASP | CB-CG-OD2 | 5.44 | 123.19 | 118.30 |
| 4 | 7 | 356 | TRP | CB-CG-CD1 | -5.44 | 119.93 | 127.00 |
| 4 | 9 | 356 | TRP | CB-CG-CD1 | -5.44 | 119.93 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | Z | 279 | TYR | CB-CG-CD2 | -5.44 | 117.74 | 121.00 |
| 4 | W | 79 | TRP | CB-CG-CD1 | -5.43 | 119.93 | 127.00 |
| 1 | A | 320 | ILE | CB-CA-C | -5.43 | 100.73 | 111.60 |
| 1 | J | 306 | THR | CA-CB-CG2 | -5.43 | 104.80 | 112.40 |
| 4 | 7 | 79 | TRP | CB-CG-CD1 | -5.43 | 119.94 | 127.00 |
| 1 | M | 218 | LEU | O-C-N | 5.43 | 131.38 | 122.70 |
| 1 | S | 326 | ASP | CB-CG-OD2 | 5.43 | 123.18 | 118.30 |
| 1 | D | 343 | PHE | CB-CG-CD2 | -5.42 | 117.00 | 120.80 |
| 4 | 1 | 356 | TRP | CB-CG-CD1 | -5.42 | 119.96 | 127.00 |
| 4 | 4 | 356 | TRP | CB-CG-CD1 | -5.41 | 119.96 | 127.00 |
| 1 | M | 306 | THR | CA-CB-CG2 | -5.41 | 104.83 | 112.40 |
| 4 | X | 279 | TYR | CB-CG-CD2 | -5.41 | 117.75 | 121.00 |
| 4 | 5 | 356 | TRP | CB-CG-CD1 | -5.41 | 119.97 | 127.00 |
| 1 | J | 384 | ASP | CB-CG-OD1 | -5.41 | 113.44 | 118.30 |
| 4 | 3 | 356 | TRP | CB-CG-CD1 | -5.41 | 119.97 | 127.00 |
| 1 | G | 723 | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 1 | M | 547 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 1 | S | 343 | PHE | CB-CG-CD2 | -5.40 | 117.02 | 120.80 |
| 4 | 2 | 356 | TRP | CB-CG-CD1 | -5.40 | 119.98 | 127.00 |
| 4 | 5 | 79 | TRP | CB-CG-CD1 | -5.40 | 119.98 | 127.00 |
| 4 | 6 | 356 | TRP | CB-CG-CD1 | -5.40 | 119.98 | 127.00 |
| 4 | X | 147 | ARG | NE-CZ-NH2 | -5.40 | 117.60 | 120.30 |
| 4 | Y | 356 | TRP | CB-CG-CD1 | -5.40 | 119.98 | 127.00 |
| 4 | Y | 356 | TRP | CG-CD2-CE3 | 5.40 | 138.76 | 133.90 |
| 1 | S | 306 | THR | CA-CB-CG2 | -5.40 | 104.84 | 112.40 |
| 1 | D | 547 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 1 | D | 326 | ASP | CB-CG-OD2 | 5.39 | 123.16 | 118.30 |
| 4 | V | 356 | TRP | CB-CG-CD1 | -5.39 | 119.99 | 127.00 |
| 1 | G | 241 | ASP | CB-CG-OD2 | 5.39 | 123.15 | 118.30 |
| 4 | 6 | 356 | TRP | CG-CD1-NE1 | -5.39 | 104.71 | 110.10 |
| 4 | X | 79 | TRP | CB-CG-CD1 | -5.39 | 119.99 | 127.00 |
| 4 | 1 | 147 | ARG | NE-CZ-NH2 | -5.39 | 117.61 | 120.30 |
| 4 | 8 | 147 | ARG | NE-CZ-NH2 | -5.39 | 117.61 | 120.30 |
| 4 | 9 | 356 | TRP | CG-CD1-NE1 | -5.38 | 104.72 | 110.10 |
| 1 | S | 384 | ASP | CB-CG-OD1 | -5.38 | 113.45 | 118.30 |
| 4 | 9 | 251 | GLY | CA-C-N | -5.38 | 105.36 | 117.20 |
| 4 | 2 | 147 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 4 | Z | 79 | TRP | CB-CG-CD1 | -5.38 | 120.01 | 127.00 |
| 4 | 1 | 79 | TRP | CB-CG-CD1 | -5.38 | 120.01 | 127.00 |
| 4 | 2 | 11 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 4 | 2 | 356 | TRP | CG-CD1-NE1 | -5.38 | 104.72 | 110.10 |
| 4 | Z | 356 | TRP | CB-CG-CD1 | -5.38 | 120.01 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | V | 79 | TRP | CB-CG-CD1 | -5.38 | 120.01 | 127.00 |
| 4 | Y | 79 | TRP | CB-CG-CD1 | -5.37 | 120.02 | 127.00 |
| 1 | G | 343 | PHE | CB-CG-CD2 | -5.37 | 117.04 | 120.80 |
| 1 | M | 241 | ASP | CB-CG-OD2 | 5.37 | 123.13 | 118.30 |
| 1 | S | 723 | ARG | NE-CZ-NH1 | 5.37 | 122.99 | 120.30 |
| 4 | W | 356 | TRP | CB-CG-CD1 | -5.37 | 120.02 | 127.00 |
| 4 | 5 | 356 | TRP | CG-CD1-NE1 | -5.37 | 104.73 | 110.10 |
| 4 | 9 | 279 | TYR | CB-CG-CD2 | -5.37 | 117.78 | 121.00 |
| 4 | X | 356 | TRP | CG-CD1-NE1 | -5.37 | 104.73 | 110.10 |
| 4 | Y | 356 | TRP | CG-CD1-NE1 | -5.37 | 104.73 | 110.10 |
| 4 | 8 | 335 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 2 | K | 136 | MET | CG-SD-CE | 5.36 | 108.78 | 100.20 |
| 4 | 3 | 79 | TRP | CB-CG-CD1 | -5.36 | 120.03 | 127.00 |
| 1 | G | 686 | MET | CG-SD-CE | -5.36 | 91.62 | 100.20 |
| 1 | M | 800 | ARG | NH1-CZ-NH2 | 5.36 | 125.30 | 119.40 |
| 4 | 3 | 251 | GLY | CA-C-N | -5.36 | 105.42 | 117.20 |
| 4 | 8 | 79 | TRP | CB-CG-CD1 | -5.36 | 120.04 | 127.00 |
| 4 | 8 | 356 | TRP | CG-CD1-NE1 | -5.36 | 104.74 | 110.10 |
| 4 | Y | 62 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 1 | G | 555 | TYR | CB-CG-CD1 | 5.36 | 124.21 | 121.00 |
| 4 | 7 | 356 | TRP | CG-CD1-NE1 | -5.36 | 104.74 | 110.10 |
| 4 | Y | 251 | GLY | CA-C-N | -5.36 | 105.42 | 117.20 |
| 1 | A | 686 | MET | CG-SD-CE | -5.35 | 91.63 | 100.20 |
| 1 | A | 326 | ASP | CB-CG-OD2 | 5.35 | 123.12 | 118.30 |
| 2 | B | 136 | MET | CG-SD-CE | 5.35 | 108.76 | 100.20 |
| 1 | J | 723 | ARG | NE-CZ-NH1 | 5.35 | 122.98 | 120.30 |
| 4 | 1 | 251 | GLY | CA-C-N | -5.35 | 105.43 | 117.20 |
| 1 | A | 384 | ASP | CB-CG-OD1 | -5.35 | 113.48 | 118.30 |
| 1 | D | 800 | ARG | NH1-CZ-NH2 | 5.35 | 125.28 | 119.40 |
| 1 | J | 170 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 4 | 1 | 335 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 1 | G | 601 | ASP | CB-CG-OD2 | 5.35 | 123.11 | 118.30 |
| 1 | J | 686 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 |
| 2 | T | 136 | MET | CG-SD-CE | 5.35 | 108.75 | 100.20 |
| 1 | J | 218 | LEU | O-C-N | 5.34 | 131.25 | 122.70 |
| 4 | 6 | 251 | GLY | CA-C-N | -5.34 | 105.44 | 117.20 |
| 4 | W | 251 | GLY | CA-C-N | -5.34 | 105.44 | 117.20 |
| 2 | N | 136 | MET | CG-SD-CE | 5.34 | 108.75 | 100.20 |
| 1 | S | 218 | LEU | O-C-N | 5.34 | 131.25 | 122.70 |
| 4 | 5 | 251 | GLY | CA-C-N | -5.34 | 105.45 | 117.20 |
| 1 | A | 343 | PHE | CB-CG-CD2 | -5.34 | 117.06 | 120.80 |
| 4 | 8 | 251 | GLY | CA-C-N | -5.34 | 105.45 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | V | 251 | GLY | CA-C-N | -5.34 | 105.45 | 117.20 |
| 4 | 2 | 251 | GLY | CA-C-N | -5.34 | 105.46 | 117.20 |
| 4 | 6 | 11 | ASP | CB-CG-OD1 | 5.34 | 123.10 | 118.30 |
| 4 | Z | 176 | MET | CG-SD-CE | 5.34 | 108.74 | 100.20 |
| 1 | M | 686 | MET | CG-SD-CE | -5.33 | 91.67 | 100.20 |
| 1 | A | 723 | ARG | NE-CZ-NH1 | 5.33 | 122.97 | 120.30 |
| 1 | G | 125 | THR | CA-CB-CG2 | -5.33 | 104.93 | 112.40 |
| 1 | S | 241 | ASP | CB-CG-OD2 | 5.33 | 123.10 | 118.30 |
| 4 | X | 251 | GLY | CA-C-N | -5.33 | 105.47 | 117.20 |
| 1 | D | 241 | ASP | CB-CG-OD2 | 5.33 | 123.10 | 118.30 |
| 1 | D | 601 | ASP | CB-CG-OD2 | 5.33 | 123.10 | 118.30 |
| 4 | 5 | 147 | ARG | NE-CZ-NH2 | -5.33 | 117.64 | 120.30 |
| 4 | V | 356 | TRP | CG-CD1-NE1 | -5.33 | 104.77 | 110.10 |
| 1 | S | 686 | MET | CG-SD-CE | -5.33 | 91.67 | 100.20 |
| 4 | 1 | 356 | TRP | CG-CD1-NE1 | -5.33 | 104.77 | 110.10 |
| 4 | 3 | 147 | ARG | NE-CZ-NH2 | -5.33 | 117.64 | 120.30 |
| 4 | 4 | 356 | TRP | CG-CD1-NE1 | -5.33 | 104.77 | 110.10 |
| 4 | V | 335 | ARG | NE-CZ-NH1 | 5.33 | 122.97 | 120.30 |
| 4 | 7 | 251 | GLY | CA-C-N | -5.33 | 105.48 | 117.20 |
| 4 | X | 176 | MET | CG-SD-CE | 5.33 | 108.72 | 100.20 |
| 4 | 7 | 176 | MET | CG-SD-CE | 5.33 | 108.72 | 100.20 |
| 4 | 4 | 251 | GLY | CA-C-N | -5.32 | 105.49 | 117.20 |
| 4 | W | 356 | TRP | CG-CD1-NE1 | -5.32 | 104.78 | 110.10 |
| 4 | Z | 251 | GLY | CA-C-N | -5.32 | 105.50 | 117.20 |
| 4 | 8 | 176 | MET | CG-SD-CE | 5.32 | 108.71 | 100.20 |
| 1 | J | 241 | ASP | CB-CG-OD2 | 5.32 | 123.09 | 118.30 |
| 4 | 9 | 147 | ARG | NE-CZ-NH2 | -5.31 | 117.64 | 120.30 |
| 4 | W | 176 | MET | CG-SD-CE | 5.31 | 108.70 | 100.20 |
| 1 | D | 354 | LEU | CB-CG-CD2 | -5.31 | 101.97 | 111.00 |
| 4 | Y | 176 | MET | CG-SD-CE | 5.31 | 108.69 | 100.20 |
| 2 | H | 136 | MET | CG-SD-CE | 5.31 | 108.69 | 100.20 |
| 4 | V | 176 | MET | CG-SD-CE | 5.31 | 108.69 | 100.20 |
| 1 | G | 354 | LEU | CB-CG-CD2 | -5.31 | 101.98 | 111.00 |
| 4 | 3 | 356 | TRP | CG-CD1-NE1 | -5.30 | 104.80 | 110.10 |
| 4 | 4 | 337 | TYR | CB-CG-CD1 | -5.30 | 117.82 | 121.00 |
| 1 | D | 686 | MET | CG-SD-CE | -5.30 | 91.72 | 100.20 |
| 1 | J | 800 | ARG | NH1-CZ-NH2 | 5.30 | 125.23 | 119.40 |
| 4 | 4 | 176 | MET | CG-SD-CE | 5.30 | 108.68 | 100.20 |
| 1 | A | 601 | ASP | CB-CG-OD2 | 5.30 | 123.07 | 118.30 |
| 4 | Z | 147 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 1 | J | 601 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 1 | G | 33 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | G | 384 | ASP | CB-CG-OD1 | -5.29 | 113.54 | 118.30 |
| 1 | G | 218 | LEU | O-C-N | 5.29 | 131.16 | 122.70 |
| 2 | E | 136 | MET | CG-SD-CE | 5.28 | 108.65 | 100.20 |
| 1 | M | 384 | ASP | CB-CG-OD1 | -5.28 | 113.55 | 118.30 |
| 4 | 5 | 176 | MET | CG-SD-CE | 5.28 | 108.65 | 100.20 |
| 1 | A | 218 | LEU | O-C-N | 5.28 | 131.15 | 122.70 |
| 1 | D | 125 | THR | CA-CB-CG2 | -5.28 | 105.01 | 112.40 |
| 4 | 2 | 176 | MET | CG-SD-CE | 5.28 | 108.65 | 100.20 |
| 4 | 1 | 176 | MET | CG-SD-CE | 5.28 | 108.64 | 100.20 |
| 4 | 6 | 176 | MET | CG-SD-CE | 5.28 | 108.64 | 100.20 |
| 1 | A | 354 | LEU | CB-CG-CD2 | -5.28 | 102.03 | 111.00 |
| 1 | M | 601 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 1 | S | 660 | LEU | CB-CG-CD2 | 5.28 | 119.97 | 111.00 |
| 1 | S | 800 | ARG | NH1-CZ-NH2 | 5.27 | 125.20 | 119.40 |
| 4 | 7 | 147 | ARG | NE-CZ-NH2 | -5.27 | 117.66 | 120.30 |
| 1 | G | 660 | LEU | CB-CG-CD2 | 5.27 | 119.96 | 111.00 |
| 4 | 3 | 176 | MET | CG-SD-CE | 5.27 | 108.63 | 100.20 |
| 1 | S | 125 | THR | CA-CB-CG2 | -5.27 | 105.03 | 112.40 |
| 4 | 9 | 176 | MET | CG-SD-CE | 5.27 | 108.63 | 100.20 |
| 4 | Z | 62 | ARG | NE-CZ-NH1 | 5.27 | 122.93 | 120.30 |
| 1 | A | 547 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 1 | A | 125 | THR | CA-CB-CG2 | -5.26 | 105.03 | 112.40 |
| 1 | D | 660 | LEU | CB-CG-CD2 | 5.26 | 119.94 | 111.00 |
| 1 | M | 125 | THR | CA-CB-CG2 | -5.26 | 105.03 | 112.40 |
| 4 | W | 335 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 1 | J | 4 | ASP | CB-CG-OD1 | -5.26 | 113.57 | 118.30 |
| 1 | M | 660 | LEU | CB-CG-CD2 | 5.26 | 119.94 | 111.00 |
| 1 | M | 346 | ASP | N-CA-CB | -5.26 | 101.14 | 110.60 |
| 4 | 4 | 335 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 4 | Z | 356 | TRP | CG-CD1-NE1 | -5.25 | 104.85 | 110.10 |
| 1 | A | 660 | LEU | CB-CG-CD2 | 5.25 | 119.92 | 111.00 |
| 1 | J | 125 | THR | CA-CB-CG2 | -5.25 | 105.05 | 112.40 |
| 1 | J | 660 | LEU | CB-CG-CD2 | 5.25 | 119.92 | 111.00 |
| 4 | 6 | 91 | TYR | CB-CG-CD2 | -5.25 | 117.85 | 121.00 |
| 4 | W | 337 | TYR | CB-CG-CD1 | -5.25 | 117.85 | 121.00 |
| 4 | 1 | 337 | TYR | CB-CG-CD1 | -5.24 | 117.86 | 121.00 |
| 1 | A | 760 | PHE | CB-CG-CD1 | 5.24 | 124.47 | 120.80 |
| 1 | J | 354 | LEU | CB-CG-CD2 | -5.24 | 102.09 | 111.00 |
| 1 | G | 547 | ASP | CB-CG-OD2 | 5.24 | 123.01 | 118.30 |
| 1 | S | 601 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 1 | M | 354 | LEU | CB-CG-CD2 | -5.23 | 102.11 | 111.00 |
| 1 | D | 760 | PHE | CB-CG-CD1 | 5.23 | 124.46 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | J | 760 | PHE | CB-CG-CD1 | 5.23 | 124.46 | 120.80 |
| 1 | S | 346 | ASP | N-CA-CB | -5.22 | 101.20 | 110.60 |
| 4 | V | 62 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | S | 170 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 4 | 5 | 335 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 4 | 7 | 62 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | A | 346 | ASP | N-CA-CB | -5.22 | 101.20 | 110.60 |
| 1 | S | 354 | LEU | CB-CG-CD2 | -5.22 | 102.13 | 111.00 |
| 4 | 5 | 337 | TYR | CB-CG-CD1 | -5.22 | 117.87 | 121.00 |
| 4 | 6 | 335 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | M | 555 | TYR | CB-CG-CD1 | 5.22 | 124.13 | 121.00 |
| 1 | G | 800 | ARG | NH1-CZ-NH2 | 5.22 | 125.14 | 119.40 |
| 4 | 9 | 335 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 4 | 1 | 53 | TYR | CB-CG-CD1 | -5.21 | 117.87 | 121.00 |
| 4 | Z | 91 | TYR | CB-CG-CD2 | -5.21 | 117.87 | 121.00 |
| 1 | G | 4 | ASP | CB-CG-OD1 | -5.20 | 113.62 | 118.30 |
| 1 | D | 346 | ASP | N-CA-CB | -5.20 | 101.24 | 110.60 |
| 1 | S | 4 | ASP | CB-CG-OD1 | -5.20 | 113.62 | 118.30 |
| 4 | X | 91 | TYR | CB-CG-CD2 | -5.19 | 117.88 | 121.00 |
| 1 | D | 170 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 1 | M | 160 | ASP | CB-CG-OD2 | -5.19 | 113.63 | 118.30 |
| 4 | W | 147 | ARG | NE-CZ-NH2 | -5.19 | 117.70 | 120.30 |
| 4 | X | 335 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 4 | Z | 335 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 1 | D | 4 | ASP | CB-CG-OD1 | -5.19 | 113.63 | 118.30 |
| 1 | M | 4 | ASP | CB-CG-OD1 | -5.19 | 113.63 | 118.30 |
| 1 | J | 346 | ASP | N-CA-CB | -5.19 | 101.26 | 110.60 |
| 4 | W | 62 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 1 | A | 90 | ASP | CB-CG-OD1 | -5.19 | 113.63 | 118.30 |
| 1 | D | 218 | LEU | O-C-N | 5.18 | 130.99 | 122.70 |
| 4 | 4 | 147 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |
| 4 | 6 | 147 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |
| 1 | A | 800 | ARG | NH1-CZ-NH2 | 5.18 | 125.10 | 119.40 |
| 4 | 4 | 290 | ARG | CA-C-N | 5.18 | 128.60 | 117.20 |
| 4 | 7 | 290 | ARG | CA-C-N | 5.18 | 128.59 | 117.20 |
| 4 | Y | 147 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |
| 1 | S | 555 | TYR | CB-CG-CD1 | 5.18 | 124.11 | 121.00 |
| 4 | 8 | 62 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 1 | S | 760 | PHE | CB-CG-CD1 | 5.17 | 124.42 | 120.80 |
| 4 | Y | 290 | ARG | CA-C-N | 5.17 | 128.58 | 117.20 |
| 4 | 7 | 337 | TYR | CB-CG-CD1 | -5.17 | 117.90 | 121.00 |
| 1 | A | 555 | TYR | CB-CG-CD1 | 5.17 | 124.10 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 1 | 290 | ARG | CA-C-N | 5.17 | 128.57 | 117.20 |
| 4 | W | 290 | ARG | CA-C-N | 5.17 | 128.57 | 117.20 |
| 4 | 3 | 62 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 1 | G | 170 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 1 | M | 170 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 4 | 3 | 335 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 4 | Z | 290 | ARG | CA-C-N | 5.16 | 128.55 | 117.20 |
| 4 | 8 | 290 | ARG | CA-C-N | 5.16 | 128.54 | 117.20 |
| 4 | X | 290 | ARG | CA-C-N | 5.15 | 128.54 | 117.20 |
| 1 | A | 160 | ASP | CB-CG-OD2 | -5.15 | 113.66 | 118.30 |
| 4 | 2 | 335 | ARG | NE-CZ-NH1 | 5.15 | 122.88 | 120.30 |
| 4 | V | 290 | ARG | CA-C-N | 5.15 | 128.54 | 117.20 |
| 4 | X | 337 | TYR | CB-CG-CD1 | -5.15 | 117.91 | 121.00 |
| 4 | 3 | 290 | ARG | CA-C-N | 5.15 | 128.53 | 117.20 |
| 4 | 3 | 337 | TYR | CB-CG-CD1 | -5.15 | 117.91 | 121.00 |
| 4 | Y | 337 | TYR | CB-CG-CD1 | -5.15 | 117.91 | 121.00 |
| 4 | 6 | 290 | ARG | CA-C-N | 5.14 | 128.50 | 117.20 |
| 4 | 6 | 337 | TYR | CB-CG-CD1 | -5.13 | 117.92 | 121.00 |
| 4 | 9 | 290 | ARG | CA-C-N | 5.13 | 128.49 | 117.20 |
| 4 | 9 | 337 | TYR | CB-CG-CD1 | -5.13 | 117.92 | 121.00 |
| 1 | G | 346 | ASP | N-CA-CB | -5.13 | 101.37 | 110.60 |
| 4 | 2 | 290 | ARG | CA-C-N | 5.13 | 128.48 | 117.20 |
| 1 | D | 82 | PRO | N-CA-CB | 5.12 | 109.45 | 103.30 |
| 1 | S | 301 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 4 | 8 | 53 | TYR | CB-CG-CD1 | -5.12 | 117.92 | 121.00 |
| 4 | 8 | 337 | TYR | CB-CG-CD1 | -5.12 | 117.92 | 121.00 |
| 1 | G | 709 | LYS | O-C-N | 5.12 | 131.91 | 123.20 |
| 4 | 2 | 86 | TRP | CG-CD1-NE1 | -5.12 | 104.98 | 110.10 |
| 4 | 5 | 62 | ARG | CA-CB-CG | 5.12 | 124.67 | 113.40 |
| 4 | 5 | 290 | ARG | CA-C-N | 5.12 | 128.47 | 117.20 |
| 4 | 7 | 91 | TYR | CB-CG-CD2 | -5.12 | 117.93 | 121.00 |
| 1 | M | 82 | PRO | N-CA-CB | 5.12 | 109.44 | 103.30 |
| 1 | D | 576 | GLU | CA-CB-CG | -5.12 | 102.15 | 113.40 |
| 1 | G | 576 | GLU | CA-CB-CG | -5.12 | 102.15 | 113.40 |
| 4 | 9 | 53 | TYR | CB-CG-CD1 | -5.12 | 117.93 | 121.00 |
| 1 | J | 628 | GLY | O-C-N | -5.11 | 114.52 | 122.70 |
| 4 | 1 | 91 | TYR | CB-CG-CD2 | -5.11 | 117.93 | 121.00 |
| 4 | 3 | 91 | TYR | CB-CG-CD2 | -5.11 | 117.93 | 121.00 |
| 1 | S | 628 | GLY | O-C-N | -5.11 | 114.52 | 122.70 |
| 4 | 2 | 62 | ARG | CA-CB-CG | 5.11 | 124.64 | 113.40 |
| 4 | 1 | 62 | ARG | NE-CZ-NH1 | 5.11 | 122.86 | 120.30 |
| 1 | A | 4 | ASP | CB-CG-OD1 | -5.11 | 113.70 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | M | 760 | PHE | CB-CG-CD1 | 5.11 | 124.37 | 120.80 |
| 4 | Y | 91 | TYR | CB-CG-CD2 | -5.11 | 117.94 | 121.00 |
| 1 | M | 218 | LEU | CA-CB-CG | 5.10 | 127.04 | 115.30 |
| 4 | Y | 53 | TYR | CB-CG-CD1 | -5.10 | 117.94 | 121.00 |
| 4 | Z | 53 | TYR | CB-CG-CD1 | -5.10 | 117.94 | 121.00 |
| 4 | 6 | 62 | ARG | CA-CB-CG | 5.10 | 124.62 | 113.40 |
| 4 | 7 | 62 | ARG | CA-CB-CG | 5.10 | 124.62 | 113.40 |
| 4 | 2 | 91 | TYR | CB-CG-CD2 | -5.10 | 117.94 | 121.00 |
| 4 | 3 | 62 | ARG | CA-CB-CG | 5.10 | 124.62 | 113.40 |
| 4 | 5 | 62 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 4 | 9 | 62 | ARG | CA-CB-CG | 5.10 | 124.62 | 113.40 |
| 1 | D | 218 | LEU | CA-CB-CG | 5.10 | 127.02 | 115.30 |
| 1 | D | 628 | GLY | O-C-N | -5.10 | 114.55 | 122.70 |
| 1 | J | 555 | TYR | CB-CG-CD1 | 5.10 | 124.06 | 121.00 |
| 1 | J | 576 | GLU | CA-CB-CG | -5.10 | 102.19 | 113.40 |
| 4 | W | 62 | ARG | CA-CB-CG | 5.10 | 124.61 | 113.40 |
| 1 | G | 90 | ASP | CB-CG-OD1 | -5.09 | 113.72 | 118.30 |
| 4 | 6 | 53 | TYR | CB-CG-CD1 | -5.09 | 117.94 | 121.00 |
| 1 | A | 576 | GLU | CA-CB-CG | -5.09 | 102.20 | 113.40 |
| 4 | V | 62 | ARG | CA-CB-CG | 5.09 | 124.60 | 113.40 |
| 4 | Y | 62 | ARG | CA-CB-CG | 5.09 | 124.60 | 113.40 |
| 4 | Z | 62 | ARG | CA-CB-CG | 5.09 | 124.60 | 113.40 |
| 1 | A | 218 | LEU | CA-CB-CG | 5.09 | 127.00 | 115.30 |
| 1 | J | 82 | PRO | N-CA-CB | 5.09 | 109.41 | 103.30 |
| 4 | 6 | 62 | ARG | NE-CZ-NH1 | 5.09 | 122.84 | 120.30 |
| 4 | 7 | 335 | ARG | NE-CZ-NH1 | 5.09 | 122.84 | 120.30 |
| 1 | M | 576 | GLU | CA-CB-CG | -5.08 | 102.22 | 113.40 |
| 1 | S | 218 | LEU | CA-CB-CG | 5.08 | 126.99 | 115.30 |
| 4 | V | 91 | TYR | CB-CG-CD2 | -5.08 | 117.95 | 121.00 |
| 1 | A | 621 | LEU | CA-CB-CG | -5.08 | 103.61 | 115.30 |
| 4 | 4 | 62 | ARG | CA-CB-CG | 5.08 | 124.58 | 113.40 |
| 4 | 8 | 62 | ARG | CA-CB-CG | 5.08 | 124.58 | 113.40 |
| 1 | M | 463 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 1 | J | 160 | ASP | CB-CG-OD2 | -5.08 | 113.73 | 118.30 |
| 1 | M | 628 | GLY | O-C-N | -5.08 | 114.57 | 122.70 |
| 1 | S | 82 | PRO | N-CA-CB | 5.08 | 109.39 | 103.30 |
| 1 | S | 576 | GLU | CA-CB-CG | -5.08 | 102.24 | 113.40 |
| 4 | V | 53 | TYR | CB-CG-CD1 | -5.08 | 117.95 | 121.00 |
| 4 | 4 | 191 | LYS | CA-C-N | 5.07 | 128.36 | 117.20 |
| 4 | 9 | 191 | LYS | CA-C-N | 5.07 | 128.36 | 117.20 |
| 4 | V | 337 | TYR | CB-CG-CD1 | -5.07 | 117.96 | 121.00 |
| 4 | Z | 191 | LYS | CA-C-N | 5.07 | 128.36 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | J | 218 | LEU | CA-CB-CG | 5.07 | 126.96 | 115.30 |
| 4 | 1 | 62 | ARG | CA-CB-CG | 5.07 | 124.55 | 113.40 |
| 4 | W | 191 | LYS | CA-C-N | 5.07 | 128.36 | 117.20 |
| 4 | X | 86 | TRP | CG-CD1-NE1 | -5.07 | 105.03 | 110.10 |
| 4 | 8 | 91 | TYR | CB-CG-CD2 | -5.07 | 117.96 | 121.00 |
| 1 | A | 235 | ALA | N-CA-CB | -5.07 | 103.00 | 110.10 |
| 4 | 2 | 191 | LYS | CA-C-N | 5.07 | 128.35 | 117.20 |
| 4 | 6 | 86 | TRP | CG-CD1-NE1 | -5.07 | 105.03 | 110.10 |
| 4 | 5 | 53 | TYR | CB-CG-CD1 | -5.07 | 117.96 | 121.00 |
| 4 | Y | 335 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 1 | G | 760 | PHE | CB-CG-CD1 | 5.06 | 124.34 | 120.80 |
| 4 | X | 62 | ARG | CA-CB-CG | 5.06 | 124.54 | 113.40 |
| 4 | 5 | 191 | LYS | CA-C-N | 5.06 | 128.34 | 117.20 |
| 4 | X | 191 | LYS | CA-C-N | 5.06 | 128.33 | 117.20 |
| 1 | G | 621 | LEU | CA-CB-CG | -5.06 | 103.66 | 115.30 |
| 4 | 1 | 191 | LYS | CA-C-N | 5.06 | 128.33 | 117.20 |
| 4 | 8 | 191 | LYS | CA-C-N | 5.06 | 128.33 | 117.20 |
| 4 | V | 191 | LYS | CA-C-N | 5.06 | 128.33 | 117.20 |
| 1 | M | 301 | ASP | CB-CG-OD2 | 5.06 | 122.85 | 118.30 |
| 4 | 9 | 86 | TRP | CG-CD1-NE1 | -5.06 | 105.04 | 110.10 |
| 1 | M | 621 | LEU | CA-CB-CG | -5.05 | 103.67 | 115.30 |
| 4 | 2 | 62 | ARG | NE-CZ-NH1 | 5.05 | 122.83 | 120.30 |
| 4 | 3 | 86 | TRP | CG-CD1-NE1 | -5.05 | 105.05 | 110.10 |
| 4 | 7 | 191 | LYS | CA-C-N | 5.05 | 128.32 | 117.20 |
| 1 | J | 90 | ASP | CB-CG-OD1 | -5.05 | 113.75 | 118.30 |
| 1 | D | 621 | LEU | CA-CB-CG | -5.05 | 103.69 | 115.30 |
| 4 | 4 | 91 | TYR | CB-CG-CD2 | -5.05 | 117.97 | 121.00 |
| 1 | A | 463 | ASP | CB-CG-OD1 | 5.05 | 122.84 | 118.30 |
| 1 | G | 160 | ASP | CB-CG-OD2 | -5.05 | 113.76 | 118.30 |
| 1 | J | 301 | ASP | CB-CG-OD2 | 5.05 | 122.84 | 118.30 |
| 4 | 3 | 191 | LYS | CA-C-N | 5.05 | 128.30 | 117.20 |
| 4 | 5 | 91 | TYR | CB-CG-CD2 | -5.05 | 117.97 | 121.00 |
| 4 | 6 | 191 | LYS | CA-C-N | 5.05 | 128.30 | 117.20 |
| 1 | A | 82 | PRO | N-CA-CB | 5.04 | 109.35 | 103.30 |
| 4 | X | 53 | TYR | CB-CG-CD1 | -5.04 | 117.97 | 121.00 |
| 1 | G | 628 | GLY | O-C-N | -5.04 | 114.63 | 122.70 |
| 1 | J | 621 | LEU | CA-CB-CG | -5.04 | 103.70 | 115.30 |
| 4 | 8 | 86 | TRP | CG-CD1-NE1 | -5.04 | 105.06 | 110.10 |
| 1 | S | 621 | LEU | CA-CB-CG | -5.04 | 103.72 | 115.30 |
| 4 | 3 | 53 | TYR | CB-CG-CD1 | -5.04 | 117.98 | 121.00 |
| 4 | 4 | 53 | TYR | CB-CG-CD1 | -5.04 | 117.98 | 121.00 |
| 4 | W | 91 | TYR | CB-CG-CD2 | -5.03 | 117.98 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | Y | 86 | TRP | CG-CD1-NE1 | -5.03 | 105.07 | 110.10 |
| 4 | Y | 191 | LYS | CA-C-N | 5.03 | 128.28 | 117.20 |
| 4 | 2 | 53 | TYR | CB-CG-CD1 | -5.03 | 117.98 | 121.00 |
| 1 | G | 218 | LEU | CA-CB-CG | 5.03 | 126.87 | 115.30 |
| 1 | S | 235 | ALA | N-CA-CB | -5.03 | 103.06 | 110.10 |
| 1 | A | 739 | ASP | CA-CB-CG | -5.03 | 102.34 | 113.40 |
| 1 | D | 739 | ASP | N-CA-CB | 5.03 | 119.65 | 110.60 |
| 1 | D | 301 | ASP | CB-CG-OD2 | 5.03 | 122.82 | 118.30 |
| 1 | J | 739 | ASP | N-CA-CB | 5.03 | 119.64 | 110.60 |
| 4 | 2 | 337 | TYR | CB-CG-CD1 | -5.02 | 117.98 | 121.00 |
| 1 | D | 160 | ASP | CB-CG-OD2 | -5.02 | 113.78 | 118.30 |
| 1 | D | 555 | TYR | CB-CG-CD1 | 5.02 | 124.01 | 121.00 |
| 1 | M | 90 | ASP | CB-CG-OD1 | -5.02 | 113.78 | 118.30 |
| 1 | S | 160 | ASP | CB-CG-OD2 | -5.02 | 113.78 | 118.30 |
| 1 | G | 739 | ASP | N-CA-CB | 5.02 | 119.63 | 110.60 |
| 1 | A | 628 | GLY | O-C-N | -5.01 | 114.69 | 122.70 |
| 4 | X | 62 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |
| 4 | 7 | 53 | TYR | CB-CG-CD1 | -5.00 | 118.00 | 121.00 |
| 4 | W | 53 | TYR | CB-CG-CD1 | -5.00 | 118.00 | 121.00 |

All (6) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 648 | THR | CB |
| 1 | D | 648 | THR | CB |
| 1 | G | 648 | THR | CB |
| 1 | J | 648 | THR | CB |
| 1 | M | 648 | THR | CB |
| 1 | S | 648 | THR | CB |

All (77) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 4 | 1 | 62 | ARG | Sidechain |
| 4 | 2 | 62 | ARG | Sidechain |
| 4 | 3 | 62 | ARG | Sidechain |
| 4 | 4 | 62 | ARG | Sidechain |
| 4 | 5 | 62 | ARG | Sidechain |
| 4 | 6 | 62 | ARG | Sidechain |
| 4 | 7 | 62 | ARG | Sidechain |
| 4 | 8 | 62 | ARG | Sidechain |
| 4 | 9 | 62 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 623 | PHE | Sidechain |
| 1 | A | 637 | LYS | Mainchain |
| 1 | A | 649 | VAL | Mainchain |
| 1 | A | 98 | HIS | Mainchain |
| 2 | B | 150 | TYR | Sidechain |
| 2 | B | 155 | TYR | Mainchain |
| 2 | B | 22 | THR | Mainchain |
| 3 | C | 75 | ALA | Mainchain |
| 3 | C | 85 | GLU | Mainchain |
| 1 | D | 623 | PHE | Sidechain |
| 1 | D | 637 | LYS | Mainchain |
| 1 | D | 649 | VAL | Mainchain |
| 1 | D | 98 | HIS | Mainchain |
| 2 | E | 150 | TYR | Sidechain |
| 2 | E | 155 | TYR | Mainchain |
| 2 | E | 22 | THR | Mainchain |
| 3 | F | 75 | ALA | Mainchain |
| 3 | F | 85 | GLU | Mainchain |
| 1 | G | 623 | PHE | Sidechain |
| 1 | G | 637 | LYS | Mainchain |
| 1 | G | 649 | VAL | Mainchain |
| 1 | G | 709 | LYS | Mainchain |
| 1 | G | 98 | HIS | Mainchain |
| 2 | H | 150 | TYR | Sidechain |
| 2 | H | 155 | TYR | Mainchain |
| 2 | H | 22 | THR | Mainchain |
| 3 | I | 75 | ALA | Mainchain |
| 3 | I | 85 | GLU | Mainchain |
| 1 | J | 623 | PHE | Sidechain |
| 1 | J | 637 | LYS | Mainchain |
| 1 | J | 649 | VAL | Mainchain |
| 1 | J | 709 | LYS | Mainchain,Peptide |
| 1 | J | 98 | HIS | Mainchain |
| 2 | K | 150 | TYR | Sidechain |
| 2 | K | 155 | TYR | Mainchain |
| 2 | K | 22 | THR | Mainchain |
| 3 | L | 75 | ALA | Mainchain |
| 3 | L | 85 | GLU | Mainchain |
| 1 | M | 623 | PHE | Sidechain |
| 1 | M | 637 | LYS | Mainchain |
| 1 | M | 649 | VAL | Mainchain |
| 1 | M | 709 | LYS | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | M | 785 | GLU | Mainchain,Peptide |
| 1 | M | 98 | HIS | Mainchain |
| 2 | N | 150 | TYR | Sidechain |
| 2 | N | 155 | TYR | Mainchain |
| 2 | N | 22 | THR | Mainchain |
| 3 | O | 75 | ALA | Mainchain |
| 3 | O | 85 | GLU | Mainchain |
| 1 | S | 623 | PHE | Sidechain |
| 1 | S | 637 | LYS | Mainchain |
| 1 | S | 649 | VAL | Mainchain |
| 1 | S | 769 | ALA | Mainchain |
| 1 | S | 785 | GLU | Mainchain,Peptide |
| 1 | S | 98 | HIS | Mainchain |
| 2 | T | 150 | TYR | Sidechain |
| 2 | T | 155 | TYR | Mainchain |
| 2 | T | 22 | THR | Mainchain |
| 3 | U | 75 | ALA | Mainchain |
| 3 | U | 85 | GLU | Mainchain |
| 4 | V | 62 | ARG | Sidechain |
| 4 | W | 62 | ARG | Sidechain |
| 4 | X | 62 | ARG | Sidechain |
| 4 | Y | 62 | ARG | Sidechain |
| 4 | Z | 62 | ARG | Sidechain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 6797 | 0 | 6755 | 1473 | 22 |
| 1 | D | 6797 | 0 | 6759 | 1500 | 23 |
| 1 | G | 6797 | 0 | 6762 | 1471 | 0 |
| 1 | J | 6797 | 0 | 6761 | 1483 | 0 |
| 1 | M | 6797 | 0 | 6766 | 1434 | 0 |
| 1 | S | 6797 | 0 | 6764 | 1607 | 0 |
| 2 | B | 1127 | 0 | 1085 | 237 | 0 |
| 2 | E | 1127 | 0 | 1088 | 272 | 0 |
| 2 | H | 1127 | 0 | 1087 | 258 | 0 |
| 2 | K | 1127 | 0 | 1088 | 282 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | N | 1127 | 0 | 1088 | 252 | 0 |
| 2 | T | 1127 | 0 | 1089 | 262 | 0 |
| 3 | C | 1123 | 0 | 1083 | 191 | 0 |
| 3 | F | 1123 | 0 | 1084 | 187 | 0 |
| 3 | I | 1123 | 0 | 1082 | 184 | 0 |
| 3 | L | 1123 | 0 | 1083 | 163 | 0 |
| 3 | O | 1123 | 0 | 1084 | 164 | 0 |
| 3 | U | 1123 | 0 | 1084 | 292 | 0 |
| 4 | 1 | 2906 | 0 | 2862 | 156 | 0 |
| 4 | 2 | 2906 | 0 | 2853 | 428 | 82 |
| 4 | 3 | 2906 | 0 | 2865 | 219 | 546 |
| 4 | 4 | 2906 | 0 | 2862 | 199 | 3082 |
| 4 | 5 | 2906 | 0 | 2866 | 124 | 3382 |
| 4 | 6 | 2906 | 0 | 2866 | 117 | 3395 |
| 4 | 7 | 2906 | 0 | 2866 | 77 | 3105 |
| 4 | 8 | 2906 | 0 | 2857 | 321 | 3475 |
| 4 | 9 | 2906 | 0 | 2855 | 339 | 3347 |
| 4 | V | 2906 | 0 | 2851 | 383 | 427 |
| 4 | W | 2906 | 0 | 2851 | 388 | 88 |
| 4 | X | 2906 | 0 | 2862 | 210 | 0 |
| 4 | Y | 2906 | 0 | 2861 | 167 | 0 |
| 4 | Z | 2906 | 0 | 2854 | 390 | 0 |
| All | All | 94966 | 0 | 93623 | 11394 | 10487 |

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 61.

All (11394) 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) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:287:ILE:CG1 | 4:3:203:THR:H | 1.06 | 1.68 |
| 1:D:797:PHE:CE2 | 3:F:126:LEU:HD22 | 1.17 | 1.68 |
| 1:S:783:LEU:CG | 1:S:786:ILE:HD11 | 1.24 | 1.68 |
| 1:D:813:ILE:HG23 | 2:E:128:PHE:CZ | 1.23 | 1.66 |
| 4:4:287:ILE:HG23 | 4:6:202:THR:CB | 1.20 | 1.65 |
| 1:D:791:GLN:HE22 | 3:F:115:GLY:CA | 1.09 | 1.65 |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CG1 | 1.17 | 1.65 |
| 1:D:508:ILE:HD11 | 1:D:766:PHE:CE1 | 1.20 | 1.65 |
| 1:D:508:ILE:CD1 | 1:D:766:PHE:CE1 | 1.78 | 1.65 |
| 4:X:291:LYS:HE3 | 4:Z:243:PRO:CB | 1.17 | 1.64 |
| 1:G:831:TRP:CH2 | 2:H:47:LEU:HD21 | 1.31 | 1.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:287:ILE:CG2 | 4:3:202:THR:HB | 1.25 | 1.63 |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CG1 | 1.17 | 1.63 |
| 1:J:84:MLY:HH11 | 1:J:720:PHE:CD1 | 1.25 | 1.63 |
| 4:3:287:ILE:CG2 | 4:5:202:THR:HB | 1.24 | 1.63 |
| 1:A:505:MLY:HB3 | 1:A:762:HIS:CD2 | 1.21 | 1.63 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:CD2 | 1.27 | 1.63 |
| 1:G:795:ARG:HG2 | 3:I:118:MET:CE | 1.19 | 1.62 |
| 1:D:508:ILE:CD1 | 1:D:766:PHE:CZ | 1.75 | 1.62 |
| 1:M:720:PHE:CE1 | 1:M:772:LEU:HD21 | 1.10 | 1.62 |
| 1:M:725:ARG:HE | 1:M:733:PRO:CB | 1.09 | 1.62 |
| 1:M:818:TYR:CE1 | 2:N:127:ARG:NH2 | 1.68 | 1.61 |
| 1:J:797:PHE:CD1 | 3:L:146:ILE:HG23 | 1.29 | 1.61 |
| 1:A:725:ARG:HE | 1:A:733:PRO:CB | 1.09 | 1.61 |
| 1:G:768:MLY:CH2 | 1:G:772:LEU:HD13 | 1.15 | 1.61 |
| 1:D:797:PHE:CD1 | 3:F:146:ILE:HG23 | 1.31 | 1.61 |
| 1:A:206:LYS:CD | 1:A:217:THR:HG23 | 1.28 | 1.61 |
| 4:4:287:ILE:CG2 | 4:6:202:THR:HB | 1.24 | 1.61 |
| 1:G:797:PHE:CE2 | 3:I:126:LEU:HD22 | 1.11 | 1.60 |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CG1 | 1.17 | 1.60 |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CD1 | 1.22 | 1.59 |
| 1:S:795:ARG:HG2 | 3:U:118:MET:CE | 1.19 | 1.59 |
| 2:T:144:VAL:HG13 | 2:T:153:ILE:CG1 | 1.17 | 1.59 |
| 1:G:725:ARG:HE | 1:G:733:PRO:CB | 1.09 | 1.58 |
| 1:J:792:ALA:CB | 3:L:42:THR:HG22 | 1.31 | 1.58 |
| 1:J:206:LYS:CD | 1:J:217:THR:HG23 | 1.28 | 1.58 |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CD1 | 1.22 | 1.58 |
| 1:G:206:LYS:CD | 1:G:217:THR:HG23 | 1.28 | 1.58 |
| 1:J:710:GLY:CA | 1:J:772:LEU:HD22 | 1.33 | 1.58 |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:CD1 | 1.22 | 1.57 |
| 1:A:538:GLU:CA | 4:8:349:LEU:CD1 | 1.78 | 1.57 |
| 1:J:725:ARG:HE | 1:J:733:PRO:CB | 1.09 | 1.57 |
| 1:J:798:LEU:CD1 | 3:L:126:LEU:HD11 | 1.24 | 1.57 |
| 1:S:727:LEU:HD23 | 1:S:783:LEU:CB | 1.26 | 1.57 |
| 1:S:795:ARG:CG | 3:U:118:MET:HE1 | 1.32 | 1.57 |
| 4:3:287:ILE:HG23 | 4:5:202:THR:CB | 1.20 | 1.57 |
| 1:D:834:LEU:CD1 | 2:E:54:MET:HG3 | 1.34 | 1.57 |
| 1:G:831:TRP:CH2 | 2:H:47:LEU:CD2 | 1.85 | 1.57 |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CD1 | 1.22 | 1.56 |
| 1:J:818:TYR:CE1 | 2:K:127:ARG:NH2 | 1.68 | 1.56 |
| 1:J:84:MLY:HD3 | 1:J:724:TYR:CE2 | 1.39 | 1.56 |
| 1:S:817:GLN:CG | 2:T:127:ARG:HD2 | 1.23 | 1.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CG | 1.35 | 1.56 |
| 1:D:206:LYS:CD | 1:D:217:THR:HG23 | 1.28 | 1.56 |
| 1:D:818:TYR:HB3 | 2:E:90:GLY:CA | 1.34 | 1.56 |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CD1 | 1.22 | 1.56 |
| 1:G:795:ARG:CG | 3:I:118:MET:HE1 | 1.32 | 1.56 |
| 1:D:538:GLU:CA | 4:9:349:LEU:CD1 | 1.78 | 1.56 |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CG1 | 1.17 | 1.56 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:HD21 | 1.09 | 1.56 |
| 1:A:736:GLN:HA | 1:A:743:ALA:CB | 1.35 | 1.55 |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:CD1 | 1.20 | 1.55 |
| 1:D:834:LEU:HD11 | 2:E:54:MET:CG | 1.22 | 1.55 |
| 1:M:538:GLU:CA | 4:Z:349:LEU:CD1 | 1.79 | 1.55 |
| 1:D:727:LEU:HB2 | 1:D:782:MLY:CH1 | 1.08 | 1.55 |
| 1:J:84:MLY:HH21 | 1:J:720:PHE:CA | 1.18 | 1.55 |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:CG1 | 1.17 | 1.55 |
| 1:S:641:LYS:HG3 | 1:S:647:GLN:CG | 1.37 | 1.55 |
| 1:G:530:MET:HG2 | 4:V:354:GLN:CB | 1.35 | 1.55 |
| 1:M:836:PHE:CE1 | 2:N:159:HIS:HA | 1.35 | 1.55 |
| 1:J:84:MLY:CH2 | 1:J:720:PHE:HA | 1.18 | 1.54 |
| 1:A:799:MET:SD | 3:C:32:ASP:HB3 | 1.46 | 1.54 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:CB | 1.70 | 1.54 |
| 1:J:530:MET:HG2 | 4:W:354:GLN:CB | 1.36 | 1.54 |
| 2:T:144:VAL:HG13 | 2:T:153:ILE:CD1 | 1.22 | 1.54 |
| 1:M:720:PHE:CE1 | 1:M:772:LEU:CD2 | 1.82 | 1.54 |
| 1:S:798:LEU:CD2 | 3:U:126:LEU:HD11 | 1.35 | 1.54 |
| 1:J:538:GLU:CA | 4:W:349:LEU:CD1 | 1.79 | 1.54 |
| 1:G:768:MLY:HH23 | 1:G:772:LEU:CD1 | 1.11 | 1.54 |
| 1:M:641:LYS:HG3 | 1:M:647:GLN:CG | 1.37 | 1.54 |
| 1:M:736:GLN:HA | 1:M:743:ALA:CB | 1.35 | 1.54 |
| 1:S:725:ARG:HE | 1:S:733:PRO:CB | 1.09 | 1.54 |
| 1:D:725:ARG:HE | 1:D:733:PRO:CB | 1.09 | 1.54 |
| 1:G:149:GLN:CG | 1:G:763:THR:HG21 | 1.10 | 1.54 |
| 1:D:641:LYS:HG3 | 1:D:647:GLN:CG | 1.36 | 1.54 |
| 1:D:736:GLN:HA | 1:D:743:ALA:CB | 1.35 | 1.54 |
| 4:1:287:ILE:HG23 | 4:3:202:THR:CB | 1.34 | 1.53 |
| 1:G:538:GLU:CA | 4:V:349:LEU:CD1 | 1.79 | 1.53 |
| 1:G:556:ASP:CG | 4:X:47:MET:CE | 1.76 | 1.53 |
| 1:S:538:GLU:CA | 4:2:349:LEU:CD1 | 1.79 | 1.53 |
| 1:M:206:LYS:CD | 1:M:217:THR:HG23 | 1.28 | 1.53 |
| 1:A:530:MET:HG2 | 4:8:354:GLN:CB | 1.35 | 1.53 |
| 1:J:736:GLN:HA | 1:J:743:ALA:CB | 1.35 | 1.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:530:MET:HG2 | 4:Z:354:GLN:CB | 1.36 | 1.53 |
| 1:S:206:LYS:CD | 1:S:217:THR:HG23 | 1.28 | 1.53 |
| 1:G:736:GLN:HA | 1:G:743:ALA:CB | 1.35 | 1.52 |
| 1:S:530:MET:HG2 | 4:2:354:GLN:CB | 1.36 | 1.52 |
| 1:G:754:ASP:HA | 1:G:779:ARG:CD | 1.31 | 1.52 |
| 1:D:818:TYR:CB | 2:E:90:GLY:HA3 | 1.07 | 1.52 |
| 1:J:710:GLY:HA2 | 1:J:772:LEU:CD2 | 1.40 | 1.52 |
| 1:J:817:GLN:CG | 2:K:127:ARG:HD2 | 1.36 | 1.52 |
| 1:J:556:ASP:CG | 4:Y:47:MET:CE | 1.76 | 1.52 |
| 1:J:641:LYS:HG3 | 1:J:647:GLN:CG | 1.37 | 1.52 |
| 1:D:836:PHE:CZ | 2:E:160:GLY:N | 1.75 | 1.52 |
| 1:S:727:LEU:CD2 | 1:S:783:LEU:HB2 | 1.40 | 1.52 |
| 1:D:508:ILE:HD11 | 1:D:766:PHE:CZ | 0.99 | 1.51 |
| 1:G:757:GLN:HG3 | 1:G:776:GLU:CG | 1.07 | 1.51 |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:CG | 1.37 | 1.51 |
| 1:G:791:GLN:HE22 | 3:I:115:GLY:CA | 1.18 | 1.51 |
| 1:M:206:LYS:HD3 | 1:M:217:THR:CG2 | 1.40 | 1.51 |
| 1:G:206:LYS:HD3 | 1:G:217:THR:CG2 | 1.40 | 1.51 |
| 1:M:799:MET:SD | 3:O:32:ASP:HB3 | 1.50 | 1.51 |
| 1:A:753:VAL:CG1 | 1:A:775:LEU:HG | 1.36 | 1.51 |
| 1:S:736:GLN:HA | 1:S:743:ALA:CB | 1.35 | 1.51 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:CG | 1.37 | 1.51 |
| 1:M:720:PHE:HE1 | 1:M:772:LEU:CD2 | 1.13 | 1.51 |
| 1:A:505:MLY:CB | 1:A:762:HIS:HD2 | 0.89 | 1.50 |
| 2:T:117:LEU:HD12 | 2:T:147:ASN:CB | 1.41 | 1.50 |
| 1:D:530:MET:HG2 | 4:9:354:GLN:CB | 1.35 | 1.50 |
| 1:D:747:LEU:CD1 | 1:D:782:MLY:HH21 | 1.39 | 1.50 |
| 1:M:783:LEU:HA | 1:M:786:ILE:CG1 | 1.37 | 1.50 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CG | 1.30 | 1.50 |
| 1:D:206:LYS:HD3 | 1:D:217:THR:CG2 | 1.40 | 1.50 |
| 1:J:95:THR:HA | 1:J:713:SER:CB | 1.41 | 1.50 |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD1 | 1.02 | 1.50 |
| 4:2:112:PRO:HG2 | 4:3:197:GLY:N | 1.19 | 1.49 |
| 1:G:149:GLN:HG2 | 1:G:763:THR:CG2 | 1.42 | 1.49 |
| 1:A:795:ARG:HB3 | 3:C:35:ARG:CZ | 1.41 | 1.49 |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CB | 1.42 | 1.49 |
| 1:G:149:GLN:CG | 1:G:763:THR:CG2 | 1.91 | 1.49 |
| 1:G:721:LYS:HG3 | 1:G:736:GLN:CG | 1.15 | 1.49 |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CB | 1.41 | 1.49 |
| 1:M:783:LEU:CG | 1:M:786:ILE:HD11 | 1.05 | 1.49 |
| 1:S:792:ALA:CB | 3:U:42:THR:HG22 | 1.41 | 1.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:797:PHE:CE1 | 3:L:146:ILE:HG23 | 1.47 | 1.48 |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CB | 1.42 | 1.48 |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CB | 1.41 | 1.48 |
| 1:G:641:LYS:CG | 1:G:647:GLN:NE2 | 1.77 | 1.48 |
| 1:J:206:LYS:HD3 | 1:J:217:THR:CG2 | 1.40 | 1.48 |
| 1:M:641:LYS:CG | 1:M:647:GLN:NE2 | 1.77 | 1.48 |
| 1:S:641:LYS:CG | 1:S:647:GLN:NE2 | 1.77 | 1.48 |
| 4:3:287:ILE:CB | 4:5:202:THR:HB | 1.44 | 1.48 |
| 1:A:206:LYS:HD3 | 1:A:217:THR:CG2 | 1.40 | 1.48 |
| 2:K:111:SER:HB2 | 2:K:148:VAL:C | 1.22 | 1.47 |
| 1:S:206:LYS:HD3 | 1:S:217:THR:CG2 | 1.40 | 1.47 |
| 1:M:721:LYS:HG3 | 1:M:736:GLN:CG | 1.15 | 1.47 |
| 1:D:641:LYS:CG | 1:D:647:GLN:NE2 | 1.77 | 1.47 |
| 1:J:792:ALA:CB | 3:L:42:THR:CG2 | 1.83 | 1.47 |
| 2:B:111:SER:HB2 | 2:B:148:VAL:C | 1.23 | 1.47 |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:CG2 | 1.42 | 1.47 |
| 4:4:287:ILE:CG2 | 4:6:202:THR:CB | 1.79 | 1.47 |
| 2:E:111:SER:HB2 | 2:E:148:VAL:C | 1.23 | 1.47 |
| 2:T:111:SER:HB2 | 2:T:148:VAL:C | 1.23 | 1.47 |
| 2:N:111:SER:HB2 | 2:N:148:VAL:C | 1.22 | 1.47 |
| 1:A:538:GLU:C | 4:8:349:LEU:CD1 | 1.84 | 1.46 |
| 1:A:641:LYS:CG | 1:A:647:GLN:NE2 | 1.76 | 1.46 |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CG | 1.29 | 1.46 |
| 1:M:821:ARG:NH2 | 2:N:127:ARG:HG2 | 1.16 | 1.46 |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CG | 1.30 | 1.46 |
| 1:D:727:LEU:CB | 1:D:782:MLY:HH13 | 1.40 | 1.46 |
| 2:H:111:SER:HB2 | 2:H:148:VAL:C | 1.23 | 1.46 |
| 4:3:287:ILE:CG2 | 4:5:202:THR:CB | 1.79 | 1.46 |
| 1:D:538:GLU:C | 4:9:349:LEU:CD1 | 1.84 | 1.46 |
| 1:S:798:LEU:HD11 | 3:U:126:LEU:CD2 | 1.45 | 1.46 |
| 1:G:757:GLN:CG | 1:G:776:GLU:HG2 | 0.98 | 1.45 |
| 1:M:641:LYS:CD | 1:M:647:GLN:CD | 1.85 | 1.45 |
| 1:M:783:LEU:CA | 1:M:786:ILE:HG13 | 1.43 | 1.45 |
| 1:D:641:LYS:CD | 1:D:647:GLN:CD | 1.85 | 1.45 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CB | 1.42 | 1.45 |
| 2:T:117:LEU:HD12 | 2:T:147:ASN:CG | 1.29 | 1.45 |
| 1:D:769:ALA:HA | 1:D:771:LEU:CA | 1.33 | 1.45 |
| 1:J:641:LYS:CD | 1:J:647:GLN:CD | 1.85 | 1.45 |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CG | 1.29 | 1.44 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:CB | 1.47 | 1.44 |
| 1:J:641:LYS:CG | 1:J:647:GLN:NE2 | 1.77 | 1.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:J:28:GLN:CA | 1:J:723:ARG:NH2 | 1.69 | 1.44 |
| 1:S:795:ARG:NH2 | 3:U:116:GLU:HB3 | 1.24 | 1.44 |
| 1:M:538:GLU:C | 4:Z:349:LEU:CD1 | 1.84 | 1.44 |
| 1:S:641:LYS:CD | 1:S:647:GLN:CD | 1.85 | 1.44 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:CD | 1.71 | 1.44 |
| 1:A:641:LYS:CD | 1:A:647:GLN:CD | 1.85 | 1.44 |
| 1:G:538:GLU:C | 4:V:349:LEU:CD1 | 1.84 | 1.44 |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CG | 1.29 | 1.43 |
| 4:4:287:ILE:CB | 4:6:202:THR:HB | 1.44 | 1.43 |
| 1:G:792:ALA:CB | 3:I:42:THR:HG22 | 1.44 | 1.43 |
| 1:J:817:GLN:CB | 2:K:127:ARG:HD2 | 1.46 | 1.43 |
| 1:G:769:ALA:CB | 1:G:770:GLY:HA2 | 1.49 | 1.43 |
| 1:J:538:GLU:C | 4:W:349:LEU:CD1 | 1.84 | 1.43 |
| 1:G:641:LYS:CD | 1:G:647:GLN:CD | 1.85 | 1.42 |
| 1:A:149:GLN:OE1 | 1:A:716:LEU:CD2 | 1.67 | 1.42 |
| 1:M:783:LEU:HG | 1:M:786:ILE:CD1 | 0.97 | 1.42 |
| 1:M:819:ASN:CG | 2:N:92:ASP:HB2 | 1.36 | 1.42 |
| 1:S:505:MLY:HH11 | 1:S:762:HIS:NE2 | 1.21 | 1.42 |
| 1:D:721:LYS:HG3 | 1:D:736:GLN:CG | 1.15 | 1.42 |
| 1:A:831:TRP:CD1 | 2:B:51:PHE:HZ | 1.37 | 1.42 |
| 1:J:792:ALA:HB2 | 3:L:42:THR:CG2 | 0.96 | 1.41 |
| 1:G:821:ARG:NH2 | 2:H:127:ARG:HG2 | 1.34 | 1.41 |
| 1:M:736:GLN:N | 1:M:743:ALA:HB1 | 1.35 | 1.41 |
| 1:G:792:ALA:HB2 | 3:I:42:THR:CG2 | 1.47 | 1.41 |
| 1:S:506:GLU:OE2 | 1:S:760:PHE:CD1 | 1.71 | 1.41 |
| 1:A:733:PRO:O | 1:A:737:PHE:CD1 | 1.73 | 1.41 |
| 1:S:796:GLY:HA2 | 3:U:35:ARG:CD | 1.50 | 1.41 |
| 1:S:538:GLU:C | 4:2:349:LEU:CD1 | 1.84 | 1.41 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:CD1 | 1.99 | 1.41 |
| 1:A:530:MET:CG | 4:8:354:GLN:HB2 | 1.50 | 1.41 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:CD1 | 1.99 | 1.41 |
| 1:G:567:LYS:NZ | 4:X:92:ASN:HD22 | 1.17 | 1.41 |
| 2:K:144:VAL:CG1 | 2:K:153:ILE:CD1 | 1.99 | 1.41 |
| 1:J:202:SER:HA | 1:J:207:LYS:CE | 1.51 | 1.41 |
| 1:M:733:PRO:O | 1:M:737:PHE:CD1 | 1.73 | 1.41 |
| 1:D:202:SER:HA | 1:D:207:LYS:CE | 1.51 | 1.40 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:CD1 | 1.99 | 1.40 |
| 1:J:733:PRO:O | 1:J:737:PHE:CD1 | 1.73 | 1.40 |
| 4:X:286:ASP:OD1 | 4:Z:202:THR:CB | 1.64 | 1.40 |
| 1:D:791:GLN:NE2 | 3:F:115:GLY:HA3 | 1.15 | 1.40 |
| 1:S:218:LEU:CB | 1:S:221:GLN:HG3 | 1.52 | 1.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:798:LEU:CD1 | 3:F:126:LEU:HD11 | 0.95 | 1.40 |
| 1:S:793:ARG:NH1 | 3:U:40:ASN:HD22 | 0.96 | 1.40 |
| 1:D:530:MET:CG | 4:9:354:GLN:HB2 | 1.50 | 1.40 |
| 1:G:797:PHE:CE2 | 3:I:126:LEU:CD2 | 2.02 | 1.40 |
| 1:M:218:LEU:CB | 1:M:221:GLN:HG3 | 1.52 | 1.40 |
| 1:D:733:PRO:O | 1:D:737:PHE:CD1 | 1.74 | 1.40 |
| 2:T:144:VAL:CG1 | 2:T:153:ILE:CD1 | 1.99 | 1.40 |
| 1:A:202:SER:HA | 1:A:207:LYS:CE | 1.51 | 1.40 |
| 1:D:769:ALA:CA | 1:D:771:LEU:HA | 1.37 | 1.40 |
| 1:G:218:LEU:CB | 1:G:221:GLN:HG3 | 1.51 | 1.40 |
| 1:A:218:LEU:CB | 1:A:221:GLN:HG3 | 1.52 | 1.40 |
| 1:A:817:GLN:NE2 | 2:B:127:ARG:CG | 1.83 | 1.40 |
| 1:S:795:ARG:NH1 | 3:U:43:ASN:HB2 | 1.30 | 1.40 |
| 1:M:537:GLU:O | 4:Z:349:LEU:CD1 | 1.70 | 1.40 |
| 1:G:754:ASP:OD2 | 1:G:779:ARG:CB | 1.70 | 1.39 |
| 1:G:733:PRO:O | 1:G:737:PHE:CD1 | 1.74 | 1.39 |
| 1:S:534:SER:O | 4:2:351:THR:CG2 | 1.64 | 1.39 |
| 4:X:291:LYS:CE | 4:Z:243:PRO:HB2 | 1.52 | 1.39 |
| 1:D:537:GLU:O | 4:9:349:LEU:CD1 | 1.70 | 1.39 |
| 1:G:736:GLN:N | 1:G:743:ALA:HB1 | 1.34 | 1.39 |
| 1:G:537:GLU:O | 4:V:349:LEU:CD1 | 1.71 | 1.39 |
| 1:S:795:ARG:NH1 | 3:U:43:ASN:CB | 1.84 | 1.39 |
| 1:A:721:LYS:HG3 | 1:A:736:GLN:CG | 1.15 | 1.39 |
| 1:D:85:TYR:OH | 1:D:772:LEU:CD2 | 1.69 | 1.39 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:CD1 | 1.99 | 1.39 |
| 1:S:798:LEU:CG | 3:U:126:LEU:HD11 | 1.51 | 1.39 |
| 1:J:530:MET:CG | 4:W:354:GLN:HB2 | 1.51 | 1.39 |
| 1:S:736:GLN:N | 1:S:743:ALA:HB1 | 1.35 | 1.39 |
| 1:S:733:PRO:O | 1:S:737:PHE:CD1 | 1.73 | 1.39 |
| 1:S:831:TRP:HH2 | 2:T:47:LEU:CD2 | 1.34 | 1.39 |
| 1:G:728:ASN:ND2 | 3:I:114:LEU:HD23 | 1.36 | 1.39 |
| 1:J:537:GLU:O | 4:W:349:LEU:CD1 | 1.70 | 1.39 |
| 1:M:736:GLN:CA | 1:M:743:ALA:CB | 2.00 | 1.39 |
| 1:G:819:ASN:CA | 2:H:90:GLY:O | 1.69 | 1.38 |
| 1:M:817:GLN:CG | 2:N:127:ARG:HD2 | 1.51 | 1.38 |
| 1:J:218:LEU:CB | 1:J:221:GLN:HG3 | 1.52 | 1.38 |
| 1:J:567:LYS:NZ | 4:Y:92:ASN:HD22 | 1.16 | 1.38 |
| 1:M:202:SER:HA | 1:M:207:LYS:CE | 1.51 | 1.38 |
| 1:S:537:GLU:O | 4:2:349:LEU:CD1 | 1.70 | 1.38 |
| 1:J:505:MLY:HD2 | 1:J:762:HIS:CE1 | 1.57 | 1.38 |
| 1:S:202:SER:HA | 1:S:207:LYS:CE | 1.51 | 1.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:721:LYS:HG3 | 1:S:736:GLN:CG | 1.15 | 1.38 |
| 1:J:736:GLN:CA | 1:J:743:ALA:CB | 2.00 | 1.38 |
| 1:S:530:MET:CG | 4:2:354:GLN:HB2 | 1.51 | 1.38 |
| 1:J:838:ILE:HD11 | 2:K:54:MET:CE | 1.48 | 1.38 |
| 1:A:537:GLU:O | 4:8:349:LEU:CD1 | 1.70 | 1.38 |
| 1:D:736:GLN:CA | 1:D:743:ALA:CB | 2.00 | 1.38 |
| 1:M:534:SER:O | 4:Z:351:THR:CG2 | 1.64 | 1.38 |
| 1:S:736:GLN:CA | 1:S:743:ALA:CB | 2.00 | 1.38 |
| 4:1:287:ILE:CG1 | 4:3:203:THR:N | 1.74 | 1.38 |
| 1:A:736:GLN:N | 1:A:743:ALA:HB1 | 1.35 | 1.38 |
| 1:M:736:GLN:CA | 1:M:743:ALA:HB1 | 1.53 | 1.38 |
| 1:D:218:LEU:CB | 1:D:221:GLN:HG3 | 1.52 | 1.38 |
| 1:D:721:LYS:CG | 1:D:736:GLN:CG | 1.96 | 1.38 |
| 2:T:144:VAL:CG1 | 2:T:153:ILE:HG12 | 1.54 | 1.38 |
| 1:S:92:ALA:O | 1:S:714:ARG:CG | 1.68 | 1.37 |
| 1:M:530:MET:CG | 4:Z:354:GLN:HB2 | 1.51 | 1.37 |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:CG | 1.51 | 1.37 |
| 1:G:202:SER:HA | 1:G:207:LYS:CE | 1.51 | 1.37 |
| 1:J:721:LYS:HG3 | 1:J:736:GLN:CG | 1.15 | 1.37 |
| 1:G:530:MET:CG | 4:V:354:GLN:HB2 | 1.51 | 1.37 |
| 1:D:813:ILE:CG2 | 2:E:128:PHE:CZ | 2.08 | 1.37 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:HG12 | 1.54 | 1.37 |
| 1:G:795:ARG:NE | 3:I:116:GLU:HB3 | 1.38 | 1.37 |
| 1:S:721:LYS:CG | 1:S:736:GLN:CG | 1.97 | 1.37 |
| 1:S:798:LEU:HD11 | 3:U:126:LEU:CD1 | 1.55 | 1.37 |
| 1:D:797:PHE:HE2 | 3:F:126:LEU:CD2 | 1.36 | 1.37 |
| 1:A:736:GLN:CA | 1:A:743:ALA:HB1 | 1.53 | 1.37 |
| 2:B:117:LEU:HB2 | 2:B:147:ASN:ND2 | 1.39 | 1.37 |
| 2:K:144:VAL:CG1 | 2:K:153:ILE:HG12 | 1.54 | 1.37 |
| 1:S:641:LYS:CG | 1:S:647:GLN:CD | 1.93 | 1.37 |
| 1:S:728:ASN:OD1 | 3:U:90:GLY:CA | 1.69 | 1.37 |
| 1:D:713:SER:OG | 1:D:771:LEU:CD2 | 1.72 | 1.37 |
| 1:J:818:TYR:CZ | 2:K:127:ARG:NH2 | 1.90 | 1.37 |
| 1:M:641:LYS:CG | 1:M:647:GLN:CD | 1.93 | 1.37 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:CD | 1.45 | 1.37 |
| 1:A:736:GLN:CA | 1:A:743:ALA:CB | 2.00 | 1.37 |
| 1:G:553:MLY:CH1 | 4:X:45:VAL:HG11 | 1.54 | 1.37 |
| 1:J:736:GLN:N | 1:J:743:ALA:HB1 | 1.35 | 1.37 |
| 1:G:791:GLN:NE2 | 3:I:115:GLY:HA3 | 1.06 | 1.36 |
| 1:M:649:VAL:O | 1:M:649:VAL:CG1 | 1.74 | 1.36 |
| 4:1:287:ILE:HG12 | 4:3:202:THR:C | 1.42 | 1.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:736:GLN:N | 1:D:743:ALA:HB1 | 1.35 | 1.36 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:O | 1.74 | 1.36 |
| 1:G:641:LYS:CG | 1:G:647:GLN:CD | 1.93 | 1.36 |
| 1:S:795:ARG:HH11 | 3:U:43:ASN:CG | 1.27 | 1.36 |
| 1:J:553:MLY:CH1 | 4:Y:45:VAL:HG11 | 1.55 | 1.36 |
| 2:E:117:LEU:HB2 | 2:E:147:ASN:ND2 | 1.40 | 1.36 |
| 1:J:84:MLY:CD | 1:J:724:TYR:CE2 | 2.08 | 1.36 |
| 1:M:641:LYS:HG3 | 1:M:647:GLN:CD | 1.46 | 1.36 |
| 1:D:641:LYS:CG | 1:D:647:GLN:CD | 1.93 | 1.36 |
| 4:2:287:ILE:CG2 | 4:4:203:THR:HG22 | 1.56 | 1.35 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:HG12 | 1.54 | 1.35 |
| 1:G:534:SER:O | 4:V:351:THR:CG2 | 1.64 | 1.35 |
| 1:S:641:LYS:HG3 | 1:S:647:GLN:CD | 1.45 | 1.35 |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:HD21 | 1.54 | 1.35 |
| 1:D:724:TYR:CA | 1:D:782:MLY:HD2 | 1.51 | 1.35 |
| 1:S:736:GLN:CA | 1:S:743:ALA:HB1 | 1.53 | 1.35 |
| 1:A:817:GLN:NE2 | 2:B:127:ARG:HG2 | 1.08 | 1.35 |
| 1:G:736:GLN:CA | 1:G:743:ALA:CB | 2.00 | 1.35 |
| 1:S:819:ASN:CG | 2:T:92:ASP:HB2 | 1.46 | 1.35 |
| 1:G:736:GLN:CA | 1:G:743:ALA:HB1 | 1.53 | 1.35 |
| 1:J:736:GLN:CA | 1:J:743:ALA:HB1 | 1.53 | 1.35 |
| 4:4:288:ASP:OD2 | 4:6:203:THR:HG21 | 1.21 | 1.35 |
| 1:A:641:LYS:CG | 1:A:647:GLN:CD | 1.93 | 1.35 |
| 1:J:641:LYS:HG3 | 1:J:647:GLN:CD | 1.45 | 1.35 |
| 1:J:829:TRP:CZ3 | 2:K:87:LYS:NZ | 1.90 | 1.35 |
| 1:S:538:GLU:CA | 4:2:349:LEU:HD12 | 0.88 | 1.35 |
| 1:J:641:LYS:CG | 1:J:647:GLN:CD | 1.93 | 1.35 |
| 1:M:795:ARG:HG2 | 3:O:118:MET:CE | 1.56 | 1.35 |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:OD1 | 1.74 | 1.35 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:HG12 | 1.54 | 1.35 |
| 2:K:117:LEU:CD1 | 2:K:147:ASN:OD1 | 1.74 | 1.35 |
| 1:M:838:ILE:HD11 | 2:N:54:MET:CE | 1.56 | 1.35 |
| 1:A:793:ARG:HH21 | 3:C:147:MET:CE | 1.39 | 1.35 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:CG1 | 2.03 | 1.35 |
| 2:N:117:LEU:CD1 | 2:N:147:ASN:OD1 | 1.74 | 1.35 |
| 1:S:642:LYS:HG3 | 4:2:23:GLY:N | 1.40 | 1.35 |
| 2:T:117:LEU:CD1 | 2:T:147:ASN:OD1 | 1.74 | 1.35 |
| 1:D:814:PHE:HD1 | 2:E:127:ARG:NH1 | 1.24 | 1.35 |
| 1:G:838:ILE:HD11 | 2:H:54:MET:CE | 1.56 | 1.35 |
| 2:T:117:LEU:HB2 | 2:T:147:ASN:ND2 | 1.40 | 1.35 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:CD | 1.54 | 1.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:797:PHE:CE2 | 3:F:126:LEU:CD2 | 2.09 | 1.34 |
| 1:G:538:GLU:CA | 4:V:349:LEU:HD12 | 0.88 | 1.34 |
| 1:S:649:VAL:CG1 | 1:S:649:VAL:O | 1.74 | 1.34 |
| 1:S:530:MET:HA | 4:2:354:GLN:CG | 1.56 | 1.34 |
| 1:A:538:GLU:CA | 4:8:349:LEU:HD12 | 0.87 | 1.34 |
| 1:D:642:LYS:HG3 | 4:9:23:GLY:N | 1.40 | 1.34 |
| 4:1:287:ILE:HG12 | 4:3:203:THR:N | 1.22 | 1.34 |
| 1:A:530:MET:HA | 4:8:354:GLN:CG | 1.56 | 1.34 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:CG1 | 2.03 | 1.34 |
| 1:M:642:LYS:HG3 | 4:Z:23:GLY:N | 1.40 | 1.34 |
| 1:M:538:GLU:CA | 4:Z:349:LEU:HD12 | 0.88 | 1.34 |
| 1:D:534:SER:O | 4:9:351:THR:CG2 | 1.64 | 1.34 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:HG12 | 1.54 | 1.34 |
| 1:S:836:PHE:CE1 | 2:T:159:HIS:HA | 1.60 | 1.34 |
| 4:3:288:ASP:OD2 | 4:5:203:THR:HG21 | 1.21 | 1.34 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:O | 1.74 | 1.34 |
| 1:J:642:LYS:HG3 | 4:W:23:GLY:N | 1.40 | 1.34 |
| 1:J:538:GLU:CA | 4:W:349:LEU:HD12 | 0.88 | 1.34 |
| 1:D:530:MET:HA | 4:9:354:GLN:CG | 1.56 | 1.34 |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:CD | 1.45 | 1.34 |
| 4:4:324:THR:OG1 | 4:6:244:ASP:CA | 1.76 | 1.34 |
| 2:T:114:LYS:CA | 2:T:146:GLY:O | 1.76 | 1.34 |
| 2:E:114:LYS:CA | 2:E:146:GLY:O | 1.76 | 1.34 |
| 1:D:795:ARG:HD3 | 3:F:43:ASN:OD1 | 1.19 | 1.34 |
| 1:G:752:ASP:O | 1:G:780:ASP:HA | 1.28 | 1.34 |
| 1:J:649:VAL:O | 1:J:649:VAL:CG1 | 1.74 | 1.34 |
| 1:J:819:ASN:HA | 2:K:90:GLY:O | 1.21 | 1.34 |
| 1:S:798:LEU:HD21 | 3:U:126:LEU:CD1 | 1.55 | 1.34 |
| 1:J:530:MET:HA | 4:W:354:GLN:CG | 1.56 | 1.33 |
| 1:A:534:SER:O | 4:8:351:THR:CG2 | 1.64 | 1.33 |
| 1:A:795:ARG:CD | 3:C:35:ARG:HH12 | 1.41 | 1.33 |
| 1:S:798:LEU:CD1 | 3:U:126:LEU:HD11 | 1.56 | 1.33 |
| 1:D:795:ARG:CD | 3:F:43:ASN:OD1 | 1.75 | 1.33 |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:OD1 | 1.74 | 1.33 |
| 1:J:836:PHE:CE1 | 2:K:159:HIS:HA | 1.62 | 1.33 |
| 1:M:795:ARG:CG | 3:O:118:MET:CE | 2.07 | 1.33 |
| 1:S:783:LEU:HA | 1:S:786:ILE:CG1 | 1.58 | 1.33 |
| 1:D:538:GLU:CA | 4:9:349:LEU:HD12 | 0.87 | 1.33 |
| 1:G:721:LYS:CG | 1:G:736:GLN:CG | 1.97 | 1.33 |
| 2:K:117:LEU:HB2 | 2:K:147:ASN:ND2 | 1.39 | 1.33 |
| 1:M:530:MET:HA | 4:Z:354:GLN:CG | 1.56 | 1.33 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:M:795:ARG:HB3 | 3:O:35:ARG:NH2 | 1.43 | 1.33 |
| 1:A:834:LEU:HD21 | 2:B:54:MET:CE | 1.57 | 1.33 |
| 1:G:530:MET:HA | 4:V:354:GLN:CG | 1.57 | 1.33 |
| 1:M:829:TRP:CZ3 | 2:N:87:LYS:NZ | 1.95 | 1.33 |
| 1:S:629:GLU:HA | 1:S:643:GLY:O | 1.17 | 1.33 |
| 2:T:144:VAL:CG1 | 2:T:153:ILE:CG1 | 2.03 | 1.33 |
| 1:S:795:ARG:CD | 3:U:43:ASN:OD1 | 1.77 | 1.33 |
| 1:M:635:GLY:CA | 4:Z:334:GLU:HG2 | 1.59 | 1.33 |
| 1:S:635:GLY:CA | 4:2:334:GLU:HG2 | 1.59 | 1.33 |
| 4:1:287:ILE:CB | 4:3:203:THR:H | 1.39 | 1.33 |
| 1:J:721:LYS:CG | 1:J:736:GLN:CG | 1.97 | 1.33 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:CG1 | 2.03 | 1.33 |
| 4:3:287:ILE:HG23 | 4:5:202:THR:OG1 | 1.29 | 1.33 |
| 4:3:324:THR:OG1 | 4:5:244:ASP:CA | 1.76 | 1.33 |
| 1:D:792:ALA:HB2 | 3:F:42:THR:CG2 | 1.59 | 1.33 |
| 1:M:819:ASN:OD1 | 2:N:92:ASP:N | 1.60 | 1.33 |
| 1:S:791:GLN:CD | 3:U:116:GLU:H | 1.32 | 1.33 |
| 1:J:635:GLY:CA | 4:W:334:GLU:HG2 | 1.59 | 1.33 |
| 1:D:635:GLY:CA | 4:9:334:GLU:HG2 | 1.59 | 1.32 |
| 1:D:641:LYS:HG3 | 1:D:647:GLN:CD | 1.46 | 1.32 |
| 2:H:117:LEU:HB2 | 2:H:147:ASN:ND2 | 1.39 | 1.32 |
| 1:J:721:LYS:CG | 1:J:736:GLN:CD | 1.98 | 1.32 |
| 1:A:799:MET:SD | 3:C:32:ASP:CB | 2.17 | 1.32 |
| 1:A:635:GLY:CA | 4:8:334:GLU:HG2 | 1.59 | 1.32 |
| 1:D:649:VAL:O | 1:D:649:VAL:CG1 | 1.74 | 1.32 |
| 1:S:93:MET:CE | 1:S:764:MLY:HB2 | 1.58 | 1.32 |
| 1:D:747:LEU:HD11 | 1:D:782:MLY:CH2 | 1.58 | 1.32 |
| 2:N:117:LEU:HB2 | 2:N:147:ASN:ND2 | 1.39 | 1.32 |
| 1:S:793:ARG:NH1 | 3:U:40:ASN:ND2 | 1.71 | 1.32 |
| 1:A:725:ARG:NE | 1:A:733:PRO:HB3 | 0.99 | 1.32 |
| 1:D:799:MET:CE | 3:F:32:ASP:HB3 | 1.59 | 1.32 |
| 1:G:725:ARG:NE | 1:G:733:PRO:HB3 | 1.00 | 1.32 |
| 2:H:114:LYS:CA | 2:H:146:GLY:O | 1.76 | 1.32 |
| 2:K:114:LYS:CA | 2:K:146:GLY:O | 1.76 | 1.32 |
| 2:N:114:LYS:CA | 2:N:146:GLY:O | 1.76 | 1.32 |
| 1:J:534:SER:O | 4:W:351:THR:CG2 | 1.64 | 1.32 |
| 1:G:635:GLY:CA | 4:V:334:GLU:HG2 | 1.59 | 1.32 |
| 1:M:629:GLU:HA | 1:M:643:GLY:O | 1.17 | 1.32 |
| 4:2:166:TYR:CE2 | 4:4:64:ILE:HG21 | 1.63 | 1.32 |
| 1:D:813:ILE:CG2 | 2:E:128:PHE:CE1 | 2.13 | 1.32 |
| 1:G:642:LYS:HG3 | 4:V:23:GLY:N | 1.39 | 1.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:144:VAL:CG1 | 2:K:153:ILE:CG1 | 2.03 | 1.32 |
| 1:M:721:LYS:CG | 1:M:736:GLN:CD | 1.98 | 1.32 |
| 4:2:112:PRO:CG | 4:3:197:GLY:N | 1.90 | 1.32 |
| 4:4:288:ASP:CG | 4:6:203:THR:CG2 | 1.98 | 1.32 |
| 1:D:721:LYS:CG | 1:D:736:GLN:CD | 1.98 | 1.32 |
| 1:G:753:VAL:O | 1:G:779:ARG:NH1 | 1.63 | 1.32 |
| 1:M:725:ARG:NE | 1:M:733:PRO:HB3 | 1.00 | 1.32 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CD2 | 1.57 | 1.31 |
| 1:S:783:LEU:HG | 1:S:786:ILE:CD1 | 1.59 | 1.31 |
| 1:D:725:ARG:NE | 1:D:733:PRO:HB3 | 1.00 | 1.31 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:CG1 | 2.03 | 1.31 |
| 2:K:121:LEU:O | 2:K:128:PHE:CB | 1.78 | 1.31 |
| 1:A:721:LYS:CG | 1:A:736:GLN:CD | 1.98 | 1.31 |
| 1:D:795:ARG:HB3 | 3:F:35:ARG:NH1 | 1.45 | 1.31 |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:OD1 | 1.74 | 1.31 |
| 1:S:721:LYS:HG2 | 1:S:736:GLN:OE1 | 1.29 | 1.31 |
| 1:S:831:TRP:CH2 | 2:T:47:LEU:CD2 | 2.14 | 1.31 |
| 1:G:721:LYS:CG | 1:G:736:GLN:CD | 1.98 | 1.31 |
| 1:S:792:ALA:HB2 | 3:U:42:THR:CG2 | 1.60 | 1.31 |
| 2:B:114:LYS:CA | 2:B:146:GLY:O | 1.76 | 1.31 |
| 1:D:599:ASN:HA | 1:D:649:VAL:CB | 1.60 | 1.31 |
| 2:E:121:LEU:O | 2:E:128:PHE:CB | 1.79 | 1.31 |
| 1:S:707:CYS:C | 1:S:714:ARG:HH22 | 1.33 | 1.31 |
| 4:3:288:ASP:CG | 4:5:203:THR:CG2 | 1.98 | 1.31 |
| 1:A:642:LYS:HG3 | 4:8:23:GLY:N | 1.40 | 1.30 |
| 1:M:721:LYS:HG2 | 1:M:736:GLN:OE1 | 1.29 | 1.30 |
| 1:A:735:GLY:O | 1:A:743:ALA:HB2 | 1.29 | 1.30 |
| 1:D:721:LYS:HG2 | 1:D:736:GLN:OE1 | 1.29 | 1.30 |
| 1:M:215:GLN:N | 1:M:340:ILE:HG12 | 1.19 | 1.30 |
| 1:S:838:ILE:HD11 | 2:T:54:MET:CE | 1.60 | 1.30 |
| 1:A:502:GLU:HG3 | 1:A:761:GLY:CA | 1.61 | 1.30 |
| 1:J:599:ASN:HA | 1:J:649:VAL:CB | 1.60 | 1.30 |
| 1:D:736:GLN:CA | 1:D:743:ALA:HB1 | 1.53 | 1.30 |
| 1:G:754:ASP:CA | 1:G:779:ARG:HD2 | 1.60 | 1.30 |
| 1:S:599:ASN:HA | 1:S:649:VAL:CB | 1.60 | 1.30 |
| 1:S:721:LYS:CG | 1:S:736:GLN:CD | 1.98 | 1.30 |
| 1:S:725:ARG:NE | 1:S:733:PRO:HB3 | 1.00 | 1.30 |
| 1:J:797:PHE:CE2 | 3:L:126:LEU:HD22 | 1.67 | 1.30 |
| 2:H:121:LEU:O | 2:H:128:PHE:CB | 1.79 | 1.30 |
| 1:D:732:ILE:HG21 | 1:D:782:MLY:CH2 | 1.61 | 1.30 |
| 1:A:599:ASN:HA | 1:A:649:VAL:CB | 1.60 | 1.29 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:121:LEU:O | 2:B:128:PHE:CB | 1.79 | 1.29 |
| 1:J:84:MLY:HA | 1:J:723:ARG:CZ | 1.30 | 1.29 |
| 1:M:599:ASN:HA | 1:M:649:VAL:CB | 1.60 | 1.29 |
| 1:S:795:ARG:NH2 | 3:U:116:GLU:CB | 1.95 | 1.29 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:HA | 1.65 | 1.29 |
| 4:X:291:LYS:CE | 4:Z:243:PRO:CB | 2.06 | 1.29 |
| 1:A:537:GLU:C | 4:8:349:LEU:HD13 | 1.52 | 1.29 |
| 1:J:725:ARG:NE | 1:J:733:PRO:HB3 | 1.00 | 1.29 |
| 1:A:215:GLN:N | 1:A:340:ILE:HG12 | 1.20 | 1.29 |
| 1:G:599:ASN:HA | 1:G:649:VAL:CB | 1.60 | 1.29 |
| 1:M:818:TYR:CZ | 2:N:127:ARG:NH2 | 2.00 | 1.29 |
| 1:S:819:ASN:ND2 | 2:T:92:ASP:HB2 | 1.47 | 1.29 |
| 1:A:800:ARG:HB3 | 3:C:149:VAL:CG2 | 1.63 | 1.29 |
| 1:D:726:VAL:CG1 | 1:D:785:GLU:HB3 | 1.61 | 1.29 |
| 1:G:819:ASN:CG | 2:H:92:ASP:HB2 | 1.38 | 1.29 |
| 1:J:829:TRP:CZ2 | 2:K:87:LYS:HE2 | 1.68 | 1.29 |
| 1:S:798:LEU:CD2 | 3:U:126:LEU:CD1 | 2.10 | 1.29 |
| 1:G:819:ASN:ND2 | 2:H:92:ASP:HB2 | 1.44 | 1.29 |
| 2:N:121:LEU:O | 2:N:128:PHE:CB | 1.79 | 1.29 |
| 1:S:818:TYR:CE1 | 2:T:127:ARG:NH2 | 2.00 | 1.29 |
| 1:D:799:MET:SD | 3:F:32:ASP:HB3 | 1.71 | 1.29 |
| 1:G:735:GLY:O | 1:G:743:ALA:HB2 | 1.29 | 1.29 |
| 1:J:721:LYS:HG3 | 1:J:736:GLN:CD | 1.54 | 1.29 |
| 1:A:538:GLU:O | 4:8:349:LEU:CD1 | 1.78 | 1.29 |
| 1:J:735:GLY:C | 1:J:743:ALA:CB | 2.01 | 1.29 |
| 1:J:538:GLU:O | 4:W:349:LEU:CD1 | 1.78 | 1.29 |
| 1:J:537:GLU:C | 4:W:349:LEU:HD13 | 1.52 | 1.29 |
| 1:A:149:GLN:NE2 | 1:A:718:ALA:HB3 | 1.44 | 1.28 |
| 1:A:721:LYS:HG3 | 1:A:736:GLN:CD | 1.53 | 1.28 |
| 1:M:28:GLN:O | 1:M:723:ARG:NH2 | 1.62 | 1.28 |
| 1:S:735:GLY:O | 1:S:743:ALA:HB2 | 1.29 | 1.28 |
| 2:T:121:LEU:O | 2:T:128:PHE:CB | 1.79 | 1.28 |
| 1:J:721:LYS:HG2 | 1:J:736:GLN:OE1 | 1.29 | 1.28 |
| 1:M:735:GLY:C | 1:M:743:ALA:CB | 2.01 | 1.28 |
| 1:A:735:GLY:C | 1:A:743:ALA:CB | 2.01 | 1.28 |
| 1:G:753:VAL:HA | 1:G:780:ASP:OD1 | 1.27 | 1.28 |
| 1:J:538:GLU:C | 4:W:349:LEU:HD12 | 1.48 | 1.28 |
| 1:M:537:GLU:C | 4:Z:349:LEU:HD13 | 1.52 | 1.28 |
| 1:D:735:GLY:C | 1:D:743:ALA:CB | 2.01 | 1.28 |
| 1:G:838:ILE:CD1 | 2:H:54:MET:HE3 | 1.63 | 1.28 |
| 1:S:834:LEU:HD13 | 2:T:51:PHE:CE1 | 1.67 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:735:GLY:C | 1:G:743:ALA:CB | 2.01 | 1.28 |
| 1:S:735:GLY:C | 1:S:743:ALA:CB | 2.01 | 1.28 |
| 1:G:537:GLU:C | 4:V:349:LEU:HD13 | 1.53 | 1.28 |
| 1:J:629:GLU:HA | 1:J:643:GLY:O | 1.17 | 1.28 |
| 1:J:817:GLN:CG | 2:K:127:ARG:CD | 2.11 | 1.28 |
| 1:M:538:GLU:O | 4:Z:349:LEU:CD1 | 1.78 | 1.28 |
| 1:J:534:SER:O | 4:W:351:THR:CA | 1.82 | 1.28 |
| 1:S:792:ALA:HB2 | 3:U:42:THR:CB | 1.64 | 1.28 |
| 4:2:112:PRO:HB3 | 4:3:196:ARG:CA | 1.62 | 1.28 |
| 1:G:721:LYS:HG3 | 1:G:736:GLN:CD | 1.54 | 1.28 |
| 1:D:799:MET:SD | 3:F:32:ASP:CB | 2.22 | 1.28 |
| 1:J:552:ASN:O | 4:Y:47:MET:SD | 1.91 | 1.28 |
| 1:D:767:PHE:O | 1:D:771:LEU:HD11 | 1.23 | 1.27 |
| 1:S:783:LEU:CB | 1:S:786:ILE:HD11 | 1.63 | 1.27 |
| 1:G:538:GLU:O | 4:V:349:LEU:CD1 | 1.78 | 1.27 |
| 1:A:721:LYS:CG | 1:A:736:GLN:OE1 | 1.82 | 1.27 |
| 1:D:534:SER:O | 4:9:351:THR:CA | 1.81 | 1.27 |
| 1:D:629:GLU:HA | 1:D:643:GLY:O | 1.17 | 1.27 |
| 1:J:721:LYS:CG | 1:J:736:GLN:OE1 | 1.83 | 1.27 |
| 1:S:795:ARG:CG | 3:U:118:MET:CE | 1.96 | 1.27 |
| 1:S:792:ALA:CB | 3:U:42:THR:CG2 | 2.11 | 1.27 |
| 1:S:537:GLU:C | 4:2:349:LEU:HD13 | 1.52 | 1.27 |
| 1:A:499:GLU:OE1 | 1:A:766:PHE:HZ | 1.08 | 1.27 |
| 1:A:795:ARG:CZ | 3:C:116:GLU:OE2 | 1.81 | 1.27 |
| 1:G:552:ASN:O | 4:X:47:MET:SD | 1.91 | 1.27 |
| 4:2:287:ILE:CB | 4:4:203:THR:HG22 | 1.62 | 1.27 |
| 1:A:707:CYS:HA | 1:A:714:ARG:NH1 | 1.45 | 1.27 |
| 1:D:537:GLU:C | 4:9:349:LEU:HD13 | 1.52 | 1.27 |
| 1:A:831:TRP:NE1 | 2:B:51:PHE:CZ | 2.03 | 1.27 |
| 1:J:799:MET:SD | 3:L:32:ASP:CG | 2.13 | 1.27 |
| 4:2:287:ILE:HB | 4:4:203:THR:CG2 | 1.62 | 1.27 |
| 1:G:728:ASN:OD1 | 3:I:114:LEU:CD2 | 1.81 | 1.27 |
| 1:A:831:TRP:CD1 | 2:B:51:PHE:CZ | 2.21 | 1.27 |
| 1:D:735:GLY:O | 1:D:743:ALA:HB2 | 1.29 | 1.27 |
| 1:D:795:ARG:HG2 | 3:F:118:MET:CE | 1.64 | 1.27 |
| 1:J:735:GLY:O | 1:J:743:ALA:HB2 | 1.29 | 1.26 |
| 1:M:721:LYS:HG3 | 1:M:736:GLN:CD | 1.54 | 1.26 |
| 1:S:534:SER:O | 4:2:351:THR:CA | 1.81 | 1.26 |
| 1:M:831:TRP:HH2 | 2:N:47:LEU:CD2 | 1.49 | 1.26 |
| 1:D:792:ALA:CB | 3:F:42:THR:HG22 | 1.64 | 1.26 |
| 1:G:730:SER:OG | 3:I:113:THR:HG21 | 1.21 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:721:LYS:CG | 1:M:736:GLN:OE1 | 1.83 | 1.26 |
| 1:S:753:VAL:HG13 | 1:S:779:ARG:CZ | 1.63 | 1.26 |
| 2:B:54:MET:HA | 2:H:21:GLU:OE1 | 1.30 | 1.26 |
| 1:D:721:LYS:CG | 1:D:736:GLN:OE1 | 1.82 | 1.26 |
| 1:G:769:ALA:HB3 | 1:G:770:GLY:CA | 1.63 | 1.26 |
| 1:S:795:ARG:HH21 | 3:U:116:GLU:CB | 1.49 | 1.26 |
| 1:A:629:GLU:HA | 1:A:643:GLY:O | 1.17 | 1.26 |
| 1:D:721:LYS:HG3 | 1:D:736:GLN:CD | 1.54 | 1.26 |
| 1:G:629:GLU:HA | 1:G:643:GLY:O | 1.17 | 1.26 |
| 1:S:721:LYS:CG | 1:S:736:GLN:OE1 | 1.83 | 1.26 |
| 1:G:538:GLU:O | 4:V:349:LEU:HD11 | 1.34 | 1.26 |
| 1:M:538:GLU:C | 4:Z:349:LEU:HD12 | 1.48 | 1.26 |
| 1:A:797:PHE:CZ | 3:C:146:ILE:HD13 | 1.68 | 1.26 |
| 1:S:786:ILE:O | 1:S:789:ALA:N | 1.67 | 1.26 |
| 4:I:247:VAL:N | 4:Y:324:THR:HG21 | 1.49 | 1.25 |
| 1:S:721:LYS:HG3 | 1:S:736:GLN:CD | 1.54 | 1.25 |
| 2:T:117:LEU:CD1 | 2:T:147:ASN:CG | 2.05 | 1.25 |
| 4:4:287:ILE:HG23 | 4:6:202:THR:OG1 | 1.28 | 1.25 |
| 1:A:534:SER:O | 4:8:351:THR:CA | 1.81 | 1.25 |
| 1:G:534:SER:O | 4:V:351:THR:CA | 1.83 | 1.25 |
| 1:S:795:ARG:CZ | 3:U:116:GLU:HB3 | 1.66 | 1.25 |
| 1:S:819:ASN:OD1 | 2:T:92:ASP:N | 1.69 | 1.25 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:HD11 | 1.65 | 1.25 |
| 1:M:721:LYS:CG | 1:M:736:GLN:CG | 1.97 | 1.25 |
| 1:S:793:ARG:CZ | 3:U:40:ASN:HD22 | 1.47 | 1.25 |
| 4:W:324:THR:HG21 | 4:Y:247:VAL:N | 1.49 | 1.25 |
| 1:A:538:GLU:C | 4:8:349:LEU:HD12 | 1.48 | 1.25 |
| 1:G:149:GLN:CD | 1:G:763:THR:CG2 | 2.00 | 1.25 |
| 1:J:84:MLY:CH1 | 1:J:720:PHE:CD1 | 2.20 | 1.25 |
| 1:M:534:SER:O | 4:Z:351:THR:CA | 1.82 | 1.25 |
| 1:M:795:ARG:CG | 3:O:118:MET:HE3 | 1.61 | 1.25 |
| 1:G:641:LYS:CD | 1:G:647:GLN:NE2 | 1.99 | 1.25 |
| 1:G:721:LYS:HG2 | 1:G:736:GLN:OE1 | 1.29 | 1.25 |
| 1:S:630:ALA:O | 4:2:25:ASP:OD2 | 1.52 | 1.25 |
| 1:G:721:LYS:CG | 1:G:736:GLN:OE1 | 1.83 | 1.24 |
| 1:G:728:ASN:CG | 3:I:114:LEU:CD2 | 2.03 | 1.24 |
| 1:M:819:ASN:CA | 2:N:90:GLY:O | 1.85 | 1.24 |
| 1:J:630:ALA:O | 4:W:25:ASP:OD2 | 1.52 | 1.24 |
| 1:D:818:TYR:CB | 2:E:90:GLY:CA | 1.98 | 1.24 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:HD11 | 1.73 | 1.24 |
| 1:S:770:GLY:O | 1:S:774:LEU:HB2 | 1.34 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:817:GLN:CB | 2:K:127:ARG:CD | 2.13 | 1.24 |
| 1:A:822:SER:OG | 2:B:88:LEU:CD2 | 1.85 | 1.24 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:HD11 | 1.73 | 1.24 |
| 1:A:733:PRO:O | 1:A:737:PHE:HD1 | 0.93 | 1.24 |
| 1:S:817:GLN:HG2 | 2:T:127:ARG:CD | 1.68 | 1.24 |
| 4:X:286:ASP:CG | 4:Z:202:THR:HB | 1.32 | 1.24 |
| 4:9:322:PRO:CB | 4:W:244:ASP:OD2 | 1.86 | 1.24 |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:CG | 2.05 | 1.24 |
| 1:J:506:GLU:OE2 | 1:J:761:GLY:HA2 | 1.36 | 1.24 |
| 2:N:117:LEU:CD1 | 2:N:147:ASN:CG | 2.05 | 1.24 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:HD11 | 1.73 | 1.24 |
| 1:J:84:MLY:HH22 | 1:J:719:ASP:O | 1.12 | 1.24 |
| 4:X:291:LYS:HD2 | 4:Z:244:ASP:N | 1.48 | 1.24 |
| 4:1:287:ILE:HG12 | 4:3:202:THR:CA | 1.66 | 1.24 |
| 1:S:538:GLU:O | 4:2:349:LEU:CD1 | 1.78 | 1.24 |
| 2:K:117:LEU:CD1 | 2:K:147:ASN:CG | 2.05 | 1.24 |
| 1:S:538:GLU:O | 4:2:349:LEU:HD11 | 1.35 | 1.24 |
| 1:D:797:PHE:CD1 | 3:F:146:ILE:CG2 | 2.21 | 1.23 |
| 1:M:646:PHE:CE2 | 1:M:652:LEU:HD11 | 1.73 | 1.23 |
| 1:M:797:PHE:CD1 | 3:O:149:VAL:CG1 | 2.18 | 1.23 |
| 1:A:502:GLU:CA | 1:A:761:GLY:HA3 | 1.69 | 1.23 |
| 1:D:630:ALA:O | 4:9:25:ASP:OD2 | 1.52 | 1.23 |
| 1:D:791:GLN:NE2 | 3:F:116:GLU:H | 1.37 | 1.23 |
| 1:D:791:GLN:NE2 | 3:F:116:GLU:N | 1.86 | 1.23 |
| 1:D:814:PHE:CD1 | 2:E:127:ARG:NH1 | 2.06 | 1.23 |
| 1:J:733:PRO:O | 1:J:737:PHE:HD1 | 0.93 | 1.23 |
| 2:K:121:LEU:C | 2:K:128:PHE:CB | 2.07 | 1.23 |
| 1:M:35:MLY:CH2 | 1:M:777:GLU:HG2 | 1.68 | 1.23 |
| 1:M:799:MET:SD | 3:O:32:ASP:CB | 2.24 | 1.23 |
| 4:2:290:ARG:HH21 | 4:4:202:THR:CG2 | 1.50 | 1.23 |
| 1:A:499:GLU:OE1 | 1:A:766:PHE:CZ | 1.92 | 1.23 |
| 1:D:641:LYS:CG | 1:D:647:GLN:CG | 2.15 | 1.23 |
| 2:H:121:LEU:C | 2:H:128:PHE:CB | 2.07 | 1.23 |
| 1:S:646:PHE:CE2 | 1:S:652:LEU:HD11 | 1.73 | 1.23 |
| 1:S:798:LEU:CD1 | 3:U:126:LEU:HD21 | 1.67 | 1.23 |
| 1:S:834:LEU:CD1 | 2:T:51:PHE:HE1 | 1.52 | 1.23 |
| 1:G:557:GLU:CB | 4:X:46:GLY:O | 1.86 | 1.23 |
| 1:D:538:GLU:O | 4:9:349:LEU:CD1 | 1.78 | 1.23 |
| 1:D:641:LYS:CD | 1:D:647:GLN:NE2 | 1.99 | 1.23 |
| 1:S:770:GLY:O | 1:S:774:LEU:N | 1.68 | 1.23 |
| 1:G:641:LYS:CG | 1:G:647:GLN:CG | 2.16 | 1.23 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:757:GLN:CG | 1:G:776:GLU:CG | 1.77 | 1.23 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:CD2 | 1.97 | 1.23 |
| 1:D:733:PRO:O | 1:D:737:PHE:HD1 | 0.93 | 1.23 |
| 1:M:215:GLN:N | 1:M:340:ILE:CG1 | 2.02 | 1.23 |
| 1:M:506:GLU:OE2 | 1:M:761:GLY:HA2 | 1.37 | 1.23 |
| 1:S:641:LYS:CD | 1:S:647:GLN:NE2 | 1.99 | 1.23 |
| 1:S:798:LEU:HD11 | 3:U:126:LEU:CG | 1.68 | 1.23 |
| 2:T:121:LEU:C | 2:T:128:PHE:CB | 2.07 | 1.23 |
| 1:G:215:GLN:N | 1:G:340:ILE:CG1 | 2.02 | 1.23 |
| 1:G:629:GLU:CA | 1:G:643:GLY:O | 1.87 | 1.23 |
| 1:M:641:LYS:CD | 1:M:647:GLN:NE2 | 1.99 | 1.23 |
| 1:S:750:GLY:HA2 | 3:U:89:GLU:CB | 1.69 | 1.23 |
| 4:V:325:MET:SD | 4:X:244:ASP:HB2 | 1.77 | 1.23 |
| 1:D:215:GLN:N | 1:D:340:ILE:HG12 | 1.20 | 1.23 |
| 1:G:733:PRO:O | 1:G:737:PHE:HD1 | 0.93 | 1.23 |
| 1:J:215:GLN:N | 1:J:340:ILE:HG12 | 1.20 | 1.23 |
| 1:S:215:GLN:N | 1:S:340:ILE:CG1 | 2.02 | 1.23 |
| 1:S:791:GLN:OE1 | 3:U:116:GLU:N | 1.70 | 1.23 |
| 4:8:322:PRO:CB | 4:V:244:ASP:OD2 | 1.86 | 1.23 |
| 1:A:630:ALA:O | 4:8:25:ASP:OD2 | 1.53 | 1.23 |
| 1:A:768:MLY:CB | 1:A:771:LEU:HB2 | 1.69 | 1.23 |
| 1:D:215:GLN:N | 1:D:340:ILE:CG1 | 2.02 | 1.23 |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:CG | 2.05 | 1.23 |
| 1:M:629:GLU:CA | 1:M:643:GLY:O | 1.87 | 1.22 |
| 2:N:121:LEU:C | 2:N:128:PHE:CB | 2.07 | 1.22 |
| 1:S:93:MET:HE2 | 1:S:764:MLY:CB | 1.69 | 1.22 |
| 4:V:324:THR:HG21 | 4:X:247:VAL:N | 1.49 | 1.22 |
| 4:7:322:PRO:CB | 4:9:244:ASP:OD2 | 1.86 | 1.22 |
| 1:D:534:SER:O | 4:9:351:THR:CB | 1.88 | 1.22 |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:CG | 2.05 | 1.22 |
| 1:D:795:ARG:CG | 3:F:118:MET:HE1 | 1.68 | 1.22 |
| 1:J:557:GLU:CB | 4:Y:46:GLY:O | 1.87 | 1.22 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:HD11 | 1.73 | 1.22 |
| 1:M:735:GLY:O | 1:M:743:ALA:HB2 | 1.29 | 1.22 |
| 1:M:821:ARG:NH2 | 2:N:127:ARG:CG | 2.01 | 1.22 |
| 1:A:641:LYS:CD | 1:A:647:GLN:NE2 | 1.99 | 1.22 |
| 2:B:121:LEU:C | 2:B:128:PHE:CB | 2.07 | 1.22 |
| 1:A:505:MLY:CA | 1:A:762:HIS:CD2 | 2.21 | 1.22 |
| 1:J:567:LYS:NZ | 4:Y:92:ASN:ND2 | 1.85 | 1.22 |
| 1:J:641:LYS:CG | 1:J:647:GLN:CG | 2.16 | 1.22 |
| 1:S:534:SER:O | 4:2:351:THR:CB | 1.87 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:629:GLU:CA | 1:S:643:GLY:O | 1.87 | 1.22 |
| 1:J:215:GLN:N | 1:J:340:ILE:CG1 | 2.02 | 1.22 |
| 1:M:534:SER:O | 4:Z:351:THR:CB | 1.87 | 1.22 |
| 1:S:641:LYS:CG | 1:S:647:GLN:CG | 2.16 | 1.22 |
| 4:1:244:ASP:HB2 | 4:Y:325:MET:SD | 1.77 | 1.22 |
| 1:A:629:GLU:CA | 1:A:643:GLY:O | 1.87 | 1.22 |
| 1:J:797:PHE:CD1 | 3:L:146:ILE:CG2 | 2.22 | 1.22 |
| 4:2:244:ASP:OD2 | 4:Z:322:PRO:CB | 1.86 | 1.22 |
| 1:A:534:SER:O | 4:8:351:THR:CB | 1.87 | 1.22 |
| 1:A:215:GLN:N | 1:A:340:ILE:CG1 | 2.02 | 1.22 |
| 1:S:783:LEU:CA | 1:S:786:ILE:HG13 | 1.68 | 1.22 |
| 1:S:817:GLN:CG | 2:T:127:ARG:CD | 2.16 | 1.22 |
| 2:E:121:LEU:C | 2:E:128:PHE:CB | 2.07 | 1.21 |
| 1:J:821:ARG:NH2 | 2:K:127:ARG:HG2 | 1.54 | 1.21 |
| 1:S:770:GLY:C | 1:S:771:LEU:C | 1.99 | 1.21 |
| 1:M:733:PRO:O | 1:M:737:PHE:HD1 | 0.93 | 1.21 |
| 1:S:819:ASN:CA | 2:T:90:GLY:O | 1.88 | 1.21 |
| 4:W:325:MET:SD | 4:Y:244:ASP:HB2 | 1.77 | 1.21 |
| 1:A:502:GLU:HG3 | 1:A:761:GLY:N | 1.52 | 1.21 |
| 1:D:629:GLU:CA | 1:D:643:GLY:O | 1.87 | 1.21 |
| 1:G:783:LEU:O | 1:G:787:ILE:N | 1.71 | 1.21 |
| 1:G:534:SER:O | 4:V:351:THR:CB | 1.89 | 1.21 |
| 1:A:641:LYS:CG | 1:A:647:GLN:HG3 | 1.71 | 1.21 |
| 1:J:84:MLY:CH1 | 1:J:720:PHE:HD1 | 1.52 | 1.21 |
| 4:3:288:ASP:OD2 | 4:5:203:THR:CG2 | 1.89 | 1.21 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:HD11 | 1.64 | 1.21 |
| 1:A:795:ARG:HD2 | 3:C:35:ARG:NH1 | 1.54 | 1.21 |
| 1:M:641:LYS:CG | 1:M:647:GLN:HG3 | 1.71 | 1.21 |
| 1:A:553:MLY:CE | 4:V:45:VAL:HA | 1.52 | 1.21 |
| 1:M:806:MET:N | 1:M:807:VAL:N | 1.88 | 1.21 |
| 1:S:797:PHE:CE1 | 3:U:146:ILE:O | 1.94 | 1.21 |
| 1:J:641:LYS:CD | 1:J:647:GLN:NE2 | 1.99 | 1.21 |
| 1:S:538:GLU:C | 4:2:349:LEU:HD12 | 1.48 | 1.21 |
| 1:D:791:GLN:HE22 | 3:F:115:GLY:C | 1.43 | 1.21 |
| 1:M:641:LYS:CG | 1:M:647:GLN:CG | 2.16 | 1.21 |
| 1:A:721:LYS:HG2 | 1:A:736:GLN:OE1 | 1.29 | 1.21 |
| 1:J:629:GLU:CA | 1:J:643:GLY:O | 1.87 | 1.21 |
| 1:M:831:TRP:CH2 | 2:N:47:LEU:CD2 | 2.23 | 1.21 |
| 1:J:534:SER:O | 4:W:351:THR:CB | 1.87 | 1.21 |
| 1:S:733:PRO:O | 1:S:737:PHE:HD1 | 0.93 | 1.21 |
| 4:X:286:ASP:OD1 | 4:Z:202:THR:HB | 1.05 | 1.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:798:LEU:CD1 | 3:U:126:LEU:CD1 | 2.12 | 1.20 |
| 1:G:567:LYS:NZ | 4:X:92:ASN:ND2 | 1.86 | 1.20 |
| 1:A:501:GLU:HG2 | 1:A:762:HIS:ND1 | 1.54 | 1.20 |
| 1:S:836:PHE:CZ | 2:T:160:GLY:N | 2.09 | 1.20 |
| 4:4:288:ASP:CG | 4:6:203:THR:HG21 | 1.60 | 1.20 |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:CB | 2.19 | 1.20 |
| 1:D:641:LYS:CG | 1:D:647:GLN:HG3 | 1.70 | 1.20 |
| 4:1:288:ASP:CG | 4:3:203:THR:HG21 | 1.62 | 1.20 |
| 1:A:641:LYS:CG | 1:A:647:GLN:CG | 2.16 | 1.20 |
| 1:J:792:ALA:CA | 3:L:42:THR:HG22 | 1.70 | 1.20 |
| 1:M:35:MLY:HH22 | 1:M:777:GLU:CG | 1.71 | 1.20 |
| 1:M:630:ALA:O | 4:Z:25:ASP:OD2 | 1.52 | 1.20 |
| 1:D:538:GLU:C | 4:9:349:LEU:HD12 | 1.48 | 1.20 |
| 1:J:819:ASN:CG | 2:K:92:ASP:HB2 | 1.62 | 1.20 |
| 1:G:538:GLU:C | 4:V:349:LEU:HD12 | 1.48 | 1.20 |
| 1:D:791:GLN:CD | 3:F:116:GLU:H | 1.45 | 1.20 |
| 1:G:754:ASP:CA | 1:G:779:ARG:CD | 2.17 | 1.20 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CD | 1.59 | 1.20 |
| 1:M:538:GLU:OE2 | 4:Z:355:MET:CE | 1.90 | 1.20 |
| 4:7:322:PRO:HB2 | 4:9:244:ASP:OD2 | 1.39 | 1.19 |
| 1:D:538:GLU:OE2 | 4:9:355:MET:CE | 1.90 | 1.19 |
| 1:J:641:LYS:CG | 1:J:647:GLN:HG3 | 1.71 | 1.19 |
| 1:S:641:LYS:CG | 1:S:647:GLN:HG3 | 1.71 | 1.19 |
| 4:4:288:ASP:OD2 | 4:6:203:THR:CG2 | 1.89 | 1.19 |
| 1:J:557:GLU:CA | 4:Y:48:GLY:N | 1.98 | 1.19 |
| 1:S:731:ALA:HB1 | 3:U:93:VAL:C | 1.61 | 1.19 |
| 1:S:783:LEU:HA | 1:S:786:ILE:HG13 | 1.20 | 1.19 |
| 4:1:287:ILE:CG2 | 4:3:202:THR:CB | 1.98 | 1.19 |
| 4:2:290:ARG:NH2 | 4:4:202:THR:HG22 | 1.58 | 1.19 |
| 1:D:538:GLU:O | 4:9:349:LEU:HD11 | 1.35 | 1.19 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:CG | 2.05 | 1.19 |
| 1:S:538:GLU:OE2 | 4:2:355:MET:CE | 1.90 | 1.19 |
| 1:D:557:GLU:H | 4:W:48:GLY:CA | 1.56 | 1.19 |
| 1:G:641:LYS:CG | 1:G:647:GLN:HG3 | 1.71 | 1.19 |
| 1:M:553:MLY:CE | 4:2:45:VAL:HA | 1.52 | 1.19 |
| 1:A:795:ARG:HB3 | 3:C:35:ARG:NH2 | 1.57 | 1.19 |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:OD1 | 1.32 | 1.19 |
| 1:S:796:GLY:CA | 3:U:35:ARG:HD3 | 1.71 | 1.19 |
| 1:A:800:ARG:CB | 3:C:149:VAL:HG22 | 1.71 | 1.19 |
| 2:K:117:LEU:CD1 | 2:K:147:ASN:CB | 2.19 | 1.19 |
| 1:J:819:ASN:ND2 | 2:K:92:ASP:HB2 | 1.53 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:557:GLU:H | 4:2:48:GLY:CA | 1.56 | 1.19 |
| 1:M:829:TRP:CZ2 | 2:N:87:LYS:HE2 | 1.78 | 1.19 |
| 1:S:798:LEU:CD1 | 3:U:126:LEU:CD2 | 2.20 | 1.19 |
| 1:A:839:MLY:HH13 | 2:B:159:HIS:CD2 | 1.76 | 1.19 |
| 1:J:538:GLU:OE2 | 4:W:355:MET:CE | 1.90 | 1.19 |
| 4:4:287:ILE:CG2 | 4:6:202:THR:OG1 | 1.84 | 1.19 |
| 2:T:117:LEU:CD1 | 2:T:147:ASN:CB | 2.19 | 1.19 |
| 1:J:95:THR:CA | 1:J:713:SER:HB3 | 1.72 | 1.18 |
| 1:M:721:LYS:HA | 1:M:736:GLN:NE2 | 1.58 | 1.18 |
| 4:2:244:ASP:OD2 | 4:Z:322:PRO:HB2 | 1.39 | 1.18 |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:CB | 2.19 | 1.18 |
| 1:M:783:LEU:CG | 1:M:786:ILE:CD1 | 1.79 | 1.18 |
| 1:S:549:SER:HA | 4:4:43:VAL:HG11 | 1.19 | 1.18 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:CG | 1.74 | 1.18 |
| 1:A:735:GLY:O | 1:A:743:ALA:CB | 1.91 | 1.18 |
| 1:G:641:LYS:CB | 1:G:647:GLN:NE2 | 2.07 | 1.18 |
| 1:J:721:LYS:HA | 1:J:736:GLN:NE2 | 1.58 | 1.18 |
| 1:G:553:MLY:CE | 4:X:45:VAL:CB | 2.22 | 1.18 |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:CB | 2.19 | 1.18 |
| 1:S:641:LYS:HD2 | 1:S:647:GLN:NE2 | 1.59 | 1.18 |
| 1:S:641:LYS:CB | 1:S:647:GLN:NE2 | 2.07 | 1.18 |
| 1:D:641:LYS:CB | 1:D:647:GLN:NE2 | 2.07 | 1.18 |
| 1:G:557:GLU:CA | 4:X:48:GLY:N | 1.99 | 1.18 |
| 1:J:739:ASP:HB3 | 1:J:742:LYS:HB3 | 1.21 | 1.18 |
| 1:S:829:TRP:CZ3 | 2:T:87:LYS:NZ | 2.12 | 1.18 |
| 1:J:553:MLY:HG3 | 4:Y:45:VAL:O | 1.01 | 1.18 |
| 1:D:538:GLU:HA | 4:9:349:LEU:CD1 | 1.55 | 1.18 |
| 1:A:791:GLN:NE2 | 3:C:116:GLU:H | 1.41 | 1.18 |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:OD1 | 1.32 | 1.18 |
| 1:G:721:LYS:HA | 1:G:736:GLN:NE2 | 1.58 | 1.18 |
| 1:J:538:GLU:HA | 4:W:349:LEU:CD1 | 1.55 | 1.18 |
| 2:N:117:LEU:CD1 | 2:N:147:ASN:CB | 2.19 | 1.18 |
| 1:D:721:LYS:HA | 1:D:736:GLN:NE2 | 1.58 | 1.18 |
| 1:J:641:LYS:CB | 1:J:647:GLN:NE2 | 2.07 | 1.18 |
| 1:M:641:LYS:CB | 1:M:647:GLN:NE2 | 2.07 | 1.18 |
| 1:A:557:GLU:H | 4:V:48:GLY:CA | 1.56 | 1.18 |
| 1:D:735:GLY:O | 1:D:743:ALA:CB | 1.91 | 1.17 |
| 1:G:817:GLN:OE1 | 2:H:127:ARG:HD2 | 1.41 | 1.17 |
| 1:S:728:ASN:OD1 | 3:U:90:GLY:HA2 | 1.00 | 1.17 |
| 1:J:538:GLU:O | 4:W:349:LEU:HD11 | 1.35 | 1.17 |
| 4:9:322:PRO:HB2 | 4:W:244:ASP:OD2 | 1.39 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:641:LYS:CB | 1:A:647:GLN:NE2 | 2.07 | 1.17 |
| 1:D:201:ALA:O | 1:D:202:SER:HB3 | 1.36 | 1.17 |
| 1:G:538:GLU:OE2 | 4:V:355:MET:CE | 1.90 | 1.17 |
| 1:J:94:MET:O | 1:J:713:SER:HB3 | 1.43 | 1.17 |
| 1:A:538:GLU:OE2 | 4:8:355:MET:CE | 1.91 | 1.17 |
| 1:A:95:THR:OG1 | 1:A:769:ALA:HA | 1.45 | 1.17 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:HD11 | 1.64 | 1.17 |
| 1:J:553:MLY:CE | 4:Y:45:VAL:CB | 2.21 | 1.17 |
| 1:M:506:GLU:OE2 | 1:M:761:GLY:CA | 1.91 | 1.17 |
| 2:T:144:VAL:CG1 | 2:T:153:ILE:HD11 | 1.64 | 1.17 |
| 1:G:553:MLY:HG3 | 4:X:45:VAL:O | 1.01 | 1.17 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:HA | 1.78 | 1.17 |
| 1:J:721:LYS:HG3 | 1:J:736:GLN:HG2 | 1.25 | 1.17 |
| 1:G:639:GLY:HA2 | 4:V:345:ILE:HA | 1.26 | 1.17 |
| 4:9:290:ARG:NH2 | 4:W:202:THR:HG23 | 1.59 | 1.17 |
| 1:J:553:MLY:HE2 | 4:Y:45:VAL:CB | 1.74 | 1.17 |
| 4:2:202:THR:HG23 | 4:Z:290:ARG:NH2 | 1.59 | 1.17 |
| 1:G:639:GLY:CA | 4:V:345:ILE:HA | 1.73 | 1.17 |
| 1:G:792:ALA:HB2 | 3:I:42:THR:CB | 1.73 | 1.17 |
| 4:7:290:ARG:NH2 | 4:9:202:THR:HG23 | 1.59 | 1.17 |
| 1:G:90:ASP:OD2 | 1:G:764:MLY:HH11 | 1.02 | 1.17 |
| 1:S:817:GLN:CB | 2:T:127:ARG:HD2 | 1.73 | 1.17 |
| 1:D:724:TYR:CA | 1:D:782:MLY:CD | 2.20 | 1.17 |
| 1:J:553:MLY:CE | 4:Y:45:VAL:HG12 | 1.69 | 1.17 |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:HB3 | 1.75 | 1.16 |
| 1:G:553:MLY:HE2 | 4:X:45:VAL:CB | 1.75 | 1.16 |
| 1:J:530:MET:HE2 | 4:W:354:GLN:HG2 | 1.24 | 1.16 |
| 1:J:640:LYS:HB3 | 1:J:645:SER:OG | 1.46 | 1.16 |
| 2:K:117:LEU:CD1 | 2:K:147:ASN:HB3 | 1.75 | 1.16 |
| 4:X:291:LYS:CD | 4:Z:244:ASP:N | 2.07 | 1.16 |
| 1:D:553:MLY:CE | 4:W:45:VAL:HA | 1.52 | 1.16 |
| 1:G:640:LYS:HB3 | 1:G:645:SER:OG | 1.46 | 1.16 |
| 1:J:641:LYS:CE | 4:W:348:SER:O | 1.93 | 1.16 |
| 1:S:819:ASN:HA | 2:T:90:GLY:O | 0.99 | 1.16 |
| 1:S:795:ARG:HD2 | 3:U:43:ASN:OD1 | 0.98 | 1.16 |
| 1:D:639:GLY:CA | 4:9:345:ILE:HA | 1.73 | 1.16 |
| 1:D:538:GLU:C | 4:9:349:LEU:HD11 | 1.54 | 1.16 |
| 1:M:735:GLY:O | 1:M:743:ALA:CB | 1.91 | 1.16 |
| 1:A:721:LYS:HA | 1:A:736:GLN:NE2 | 1.59 | 1.16 |
| 1:D:649:VAL:HA | 1:D:649:VAL:CG2 | 1.76 | 1.16 |
| 1:M:641:LYS:CE | 4:Z:348:SER:O | 1.93 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:721:LYS:HA | 1:S:736:GLN:NE2 | 1.58 | 1.16 |
| 4:V:325:MET:SD | 4:X:244:ASP:CB | 2.33 | 1.16 |
| 1:A:642:LYS:CG | 4:8:23:GLY:N | 2.09 | 1.16 |
| 1:D:721:LYS:HG3 | 1:D:736:GLN:HG2 | 1.25 | 1.16 |
| 1:S:797:PHE:CE2 | 3:U:146:ILE:HD12 | 1.78 | 1.16 |
| 4:1:288:ASP:OD2 | 4:3:203:THR:HG21 | 1.46 | 1.16 |
| 1:A:768:MLY:HB3 | 1:A:771:LEU:CB | 1.75 | 1.16 |
| 1:D:85:TYR:OH | 1:D:772:LEU:HD23 | 1.24 | 1.16 |
| 1:G:642:LYS:CG | 4:V:23:GLY:N | 2.08 | 1.16 |
| 1:G:831:TRP:HH2 | 2:H:47:LEU:CD2 | 1.36 | 1.16 |
| 1:J:557:GLU:HB3 | 4:Y:46:GLY:O | 0.99 | 1.16 |
| 4:X:291:LYS:HE3 | 4:Z:243:PRO:HB3 | 1.24 | 1.16 |
| 1:A:502:GLU:CG | 1:A:761:GLY:HA3 | 1.76 | 1.16 |
| 1:A:641:LYS:CE | 4:8:348:SER:O | 1.93 | 1.16 |
| 1:D:215:GLN:HA | 1:D:340:ILE:CG2 | 1.76 | 1.16 |
| 1:G:530:MET:HE2 | 4:V:354:GLN:CG | 1.74 | 1.16 |
| 4:7:287:ILE:HG21 | 4:9:205:GLU:HG2 | 1.17 | 1.16 |
| 1:D:712:PRO:CG | 1:D:771:LEU:HB2 | 1.76 | 1.16 |
| 1:J:201:ALA:O | 1:J:202:SER:HB3 | 1.35 | 1.16 |
| 1:J:735:GLY:O | 1:J:743:ALA:CB | 1.91 | 1.16 |
| 2:K:144:VAL:CG1 | 2:K:153:ILE:HD11 | 1.65 | 1.16 |
| 1:G:641:LYS:CE | 4:V:348:SER:O | 1.93 | 1.16 |
| 1:J:642:LYS:CG | 4:W:23:GLY:N | 2.08 | 1.16 |
| 1:D:642:LYS:CG | 4:9:23:GLY:N | 2.08 | 1.16 |
| 1:A:792:ALA:HB2 | 3:C:42:THR:HG22 | 1.24 | 1.16 |
| 1:D:747:LEU:CD1 | 1:D:782:MLY:CH2 | 2.18 | 1.16 |
| 1:M:640:LYS:HB3 | 1:M:645:SER:OG | 1.45 | 1.16 |
| 1:S:727:LEU:HD23 | 1:S:783:LEU:HB3 | 1.20 | 1.16 |
| 1:S:831:TRP:CH2 | 2:T:47:LEU:HD22 | 1.76 | 1.16 |
| 1:S:530:MET:HE2 | 4:2:354:GLN:HG2 | 1.24 | 1.15 |
| 1:G:556:ASP:CG | 4:X:47:MET:HE3 | 1.44 | 1.15 |
| 1:G:735:GLY:O | 1:G:743:ALA:CB | 1.91 | 1.15 |
| 1:G:757:GLN:HG2 | 1:G:776:GLU:OE2 | 1.43 | 1.15 |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:HA | 1.76 | 1.15 |
| 1:J:95:THR:HA | 1:J:713:SER:OG | 1.43 | 1.15 |
| 1:M:639:GLY:CA | 4:Z:345:ILE:HA | 1.73 | 1.15 |
| 1:S:752:ASP:HB3 | 3:U:86:ASP:OD2 | 1.46 | 1.15 |
| 4:8:322:PRO:HB2 | 4:V:244:ASP:OD2 | 1.39 | 1.15 |
| 1:S:641:LYS:CE | 4:2:348:SER:O | 1.93 | 1.15 |
| 1:A:639:GLY:CA | 4:8:345:ILE:HA | 1.74 | 1.15 |
| 1:A:707:CYS:HA | 1:A:714:ARG:CZ | 1.65 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:640:LYS:HB3 | 1:D:645:SER:OG | 1.46 | 1.15 |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:HB3 | 1.76 | 1.15 |
| 1:D:530:MET:HE2 | 4:9:354:GLN:HG2 | 1.25 | 1.15 |
| 1:A:538:GLU:O | 4:8:349:LEU:HD11 | 1.35 | 1.15 |
| 1:S:215:GLN:HA | 1:S:340:ILE:CG2 | 1.75 | 1.15 |
| 1:S:731:ALA:O | 3:U:93:VAL:HG12 | 1.45 | 1.15 |
| 1:S:750:GLY:HA2 | 3:U:89:GLU:HB3 | 1.17 | 1.15 |
| 4:1:244:ASP:CB | 4:Y:325:MET:SD | 2.33 | 1.15 |
| 1:D:201:ALA:O | 1:D:202:SER:CB | 1.92 | 1.15 |
| 1:D:507:GLY:HA3 | 1:D:762:HIS:CG | 1.80 | 1.15 |
| 1:J:768:MLY:HB2 | 1:J:773:GLY:CA | 1.74 | 1.15 |
| 1:J:801:VAL:HG21 | 3:L:126:LEU:CD2 | 1.76 | 1.15 |
| 2:N:117:LEU:CD1 | 2:N:147:ASN:HB3 | 1.76 | 1.15 |
| 1:M:642:LYS:CG | 4:Z:23:GLY:N | 2.08 | 1.15 |
| 1:A:201:ALA:O | 1:A:202:SER:CB | 1.92 | 1.15 |
| 1:A:640:LYS:HB3 | 1:A:645:SER:OG | 1.46 | 1.15 |
| 1:D:836:PHE:CE1 | 2:E:159:HIS:HB2 | 1.80 | 1.15 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:HD11 | 1.64 | 1.15 |
| 1:S:218:LEU:HB2 | 1:S:221:GLN:HG3 | 1.17 | 1.15 |
| 1:S:735:GLY:O | 1:S:743:ALA:CB | 1.91 | 1.15 |
| 1:M:201:ALA:O | 1:M:202:SER:CB | 1.92 | 1.15 |
| 1:S:201:ALA:O | 1:S:202:SER:HB3 | 1.35 | 1.15 |
| 1:S:639:GLY:HA2 | 4:2:345:ILE:HA | 1.26 | 1.15 |
| 1:S:639:GLY:HA3 | 4:2:344:SER:O | 1.46 | 1.15 |
| 4:3:324:THR:CB | 4:5:244:ASP:HA | 1.77 | 1.15 |
| 1:D:641:LYS:CE | 4:9:348:SER:O | 1.93 | 1.15 |
| 1:D:713:SER:HB2 | 1:D:775:LEU:CD2 | 1.77 | 1.15 |
| 1:G:215:GLN:HA | 1:G:340:ILE:CG2 | 1.76 | 1.15 |
| 1:G:817:GLN:CD | 2:H:127:ARG:HD2 | 1.66 | 1.15 |
| 1:J:641:LYS:HD2 | 1:J:647:GLN:NE2 | 1.58 | 1.15 |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:HG22 | 1.21 | 1.15 |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HE2 | 1.00 | 1.15 |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:HB3 | 1.76 | 1.15 |
| 1:M:215:GLN:HA | 1:M:340:ILE:CG2 | 1.75 | 1.15 |
| 1:S:792:ALA:CB | 3:U:42:THR:HA | 1.76 | 1.15 |
| 1:G:639:GLY:HA3 | 4:V:344:SER:O | 1.47 | 1.15 |
| 4:9:287:ILE:HG21 | 4:W:205:GLU:HG2 | 1.17 | 1.15 |
| 1:A:639:GLY:HA3 | 4:8:344:SER:O | 1.47 | 1.15 |
| 1:D:736:GLN:N | 1:D:743:ALA:CB | 2.05 | 1.15 |
| 1:J:538:GLU:C | 4:W:349:LEU:HD11 | 1.54 | 1.15 |
| 1:J:556:ASP:CG | 4:Y:47:MET:HE3 | 1.42 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:111:SER:CA | 2:K:148:VAL:O | 1.95 | 1.15 |
| 4:8:290:ARG:NH2 | 4:V:202:THR:HG23 | 1.59 | 1.15 |
| 2:H:111:SER:CA | 2:H:148:VAL:O | 1.95 | 1.14 |
| 2:K:112:ILE:O | 2:K:147:ASN:O | 1.65 | 1.14 |
| 1:S:642:LYS:CG | 4:2:23:GLY:N | 2.08 | 1.14 |
| 1:A:641:LYS:HD2 | 1:A:647:GLN:NE2 | 1.59 | 1.14 |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:HB3 | 1.08 | 1.14 |
| 1:G:201:ALA:O | 1:G:202:SER:HB3 | 1.35 | 1.14 |
| 1:J:799:MET:SD | 3:L:32:ASP:CB | 2.35 | 1.14 |
| 1:M:218:LEU:HB2 | 1:M:221:GLN:HG3 | 1.17 | 1.14 |
| 2:N:121:LEU:CA | 2:N:128:PHE:HB3 | 1.78 | 1.14 |
| 1:S:538:GLU:C | 4:2:349:LEU:HD11 | 1.54 | 1.14 |
| 1:S:505:MLY:HH11 | 1:S:762:HIS:CE1 | 1.81 | 1.14 |
| 1:J:553:MLY:CE | 4:Y:45:VAL:HG11 | 1.53 | 1.14 |
| 1:S:542:PHE:HA | 4:2:143:TYR:CE1 | 1.82 | 1.14 |
| 2:E:111:SER:CB | 2:E:148:VAL:C | 1.93 | 1.14 |
| 1:J:215:GLN:HA | 1:J:340:ILE:CG2 | 1.75 | 1.14 |
| 1:M:95:THR:HA | 1:M:713:SER:CB | 1.77 | 1.14 |
| 2:N:111:SER:CA | 2:N:148:VAL:O | 1.95 | 1.14 |
| 1:A:215:GLN:HA | 1:A:340:ILE:CG2 | 1.76 | 1.14 |
| 1:A:817:GLN:CD | 2:B:127:ARG:NE | 1.99 | 1.14 |
| 1:D:713:SER:CB | 1:D:775:LEU:HD22 | 1.76 | 1.14 |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:CB | 1.78 | 1.14 |
| 2:H:121:LEU:CA | 2:H:128:PHE:HB3 | 1.78 | 1.14 |
| 1:M:639:GLY:HA3 | 4:Z:344:SER:O | 1.46 | 1.14 |
| 1:M:805:ALA:C | 1:M:807:VAL:N | 2.00 | 1.14 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:HB3 | 0.81 | 1.14 |
| 1:M:542:PHE:HA | 4:Z:143:TYR:CE1 | 1.82 | 1.14 |
| 4:X:325:MET:SD | 4:Z:244:ASP:OD2 | 2.04 | 1.14 |
| 4:2:112:PRO:HG2 | 4:3:197:GLY:CA | 1.76 | 1.14 |
| 4:4:324:THR:CB | 4:6:244:ASP:HA | 1.77 | 1.14 |
| 2:B:121:LEU:CA | 2:B:128:PHE:HB3 | 1.77 | 1.14 |
| 1:G:557:GLU:HB3 | 4:X:46:GLY:O | 0.99 | 1.14 |
| 2:K:121:LEU:CA | 2:K:128:PHE:HB3 | 1.77 | 1.14 |
| 1:S:640:LYS:HB3 | 1:S:645:SER:OG | 1.45 | 1.14 |
| 1:S:792:ALA:HB2 | 3:U:42:THR:CA | 1.78 | 1.14 |
| 1:A:795:ARG:CB | 3:C:35:ARG:NH1 | 2.10 | 1.14 |
| 1:J:831:TRP:CH2 | 2:K:47:LEU:HD21 | 1.83 | 1.14 |
| 1:S:736:GLN:N | 1:S:743:ALA:CB | 2.05 | 1.14 |
| 1:S:795:ARG:HB3 | 3:U:35:ARG:NH2 | 1.62 | 1.14 |
| 1:A:800:ARG:HD2 | 3:C:149:VAL:C | 1.68 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:506:GLU:OE2 | 1:D:764:MLY:HH22 | 1.46 | 1.14 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:OD1 | 1.32 | 1.14 |
| 1:M:817:GLN:CB | 2:N:127:ARG:HD2 | 1.77 | 1.14 |
| 4:W:325:MET:SD | 4:Y:244:ASP:CB | 2.33 | 1.14 |
| 2:B:111:SER:CA | 2:B:148:VAL:O | 1.95 | 1.14 |
| 2:K:111:SER:CB | 2:K:148:VAL:C | 1.92 | 1.14 |
| 1:S:821:ARG:NH2 | 2:T:127:ARG:HG2 | 1.62 | 1.14 |
| 1:A:635:GLY:HA2 | 4:8:334:GLU:HG2 | 1.16 | 1.14 |
| 1:A:641:LYS:NZ | 4:8:348:SER:O | 1.80 | 1.14 |
| 1:D:641:LYS:NZ | 4:9:348:SER:O | 1.80 | 1.14 |
| 1:J:28:GLN:C | 1:J:723:ARG:NH2 | 1.99 | 1.14 |
| 1:S:817:GLN:HB3 | 2:T:127:ARG:NH1 | 1.61 | 1.14 |
| 4:2:112:PRO:HB3 | 4:3:196:ARG:HA | 1.19 | 1.14 |
| 1:A:502:GLU:CG | 1:A:761:GLY:CA | 2.20 | 1.14 |
| 1:D:724:TYR:HA | 1:D:782:MLY:CD | 1.74 | 1.14 |
| 1:G:215:GLN:N | 1:G:340:ILE:HG12 | 1.19 | 1.14 |
| 2:T:111:SER:CA | 2:T:148:VAL:O | 1.95 | 1.14 |
| 1:J:768:MLY:CB | 1:J:773:GLY:CA | 2.23 | 1.13 |
| 2:T:121:LEU:C | 2:T:128:PHE:HB2 | 1.67 | 1.13 |
| 2:E:112:ILE:O | 2:E:147:ASN:O | 1.65 | 1.13 |
| 1:J:817:GLN:CG | 2:K:127:ARG:HB2 | 1.78 | 1.13 |
| 1:M:786:ILE:C | 1:M:787:ILE:N | 2.02 | 1.13 |
| 1:S:599:ASN:OD1 | 1:S:649:VAL:CB | 1.96 | 1.13 |
| 4:4:287:ILE:HD13 | 4:6:203:THR:HB | 1.15 | 1.13 |
| 1:A:839:MLY:CH1 | 2:B:159:HIS:HD2 | 1.62 | 1.13 |
| 1:D:542:PHE:HA | 4:9:143:TYR:CE1 | 1.82 | 1.13 |
| 1:G:84:MLY:HH22 | 1:G:719:ASP:O | 1.22 | 1.13 |
| 1:J:795:ARG:NE | 3:L:116:GLU:OE2 | 1.81 | 1.13 |
| 1:J:641:LYS:NZ | 4:W:348:SER:O | 1.80 | 1.13 |
| 1:M:541:MET:C | 4:Z:143:TYR:OH | 1.87 | 1.13 |
| 1:A:639:GLY:HA2 | 4:8:345:ILE:HA | 1.26 | 1.13 |
| 1:G:649:VAL:HG22 | 1:G:649:VAL:HG13 | 1.21 | 1.13 |
| 1:J:599:ASN:OD1 | 1:J:649:VAL:CB | 1.96 | 1.13 |
| 1:J:817:GLN:CD | 2:K:127:ARG:HD2 | 1.69 | 1.13 |
| 1:S:783:LEU:CG | 1:S:786:ILE:CD1 | 2.20 | 1.13 |
| 2:T:117:LEU:CD1 | 2:T:147:ASN:HB3 | 1.76 | 1.13 |
| 1:A:542:PHE:HA | 4:8:143:TYR:CE1 | 1.82 | 1.13 |
| 1:A:149:GLN:NE2 | 1:A:718:ALA:CB | 2.10 | 1.13 |
| 1:D:218:LEU:HB2 | 1:D:221:GLN:HG3 | 1.17 | 1.13 |
| 1:J:84:MLY:CD | 1:J:724:TYR:HE2 | 1.50 | 1.13 |
| 1:J:542:PHE:HA | 4:W:143:TYR:CE1 | 1.82 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:530:MET:HE2 | 4:8:354:GLN:HG2 | 1.18 | 1.13 |
| 2:B:121:LEU:C | 2:B:128:PHE:HB2 | 1.67 | 1.13 |
| 1:M:641:LYS:NZ | 4:Z:348:SER:O | 1.80 | 1.13 |
| 1:M:836:PHE:CE1 | 2:N:159:HIS:CA | 2.30 | 1.13 |
| 1:S:148:ARG:HH22 | 1:S:764:MLY:CH2 | 1.60 | 1.13 |
| 4:3:287:ILE:CG2 | 4:5:202:THR:OG1 | 1.84 | 1.13 |
| 1:A:641:LYS:CE | 1:A:647:GLN:OE1 | 1.97 | 1.13 |
| 2:E:121:LEU:CA | 2:E:128:PHE:HB3 | 1.77 | 1.13 |
| 1:G:541:MET:C | 4:V:143:TYR:OH | 1.87 | 1.13 |
| 1:S:739:ASP:HB3 | 1:S:742:LYS:HB3 | 1.21 | 1.13 |
| 2:B:112:ILE:O | 2:B:147:ASN:O | 1.65 | 1.13 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:HB3 | 1.79 | 1.13 |
| 1:J:768:MLY:HB2 | 1:J:773:GLY:HA3 | 1.30 | 1.13 |
| 1:M:649:VAL:CG2 | 1:M:649:VAL:HA | 1.76 | 1.13 |
| 2:T:121:LEU:CA | 2:T:128:PHE:HB3 | 1.78 | 1.13 |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:OD1 | 1.32 | 1.13 |
| 2:E:111:SER:CA | 2:E:148:VAL:O | 1.95 | 1.13 |
| 1:G:649:VAL:HA | 1:G:649:VAL:CG2 | 1.76 | 1.13 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:CB | 1.96 | 1.13 |
| 1:S:93:MET:HE1 | 1:S:764:MLY:HB2 | 1.26 | 1.13 |
| 1:D:639:GLY:HA3 | 4:9:344:SER:O | 1.46 | 1.12 |
| 1:G:542:PHE:HA | 4:V:143:TYR:CE1 | 1.82 | 1.12 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:CB | 1.96 | 1.12 |
| 2:N:121:LEU:C | 2:N:128:PHE:HB2 | 1.67 | 1.12 |
| 2:T:112:ILE:O | 2:T:147:ASN:O | 1.65 | 1.12 |
| 1:A:799:MET:CE | 3:C:32:ASP:HB3 | 1.78 | 1.12 |
| 1:D:641:LYS:CE | 1:D:647:GLN:OE1 | 1.97 | 1.12 |
| 2:K:111:SER:HB3 | 2:K:148:VAL:O | 1.50 | 1.12 |
| 1:M:201:ALA:O | 1:M:202:SER:HB3 | 1.35 | 1.12 |
| 1:M:720:PHE:HE1 | 1:M:772:LEU:HD22 | 1.07 | 1.12 |
| 2:N:163:ALA:C | 2:T:21:GLU:HB2 | 1.69 | 1.12 |
| 4:1:287:ILE:CB | 4:3:202:THR:HB | 1.77 | 1.12 |
| 1:S:641:LYS:NZ | 4:2:348:SER:O | 1.80 | 1.12 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:CB | 1.96 | 1.12 |
| 1:J:639:GLY:HA2 | 4:W:345:ILE:HA | 1.26 | 1.12 |
| 1:A:505:MLY:CA | 1:A:762:HIS:HD2 | 1.56 | 1.12 |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:CB | 1.96 | 1.12 |
| 1:G:795:ARG:CB | 3:I:118:MET:HE1 | 1.78 | 1.12 |
| 3:I:48:LYS:C | 3:I:52:ASN:ND2 | 2.03 | 1.12 |
| 1:J:757:GLN:HA | 1:J:776:GLU:HG3 | 1.16 | 1.12 |
| 1:J:541:MET:C | 4:W:143:TYR:OH | 1.87 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:557:GLU:HA | 4:X:48:GLY:N | 1.13 | 1.12 |
| 3:C:48:LYS:C | 3:C:52:ASN:ND2 | 2.03 | 1.12 |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CG | 1.79 | 1.12 |
| 1:M:739:ASP:HB3 | 1:M:742:LYS:HB3 | 1.21 | 1.12 |
| 2:T:111:SER:CB | 2:T:148:VAL:C | 1.92 | 1.12 |
| 3:U:48:LYS:C | 3:U:52:ASN:ND2 | 2.03 | 1.12 |
| 1:A:530:MET:HE2 | 4:8:354:GLN:CG | 1.78 | 1.12 |
| 1:D:541:MET:C | 4:9:143:TYR:OH | 1.87 | 1.12 |
| 1:D:726:VAL:HG11 | 1:D:785:GLU:HB3 | 1.16 | 1.12 |
| 1:G:641:LYS:NZ | 4:V:348:SER:O | 1.80 | 1.12 |
| 1:J:218:LEU:HB2 | 1:J:221:GLN:HG3 | 1.17 | 1.12 |
| 1:J:788:THR:O | 3:L:42:THR:HG21 | 1.49 | 1.12 |
| 3:L:48:LYS:C | 3:L:52:ASN:ND2 | 2.03 | 1.12 |
| 1:M:95:THR:CA | 1:M:713:SER:HB3 | 1.80 | 1.12 |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:OD1 | 1.32 | 1.12 |
| 3:O:48:LYS:C | 3:O:52:ASN:ND2 | 2.03 | 1.12 |
| 1:S:215:GLN:N | 1:S:340:ILE:HG12 | 1.20 | 1.12 |
| 1:M:623:PHE:CG | 1:M:623:PHE:CB | 2.33 | 1.12 |
| 1:S:649:VAL:CG2 | 1:S:649:VAL:HA | 1.77 | 1.12 |
| 1:S:836:PHE:CE1 | 2:T:160:GLY:N | 2.16 | 1.12 |
| 4:2:205:GLU:HG2 | 4:Z:287:ILE:HG21 | 1.17 | 1.12 |
| 2:B:121:LEU:O | 2:B:128:PHE:HB2 | 0.94 | 1.12 |
| 1:D:739:ASP:HB3 | 1:D:742:LYS:HB3 | 1.21 | 1.12 |
| 1:J:623:PHE:CG | 1:J:623:PHE:CB | 2.33 | 1.12 |
| 1:M:819:ASN:HA | 2:N:90:GLY:O | 0.95 | 1.12 |
| 1:J:639:GLY:HA3 | 4:W:344:SER:O | 1.46 | 1.12 |
| 1:A:649:VAL:CG2 | 1:A:649:VAL:HA | 1.76 | 1.12 |
| 1:A:791:GLN:HE22 | 3:C:116:GLU:N | 1.47 | 1.12 |
| 1:D:813:ILE:HG21 | 2:E:128:PHE:CE1 | 1.76 | 1.12 |
| 1:G:641:LYS:HD2 | 1:G:647:GLN:NE2 | 1.59 | 1.12 |
| 1:S:721:LYS:HG3 | 1:S:736:GLN:HG2 | 1.25 | 1.12 |
| 1:G:538:GLU:C | 4:V:349:LEU:HD11 | 1.54 | 1.12 |
| 4:X:324:THR:CG2 | 4:Z:247:VAL:CG2 | 2.26 | 1.12 |
| 1:G:641:LYS:CE | 1:G:647:GLN:OE1 | 1.97 | 1.12 |
| 1:G:728:ASN:OD1 | 3:I:114:LEU:HD21 | 1.43 | 1.12 |
| 1:J:831:TRP:CH2 | 2:K:47:LEU:CD2 | 2.33 | 1.12 |
| 2:K:121:LEU:C | 2:K:128:PHE:HB2 | 1.67 | 1.12 |
| 1:M:635:GLY:HA2 | 4:Z:334:GLU:HG2 | 1.16 | 1.12 |
| 1:M:641:LYS:CE | 1:M:647:GLN:OE1 | 1.97 | 1.12 |
| 1:S:93:MET:HE3 | 1:S:764:MLY:HD2 | 1.27 | 1.12 |
| 1:A:538:GLU:C | 4:8:349:LEU:HD11 | 1.54 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:795:ARG:HB3 | 3:C:35:ARG:NH1 | 1.62 | 1.11 |
| 1:J:641:LYS:CE | 1:J:647:GLN:OE1 | 1.97 | 1.11 |
| 4:3:287:ILE:HD13 | 4:5:203:THR:HB | 1.15 | 1.11 |
| 1:D:641:LYS:CE | 1:D:647:GLN:CD | 2.18 | 1.11 |
| 1:D:641:LYS:HD2 | 1:D:647:GLN:NE2 | 1.59 | 1.11 |
| 2:E:117:LEU:HB2 | 2:E:147:ASN:CG | 1.70 | 1.11 |
| 1:G:635:GLY:HA2 | 4:V:334:GLU:HG2 | 1.16 | 1.11 |
| 1:G:754:ASP:CG | 1:G:779:ARG:HD2 | 1.69 | 1.11 |
| 1:S:641:LYS:CE | 1:S:647:GLN:OE1 | 1.97 | 1.11 |
| 1:J:635:GLY:HA2 | 4:W:334:GLU:HG2 | 1.16 | 1.11 |
| 1:S:541:MET:C | 4:2:143:TYR:OH | 1.87 | 1.11 |
| 1:A:839:MLY:CH1 | 2:B:159:HIS:CD2 | 2.33 | 1.11 |
| 2:H:121:LEU:O | 2:H:128:PHE:HB2 | 0.94 | 1.11 |
| 1:S:641:LYS:HG3 | 1:S:647:GLN:HG3 | 1.20 | 1.11 |
| 1:S:641:LYS:CE | 1:S:647:GLN:CD | 2.18 | 1.11 |
| 1:S:93:MET:CE | 1:S:764:MLY:HD2 | 1.80 | 1.11 |
| 2:T:117:LEU:HD12 | 2:T:147:ASN:OD1 | 1.32 | 1.11 |
| 1:S:791:GLN:HE22 | 3:U:115:GLY:CA | 1.61 | 1.11 |
| 1:A:795:ARG:CD | 3:C:43:ASN:OD1 | 1.98 | 1.11 |
| 1:D:623:PHE:CG | 1:D:623:PHE:CB | 2.33 | 1.11 |
| 1:D:797:PHE:HE1 | 3:F:146:ILE:HA | 1.00 | 1.11 |
| 4:9:290:ARG:CZ | 4:W:202:THR:HG21 | 1.81 | 1.11 |
| 1:A:641:LYS:CE | 1:A:647:GLN:CD | 2.18 | 1.11 |
| 1:A:721:LYS:CG | 1:A:736:GLN:CG | 1.97 | 1.11 |
| 1:G:218:LEU:HB2 | 1:G:221:GLN:HG3 | 1.17 | 1.11 |
| 2:K:121:LEU:O | 2:K:128:PHE:HB2 | 0.94 | 1.11 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:OE1 | 1.50 | 1.11 |
| 2:T:117:LEU:HB2 | 2:T:147:ASN:CG | 1.70 | 1.11 |
| 1:D:734:GLU:O | 1:D:738:MET:HG2 | 1.51 | 1.11 |
| 1:G:148:ARG:HH21 | 1:G:764:MLY:HH21 | 1.11 | 1.11 |
| 1:G:795:ARG:CG | 3:I:118:MET:CE | 2.04 | 1.11 |
| 1:J:639:GLY:CA | 4:W:345:ILE:HA | 1.73 | 1.11 |
| 1:M:838:ILE:HD11 | 2:N:54:MET:HE1 | 1.17 | 1.11 |
| 3:U:24:LYS:CB | 3:U:63:ILE:O | 1.99 | 1.11 |
| 1:A:95:THR:OG1 | 1:A:769:ALA:CA | 1.99 | 1.11 |
| 1:M:798:LEU:HD12 | 3:O:126:LEU:HD21 | 1.28 | 1.11 |
| 1:A:541:MET:C | 4:8:143:TYR:OH | 1.87 | 1.11 |
| 1:A:218:LEU:HB2 | 1:A:221:GLN:HG3 | 1.17 | 1.11 |
| 1:A:623:PHE:CG | 1:A:623:PHE:CB | 2.33 | 1.11 |
| 1:A:831:TRP:CZ2 | 2:B:47:LEU:HA | 1.84 | 1.11 |
| 2:H:117:LEU:HB2 | 2:H:147:ASN:CG | 1.70 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:795:ARG:HH21 | 3:I:116:GLU:CB | 1.63 | 1.11 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:HH11 | 1.13 | 1.11 |
| 1:S:806:MET:N | 1:S:807:VAL:N | 1.97 | 1.11 |
| 2:B:117:LEU:HB2 | 2:B:147:ASN:CG | 1.71 | 1.11 |
| 3:C:24:LYS:CB | 3:C:63:ILE:O | 1.99 | 1.11 |
| 1:G:754:ASP:OD2 | 1:G:779:ARG:HB2 | 1.42 | 1.11 |
| 3:O:24:LYS:CB | 3:O:63:ILE:O | 1.99 | 1.11 |
| 1:S:530:MET:CE | 4:2:354:GLN:HG2 | 1.80 | 1.11 |
| 1:A:795:ARG:NE | 3:C:43:ASN:OD1 | 1.82 | 1.11 |
| 1:D:797:PHE:CG | 3:F:146:ILE:HG23 | 1.86 | 1.11 |
| 3:F:48:LYS:C | 3:F:52:ASN:ND2 | 2.03 | 1.11 |
| 1:G:641:LYS:CE | 1:G:647:GLN:CD | 2.18 | 1.11 |
| 1:G:795:ARG:HG2 | 3:I:118:MET:HE2 | 1.32 | 1.11 |
| 2:N:112:ILE:O | 2:N:147:ASN:O | 1.65 | 1.11 |
| 1:S:709:LYS:O | 1:S:710:GLY:N | 1.84 | 1.11 |
| 4:4:288:ASP:CG | 4:6:203:THR:HG23 | 1.66 | 1.10 |
| 1:A:721:LYS:HG3 | 1:A:736:GLN:HG2 | 1.25 | 1.10 |
| 1:J:95:THR:CA | 1:J:713:SER:CB | 2.29 | 1.10 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:CG2 | 2.30 | 1.10 |
| 1:M:797:PHE:CD1 | 3:O:149:VAL:HG11 | 1.83 | 1.10 |
| 2:N:117:LEU:HB2 | 2:N:147:ASN:CG | 1.70 | 1.10 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:OE1 | 1.50 | 1.10 |
| 3:L:24:LYS:CB | 3:L:63:ILE:O | 1.99 | 1.10 |
| 4:8:290:ARG:CZ | 4:V:202:THR:HG21 | 1.81 | 1.10 |
| 2:E:121:LEU:C | 2:E:128:PHE:HB2 | 1.67 | 1.10 |
| 1:G:149:GLN:CD | 1:G:763:THR:HG21 | 1.60 | 1.10 |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:HG13 | 1.21 | 1.10 |
| 1:M:649:VAL:O | 1:M:649:VAL:HG12 | 0.94 | 1.10 |
| 1:S:639:GLY:CA | 4:2:345:ILE:HA | 1.73 | 1.10 |
| 1:D:639:GLY:HA2 | 4:9:345:ILE:HA | 1.26 | 1.10 |
| 3:F:24:LYS:CB | 3:F:63:ILE:O | 1.99 | 1.10 |
| 1:G:553:MLY:CE | 4:X:45:VAL:HG12 | 1.69 | 1.10 |
| 1:S:783:LEU:CB | 1:S:786:ILE:CD1 | 2.29 | 1.10 |
| 1:D:202:SER:CA | 1:D:207:LYS:HE2 | 1.82 | 1.10 |
| 1:G:530:MET:CE | 4:V:354:GLN:HG2 | 1.80 | 1.10 |
| 1:G:754:ASP:OD2 | 1:G:779:ARG:HB3 | 1.35 | 1.10 |
| 1:J:571:ALA:O | 1:J:572:LYS:HG3 | 1.52 | 1.10 |
| 1:M:530:MET:CE | 4:Z:354:GLN:HG2 | 1.80 | 1.10 |
| 4:8:287:ILE:HG21 | 4:V:205:GLU:HG2 | 1.17 | 1.10 |
| 1:G:734:GLU:O | 1:G:738:MET:HG2 | 1.51 | 1.10 |
| 2:H:111:SER:CB | 2:H:148:VAL:C | 1.93 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:641:LYS:CE | 1:M:647:GLN:CD | 2.18 | 1.10 |
| 1:M:831:TRP:HH2 | 2:N:47:LEU:HD21 | 1.15 | 1.10 |
| 1:S:635:GLY:HA2 | 4:2:334:GLU:HG2 | 1.16 | 1.10 |
| 1:D:795:ARG:CB | 3:F:35:ARG:NH1 | 2.14 | 1.10 |
| 1:G:649:VAL:HG12 | 1:G:649:VAL:O | 0.94 | 1.10 |
| 1:D:635:GLY:HA2 | 4:9:334:GLU:HG2 | 1.16 | 1.10 |
| 1:S:623:PHE:CG | 1:S:623:PHE:CB | 2.33 | 1.10 |
| 1:S:734:GLU:O | 1:S:738:MET:HG2 | 1.51 | 1.10 |
| 1:A:739:ASP:HB3 | 1:A:742:LYS:HB3 | 1.22 | 1.10 |
| 1:J:710:GLY:CA | 1:J:772:LEU:CD2 | 2.06 | 1.10 |
| 1:M:571:ALA:O | 1:M:572:LYS:HG3 | 1.52 | 1.10 |
| 1:M:734:GLU:O | 1:M:738:MET:HG2 | 1.51 | 1.10 |
| 1:M:800:ARG:NH2 | 3:O:40:ASN:OD1 | 1.84 | 1.10 |
| 1:S:649:VAL:HG12 | 1:S:649:VAL:O | 0.94 | 1.10 |
| 1:D:800:ARG:NH2 | 3:F:40:ASN:ND2 | 2.00 | 1.10 |
| 1:G:623:PHE:CG | 1:G:623:PHE:CB | 2.33 | 1.10 |
| 3:I:24:LYS:CB | 3:I:63:ILE:O | 1.99 | 1.10 |
| 1:J:641:LYS:CE | 1:J:647:GLN:CD | 2.18 | 1.10 |
| 1:J:649:VAL:O | 1:J:649:VAL:HG12 | 0.94 | 1.10 |
| 1:M:641:LYS:HG3 | 1:M:647:GLN:HG3 | 1.20 | 1.10 |
| 1:S:805:ALA:O | 1:S:809:ARG:N | 1.84 | 1.10 |
| 4:2:202:THR:HG21 | 4:Z:290:ARG:CZ | 1.81 | 1.10 |
| 1:A:757:GLN:OE1 | 1:A:771:LEU:HD12 | 1.49 | 1.09 |
| 1:D:649:VAL:O | 1:D:649:VAL:HG12 | 0.94 | 1.09 |
| 2:E:121:LEU:O | 2:E:128:PHE:HB2 | 0.94 | 1.09 |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:HG3 | 1.21 | 1.09 |
| 1:J:202:SER:CA | 1:J:207:LYS:HE2 | 1.82 | 1.09 |
| 1:J:768:MLY:HH11 | 1:J:772:LEU:HD12 | 1.19 | 1.09 |
| 2:N:121:LEU:O | 2:N:128:PHE:HB2 | 0.94 | 1.09 |
| 2:T:121:LEU:O | 2:T:128:PHE:HB2 | 0.94 | 1.09 |
| 1:M:538:GLU:O | 4:Z:349:LEU:HD11 | 1.35 | 1.09 |
| 4:3:288:ASP:CG | 4:5:203:THR:HG23 | 1.66 | 1.09 |
| 1:A:201:ALA:O | 1:A:202:SER:HB3 | 1.35 | 1.09 |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:HG2 | 1.33 | 1.09 |
| 2:E:111:SER:HB3 | 2:E:148:VAL:O | 1.50 | 1.09 |
| 1:G:721:LYS:HA | 1:G:736:GLN:CD | 1.73 | 1.09 |
| 1:J:797:PHE:CZ | 3:L:126:LEU:HD22 | 1.87 | 1.09 |
| 1:S:538:GLU:HA | 4:2:349:LEU:CD1 | 1.55 | 1.09 |
| 1:D:530:MET:CE | 4:9:354:GLN:HG2 | 1.80 | 1.09 |
| 1:D:571:ALA:O | 1:D:572:LYS:HG3 | 1.52 | 1.09 |
| 1:J:557:GLU:HA | 4:Y:48:GLY:N | 1.13 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:799:MET:SD | 3:L:32:ASP:HB3 | 1.92 | 1.09 |
| 1:S:641:LYS:HD2 | 1:S:647:GLN:CD | 1.70 | 1.09 |
| 1:A:721:LYS:HA | 1:A:736:GLN:CD | 1.73 | 1.09 |
| 1:A:834:LEU:HD21 | 2:B:54:MET:HE2 | 1.26 | 1.09 |
| 2:H:111:SER:HB3 | 2:H:148:VAL:O | 1.49 | 1.09 |
| 1:G:201:ALA:O | 1:G:202:SER:CB | 1.92 | 1.09 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:OE1 | 1.50 | 1.09 |
| 1:A:649:VAL:O | 1:A:649:VAL:HG12 | 0.94 | 1.09 |
| 1:A:817:GLN:CD | 2:B:127:ARG:CD | 2.20 | 1.09 |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:CB | 1.65 | 1.09 |
| 1:A:797:PHE:HE2 | 3:C:126:LEU:HD22 | 1.11 | 1.09 |
| 1:G:553:MLY:HE2 | 4:X:45:VAL:HB | 1.09 | 1.09 |
| 1:G:721:LYS:HG3 | 1:G:736:GLN:HG2 | 1.25 | 1.09 |
| 1:J:756:THR:HG21 | 1:J:776:GLU:O | 1.50 | 1.09 |
| 1:A:505:MLY:HB3 | 1:A:762:HIS:H | 1.14 | 1.09 |
| 1:D:834:LEU:HD11 | 2:E:54:MET:CB | 1.81 | 1.09 |
| 1:G:739:ASP:HB3 | 1:G:742:LYS:HB3 | 1.21 | 1.09 |
| 1:G:736:GLN:N | 1:G:743:ALA:CB | 2.04 | 1.09 |
| 1:J:84:MLY:CA | 1:J:723:ARG:CZ | 2.19 | 1.09 |
| 1:S:92:ALA:HB3 | 1:S:764:MLY:CH1 | 1.80 | 1.09 |
| 4:7:290:ARG:CZ | 4:9:202:THR:HG21 | 1.81 | 1.09 |
| 1:A:538:GLU:HA | 4:8:349:LEU:CD1 | 1.54 | 1.09 |
| 1:A:571:ALA:O | 1:A:572:LYS:HG3 | 1.52 | 1.09 |
| 1:A:501:GLU:CG | 1:A:762:HIS:HD1 | 1.64 | 1.09 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:OE1 | 1.50 | 1.09 |
| 2:K:117:LEU:HB2 | 2:K:147:ASN:CG | 1.70 | 1.09 |
| 4:3:288:ASP:CG | 4:5:203:THR:HG21 | 1.60 | 1.09 |
| 1:A:643:GLY:O | 1:A:644:SER:OG | 1.70 | 1.09 |
| 1:D:727:LEU:CB | 1:D:782:MLY:HH12 | 1.77 | 1.09 |
| 1:G:92:ALA:O | 1:G:714:ARG:CG | 2.01 | 1.09 |
| 1:J:530:MET:CE | 4:W:354:GLN:HG2 | 1.80 | 1.09 |
| 1:A:530:MET:CE | 4:8:354:GLN:HG2 | 1.80 | 1.09 |
| 1:A:734:GLU:O | 1:A:738:MET:HG2 | 1.51 | 1.09 |
| 1:A:505:MLY:N | 1:A:762:HIS:CD2 | 2.21 | 1.09 |
| 1:D:649:VAL:HG13 | 1:D:649:VAL:HG22 | 1.21 | 1.09 |
| 1:G:831:TRP:HE1 | 2:H:67:MET:HB3 | 1.02 | 1.09 |
| 1:G:797:PHE:CZ | 3:I:126:LEU:HD22 | 1.87 | 1.09 |
| 1:J:201:ALA:O | 1:J:202:SER:CB | 1.92 | 1.09 |
| 2:E:162:ASP:O | 2:K:21:GLU:HB2 | 1.49 | 1.09 |
| 1:S:721:LYS:HA | 1:S:736:GLN:CD | 1.73 | 1.09 |
| 1:A:822:SER:OG | 2:B:88:LEU:HD23 | 0.93 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:202:SER:CA | 1:G:207:LYS:HE2 | 1.82 | 1.08 |
| 1:G:797:PHE:CD1 | 3:I:146:ILE:HG23 | 1.88 | 1.08 |
| 1:J:643:GLY:O | 1:J:644:SER:OG | 1.69 | 1.08 |
| 1:J:799:MET:SD | 3:L:32:ASP:OD2 | 2.07 | 1.08 |
| 1:M:97:LEU:CD2 | 1:M:712:PRO:HB3 | 1.81 | 1.08 |
| 1:S:538:GLU:OE2 | 4:2:355:MET:HE1 | 1.48 | 1.08 |
| 1:D:638:GLY:CA | 4:9:341:ILE:O | 2.01 | 1.08 |
| 1:A:831:TRP:CE2 | 2:B:51:PHE:CZ | 2.41 | 1.08 |
| 1:D:712:PRO:HG2 | 1:D:771:LEU:CB | 1.82 | 1.08 |
| 1:G:571:ALA:O | 1:G:572:LYS:HG3 | 1.52 | 1.08 |
| 2:H:112:ILE:O | 2:H:147:ASN:O | 1.65 | 1.08 |
| 1:M:530:MET:HE2 | 4:Z:354:GLN:HG2 | 1.31 | 1.08 |
| 1:S:643:GLY:O | 1:S:644:SER:OG | 1.70 | 1.08 |
| 1:S:649:VAL:HG13 | 1:S:649:VAL:HG22 | 1.21 | 1.08 |
| 1:S:770:GLY:O | 1:S:774:LEU:CB | 1.99 | 1.08 |
| 1:S:817:GLN:HG2 | 2:T:127:ARG:HD2 | 1.10 | 1.08 |
| 1:M:639:GLY:HA2 | 4:Z:345:ILE:HA | 1.26 | 1.08 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:CD1 | 1.55 | 1.08 |
| 1:D:836:PHE:HZ | 2:E:160:GLY:N | 1.23 | 1.08 |
| 1:J:638:GLY:CA | 4:W:341:ILE:O | 2.01 | 1.08 |
| 1:M:641:LYS:HD2 | 1:M:647:GLN:NE2 | 1.59 | 1.08 |
| 1:A:709:LYS:C | 1:A:710:GLY:HA3 | 1.73 | 1.08 |
| 1:D:800:ARG:NH2 | 3:F:40:ASN:HD21 | 1.51 | 1.08 |
| 1:G:819:ASN:CG | 2:H:92:ASP:CB | 2.14 | 1.08 |
| 1:M:202:SER:CA | 1:M:207:LYS:HE2 | 1.82 | 1.08 |
| 1:A:202:SER:CA | 1:A:207:LYS:HE2 | 1.82 | 1.08 |
| 1:A:505:MLY:HG3 | 1:A:741:LYS:NZ | 1.67 | 1.08 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:OE1 | 1.50 | 1.08 |
| 1:G:800:ARG:NH2 | 3:I:40:ASN:OD1 | 1.87 | 1.08 |
| 1:J:721:LYS:HA | 1:J:736:GLN:CD | 1.73 | 1.08 |
| 1:M:836:PHE:CE2 | 2:N:160:GLY:N | 2.18 | 1.08 |
| 1:D:747:LEU:HD13 | 1:D:782:MLY:HH21 | 1.22 | 1.08 |
| 1:J:28:GLN:O | 1:J:723:ARG:NH2 | 1.86 | 1.08 |
| 1:J:94:MET:C | 1:J:713:SER:HB3 | 1.72 | 1.08 |
| 1:J:838:ILE:HD11 | 2:K:54:MET:HE1 | 1.16 | 1.08 |
| 1:M:553:MLY:HB3 | 4:2:46:GLY:CA | 1.51 | 1.08 |
| 2:N:111:SER:OG | 2:N:148:VAL:O | 1.71 | 1.08 |
| 1:S:817:GLN:CB | 2:T:127:ARG:HH11 | 1.65 | 1.08 |
| 1:S:529:PRO:HB3 | 4:2:353:GLN:OE1 | 1.53 | 1.08 |
| 1:M:721:LYS:HA | 1:M:736:GLN:CD | 1.73 | 1.08 |
| 1:S:836:PHE:CE2 | 2:T:160:GLY:HA3 | 1.88 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:529:PRO:HB3 | 4:Z:353:GLN:OE1 | 1.53 | 1.08 |
| 4:4:324:THR:OG1 | 4:6:244:ASP:HA | 1.44 | 1.08 |
| 2:B:111:SER:CB | 2:B:148:VAL:C | 1.93 | 1.08 |
| 1:D:641:LYS:HG3 | 1:D:647:GLN:HG3 | 1.20 | 1.08 |
| 1:J:28:GLN:HA | 1:J:723:ARG:NH2 | 1.17 | 1.08 |
| 1:J:820:VAL:HG11 | 2:K:136:MET:HE3 | 1.25 | 1.08 |
| 1:S:792:ALA:CB | 3:U:42:THR:CA | 2.32 | 1.08 |
| 4:1:287:ILE:HB | 4:3:203:THR:HG22 | 1.16 | 1.08 |
| 2:E:123:THR:HA | 3:F:19:ARG:HH22 | 1.18 | 1.08 |
| 1:J:838:ILE:HD11 | 2:K:54:MET:HE3 | 1.31 | 1.08 |
| 1:M:409:GLY:N | 1:M:636:LYS:HG3 | 1.69 | 1.08 |
| 1:S:839:MLY:HH13 | 2:T:159:HIS:HD2 | 1.17 | 1.08 |
| 1:S:638:GLY:CA | 4:2:341:ILE:O | 2.01 | 1.08 |
| 1:J:576:GLU:HG2 | 1:J:577:ALA:N | 1.66 | 1.08 |
| 1:M:643:GLY:O | 1:M:644:SER:OG | 1.70 | 1.08 |
| 1:J:556:ASP:OD1 | 4:Y:47:MET:HE3 | 1.51 | 1.08 |
| 4:1:287:ILE:HD13 | 4:3:203:THR:HB | 1.08 | 1.07 |
| 1:A:538:GLU:OE2 | 4:8:355:MET:HE1 | 1.54 | 1.07 |
| 1:A:736:GLN:HA | 1:A:743:ALA:HB3 | 1.35 | 1.07 |
| 2:B:111:SER:CB | 2:B:148:VAL:O | 0.78 | 1.07 |
| 1:A:831:TRP:CH2 | 2:B:50:THR:HB | 1.89 | 1.07 |
| 1:J:734:GLU:O | 1:J:738:MET:HG2 | 1.51 | 1.07 |
| 2:E:111:SER:OG | 2:E:148:VAL:O | 1.71 | 1.07 |
| 1:D:791:GLN:NE2 | 3:F:115:GLY:CA | 1.84 | 1.07 |
| 1:G:530:MET:HE2 | 4:V:354:GLN:HG2 | 1.15 | 1.07 |
| 2:H:111:SER:CB | 2:H:148:VAL:O | 0.78 | 1.07 |
| 1:G:829:TRP:CZ3 | 2:H:87:LYS:NZ | 2.21 | 1.07 |
| 1:J:820:VAL:HG11 | 2:K:136:MET:CE | 1.84 | 1.07 |
| 1:S:202:SER:CA | 1:S:207:LYS:HE2 | 1.82 | 1.07 |
| 1:S:795:ARG:HB3 | 3:U:35:ARG:HH22 | 0.95 | 1.07 |
| 1:A:93:MET:CE | 1:A:715:VAL:HA | 1.84 | 1.07 |
| 2:B:121:LEU:C | 2:B:128:PHE:HB3 | 1.72 | 1.07 |
| 2:E:111:SER:CB | 2:E:148:VAL:O | 0.78 | 1.07 |
| 1:D:795:ARG:HB3 | 3:F:35:ARG:CZ | 1.84 | 1.07 |
| 1:G:72:VAL:HG13 | 1:G:76:GLN:HB3 | 1.36 | 1.07 |
| 1:G:792:ALA:HB2 | 3:I:42:THR:CA | 1.84 | 1.07 |
| 1:M:649:VAL:HG13 | 1:M:649:VAL:HG22 | 1.21 | 1.07 |
| 1:M:736:GLN:HA | 1:M:743:ALA:HB3 | 1.35 | 1.07 |
| 4:6:3:ASP:HA | 4:6:6:THR:HB | 1.36 | 1.07 |
| 1:A:541:MET:SD | 4:8:345:ILE:O | 2.12 | 1.07 |
| 1:D:409:GLY:N | 1:D:636:LYS:HG3 | 1.70 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:638:GLY:CA | 4:Z:341:ILE:O | 2.01 | 1.07 |
| 1:S:72:VAL:HG13 | 1:S:76:GLN:HB3 | 1.36 | 1.07 |
| 2:T:111:SER:CB | 2:T:148:VAL:O | 0.78 | 1.07 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:HG3 | 1.21 | 1.07 |
| 1:D:541:MET:SD | 4:9:345:ILE:O | 2.12 | 1.07 |
| 1:G:638:GLY:CA | 4:V:341:ILE:O | 2.02 | 1.07 |
| 1:S:571:ALA:O | 1:S:572:LYS:HG3 | 1.52 | 1.07 |
| 1:S:783:LEU:C | 1:S:786:ILE:HG13 | 1.72 | 1.07 |
| 4:2:3:ASP:HA | 4:2:6:THR:HB | 1.36 | 1.07 |
| 1:A:409:GLY:N | 1:A:636:LYS:HG3 | 1.69 | 1.07 |
| 1:A:817:GLN:OE1 | 2:B:127:ARG:NE | 1.87 | 1.07 |
| 1:D:813:ILE:HG21 | 2:E:128:PHE:HE1 | 1.02 | 1.07 |
| 1:G:538:GLU:HA | 4:V:349:LEU:CD1 | 1.55 | 1.07 |
| 1:G:641:LYS:HB2 | 1:G:647:GLN:NE2 | 1.68 | 1.07 |
| 1:M:721:LYS:HG3 | 1:M:736:GLN:HG2 | 1.25 | 1.07 |
| 4:X:3:ASP:HA | 4:X:6:THR:HB | 1.36 | 1.07 |
| 1:M:541:MET:SD | 4:Z:345:ILE:O | 2.13 | 1.07 |
| 4:2:290:ARG:HH21 | 4:4:202:THR:HG21 | 1.16 | 1.07 |
| 1:D:529:PRO:HB3 | 4:9:353:GLN:OE1 | 1.53 | 1.07 |
| 1:D:553:MLY:HB3 | 4:W:46:GLY:CA | 1.51 | 1.07 |
| 1:G:556:ASP:OD1 | 4:X:47:MET:HE3 | 1.53 | 1.07 |
| 1:S:148:ARG:NH2 | 1:S:764:MLY:CH2 | 2.16 | 1.07 |
| 1:S:792:ALA:HB3 | 3:U:42:THR:HG22 | 1.14 | 1.07 |
| 2:T:121:LEU:C | 2:T:128:PHE:HB3 | 1.72 | 1.07 |
| 2:T:111:SER:HB3 | 2:T:148:VAL:O | 1.50 | 1.07 |
| 4:3:324:THR:OG1 | 4:5:244:ASP:HA | 1.45 | 1.07 |
| 1:D:721:LYS:HA | 1:D:736:GLN:CD | 1.73 | 1.07 |
| 1:D:799:MET:HE1 | 3:F:32:ASP:HB3 | 1.37 | 1.07 |
| 1:G:752:ASP:OD1 | 1:G:780:ASP:O | 1.71 | 1.07 |
| 1:G:796:GLY:HA2 | 3:I:35:ARG:HD3 | 1.08 | 1.07 |
| 1:J:541:MET:SD | 4:W:345:ILE:O | 2.13 | 1.07 |
| 2:K:111:SER:CB | 2:K:148:VAL:O | 0.78 | 1.07 |
| 1:M:783:LEU:CB | 1:M:786:ILE:CD1 | 2.32 | 1.07 |
| 1:S:530:MET:HE2 | 4:2:354:GLN:CG | 1.84 | 1.07 |
| 1:D:724:TYR:CB | 1:D:782:MLY:CD | 2.31 | 1.07 |
| 2:N:111:SER:CB | 2:N:148:VAL:O | 0.78 | 1.07 |
| 1:S:201:ALA:O | 1:S:202:SER:CB | 1.92 | 1.07 |
| 2:T:111:SER:OG | 2:T:148:VAL:O | 1.72 | 1.07 |
| 1:G:641:LYS:HD2 | 1:G:647:GLN:CD | 1.70 | 1.07 |
| 1:G:643:GLY:O | 1:G:644:SER:OG | 1.70 | 1.07 |
| 1:M:538:GLU:C | 4:Z:349:LEU:HD11 | 1.54 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:792:ALA:HB2 | 3:O:42:THR:HG22 | 1.36 | 1.07 |
| 1:G:541:MET:SD | 4:V:345:ILE:O | 2.13 | 1.07 |
| 4:4:3:ASP:HA | 4:4:6:THR:HB | 1.36 | 1.06 |
| 1:S:736:GLN:HA | 1:S:743:ALA:HB3 | 1.35 | 1.06 |
| 1:S:834:LEU:CD1 | 2:T:51:PHE:CE1 | 2.31 | 1.06 |
| 1:J:529:PRO:HB3 | 4:W:353:GLN:OE1 | 1.53 | 1.06 |
| 1:S:541:MET:SD | 4:2:345:ILE:O | 2.13 | 1.06 |
| 1:A:638:GLY:CA | 4:8:341:ILE:O | 2.01 | 1.06 |
| 1:D:643:GLY:O | 1:D:644:SER:OG | 1.70 | 1.06 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:HG2 | 1.68 | 1.06 |
| 2:K:114:LYS:HA | 2:K:146:GLY:O | 0.89 | 1.06 |
| 1:S:798:LEU:HD21 | 3:U:126:LEU:HD12 | 1.36 | 1.06 |
| 1:A:641:LYS:HB2 | 1:A:647:GLN:NE2 | 1.68 | 1.06 |
| 1:M:791:GLN:NE2 | 3:O:114:LEU:O | 1.88 | 1.06 |
| 1:G:529:PRO:HB3 | 4:V:353:GLN:OE1 | 1.53 | 1.06 |
| 1:J:530:MET:HE2 | 4:W:354:GLN:CG | 1.84 | 1.06 |
| 1:A:529:PRO:HB3 | 4:8:353:GLN:OE1 | 1.53 | 1.06 |
| 1:D:736:GLN:HA | 1:D:743:ALA:HB3 | 1.35 | 1.06 |
| 2:K:111:SER:OG | 2:K:148:VAL:O | 1.71 | 1.06 |
| 2:N:111:SER:HB3 | 2:N:148:VAL:O | 1.50 | 1.06 |
| 1:S:93:MET:CE | 1:S:764:MLY:CB | 2.27 | 1.06 |
| 1:D:542:PHE:CG | 4:9:143:TYR:HE1 | 1.73 | 1.06 |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:HB2 | 1.14 | 1.06 |
| 1:G:635:GLY:HA3 | 4:V:341:ILE:HD13 | 1.37 | 1.06 |
| 2:H:121:LEU:C | 2:H:128:PHE:HB2 | 1.67 | 1.06 |
| 1:S:641:LYS:HE3 | 1:S:647:GLN:OE1 | 1.50 | 1.06 |
| 1:A:791:GLN:OE1 | 3:C:116:GLU:HG3 | 1.54 | 1.06 |
| 1:A:797:PHE:CZ | 3:C:146:ILE:CD1 | 2.37 | 1.06 |
| 1:D:576:GLU:HG2 | 1:D:577:ALA:N | 1.66 | 1.06 |
| 1:D:72:VAL:HG13 | 1:D:76:GLN:HB3 | 1.36 | 1.06 |
| 2:E:114:LYS:HA | 2:E:146:GLY:O | 0.89 | 1.06 |
| 1:G:792:ALA:HB3 | 3:I:42:THR:HG22 | 1.36 | 1.06 |
| 1:G:831:TRP:CZ2 | 2:H:47:LEU:CD2 | 2.39 | 1.06 |
| 4:1:288:ASP:CG | 4:3:203:THR:CG2 | 2.22 | 1.06 |
| 1:A:817:GLN:HE21 | 2:B:127:ARG:CG | 1.57 | 1.06 |
| 2:E:123:THR:HA | 3:F:19:ARG:NH2 | 1.71 | 1.06 |
| 1:G:821:ARG:NH2 | 2:H:127:ARG:CG | 2.19 | 1.06 |
| 4:Z:3:ASP:HA | 4:Z:6:THR:HB | 1.36 | 1.06 |
| 1:A:93:MET:HG2 | 1:A:715:VAL:HG22 | 1.37 | 1.06 |
| 2:B:54:MET:CA | 2:H:21:GLU:OE1 | 2.04 | 1.06 |
| 1:D:769:ALA:C | 1:D:774:LEU:HB2 | 1.74 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:821:ARG:HH22 | 2:H:127:ARG:CG | 1.68 | 1.06 |
| 2:H:111:SER:OG | 2:H:148:VAL:O | 1.71 | 1.06 |
| 1:J:557:GLU:HB3 | 4:Y:46:GLY:C | 1.75 | 1.06 |
| 1:J:84:MLY:CE | 1:J:724:TYR:HE2 | 1.69 | 1.06 |
| 1:S:409:GLY:N | 1:S:636:LYS:HG3 | 1.69 | 1.06 |
| 4:2:290:ARG:NH2 | 4:4:202:THR:CG2 | 2.15 | 1.06 |
| 2:B:114:LYS:HA | 2:B:146:GLY:O | 0.89 | 1.06 |
| 1:D:793:ARG:HH21 | 3:F:147:MET:CE | 1.68 | 1.06 |
| 1:G:97:LEU:CD2 | 1:G:712:PRO:HB3 | 1.85 | 1.06 |
| 1:J:552:ASN:O | 4:Y:47:MET:CE | 2.04 | 1.06 |
| 1:M:542:PHE:CG | 4:Z:143:TYR:HE1 | 1.73 | 1.06 |
| 1:M:84:MLY:HH11 | 1:M:715:VAL:CG1 | 1.83 | 1.06 |
| 4:X:324:THR:CG2 | 4:Z:247:VAL:HG22 | 1.82 | 1.06 |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:N | 1.69 | 1.06 |
| 1:A:635:GLY:HA3 | 4:8:341:ILE:HD13 | 1.37 | 1.05 |
| 1:A:641:LYS:HE3 | 4:8:348:SER:O | 1.56 | 1.05 |
| 1:A:542:PHE:CG | 4:8:143:TYR:HE1 | 1.73 | 1.05 |
| 1:G:795:ARG:CA | 3:I:118:MET:HE1 | 1.86 | 1.05 |
| 2:N:111:SER:CB | 2:N:148:VAL:C | 1.92 | 1.05 |
| 1:J:553:MLY:HE2 | 4:Y:45:VAL:HB | 1.09 | 1.05 |
| 1:A:817:GLN:CG | 2:B:127:ARG:HD3 | 1.86 | 1.05 |
| 1:A:799:MET:SD | 3:C:32:ASP:CA | 2.44 | 1.05 |
| 1:G:542:PHE:CG | 4:V:143:TYR:HE1 | 1.74 | 1.05 |
| 1:S:506:GLU:OE2 | 1:S:760:PHE:HD1 | 1.10 | 1.05 |
| 1:S:805:ALA:C | 1:S:807:VAL:N | 2.09 | 1.05 |
| 2:T:114:LYS:HA | 2:T:146:GLY:O | 0.89 | 1.05 |
| 4:3:324:THR:CG2 | 4:5:244:ASP:HA | 1.86 | 1.05 |
| 1:D:767:PHE:O | 1:D:771:LEU:CD1 | 2.03 | 1.05 |
| 1:G:736:GLN:HA | 1:G:743:ALA:HB3 | 1.35 | 1.05 |
| 1:G:795:ARG:HE | 3:I:116:GLU:CB | 1.68 | 1.05 |
| 2:K:140:PHE:O | 2:K:141:PRO:O | 1.75 | 1.05 |
| 1:J:798:LEU:HD12 | 3:L:126:LEU:HD11 | 1.28 | 1.05 |
| 1:M:576:GLU:HG2 | 1:M:577:ALA:N | 1.66 | 1.05 |
| 1:S:783:LEU:O | 1:S:786:ILE:HG13 | 1.54 | 1.05 |
| 2:B:111:SER:OG | 2:B:148:VAL:O | 1.71 | 1.05 |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:HH21 | 1.37 | 1.05 |
| 1:D:747:LEU:HD11 | 1:D:782:MLY:HH21 | 1.15 | 1.05 |
| 2:E:140:PHE:O | 2:E:141:PRO:O | 1.74 | 1.05 |
| 1:G:409:GLY:N | 1:G:636:LYS:HG3 | 1.70 | 1.05 |
| 1:J:834:LEU:CD1 | 2:K:51:PHE:HE1 | 1.68 | 1.05 |
| 1:M:553:MLY:CB | 4:2:46:GLY:CA | 2.33 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:731:ALA:C | 3:U:93:VAL:HG12 | 1.75 | 1.05 |
| 1:S:746:LYS:NZ | 3:U:96:LYS:HA | 1.70 | 1.05 |
| 1:A:641:LYS:HD2 | 1:A:647:GLN:CD | 1.70 | 1.05 |
| 1:A:72:VAL:HG13 | 1:A:76:GLN:HB3 | 1.36 | 1.05 |
| 2:E:163:ALA:HA | 2:K:21:GLU:HB3 | 1.39 | 1.05 |
| 1:G:553:MLY:HH13 | 4:X:45:VAL:HG11 | 1.37 | 1.05 |
| 1:G:728:ASN:CG | 3:I:114:LEU:HD21 | 1.66 | 1.05 |
| 1:J:409:GLY:N | 1:J:636:LYS:HG3 | 1.69 | 1.05 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:CG | 1.86 | 1.05 |
| 1:M:97:LEU:HD22 | 1:M:712:PRO:HB3 | 1.35 | 1.05 |
| 1:J:530:MET:CA | 4:W:354:GLN:HG3 | 1.87 | 1.05 |
| 1:J:538:GLU:OE2 | 4:W:355:MET:HE1 | 1.52 | 1.05 |
| 1:D:530:MET:CA | 4:9:354:GLN:HG3 | 1.87 | 1.05 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:CD | 1.77 | 1.05 |
| 1:D:641:LYS:HB2 | 1:D:647:GLN:NE2 | 1.68 | 1.05 |
| 1:G:753:VAL:CA | 1:G:780:ASP:OD1 | 2.03 | 1.05 |
| 1:M:795:ARG:CZ | 3:O:116:GLU:HB3 | 1.85 | 1.05 |
| 1:J:638:GLY:HA2 | 4:W:341:ILE:O | 1.57 | 1.05 |
| 4:2:112:PRO:CB | 4:3:196:ARG:C | 2.25 | 1.05 |
| 4:2:112:PRO:HB3 | 4:3:196:ARG:C | 1.76 | 1.05 |
| 1:A:795:ARG:CB | 3:C:35:ARG:CZ | 2.32 | 1.05 |
| 1:D:713:SER:HB2 | 1:D:775:LEU:HD22 | 1.35 | 1.05 |
| 1:J:641:LYS:HE3 | 4:W:348:SER:O | 1.55 | 1.05 |
| 1:M:635:GLY:HA3 | 4:Z:341:ILE:HD13 | 1.36 | 1.05 |
| 1:M:530:MET:CA | 4:Z:354:GLN:HG3 | 1.87 | 1.05 |
| 4:4:324:THR:CG2 | 4:6:244:ASP:HA | 1.86 | 1.05 |
| 1:D:530:MET:HE2 | 4:9:354:GLN:CG | 1.85 | 1.05 |
| 1:D:638:GLY:HA2 | 4:9:341:ILE:O | 1.57 | 1.05 |
| 2:E:121:LEU:C | 2:E:128:PHE:HB3 | 1.72 | 1.05 |
| 2:N:114:LYS:HA | 2:N:146:GLY:O | 0.89 | 1.05 |
| 1:S:542:PHE:CG | 4:2:143:TYR:HE1 | 1.73 | 1.05 |
| 1:J:553:MLY:HH13 | 4:Y:45:VAL:HG11 | 1.37 | 1.05 |
| 1:S:635:GLY:HA3 | 4:2:341:ILE:HD13 | 1.37 | 1.04 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:CD | 1.77 | 1.04 |
| 1:M:641:LYS:HD2 | 1:M:647:GLN:CD | 1.70 | 1.04 |
| 2:H:114:LYS:HA | 2:H:146:GLY:O | 0.89 | 1.04 |
| 1:J:795:ARG:NH2 | 3:L:116:GLU:OE1 | 1.90 | 1.04 |
| 1:M:638:GLY:HA2 | 4:Z:341:ILE:O | 1.57 | 1.04 |
| 1:A:576:GLU:HG2 | 1:A:577:ALA:N | 1.66 | 1.04 |
| 1:A:831:TRP:CH2 | 2:B:34:ILE:HG23 | 1.91 | 1.04 |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CE1 | 1.87 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:49:ILE:HA | 3:F:52:ASN:HD22 | 1.23 | 1.04 |
| 2:K:121:LEU:HG | 2:K:128:PHE:CA | 1.60 | 1.04 |
| 1:J:795:ARG:HG2 | 3:L:118:MET:HE1 | 1.36 | 1.04 |
| 1:S:829:TRP:CZ2 | 2:T:87:LYS:HE2 | 1.91 | 1.04 |
| 1:S:795:ARG:NH1 | 3:U:43:ASN:OD1 | 1.87 | 1.04 |
| 1:A:599:ASN:HA | 1:A:649:VAL:HB | 1.06 | 1.04 |
| 1:A:709:LYS:O | 1:A:710:GLY:HA3 | 1.56 | 1.04 |
| 1:A:97:LEU:CD2 | 1:A:712:PRO:HB3 | 1.86 | 1.04 |
| 1:D:641:LYS:HE3 | 4:9:348:SER:O | 1.56 | 1.04 |
| 2:E:144:VAL:HG11 | 2:E:153:ILE:HG12 | 1.38 | 1.04 |
| 3:I:49:ILE:CA | 3:I:52:ASN:HD22 | 1.71 | 1.04 |
| 2:K:121:LEU:C | 2:K:128:PHE:HB3 | 1.71 | 1.04 |
| 1:M:834:LEU:HD13 | 2:N:51:PHE:HE1 | 1.22 | 1.04 |
| 1:S:638:GLY:HA2 | 4:2:341:ILE:O | 1.57 | 1.04 |
| 1:A:93:MET:HE2 | 1:A:715:VAL:CA | 1.87 | 1.04 |
| 1:D:726:VAL:CG1 | 1:D:785:GLU:CB | 2.33 | 1.04 |
| 1:G:552:ASN:O | 4:X:47:MET:CE | 2.05 | 1.04 |
| 1:J:542:PHE:CG | 4:W:143:TYR:HE1 | 1.73 | 1.04 |
| 1:J:72:VAL:HG13 | 1:J:76:GLN:HB3 | 1.36 | 1.04 |
| 2:N:140:PHE:O | 2:N:141:PRO:O | 1.75 | 1.04 |
| 1:A:202:SER:CA | 1:A:207:LYS:CE | 2.36 | 1.04 |
| 1:A:498:LEU:CD2 | 1:A:764:MLY:HH22 | 1.88 | 1.04 |
| 1:D:727:LEU:CB | 1:D:782:MLY:HE2 | 1.74 | 1.04 |
| 1:J:736:GLN:HA | 1:J:743:ALA:HB3 | 1.35 | 1.04 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:CD | 1.77 | 1.04 |
| 2:T:140:PHE:O | 2:T:141:PRO:O | 1.75 | 1.04 |
| 1:G:553:MLY:CE | 4:X:45:VAL:HG11 | 1.53 | 1.04 |
| 4:1:322:PRO:HB3 | 4:3:244:ASP:CB | 1.88 | 1.04 |
| 4:3:324:THR:CG2 | 4:5:244:ASP:CA | 2.36 | 1.04 |
| 1:A:797:PHE:CE2 | 3:C:126:LEU:HD22 | 1.92 | 1.04 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:CD | 1.77 | 1.04 |
| 1:G:832:MET:SD | 2:H:84:PHE:HE2 | 1.81 | 1.04 |
| 1:J:641:LYS:HB2 | 1:J:647:GLN:NE2 | 1.68 | 1.04 |
| 2:K:149:ASP:OD2 | 2:K:150:TYR:N | 1.91 | 1.04 |
| 1:M:639:GLY:HA3 | 4:Z:344:SER:C | 1.78 | 1.04 |
| 1:G:530:MET:CA | 4:V:354:GLN:HG3 | 1.88 | 1.04 |
| 1:S:530:MET:CA | 4:2:354:GLN:HG3 | 1.86 | 1.04 |
| 1:A:638:GLY:HA2 | 4:8:341:ILE:O | 1.56 | 1.04 |
| 1:D:635:GLY:HA3 | 4:9:341:ILE:HD13 | 1.37 | 1.04 |
| 1:G:557:GLU:HB3 | 4:X:46:GLY:C | 1.76 | 1.04 |
| 1:G:599:ASN:HA | 1:G:649:VAL:HB | 1.05 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:641:LYS:HB2 | 1:M:647:GLN:NE2 | 1.68 | 1.04 |
| 1:M:829:TRP:CH2 | 2:N:87:LYS:HE2 | 1.92 | 1.04 |
| 1:S:793:ARG:CZ | 3:U:40:ASN:ND2 | 2.12 | 1.04 |
| 1:S:817:GLN:HB3 | 2:T:127:ARG:HH11 | 0.88 | 1.04 |
| 1:A:530:MET:CA | 4:8:354:GLN:HG3 | 1.86 | 1.04 |
| 1:G:202:SER:CA | 1:G:207:LYS:CE | 2.36 | 1.04 |
| 3:L:49:ILE:CA | 3:L:52:ASN:HD22 | 1.71 | 1.04 |
| 1:A:736:GLN:N | 1:A:743:ALA:CB | 2.05 | 1.04 |
| 1:D:827:MLY:HH21 | 2:E:139:ALA:HB3 | 1.37 | 1.04 |
| 1:G:754:ASP:HB2 | 1:G:776:GLU:HA | 1.37 | 1.04 |
| 2:H:121:LEU:C | 2:H:128:PHE:HB3 | 1.72 | 1.04 |
| 3:I:49:ILE:HA | 3:I:52:ASN:HD22 | 1.23 | 1.04 |
| 1:J:635:GLY:HA3 | 4:W:341:ILE:HD13 | 1.36 | 1.04 |
| 1:J:819:ASN:OD1 | 2:K:92:ASP:N | 1.90 | 1.04 |
| 1:M:829:TRP:CH2 | 2:N:87:LYS:NZ | 2.24 | 1.04 |
| 1:S:576:GLU:HG2 | 1:S:577:ALA:N | 1.66 | 1.04 |
| 4:8:290:ARG:CZ | 4:V:202:THR:CG2 | 2.36 | 1.04 |
| 1:G:638:GLY:HA2 | 4:V:341:ILE:O | 1.58 | 1.04 |
| 1:S:639:GLY:HA3 | 4:2:344:SER:C | 1.78 | 1.03 |
| 1:A:795:ARG:CZ | 3:C:43:ASN:OD1 | 1.98 | 1.03 |
| 1:A:831:TRP:HZ3 | 2:B:50:THR:HG21 | 1.18 | 1.03 |
| 1:J:798:LEU:CD1 | 3:L:126:LEU:CD1 | 1.99 | 1.03 |
| 1:S:641:LYS:HE3 | 4:2:348:SER:O | 1.55 | 1.03 |
| 2:T:121:LEU:HG | 2:T:128:PHE:CA | 1.60 | 1.03 |
| 1:G:641:LYS:HE3 | 4:V:348:SER:O | 1.56 | 1.03 |
| 4:W:3:ASP:HA | 4:W:6:THR:HB | 1.36 | 1.03 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:HB2 | 1.07 | 1.03 |
| 1:S:770:GLY:C | 1:S:771:LEU:O | 1.96 | 1.03 |
| 1:D:732:ILE:CD1 | 1:D:782:MLY:CH1 | 2.36 | 1.03 |
| 1:J:505:MLY:CD | 1:J:762:HIS:CE1 | 2.41 | 1.03 |
| 1:J:56:GLU:HB2 | 1:J:59:MLY:HB3 | 1.40 | 1.03 |
| 1:M:84:MLY:HH11 | 1:M:715:VAL:HG11 | 1.35 | 1.03 |
| 1:D:798:LEU:CD1 | 3:F:126:LEU:CD1 | 1.82 | 1.03 |
| 1:G:557:GLU:CB | 4:X:46:GLY:C | 2.26 | 1.03 |
| 2:H:140:PHE:O | 2:H:141:PRO:O | 1.75 | 1.03 |
| 1:M:529:PRO:C | 4:Z:354:GLN:HB3 | 1.77 | 1.03 |
| 3:O:49:ILE:CA | 3:O:52:ASN:HD22 | 1.71 | 1.03 |
| 2:T:149:ASP:OD2 | 2:T:150:TYR:N | 1.91 | 1.03 |
| 1:J:557:GLU:CB | 4:Y:46:GLY:C | 2.26 | 1.03 |
| 1:A:797:PHE:HE2 | 3:C:126:LEU:CD2 | 1.72 | 1.03 |
| 2:E:121:LEU:HG | 2:E:128:PHE:CA | 1.59 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:798:LEU:HD13 | 3:F:126:LEU:HD11 | 1.37 | 1.03 |
| 1:G:538:GLU:OE2 | 4:V:355:MET:HE1 | 1.55 | 1.03 |
| 1:G:576:GLU:HG2 | 1:G:577:ALA:N | 1.66 | 1.03 |
| 2:H:150:TYR:O | 2:H:151:LYS:CB | 2.06 | 1.03 |
| 1:M:639:GLY:N | 4:Z:345:ILE:N | 1.94 | 1.03 |
| 1:J:639:GLY:HA3 | 4:W:344:SER:C | 1.78 | 1.03 |
| 1:S:836:PHE:CE1 | 2:T:159:HIS:CA | 2.42 | 1.03 |
| 4:9:3:ASP:HA | 4:9:6:THR:HB | 1.36 | 1.03 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:CD | 1.77 | 1.03 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:CB | 2.21 | 1.03 |
| 1:J:202:SER:CA | 1:J:207:LYS:CE | 2.36 | 1.03 |
| 1:J:641:LYS:HG3 | 1:J:647:GLN:HG3 | 1.20 | 1.03 |
| 1:M:72:VAL:HG13 | 1:M:76:GLN:HB3 | 1.36 | 1.03 |
| 1:M:795:ARG:CG | 3:O:118:MET:HE1 | 1.86 | 1.03 |
| 1:S:641:LYS:CG | 4:2:348:SER:HB2 | 1.87 | 1.03 |
| 1:S:84:MLY:HH11 | 1:S:724:TYR:CE2 | 1.94 | 1.03 |
| 1:M:557:GLU:N | 4:2:48:GLY:CA | 2.12 | 1.03 |
| 4:4:324:THR:CG2 | 4:6:244:ASP:CA | 2.36 | 1.03 |
| 4:4:287:ILE:CG1 | 4:6:202:THR:HB | 1.89 | 1.03 |
| 4:7:290:ARG:CZ | 4:9:202:THR:CG2 | 2.36 | 1.03 |
| 1:A:149:GLN:HB2 | 1:A:718:ALA:CB | 1.89 | 1.03 |
| 1:A:56:GLU:HB2 | 1:A:59:MLY:HB3 | 1.40 | 1.03 |
| 1:D:202:SER:CA | 1:D:207:LYS:CE | 2.36 | 1.03 |
| 1:S:839:MLY:HH13 | 2:T:159:HIS:CD2 | 1.94 | 1.03 |
| 1:J:529:PRO:C | 4:W:354:GLN:HB3 | 1.77 | 1.03 |
| 1:M:553:MLY:HG2 | 4:2:44:MET:O | 1.59 | 1.03 |
| 4:3:3:ASP:HA | 4:3:6:THR:HB | 1.36 | 1.03 |
| 2:B:140:PHE:O | 2:B:141:PRO:O | 1.74 | 1.03 |
| 1:G:206:LYS:HD2 | 1:G:217:THR:HG23 | 1.41 | 1.03 |
| 1:J:818:TYR:CE1 | 2:K:127:ARG:CZ | 2.42 | 1.03 |
| 3:O:24:LYS:HG2 | 3:O:63:ILE:O | 1.59 | 1.03 |
| 4:9:290:ARG:CZ | 4:W:202:THR:CG2 | 2.36 | 1.03 |
| 4:W:325:MET:HE2 | 4:Y:244:ASP:OD2 | 1.57 | 1.03 |
| 1:M:642:LYS:HG3 | 4:Z:23:GLY:H | 0.86 | 1.03 |
| 4:2:202:THR:CG2 | 4:Z:290:ARG:CZ | 2.36 | 1.02 |
| 4:3:322:PRO:HB3 | 4:5:244:ASP:CG | 1.80 | 1.02 |
| 2:B:111:SER:HB3 | 2:B:148:VAL:O | 1.49 | 1.02 |
| 3:F:24:LYS:HG2 | 3:F:63:ILE:O | 1.59 | 1.02 |
| 1:G:56:GLU:HB2 | 1:G:59:MLY:HB3 | 1.40 | 1.02 |
| 1:M:806:MET:C | 1:M:807:VAL:N | 2.12 | 1.02 |
| 2:T:144:VAL:HG11 | 2:T:153:ILE:HG12 | 1.38 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:639:GLY:N | 4:V:345:ILE:N | 1.94 | 1.02 |
| 4:3:287:ILE:CG1 | 4:5:202:THR:HB | 1.89 | 1.02 |
| 3:C:49:ILE:CA | 3:C:52:ASN:HD22 | 1.71 | 1.02 |
| 1:D:599:ASN:HA | 1:D:649:VAL:HB | 1.05 | 1.02 |
| 1:G:95:THR:HA | 1:G:713:SER:HB3 | 1.38 | 1.02 |
| 1:S:791:GLN:NE2 | 3:U:115:GLY:HA3 | 1.72 | 1.02 |
| 1:S:817:GLN:CD | 2:T:127:ARG:HD2 | 1.78 | 1.02 |
| 4:1:3:ASP:HA | 4:1:6:THR:HB | 1.36 | 1.02 |
| 1:A:599:ASN:CA | 1:A:649:VAL:HB | 1.89 | 1.02 |
| 1:A:95:THR:HG1 | 1:A:769:ALA:CA | 1.69 | 1.02 |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:N | 1.91 | 1.02 |
| 1:D:642:LYS:HG3 | 4:9:23:GLY:H | 0.86 | 1.02 |
| 2:E:149:ASP:OD2 | 2:E:150:TYR:N | 1.91 | 1.02 |
| 2:N:121:LEU:C | 2:N:128:PHE:HB3 | 1.72 | 1.02 |
| 1:S:549:SER:CA | 4:4:43:VAL:HG11 | 1.89 | 1.02 |
| 1:D:639:GLY:HA3 | 4:9:344:SER:C | 1.78 | 1.02 |
| 1:G:819:ASN:HA | 2:H:90:GLY:O | 0.84 | 1.02 |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:HD12 | 1.38 | 1.02 |
| 1:S:641:LYS:HB2 | 1:S:647:GLN:NE2 | 1.68 | 1.02 |
| 1:S:751:GLY:HA2 | 3:U:86:ASP:OD1 | 1.60 | 1.02 |
| 3:U:49:ILE:CA | 3:U:52:ASN:HD22 | 1.71 | 1.02 |
| 4:1:246:GLN:C | 4:Y:324:THR:HG21 | 1.70 | 1.02 |
| 1:A:501:GLU:O | 1:A:762:HIS:CD2 | 2.12 | 1.02 |
| 1:A:639:GLY:HA3 | 4:8:344:SER:C | 1.78 | 1.02 |
| 1:D:836:PHE:CZ | 2:E:159:HIS:C | 2.32 | 1.02 |
| 1:G:599:ASN:CA | 1:G:649:VAL:HB | 1.89 | 1.02 |
| 1:M:599:ASN:CA | 1:M:649:VAL:HB | 1.89 | 1.02 |
| 1:S:642:LYS:HG3 | 4:2:23:GLY:H | 0.86 | 1.02 |
| 1:S:508:ILE:CD1 | 1:S:759:ALA:HB2 | 1.90 | 1.02 |
| 1:M:538:GLU:OE2 | 4:Z:355:MET:HE1 | 1.55 | 1.02 |
| 4:1:287:ILE:CG1 | 4:3:202:THR:CA | 2.36 | 1.02 |
| 1:A:501:GLU:O | 1:A:762:HIS:NE2 | 1.92 | 1.02 |
| 1:G:757:GLN:HG2 | 1:G:776:GLU:HG2 | 1.33 | 1.02 |
| 1:J:813:ILE:HG23 | 2:K:128:PHE:CE1 | 1.93 | 1.02 |
| 1:M:56:GLU:HB2 | 1:M:59:MLY:HB3 | 1.40 | 1.02 |
| 1:M:599:ASN:HA | 1:M:649:VAL:HB | 1.05 | 1.02 |
| 1:M:793:ARG:HH11 | 3:O:40:ASN:ND2 | 1.58 | 1.02 |
| 1:J:642:LYS:HG3 | 4:W:23:GLY:H | 0.86 | 1.02 |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:HG23 | 1.38 | 1.02 |
| 1:A:149:GLN:CD | 1:A:716:LEU:HD23 | 1.77 | 1.02 |
| 1:M:736:GLN:N | 1:M:743:ALA:CB | 2.05 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:817:GLN:HB3 | 2:N:127:ARG:CD | 1.89 | 1.02 |
| 1:M:819:ASN:ND2 | 2:N:92:ASP:HB2 | 1.75 | 1.02 |
| 2:B:121:LEU:HG | 2:B:128:PHE:CA | 1.59 | 1.02 |
| 2:B:144:VAL:HG11 | 2:B:153:ILE:HG12 | 1.38 | 1.02 |
| 1:G:639:GLY:HA3 | 4:V:344:SER:C | 1.78 | 1.02 |
| 1:G:642:LYS:HG3 | 4:V:23:GLY:H | 0.85 | 1.02 |
| 1:G:831:TRP:CH2 | 2:H:47:LEU:HD22 | 1.89 | 1.02 |
| 1:M:641:LYS:HE3 | 4:Z:348:SER:O | 1.55 | 1.02 |
| 1:S:641:LYS:HE3 | 1:S:647:GLN:CD | 1.77 | 1.02 |
| 4:V:3:ASP:HA | 4:V:6:THR:HB | 1.36 | 1.02 |
| 4:W:324:THR:HG21 | 4:Y:246:GLN:C | 1.70 | 1.02 |
| 1:S:541:MET:HB3 | 4:2:143:TYR:OH | 1.59 | 1.02 |
| 1:A:553:MLY:HB3 | 4:V:46:GLY:CA | 1.51 | 1.02 |
| 1:A:576:GLU:HG2 | 1:A:577:ALA:H | 0.85 | 1.02 |
| 3:C:24:LYS:CG | 3:C:63:ILE:O | 2.08 | 1.02 |
| 1:D:529:PRO:C | 4:9:354:GLN:HB3 | 1.78 | 1.02 |
| 3:F:49:ILE:CA | 3:F:52:ASN:HD22 | 1.71 | 1.02 |
| 3:F:24:LYS:CG | 3:F:63:ILE:O | 2.08 | 1.02 |
| 1:G:541:MET:HB3 | 4:V:143:TYR:OH | 1.60 | 1.02 |
| 1:G:576:GLU:HG2 | 1:G:577:ALA:H | 0.85 | 1.02 |
| 1:G:84:MLY:HH21 | 1:G:719:ASP:O | 1.56 | 1.02 |
| 1:J:541:MET:HB3 | 4:W:143:TYR:OH | 1.60 | 1.02 |
| 1:S:786:ILE:C | 1:S:787:ILE:N | 2.14 | 1.02 |
| 4:5:3:ASP:HA | 4:5:6:THR:HB | 1.36 | 1.02 |
| 1:A:149:GLN:HB2 | 1:A:718:ALA:HB3 | 1.37 | 1.02 |
| 1:A:642:LYS:HG3 | 4:8:23:GLY:H | 0.87 | 1.02 |
| 2:K:144:VAL:HG11 | 2:K:153:ILE:HG12 | 1.38 | 1.02 |
| 1:S:707:CYS:O | 1:S:714:ARG:NH2 | 1.92 | 1.02 |
| 1:S:791:GLN:NE2 | 3:U:114:LEU:O | 1.93 | 1.02 |
| 4:V:325:MET:HE2 | 4:X:244:ASP:OD2 | 1.58 | 1.02 |
| 1:S:529:PRO:C | 4:2:354:GLN:HB3 | 1.77 | 1.01 |
| 4:7:3:ASP:HA | 4:7:6:THR:HB | 1.36 | 1.01 |
| 1:A:639:GLY:N | 4:8:345:ILE:N | 1.94 | 1.01 |
| 1:D:838:ILE:CD1 | 2:E:54:MET:SD | 2.47 | 1.01 |
| 1:M:202:SER:CA | 1:M:207:LYS:CE | 2.36 | 1.01 |
| 1:M:206:LYS:HD2 | 1:M:217:THR:HG23 | 1.41 | 1.01 |
| 1:M:753:VAL:CG1 | 1:M:775:LEU:HD11 | 1.90 | 1.01 |
| 1:S:599:ASN:CA | 1:S:649:VAL:HB | 1.89 | 1.01 |
| 1:G:534:SER:O | 4:V:351:THR:HG23 | 1.12 | 1.01 |
| 4:8:3:ASP:HA | 4:8:6:THR:HB | 1.36 | 1.01 |
| 1:A:206:LYS:CD | 1:A:217:THR:CG2 | 2.16 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:817:GLN:HG3 | 2:B:127:ARG:HD3 | 1.35 | 1.01 |
| 1:D:98:HIS:HB3 | 1:D:100:PRO:HD2 | 1.42 | 1.01 |
| 1:G:796:GLY:HA2 | 3:I:35:ARG:CD | 1.89 | 1.01 |
| 1:G:836:PHE:CE1 | 2:H:159:HIS:HA | 1.93 | 1.01 |
| 1:J:795:ARG:CZ | 3:L:116:GLU:CD | 2.27 | 1.01 |
| 2:N:149:ASP:OD2 | 2:N:150:TYR:N | 1.91 | 1.01 |
| 1:M:795:ARG:NE | 3:O:118:MET:HE1 | 1.75 | 1.01 |
| 1:M:795:ARG:HG2 | 3:O:118:MET:HE3 | 1.14 | 1.01 |
| 1:S:639:GLY:N | 4:2:345:ILE:N | 1.94 | 1.01 |
| 1:D:541:MET:HB3 | 4:9:143:TYR:OH | 1.60 | 1.01 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:OE2 | 1.81 | 1.01 |
| 1:G:792:ALA:CB | 3:I:42:THR:CG2 | 2.17 | 1.01 |
| 1:J:599:ASN:HA | 1:J:649:VAL:HB | 1.05 | 1.01 |
| 1:J:736:GLN:N | 1:J:743:ALA:CB | 2.05 | 1.01 |
| 1:S:98:HIS:HB3 | 1:S:100:PRO:HD2 | 1.42 | 1.01 |
| 3:U:24:LYS:CG | 3:U:63:ILE:O | 2.08 | 1.01 |
| 2:B:150:TYR:O | 2:B:151:LYS:CB | 2.07 | 1.01 |
| 1:D:534:SER:O | 4:9:351:THR:HA | 1.59 | 1.01 |
| 1:J:599:ASN:CA | 1:J:649:VAL:HB | 1.89 | 1.01 |
| 1:M:646:PHE:HE2 | 1:M:652:LEU:HD21 | 1.24 | 1.01 |
| 1:A:553:MLY:HG2 | 4:V:44:MET:O | 1.59 | 1.01 |
| 1:A:557:GLU:N | 4:V:48:GLY:CA | 2.12 | 1.01 |
| 4:Y:3:ASP:HA | 4:Y:6:THR:HB | 1.36 | 1.01 |
| 1:A:642:LYS:HD3 | 4:8:340:TRP:CH2 | 1.95 | 1.01 |
| 1:A:541:MET:HB3 | 4:8:143:TYR:OH | 1.60 | 1.01 |
| 1:D:56:GLU:HB2 | 1:D:59:MLY:HB3 | 1.40 | 1.01 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:HB2 | 1.42 | 1.01 |
| 1:G:791:GLN:OE1 | 3:I:116:GLU:HG3 | 1.60 | 1.01 |
| 3:I:24:LYS:HG2 | 3:I:63:ILE:O | 1.60 | 1.01 |
| 1:M:534:SER:C | 4:Z:351:THR:HA | 1.81 | 1.01 |
| 3:O:48:LYS:O | 3:O:52:ASN:ND2 | 1.94 | 1.01 |
| 1:S:599:ASN:HA | 1:S:649:VAL:HB | 1.05 | 1.01 |
| 3:U:49:ILE:HA | 3:U:52:ASN:HD22 | 1.23 | 1.01 |
| 1:M:642:LYS:HD3 | 4:Z:340:TRP:CH2 | 1.96 | 1.01 |
| 1:A:642:LYS:HD3 | 4:8:340:TRP:CZ3 | 1.95 | 1.01 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:HB2 | 1.42 | 1.01 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:O | 2.14 | 1.01 |
| 1:D:813:ILE:HG23 | 2:E:128:PHE:CE1 | 1.83 | 1.01 |
| 2:H:149:ASP:OD2 | 2:H:150:TYR:N | 1.91 | 1.01 |
| 1:J:834:LEU:CD1 | 2:K:51:PHE:CE1 | 2.44 | 1.01 |
| 4:2:204:ALA:H | 4:Z:287:ILE:HB | 1.25 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:206:LYS:HD2 | 1:A:217:THR:HG23 | 1.41 | 1.01 |
| 1:A:797:PHE:HD1 | 3:C:146:ILE:O | 1.42 | 1.01 |
| 3:F:48:LYS:O | 3:F:52:ASN:ND2 | 1.94 | 1.01 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:HD3 | 1.36 | 1.01 |
| 3:U:24:LYS:HG2 | 3:U:63:ILE:O | 1.59 | 1.01 |
| 4:4:287:ILE:CG1 | 4:6:202:THR:CB | 2.33 | 1.01 |
| 1:A:149:GLN:HB3 | 1:A:719:ASP:N | 1.76 | 1.01 |
| 1:D:791:GLN:OE1 | 3:F:116:GLU:HG3 | 1.60 | 1.01 |
| 1:J:641:LYS:HD2 | 1:J:647:GLN:CD | 1.70 | 1.01 |
| 1:J:642:LYS:HD3 | 4:W:340:TRP:CZ3 | 1.96 | 1.01 |
| 1:M:720:PHE:CD1 | 1:M:772:LEU:HD21 | 1.96 | 1.01 |
| 1:S:839:MLY:HH21 | 2:T:158:THR:HG22 | 1.42 | 1.01 |
| 4:1:287:ILE:HB | 4:3:203:THR:CG2 | 1.90 | 1.01 |
| 1:G:98:HIS:HB3 | 1:G:100:PRO:HD2 | 1.42 | 1.01 |
| 1:G:642:LYS:HD3 | 4:V:340:TRP:CH2 | 1.96 | 1.01 |
| 1:G:730:SER:OG | 3:I:113:THR:CG2 | 2.09 | 1.01 |
| 3:L:48:LYS:O | 3:L:52:ASN:ND2 | 1.94 | 1.01 |
| 1:M:797:PHE:HD1 | 3:O:149:VAL:CG1 | 1.74 | 1.01 |
| 1:S:56:GLU:HB2 | 1:S:59:MLY:HB3 | 1.40 | 1.01 |
| 1:A:793:ARG:NH2 | 3:C:147:MET:CE | 2.23 | 1.01 |
| 3:C:49:ILE:HA | 3:C:52:ASN:HD22 | 1.23 | 1.01 |
| 3:I:24:LYS:CG | 3:I:63:ILE:O | 2.08 | 1.01 |
| 1:J:534:SER:O | 4:W:351:THR:HA | 1.60 | 1.01 |
| 2:E:163:ALA:CA | 2:K:21:GLU:HB3 | 1.91 | 1.01 |
| 1:M:642:LYS:HD3 | 4:Z:340:TRP:CZ3 | 1.96 | 1.01 |
| 1:M:783:LEU:CG | 1:M:786:ILE:HD12 | 1.91 | 1.01 |
| 1:M:795:ARG:CD | 3:O:43:ASN:OD1 | 2.07 | 1.01 |
| 1:S:752:ASP:N | 3:U:86:ASP:OD1 | 1.94 | 1.01 |
| 1:J:642:LYS:HD3 | 4:W:340:TRP:CH2 | 1.95 | 1.01 |
| 1:S:534:SER:C | 4:2:351:THR:HA | 1.81 | 1.00 |
| 3:C:48:LYS:O | 3:C:52:ASN:ND2 | 1.94 | 1.00 |
| 1:D:713:SER:OG | 1:D:771:LEU:CG | 2.08 | 1.00 |
| 1:D:836:PHE:HE1 | 2:E:159:HIS:HB2 | 1.21 | 1.00 |
| 1:M:541:MET:HB3 | 4:Z:143:TYR:OH | 1.59 | 1.00 |
| 1:M:819:ASN:CG | 2:N:92:ASP:CB | 2.28 | 1.00 |
| 2:N:121:LEU:HG | 2:N:128:PHE:CA | 1.60 | 1.00 |
| 1:S:92:ALA:HB3 | 1:S:764:MLY:HH12 | 1.43 | 1.00 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:CB | 1.91 | 1.00 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:CB | 1.91 | 1.00 |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HD11 | 1.22 | 1.00 |
| 1:J:757:GLN:HA | 1:J:776:GLU:CG | 1.91 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:797:PHE:CZ | 3:U:146:ILE:HA | 1.96 | 1.00 |
| 4:8:290:ARG:NH2 | 4:V:202:THR:CG2 | 2.23 | 1.00 |
| 4:2:202:THR:CG2 | 4:Z:290:ARG:NH2 | 2.24 | 1.00 |
| 3:C:24:LYS:HG2 | 3:C:63:ILE:O | 1.59 | 1.00 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:HB2 | 1.42 | 1.00 |
| 1:J:639:GLY:N | 4:W:345:ILE:N | 1.94 | 1.00 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:HB2 | 1.43 | 1.00 |
| 2:N:150:TYR:O | 2:N:151:LYS:CB | 2.07 | 1.00 |
| 1:S:576:GLU:HG2 | 1:S:577:ALA:H | 0.85 | 1.00 |
| 1:M:530:MET:HE2 | 4:Z:354:GLN:CG | 1.91 | 1.00 |
| 1:A:505:MLY:CG | 1:A:762:HIS:CD2 | 2.44 | 1.00 |
| 1:A:95:THR:HG1 | 1:A:769:ALA:HA | 0.86 | 1.00 |
| 1:D:508:ILE:HD11 | 1:D:766:PHE:HZ | 1.26 | 1.00 |
| 1:D:599:ASN:CA | 1:D:649:VAL:HB | 1.89 | 1.00 |
| 3:L:24:LYS:CG | 3:L:63:ILE:O | 2.08 | 1.00 |
| 4:7:290:ARG:NH2 | 4:9:202:THR:CG2 | 2.23 | 1.00 |
| 1:A:646:PHE:HE2 | 1:A:652:LEU:HD21 | 1.24 | 1.00 |
| 1:D:218:LEU:CA | 1:D:221:GLN:HG3 | 1.90 | 1.00 |
| 1:D:642:LYS:HD3 | 4:9:340:TRP:CH2 | 1.96 | 1.00 |
| 1:D:642:LYS:HD3 | 4:9:340:TRP:CZ3 | 1.96 | 1.00 |
| 1:D:827:MLY:HH21 | 2:E:139:ALA:CB | 1.90 | 1.00 |
| 1:J:792:ALA:N | 3:L:42:THR:HG22 | 1.75 | 1.00 |
| 1:M:818:TYR:CE1 | 2:N:127:ARG:CZ | 2.45 | 1.00 |
| 1:S:215:GLN:CA | 1:S:340:ILE:HG23 | 1.92 | 1.00 |
| 1:S:642:LYS:HD3 | 4:2:340:TRP:CZ3 | 1.96 | 1.00 |
| 4:4:322:PRO:HB3 | 4:6:244:ASP:CG | 1.80 | 1.00 |
| 1:G:84:MLY:HD3 | 1:G:723:ARG:HD2 | 1.40 | 1.00 |
| 1:J:641:LYS:CG | 4:W:348:SER:HB2 | 1.87 | 1.00 |
| 3:L:24:LYS:HG2 | 3:L:63:ILE:O | 1.59 | 1.00 |
| 2:T:150:TYR:O | 2:T:151:LYS:CB | 2.07 | 1.00 |
| 1:G:503:TYR:OH | 1:G:711:PHE:HD2 | 1.43 | 1.00 |
| 1:G:769:ALA:CB | 1:G:770:GLY:CA | 2.29 | 1.00 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:HB2 | 1.42 | 1.00 |
| 1:M:534:SER:O | 4:Z:351:THR:HA | 1.60 | 1.00 |
| 2:N:144:VAL:HG11 | 2:N:153:ILE:HG12 | 1.38 | 1.00 |
| 1:S:641:LYS:HE3 | 1:S:647:GLN:HB2 | 1.42 | 1.00 |
| 1:A:218:LEU:CA | 1:A:221:GLN:HG3 | 1.91 | 1.00 |
| 1:A:576:GLU:CG | 1:A:577:ALA:H | 1.75 | 1.00 |
| 1:G:215:GLN:CA | 1:G:340:ILE:HG23 | 1.92 | 1.00 |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:CB | 1.92 | 1.00 |
| 1:G:755:HIS:ND1 | 1:G:779:ARG:NH1 | 2.10 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:144:VAL:HG11 | 2:H:153:ILE:HG12 | 1.38 | 1.00 |
| 1:J:646:PHE:HE2 | 1:J:652:LEU:HD21 | 1.24 | 1.00 |
| 1:J:94:MET:O | 1:J:713:SER:CB | 2.09 | 1.00 |
| 1:S:202:SER:CA | 1:S:207:LYS:CE | 2.36 | 1.00 |
| 1:S:642:LYS:HD3 | 4:2:340:TRP:CH2 | 1.96 | 1.00 |
| 4:9:286:ASP:OD1 | 4:W:203:THR:HG22 | 1.62 | 1.00 |
| 4:7:287:ILE:HB | 4:9:204:ALA:H | 1.26 | 1.00 |
| 4:9:290:ARG:NH2 | 4:W:202:THR:CG2 | 2.23 | 1.00 |
| 1:A:502:GLU:CB | 1:A:761:GLY:HA3 | 1.91 | 1.00 |
| 1:G:97:LEU:HD23 | 1:G:712:PRO:HB3 | 1.43 | 1.00 |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:HG12 | 1.14 | 1.00 |
| 1:S:534:SER:O | 4:2:351:THR:HA | 1.59 | 1.00 |
| 1:S:804:ARG:CA | 1:S:807:VAL:HB | 1.91 | 1.00 |
| 4:8:286:ASP:OD1 | 4:V:203:THR:HG22 | 1.62 | 1.00 |
| 4:8:287:ILE:HB | 4:V:204:ALA:H | 1.25 | 1.00 |
| 4:2:203:THR:HG22 | 4:Z:286:ASP:OD1 | 1.62 | 1.00 |
| 1:G:754:ASP:CB | 1:G:779:ARG:HD2 | 1.91 | 1.00 |
| 1:J:98:HIS:HB3 | 1:J:100:PRO:HD2 | 1.42 | 1.00 |
| 1:J:819:ASN:CA | 2:K:90:GLY:O | 2.09 | 1.00 |
| 4:7:286:ASP:OD1 | 4:9:203:THR:HG22 | 1.62 | 0.99 |
| 1:A:215:GLN:CA | 1:A:340:ILE:HG23 | 1.92 | 0.99 |
| 2:B:139:ALA:O | 2:B:141:PRO:HD3 | 1.62 | 0.99 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:CB | 1.91 | 0.99 |
| 2:E:150:TYR:O | 2:E:151:LYS:CB | 2.07 | 0.99 |
| 1:J:174:SER:HB3 | 1:J:667:THR:HG21 | 1.44 | 0.99 |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:HD11 | 1.21 | 0.99 |
| 1:J:795:ARG:NH2 | 3:L:116:GLU:CD | 2.14 | 0.99 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:CB | 1.91 | 0.99 |
| 2:N:149:ASP:OD2 | 2:N:150:TYR:O | 1.80 | 0.99 |
| 1:J:639:GLY:CA | 4:W:345:ILE:CA | 2.40 | 0.99 |
| 1:D:553:MLY:HG2 | 4:W:44:MET:O | 1.59 | 0.99 |
| 4:3:288:ASP:N | 4:5:203:THR:HG22 | 1.77 | 0.99 |
| 1:D:713:SER:OG | 1:D:771:LEU:HG | 1.61 | 0.99 |
| 1:G:218:LEU:CA | 1:G:221:GLN:HG3 | 1.91 | 0.99 |
| 1:G:831:TRP:CZ2 | 2:H:47:LEU:HD21 | 1.97 | 0.99 |
| 1:J:218:LEU:CA | 1:J:221:GLN:HG3 | 1.91 | 0.99 |
| 1:M:35:MLY:HE2 | 1:M:777:GLU:CD | 1.82 | 0.99 |
| 1:S:576:GLU:CG | 1:S:577:ALA:H | 1.75 | 0.99 |
| 1:S:646:PHE:HE2 | 1:S:652:LEU:HD21 | 1.24 | 0.99 |
| 1:S:641:LYS:HE3 | 1:S:647:GLN:CB | 1.91 | 0.99 |
| 1:S:831:TRP:HH2 | 2:T:47:LEU:HD21 | 1.27 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:534:SER:C | 4:8:351:THR:HA | 1.81 | 0.99 |
| 1:D:639:GLY:CA | 4:9:345:ILE:CA | 2.41 | 0.99 |
| 1:A:93:MET:HE1 | 1:A:715:VAL:HG13 | 1.39 | 0.99 |
| 1:D:646:PHE:HE2 | 1:D:652:LEU:HD21 | 1.24 | 0.99 |
| 1:G:529:PRO:C | 4:V:354:GLN:HB3 | 1.79 | 0.99 |
| 1:G:728:ASN:ND2 | 3:I:114:LEU:CD2 | 2.21 | 0.99 |
| 1:M:215:GLN:CA | 1:M:340:ILE:HG23 | 1.92 | 0.99 |
| 1:S:120:GLY:HA2 | 1:S:764:MLY:CH1 | 1.93 | 0.99 |
| 4:X:287:ILE:CG1 | 4:Z:201:VAL:HG23 | 1.91 | 0.99 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:HG22 | 1.92 | 0.99 |
| 1:D:174:SER:HB3 | 1:D:667:THR:HG21 | 1.44 | 0.99 |
| 1:D:831:TRP:CE2 | 2:E:51:PHE:CZ | 2.49 | 0.99 |
| 1:G:757:GLN:HG3 | 1:G:776:GLU:HG3 | 1.40 | 0.99 |
| 1:M:218:LEU:CA | 1:M:221:GLN:HG3 | 1.91 | 0.99 |
| 1:M:576:GLU:CG | 1:M:577:ALA:H | 1.75 | 0.99 |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:CA | 1.75 | 0.99 |
| 1:M:829:TRP:CH2 | 2:N:87:LYS:CE | 2.44 | 0.99 |
| 2:N:141:PRO:HB2 | 2:N:142:PRO:HD2 | 1.44 | 0.99 |
| 1:M:639:GLY:CA | 4:Z:345:ILE:CA | 2.40 | 0.99 |
| 4:2:287:ILE:HB | 4:4:203:THR:HG22 | 1.24 | 0.99 |
| 1:G:576:GLU:CG | 1:G:577:ALA:H | 1.75 | 0.99 |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE3 | 1.26 | 0.99 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:CB | 1.91 | 0.99 |
| 3:O:24:LYS:CG | 3:O:63:ILE:O | 2.08 | 0.99 |
| 1:S:797:PHE:CZ | 3:U:146:ILE:HD13 | 1.96 | 0.99 |
| 4:9:287:ILE:HB | 4:W:204:ALA:H | 1.25 | 0.99 |
| 4:3:322:PRO:CB | 4:5:244:ASP:CB | 2.40 | 0.99 |
| 1:D:795:ARG:HB3 | 3:F:35:ARG:HH12 | 1.20 | 0.99 |
| 1:G:754:ASP:HA | 1:G:779:ARG:HD3 | 1.42 | 0.99 |
| 1:J:757:GLN:NE2 | 1:J:777:GLU:N | 1.95 | 0.99 |
| 1:M:649:VAL:CG1 | 1:M:649:VAL:HG22 | 1.92 | 0.99 |
| 1:M:817:GLN:CG | 2:N:127:ARG:CD | 2.40 | 0.99 |
| 1:S:804:ARG:HA | 1:S:807:VAL:HB | 1.44 | 0.99 |
| 1:G:534:SER:C | 4:V:351:THR:HA | 1.82 | 0.99 |
| 1:A:793:ARG:NH2 | 3:C:147:MET:HE2 | 1.78 | 0.99 |
| 1:G:754:ASP:HA | 1:G:779:ARG:HD2 | 1.01 | 0.99 |
| 1:J:534:SER:C | 4:W:351:THR:HA | 1.81 | 0.99 |
| 1:J:576:GLU:HG2 | 1:J:577:ALA:H | 0.85 | 0.99 |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:CA | 1.76 | 0.99 |
| 4:W:324:THR:CG2 | 4:Y:247:VAL:N | 2.24 | 0.99 |
| 4:1:247:VAL:N | 4:Y:324:THR:CG2 | 2.24 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:639:GLY:CA | 4:2:345:ILE:CA | 2.40 | 0.99 |
| 1:A:836:PHE:CZ | 2:B:160:GLY:N | 2.31 | 0.99 |
| 1:A:97:LEU:CD2 | 1:A:712:PRO:CB | 2.40 | 0.99 |
| 1:D:534:SER:C | 4:9:351:THR:HA | 1.81 | 0.99 |
| 2:H:121:LEU:HG | 2:H:128:PHE:CA | 1.60 | 0.99 |
| 1:M:576:GLU:HG2 | 1:M:577:ALA:H | 0.85 | 0.99 |
| 3:O:49:ILE:HA | 3:O:52:ASN:HD22 | 1.23 | 0.99 |
| 3:U:48:LYS:O | 3:U:52:ASN:ND2 | 1.94 | 0.99 |
| 4:V:324:THR:CG2 | 4:X:247:VAL:N | 2.24 | 0.99 |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:O | 1.80 | 0.99 |
| 1:G:503:TYR:CE1 | 1:G:711:PHE:CE2 | 2.51 | 0.99 |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:CA | 1.75 | 0.99 |
| 1:G:639:GLY:CA | 4:V:345:ILE:CA | 2.40 | 0.99 |
| 1:A:639:GLY:CA | 4:8:345:ILE:CA | 2.41 | 0.99 |
| 1:A:529:PRO:C | 4:8:354:GLN:HB3 | 1.78 | 0.99 |
| 1:A:839:MLY:HH11 | 2:B:159:HIS:HD2 | 1.23 | 0.99 |
| 1:G:642:LYS:HD3 | 4:V:340:TRP:CZ3 | 1.96 | 0.99 |
| 2:K:121:LEU:CB | 2:K:128:PHE:HB3 | 1.69 | 0.99 |
| 2:K:139:ALA:O | 2:K:141:PRO:HD3 | 1.62 | 0.99 |
| 1:M:84:MLY:CH1 | 1:M:715:VAL:CG1 | 2.41 | 0.99 |
| 1:S:508:ILE:HD11 | 1:S:759:ALA:HB2 | 1.01 | 0.99 |
| 4:2:244:ASP:OD2 | 4:Z:322:PRO:HB3 | 1.62 | 0.98 |
| 1:D:538:GLU:OE2 | 4:9:355:MET:HE1 | 1.61 | 0.98 |
| 1:G:646:PHE:HE2 | 1:G:652:LEU:HD21 | 1.24 | 0.98 |
| 1:G:784:ALA:O | 1:G:788:THR:N | 1.96 | 0.98 |
| 1:J:768:MLY:HH11 | 1:J:772:LEU:CD1 | 1.78 | 0.98 |
| 1:M:95:THR:HA | 1:M:713:SER:HB3 | 1.34 | 0.98 |
| 2:N:130:PRO:O | 2:N:133:ILE:N | 1.96 | 0.98 |
| 1:S:218:LEU:CA | 1:S:221:GLN:HG3 | 1.91 | 0.98 |
| 4:4:322:PRO:CB | 4:6:244:ASP:CB | 2.40 | 0.98 |
| 1:D:767:PHE:C | 1:D:771:LEU:HD11 | 1.62 | 0.98 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:HG22 | 1.92 | 0.98 |
| 2:H:149:ASP:OD2 | 2:H:150:TYR:O | 1.80 | 0.98 |
| 1:A:98:HIS:HB3 | 1:A:100:PRO:HD2 | 1.42 | 0.98 |
| 1:D:649:VAL:CG1 | 1:D:649:VAL:HG22 | 1.92 | 0.98 |
| 1:G:752:ASP:O | 1:G:780:ASP:OD1 | 1.80 | 0.98 |
| 3:I:48:LYS:O | 3:I:52:ASN:ND2 | 1.94 | 0.98 |
| 2:K:150:TYR:O | 2:K:151:LYS:CB | 2.06 | 0.98 |
| 1:S:786:ILE:CB | 1:S:787:ILE:N | 2.26 | 0.98 |
| 1:D:206:LYS:HD2 | 1:D:217:THR:HG23 | 1.41 | 0.98 |
| 1:D:215:GLN:CA | 1:D:340:ILE:HG23 | 1.92 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:823:PHE:CE1 | 2:E:160:GLY:HA2 | 1.97 | 0.98 |
| 1:M:831:TRP:CH2 | 2:N:47:LEU:HD21 | 1.94 | 0.98 |
| 2:B:112:ILE:O | 2:B:147:ASN:C | 2.01 | 0.98 |
| 1:G:728:ASN:OD1 | 3:I:114:LEU:CG | 2.10 | 0.98 |
| 2:N:117:LEU:CB | 2:N:147:ASN:CG | 2.32 | 0.98 |
| 2:N:139:ALA:O | 2:N:141:PRO:HD3 | 1.62 | 0.98 |
| 1:S:206:LYS:HD2 | 1:S:217:THR:HG23 | 1.41 | 0.98 |
| 1:S:546:THR:HB | 4:4:47:MET:O | 1.62 | 0.98 |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:CA | 1.75 | 0.98 |
| 3:L:49:ILE:HA | 3:L:52:ASN:HD22 | 1.23 | 0.98 |
| 1:M:530:MET:CE | 4:Z:354:GLN:CG | 2.40 | 0.98 |
| 1:M:795:ARG:HG3 | 3:O:118:MET:CE | 1.92 | 0.98 |
| 1:S:612:GLN:HE22 | 1:S:627:GLY:CA | 1.76 | 0.98 |
| 4:1:287:ILE:CB | 4:3:203:THR:N | 2.06 | 0.98 |
| 2:B:117:LEU:CB | 2:B:147:ASN:CG | 2.32 | 0.98 |
| 2:B:141:PRO:HB2 | 2:B:142:PRO:HD2 | 1.44 | 0.98 |
| 1:J:215:GLN:CA | 1:J:340:ILE:HG23 | 1.92 | 0.98 |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:CG1 | 1.92 | 0.98 |
| 1:J:829:TRP:CH2 | 2:K:87:LYS:NZ | 2.30 | 0.98 |
| 2:K:117:LEU:CB | 2:K:147:ASN:CG | 2.32 | 0.98 |
| 1:M:791:GLN:OE1 | 3:O:116:GLU:N | 1.95 | 0.98 |
| 1:M:84:MLY:HH21 | 1:M:719:ASP:C | 1.84 | 0.98 |
| 1:M:98:HIS:HB3 | 1:M:100:PRO:HD2 | 1.42 | 0.98 |
| 2:N:112:ILE:O | 2:N:147:ASN:C | 2.02 | 0.98 |
| 1:S:792:ALA:HB2 | 3:U:42:THR:HG22 | 1.19 | 0.98 |
| 2:T:117:LEU:HD13 | 2:T:147:ASN:OD1 | 1.64 | 0.98 |
| 2:T:144:VAL:HG13 | 2:T:153:ILE:HD11 | 1.21 | 0.98 |
| 4:9:322:PRO:HB3 | 4:W:244:ASP:OD2 | 1.62 | 0.98 |
| 1:J:206:LYS:HD2 | 1:J:217:THR:HG23 | 1.41 | 0.98 |
| 1:J:769:ALA:CB | 1:J:770:GLY:HA2 | 1.93 | 0.98 |
| 2:K:150:TYR:C | 2:K:151:LYS:HG3 | 1.83 | 0.98 |
| 3:L:46:ILE:O | 3:L:50:LEU:HG | 1.64 | 0.98 |
| 1:M:786:ILE:O | 1:M:790:THR:N | 1.96 | 0.98 |
| 1:M:795:ARG:HE | 3:O:118:MET:HE1 | 1.26 | 0.98 |
| 1:M:793:ARG:NH1 | 3:O:40:ASN:ND2 | 2.12 | 0.98 |
| 2:B:130:PRO:O | 2:B:133:ILE:N | 1.96 | 0.98 |
| 2:E:149:ASP:OD2 | 2:E:150:TYR:O | 1.80 | 0.98 |
| 2:E:150:TYR:C | 2:E:151:LYS:HG3 | 1.83 | 0.98 |
| 3:L:52:ASN:HB2 | 3:L:53:PRO:HD3 | 1.46 | 0.98 |
| 2:N:150:TYR:C | 2:N:151:LYS:HG3 | 1.83 | 0.98 |
| 2:T:139:ALA:O | 2:T:141:PRO:HD3 | 1.62 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:288:ASP:N | 4:6:203:THR:HG22 | 1.77 | 0.98 |
| 2:E:117:LEU:HD13 | 2:E:147:ASN:OD1 | 1.64 | 0.98 |
| 2:H:112:ILE:O | 2:H:147:ASN:C | 2.01 | 0.98 |
| 1:J:797:PHE:CE2 | 3:L:126:LEU:CD2 | 2.47 | 0.98 |
| 1:M:32:PHE:O | 1:M:780:ASP:OD2 | 1.82 | 0.98 |
| 1:S:508:ILE:HD11 | 1:S:759:ALA:CB | 1.93 | 0.98 |
| 1:S:817:GLN:HB3 | 2:T:127:ARG:CD | 1.93 | 0.98 |
| 4:V:324:THR:HG21 | 4:X:246:GLN:C | 1.70 | 0.98 |
| 1:D:553:MLY:CB | 4:W:46:GLY:CA | 2.32 | 0.98 |
| 1:A:505:MLY:CB | 1:A:762:HIS:N | 2.26 | 0.97 |
| 2:B:150:TYR:C | 2:B:151:LYS:HG3 | 1.83 | 0.97 |
| 1:D:508:ILE:CG1 | 1:D:766:PHE:CE1 | 2.46 | 0.97 |
| 2:E:130:PRO:O | 2:E:133:ILE:N | 1.97 | 0.97 |
| 3:F:52:ASN:HB2 | 3:F:53:PRO:HD3 | 1.46 | 0.97 |
| 1:J:576:GLU:CG | 1:J:577:ALA:H | 1.75 | 0.97 |
| 2:K:130:PRO:O | 2:K:133:ILE:N | 1.96 | 0.97 |
| 1:S:649:VAL:CG1 | 1:S:649:VAL:HG22 | 1.92 | 0.97 |
| 1:S:819:ASN:CG | 2:T:92:ASP:CB | 2.32 | 0.97 |
| 3:U:46:ILE:O | 3:U:50:LEU:HG | 1.64 | 0.97 |
| 1:A:218:LEU:CA | 1:A:221:GLN:CG | 2.42 | 0.97 |
| 1:M:838:ILE:HD11 | 2:N:54:MET:HE3 | 1.43 | 0.97 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:HB2 | 1.45 | 0.97 |
| 1:J:534:SER:O | 4:W:351:THR:HG23 | 1.13 | 0.97 |
| 4:7:322:PRO:HB3 | 4:9:244:ASP:OD2 | 1.62 | 0.97 |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:CA | 1.76 | 0.97 |
| 1:D:649:VAL:CG2 | 1:D:649:VAL:CA | 2.42 | 0.97 |
| 1:G:831:TRP:HE1 | 2:H:67:MET:CB | 1.77 | 0.97 |
| 1:J:553:MLY:HH12 | 4:Y:45:VAL:HG21 | 1.46 | 0.97 |
| 2:K:149:ASP:OD2 | 2:K:150:TYR:O | 1.80 | 0.97 |
| 1:S:174:SER:HB3 | 1:S:667:THR:HG21 | 1.44 | 0.97 |
| 1:J:642:LYS:HD2 | 4:W:24:ASP:O | 1.65 | 0.97 |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:HG22 | 1.00 | 0.97 |
| 1:A:502:GLU:C | 1:A:761:GLY:HA3 | 1.84 | 0.97 |
| 1:A:534:SER:O | 4:8:351:THR:HA | 1.60 | 0.97 |
| 1:D:530:MET:CE | 4:9:354:GLN:CG | 2.40 | 0.97 |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:CH2 | 1.92 | 0.97 |
| 1:J:530:MET:CE | 4:W:354:GLN:CG | 2.41 | 0.97 |
| 1:S:805:ALA:HA | 1:S:808:GLU:HB2 | 1.44 | 0.97 |
| 2:T:121:LEU:CB | 2:T:128:PHE:HB3 | 1.69 | 0.97 |
| 2:T:149:ASP:OD2 | 2:T:150:TYR:O | 1.80 | 0.97 |
| 1:A:800:ARG:HH22 | 3:C:40:ASN:HD21 | 1.10 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:139:ALA:O | 2:E:141:PRO:HD3 | 1.62 | 0.97 |
| 2:H:130:PRO:O | 2:H:133:ILE:N | 1.97 | 0.97 |
| 1:G:792:ALA:CB | 3:I:42:THR:HA | 1.94 | 0.97 |
| 1:M:542:PHE:CG | 4:Z:143:TYR:CE1 | 2.53 | 0.97 |
| 1:J:642:LYS:HG2 | 4:W:21:PHE:O | 1.65 | 0.97 |
| 1:A:642:LYS:HG2 | 4:8:21:PHE:O | 1.65 | 0.97 |
| 2:E:117:LEU:CB | 2:E:147:ASN:CG | 2.32 | 0.97 |
| 2:E:141:PRO:HB2 | 2:E:142:PRO:HD2 | 1.44 | 0.97 |
| 1:J:95:THR:HA | 1:J:713:SER:HB3 | 1.11 | 0.97 |
| 2:K:117:LEU:HD13 | 2:K:147:ASN:OD1 | 1.64 | 0.97 |
| 1:M:174:SER:HB3 | 1:M:667:THR:HG21 | 1.44 | 0.97 |
| 1:S:93:MET:HE2 | 1:S:764:MLY:CD | 1.93 | 0.97 |
| 2:T:112:ILE:O | 2:T:147:ASN:C | 2.01 | 0.97 |
| 1:A:707:CYS:CA | 1:A:714:ARG:CZ | 2.39 | 0.97 |
| 1:D:726:VAL:O | 1:D:785:GLU:HG2 | 1.64 | 0.97 |
| 2:E:112:ILE:O | 2:E:147:ASN:C | 2.01 | 0.97 |
| 1:M:831:TRP:CH2 | 2:N:47:LEU:HD22 | 1.97 | 0.97 |
| 1:S:93:MET:HE3 | 1:S:716:LEU:HD12 | 1.46 | 0.97 |
| 2:T:141:PRO:HB2 | 2:T:142:PRO:HD2 | 1.44 | 0.97 |
| 1:S:542:PHE:CG | 4:2:143:TYR:CE1 | 2.53 | 0.97 |
| 1:A:174:SER:HB3 | 1:A:667:THR:HG21 | 1.44 | 0.97 |
| 1:A:502:GLU:OE1 | 1:A:763:THR:N | 1.97 | 0.97 |
| 1:D:736:GLN:CA | 1:D:743:ALA:HB2 | 1.95 | 0.97 |
| 1:D:836:PHE:HE1 | 2:E:159:HIS:CB | 1.78 | 0.97 |
| 1:D:799:MET:SD | 3:F:32:ASP:CA | 2.51 | 0.97 |
| 1:G:649:VAL:CA | 1:G:649:VAL:CG2 | 2.43 | 0.97 |
| 2:H:117:LEU:CB | 2:H:147:ASN:CG | 2.32 | 0.97 |
| 2:H:117:LEU:HD13 | 2:H:147:ASN:OD1 | 1.64 | 0.97 |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:CA | 2.43 | 0.97 |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:CD2 | 1.95 | 0.97 |
| 1:S:649:VAL:CA | 1:S:649:VAL:CG2 | 2.43 | 0.97 |
| 2:T:130:PRO:O | 2:T:133:ILE:N | 1.96 | 0.97 |
| 1:A:538:GLU:N | 4:8:349:LEU:CD1 | 2.28 | 0.97 |
| 1:D:576:GLU:CG | 1:D:577:ALA:H | 1.75 | 0.97 |
| 1:D:747:LEU:HD21 | 1:D:782:MLY:HH11 | 1.45 | 0.97 |
| 1:D:838:ILE:HD12 | 2:E:54:MET:SD | 2.04 | 0.97 |
| 1:G:218:LEU:CA | 1:G:221:GLN:CG | 2.42 | 0.97 |
| 4:1:287:ILE:CG2 | 4:3:204:ALA:H | 1.78 | 0.97 |
| 1:A:649:VAL:CA | 1:A:649:VAL:CG2 | 2.43 | 0.97 |
| 1:D:818:TYR:HB2 | 2:E:90:GLY:HA3 | 1.41 | 0.97 |
| 2:H:139:ALA:O | 2:H:141:PRO:HD3 | 1.62 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:831:TRP:HH2 | 2:K:47:LEU:HD21 | 1.24 | 0.97 |
| 1:M:805:ALA:O | 1:M:809:ARG:HB2 | 1.63 | 0.97 |
| 3:O:46:ILE:O | 3:O:50:LEU:HG | 1.64 | 0.97 |
| 1:S:707:CYS:C | 1:S:714:ARG:NH2 | 2.17 | 0.97 |
| 1:S:770:GLY:C | 1:S:771:LEU:CA | 2.33 | 0.97 |
| 2:T:117:LEU:CB | 2:T:147:ASN:CG | 2.32 | 0.97 |
| 1:D:642:LYS:HG2 | 4:9:21:PHE:O | 1.65 | 0.96 |
| 1:A:542:PHE:CG | 4:8:143:TYR:CE1 | 2.52 | 0.96 |
| 1:D:576:GLU:HG2 | 1:D:577:ALA:H | 0.85 | 0.96 |
| 1:G:534:SER:O | 4:V:351:THR:HA | 1.60 | 0.96 |
| 2:H:121:LEU:HG | 2:H:128:PHE:HA | 1.47 | 0.96 |
| 2:H:150:TYR:C | 2:H:151:LYS:HG3 | 1.83 | 0.96 |
| 3:I:46:ILE:O | 3:I:50:LEU:HG | 1.64 | 0.96 |
| 1:J:792:ALA:CB | 3:L:42:THR:HG23 | 1.70 | 0.96 |
| 1:J:84:MLY:HD3 | 1:J:724:TYR:CZ | 2.00 | 0.96 |
| 2:K:112:ILE:O | 2:K:147:ASN:C | 2.02 | 0.96 |
| 1:S:218:LEU:CA | 1:S:221:GLN:CG | 2.42 | 0.96 |
| 1:S:753:VAL:HG22 | 1:S:779:ARG:NH2 | 1.79 | 0.96 |
| 1:S:838:ILE:HD11 | 2:T:54:MET:SD | 2.04 | 0.96 |
| 4:8:322:PRO:HB3 | 4:V:244:ASP:OD2 | 1.62 | 0.96 |
| 1:J:567:LYS:HZ1 | 4:Y:92:ASN:HD22 | 1.07 | 0.96 |
| 1:S:637:LYS:NZ | 4:2:141:SER:O | 1.98 | 0.96 |
| 1:A:498:LEU:HD23 | 1:A:764:MLY:HH22 | 1.44 | 0.96 |
| 1:A:642:LYS:HD2 | 4:8:24:ASP:O | 1.64 | 0.96 |
| 2:H:141:PRO:HB2 | 2:H:142:PRO:HD2 | 1.44 | 0.96 |
| 2:K:141:PRO:HB2 | 2:K:142:PRO:HD2 | 1.44 | 0.96 |
| 1:G:642:LYS:HG2 | 4:V:21:PHE:O | 1.65 | 0.96 |
| 1:J:218:LEU:CA | 1:J:221:GLN:CG | 2.42 | 0.96 |
| 1:J:542:PHE:CG | 4:W:143:TYR:CE1 | 2.53 | 0.96 |
| 2:K:121:LEU:HG | 2:K:128:PHE:HA | 1.47 | 0.96 |
| 1:M:218:LEU:CA | 1:M:221:GLN:CG | 2.42 | 0.96 |
| 1:S:795:ARG:HH21 | 3:U:116:GLU:CA | 1.78 | 0.96 |
| 1:M:635:GLY:HA3 | 4:Z:334:GLU:HG2 | 1.47 | 0.96 |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:HD11 | 1.94 | 0.96 |
| 1:D:795:ARG:NE | 3:F:116:GLU:OE2 | 1.77 | 0.96 |
| 1:G:642:LYS:HD2 | 4:V:24:ASP:O | 1.65 | 0.96 |
| 1:J:84:MLY:HH12 | 1:J:715:VAL:HG11 | 1.44 | 0.96 |
| 1:M:783:LEU:CB | 1:M:786:ILE:HD12 | 1.96 | 0.96 |
| 1:S:215:GLN:H | 1:S:340:ILE:CG1 | 1.72 | 0.96 |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:HD11 | 1.22 | 0.96 |
| 2:B:150:TYR:O | 2:B:151:LYS:HG3 | 1.65 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:649:VAL:CG1 | 1:D:649:VAL:CG2 | 2.43 | 0.96 |
| 3:I:52:ASN:HB2 | 3:I:53:PRO:HD3 | 1.46 | 0.96 |
| 1:M:649:VAL:CA | 1:M:649:VAL:CG2 | 2.43 | 0.96 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:HD2 | 1.45 | 0.96 |
| 1:M:796:GLY:HA2 | 3:O:35:ARG:HD3 | 1.45 | 0.96 |
| 1:S:727:LEU:HD21 | 1:S:783:LEU:HB2 | 1.44 | 0.96 |
| 1:D:642:LYS:HD2 | 4:9:24:ASP:O | 1.64 | 0.96 |
| 1:A:649:VAL:CG2 | 1:A:649:VAL:CG1 | 2.44 | 0.96 |
| 1:D:218:LEU:CA | 1:D:221:GLN:CG | 2.42 | 0.96 |
| 1:G:174:SER:HB3 | 1:G:667:THR:HG21 | 1.44 | 0.96 |
| 1:M:637:LYS:NZ | 4:Z:141:SER:O | 1.98 | 0.96 |
| 1:S:537:GLU:C | 4:2:349:LEU:CD1 | 2.20 | 0.96 |
| 1:A:149:GLN:CD | 1:A:718:ALA:HB3 | 1.84 | 0.96 |
| 1:G:93:MET:HA | 1:G:714:ARG:H | 1.29 | 0.96 |
| 2:H:121:LEU:CB | 2:H:128:PHE:HB3 | 1.69 | 0.96 |
| 1:J:829:TRP:CH2 | 2:K:87:LYS:CE | 2.49 | 0.96 |
| 1:M:642:LYS:HG2 | 4:Z:21:PHE:O | 1.65 | 0.96 |
| 1:S:549:SER:HB2 | 4:4:43:VAL:HG21 | 1.44 | 0.96 |
| 4:4:287:ILE:HD13 | 4:6:203:THR:CB | 1.91 | 0.96 |
| 1:D:542:PHE:CG | 4:9:143:TYR:CE1 | 2.52 | 0.96 |
| 2:B:121:LEU:HG | 2:B:128:PHE:HA | 1.46 | 0.96 |
| 1:D:798:LEU:CG | 3:F:126:LEU:HD11 | 1.96 | 0.96 |
| 1:G:542:PHE:CG | 4:V:143:TYR:CE1 | 2.53 | 0.96 |
| 1:J:721:LYS:CA | 1:J:736:GLN:CD | 2.34 | 0.96 |
| 1:D:538:GLU:N | 4:9:349:LEU:CD1 | 2.28 | 0.96 |
| 3:C:46:ILE:O | 3:C:50:LEU:HG | 1.64 | 0.96 |
| 1:D:543:PRO:CG | 4:9:143:TYR:O | 2.14 | 0.96 |
| 1:J:710:GLY:C | 1:J:772:LEU:CD2 | 2.35 | 0.96 |
| 1:J:84:MLY:CH2 | 1:J:719:ASP:C | 2.34 | 0.96 |
| 1:S:502:GLU:OE1 | 1:S:761:GLY:HA3 | 1.65 | 0.96 |
| 1:S:797:PHE:CZ | 3:U:146:ILE:CD1 | 2.48 | 0.96 |
| 2:T:150:TYR:C | 2:T:151:LYS:HG3 | 1.83 | 0.96 |
| 3:U:52:ASN:HB2 | 3:U:53:PRO:HD3 | 1.46 | 0.96 |
| 1:S:635:GLY:HA3 | 4:2:334:GLU:HG2 | 1.47 | 0.96 |
| 1:A:635:GLY:HA3 | 4:8:334:GLU:HG2 | 1.47 | 0.96 |
| 1:A:530:MET:CE | 4:8:354:GLN:CG | 2.41 | 0.96 |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CZ | 2.00 | 0.96 |
| 1:G:728:ASN:CG | 3:I:114:LEU:HD23 | 1.73 | 0.96 |
| 1:S:543:PRO:CG | 4:2:143:TYR:O | 2.14 | 0.95 |
| 1:A:637:LYS:NZ | 4:8:141:SER:O | 1.99 | 0.95 |
| 1:A:502:GLU:CA | 1:A:761:GLY:CA | 2.44 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CG | 1.95 | 0.95 |
| 3:F:46:ILE:O | 3:F:50:LEU:HG | 1.65 | 0.95 |
| 1:G:92:ALA:O | 1:G:714:ARG:HG2 | 1.65 | 0.95 |
| 1:J:710:GLY:HA2 | 1:J:772:LEU:HD21 | 1.46 | 0.95 |
| 1:M:543:PRO:CG | 4:Z:143:TYR:O | 2.14 | 0.95 |
| 2:N:121:LEU:HG | 2:N:128:PHE:HA | 1.47 | 0.95 |
| 2:N:150:TYR:O | 2:N:151:LYS:HG3 | 1.65 | 0.95 |
| 1:S:795:ARG:HH11 | 3:U:43:ASN:CB | 1.62 | 0.95 |
| 1:G:538:GLU:N | 4:V:349:LEU:CD1 | 2.29 | 0.95 |
| 1:A:534:SER:O | 4:8:351:THR:HG23 | 1.13 | 0.95 |
| 1:A:735:GLY:C | 1:A:743:ALA:CA | 2.34 | 0.95 |
| 1:A:817:GLN:CD | 2:B:127:ARG:HG2 | 1.85 | 0.95 |
| 1:D:727:LEU:HB2 | 1:D:782:MLY:NZ | 1.81 | 0.95 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:CG2 | 2.44 | 0.95 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:CD | 1.89 | 0.95 |
| 2:T:150:TYR:O | 2:T:151:LYS:HG3 | 1.65 | 0.95 |
| 1:S:795:ARG:HH12 | 3:U:43:ASN:CB | 1.64 | 0.95 |
| 1:G:637:LYS:NZ | 4:V:141:SER:O | 1.99 | 0.95 |
| 4:W:286:ASP:CG | 4:Y:203:THR:HG22 | 1.87 | 0.95 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:CG | 2.29 | 0.95 |
| 3:C:52:ASN:HB2 | 3:C:53:PRO:HD3 | 1.45 | 0.95 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:HB3 | 1.41 | 0.95 |
| 1:S:649:VAL:CG1 | 1:S:649:VAL:CG2 | 2.44 | 0.95 |
| 1:S:735:GLY:C | 1:S:743:ALA:CA | 2.35 | 0.95 |
| 1:S:120:GLY:HA2 | 1:S:764:MLY:HH13 | 1.45 | 0.95 |
| 1:S:797:PHE:CE2 | 3:U:146:ILE:CD1 | 2.48 | 0.95 |
| 4:1:287:ILE:HD13 | 4:3:203:THR:CB | 1.96 | 0.95 |
| 1:A:754:ASP:OD2 | 1:A:778:MET:CE | 2.14 | 0.95 |
| 1:D:800:ARG:HH22 | 3:F:40:ASN:ND2 | 1.64 | 0.95 |
| 1:M:537:GLU:C | 4:Z:349:LEU:CD1 | 2.20 | 0.95 |
| 1:M:538:GLU:HG3 | 4:Z:352:PHE:N | 1.81 | 0.95 |
| 1:M:84:MLY:CH1 | 1:M:715:VAL:HG13 | 1.96 | 0.95 |
| 1:M:35:MLY:HE2 | 1:M:777:GLU:CG | 1.97 | 0.95 |
| 1:S:530:MET:CE | 4:2:354:GLN:CG | 2.40 | 0.95 |
| 1:S:721:LYS:CA | 1:S:736:GLN:CD | 2.34 | 0.95 |
| 1:D:637:LYS:NZ | 4:9:141:SER:O | 1.99 | 0.95 |
| 1:A:502:GLU:HG3 | 1:A:761:GLY:HA3 | 1.33 | 0.95 |
| 1:D:732:ILE:HG21 | 1:D:782:MLY:HH21 | 0.97 | 0.95 |
| 1:M:642:LYS:HD2 | 4:Z:24:ASP:O | 1.64 | 0.95 |
| 1:S:746:LYS:HZ1 | 3:U:96:LYS:HA | 1.26 | 0.95 |
| 1:A:831:TRP:HZ2 | 2:B:47:LEU:HA | 1.22 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:537:GLU:C | 4:9:349:LEU:CD1 | 2.20 | 0.95 |
| 1:D:712:PRO:HD2 | 1:D:771:LEU:HD13 | 1.46 | 0.95 |
| 1:D:712:PRO:HG2 | 1:D:771:LEU:HB2 | 0.97 | 0.95 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:HG23 | 2.02 | 0.95 |
| 1:J:735:GLY:C | 1:J:743:ALA:CA | 2.34 | 0.95 |
| 1:J:756:THR:HG23 | 1:J:779:ARG:CD | 1.96 | 0.95 |
| 1:M:795:ARG:HB3 | 3:O:35:ARG:HH22 | 1.13 | 0.95 |
| 1:G:530:MET:CE | 4:V:354:GLN:CG | 2.39 | 0.95 |
| 1:S:538:GLU:HG3 | 4:2:352:PHE:N | 1.82 | 0.95 |
| 2:E:121:LEU:HG | 2:E:128:PHE:HA | 1.47 | 0.95 |
| 1:J:543:PRO:CG | 4:W:143:TYR:O | 2.14 | 0.95 |
| 1:S:727:LEU:CD2 | 1:S:783:LEU:CB | 2.14 | 0.95 |
| 1:S:804:ARG:O | 1:S:808:GLU:N | 2.00 | 0.95 |
| 1:A:553:MLY:CB | 4:V:46:GLY:CA | 2.32 | 0.95 |
| 1:J:635:GLY:HA3 | 4:W:334:GLU:HG2 | 1.47 | 0.95 |
| 4:X:291:LYS:HE2 | 4:Z:243:PRO:C | 1.85 | 0.95 |
| 1:D:635:GLY:HA3 | 4:9:334:GLU:HG2 | 1.47 | 0.95 |
| 2:B:121:LEU:CB | 2:B:128:PHE:HB3 | 1.69 | 0.95 |
| 2:E:150:TYR:O | 2:E:151:LYS:HG3 | 1.65 | 0.95 |
| 1:J:791:GLN:CD | 3:L:116:GLU:HG3 | 1.87 | 0.95 |
| 1:M:649:VAL:CG2 | 1:M:649:VAL:CG1 | 2.43 | 0.95 |
| 1:S:817:GLN:CB | 2:T:127:ARG:CD | 2.41 | 0.95 |
| 1:S:791:GLN:HE22 | 3:U:115:GLY:HA3 | 1.21 | 0.95 |
| 4:X:291:LYS:CE | 4:Z:243:PRO:C | 2.34 | 0.95 |
| 1:M:538:GLU:N | 4:Z:349:LEU:CD1 | 2.28 | 0.95 |
| 1:A:502:GLU:HA | 1:A:762:HIS:N | 1.82 | 0.95 |
| 1:A:95:THR:OG1 | 1:A:769:ALA:C | 2.03 | 0.95 |
| 1:G:735:GLY:C | 1:G:743:ALA:CA | 2.34 | 0.95 |
| 1:M:546:THR:HG22 | 1:M:548:THR:H | 1.32 | 0.95 |
| 1:G:543:PRO:CG | 4:V:143:TYR:O | 2.15 | 0.95 |
| 1:J:637:LYS:NZ | 4:W:141:SER:O | 1.99 | 0.95 |
| 1:S:642:LYS:HD2 | 4:2:24:ASP:O | 1.65 | 0.95 |
| 1:S:538:GLU:N | 4:2:349:LEU:CD1 | 2.28 | 0.95 |
| 4:4:324:THR:OG1 | 4:6:244:ASP:N | 1.96 | 0.95 |
| 1:A:541:MET:N | 4:8:349:LEU:HD21 | 1.80 | 0.95 |
| 1:A:530:MET:CA | 4:8:354:GLN:CG | 2.44 | 0.95 |
| 1:A:543:PRO:CG | 4:8:143:TYR:O | 2.14 | 0.95 |
| 1:A:791:GLN:NE2 | 3:C:116:GLU:N | 2.10 | 0.95 |
| 1:G:635:GLY:HA3 | 4:V:334:GLU:HG2 | 1.47 | 0.95 |
| 2:K:150:TYR:O | 2:K:151:LYS:HG3 | 1.65 | 0.95 |
| 1:M:206:LYS:CD | 1:M:217:THR:CG2 | 2.16 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:721:LYS:CA | 1:M:736:GLN:CD | 2.34 | 0.95 |
| 1:S:534:SER:O | 4:2:351:THR:HG23 | 1.13 | 0.95 |
| 1:S:786:ILE:C | 1:S:789:ALA:H | 1.69 | 0.95 |
| 1:S:803:TYR:O | 1:S:807:VAL:N | 2.00 | 0.95 |
| 4:V:286:ASP:CG | 4:X:203:THR:HG22 | 1.87 | 0.95 |
| 1:D:641:LYS:HD2 | 1:D:647:GLN:CD | 1.70 | 0.94 |
| 1:D:721:LYS:CA | 1:D:736:GLN:CD | 2.34 | 0.94 |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:HD11 | 1.21 | 0.94 |
| 1:G:754:ASP:N | 1:G:776:GLU:OE1 | 1.85 | 0.94 |
| 1:S:786:ILE:HB | 1:S:787:ILE:N | 1.82 | 0.94 |
| 4:3:322:PRO:HB2 | 4:5:244:ASP:HB3 | 1.49 | 0.94 |
| 1:A:502:GLU:CG | 1:A:764:MLY:O | 2.14 | 0.94 |
| 1:D:553:MLY:HB3 | 4:W:46:GLY:HA2 | 1.47 | 0.94 |
| 1:D:823:PHE:CE1 | 2:E:156:VAL:HG12 | 2.02 | 0.94 |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:HG21 | 1.46 | 0.94 |
| 1:G:795:ARG:HE | 3:I:116:GLU:HB3 | 0.85 | 0.94 |
| 1:J:538:GLU:HG3 | 4:W:352:PHE:N | 1.81 | 0.94 |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:CG1 | 2.43 | 0.94 |
| 1:S:642:LYS:HG2 | 4:2:21:PHE:O | 1.65 | 0.94 |
| 4:8:288:ASP:HA | 4:V:204:ALA:HB2 | 1.48 | 0.94 |
| 4:1:244:ASP:OD2 | 4:Y:325:MET:HE2 | 1.67 | 0.94 |
| 1:A:721:LYS:CA | 1:A:736:GLN:CD | 2.34 | 0.94 |
| 2:B:117:LEU:HD13 | 2:B:147:ASN:OD1 | 1.64 | 0.94 |
| 1:D:735:GLY:C | 1:D:743:ALA:CA | 2.35 | 0.94 |
| 1:G:721:LYS:CA | 1:G:736:GLN:CD | 2.34 | 0.94 |
| 1:J:710:GLY:N | 1:J:772:LEU:HD22 | 1.81 | 0.94 |
| 1:M:735:GLY:C | 1:M:743:ALA:CA | 2.35 | 0.94 |
| 1:M:819:ASN:OD1 | 2:N:92:ASP:HB2 | 1.67 | 0.94 |
| 1:G:538:GLU:HG3 | 4:V:352:PHE:N | 1.81 | 0.94 |
| 1:S:530:MET:HA | 4:2:354:GLN:HG3 | 0.96 | 0.94 |
| 2:E:163:ALA:O | 2:K:22:THR:N | 1.99 | 0.94 |
| 1:G:831:TRP:NE1 | 2:H:67:MET:HB3 | 1.81 | 0.94 |
| 1:J:792:ALA:HB2 | 3:L:42:THR:CB | 1.98 | 0.94 |
| 3:O:52:ASN:HB2 | 3:O:53:PRO:HD3 | 1.45 | 0.94 |
| 1:S:541:MET:N | 4:2:349:LEU:HD21 | 1.80 | 0.94 |
| 2:T:150:TYR:O | 2:T:151:LYS:CG | 2.16 | 0.94 |
| 1:G:642:LYS:CG | 4:V:23:GLY:H | 1.76 | 0.94 |
| 1:J:541:MET:N | 4:W:349:LEU:HD21 | 1.80 | 0.94 |
| 1:D:538:GLU:HG3 | 4:9:352:PHE:N | 1.82 | 0.94 |
| 1:A:93:MET:HE2 | 1:A:715:VAL:HA | 0.95 | 0.94 |
| 1:D:747:LEU:HD11 | 1:D:782:MLY:HH22 | 1.49 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:162:ASP:O | 2:K:21:GLU:CB | 2.15 | 0.94 |
| 1:A:546:THR:HG22 | 1:A:548:THR:H | 1.32 | 0.94 |
| 1:A:641:LYS:CD | 4:8:348:SER:HB2 | 1.92 | 0.94 |
| 1:A:505:MLY:HB3 | 1:A:762:HIS:N | 1.80 | 0.94 |
| 1:G:754:ASP:OD2 | 1:G:776:GLU:HA | 1.67 | 0.94 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:HA | 1.97 | 0.94 |
| 1:M:795:ARG:HD2 | 3:O:43:ASN:OD1 | 1.64 | 0.94 |
| 1:M:818:TYR:HE1 | 2:N:127:ARG:NH2 | 1.66 | 0.94 |
| 1:G:530:MET:HA | 4:V:354:GLN:HG3 | 0.97 | 0.94 |
| 4:1:287:ILE:CD1 | 4:3:203:THR:HB | 1.96 | 0.94 |
| 1:D:541:MET:N | 4:9:349:LEU:HD21 | 1.80 | 0.94 |
| 1:A:97:LEU:HD23 | 1:A:712:PRO:HB3 | 1.49 | 0.94 |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HE3 | 1.31 | 0.94 |
| 2:B:150:TYR:O | 2:B:151:LYS:HB2 | 1.67 | 0.94 |
| 1:G:546:THR:HG22 | 1:G:548:THR:H | 1.32 | 0.94 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:OE1 | 1.67 | 0.94 |
| 1:J:783:LEU:O | 1:J:787:ILE:N | 1.99 | 0.94 |
| 1:J:834:LEU:HD13 | 2:K:51:PHE:HE1 | 1.33 | 0.94 |
| 1:M:817:GLN:CD | 2:N:127:ARG:HD2 | 1.87 | 0.94 |
| 2:N:150:TYR:O | 2:N:151:LYS:CG | 2.16 | 0.94 |
| 1:S:218:LEU:CB | 1:S:221:GLN:CG | 2.46 | 0.94 |
| 1:D:557:GLU:N | 4:W:48:GLY:CA | 2.12 | 0.94 |
| 1:M:530:MET:CA | 4:Z:354:GLN:CG | 2.45 | 0.94 |
| 4:2:112:PRO:CB | 4:3:196:ARG:CA | 2.44 | 0.94 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HD21 | 0.95 | 0.94 |
| 1:D:206:LYS:CD | 1:D:217:THR:CG2 | 2.16 | 0.94 |
| 1:D:612:GLN:NE2 | 1:D:627:GLY:CA | 2.31 | 0.94 |
| 1:D:724:TYR:HB3 | 1:D:782:MLY:CD | 1.96 | 0.94 |
| 1:D:732:ILE:CD1 | 1:D:782:MLY:HH11 | 1.95 | 0.94 |
| 1:G:838:ILE:CD1 | 2:H:54:MET:CE | 2.29 | 0.94 |
| 1:J:756:THR:HG23 | 1:J:779:ARG:HD2 | 1.47 | 0.94 |
| 2:N:121:LEU:CB | 2:N:128:PHE:HB3 | 1.69 | 0.94 |
| 1:A:553:MLY:HB3 | 4:V:46:GLY:HA2 | 1.47 | 0.94 |
| 1:J:538:GLU:N | 4:W:349:LEU:CD1 | 2.28 | 0.94 |
| 1:D:215:GLN:HA | 1:D:340:ILE:HG23 | 0.95 | 0.94 |
| 2:E:150:TYR:O | 2:E:151:LYS:CG | 2.15 | 0.94 |
| 1:J:612:GLN:NE2 | 1:J:627:GLY:CA | 2.31 | 0.94 |
| 1:M:800:ARG:HB3 | 3:O:149:VAL:HG22 | 1.47 | 0.94 |
| 4:9:288:ASP:HA | 4:W:204:ALA:HB2 | 1.48 | 0.94 |
| 1:G:553:MLY:CE | 4:X:45:VAL:HB | 1.91 | 0.94 |
| 4:7:288:ASP:HA | 4:9:204:ALA:HB2 | 1.48 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:612:GLN:NE2 | 1:A:627:GLY:HA3 | 1.83 | 0.94 |
| 1:G:215:GLN:HA | 1:G:340:ILE:HG23 | 0.95 | 0.94 |
| 2:H:150:TYR:O | 2:H:151:LYS:HG3 | 1.65 | 0.94 |
| 1:J:546:THR:HG22 | 1:J:548:THR:H | 1.32 | 0.94 |
| 2:K:150:TYR:O | 2:K:151:LYS:CG | 2.15 | 0.94 |
| 1:S:612:GLN:NE2 | 1:S:627:GLY:HA3 | 1.83 | 0.94 |
| 1:S:736:GLN:CA | 1:S:743:ALA:HB2 | 1.95 | 0.94 |
| 1:S:795:ARG:HB2 | 3:U:35:ARG:NH1 | 1.83 | 0.94 |
| 1:S:84:MLY:CH1 | 1:S:724:TYR:HE2 | 1.80 | 0.94 |
| 4:2:287:ILE:HG12 | 4:4:203:THR:H | 1.30 | 0.94 |
| 4:4:322:PRO:HB3 | 4:6:244:ASP:CB | 1.98 | 0.94 |
| 1:A:538:GLU:HG3 | 4:8:352:PHE:N | 1.82 | 0.94 |
| 1:D:557:GLU:H | 4:W:48:GLY:HA2 | 1.32 | 0.94 |
| 1:J:612:GLN:NE2 | 1:J:627:GLY:HA3 | 1.83 | 0.94 |
| 1:J:84:MLY:NZ | 1:J:724:TYR:CE2 | 2.35 | 0.94 |
| 1:M:218:LEU:CB | 1:M:221:GLN:CG | 2.46 | 0.94 |
| 1:M:612:GLN:NE2 | 1:M:627:GLY:HA3 | 1.83 | 0.94 |
| 4:X:324:THR:HB | 4:Z:246:GLN:HA | 1.50 | 0.94 |
| 1:A:530:MET:HA | 4:8:354:GLN:HG3 | 0.96 | 0.93 |
| 1:G:795:ARG:NE | 3:I:116:GLU:CB | 2.27 | 0.93 |
| 1:S:795:ARG:CG | 3:U:118:MET:HE2 | 1.95 | 0.93 |
| 1:S:93:MET:CE | 1:S:764:MLY:CD | 2.45 | 0.93 |
| 1:S:838:ILE:CD1 | 2:T:54:MET:CE | 2.44 | 0.93 |
| 4:X:287:ILE:C | 4:Z:205:GLU:CD | 2.27 | 0.93 |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:H | 1.29 | 0.93 |
| 1:A:768:MLY:HG2 | 1:A:771:LEU:HD13 | 1.49 | 0.93 |
| 1:D:818:TYR:CG | 2:E:90:GLY:HA3 | 2.03 | 0.93 |
| 1:G:612:GLN:NE2 | 1:G:627:GLY:HA3 | 1.83 | 0.93 |
| 1:G:754:ASP:CB | 1:G:776:GLU:HA | 1.97 | 0.93 |
| 1:J:829:TRP:CE3 | 2:K:87:LYS:NZ | 2.29 | 0.93 |
| 1:M:553:MLY:HB3 | 4:2:46:GLY:HA2 | 1.48 | 0.93 |
| 2:N:117:LEU:HD13 | 2:N:147:ASN:OD1 | 1.64 | 0.93 |
| 1:G:530:MET:CA | 4:V:354:GLN:CG | 2.45 | 0.93 |
| 1:G:567:LYS:HZ2 | 4:X:92:ASN:HD22 | 1.11 | 0.93 |
| 1:M:541:MET:N | 4:Z:349:LEU:HD21 | 1.80 | 0.93 |
| 4:3:322:PRO:HB3 | 4:5:244:ASP:CB | 1.97 | 0.93 |
| 4:3:287:ILE:CG2 | 4:5:204:ALA:H | 1.81 | 0.93 |
| 1:D:642:LYS:CG | 4:9:23:GLY:H | 1.77 | 0.93 |
| 1:D:612:GLN:NE2 | 1:D:627:GLY:HA3 | 1.83 | 0.93 |
| 1:G:215:GLN:H | 1:G:340:ILE:CG1 | 1.73 | 0.93 |
| 1:G:206:LYS:CD | 1:G:217:THR:CG2 | 2.16 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:819:ASN:ND2 | 2:H:92:ASP:CB | 2.30 | 0.93 |
| 2:T:121:LEU:HG | 2:T:128:PHE:HA | 1.47 | 0.93 |
| 1:S:750:GLY:CA | 3:U:89:GLU:HB3 | 1.97 | 0.93 |
| 4:X:324:THR:CG2 | 4:Z:247:VAL:HG23 | 1.93 | 0.93 |
| 1:S:530:MET:CA | 4:2:354:GLN:CG | 2.44 | 0.93 |
| 4:4:287:ILE:CG2 | 4:6:204:ALA:H | 1.81 | 0.93 |
| 1:D:538:GLU:OE2 | 4:9:355:MET:HE3 | 1.66 | 0.93 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:NE2 | 1.58 | 0.93 |
| 1:D:546:THR:HG22 | 1:D:548:THR:H | 1.32 | 0.93 |
| 1:D:747:LEU:CD2 | 1:D:782:MLY:HH11 | 1.96 | 0.93 |
| 1:G:84:MLY:HH21 | 1:G:720:PHE:HA | 1.51 | 0.93 |
| 1:M:530:MET:HA | 4:Z:354:GLN:HG3 | 0.96 | 0.93 |
| 2:T:150:TYR:O | 2:T:151:LYS:HB2 | 1.67 | 0.93 |
| 1:S:831:TRP:CH2 | 2:T:47:LEU:HD21 | 2.00 | 0.93 |
| 2:B:150:TYR:O | 2:B:151:LYS:CG | 2.15 | 0.93 |
| 1:D:726:VAL:CG1 | 1:D:785:GLU:CG | 2.44 | 0.93 |
| 1:J:530:MET:HA | 4:W:354:GLN:HG3 | 0.96 | 0.93 |
| 1:S:770:GLY:O | 1:S:774:LEU:CA | 2.15 | 0.93 |
| 1:J:739:ASP:HB3 | 1:J:742:LYS:CB | 1.99 | 0.93 |
| 1:M:798:LEU:CD2 | 3:O:126:LEU:HD11 | 1.98 | 0.93 |
| 1:S:749:GLY:O | 3:U:89:GLU:HB3 | 1.69 | 0.93 |
| 4:W:325:MET:CE | 4:Y:244:ASP:CG | 2.37 | 0.93 |
| 4:1:203:THR:HG22 | 4:Y:286:ASP:CG | 1.87 | 0.93 |
| 1:D:739:ASP:HB3 | 1:D:742:LYS:CB | 1.98 | 0.93 |
| 1:G:757:GLN:HG2 | 1:G:776:GLU:CD | 1.88 | 0.93 |
| 1:G:792:ALA:CB | 3:I:42:THR:CA | 2.47 | 0.93 |
| 1:J:84:MLY:HH11 | 1:J:720:PHE:CE1 | 2.04 | 0.93 |
| 1:M:799:MET:SD | 3:O:32:ASP:CG | 2.47 | 0.93 |
| 1:S:642:LYS:CB | 4:2:21:PHE:O | 2.17 | 0.93 |
| 1:S:836:PHE:CE2 | 2:T:160:GLY:CA | 2.52 | 0.93 |
| 1:M:642:LYS:CG | 4:Z:23:GLY:H | 1.77 | 0.93 |
| 4:3:287:ILE:HD13 | 4:5:203:THR:CB | 1.91 | 0.93 |
| 4:4:287:ILE:HG21 | 4:6:202:THR:CB | 1.99 | 0.93 |
| 1:A:642:LYS:CB | 4:8:21:PHE:O | 2.17 | 0.93 |
| 1:D:530:MET:HA | 4:9:354:GLN:HG3 | 0.96 | 0.93 |
| 1:A:28:GLN:HE22 | 1:A:723:ARG:HH21 | 0.97 | 0.93 |
| 1:A:739:ASP:HB3 | 1:A:742:LYS:CB | 1.99 | 0.93 |
| 1:A:502:GLU:O | 1:A:761:GLY:HA2 | 1.69 | 0.93 |
| 1:A:831:TRP:CZ3 | 2:B:50:THR:HG21 | 2.04 | 0.93 |
| 1:D:639:GLY:N | 4:9:345:ILE:N | 1.94 | 0.93 |
| 1:G:629:GLU:CB | 1:G:643:GLY:O | 2.17 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:797:PHE:HE2 | 3:I:126:LEU:CD2 | 1.61 | 0.93 |
| 1:J:215:GLN:H | 1:J:340:ILE:CG1 | 1.72 | 0.93 |
| 1:J:836:PHE:HE1 | 2:K:159:HIS:HA | 1.23 | 0.93 |
| 1:M:612:GLN:NE2 | 1:M:627:GLY:CA | 2.31 | 0.93 |
| 1:M:641:LYS:HG3 | 1:M:647:GLN:NE2 | 1.58 | 0.93 |
| 1:S:215:GLN:HA | 1:S:340:ILE:HG23 | 0.95 | 0.93 |
| 1:S:821:ARG:HH21 | 2:T:127:ARG:HG2 | 1.27 | 0.93 |
| 4:4:322:PRO:HB2 | 4:6:244:ASP:HB3 | 1.49 | 0.93 |
| 1:A:648:THR:HG21 | 1:A:651:ALA:HB2 | 1.50 | 0.93 |
| 1:J:791:GLN:HE21 | 3:L:115:GLY:HA3 | 1.31 | 0.93 |
| 1:J:836:PHE:CZ | 2:K:160:GLY:N | 2.35 | 0.93 |
| 1:M:215:GLN:HA | 1:M:340:ILE:HG23 | 0.95 | 0.93 |
| 1:M:797:PHE:HE2 | 3:O:126:LEU:CD2 | 1.81 | 0.93 |
| 1:J:642:LYS:CB | 4:W:21:PHE:O | 2.17 | 0.93 |
| 4:1:244:ASP:CG | 4:Y:325:MET:CE | 2.37 | 0.93 |
| 1:G:739:ASP:HB3 | 1:G:742:LYS:CB | 1.99 | 0.93 |
| 2:H:150:TYR:O | 2:H:151:LYS:CG | 2.15 | 0.93 |
| 1:M:549:SER:C | 4:2:46:GLY:HA3 | 1.90 | 0.93 |
| 1:S:149:GLN:OE1 | 1:S:763:THR:HA | 1.69 | 0.93 |
| 4:2:204:ALA:HB2 | 4:Z:288:ASP:HA | 1.48 | 0.93 |
| 4:3:287:ILE:CG1 | 4:5:202:THR:CB | 2.33 | 0.92 |
| 1:A:502:GLU:HA | 1:A:761:GLY:CA | 1.99 | 0.92 |
| 1:J:538:GLU:N | 4:W:351:THR:H | 1.67 | 0.92 |
| 1:J:838:ILE:CD1 | 2:K:54:MET:CE | 2.44 | 0.92 |
| 1:S:804:ARG:C | 1:S:807:VAL:HB | 1.88 | 0.92 |
| 4:3:287:ILE:HG21 | 4:5:202:THR:CB | 1.99 | 0.92 |
| 4:3:287:ILE:HB | 4:5:203:THR:HG22 | 1.50 | 0.92 |
| 1:A:215:GLN:HA | 1:A:340:ILE:HG23 | 0.96 | 0.92 |
| 1:A:800:ARG:CD | 3:C:149:VAL:C | 2.37 | 0.92 |
| 2:E:150:TYR:O | 2:E:151:LYS:HB2 | 1.67 | 0.92 |
| 1:G:834:LEU:CD1 | 2:H:51:PHE:CE1 | 2.52 | 0.92 |
| 1:J:537:GLU:C | 4:W:349:LEU:CD1 | 2.20 | 0.92 |
| 2:K:150:TYR:O | 2:K:151:LYS:HB2 | 1.67 | 0.92 |
| 1:J:834:LEU:HD13 | 2:K:51:PHE:CE1 | 2.02 | 0.92 |
| 1:M:629:GLU:CB | 1:M:643:GLY:O | 2.17 | 0.92 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:HD2 | 1.45 | 0.92 |
| 1:A:557:GLU:H | 4:V:48:GLY:HA2 | 1.32 | 0.92 |
| 1:J:530:MET:CA | 4:W:354:GLN:CG | 2.44 | 0.92 |
| 1:D:549:SER:C | 4:W:46:GLY:HA3 | 1.90 | 0.92 |
| 4:1:287:ILE:CB | 4:3:203:THR:HG22 | 2.00 | 0.92 |
| 1:A:831:TRP:HZ2 | 2:B:47:LEU:CA | 1.80 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:820:VAL:HG11 | 2:E:136:MET:CE | 1.99 | 0.92 |
| 1:G:537:GLU:C | 4:V:349:LEU:CD1 | 2.21 | 0.92 |
| 1:J:829:TRP:CH2 | 2:K:87:LYS:HE2 | 2.03 | 0.92 |
| 1:M:836:PHE:CZ | 2:N:160:GLY:N | 2.34 | 0.92 |
| 1:M:797:PHE:CE1 | 3:O:149:VAL:CG1 | 2.52 | 0.92 |
| 1:S:612:GLN:NE2 | 1:S:627:GLY:CA | 2.31 | 0.92 |
| 1:S:629:GLU:CB | 1:S:643:GLY:O | 2.17 | 0.92 |
| 1:D:642:LYS:CB | 4:9:21:PHE:O | 2.17 | 0.92 |
| 1:D:508:ILE:CD1 | 1:D:766:PHE:CE2 | 2.52 | 0.92 |
| 1:D:834:LEU:CG | 2:E:54:MET:HG3 | 1.99 | 0.92 |
| 1:J:801:VAL:HG21 | 3:L:126:LEU:HD23 | 1.47 | 0.92 |
| 1:M:834:LEU:HD13 | 2:N:51:PHE:CE1 | 2.05 | 0.92 |
| 4:W:286:ASP:OD2 | 4:Y:203:THR:HG22 | 1.69 | 0.92 |
| 4:2:287:ILE:HG21 | 4:4:203:THR:N | 1.84 | 0.92 |
| 1:J:84:MLY:NZ | 1:J:724:TYR:HE2 | 1.66 | 0.92 |
| 1:J:791:GLN:NE2 | 3:L:115:GLY:HA3 | 1.84 | 0.92 |
| 1:S:834:LEU:HD13 | 2:T:51:PHE:HE1 | 0.75 | 0.92 |
| 4:V:325:MET:CE | 4:X:244:ASP:CG | 2.37 | 0.92 |
| 4:X:291:LYS:CG | 4:Z:244:ASP:N | 2.24 | 0.92 |
| 2:H:150:TYR:O | 2:H:151:LYS:HB2 | 1.67 | 0.92 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:CG | 2.00 | 0.92 |
| 1:S:638:GLY:HA3 | 4:2:341:ILE:O | 1.70 | 0.92 |
| 1:D:278:GLN:HG2 | 1:D:317:GLU:HB2 | 1.52 | 0.92 |
| 1:G:783:LEU:O | 1:G:787:ILE:HB | 1.70 | 0.92 |
| 1:J:505:MLY:HD2 | 1:J:762:HIS:HE1 | 1.17 | 0.92 |
| 1:J:648:THR:HG21 | 1:J:651:ALA:HB2 | 1.50 | 0.92 |
| 1:M:834:LEU:CD1 | 2:N:51:PHE:HE1 | 1.82 | 0.92 |
| 1:S:838:ILE:HD11 | 2:T:54:MET:HE3 | 1.48 | 0.92 |
| 4:V:286:ASP:OD2 | 4:X:203:THR:HG22 | 1.69 | 0.92 |
| 1:M:642:LYS:CB | 4:Z:21:PHE:O | 2.17 | 0.92 |
| 1:A:149:GLN:CB | 1:A:718:ALA:HB3 | 2.00 | 0.92 |
| 1:A:638:GLY:HA3 | 4:8:341:ILE:O | 1.70 | 0.92 |
| 1:A:629:GLU:CB | 1:A:643:GLY:O | 2.17 | 0.92 |
| 1:A:795:ARG:HD2 | 3:C:35:ARG:HH12 | 0.77 | 0.92 |
| 1:G:648:THR:HG21 | 1:G:651:ALA:HB2 | 1.50 | 0.92 |
| 1:G:707:CYS:SG | 1:G:714:ARG:NH2 | 2.43 | 0.92 |
| 1:J:278:GLN:HG2 | 1:J:317:GLU:HB2 | 1.52 | 0.92 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:CA | 2.48 | 0.92 |
| 1:G:537:GLU:O | 4:V:349:LEU:HD13 | 0.74 | 0.92 |
| 1:A:502:GLU:HG2 | 1:A:764:MLY:O | 1.69 | 0.92 |
| 1:A:612:GLN:NE2 | 1:A:627:GLY:CA | 2.31 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:629:GLU:CB | 1:D:643:GLY:O | 2.17 | 0.92 |
| 1:G:728:ASN:HD21 | 3:I:114:LEU:HD23 | 1.16 | 0.92 |
| 1:G:831:TRP:CZ2 | 2:H:47:LEU:HD22 | 2.01 | 0.92 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:CG | 2.00 | 0.92 |
| 1:S:641:LYS:HE3 | 1:S:647:GLN:CG | 2.00 | 0.92 |
| 1:G:642:LYS:CB | 4:V:21:PHE:O | 2.17 | 0.92 |
| 1:M:542:PHE:HA | 4:Z:143:TYR:HE1 | 1.34 | 0.92 |
| 4:1:203:THR:HG22 | 4:Y:286:ASP:OD2 | 1.70 | 0.92 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:CG | 2.00 | 0.92 |
| 1:D:648:THR:HG21 | 1:D:651:ALA:HB2 | 1.50 | 0.92 |
| 1:D:649:VAL:C | 1:D:649:VAL:CG1 | 2.38 | 0.92 |
| 1:G:612:GLN:NE2 | 1:G:627:GLY:CA | 2.31 | 0.92 |
| 1:G:817:GLN:HG2 | 2:H:127:ARG:CB | 2.00 | 0.92 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:C | 2.38 | 0.92 |
| 1:M:213:LYS:HA | 1:M:220:ASP:CG | 1.90 | 0.92 |
| 1:M:538:GLU:N | 4:Z:351:THR:H | 1.67 | 0.92 |
| 1:S:735:GLY:C | 1:S:743:ALA:HA | 1.90 | 0.92 |
| 4:X:291:LYS:HD2 | 4:Z:244:ASP:H | 1.23 | 0.92 |
| 4:1:287:ILE:HG23 | 4:3:202:THR:OG1 | 1.68 | 0.91 |
| 1:A:544:LYS:HD2 | 4:8:147:ARG:HB3 | 1.53 | 0.91 |
| 1:A:537:GLU:O | 4:8:349:LEU:HD13 | 0.74 | 0.91 |
| 1:D:641:LYS:HG3 | 1:D:647:GLN:NE2 | 1.59 | 0.91 |
| 1:D:818:TYR:HB2 | 2:E:90:GLY:CA | 1.95 | 0.91 |
| 1:J:213:LYS:HA | 1:J:220:ASP:CG | 1.90 | 0.91 |
| 1:M:648:THR:HG21 | 1:M:651:ALA:HB2 | 1.50 | 0.91 |
| 1:S:213:LYS:HA | 1:S:220:ASP:CG | 1.90 | 0.91 |
| 1:S:739:ASP:HB3 | 1:S:742:LYS:CB | 1.98 | 0.91 |
| 1:G:541:MET:N | 4:V:349:LEU:HD21 | 1.80 | 0.91 |
| 1:S:542:PHE:HA | 4:2:143:TYR:HE1 | 1.34 | 0.91 |
| 1:D:537:GLU:O | 4:9:349:LEU:HD13 | 0.74 | 0.91 |
| 1:A:549:SER:C | 4:V:46:GLY:HA3 | 1.89 | 0.91 |
| 1:D:213:LYS:HA | 1:D:220:ASP:CG | 1.90 | 0.91 |
| 1:G:829:TRP:CZ2 | 2:H:87:LYS:HE2 | 2.04 | 0.91 |
| 1:J:218:LEU:CB | 1:J:221:GLN:CG | 2.46 | 0.91 |
| 1:M:795:ARG:HG3 | 3:O:118:MET:HE3 | 1.46 | 0.91 |
| 1:M:800:ARG:HB3 | 3:O:149:VAL:CG2 | 2.00 | 0.91 |
| 1:S:218:LEU:HA | 1:S:221:GLN:CG | 2.01 | 0.91 |
| 1:S:791:GLN:OE1 | 3:U:116:GLU:HG3 | 1.70 | 0.91 |
| 1:S:797:PHE:HE1 | 3:U:146:ILE:O | 1.48 | 0.91 |
| 1:S:537:GLU:O | 4:2:349:LEU:HD13 | 0.73 | 0.91 |
| 1:A:538:GLU:N | 4:8:349:LEU:HD12 | 1.86 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:LEU:HA | 1:A:221:GLN:CG | 2.01 | 0.91 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:C | 2.38 | 0.91 |
| 1:D:836:PHE:CE2 | 2:E:160:GLY:N | 2.39 | 0.91 |
| 1:G:649:VAL:C | 1:G:649:VAL:CG1 | 2.38 | 0.91 |
| 1:M:218:LEU:HA | 1:M:221:GLN:CG | 2.01 | 0.91 |
| 1:M:797:PHE:CD1 | 3:O:149:VAL:HG12 | 2.03 | 0.91 |
| 1:M:798:LEU:HD23 | 3:O:122:GLU:HB3 | 1.53 | 0.91 |
| 1:S:641:LYS:HG3 | 1:S:647:GLN:NE2 | 1.59 | 0.91 |
| 1:S:831:TRP:CZ2 | 2:T:47:LEU:HD22 | 2.05 | 0.91 |
| 1:M:537:GLU:O | 4:Z:349:LEU:HD13 | 0.73 | 0.91 |
| 1:D:538:GLU:N | 4:9:351:THR:H | 1.68 | 0.91 |
| 1:D:530:MET:CA | 4:9:354:GLN:CG | 2.45 | 0.91 |
| 1:A:501:GLU:O | 1:A:762:HIS:CE1 | 2.22 | 0.91 |
| 1:A:538:GLU:N | 4:8:351:THR:H | 1.68 | 0.91 |
| 1:A:735:GLY:C | 1:A:743:ALA:HA | 1.91 | 0.91 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:CG | 2.00 | 0.91 |
| 1:G:218:LEU:CB | 1:G:221:GLN:CG | 2.46 | 0.91 |
| 1:J:792:ALA:H | 3:L:42:THR:HG22 | 1.36 | 0.91 |
| 1:J:537:GLU:O | 4:W:349:LEU:HD13 | 0.73 | 0.91 |
| 1:M:538:GLU:N | 4:Z:349:LEU:HD12 | 1.86 | 0.91 |
| 1:A:537:GLU:C | 4:8:349:LEU:CD1 | 2.20 | 0.91 |
| 1:D:799:MET:SD | 3:F:32:ASP:HA | 2.11 | 0.91 |
| 1:J:829:TRP:CE2 | 2:K:87:LYS:HE2 | 2.04 | 0.91 |
| 1:M:544:LYS:HD2 | 4:Z:147:ARG:HB3 | 1.53 | 0.91 |
| 1:M:739:ASP:HB3 | 1:M:742:LYS:CB | 1.99 | 0.91 |
| 1:M:735:GLY:C | 1:M:743:ALA:HA | 1.91 | 0.91 |
| 2:N:150:TYR:O | 2:N:151:LYS:HB2 | 1.67 | 0.91 |
| 1:M:836:PHE:HE1 | 2:N:159:HIS:HA | 1.32 | 0.91 |
| 1:S:546:THR:HG22 | 1:S:548:THR:H | 1.32 | 0.91 |
| 1:S:502:GLU:OE1 | 1:S:761:GLY:CA | 2.18 | 0.91 |
| 4:W:324:THR:CG2 | 4:Y:247:VAL:H | 1.84 | 0.91 |
| 4:1:247:VAL:H | 4:Y:324:THR:CG2 | 1.84 | 0.91 |
| 1:M:636:LYS:HD2 | 4:Z:332:PRO:HB3 | 1.52 | 0.91 |
| 1:D:813:ILE:CG2 | 2:E:128:PHE:HZ | 1.60 | 0.91 |
| 2:H:149:ASP:CG | 2:H:150:TYR:H | 1.73 | 0.91 |
| 1:J:218:LEU:HA | 1:J:221:GLN:CG | 2.01 | 0.91 |
| 1:J:629:GLU:CB | 1:J:643:GLY:O | 2.17 | 0.91 |
| 1:M:649:VAL:C | 1:M:649:VAL:CG1 | 2.38 | 0.91 |
| 4:2:287:ILE:CB | 4:4:203:THR:CG2 | 2.35 | 0.91 |
| 1:D:538:GLU:N | 4:9:349:LEU:HD12 | 1.86 | 0.91 |
| 1:A:817:GLN:CG | 2:B:127:ARG:CD | 2.47 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:735:GLY:C | 1:J:743:ALA:HA | 1.90 | 0.91 |
| 1:S:829:TRP:CH2 | 2:T:87:LYS:HE2 | 2.06 | 0.91 |
| 4:V:324:THR:CG2 | 4:X:247:VAL:H | 1.84 | 0.91 |
| 1:D:712:PRO:HB2 | 1:D:771:LEU:CB | 2.01 | 0.91 |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:HH12 | 1.99 | 0.91 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:CA | 2.53 | 0.91 |
| 1:G:795:ARG:HB3 | 3:I:35:ARG:HH22 | 1.34 | 0.91 |
| 1:S:630:ALA:O | 4:2:25:ASP:CG | 2.09 | 0.91 |
| 1:S:752:ASP:CB | 3:U:86:ASP:OD2 | 2.19 | 0.91 |
| 1:S:92:ALA:HB3 | 1:S:764:MLY:HH11 | 1.53 | 0.91 |
| 4:1:287:ILE:HG21 | 4:3:204:ALA:H | 1.33 | 0.91 |
| 1:D:218:LEU:CB | 1:D:221:GLN:CG | 2.46 | 0.91 |
| 1:D:735:GLY:O | 1:D:743:ALA:CA | 2.19 | 0.91 |
| 1:J:831:TRP:HE1 | 2:K:67:MET:HB3 | 1.35 | 0.91 |
| 1:M:736:GLN:CA | 1:M:743:ALA:HB2 | 1.95 | 0.91 |
| 1:S:649:VAL:C | 1:S:649:VAL:CG1 | 2.38 | 0.91 |
| 1:S:798:LEU:HD12 | 3:U:126:LEU:HD21 | 1.52 | 0.91 |
| 1:S:544:LYS:HD2 | 4:2:147:ARG:HB3 | 1.53 | 0.91 |
| 4:2:112:PRO:CG | 4:3:196:ARG:C | 2.40 | 0.91 |
| 1:A:218:LEU:CB | 1:A:221:GLN:CG | 2.46 | 0.91 |
| 1:A:502:GLU:CD | 1:A:764:MLY:O | 2.09 | 0.91 |
| 1:G:213:LYS:HA | 1:G:220:ASP:CG | 1.90 | 0.91 |
| 1:G:649:VAL:CB | 1:G:649:VAL:CG2 | 2.49 | 0.91 |
| 1:J:768:MLY:CH1 | 1:J:772:LEU:HD12 | 1.95 | 0.91 |
| 1:S:278:GLN:HG2 | 1:S:317:GLU:HB2 | 1.52 | 0.91 |
| 1:S:649:VAL:CG2 | 1:S:649:VAL:CB | 2.49 | 0.91 |
| 1:S:829:TRP:CH2 | 2:T:87:LYS:NZ | 2.39 | 0.91 |
| 1:J:552:ASN:O | 4:Y:47:MET:HE1 | 1.69 | 0.91 |
| 4:3:324:THR:HG23 | 4:5:244:ASP:CA | 2.01 | 0.90 |
| 1:A:505:MLY:HB3 | 1:A:762:HIS:CG | 2.03 | 0.90 |
| 1:A:550:PHE:HA | 4:V:46:GLY:CA | 2.01 | 0.90 |
| 1:A:649:VAL:CG2 | 1:A:649:VAL:CB | 2.50 | 0.90 |
| 1:A:791:GLN:CD | 3:C:116:GLU:H | 1.74 | 0.90 |
| 1:D:735:GLY:C | 1:D:743:ALA:HA | 1.91 | 0.90 |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:NE2 | 1.58 | 0.90 |
| 1:M:649:VAL:CB | 1:M:649:VAL:CG2 | 2.49 | 0.90 |
| 1:S:92:ALA:C | 1:S:714:ARG:HG3 | 1.91 | 0.90 |
| 1:G:410:ASN:OD1 | 4:V:334:GLU:C | 2.09 | 0.90 |
| 1:G:638:GLY:HA3 | 4:V:341:ILE:O | 1.70 | 0.90 |
| 4:X:291:LYS:CD | 4:Z:243:PRO:HB2 | 1.99 | 0.90 |
| 4:2:166:TYR:CZ | 4:4:64:ILE:HG21 | 2.05 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:LYS:HA | 1:A:220:ASP:CG | 1.90 | 0.90 |
| 1:A:149:GLN:OE1 | 1:A:716:LEU:HD23 | 0.73 | 0.90 |
| 1:D:544:LYS:HD2 | 4:9:147:ARG:HB3 | 1.53 | 0.90 |
| 1:D:713:SER:HB3 | 1:D:775:LEU:HD22 | 1.51 | 0.90 |
| 1:D:800:ARG:O | 3:F:149:VAL:HG21 | 1.69 | 0.90 |
| 1:G:544:LYS:HD2 | 4:V:147:ARG:HB3 | 1.53 | 0.90 |
| 1:G:834:LEU:HD13 | 2:H:51:PHE:CE1 | 2.05 | 0.90 |
| 1:M:278:GLN:HG2 | 1:M:317:GLU:HB2 | 1.52 | 0.90 |
| 1:S:636:LYS:HD2 | 4:2:332:PRO:HB3 | 1.52 | 0.90 |
| 3:U:62:ALA:O | 3:U:63:ILE:HG12 | 1.71 | 0.90 |
| 4:3:287:ILE:CD1 | 4:5:203:THR:HB | 2.01 | 0.90 |
| 2:B:149:ASP:CG | 2:B:150:TYR:H | 1.73 | 0.90 |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CD1 | 2.06 | 0.90 |
| 1:G:538:GLU:N | 4:V:351:THR:H | 1.68 | 0.90 |
| 1:G:813:ILE:HG23 | 2:H:128:PHE:CZ | 2.06 | 0.90 |
| 1:J:215:GLN:HA | 1:J:340:ILE:HG23 | 0.95 | 0.90 |
| 1:M:819:ASN:OD1 | 2:N:92:ASP:CB | 2.18 | 0.90 |
| 1:S:648:THR:HG21 | 1:S:651:ALA:HB2 | 1.50 | 0.90 |
| 1:A:553:MLY:HE2 | 4:V:45:VAL:HA | 1.53 | 0.90 |
| 1:S:538:GLU:N | 4:2:351:THR:H | 1.68 | 0.90 |
| 1:A:636:LYS:HD2 | 4:8:332:PRO:HB3 | 1.51 | 0.90 |
| 1:G:218:LEU:HA | 1:G:221:GLN:CG | 2.01 | 0.90 |
| 1:G:542:PHE:HA | 4:V:143:TYR:HE1 | 1.34 | 0.90 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:CG | 2.00 | 0.90 |
| 1:G:97:LEU:CD2 | 1:G:712:PRO:CB | 2.50 | 0.90 |
| 1:G:728:ASN:ND2 | 3:I:113:THR:O | 2.04 | 0.90 |
| 1:G:838:ILE:HD12 | 2:H:54:MET:HE3 | 1.49 | 0.90 |
| 1:J:95:THR:N | 1:J:713:SER:HB3 | 1.84 | 0.90 |
| 1:J:735:GLY:O | 1:J:743:ALA:CA | 2.19 | 0.90 |
| 1:M:553:MLY:HE2 | 4:2:45:VAL:HA | 1.53 | 0.90 |
| 1:M:638:GLY:HA3 | 4:Z:341:ILE:O | 1.70 | 0.90 |
| 1:M:735:GLY:O | 1:M:743:ALA:CA | 2.19 | 0.90 |
| 1:M:804:ARG:O | 1:M:808:GLU:N | 2.04 | 0.90 |
| 3:O:62:ALA:O | 3:O:63:ILE:CG1 | 2.19 | 0.90 |
| 1:S:709:LYS:C | 1:S:710:GLY:HA3 | 1.92 | 0.90 |
| 1:G:567:LYS:HZ1 | 4:X:92:ASN:HD22 | 1.11 | 0.90 |
| 1:A:809:ARG:NH1 | 2:B:124:GLY:HA2 | 1.85 | 0.90 |
| 2:E:137:TRP:HA | 2:E:145:ALA:HB2 | 1.54 | 0.90 |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE1 | 1.51 | 0.90 |
| 1:J:641:LYS:HG3 | 1:J:647:GLN:NE2 | 1.59 | 0.90 |
| 1:M:721:LYS:CB | 1:M:736:GLN:OE1 | 2.20 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:24:LYS:HB3 | 3:O:63:ILE:O | 1.72 | 0.90 |
| 1:M:630:ALA:O | 4:Z:25:ASP:CG | 2.09 | 0.90 |
| 4:4:287:ILE:HB | 4:6:203:THR:HG22 | 1.50 | 0.90 |
| 1:D:538:GLU:O | 4:9:349:LEU:CG | 2.20 | 0.90 |
| 1:G:278:GLN:HG2 | 1:G:317:GLU:HB2 | 1.52 | 0.90 |
| 1:G:796:GLY:CA | 3:I:35:ARG:HD3 | 1.99 | 0.90 |
| 3:I:24:LYS:HB3 | 3:I:63:ILE:O | 1.72 | 0.90 |
| 1:M:557:GLU:H | 4:2:48:GLY:HA2 | 1.32 | 0.90 |
| 1:S:721:LYS:CB | 1:S:736:GLN:OE1 | 2.20 | 0.90 |
| 1:S:549:SER:HA | 4:4:43:VAL:CG1 | 2.01 | 0.90 |
| 1:D:795:ARG:CB | 3:F:35:ARG:HH12 | 1.76 | 0.90 |
| 1:G:736:GLN:HA | 1:G:743:ALA:HB2 | 1.51 | 0.90 |
| 1:J:538:GLU:O | 4:W:349:LEU:CG | 2.20 | 0.90 |
| 1:M:649:VAL:HG13 | 1:M:649:VAL:CG2 | 2.02 | 0.90 |
| 1:S:641:LYS:CD | 1:S:647:GLN:OE1 | 2.18 | 0.90 |
| 1:S:649:VAL:HG13 | 1:S:649:VAL:CG2 | 2.02 | 0.90 |
| 3:U:62:ALA:O | 3:U:63:ILE:CG1 | 2.19 | 0.90 |
| 1:J:544:LYS:HD2 | 4:W:147:ARG:HB3 | 1.53 | 0.90 |
| 1:A:530:MET:N | 4:8:354:GLN:HB3 | 1.87 | 0.90 |
| 1:A:735:GLY:O | 1:A:743:ALA:CA | 2.19 | 0.90 |
| 1:A:795:ARG:HD3 | 3:C:43:ASN:OD1 | 1.70 | 0.90 |
| 1:A:797:PHE:CE2 | 3:C:146:ILE:HD12 | 2.06 | 0.90 |
| 1:D:721:LYS:CB | 1:D:736:GLN:OE1 | 2.20 | 0.90 |
| 1:G:735:GLY:C | 1:G:743:ALA:HA | 1.90 | 0.90 |
| 1:G:752:ASP:CG | 1:G:780:ASP:O | 2.08 | 0.90 |
| 1:J:638:GLY:HA3 | 4:W:341:ILE:O | 1.70 | 0.90 |
| 1:J:820:VAL:CG1 | 2:K:136:MET:CE | 2.48 | 0.90 |
| 1:A:553:MLY:CG | 4:V:44:MET:O | 2.20 | 0.90 |
| 1:J:636:LYS:HD2 | 4:W:332:PRO:HB3 | 1.52 | 0.90 |
| 1:M:550:PHE:CA | 4:2:46:GLY:HA3 | 2.02 | 0.90 |
| 1:A:542:PHE:HA | 4:8:143:TYR:HE1 | 1.34 | 0.90 |
| 1:D:218:LEU:HA | 1:D:221:GLN:CG | 2.01 | 0.90 |
| 1:D:85:TYR:HH | 1:D:772:LEU:HD23 | 0.94 | 0.90 |
| 1:G:817:GLN:HG2 | 2:H:127:ARG:HB2 | 1.53 | 0.90 |
| 1:M:550:PHE:HA | 4:2:46:GLY:CA | 2.00 | 0.90 |
| 1:S:410:ASN:OD1 | 4:2:334:GLU:C | 2.10 | 0.90 |
| 1:S:805:ALA:O | 1:S:809:ARG:HB2 | 1.72 | 0.90 |
| 1:D:550:PHE:CA | 4:W:46:GLY:HA3 | 2.02 | 0.90 |
| 1:S:538:GLU:O | 4:2:349:LEU:CG | 2.20 | 0.90 |
| 1:A:410:ASN:OD1 | 4:8:334:GLU:C | 2.11 | 0.90 |
| 1:A:831:TRP:CZ3 | 2:B:34:ILE:HG23 | 2.06 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:62:ALA:O | 3:C:63:ILE:HG12 | 1.71 | 0.90 |
| 1:D:530:MET:N | 4:9:354:GLN:HB3 | 1.87 | 0.90 |
| 1:J:206:LYS:CD | 1:J:217:THR:CG2 | 2.16 | 0.90 |
| 1:J:534:SER:HA | 4:W:350:SER:O | 1.71 | 0.90 |
| 1:J:839:MLY:HH21 | 2:K:158:THR:HG22 | 1.53 | 0.90 |
| 1:M:534:SER:HA | 4:Z:350:SER:O | 1.71 | 0.90 |
| 1:M:538:GLU:O | 4:Z:349:LEU:CG | 2.20 | 0.90 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:NH1 | 1.87 | 0.90 |
| 1:S:783:LEU:HB3 | 1:S:786:ILE:CD1 | 1.99 | 0.90 |
| 1:A:736:GLN:CA | 1:A:743:ALA:HB2 | 1.95 | 0.89 |
| 1:D:641:LYS:CD | 1:D:647:GLN:OE1 | 2.17 | 0.89 |
| 1:D:649:VAL:CB | 1:D:649:VAL:CG2 | 2.49 | 0.89 |
| 1:G:649:VAL:CG2 | 1:G:649:VAL:HG13 | 2.02 | 0.89 |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:HD21 | 1.54 | 0.89 |
| 2:K:137:TRP:HA | 2:K:145:ALA:HB2 | 1.53 | 0.89 |
| 3:L:62:ALA:O | 3:L:63:ILE:CG1 | 2.19 | 0.89 |
| 1:M:793:ARG:NH1 | 3:O:40:ASN:HD22 | 1.66 | 0.89 |
| 3:O:62:ALA:O | 3:O:63:ILE:HG12 | 1.71 | 0.89 |
| 1:S:753:VAL:HG22 | 1:S:779:ARG:HH22 | 1.34 | 0.89 |
| 1:S:791:GLN:CD | 3:U:116:GLU:N | 2.17 | 0.89 |
| 1:A:550:PHE:CA | 4:V:46:GLY:HA3 | 2.02 | 0.89 |
| 1:J:630:ALA:O | 4:W:25:ASP:CG | 2.09 | 0.89 |
| 1:S:546:THR:OG1 | 4:4:46:GLY:C | 2.09 | 0.89 |
| 1:D:636:LYS:HD2 | 4:9:332:PRO:HB3 | 1.52 | 0.89 |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:CG2 | 2.02 | 0.89 |
| 3:C:62:ALA:O | 3:C:63:ILE:CG1 | 2.19 | 0.89 |
| 1:G:538:GLU:OE2 | 4:V:355:MET:HE3 | 1.72 | 0.89 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:HB3 | 1.84 | 0.89 |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:HG13 | 2.02 | 0.89 |
| 1:J:836:PHE:CE1 | 2:K:159:HIS:CA | 2.52 | 0.89 |
| 1:S:92:ALA:O | 1:S:714:ARG:HG3 | 0.72 | 0.89 |
| 1:D:550:PHE:HA | 4:W:46:GLY:CA | 2.00 | 0.89 |
| 1:G:553:MLY:NZ | 4:X:45:VAL:HG11 | 1.88 | 0.89 |
| 1:M:410:ASN:OD1 | 4:Z:334:GLU:C | 2.10 | 0.89 |
| 1:D:649:VAL:HG13 | 1:D:649:VAL:CG2 | 2.02 | 0.89 |
| 3:F:62:ALA:O | 3:F:63:ILE:CG1 | 2.19 | 0.89 |
| 1:G:534:SER:HA | 4:V:350:SER:O | 1.71 | 0.89 |
| 1:G:636:LYS:HD2 | 4:V:332:PRO:HB3 | 1.52 | 0.89 |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:CB | 2.49 | 0.89 |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:CD2 | 2.02 | 0.89 |
| 1:S:735:GLY:O | 1:S:743:ALA:CA | 2.19 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:746:LYS:O | 3:U:93:VAL:HG22 | 1.70 | 0.89 |
| 1:D:553:MLY:HE2 | 4:W:45:VAL:HA | 1.53 | 0.89 |
| 1:J:567:LYS:HZ2 | 4:Y:92:ASN:HD22 | 1.14 | 0.89 |
| 1:S:541:MET:CB | 4:2:143:TYR:OH | 2.20 | 0.89 |
| 3:C:24:LYS:HB3 | 3:C:63:ILE:O | 1.72 | 0.89 |
| 1:G:92:ALA:O | 1:G:714:ARG:HG3 | 1.72 | 0.89 |
| 1:G:829:TRP:CH2 | 2:H:87:LYS:HE2 | 2.06 | 0.89 |
| 1:J:813:ILE:CG2 | 2:K:128:PHE:HE1 | 1.86 | 0.89 |
| 1:M:530:MET:N | 4:Z:354:GLN:HB3 | 1.87 | 0.89 |
| 1:S:793:ARG:HD3 | 3:U:40:ASN:ND2 | 1.87 | 0.89 |
| 1:M:553:MLY:CG | 4:2:44:MET:O | 2.20 | 0.89 |
| 1:G:735:GLY:O | 1:G:743:ALA:CA | 2.20 | 0.89 |
| 3:I:62:ALA:O | 3:I:63:ILE:CG1 | 2.19 | 0.89 |
| 1:J:710:GLY:C | 1:J:772:LEU:HD22 | 1.90 | 0.89 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:HB | 1.73 | 0.89 |
| 2:N:137:TRP:HA | 2:N:145:ALA:HB2 | 1.54 | 0.89 |
| 1:J:410:ASN:OD1 | 4:W:334:GLU:C | 2.10 | 0.89 |
| 1:A:278:GLN:HG2 | 1:A:317:GLU:HB2 | 1.52 | 0.89 |
| 1:A:534:SER:HA | 4:8:350:SER:O | 1.71 | 0.89 |
| 1:A:502:GLU:CG | 1:A:761:GLY:N | 2.35 | 0.89 |
| 1:D:215:GLN:H | 1:D:340:ILE:CG1 | 1.73 | 0.89 |
| 1:J:530:MET:N | 4:W:354:GLN:HB3 | 1.87 | 0.89 |
| 1:J:721:LYS:CB | 1:J:736:GLN:OE1 | 2.20 | 0.89 |
| 1:J:84:MLY:HA | 1:J:723:ARG:NH1 | 1.86 | 0.89 |
| 1:S:793:ARG:HH11 | 3:U:40:ASN:ND2 | 1.48 | 0.89 |
| 1:G:642:LYS:HG2 | 4:V:22:ALA:CA | 2.03 | 0.89 |
| 1:M:635:GLY:CA | 4:Z:341:ILE:HD13 | 2.02 | 0.89 |
| 1:A:709:LYS:O | 1:A:710:GLY:CA | 2.20 | 0.89 |
| 1:D:638:GLY:HA3 | 4:9:341:ILE:O | 1.70 | 0.89 |
| 3:F:62:ALA:O | 3:F:63:ILE:HG12 | 1.71 | 0.89 |
| 2:N:149:ASP:CG | 2:N:150:TYR:H | 1.73 | 0.89 |
| 1:S:635:GLY:CA | 4:2:341:ILE:HD13 | 2.02 | 0.89 |
| 1:A:630:ALA:O | 4:8:25:ASP:CG | 2.10 | 0.89 |
| 1:A:215:GLN:H | 1:A:340:ILE:HG12 | 1.06 | 0.89 |
| 1:D:534:SER:O | 4:9:351:THR:HG23 | 1.13 | 0.89 |
| 1:D:727:LEU:CB | 1:D:782:MLY:CE | 2.51 | 0.89 |
| 1:J:635:GLY:CA | 4:W:341:ILE:HD13 | 2.02 | 0.89 |
| 1:M:557:GLU:H | 4:2:48:GLY:HA3 | 1.28 | 0.89 |
| 1:S:641:LYS:HD2 | 4:2:348:SER:CB | 2.03 | 0.89 |
| 4:3:324:THR:HG23 | 4:5:244:ASP:HA | 1.52 | 0.89 |
| 1:A:641:LYS:HD2 | 4:8:348:SER:CB | 2.02 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:149:GLN:HE21 | 1:A:718:ALA:HB3 | 1.34 | 0.89 |
| 1:A:721:LYS:CB | 1:A:736:GLN:OE1 | 2.20 | 0.89 |
| 1:G:538:GLU:O | 4:V:349:LEU:CG | 2.20 | 0.89 |
| 2:H:137:TRP:HA | 2:H:145:ALA:HB2 | 1.54 | 0.89 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:OE1 | 2.19 | 0.89 |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:HG12 | 1.14 | 0.89 |
| 3:L:24:LYS:HB3 | 3:L:63:ILE:O | 1.72 | 0.89 |
| 1:M:642:LYS:HG2 | 4:Z:22:ALA:CA | 2.03 | 0.89 |
| 1:M:806:MET:CA | 1:M:807:VAL:N | 2.35 | 0.89 |
| 1:S:629:GLU:HG2 | 1:S:643:GLY:O | 1.72 | 0.89 |
| 4:2:166:TYR:CE2 | 4:4:64:ILE:CG2 | 2.53 | 0.89 |
| 4:4:287:ILE:CD1 | 4:6:203:THR:HB | 2.01 | 0.89 |
| 1:A:215:GLN:H | 1:A:340:ILE:CG1 | 1.73 | 0.89 |
| 1:A:629:GLU:HG2 | 1:A:643:GLY:O | 1.72 | 0.89 |
| 2:E:149:ASP:CG | 2:E:150:TYR:H | 1.72 | 0.89 |
| 1:J:792:ALA:HB2 | 3:L:42:THR:HG23 | 0.90 | 0.89 |
| 1:J:795:ARG:NE | 3:L:116:GLU:CD | 2.25 | 0.89 |
| 3:L:62:ALA:O | 3:L:63:ILE:HG12 | 1.71 | 0.89 |
| 1:M:538:GLU:OE2 | 4:Z:355:MET:HE3 | 1.72 | 0.89 |
| 1:M:84:MLY:CH2 | 1:M:719:ASP:O | 2.20 | 0.89 |
| 4:4:324:THR:HG23 | 4:6:244:ASP:HA | 1.52 | 0.88 |
| 1:D:727:LEU:HD13 | 1:D:782:MLY:HH12 | 1.54 | 0.88 |
| 1:D:836:PHE:CE2 | 2:E:160:GLY:CA | 2.56 | 0.88 |
| 1:J:505:MLY:CD | 1:J:762:HIS:HE1 | 1.84 | 0.88 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:HH11 | 1.36 | 0.88 |
| 1:J:801:VAL:HG21 | 3:L:126:LEU:HD21 | 1.54 | 0.88 |
| 1:M:629:GLU:HG2 | 1:M:643:GLY:O | 1.72 | 0.88 |
| 1:S:84:MLY:HH11 | 1:S:724:TYR:HE2 | 1.29 | 0.88 |
| 1:D:534:SER:HA | 4:9:350:SER:O | 1.71 | 0.88 |
| 1:A:28:GLN:HE22 | 1:A:723:ARG:NH2 | 1.70 | 0.88 |
| 1:D:508:ILE:CD1 | 1:D:766:PHE:CD1 | 2.55 | 0.88 |
| 1:D:507:GLY:HA2 | 1:D:762:HIS:CE1 | 2.08 | 0.88 |
| 1:G:721:LYS:CB | 1:G:736:GLN:OE1 | 2.20 | 0.88 |
| 1:J:94:MET:O | 1:J:713:SER:HA | 1.72 | 0.88 |
| 1:M:641:LYS:HD2 | 4:Z:348:SER:CB | 2.02 | 0.88 |
| 1:M:836:PHE:CD1 | 2:N:159:HIS:HA | 2.07 | 0.88 |
| 1:S:709:LYS:C | 1:S:710:GLY:CA | 2.41 | 0.88 |
| 1:G:635:GLY:CA | 4:V:341:ILE:HD13 | 2.03 | 0.88 |
| 1:A:635:GLY:CA | 4:8:341:ILE:HD13 | 2.03 | 0.88 |
| 1:D:630:ALA:O | 4:9:25:ASP:CG | 2.09 | 0.88 |
| 2:H:121:LEU:CA | 2:H:128:PHE:CB | 2.46 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:756:THR:HG21 | 1:J:776:GLU:C | 1.92 | 0.88 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:CB | 2.01 | 0.88 |
| 1:S:753:VAL:CG1 | 1:S:779:ARG:CZ | 2.50 | 0.88 |
| 1:S:797:PHE:CE1 | 3:U:149:VAL:HG12 | 2.08 | 0.88 |
| 1:S:642:LYS:CG | 4:2:21:PHE:O | 2.22 | 0.88 |
| 1:S:534:SER:HA | 4:2:350:SER:O | 1.71 | 0.88 |
| 1:D:635:GLY:HA2 | 4:9:334:GLU:CG | 2.03 | 0.88 |
| 1:G:215:GLN:H | 1:G:340:ILE:HG12 | 1.06 | 0.88 |
| 1:G:754:ASP:HB2 | 1:G:776:GLU:CA | 2.00 | 0.88 |
| 1:J:541:MET:CB | 4:W:143:TYR:OH | 2.20 | 0.88 |
| 1:M:215:GLN:H | 1:M:340:ILE:CG1 | 1.72 | 0.88 |
| 1:S:817:GLN:HG2 | 2:T:127:ARG:CB | 2.03 | 0.88 |
| 4:1:322:PRO:CB | 4:3:244:ASP:HB3 | 2.02 | 0.88 |
| 2:B:137:TRP:HA | 2:B:145:ALA:HB2 | 1.54 | 0.88 |
| 1:D:635:GLY:CA | 4:9:341:ILE:HD13 | 2.03 | 0.88 |
| 1:G:629:GLU:HG2 | 1:G:643:GLY:O | 1.72 | 0.88 |
| 2:T:121:LEU:CA | 2:T:128:PHE:CB | 2.46 | 0.88 |
| 4:V:286:ASP:OD1 | 4:X:203:THR:HG22 | 1.74 | 0.88 |
| 4:1:203:THR:HG22 | 4:Y:286:ASP:OD1 | 1.74 | 0.88 |
| 1:D:541:MET:CB | 4:9:143:TYR:OH | 2.20 | 0.88 |
| 1:D:410:ASN:OD1 | 4:9:334:GLU:C | 2.10 | 0.88 |
| 1:D:553:MLY:CG | 4:W:44:MET:O | 2.20 | 0.88 |
| 1:G:728:ASN:OD1 | 3:I:114:LEU:HG | 1.74 | 0.88 |
| 1:J:642:LYS:HG2 | 4:W:22:ALA:CA | 2.03 | 0.88 |
| 1:J:599:ASN:OD1 | 1:J:649:VAL:HB | 1.73 | 0.88 |
| 2:T:149:ASP:CG | 2:T:150:TYR:H | 1.73 | 0.88 |
| 1:S:797:PHE:CE1 | 3:U:146:ILE:HA | 2.07 | 0.88 |
| 4:2:112:PRO:CG | 4:3:197:GLY:H | 1.76 | 0.88 |
| 1:A:642:LYS:CG | 4:8:21:PHE:O | 2.22 | 0.88 |
| 1:A:505:MLY:HG3 | 1:A:741:LYS:HZ2 | 1.35 | 0.88 |
| 1:A:538:GLU:O | 4:8:349:LEU:CG | 2.20 | 0.88 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:HB | 1.72 | 0.88 |
| 1:D:836:PHE:CE1 | 2:E:159:HIS:CB | 2.52 | 0.88 |
| 1:G:552:ASN:O | 4:X:47:MET:HE1 | 1.72 | 0.88 |
| 1:G:735:GLY:C | 1:G:743:ALA:HB2 | 1.82 | 0.88 |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:HG2 | 0.81 | 0.88 |
| 1:J:629:GLU:HG2 | 1:J:643:GLY:O | 1.72 | 0.88 |
| 2:N:137:TRP:HA | 2:N:145:ALA:CB | 2.04 | 0.88 |
| 1:S:206:LYS:CD | 1:S:217:THR:CG2 | 2.16 | 0.88 |
| 1:S:530:MET:N | 4:2:354:GLN:HB3 | 1.87 | 0.88 |
| 2:T:137:TRP:HA | 2:T:145:ALA:CB | 2.04 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:642:LYS:CG | 4:W:21:PHE:O | 2.22 | 0.88 |
| 1:A:792:ALA:HB2 | 3:C:42:THR:CG2 | 2.04 | 0.88 |
| 1:D:819:ASN:N | 2:E:90:GLY:O | 2.06 | 0.88 |
| 3:I:62:ALA:O | 3:I:63:ILE:HG12 | 1.71 | 0.88 |
| 1:M:541:MET:CB | 4:Z:143:TYR:OH | 2.20 | 0.88 |
| 1:G:530:MET:N | 4:V:354:GLN:HB3 | 1.88 | 0.88 |
| 4:X:291:LYS:CD | 4:Z:243:PRO:C | 2.41 | 0.88 |
| 4:3:324:THR:OG1 | 4:5:244:ASP:N | 1.96 | 0.88 |
| 1:D:641:LYS:HD2 | 4:9:348:SER:CB | 2.02 | 0.88 |
| 1:J:635:GLY:HA2 | 4:W:334:GLU:CG | 2.03 | 0.88 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:HD11 | 2.04 | 0.88 |
| 1:S:642:LYS:HG2 | 4:2:22:ALA:CA | 2.03 | 0.88 |
| 1:S:839:MLY:CH1 | 2:T:159:HIS:HD2 | 1.87 | 0.88 |
| 4:X:324:THR:CB | 4:Z:246:GLN:HA | 2.03 | 0.88 |
| 1:S:538:GLU:N | 4:2:349:LEU:HD12 | 1.86 | 0.88 |
| 1:A:541:MET:CB | 4:8:143:TYR:OH | 2.20 | 0.88 |
| 1:D:642:LYS:HG2 | 4:9:22:ALA:CA | 2.04 | 0.88 |
| 2:E:137:TRP:HA | 2:E:145:ALA:CB | 2.03 | 0.88 |
| 1:G:641:LYS:HD2 | 4:V:348:SER:CB | 2.03 | 0.88 |
| 3:L:139:TYR:HA | 3:L:142:PHE:HB3 | 1.56 | 0.88 |
| 1:M:215:GLN:H | 1:M:340:ILE:HG12 | 1.05 | 0.88 |
| 1:M:635:GLY:HA2 | 4:Z:334:GLU:CG | 2.03 | 0.88 |
| 1:M:641:LYS:CD | 1:M:647:GLN:OE1 | 2.18 | 0.88 |
| 1:S:215:GLN:H | 1:S:340:ILE:HG12 | 1.05 | 0.88 |
| 3:U:24:LYS:HB3 | 3:U:63:ILE:O | 1.72 | 0.88 |
| 1:G:642:LYS:CG | 4:V:21:PHE:O | 2.22 | 0.88 |
| 1:A:93:MET:CG | 1:A:715:VAL:HG22 | 2.02 | 0.87 |
| 2:E:121:LEU:CB | 2:E:128:PHE:HB3 | 1.69 | 0.87 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:CD1 | 2.58 | 0.87 |
| 1:J:567:LYS:HZ3 | 4:Y:92:ASN:ND2 | 1.71 | 0.87 |
| 1:J:641:LYS:HD2 | 4:W:348:SER:CB | 2.03 | 0.87 |
| 1:S:599:ASN:OD1 | 1:S:649:VAL:HB | 1.73 | 0.87 |
| 1:S:635:GLY:HA2 | 4:2:334:GLU:CG | 2.03 | 0.87 |
| 1:S:786:ILE:O | 1:S:789:ALA:CA | 2.21 | 0.87 |
| 1:S:731:ALA:CB | 3:U:93:VAL:C | 2.43 | 0.87 |
| 4:4:287:ILE:HG21 | 4:6:202:THR:OG1 | 1.75 | 0.87 |
| 1:A:636:LYS:H | 4:8:334:GLU:CD | 1.77 | 0.87 |
| 1:A:817:GLN:CD | 2:B:127:ARG:CG | 2.39 | 0.87 |
| 1:A:97:LEU:HD22 | 1:A:712:PRO:CB | 2.03 | 0.87 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:CD1 | 2.58 | 0.87 |
| 1:J:769:ALA:CB | 1:J:770:GLY:CA | 2.51 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:646:PHE:CE2 | 1:M:652:LEU:CD1 | 2.58 | 0.87 |
| 1:S:736:GLN:HA | 1:S:743:ALA:HB2 | 1.51 | 0.87 |
| 1:M:642:LYS:CG | 4:Z:21:PHE:O | 2.22 | 0.87 |
| 4:2:287:ILE:CG2 | 4:4:203:THR:CG2 | 2.50 | 0.87 |
| 1:G:752:ASP:OD1 | 1:G:783:LEU:HB2 | 1.74 | 0.87 |
| 1:J:820:VAL:CG1 | 2:K:136:MET:HE3 | 2.05 | 0.87 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:CG | 2.37 | 0.87 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CD1 | 2.04 | 0.87 |
| 1:D:506:GLU:OE2 | 1:D:764:MLY:CH2 | 2.22 | 0.87 |
| 1:D:793:ARG:NH2 | 3:F:147:MET:CE | 2.36 | 0.87 |
| 1:G:791:GLN:CD | 3:I:116:GLU:H | 1.77 | 0.87 |
| 1:M:28:GLN:C | 1:M:723:ARG:HH22 | 1.77 | 0.87 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:CD | 2.03 | 0.87 |
| 1:S:751:GLY:CA | 3:U:86:ASP:OD1 | 2.22 | 0.87 |
| 1:J:553:MLY:NZ | 4:Y:45:VAL:HG11 | 1.88 | 0.87 |
| 4:1:322:PRO:CB | 4:3:244:ASP:CB | 2.52 | 0.87 |
| 1:A:642:LYS:HG2 | 4:8:22:ALA:CA | 2.04 | 0.87 |
| 1:A:72:VAL:CG1 | 1:A:76:GLN:HB3 | 2.05 | 0.87 |
| 1:D:629:GLU:HG2 | 1:D:643:GLY:O | 1.72 | 0.87 |
| 1:D:708:ARG:C | 1:D:710:GLY:N | 2.28 | 0.87 |
| 1:M:720:PHE:CD1 | 1:M:772:LEU:CD2 | 2.56 | 0.87 |
| 2:T:137:TRP:HA | 2:T:145:ALA:HB2 | 1.53 | 0.87 |
| 1:J:538:GLU:N | 4:W:349:LEU:HD12 | 1.86 | 0.87 |
| 4:3:324:THR:OG1 | 4:5:244:ASP:CB | 2.22 | 0.87 |
| 4:4:324:THR:OG1 | 4:6:244:ASP:CB | 2.22 | 0.87 |
| 1:D:642:LYS:CG | 4:9:21:PHE:O | 2.22 | 0.87 |
| 1:A:505:MLY:CB | 1:A:762:HIS:H | 1.87 | 0.87 |
| 2:B:137:TRP:HA | 2:B:145:ALA:CB | 2.04 | 0.87 |
| 3:C:139:TYR:HA | 3:C:142:PHE:HB3 | 1.56 | 0.87 |
| 1:G:755:HIS:HA | 1:G:758:TYR:CE1 | 2.10 | 0.87 |
| 1:G:72:VAL:CG1 | 1:G:76:GLN:HB3 | 2.05 | 0.87 |
| 1:G:792:ALA:HB2 | 3:I:42:THR:HG22 | 1.03 | 0.87 |
| 1:J:553:MLY:CH1 | 4:Y:45:VAL:CG1 | 2.49 | 0.87 |
| 1:J:813:ILE:CG2 | 2:K:128:PHE:CE1 | 2.57 | 0.87 |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:HB2 | 1.57 | 0.87 |
| 1:M:798:LEU:HD22 | 3:O:126:LEU:HD11 | 1.57 | 0.87 |
| 1:S:797:PHE:CE1 | 3:U:149:VAL:CG1 | 2.57 | 0.87 |
| 1:A:557:GLU:H | 4:V:48:GLY:HA3 | 1.28 | 0.87 |
| 4:W:286:ASP:OD1 | 4:Y:203:THR:HG22 | 1.74 | 0.87 |
| 1:D:755:HIS:HA | 1:D:758:TYR:CE1 | 2.10 | 0.87 |
| 1:D:800:ARG:NH2 | 3:F:40:ASN:CG | 2.28 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:F:24:LYS:HB3 | 3:F:63:ILE:O | 1.72 | 0.87 |
| 1:G:503:TYR:OH | 1:G:711:PHE:CD2 | 2.23 | 0.87 |
| 1:J:553:MLY:HG3 | 4:Y:45:VAL:C | 1.95 | 0.87 |
| 1:J:636:LYS:H | 4:W:334:GLU:CD | 1.78 | 0.87 |
| 1:J:641:LYS:CD | 1:J:647:GLN:OE1 | 2.18 | 0.87 |
| 2:K:149:ASP:CG | 2:K:150:TYR:H | 1.73 | 0.87 |
| 1:J:797:PHE:HE2 | 3:L:126:LEU:HD13 | 1.39 | 0.87 |
| 4:X:288:ASP:N | 4:Z:202:THR:OG1 | 2.03 | 0.87 |
| 1:A:822:SER:CB | 2:B:88:LEU:HD23 | 2.04 | 0.87 |
| 1:D:649:VAL:CG1 | 1:D:649:VAL:CA | 2.53 | 0.87 |
| 1:D:712:PRO:HB2 | 1:D:771:LEU:HB3 | 1.54 | 0.87 |
| 1:D:72:VAL:CG1 | 1:D:76:GLN:HB3 | 2.05 | 0.87 |
| 1:G:541:MET:CB | 4:V:143:TYR:OH | 2.21 | 0.87 |
| 1:G:636:LYS:H | 4:V:334:GLU:CD | 1.78 | 0.87 |
| 1:G:646:PHE:CD2 | 1:G:652:LEU:HD11 | 2.09 | 0.87 |
| 1:G:649:VAL:CA | 1:G:649:VAL:CG1 | 2.53 | 0.87 |
| 2:K:137:TRP:HA | 2:K:145:ALA:CB | 2.04 | 0.87 |
| 1:M:72:VAL:CG1 | 1:M:76:GLN:HB3 | 2.05 | 0.87 |
| 1:S:731:ALA:HB1 | 3:U:93:VAL:CB | 2.05 | 0.87 |
| 1:G:538:GLU:N | 4:V:349:LEU:HD12 | 1.87 | 0.87 |
| 4:8:322:PRO:HB2 | 4:V:244:ASP:CG | 1.94 | 0.87 |
| 1:A:831:TRP:NE1 | 2:B:51:PHE:CE2 | 2.42 | 0.87 |
| 1:G:641:LYS:CD | 1:G:647:GLN:OE1 | 2.17 | 0.87 |
| 1:G:819:ASN:HA | 2:H:90:GLY:C | 1.95 | 0.87 |
| 2:K:121:LEU:CA | 2:K:128:PHE:CB | 2.46 | 0.87 |
| 1:S:546:THR:CG2 | 4:4:46:GLY:O | 2.23 | 0.87 |
| 1:S:795:ARG:HG3 | 3:U:118:MET:CE | 2.03 | 0.87 |
| 1:S:546:THR:OG1 | 4:4:46:GLY:CA | 2.21 | 0.86 |
| 4:7:322:PRO:HB2 | 4:9:244:ASP:CG | 1.94 | 0.86 |
| 1:A:635:GLY:HA2 | 4:8:334:GLU:CG | 2.03 | 0.86 |
| 1:A:649:VAL:CA | 1:A:649:VAL:CG1 | 2.53 | 0.86 |
| 1:M:636:LYS:H | 4:Z:334:GLU:CD | 1.78 | 0.86 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:CA | 2.55 | 0.86 |
| 1:A:797:PHE:CE2 | 3:C:146:ILE:CD1 | 2.58 | 0.86 |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:CD2 | 2.33 | 0.86 |
| 1:D:723:ARG:NH2 | 1:D:779:ARG:NH2 | 2.23 | 0.86 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:CA | 2.53 | 0.86 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:CD | 2.43 | 0.86 |
| 1:J:93:MET:HE1 | 1:J:764:MLY:HD2 | 1.57 | 0.86 |
| 1:S:646:PHE:CE2 | 1:S:652:LEU:CD1 | 2.58 | 0.86 |
| 1:S:791:GLN:NE2 | 3:U:116:GLU:H | 1.73 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:9:322:PRO:HB2 | 4:W:244:ASP:CG | 1.94 | 0.86 |
| 4:2:244:ASP:CG | 4:Z:322:PRO:HB2 | 1.94 | 0.86 |
| 1:S:636:LYS:H | 4:2:334:GLU:CD | 1.78 | 0.86 |
| 1:A:538:GLU:OE2 | 4:8:355:MET:HE3 | 1.74 | 0.86 |
| 1:D:206:LYS:HD3 | 1:D:217:THR:CB | 2.06 | 0.86 |
| 1:D:636:LYS:H | 4:9:334:GLU:CD | 1.78 | 0.86 |
| 2:H:137:TRP:HA | 2:H:145:ALA:CB | 2.04 | 0.86 |
| 1:M:649:VAL:CA | 1:M:649:VAL:CG1 | 2.53 | 0.86 |
| 1:M:95:THR:HG1 | 1:M:770:GLY:N | 1.73 | 0.86 |
| 1:M:817:GLN:CB | 2:N:127:ARG:HH11 | 1.88 | 0.86 |
| 1:J:553:MLY:CE | 4:Y:45:VAL:HB | 1.91 | 0.86 |
| 4:1:287:ILE:HG12 | 4:3:202:THR:HA | 1.57 | 0.86 |
| 1:D:310:TYR:CZ | 1:D:320:ILE:HD11 | 2.11 | 0.86 |
| 1:G:707:CYS:SG | 1:G:714:ARG:NH1 | 2.48 | 0.86 |
| 1:J:829:TRP:CZ2 | 2:K:87:LYS:CE | 2.55 | 0.86 |
| 1:M:783:LEU:HB3 | 1:M:786:ILE:HD12 | 1.56 | 0.86 |
| 1:S:646:PHE:CD2 | 1:S:652:LEU:HD11 | 2.09 | 0.86 |
| 1:S:552:ASN:OD1 | 4:4:49:GLN:O | 1.70 | 0.86 |
| 1:G:635:GLY:HA2 | 4:V:334:GLU:CG | 2.03 | 0.86 |
| 1:S:206:LYS:HD3 | 1:S:217:THR:CB | 2.06 | 0.86 |
| 1:S:649:VAL:CA | 1:S:649:VAL:CG1 | 2.53 | 0.86 |
| 3:U:139:TYR:HA | 3:U:142:PHE:HB3 | 1.56 | 0.86 |
| 4:2:112:PRO:HG2 | 4:3:197:GLY:H | 1.26 | 0.86 |
| 1:A:206:LYS:HD3 | 1:A:217:THR:CB | 2.06 | 0.86 |
| 1:D:646:PHE:CD2 | 1:D:652:LEU:HD11 | 2.09 | 0.86 |
| 1:D:798:LEU:HD13 | 3:F:126:LEU:CD1 | 1.99 | 0.86 |
| 3:F:139:TYR:HA | 3:F:142:PHE:HB3 | 1.56 | 0.86 |
| 1:J:72:VAL:CG1 | 1:J:76:GLN:HB3 | 2.05 | 0.86 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:HG2 | 1.37 | 0.86 |
| 1:M:795:ARG:HH22 | 3:O:116:GLU:HB3 | 1.40 | 0.86 |
| 1:S:530:MET:HG2 | 4:2:354:GLN:CG | 2.05 | 0.86 |
| 1:S:725:ARG:CZ | 1:S:733:PRO:HB3 | 2.06 | 0.86 |
| 4:8:287:ILE:CG2 | 4:V:205:GLU:HG2 | 2.05 | 0.86 |
| 1:J:538:GLU:OE2 | 4:W:355:MET:HE3 | 1.75 | 0.86 |
| 1:J:757:GLN:CA | 1:J:776:GLU:HG3 | 2.03 | 0.86 |
| 1:M:206:LYS:HD3 | 1:M:217:THR:CB | 2.06 | 0.86 |
| 1:A:646:PHE:CD2 | 1:A:652:LEU:HD11 | 2.10 | 0.86 |
| 1:A:834:LEU:CD2 | 2:B:54:MET:CE | 2.49 | 0.86 |
| 1:G:817:GLN:CG | 2:H:127:ARG:HD2 | 2.05 | 0.86 |
| 1:J:310:TYR:CZ | 1:J:320:ILE:HD11 | 2.11 | 0.86 |
| 1:J:817:GLN:CD | 2:K:127:ARG:CD | 2.41 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:793:ARG:HH11 | 3:O:40:ASN:HD22 | 1.14 | 0.86 |
| 1:S:783:LEU:CA | 1:S:786:ILE:CG1 | 2.36 | 0.86 |
| 1:S:795:ARG:HG2 | 3:U:118:MET:SD | 2.14 | 0.86 |
| 1:S:836:PHE:CE2 | 2:T:160:GLY:N | 2.41 | 0.86 |
| 4:4:288:ASP:OD1 | 4:6:203:THR:HG23 | 1.76 | 0.86 |
| 1:A:641:LYS:CD | 1:A:647:GLN:OE1 | 2.17 | 0.86 |
| 2:B:117:LEU:CG | 2:B:147:ASN:CG | 2.44 | 0.86 |
| 1:D:107:MLY:HB3 | 1:D:686:MET:HE2 | 1.58 | 0.86 |
| 1:G:148:ARG:HH21 | 1:G:764:MLY:CH2 | 1.89 | 0.86 |
| 1:G:206:LYS:HD3 | 1:G:217:THR:CB | 2.06 | 0.86 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:CB | 2.54 | 0.86 |
| 1:J:646:PHE:CD2 | 1:J:652:LEU:HD11 | 2.10 | 0.86 |
| 1:M:35:MLY:HE2 | 1:M:777:GLU:OE2 | 1.75 | 0.86 |
| 1:M:797:PHE:CE2 | 3:O:126:LEU:HD22 | 2.11 | 0.86 |
| 1:S:709:LYS:O | 1:S:710:GLY:CA | 2.23 | 0.86 |
| 1:S:821:ARG:NH2 | 2:T:127:ARG:CG | 2.37 | 0.86 |
| 1:S:820:VAL:HG11 | 2:T:136:MET:HE3 | 1.57 | 0.86 |
| 4:1:288:ASP:N | 4:3:203:THR:HG22 | 1.90 | 0.85 |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:HH11 | 1.56 | 0.85 |
| 2:E:117:LEU:CG | 2:E:147:ASN:CG | 2.44 | 0.85 |
| 1:G:149:GLN:CD | 1:G:763:THR:HG23 | 1.96 | 0.85 |
| 1:G:310:TYR:CZ | 1:G:320:ILE:HD11 | 2.11 | 0.85 |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:HB2 | 1.57 | 0.85 |
| 1:J:755:HIS:HA | 1:J:758:TYR:CE1 | 2.10 | 0.85 |
| 1:J:838:ILE:CD1 | 2:K:54:MET:HE1 | 2.05 | 0.85 |
| 1:J:819:ASN:CG | 2:K:90:GLY:O | 2.14 | 0.85 |
| 1:M:646:PHE:CD2 | 1:M:652:LEU:HD11 | 2.09 | 0.85 |
| 1:M:755:HIS:HA | 1:M:758:TYR:CE1 | 2.10 | 0.85 |
| 2:N:117:LEU:CG | 2:N:147:ASN:CG | 2.44 | 0.85 |
| 1:G:538:GLU:N | 4:V:351:THR:N | 2.24 | 0.85 |
| 1:M:538:GLU:N | 4:Z:351:THR:N | 2.24 | 0.85 |
| 4:1:287:ILE:CG1 | 4:3:202:THR:HA | 2.05 | 0.85 |
| 4:4:324:THR:HG23 | 4:6:244:ASP:CA | 2.01 | 0.85 |
| 1:D:530:MET:HG2 | 4:9:354:GLN:CG | 2.05 | 0.85 |
| 2:E:121:LEU:CA | 2:E:128:PHE:CB | 2.46 | 0.85 |
| 1:J:94:MET:O | 1:J:713:SER:CA | 2.23 | 0.85 |
| 1:M:530:MET:HG2 | 4:Z:354:GLN:CG | 2.06 | 0.85 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:CA | 2.25 | 0.85 |
| 1:S:310:TYR:CZ | 1:S:320:ILE:HD11 | 2.11 | 0.85 |
| 1:G:797:PHE:CE1 | 3:I:146:ILE:HG23 | 2.10 | 0.85 |
| 1:G:84:MLY:CH2 | 1:G:719:ASP:C | 2.45 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:215:GLN:H | 1:J:340:ILE:HG12 | 1.05 | 0.85 |
| 1:M:84:MLY:HH12 | 1:M:715:VAL:HG13 | 1.57 | 0.85 |
| 3:O:139:TYR:HA | 3:O:142:PHE:HB3 | 1.56 | 0.85 |
| 1:M:797:PHE:CE1 | 3:O:149:VAL:HG11 | 2.10 | 0.85 |
| 1:A:755:HIS:HA | 1:A:758:TYR:CE1 | 2.10 | 0.85 |
| 1:A:768:MLY:HB3 | 1:A:771:LEU:HB2 | 0.89 | 0.85 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:CA | 2.25 | 0.85 |
| 2:K:117:LEU:CG | 2:K:147:ASN:CG | 2.44 | 0.85 |
| 1:M:753:VAL:HG13 | 1:M:775:LEU:HD11 | 1.57 | 0.85 |
| 1:M:803:TYR:CD2 | 3:O:17:PHE:CZ | 2.65 | 0.85 |
| 1:S:752:ASP:N | 1:S:779:ARG:NH2 | 2.24 | 0.85 |
| 1:S:72:VAL:CG1 | 1:S:76:GLN:HB3 | 2.05 | 0.85 |
| 1:S:410:ASN:OD1 | 4:2:334:GLU:CA | 2.24 | 0.85 |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:CG | 1.88 | 0.85 |
| 1:M:204:GLU:H | 1:M:207:LYS:HE3 | 1.42 | 0.85 |
| 1:M:310:TYR:CZ | 1:M:320:ILE:HD11 | 2.11 | 0.85 |
| 1:M:797:PHE:CE2 | 3:O:126:LEU:CD2 | 2.59 | 0.85 |
| 1:S:793:ARG:CD | 3:U:40:ASN:ND2 | 2.38 | 0.85 |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:HG11 | 1.58 | 0.85 |
| 4:1:244:ASP:CG | 4:Y:325:MET:HE1 | 1.97 | 0.85 |
| 4:2:205:GLU:HG2 | 4:Z:287:ILE:CG2 | 2.05 | 0.85 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:CA | 2.25 | 0.85 |
| 1:A:97:LEU:HD22 | 1:A:712:PRO:HB3 | 1.57 | 0.85 |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:CA | 2.25 | 0.85 |
| 1:D:834:LEU:HD21 | 2:E:54:MET:CE | 2.05 | 0.85 |
| 1:G:204:GLU:H | 1:G:207:LYS:HE3 | 1.42 | 0.85 |
| 1:J:769:ALA:HB2 | 1:J:770:GLY:CA | 2.06 | 0.85 |
| 1:J:839:MLY:HH21 | 2:K:158:THR:CG2 | 2.07 | 0.85 |
| 1:M:84:MLY:HH21 | 1:M:719:ASP:O | 1.75 | 0.85 |
| 1:M:819:ASN:OD1 | 2:N:91:ALA:C | 2.14 | 0.85 |
| 1:S:204:GLU:H | 1:S:207:LYS:HE3 | 1.42 | 0.85 |
| 1:S:599:ASN:OD1 | 1:S:649:VAL:CA | 2.25 | 0.85 |
| 1:S:728:ASN:OD1 | 3:U:90:GLY:HA3 | 1.74 | 0.85 |
| 1:S:795:ARG:CB | 3:U:35:ARG:NH2 | 2.40 | 0.85 |
| 1:D:732:ILE:CG2 | 1:D:747:LEU:HD13 | 1.34 | 0.85 |
| 1:D:834:LEU:CD1 | 2:E:54:MET:CB | 2.52 | 0.85 |
| 1:G:567:LYS:HZ3 | 4:X:92:ASN:ND2 | 1.74 | 0.85 |
| 1:G:732:ILE:CG2 | 1:G:747:LEU:HD13 | 1.34 | 0.85 |
| 1:J:202:SER:HA | 1:J:207:LYS:HE2 | 0.85 | 0.85 |
| 4:2:287:ILE:HG21 | 4:4:203:THR:H | 1.41 | 0.85 |
| 4:3:287:ILE:HG21 | 4:5:202:THR:OG1 | 1.74 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:310:TYR:CZ | 1:A:320:ILE:HD11 | 2.11 | 0.85 |
| 1:A:530:MET:HG2 | 4:8:354:GLN:CG | 2.05 | 0.85 |
| 1:A:735:GLY:C | 1:A:743:ALA:HB2 | 1.82 | 0.85 |
| 2:B:121:LEU:CA | 2:B:128:PHE:CB | 2.46 | 0.85 |
| 1:D:202:SER:HA | 1:D:207:LYS:HE2 | 0.85 | 0.85 |
| 1:D:215:GLN:H | 1:D:340:ILE:HG12 | 1.06 | 0.85 |
| 3:I:139:TYR:HA | 3:I:142:PHE:HB3 | 1.56 | 0.85 |
| 2:E:163:ALA:O | 2:K:21:GLU:N | 2.09 | 0.85 |
| 1:M:785:GLU:O | 1:M:788:THR:N | 2.09 | 0.85 |
| 1:M:798:LEU:CD2 | 3:O:122:GLU:HB3 | 2.07 | 0.85 |
| 1:S:755:HIS:HA | 1:S:758:TYR:CE1 | 2.10 | 0.85 |
| 1:S:817:GLN:HG2 | 2:T:127:ARG:CG | 2.07 | 0.85 |
| 1:S:819:ASN:ND2 | 2:T:92:ASP:CB | 2.39 | 0.85 |
| 2:T:117:LEU:CG | 2:T:147:ASN:CG | 2.44 | 0.85 |
| 1:M:410:ASN:OD1 | 4:Z:334:GLU:CA | 2.24 | 0.85 |
| 1:M:530:MET:HE1 | 4:Z:355:MET:SD | 2.17 | 0.85 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HB2 | 1.58 | 0.85 |
| 1:D:204:GLU:H | 1:D:207:LYS:HE3 | 1.42 | 0.85 |
| 1:D:630:ALA:C | 4:9:25:ASP:OD2 | 2.15 | 0.85 |
| 1:D:791:GLN:NE2 | 3:F:115:GLY:C | 2.15 | 0.85 |
| 1:G:530:MET:HG2 | 4:V:354:GLN:CG | 2.05 | 0.85 |
| 1:G:792:ALA:HB2 | 3:I:42:THR:HA | 1.57 | 0.85 |
| 1:M:783:LEU:CD1 | 1:M:786:ILE:HD11 | 2.06 | 0.85 |
| 1:S:797:PHE:CD1 | 3:U:146:ILE:O | 2.29 | 0.85 |
| 1:J:630:ALA:C | 4:W:25:ASP:OD2 | 2.15 | 0.85 |
| 1:J:529:PRO:CB | 4:W:353:GLN:OE1 | 2.25 | 0.85 |
| 1:M:640:LYS:C | 4:Z:23:GLY:O | 2.15 | 0.85 |
| 1:S:548:THR:O | 4:4:49:GLN:N | 2.06 | 0.85 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:CD1 | 2.58 | 0.85 |
| 1:A:817:GLN:HG3 | 2:B:127:ARG:CD | 2.05 | 0.85 |
| 1:D:725:ARG:CD | 1:D:733:PRO:HB3 | 2.07 | 0.85 |
| 1:J:725:ARG:CD | 1:J:733:PRO:HB3 | 2.07 | 0.85 |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HB2 | 1.57 | 0.85 |
| 1:M:549:SER:O | 4:2:46:GLY:HA3 | 1.77 | 0.85 |
| 1:M:735:GLY:C | 1:M:743:ALA:HB1 | 1.84 | 0.85 |
| 1:M:95:THR:HA | 1:M:713:SER:OG | 1.77 | 0.85 |
| 1:J:410:ASN:ND2 | 4:W:336:LYS:HG2 | 1.92 | 0.85 |
| 4:X:287:ILE:CG2 | 4:Z:201:VAL:HG23 | 2.06 | 0.85 |
| 4:X:286:ASP:OD1 | 4:Z:202:THR:OG1 | 1.95 | 0.85 |
| 1:A:640:LYS:CB | 1:A:645:SER:OG | 2.25 | 0.84 |
| 1:A:800:ARG:HB3 | 3:C:149:VAL:HG22 | 0.88 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:823:PHE:HE1 | 2:E:160:GLY:HA2 | 1.36 | 0.84 |
| 1:G:95:THR:HA | 1:G:713:SER:CB | 2.06 | 0.84 |
| 1:J:204:GLU:H | 1:J:207:LYS:HE3 | 1.42 | 0.84 |
| 1:J:206:LYS:HD3 | 1:J:217:THR:CB | 2.06 | 0.84 |
| 1:J:530:MET:HG2 | 4:W:354:GLN:CG | 2.06 | 0.84 |
| 1:J:756:THR:HG21 | 1:J:776:GLU:CA | 2.07 | 0.84 |
| 1:S:538:GLU:N | 4:2:351:THR:N | 2.24 | 0.84 |
| 4:1:287:ILE:HB | 4:3:203:THR:H | 1.38 | 0.84 |
| 1:A:630:ALA:C | 4:8:25:ASP:OD2 | 2.15 | 0.84 |
| 1:A:202:SER:HA | 1:A:207:LYS:HE2 | 0.85 | 0.84 |
| 1:A:725:ARG:CD | 1:A:733:PRO:HB3 | 2.07 | 0.84 |
| 1:A:795:ARG:CG | 3:C:35:ARG:HH12 | 1.90 | 0.84 |
| 1:D:732:ILE:CD1 | 1:D:782:MLY:CH2 | 2.54 | 0.84 |
| 1:D:736:GLN:HA | 1:D:743:ALA:HB2 | 1.51 | 0.84 |
| 1:G:752:ASP:O | 1:G:780:ASP:CA | 2.20 | 0.84 |
| 1:G:754:ASP:O | 1:G:776:GLU:OE1 | 1.94 | 0.84 |
| 1:G:813:ILE:CG2 | 2:H:128:PHE:CE1 | 2.60 | 0.84 |
| 1:S:107:MLY:HB3 | 1:S:686:MET:HE2 | 1.59 | 0.84 |
| 1:S:731:ALA:O | 3:U:93:VAL:CG1 | 2.24 | 0.84 |
| 1:A:640:LYS:C | 4:8:23:GLY:O | 2.15 | 0.84 |
| 4:7:287:ILE:CG2 | 4:9:205:GLU:HG2 | 2.05 | 0.84 |
| 1:A:800:ARG:NH2 | 3:C:40:ASN:HD21 | 1.75 | 0.84 |
| 1:G:553:MLY:HG3 | 4:X:45:VAL:C | 1.96 | 0.84 |
| 1:J:640:LYS:CB | 1:J:645:SER:OG | 2.25 | 0.84 |
| 1:M:84:MLY:HH12 | 1:M:715:VAL:HG22 | 1.57 | 0.84 |
| 1:S:829:TRP:CH2 | 2:T:87:LYS:CE | 2.61 | 0.84 |
| 1:S:819:ASN:CG | 2:T:90:GLY:O | 2.14 | 0.84 |
| 4:3:287:ILE:CB | 4:5:202:THR:CB | 2.33 | 0.84 |
| 4:2:287:ILE:HG12 | 4:4:203:THR:N | 1.93 | 0.84 |
| 1:D:410:ASN:ND2 | 4:9:336:LYS:HG2 | 1.93 | 0.84 |
| 1:A:502:GLU:HA | 1:A:761:GLY:C | 1.96 | 0.84 |
| 1:D:834:LEU:CD1 | 2:E:54:MET:CG | 2.16 | 0.84 |
| 1:J:599:ASN:OD1 | 1:J:649:VAL:CA | 2.25 | 0.84 |
| 1:J:831:TRP:HH2 | 2:K:47:LEU:CD2 | 1.82 | 0.84 |
| 1:S:732:ILE:HG23 | 1:S:747:LEU:HB2 | 1.57 | 0.84 |
| 4:3:288:ASP:OD1 | 4:5:203:THR:HG23 | 1.76 | 0.84 |
| 1:A:543:PRO:HG3 | 4:8:143:TYR:O | 1.77 | 0.84 |
| 1:A:538:GLU:N | 4:8:351:THR:N | 2.24 | 0.84 |
| 1:D:543:PRO:HG3 | 4:9:143:TYR:O | 1.77 | 0.84 |
| 2:H:117:LEU:CG | 2:H:147:ASN:CG | 2.45 | 0.84 |
| 1:S:795:ARG:HH12 | 3:U:43:ASN:HB2 | 1.05 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:754:ASP:OD2 | 1:A:778:MET:HE3 | 1.75 | 0.84 |
| 1:G:95:THR:CA | 1:G:713:SER:HB3 | 2.07 | 0.84 |
| 1:J:107:MLY:HB3 | 1:J:686:MET:HE2 | 1.60 | 0.84 |
| 1:J:732:ILE:CG2 | 1:J:747:LEU:HD13 | 1.34 | 0.84 |
| 1:J:538:GLU:N | 4:W:351:THR:N | 2.24 | 0.84 |
| 1:A:410:ASN:OD1 | 4:8:334:GLU:CA | 2.24 | 0.84 |
| 1:A:648:THR:CG2 | 1:A:651:ALA:HB2 | 2.08 | 0.84 |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HB2 | 1.57 | 0.84 |
| 1:D:85:TYR:OH | 1:D:772:LEU:HD22 | 1.77 | 0.84 |
| 2:K:121:LEU:CG | 2:K:128:PHE:CA | 2.48 | 0.84 |
| 2:K:141:PRO:CB | 2:K:142:PRO:CD | 2.56 | 0.84 |
| 1:A:549:SER:O | 4:V:46:GLY:HA3 | 1.77 | 0.84 |
| 1:J:410:ASN:OD1 | 4:W:334:GLU:CA | 2.24 | 0.84 |
| 1:S:543:PRO:HG3 | 4:2:143:TYR:O | 1.77 | 0.84 |
| 4:1:322:PRO:HB3 | 4:3:244:ASP:HB3 | 1.60 | 0.84 |
| 1:A:94:MET:O | 1:A:713:SER:HB3 | 1.78 | 0.84 |
| 1:D:640:LYS:C | 4:9:23:GLY:O | 2.15 | 0.84 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:CD1 | 2.57 | 0.84 |
| 1:G:553:MLY:CH1 | 4:X:45:VAL:CG1 | 2.49 | 0.84 |
| 1:G:754:ASP:HA | 1:G:779:ARG:NE | 1.92 | 0.84 |
| 1:J:769:ALA:HB3 | 1:J:770:GLY:HA2 | 1.59 | 0.84 |
| 1:M:648:THR:CG2 | 1:M:651:ALA:HB2 | 2.08 | 0.84 |
| 1:J:640:LYS:C | 4:W:23:GLY:O | 2.15 | 0.84 |
| 4:7:286:ASP:OD1 | 4:9:203:THR:CG2 | 2.26 | 0.84 |
| 1:A:800:ARG:HH22 | 3:C:40:ASN:ND2 | 1.76 | 0.84 |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:HB | 1.73 | 0.84 |
| 1:D:727:LEU:HB2 | 1:D:782:MLY:CE | 2.07 | 0.84 |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:CH1 | 2.06 | 0.84 |
| 4:Y:237:GLU:HA | 4:Y:251:GLY:HA2 | 1.60 | 0.84 |
| 4:1:237:GLU:HA | 4:1:251:GLY:HA2 | 1.60 | 0.84 |
| 1:S:640:LYS:C | 4:2:23:GLY:O | 2.15 | 0.84 |
| 1:S:630:ALA:C | 4:2:25:ASP:OD2 | 2.15 | 0.84 |
| 1:A:204:GLU:H | 1:A:207:LYS:HE3 | 1.42 | 0.84 |
| 1:A:279:LEU:HB2 | 1:A:282:GLU:HG3 | 1.60 | 0.84 |
| 1:D:529:PRO:CB | 4:9:353:GLN:OE1 | 2.25 | 0.84 |
| 1:J:279:LEU:HB2 | 1:J:282:GLU:HG3 | 1.60 | 0.84 |
| 1:S:410:ASN:ND2 | 4:2:336:LYS:HG2 | 1.92 | 0.84 |
| 1:S:732:ILE:HG21 | 1:S:747:LEU:HD13 | 0.91 | 0.84 |
| 4:4:288:ASP:H | 4:6:203:THR:HG22 | 1.41 | 0.83 |
| 4:6:237:GLU:HA | 4:6:251:GLY:HA2 | 1.60 | 0.83 |
| 1:D:279:LEU:HB2 | 1:D:282:GLU:HG3 | 1.60 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:713:SER:HB2 | 1:D:775:LEU:HD21 | 1.58 | 0.83 |
| 1:G:279:LEU:HB2 | 1:G:282:GLU:HG3 | 1.60 | 0.83 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:CD | 2.46 | 0.83 |
| 1:J:796:GLY:HA2 | 3:L:35:ARG:CD | 2.08 | 0.83 |
| 1:M:279:LEU:HB2 | 1:M:282:GLU:HG3 | 1.60 | 0.83 |
| 1:M:736:GLN:HA | 1:M:743:ALA:HB2 | 1.51 | 0.83 |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:HD11 | 1.21 | 0.83 |
| 1:S:753:VAL:HG13 | 1:S:779:ARG:NE | 1.93 | 0.83 |
| 1:S:831:TRP:HE1 | 2:T:67:MET:HB3 | 1.42 | 0.83 |
| 1:M:542:PHE:CA | 4:Z:143:TYR:CE1 | 2.61 | 0.83 |
| 4:7:237:GLU:HA | 4:7:251:GLY:HA2 | 1.60 | 0.83 |
| 4:9:237:GLU:HA | 4:9:251:GLY:HA2 | 1.60 | 0.83 |
| 1:D:542:PHE:CA | 4:9:143:TYR:CE1 | 2.61 | 0.83 |
| 1:G:202:SER:HA | 1:G:207:LYS:HE2 | 0.85 | 0.83 |
| 1:G:819:ASN:CG | 2:H:90:GLY:O | 2.17 | 0.83 |
| 1:S:218:LEU:HB3 | 1:S:221:GLN:HG3 | 1.61 | 0.83 |
| 1:S:279:LEU:HB2 | 1:S:282:GLU:HG3 | 1.60 | 0.83 |
| 1:S:795:ARG:NE | 3:U:116:GLU:HB3 | 1.93 | 0.83 |
| 1:J:542:PHE:CA | 4:W:143:TYR:CE1 | 2.61 | 0.83 |
| 4:9:286:ASP:OD1 | 4:W:203:THR:CG2 | 2.26 | 0.83 |
| 4:9:287:ILE:CG2 | 4:W:205:GLU:HG2 | 2.05 | 0.83 |
| 4:W:237:GLU:HA | 4:W:251:GLY:HA2 | 1.60 | 0.83 |
| 1:M:410:ASN:ND2 | 4:Z:336:LYS:HG2 | 1.92 | 0.83 |
| 1:A:643:GLY:N | 4:8:24:ASP:HA | 1.93 | 0.83 |
| 1:D:538:GLU:N | 4:9:351:THR:N | 2.24 | 0.83 |
| 1:G:648:THR:CG2 | 1:G:651:ALA:HB2 | 2.08 | 0.83 |
| 1:G:725:ARG:CD | 1:G:733:PRO:HB3 | 2.08 | 0.83 |
| 1:J:649:VAL:HG12 | 1:J:649:VAL:C | 1.98 | 0.83 |
| 1:J:839:MLY:HH13 | 2:K:159:HIS:HD2 | 1.41 | 0.83 |
| 1:J:791:GLN:NE2 | 3:L:115:GLY:CA | 2.42 | 0.83 |
| 1:A:732:ILE:CG2 | 1:A:747:LEU:HD13 | 1.34 | 0.83 |
| 1:D:538:GLU:CD | 4:9:355:MET:HE3 | 1.98 | 0.83 |
| 1:G:410:ASN:OD1 | 4:V:334:GLU:CA | 2.24 | 0.83 |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:CG | 1.77 | 0.83 |
| 1:M:725:ARG:CD | 1:M:733:PRO:HB3 | 2.08 | 0.83 |
| 1:M:797:PHE:CE1 | 3:O:149:VAL:HG12 | 2.13 | 0.83 |
| 1:M:803:TYR:CD2 | 3:O:17:PHE:HZ | 1.96 | 0.83 |
| 1:S:640:LYS:CB | 1:S:645:SER:OG | 2.25 | 0.83 |
| 1:S:770:GLY:O | 1:S:771:LEU:O | 1.94 | 0.83 |
| 1:G:529:PRO:CB | 4:V:353:GLN:OE1 | 2.25 | 0.83 |
| 4:2:287:ILE:HB | 4:4:203:THR:HG21 | 1.59 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:529:PRO:CB | 4:8:353:GLN:OE1 | 2.25 | 0.83 |
| 1:D:410:ASN:OD1 | 4:9:334:GLU:CA | 2.24 | 0.83 |
| 1:A:629:GLU:CG | 1:A:643:GLY:O | 2.26 | 0.83 |
| 1:A:502:GLU:O | 1:A:761:GLY:CA | 2.26 | 0.83 |
| 1:D:418:THR:HB | 1:D:421:GLU:HG3 | 1.59 | 0.83 |
| 1:D:507:GLY:HA3 | 1:D:762:HIS:CD2 | 2.14 | 0.83 |
| 1:D:813:ILE:CG2 | 2:E:128:PHE:HE1 | 1.71 | 0.83 |
| 2:H:141:PRO:CB | 2:H:142:PRO:CD | 2.56 | 0.83 |
| 1:J:648:THR:CG2 | 1:J:651:ALA:HB2 | 2.08 | 0.83 |
| 1:M:725:ARG:CZ | 1:M:733:PRO:HB3 | 2.06 | 0.83 |
| 4:1:287:ILE:CG2 | 4:3:202:THR:OG1 | 2.23 | 0.83 |
| 1:S:529:PRO:CB | 4:2:353:GLN:OE1 | 2.25 | 0.83 |
| 1:A:542:PHE:CA | 4:8:143:TYR:CE1 | 2.61 | 0.83 |
| 1:A:553:MLY:HG2 | 4:V:47:MET:H | 1.44 | 0.83 |
| 1:D:831:TRP:NE1 | 2:E:51:PHE:HZ | 1.76 | 0.83 |
| 1:G:820:VAL:HG11 | 2:H:136:MET:HE3 | 1.60 | 0.83 |
| 1:J:730:SER:O | 1:J:734:GLU:HG3 | 1.78 | 0.83 |
| 1:J:831:TRP:CZ2 | 2:K:47:LEU:HD21 | 2.14 | 0.83 |
| 1:M:720:PHE:CE1 | 1:M:772:LEU:HD22 | 1.90 | 0.83 |
| 1:S:542:PHE:CA | 4:2:143:TYR:CE1 | 2.61 | 0.83 |
| 1:S:749:GLY:HA3 | 3:U:93:VAL:CG2 | 2.09 | 0.83 |
| 1:M:630:ALA:C | 4:Z:25:ASP:OD2 | 2.15 | 0.83 |
| 1:S:530:MET:CG | 4:2:354:GLN:CB | 2.30 | 0.83 |
| 4:1:287:ILE:CD1 | 4:3:203:THR:H | 1.92 | 0.83 |
| 4:2:287:ILE:HG22 | 4:4:203:THR:HG22 | 1.60 | 0.83 |
| 1:A:707:CYS:HA | 1:A:714:ARG:HH12 | 1.39 | 0.83 |
| 1:D:629:GLU:CG | 1:D:643:GLY:O | 2.26 | 0.83 |
| 1:D:648:THR:CG2 | 1:D:651:ALA:HB2 | 2.08 | 0.83 |
| 1:D:730:SER:O | 1:D:734:GLU:HG3 | 1.78 | 0.83 |
| 1:J:641:LYS:HG2 | 1:J:647:GLN:HG3 | 1.61 | 0.83 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CB | 2.08 | 0.83 |
| 1:J:838:ILE:CD1 | 2:K:54:MET:HE3 | 2.08 | 0.83 |
| 1:M:629:GLU:CG | 1:M:643:GLY:O | 2.26 | 0.83 |
| 1:M:783:LEU:HG | 1:M:786:ILE:CG1 | 2.08 | 0.83 |
| 1:G:640:LYS:C | 4:V:23:GLY:O | 2.16 | 0.83 |
| 1:G:410:ASN:ND2 | 4:V:336:LYS:HG2 | 1.92 | 0.83 |
| 4:5:237:GLU:HA | 4:5:251:GLY:HA2 | 1.60 | 0.83 |
| 1:G:735:GLY:C | 1:G:743:ALA:HB1 | 1.84 | 0.83 |
| 1:G:769:ALA:O | 1:G:773:GLY:HA3 | 1.79 | 0.83 |
| 1:J:629:GLU:CG | 1:J:643:GLY:O | 2.26 | 0.83 |
| 1:S:202:SER:HA | 1:S:207:LYS:HE2 | 0.85 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:648:THR:CG2 | 1:S:651:ALA:HB2 | 2.08 | 0.83 |
| 1:S:502:GLU:CD | 1:S:761:GLY:CA | 2.47 | 0.83 |
| 1:A:556:ASP:HA | 4:V:49:GLN:O | 1.70 | 0.83 |
| 4:2:203:THR:CG2 | 4:Z:286:ASP:OD1 | 2.26 | 0.83 |
| 1:M:529:PRO:CB | 4:Z:353:GLN:OE1 | 2.25 | 0.83 |
| 4:1:244:ASP:HB3 | 4:Y:325:MET:SD | 2.19 | 0.83 |
| 4:3:237:GLU:HA | 4:3:251:GLY:HA2 | 1.60 | 0.83 |
| 1:G:149:GLN:CG | 1:G:763:THR:HG23 | 2.09 | 0.83 |
| 1:G:542:PHE:CA | 4:V:143:TYR:CE1 | 2.61 | 0.83 |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD13 | 0.91 | 0.83 |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:CD1 | 2.09 | 0.83 |
| 1:M:649:VAL:C | 1:M:649:VAL:HG12 | 1.98 | 0.83 |
| 4:4:322:PRO:HB2 | 4:6:244:ASP:CB | 2.08 | 0.83 |
| 1:A:769:ALA:O | 1:A:772:LEU:N | 2.08 | 0.83 |
| 2:B:141:PRO:CB | 2:B:142:PRO:CD | 2.56 | 0.83 |
| 1:D:218:LEU:HB3 | 1:D:221:GLN:HG3 | 1.61 | 0.83 |
| 1:D:549:SER:O | 4:W:46:GLY:HA3 | 1.77 | 0.83 |
| 1:J:543:PRO:HG3 | 4:W:143:TYR:O | 1.77 | 0.83 |
| 1:M:819:ASN:HA | 2:N:90:GLY:C | 1.98 | 0.83 |
| 2:N:141:PRO:CB | 2:N:142:PRO:CD | 2.56 | 0.83 |
| 1:S:641:LYS:HD2 | 4:2:348:SER:CA | 2.09 | 0.83 |
| 1:S:725:ARG:CD | 1:S:733:PRO:HB3 | 2.08 | 0.83 |
| 4:8:286:ASP:OD1 | 4:V:203:THR:CG2 | 2.26 | 0.83 |
| 1:A:838:ILE:HD12 | 2:B:54:MET:SD | 2.19 | 0.82 |
| 1:D:507:GLY:CA | 1:D:762:HIS:CG | 2.62 | 0.82 |
| 1:J:418:THR:HB | 1:J:421:GLU:HG3 | 1.60 | 0.82 |
| 1:J:84:MLY:CH1 | 1:J:715:VAL:HG11 | 2.08 | 0.82 |
| 1:S:649:VAL:C | 1:S:649:VAL:HG12 | 1.98 | 0.82 |
| 1:S:750:GLY:HA2 | 3:U:89:GLU:HB2 | 1.60 | 0.82 |
| 1:J:542:PHE:CA | 4:W:143:TYR:HE1 | 1.92 | 0.82 |
| 4:1:287:ILE:HG21 | 4:3:202:THR:CB | 2.07 | 0.82 |
| 1:A:410:ASN:ND2 | 4:8:336:LYS:HG2 | 1.93 | 0.82 |
| 2:E:141:PRO:CB | 2:E:142:PRO:CD | 2.56 | 0.82 |
| 1:D:800:ARG:HH21 | 3:F:40:ASN:CG | 1.81 | 0.82 |
| 1:M:97:LEU:HD22 | 1:M:712:PRO:CB | 2.08 | 0.82 |
| 1:M:820:VAL:HG11 | 2:N:136:MET:HE3 | 1.60 | 0.82 |
| 1:S:817:GLN:HG2 | 2:T:127:ARG:HB2 | 1.60 | 0.82 |
| 1:G:543:PRO:HG3 | 4:V:143:TYR:O | 1.78 | 0.82 |
| 1:A:107:MLY:HB3 | 1:A:686:MET:HE2 | 1.60 | 0.82 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HD11 | 1.60 | 0.82 |
| 1:D:640:LYS:CB | 1:D:645:SER:OG | 2.25 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:629:GLU:CG | 1:S:643:GLY:O | 2.26 | 0.82 |
| 4:2:287:ILE:HG21 | 4:4:203:THR:HG22 | 1.60 | 0.82 |
| 4:8:290:ARG:NH1 | 4:V:202:THR:HG21 | 1.94 | 0.82 |
| 1:D:542:PHE:CA | 4:9:143:TYR:HE1 | 1.92 | 0.82 |
| 1:A:798:LEU:HD12 | 3:C:126:LEU:HD21 | 1.56 | 0.82 |
| 1:J:218:LEU:HA | 1:J:221:GLN:HG2 | 1.62 | 0.82 |
| 1:J:506:GLU:OE2 | 1:J:761:GLY:CA | 2.25 | 0.82 |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:CD1 | 2.10 | 0.82 |
| 1:M:640:LYS:CB | 1:M:645:SER:OG | 2.25 | 0.82 |
| 1:S:505:MLY:NZ | 1:S:762:HIS:NE2 | 2.27 | 0.82 |
| 1:S:730:SER:O | 1:S:734:GLU:HG3 | 1.79 | 0.82 |
| 1:S:792:ALA:HB1 | 3:U:42:THR:HA | 1.59 | 0.82 |
| 1:G:567:LYS:HZ1 | 4:X:92:ASN:ND2 | 1.69 | 0.82 |
| 4:4:237:GLU:HA | 4:4:251:GLY:HA2 | 1.60 | 0.82 |
| 1:A:795:ARG:HG2 | 3:C:118:MET:CE | 2.09 | 0.82 |
| 2:E:111:SER:OG | 2:E:148:VAL:C | 2.15 | 0.82 |
| 1:G:578:HIS:HB3 | 1:G:592:ILE:HD12 | 1.62 | 0.82 |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:CG1 | 2.10 | 0.82 |
| 1:J:818:TYR:HE1 | 2:K:127:ARG:NH2 | 1.71 | 0.82 |
| 1:M:549:SER:O | 4:2:46:GLY:C | 2.18 | 0.82 |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:HD21 | 1.58 | 0.82 |
| 2:T:144:VAL:HG12 | 2:T:153:ILE:CD1 | 2.10 | 0.82 |
| 1:S:639:GLY:CA | 4:2:344:SER:C | 2.48 | 0.82 |
| 4:2:110:LEU:O | 4:3:195:GLU:HA | 1.79 | 0.82 |
| 1:A:292:MET:HE3 | 1:A:309:PRO:HA | 1.60 | 0.82 |
| 1:A:549:SER:O | 4:V:46:GLY:CA | 2.27 | 0.82 |
| 1:A:578:HIS:HB3 | 1:A:592:ILE:HD12 | 1.62 | 0.82 |
| 1:A:93:MET:CE | 1:A:715:VAL:HG13 | 2.09 | 0.82 |
| 1:G:629:GLU:CG | 1:G:643:GLY:O | 2.26 | 0.82 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CA | 2.09 | 0.82 |
| 1:M:35:MLY:HH22 | 1:M:777:GLU:HG2 | 0.85 | 0.82 |
| 1:M:643:GLY:N | 4:Z:24:ASP:HA | 1.93 | 0.82 |
| 1:M:641:LYS:HG2 | 1:M:647:GLN:HG3 | 1.61 | 0.82 |
| 2:T:141:PRO:CB | 2:T:142:PRO:CD | 2.56 | 0.82 |
| 1:D:218:LEU:HA | 1:D:221:GLN:HG2 | 1.62 | 0.82 |
| 1:D:549:SER:O | 4:W:46:GLY:C | 2.18 | 0.82 |
| 1:G:752:ASP:C | 1:G:780:ASP:OD1 | 2.17 | 0.82 |
| 1:J:795:ARG:CZ | 3:L:116:GLU:OE1 | 2.27 | 0.82 |
| 1:M:202:SER:HA | 1:M:207:LYS:HE2 | 0.85 | 0.82 |
| 1:M:549:SER:O | 4:2:46:GLY:CA | 2.27 | 0.82 |
| 1:A:831:TRP:CG | 2:B:51:PHE:CZ | 2.68 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:218:LEU:HD22 | 1:D:222:ILE:CG1 | 2.10 | 0.82 |
| 1:D:557:GLU:H | 4:W:48:GLY:HA3 | 1.28 | 0.82 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:HB | 1.72 | 0.82 |
| 1:G:730:SER:O | 1:G:734:GLU:HG3 | 1.79 | 0.82 |
| 1:G:94:MET:O | 1:G:713:SER:HA | 1.79 | 0.82 |
| 1:M:795:ARG:CD | 3:O:118:MET:HE1 | 2.10 | 0.82 |
| 1:S:793:ARG:HH11 | 3:U:40:ASN:HD22 | 0.85 | 0.82 |
| 1:D:549:SER:O | 4:W:46:GLY:CA | 2.27 | 0.82 |
| 1:J:553:MLY:HH12 | 4:Y:45:VAL:HG11 | 1.59 | 0.82 |
| 2:E:121:LEU:CG | 2:E:128:PHE:CA | 2.49 | 0.82 |
| 1:G:557:GLU:HB2 | 4:X:46:GLY:C | 2.00 | 0.82 |
| 1:G:639:GLY:CA | 4:V:344:SER:C | 2.49 | 0.82 |
| 1:G:640:LYS:CB | 1:G:645:SER:OG | 2.25 | 0.82 |
| 1:G:817:GLN:CG | 2:H:127:ARG:HB2 | 2.10 | 0.82 |
| 1:J:783:LEU:O | 1:J:787:ILE:HB | 1.78 | 0.82 |
| 1:S:578:HIS:HB3 | 1:S:592:ILE:HD12 | 1.61 | 0.82 |
| 1:S:796:GLY:CA | 3:U:35:ARG:CD | 2.43 | 0.82 |
| 1:D:553:MLY:HG2 | 4:W:47:MET:H | 1.44 | 0.82 |
| 4:1:287:ILE:HB | 4:3:203:THR:N | 1.93 | 0.82 |
| 4:7:290:ARG:NH1 | 4:9:202:THR:HG21 | 1.94 | 0.82 |
| 1:A:730:SER:O | 1:A:734:GLU:HG3 | 1.78 | 0.82 |
| 2:B:111:SER:OG | 2:B:148:VAL:C | 2.15 | 0.82 |
| 1:D:599:ASN:CA | 1:D:649:VAL:CB | 2.53 | 0.82 |
| 1:G:418:THR:HB | 1:G:421:GLU:HG3 | 1.59 | 0.82 |
| 1:J:639:GLY:CA | 4:W:344:SER:C | 2.48 | 0.82 |
| 1:J:796:GLY:HA2 | 3:L:35:ARG:HD3 | 1.59 | 0.82 |
| 1:M:84:MLY:CH1 | 1:M:715:VAL:CG2 | 2.57 | 0.82 |
| 1:M:553:MLY:HG2 | 4:2:47:MET:H | 1.44 | 0.81 |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:CG1 | 2.10 | 0.81 |
| 1:A:28:GLN:NE2 | 1:A:723:ARG:HH21 | 1.77 | 0.81 |
| 1:D:823:PHE:CZ | 2:E:156:VAL:HG12 | 2.15 | 0.81 |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:CG1 | 2.10 | 0.81 |
| 1:G:578:HIS:HD2 | 1:G:591:ASN:HA | 1.45 | 0.81 |
| 1:G:643:GLY:N | 4:V:24:ASP:HA | 1.94 | 0.81 |
| 1:J:218:LEU:CA | 1:J:221:GLN:HG2 | 2.10 | 0.81 |
| 1:J:641:LYS:HD2 | 4:W:348:SER:CA | 2.09 | 0.81 |
| 1:M:543:PRO:HG3 | 4:Z:143:TYR:O | 1.77 | 0.81 |
| 4:X:237:GLU:HA | 4:X:251:GLY:HA2 | 1.60 | 0.81 |
| 1:A:639:GLY:CA | 4:8:344:SER:C | 2.48 | 0.81 |
| 1:A:641:LYS:HD2 | 4:8:348:SER:CA | 2.09 | 0.81 |
| 1:A:641:LYS:HG2 | 1:A:647:GLN:HG3 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:791:GLN:HE22 | 3:F:116:GLU:N | 1.63 | 0.81 |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:HD22 | 1.45 | 0.81 |
| 1:G:107:MLY:HB3 | 1:G:686:MET:HE2 | 1.62 | 0.81 |
| 1:G:795:ARG:CA | 3:I:118:MET:CE | 2.58 | 0.81 |
| 1:J:218:LEU:HB3 | 1:J:221:GLN:HG3 | 1.61 | 0.81 |
| 1:J:84:MLY:CD | 1:J:724:TYR:CZ | 2.59 | 0.81 |
| 1:J:821:ARG:NH2 | 2:K:127:ARG:CG | 2.42 | 0.81 |
| 1:J:84:MLY:HH12 | 1:J:715:VAL:CG1 | 2.09 | 0.81 |
| 1:M:218:LEU:HA | 1:M:221:GLN:HG2 | 1.62 | 0.81 |
| 1:M:721:LYS:CA | 1:M:736:GLN:NE2 | 2.43 | 0.81 |
| 2:N:121:LEU:CA | 2:N:128:PHE:CB | 2.46 | 0.81 |
| 1:S:546:THR:HG21 | 4:4:46:GLY:O | 1.80 | 0.81 |
| 1:S:571:ALA:O | 1:S:572:LYS:CG | 2.28 | 0.81 |
| 4:2:202:THR:HG21 | 4:Z:290:ARG:NH1 | 1.94 | 0.81 |
| 2:B:121:LEU:CG | 2:B:128:PHE:CA | 2.48 | 0.81 |
| 1:G:538:GLU:CA | 4:V:351:THR:H | 1.92 | 0.81 |
| 1:G:768:MLY:HH23 | 1:G:772:LEU:CG | 2.05 | 0.81 |
| 1:J:829:TRP:CZ3 | 2:K:84:PHE:CZ | 2.68 | 0.81 |
| 1:S:599:ASN:CA | 1:S:649:VAL:CB | 2.53 | 0.81 |
| 1:S:721:LYS:CA | 1:S:736:GLN:NE2 | 2.43 | 0.81 |
| 1:S:786:ILE:C | 1:S:787:ILE:C | 2.39 | 0.81 |
| 1:S:839:MLY:HH21 | 2:T:158:THR:CG2 | 2.10 | 0.81 |
| 1:M:641:LYS:HD2 | 4:Z:348:SER:CA | 2.09 | 0.81 |
| 1:M:530:MET:CG | 4:Z:354:GLN:CB | 2.30 | 0.81 |
| 1:A:831:TRP:HH2 | 2:B:50:THR:HB | 1.40 | 0.81 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:HD21 | 2.14 | 0.81 |
| 1:J:734:GLU:O | 1:J:738:MET:CG | 2.28 | 0.81 |
| 1:J:791:GLN:OE1 | 3:L:116:GLU:HG3 | 1.79 | 0.81 |
| 1:M:599:ASN:CA | 1:M:649:VAL:CB | 2.53 | 0.81 |
| 1:S:215:GLN:N | 1:S:340:ILE:CD1 | 2.44 | 0.81 |
| 1:S:418:THR:HB | 1:S:421:GLU:HG3 | 1.60 | 0.81 |
| 1:S:732:ILE:CG2 | 1:S:747:LEU:HD13 | 1.34 | 0.81 |
| 4:V:325:MET:SD | 4:X:244:ASP:HB3 | 2.19 | 0.81 |
| 4:Z:237:GLU:HA | 4:Z:251:GLY:HA2 | 1.60 | 0.81 |
| 4:2:237:GLU:HA | 4:2:251:GLY:HA2 | 1.60 | 0.81 |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:HD2 | 1.45 | 0.81 |
| 1:A:725:ARG:CZ | 1:A:733:PRO:HB3 | 2.06 | 0.81 |
| 1:D:571:ALA:O | 1:D:572:LYS:CG | 2.28 | 0.81 |
| 1:M:215:GLN:N | 1:M:340:ILE:CD1 | 2.44 | 0.81 |
| 1:M:639:GLY:CA | 4:Z:344:SER:C | 2.48 | 0.81 |
| 1:M:795:ARG:HB3 | 3:O:35:ARG:CZ | 2.10 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:288:ASP:OD2 | 4:3:203:THR:CG2 | 2.25 | 0.81 |
| 4:8:237:GLU:HA | 4:8:251:GLY:HA2 | 1.60 | 0.81 |
| 1:A:734:GLU:O | 1:A:738:MET:CG | 2.28 | 0.81 |
| 1:A:754:ASP:OD2 | 1:A:774:LEU:HD23 | 1.80 | 0.81 |
| 1:A:795:ARG:CD | 3:C:35:ARG:NH1 | 2.24 | 0.81 |
| 1:G:757:GLN:HG2 | 1:G:776:GLU:CG | 1.85 | 0.81 |
| 1:J:578:HIS:HB3 | 1:J:592:ILE:HD12 | 1.62 | 0.81 |
| 1:J:721:LYS:CA | 1:J:736:GLN:NE2 | 2.43 | 0.81 |
| 1:M:418:THR:HB | 1:M:421:GLU:HG3 | 1.60 | 0.81 |
| 1:M:534:SER:O | 4:Z:351:THR:HG23 | 1.13 | 0.81 |
| 1:S:218:LEU:HA | 1:S:221:GLN:HG2 | 1.61 | 0.81 |
| 1:S:93:MET:HE2 | 1:S:764:MLY:HB3 | 1.62 | 0.81 |
| 4:7:223:PHE:HE1 | 4:7:255:PHE:HB2 | 1.46 | 0.81 |
| 1:A:418:THR:HB | 1:A:421:GLU:HG3 | 1.60 | 0.81 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:HD21 | 2.14 | 0.81 |
| 1:A:795:ARG:HG2 | 3:C:118:MET:HE3 | 1.61 | 0.81 |
| 1:D:218:LEU:CA | 1:D:221:GLN:HG2 | 2.10 | 0.81 |
| 1:G:232:PHE:CZ | 1:G:287:ILE:HD13 | 2.16 | 0.81 |
| 2:H:121:LEU:CG | 2:H:128:PHE:CA | 2.49 | 0.81 |
| 1:G:791:GLN:NE2 | 3:I:115:GLY:CA | 1.96 | 0.81 |
| 1:J:831:TRP:CZ2 | 2:K:47:LEU:CD2 | 2.64 | 0.81 |
| 1:M:720:PHE:CZ | 1:M:772:LEU:HD21 | 2.08 | 0.81 |
| 1:S:480:ILE:HG22 | 1:S:481:ASN:HD22 | 1.45 | 0.81 |
| 1:S:805:ALA:HA | 1:S:808:GLU:H | 1.43 | 0.81 |
| 1:S:93:MET:HG2 | 1:S:715:VAL:CA | 2.05 | 0.81 |
| 4:V:237:GLU:HA | 4:V:251:GLY:HA2 | 1.60 | 0.81 |
| 4:1:223:PHE:HE1 | 4:1:255:PHE:HB2 | 1.46 | 0.81 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:HB3 | 1.93 | 0.81 |
| 1:D:793:ARG:HH21 | 3:F:147:MET:HE1 | 1.46 | 0.81 |
| 1:D:799:MET:CE | 3:F:32:ASP:CB | 2.51 | 0.81 |
| 1:G:791:GLN:HE21 | 3:I:115:GLY:HA3 | 1.44 | 0.81 |
| 1:J:784:ALA:O | 1:J:788:THR:N | 2.14 | 0.81 |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:CG1 | 2.10 | 0.81 |
| 1:M:730:SER:O | 1:M:734:GLU:HG3 | 1.79 | 0.81 |
| 1:S:232:PHE:CZ | 1:S:287:ILE:HD13 | 2.16 | 0.81 |
| 1:G:641:LYS:HD2 | 4:V:348:SER:CA | 2.10 | 0.81 |
| 1:J:538:GLU:CA | 4:W:351:THR:H | 1.93 | 0.81 |
| 1:D:641:LYS:HD2 | 1:D:647:GLN:OE1 | 1.81 | 0.81 |
| 1:D:709:LYS:C | 1:D:710:GLY:HA2 | 2.01 | 0.81 |
| 1:G:725:ARG:CZ | 1:G:733:PRO:HB3 | 2.05 | 0.81 |
| 1:J:831:TRP:HZ3 | 2:K:34:ILE:HD13 | 1.46 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:232:PHE:CZ | 1:M:287:ILE:HD13 | 2.16 | 0.81 |
| 1:M:834:LEU:CD1 | 2:N:51:PHE:CE1 | 2.63 | 0.81 |
| 4:9:290:ARG:NH1 | 4:W:202:THR:HG21 | 1.94 | 0.81 |
| 4:9:223:PHE:HE1 | 4:9:255:PHE:HB2 | 1.46 | 0.81 |
| 1:A:232:PHE:CZ | 1:A:287:ILE:HD13 | 2.16 | 0.81 |
| 1:A:578:HIS:HD2 | 1:A:591:ASN:HA | 1.44 | 0.81 |
| 1:A:831:TRP:CZ3 | 2:B:50:THR:CG2 | 2.63 | 0.81 |
| 1:D:641:LYS:HD2 | 4:9:348:SER:CA | 2.09 | 0.81 |
| 1:D:641:LYS:HG2 | 1:D:647:GLN:HG3 | 1.60 | 0.81 |
| 1:J:215:GLN:N | 1:J:340:ILE:CD1 | 2.44 | 0.81 |
| 1:M:538:GLU:CA | 4:Z:351:THR:H | 1.93 | 0.81 |
| 1:S:374:GLN:HG3 | 1:S:375:ALA:N | 1.96 | 0.81 |
| 1:S:409:GLY:N | 1:S:636:LYS:CG | 2.44 | 0.81 |
| 1:S:795:ARG:HG3 | 3:U:118:MET:HE1 | 1.55 | 0.81 |
| 1:M:557:GLU:N | 4:2:48:GLY:HA2 | 1.90 | 0.81 |
| 1:D:639:GLY:CA | 4:9:344:SER:C | 2.48 | 0.81 |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD13 | 0.91 | 0.81 |
| 2:B:144:VAL:CA | 2:B:153:ILE:HD11 | 2.11 | 0.81 |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:HD22 | 1.45 | 0.81 |
| 1:D:643:GLY:N | 4:9:24:ASP:HA | 1.94 | 0.81 |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:HD2 | 1.45 | 0.81 |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:HD12 | 0.81 | 0.81 |
| 1:G:788:THR:O | 3:I:42:THR:HG21 | 1.80 | 0.81 |
| 1:J:374:GLN:HG3 | 1:J:375:ALA:N | 1.96 | 0.81 |
| 1:M:578:HIS:HB3 | 1:M:592:ILE:HD12 | 1.62 | 0.81 |
| 1:M:821:ARG:HH21 | 2:N:127:ARG:HG2 | 1.01 | 0.81 |
| 2:N:144:VAL:CA | 2:N:153:ILE:HD11 | 2.11 | 0.81 |
| 1:S:791:GLN:NE2 | 3:U:116:GLU:N | 2.27 | 0.81 |
| 1:S:93:MET:HE2 | 1:S:764:MLY:CG | 2.11 | 0.81 |
| 4:X:223:PHE:HE1 | 4:X:255:PHE:HB2 | 1.46 | 0.81 |
| 4:4:324:THR:CB | 4:6:244:ASP:CA | 2.48 | 0.80 |
| 1:A:502:GLU:CD | 1:A:764:MLY:N | 2.34 | 0.80 |
| 1:D:374:GLN:HG3 | 1:D:375:ALA:N | 1.96 | 0.80 |
| 1:D:734:GLU:O | 1:D:738:MET:CG | 2.28 | 0.80 |
| 1:D:800:ARG:NH2 | 3:F:40:ASN:OD1 | 2.13 | 0.80 |
| 1:J:793:ARG:NH1 | 3:L:40:ASN:HD22 | 1.79 | 0.80 |
| 2:K:111:SER:OG | 2:K:148:VAL:C | 2.15 | 0.80 |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:HD13 | 0.90 | 0.80 |
| 2:N:141:PRO:CB | 2:N:142:PRO:HD2 | 2.12 | 0.80 |
| 2:N:144:VAL:HG12 | 2:N:153:ILE:CD1 | 2.10 | 0.80 |
| 1:S:218:LEU:HD22 | 1:S:222:ILE:CG1 | 2.10 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:549:SER:O | 4:V:46:GLY:C | 2.19 | 0.80 |
| 4:W:223:PHE:HE1 | 4:W:255:PHE:HB2 | 1.46 | 0.80 |
| 1:S:538:GLU:CA | 4:2:351:THR:H | 1.93 | 0.80 |
| 3:C:49:ILE:N | 3:C:52:ASN:ND2 | 2.29 | 0.80 |
| 1:D:530:MET:HE1 | 4:9:355:MET:SD | 2.21 | 0.80 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:HD21 | 2.14 | 0.80 |
| 1:J:232:PHE:CZ | 1:J:287:ILE:HD13 | 2.16 | 0.80 |
| 2:K:141:PRO:HB2 | 2:K:142:PRO:CD | 2.12 | 0.80 |
| 1:M:480:ILE:HG22 | 1:M:481:ASN:HD22 | 1.45 | 0.80 |
| 1:M:84:MLY:CH2 | 1:M:719:ASP:HB3 | 2.10 | 0.80 |
| 1:S:542:PHE:CA | 4:2:143:TYR:HE1 | 1.92 | 0.80 |
| 4:3:223:PHE:HE1 | 4:3:255:PHE:HB2 | 1.46 | 0.80 |
| 1:A:798:LEU:CD2 | 3:C:126:LEU:HD11 | 2.12 | 0.80 |
| 2:H:141:PRO:CB | 2:H:142:PRO:HD2 | 2.11 | 0.80 |
| 2:H:144:VAL:CA | 2:H:153:ILE:HD11 | 2.11 | 0.80 |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:HD2 | 1.45 | 0.80 |
| 1:S:218:LEU:CA | 1:S:221:GLN:HG2 | 2.10 | 0.80 |
| 1:J:643:GLY:N | 4:W:24:ASP:HA | 1.94 | 0.80 |
| 1:J:530:MET:CG | 4:W:354:GLN:CB | 2.30 | 0.80 |
| 4:2:223:PHE:HE1 | 4:2:255:PHE:HB2 | 1.46 | 0.80 |
| 4:8:223:PHE:HE1 | 4:8:255:PHE:HB2 | 1.46 | 0.80 |
| 1:D:538:GLU:CA | 4:9:351:THR:H | 1.93 | 0.80 |
| 1:D:578:HIS:HB3 | 1:D:592:ILE:HD12 | 1.62 | 0.80 |
| 1:D:721:LYS:CA | 1:D:736:GLN:NE2 | 2.43 | 0.80 |
| 1:G:215:GLN:N | 1:G:340:ILE:CD1 | 2.44 | 0.80 |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:CD2 | 2.12 | 0.80 |
| 1:J:529:PRO:C | 4:W:354:GLN:CB | 2.48 | 0.80 |
| 1:J:710:GLY:O | 1:J:772:LEU:HB2 | 1.81 | 0.80 |
| 1:S:291:ILE:HA | 1:S:331:LEU:HD11 | 1.64 | 0.80 |
| 1:A:550:PHE:CA | 4:V:46:GLY:CA | 2.59 | 0.80 |
| 4:W:325:MET:SD | 4:Y:244:ASP:HB3 | 2.19 | 0.80 |
| 1:J:557:GLU:HB2 | 4:Y:46:GLY:C | 2.00 | 0.80 |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:HD2 | 1.45 | 0.80 |
| 1:D:727:LEU:CG | 1:D:782:MLY:HH12 | 2.10 | 0.80 |
| 3:F:49:ILE:N | 3:F:52:ASN:ND2 | 2.29 | 0.80 |
| 1:J:829:TRP:HZ3 | 2:K:84:PHE:CZ | 2.00 | 0.80 |
| 2:K:144:VAL:CA | 2:K:153:ILE:HD11 | 2.11 | 0.80 |
| 1:S:643:GLY:N | 4:2:24:ASP:HA | 1.93 | 0.80 |
| 1:S:734:GLU:O | 1:S:738:MET:CG | 2.28 | 0.80 |
| 1:S:783:LEU:HG | 1:S:786:ILE:HD11 | 0.81 | 0.80 |
| 1:S:747:LEU:HA | 3:U:93:VAL:HG11 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:550:PHE:N | 4:2:46:GLY:HA3 | 1.97 | 0.80 |
| 4:3:288:ASP:H | 4:5:203:THR:HG22 | 1.40 | 0.80 |
| 1:D:291:ILE:HA | 1:D:331:LEU:HD11 | 1.64 | 0.80 |
| 2:E:117:LEU:HB2 | 2:E:147:ASN:HD21 | 1.47 | 0.80 |
| 2:E:117:LEU:CB | 2:E:147:ASN:ND2 | 2.35 | 0.80 |
| 1:D:823:PHE:CD1 | 2:E:156:VAL:O | 2.35 | 0.80 |
| 1:G:795:ARG:HB2 | 3:I:35:ARG:HH12 | 1.44 | 0.80 |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:HD22 | 1.45 | 0.80 |
| 1:J:736:GLN:HA | 1:J:743:ALA:HB2 | 1.51 | 0.80 |
| 1:J:769:ALA:HB2 | 1:J:770:GLY:HA2 | 1.61 | 0.80 |
| 1:M:291:ILE:HA | 1:M:331:LEU:HD11 | 1.64 | 0.80 |
| 1:M:578:HIS:HD2 | 1:M:591:ASN:HA | 1.45 | 0.80 |
| 1:M:732:ILE:HG22 | 1:M:747:LEU:HD12 | 0.81 | 0.80 |
| 3:O:49:ILE:N | 3:O:52:ASN:ND2 | 2.29 | 0.80 |
| 1:S:735:GLY:C | 1:S:743:ALA:HB1 | 1.84 | 0.80 |
| 1:S:792:ALA:HB3 | 3:U:42:THR:CG2 | 1.96 | 0.80 |
| 4:X:291:LYS:HE3 | 4:Z:243:PRO:HB2 | 0.80 | 0.80 |
| 1:A:218:LEU:HA | 1:A:221:GLN:HG2 | 1.62 | 0.80 |
| 1:A:374:GLN:HG3 | 1:A:375:ALA:N | 1.96 | 0.80 |
| 1:D:831:TRP:CE2 | 2:E:51:PHE:HZ | 1.99 | 0.80 |
| 1:G:734:GLU:O | 1:G:738:MET:CG | 2.28 | 0.80 |
| 1:G:755:HIS:H | 1:G:779:ARG:CZ | 1.94 | 0.80 |
| 1:G:148:ARG:NH2 | 1:G:764:MLY:HH21 | 1.94 | 0.80 |
| 1:J:578:HIS:HD2 | 1:J:591:ASN:HA | 1.45 | 0.80 |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD13 | 0.91 | 0.80 |
| 1:M:218:LEU:CA | 1:M:221:GLN:HG2 | 2.10 | 0.80 |
| 1:M:734:GLU:O | 1:M:738:MET:CG | 2.28 | 0.80 |
| 2:T:141:PRO:CB | 2:T:142:PRO:HD2 | 2.12 | 0.80 |
| 2:T:144:VAL:CA | 2:T:153:ILE:HD11 | 2.11 | 0.80 |
| 1:G:542:PHE:CA | 4:V:143:TYR:HE1 | 1.93 | 0.80 |
| 1:M:550:PHE:CA | 4:2:46:GLY:CA | 2.59 | 0.80 |
| 2:B:141:PRO:CB | 2:B:142:PRO:HD2 | 2.12 | 0.80 |
| 2:E:144:VAL:CA | 2:E:153:ILE:HD11 | 2.11 | 0.80 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:HD21 | 2.14 | 0.80 |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:HD12 | 0.81 | 0.80 |
| 1:J:84:MLY:HD2 | 1:J:724:TYR:OH | 1.82 | 0.80 |
| 1:M:818:TYR:CD1 | 2:N:127:ARG:NH1 | 2.50 | 0.80 |
| 1:S:578:HIS:HD2 | 1:S:591:ASN:HA | 1.45 | 0.80 |
| 1:A:215:GLN:N | 1:A:340:ILE:CD1 | 2.44 | 0.80 |
| 1:A:218:LEU:CA | 1:A:221:GLN:HG2 | 2.10 | 0.80 |
| 1:D:215:GLN:N | 1:D:340:ILE:CD1 | 2.44 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:141:PRO:HB2 | 2:H:142:PRO:CD | 2.12 | 0.80 |
| 1:J:291:ILE:HA | 1:J:331:LEU:HD11 | 1.64 | 0.80 |
| 1:J:834:LEU:HD12 | 2:K:51:PHE:HE1 | 1.47 | 0.80 |
| 1:M:803:TYR:HD2 | 3:O:17:PHE:CZ | 1.99 | 0.80 |
| 1:S:709:LYS:C | 1:S:710:GLY:N | 2.35 | 0.80 |
| 1:S:836:PHE:HE1 | 2:T:159:HIS:HA | 1.03 | 0.80 |
| 1:A:538:GLU:CA | 4:8:351:THR:H | 1.93 | 0.80 |
| 1:D:578:HIS:HD2 | 1:D:591:ASN:HA | 1.45 | 0.80 |
| 1:D:727:LEU:HB3 | 1:D:782:MLY:CH1 | 2.09 | 0.80 |
| 1:G:218:LEU:CA | 1:G:221:GLN:HG2 | 2.10 | 0.80 |
| 1:J:599:ASN:CA | 1:J:649:VAL:CB | 2.53 | 0.80 |
| 1:J:725:ARG:CZ | 1:J:733:PRO:HB3 | 2.06 | 0.80 |
| 1:M:127:ASN:HD22 | 1:M:128:PRO:HD2 | 1.44 | 0.80 |
| 2:T:141:PRO:HB2 | 2:T:142:PRO:CD | 2.12 | 0.80 |
| 1:A:817:GLN:OE1 | 2:B:127:ARG:CZ | 2.30 | 0.79 |
| 1:D:232:PHE:CZ | 1:D:287:ILE:HD13 | 2.16 | 0.79 |
| 1:G:820:VAL:HG11 | 2:H:136:MET:CE | 2.11 | 0.79 |
| 1:M:735:GLY:C | 1:M:743:ALA:HB2 | 1.82 | 0.79 |
| 1:S:127:ASN:HD22 | 1:S:128:PRO:HD2 | 1.44 | 0.79 |
| 1:S:792:ALA:HB1 | 3:U:42:THR:CA | 2.09 | 0.79 |
| 1:G:538:GLU:HG3 | 4:V:351:THR:C | 2.02 | 0.79 |
| 4:Z:223:PHE:HE1 | 4:Z:255:PHE:HB2 | 1.46 | 0.79 |
| 1:A:797:PHE:CE2 | 3:C:126:LEU:CD2 | 2.60 | 0.79 |
| 1:D:409:GLY:N | 1:D:636:LYS:CG | 2.44 | 0.79 |
| 1:D:550:PHE:HA | 4:W:46:GLY:HA2 | 1.64 | 0.79 |
| 1:D:724:TYR:HA | 1:D:782:MLY:HD2 | 0.81 | 0.79 |
| 1:G:374:GLN:HG3 | 1:G:375:ALA:N | 1.96 | 0.79 |
| 3:L:50:LEU:C | 3:L:53:PRO:HD2 | 2.03 | 0.79 |
| 1:M:571:ALA:O | 1:M:572:LYS:CG | 2.28 | 0.79 |
| 1:S:797:PHE:HZ | 3:U:146:ILE:HD13 | 1.43 | 0.79 |
| 1:S:530:MET:HE1 | 4:2:355:MET:SD | 2.23 | 0.79 |
| 4:4:288:ASP:N | 4:6:203:THR:CG2 | 2.45 | 0.79 |
| 1:S:544:LYS:HD3 | 4:4:45:VAL:HG21 | 1.63 | 0.79 |
| 1:A:542:PHE:CA | 4:8:143:TYR:HE1 | 1.92 | 0.79 |
| 1:A:409:GLY:N | 1:A:636:LYS:CG | 2.44 | 0.79 |
| 1:A:641:LYS:HD2 | 1:A:647:GLN:OE1 | 1.81 | 0.79 |
| 1:A:793:ARG:NH2 | 3:C:147:MET:HE3 | 1.92 | 0.79 |
| 1:A:93:MET:HG2 | 1:A:715:VAL:CG2 | 2.12 | 0.79 |
| 1:D:550:PHE:N | 4:W:46:GLY:HA3 | 1.97 | 0.79 |
| 1:G:829:TRP:HZ3 | 2:H:84:PHE:CZ | 2.00 | 0.79 |
| 1:G:817:GLN:CD | 2:H:127:ARG:CD | 2.50 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:710:GLY:C | 1:J:772:LEU:HD23 | 2.01 | 0.79 |
| 1:M:374:GLN:HG3 | 1:M:375:ALA:N | 1.96 | 0.79 |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:CB | 1.85 | 0.79 |
| 2:N:121:LEU:CG | 2:N:128:PHE:CA | 2.48 | 0.79 |
| 1:S:641:LYS:HG2 | 1:S:647:GLN:HG3 | 1.61 | 0.79 |
| 3:U:50:LEU:C | 3:U:53:PRO:HD2 | 2.03 | 0.79 |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:HD12 | 0.81 | 0.79 |
| 1:D:712:PRO:CG | 1:D:771:LEU:CB | 2.53 | 0.79 |
| 2:E:141:PRO:HB2 | 2:E:142:PRO:CD | 2.12 | 0.79 |
| 3:L:49:ILE:N | 3:L:52:ASN:ND2 | 2.30 | 0.79 |
| 1:M:407:GLY:HA2 | 1:M:412:ALA:HA | 1.65 | 0.79 |
| 2:N:141:PRO:HB2 | 2:N:142:PRO:CD | 2.12 | 0.79 |
| 4:Y:223:PHE:HE1 | 4:Y:255:PHE:HB2 | 1.46 | 0.79 |
| 4:2:204:ALA:N | 4:Z:287:ILE:HB | 1.98 | 0.79 |
| 4:1:287:ILE:CG1 | 4:3:202:THR:HB | 2.13 | 0.79 |
| 1:A:799:MET:SD | 3:C:32:ASP:HA | 2.23 | 0.79 |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:CD1 | 2.09 | 0.79 |
| 1:D:725:ARG:CZ | 1:D:733:PRO:HB3 | 2.05 | 0.79 |
| 2:K:141:PRO:CB | 2:K:142:PRO:HD2 | 2.12 | 0.79 |
| 1:J:530:MET:HE1 | 4:W:355:MET:SD | 2.23 | 0.79 |
| 4:3:288:ASP:N | 4:5:203:THR:CG2 | 2.45 | 0.79 |
| 4:5:223:PHE:HE1 | 4:5:255:PHE:HB2 | 1.46 | 0.79 |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:HD22 | 1.45 | 0.79 |
| 1:A:571:ALA:O | 1:A:572:LYS:CG | 2.28 | 0.79 |
| 1:G:641:LYS:HG2 | 1:G:647:GLN:HG3 | 1.61 | 0.79 |
| 1:G:757:GLN:CG | 1:G:776:GLU:CD | 2.45 | 0.79 |
| 1:J:537:GLU:O | 4:W:350:SER:N | 2.16 | 0.79 |
| 1:M:786:ILE:CA | 1:M:787:ILE:N | 2.45 | 0.79 |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:HD23 | 1.63 | 0.79 |
| 1:S:174:SER:CB | 1:S:667:THR:HG21 | 2.13 | 0.79 |
| 1:G:530:MET:CG | 4:V:354:GLN:CB | 2.30 | 0.79 |
| 1:M:542:PHE:CA | 4:Z:143:TYR:HE1 | 1.92 | 0.79 |
| 1:A:550:PHE:N | 4:V:46:GLY:HA3 | 1.97 | 0.79 |
| 1:A:721:LYS:CA | 1:A:736:GLN:NE2 | 2.43 | 0.79 |
| 1:G:166:MET:HE1 | 1:G:254:PHE:HB2 | 1.65 | 0.79 |
| 1:G:641:LYS:CE | 1:G:647:GLN:CG | 2.61 | 0.79 |
| 3:I:50:LEU:C | 3:I:53:PRO:HD2 | 2.03 | 0.79 |
| 1:J:819:ASN:CG | 2:K:92:ASP:CB | 2.48 | 0.79 |
| 1:M:753:VAL:HG11 | 1:M:775:LEU:HD11 | 1.64 | 0.79 |
| 1:S:84:MLY:CH1 | 1:S:724:TYR:CE2 | 2.60 | 0.79 |
| 4:4:287:ILE:HG23 | 4:6:202:THR:HG1 | 1.48 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:721:LYS:HG2 | 1:A:736:GLN:CD | 1.86 | 0.79 |
| 1:A:501:GLU:HG2 | 1:A:762:HIS:HD1 | 0.71 | 0.79 |
| 1:G:571:ALA:O | 1:G:572:LYS:CG | 2.28 | 0.79 |
| 1:G:721:LYS:CA | 1:G:736:GLN:NE2 | 2.43 | 0.79 |
| 1:J:571:ALA:O | 1:J:572:LYS:CG | 2.28 | 0.79 |
| 1:M:174:SER:CB | 1:M:667:THR:HG21 | 2.13 | 0.79 |
| 1:S:727:LEU:HD23 | 1:S:783:LEU:HB2 | 0.89 | 0.79 |
| 1:S:732:ILE:HG22 | 1:S:747:LEU:HD12 | 0.81 | 0.79 |
| 1:S:805:ALA:CA | 1:S:808:GLU:H | 1.95 | 0.79 |
| 1:D:550:PHE:CA | 4:W:46:GLY:CA | 2.59 | 0.79 |
| 4:3:287:ILE:HG13 | 4:5:202:THR:CB | 2.12 | 0.79 |
| 4:6:223:PHE:HE1 | 4:6:255:PHE:HB2 | 1.46 | 0.79 |
| 1:D:537:GLU:O | 4:9:350:SER:N | 2.16 | 0.79 |
| 1:A:797:PHE:HE1 | 3:C:146:ILE:HA | 1.45 | 0.79 |
| 1:D:407:GLY:HA2 | 1:D:412:ALA:HA | 1.65 | 0.79 |
| 1:D:713:SER:HG | 1:D:771:LEU:CD2 | 1.94 | 0.79 |
| 2:E:141:PRO:CB | 2:E:142:PRO:HD2 | 2.12 | 0.79 |
| 1:G:291:ILE:HA | 1:G:331:LEU:HD11 | 1.64 | 0.79 |
| 1:G:409:GLY:N | 1:G:636:LYS:CG | 2.44 | 0.79 |
| 3:I:49:ILE:N | 3:I:52:ASN:ND2 | 2.29 | 0.79 |
| 1:J:818:TYR:CD1 | 2:K:127:ARG:NH1 | 2.50 | 0.79 |
| 1:M:642:LYS:HG2 | 4:Z:22:ALA:HA | 1.65 | 0.79 |
| 1:M:805:ALA:HA | 1:M:808:GLU:HB2 | 1.64 | 0.79 |
| 1:M:550:PHE:HA | 4:2:46:GLY:HA2 | 1.64 | 0.79 |
| 1:A:291:ILE:HA | 1:A:331:LEU:HD11 | 1.64 | 0.79 |
| 1:A:831:TRP:HZ3 | 2:B:50:THR:CG2 | 1.95 | 0.79 |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:HD12 | 0.81 | 0.79 |
| 1:D:724:TYR:HB3 | 1:D:782:MLY:NZ | 1.99 | 0.79 |
| 1:G:791:GLN:NE2 | 3:I:116:GLU:H | 1.81 | 0.79 |
| 1:S:505:MLY:HH21 | 1:S:762:HIS:CD2 | 2.17 | 0.79 |
| 1:S:795:ARG:HB2 | 3:U:35:ARG:HH12 | 1.45 | 0.79 |
| 3:U:49:ILE:N | 3:U:52:ASN:ND2 | 2.29 | 0.79 |
| 4:V:223:PHE:HE1 | 4:V:255:PHE:HB2 | 1.46 | 0.79 |
| 4:X:291:LYS:HE2 | 4:Z:243:PRO:O | 1.82 | 0.79 |
| 1:A:642:LYS:HG2 | 4:8:22:ALA:HA | 1.65 | 0.78 |
| 1:A:174:SER:CB | 1:A:667:THR:HG21 | 2.13 | 0.78 |
| 1:A:407:GLY:HA2 | 1:A:412:ALA:HA | 1.65 | 0.78 |
| 2:K:117:LEU:HB2 | 2:K:147:ASN:HD21 | 1.47 | 0.78 |
| 4:8:287:ILE:HB | 4:V:204:ALA:N | 1.97 | 0.78 |
| 1:A:505:MLY:H | 1:A:762:HIS:CD2 | 1.97 | 0.78 |
| 1:D:641:LYS:CE | 1:D:647:GLN:HB2 | 2.13 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:726:VAL:HG12 | 1:D:785:GLU:HG3 | 1.61 | 0.78 |
| 1:D:732:ILE:CD1 | 1:D:782:MLY:HH13 | 2.13 | 0.78 |
| 1:J:174:SER:CB | 1:J:667:THR:HG21 | 2.13 | 0.78 |
| 1:J:820:VAL:CG1 | 2:K:136:MET:HE1 | 2.12 | 0.78 |
| 1:M:409:GLY:N | 1:M:636:LYS:CG | 2.44 | 0.78 |
| 1:S:529:PRO:C | 4:2:354:GLN:CB | 2.49 | 0.78 |
| 1:S:537:GLU:O | 4:2:350:SER:N | 2.16 | 0.78 |
| 1:M:553:MLY:NZ | 4:2:45:VAL:HA | 1.84 | 0.78 |
| 3:F:50:LEU:C | 3:F:53:PRO:HD2 | 2.03 | 0.78 |
| 1:G:754:ASP:CG | 1:G:776:GLU:HA | 2.03 | 0.78 |
| 1:G:757:GLN:CG | 1:G:776:GLU:HG3 | 2.03 | 0.78 |
| 1:G:823:PHE:CE1 | 2:H:156:VAL:O | 2.37 | 0.78 |
| 1:J:538:GLU:HG3 | 4:W:351:THR:C | 2.03 | 0.78 |
| 4:2:166:TYR:HE2 | 4:4:64:ILE:HG21 | 1.48 | 0.78 |
| 1:A:538:GLU:HG3 | 4:8:351:THR:C | 2.03 | 0.78 |
| 2:B:141:PRO:HB2 | 2:B:142:PRO:CD | 2.12 | 0.78 |
| 1:D:769:ALA:C | 1:D:774:LEU:CB | 2.48 | 0.78 |
| 1:D:836:PHE:CE1 | 2:E:159:HIS:CA | 2.66 | 0.78 |
| 1:G:817:GLN:HB3 | 2:H:127:ARG:CD | 2.14 | 0.78 |
| 1:J:639:GLY:CA | 4:W:345:ILE:N | 2.47 | 0.78 |
| 1:M:97:LEU:CD2 | 1:M:712:PRO:CB | 2.61 | 0.78 |
| 1:S:642:LYS:HG2 | 4:2:22:ALA:HA | 1.65 | 0.78 |
| 4:4:223:PHE:HE1 | 4:4:255:PHE:HB2 | 1.46 | 0.78 |
| 1:D:174:SER:CB | 1:D:667:THR:HG21 | 2.13 | 0.78 |
| 1:D:836:PHE:CE2 | 2:E:160:GLY:C | 2.57 | 0.78 |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:CD1 | 2.10 | 0.78 |
| 1:D:823:PHE:CE1 | 2:E:156:VAL:CG1 | 2.67 | 0.78 |
| 1:G:646:PHE:HE2 | 1:G:652:LEU:CD2 | 1.97 | 0.78 |
| 1:S:839:MLY:HD2 | 2:T:159:HIS:HB3 | 1.66 | 0.78 |
| 4:X:291:LYS:CE | 4:Z:243:PRO:CA | 2.61 | 0.78 |
| 1:M:530:MET:HE3 | 4:Z:354:GLN:HG2 | 1.65 | 0.78 |
| 1:D:639:GLY:CA | 4:9:345:ILE:N | 2.47 | 0.78 |
| 1:A:219:GLU:O | 1:A:223:ILE:HG13 | 1.84 | 0.78 |
| 1:A:537:GLU:O | 4:8:350:SER:N | 2.16 | 0.78 |
| 1:A:639:GLY:CA | 4:8:345:ILE:N | 2.47 | 0.78 |
| 1:D:649:VAL:C | 1:D:649:VAL:HG12 | 1.98 | 0.78 |
| 1:G:219:GLU:O | 1:G:223:ILE:HG13 | 1.84 | 0.78 |
| 1:G:537:GLU:O | 4:V:350:SER:N | 2.16 | 0.78 |
| 1:G:801:VAL:HG21 | 3:I:126:LEU:HD23 | 1.64 | 0.78 |
| 1:J:409:GLY:N | 1:J:636:LYS:CG | 2.44 | 0.78 |
| 1:J:646:PHE:HE2 | 1:J:652:LEU:CD2 | 1.97 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:797:PHE:CE2 | 3:L:126:LEU:HD13 | 2.19 | 0.78 |
| 1:M:51:THR:O | 1:M:62:VAL:HG13 | 1.84 | 0.78 |
| 1:M:538:GLU:HG3 | 4:Z:351:THR:C | 2.03 | 0.78 |
| 1:S:646:PHE:HE2 | 1:S:652:LEU:CD2 | 1.97 | 0.78 |
| 1:S:731:ALA:HB1 | 3:U:93:VAL:CA | 2.14 | 0.78 |
| 1:S:753:VAL:HG13 | 1:S:779:ARG:NH1 | 1.98 | 0.78 |
| 4:2:173:HIS:CD2 | 4:3:268:GLY:HA3 | 2.18 | 0.78 |
| 4:3:287:ILE:HG23 | 4:5:202:THR:HG1 | 1.47 | 0.78 |
| 4:7:287:ILE:HB | 4:9:204:ALA:N | 1.98 | 0.78 |
| 1:A:498:LEU:HD21 | 1:A:764:MLY:HH22 | 1.66 | 0.78 |
| 1:D:51:THR:O | 1:D:62:VAL:HG13 | 1.84 | 0.78 |
| 1:G:817:GLN:HG3 | 2:H:128:PHE:CE1 | 2.19 | 0.78 |
| 1:J:756:THR:HG21 | 1:J:779:ARG:HB3 | 1.65 | 0.78 |
| 1:M:819:ASN:CG | 2:N:90:GLY:O | 2.22 | 0.78 |
| 3:O:50:LEU:C | 3:O:53:PRO:HD2 | 2.03 | 0.78 |
| 1:S:537:GLU:HG3 | 4:2:350:SER:O | 1.78 | 0.78 |
| 1:S:641:LYS:HD2 | 1:S:647:GLN:OE1 | 1.81 | 0.78 |
| 1:S:803:TYR:CE2 | 3:U:17:PHE:CZ | 2.72 | 0.78 |
| 4:9:287:ILE:HB | 4:W:204:ALA:N | 1.97 | 0.78 |
| 1:J:642:LYS:CG | 4:W:23:GLY:H | 1.77 | 0.78 |
| 1:A:530:MET:CG | 4:8:354:GLN:CB | 2.30 | 0.78 |
| 1:A:550:PHE:HA | 4:V:46:GLY:HA2 | 1.65 | 0.78 |
| 1:A:646:PHE:HE2 | 1:A:652:LEU:CD2 | 1.97 | 0.78 |
| 1:A:834:LEU:HD21 | 2:B:54:MET:SD | 2.21 | 0.78 |
| 2:B:121:LEU:CG | 2:B:128:PHE:HA | 2.14 | 0.78 |
| 2:B:117:LEU:HB2 | 2:B:147:ASN:HD21 | 1.47 | 0.78 |
| 1:D:481:ASN:N | 1:D:481:ASN:HD22 | 1.82 | 0.78 |
| 1:D:646:PHE:HE2 | 1:D:652:LEU:CD2 | 1.97 | 0.78 |
| 1:D:799:MET:SD | 3:F:32:ASP:CG | 2.63 | 0.78 |
| 1:G:641:LYS:CE | 1:G:647:GLN:HB2 | 2.13 | 0.78 |
| 1:G:736:GLN:CA | 1:G:743:ALA:HB2 | 1.95 | 0.78 |
| 1:M:219:GLU:O | 1:M:223:ILE:HG13 | 1.84 | 0.78 |
| 1:M:537:GLU:O | 4:Z:350:SER:N | 2.16 | 0.78 |
| 1:S:753:VAL:CG1 | 1:S:779:ARG:NH1 | 2.47 | 0.78 |
| 3:C:3:SER:O | 3:C:4:LYS:HB2 | 1.84 | 0.78 |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG12 | 1.66 | 0.78 |
| 1:G:496:PHE:CD2 | 1:G:514:ASP:HA | 2.19 | 0.78 |
| 1:G:642:LYS:HG2 | 4:V:22:ALA:HA | 1.65 | 0.78 |
| 1:S:51:THR:O | 1:S:62:VAL:HG13 | 1.84 | 0.78 |
| 1:S:84:MLY:NZ | 1:S:724:TYR:HE2 | 1.82 | 0.78 |
| 4:1:223:PHE:HD2 | 4:1:312:ARG:HH21 | 1.33 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:538:GLU:HG3 | 4:9:351:THR:C | 2.03 | 0.77 |
| 1:A:51:THR:O | 1:A:62:VAL:HG13 | 1.84 | 0.77 |
| 1:A:641:LYS:CE | 1:A:647:GLN:HB2 | 2.13 | 0.77 |
| 1:D:641:LYS:CE | 1:D:647:GLN:CG | 2.60 | 0.77 |
| 1:D:712:PRO:CB | 1:D:771:LEU:CB | 2.62 | 0.77 |
| 1:G:174:SER:CB | 1:G:667:THR:HG21 | 2.13 | 0.77 |
| 1:G:836:PHE:CZ | 2:H:159:HIS:HA | 2.17 | 0.77 |
| 1:M:639:GLY:CA | 4:Z:345:ILE:N | 2.46 | 0.77 |
| 1:M:783:LEU:CD2 | 1:M:786:ILE:HD11 | 2.10 | 0.77 |
| 1:M:795:ARG:HG2 | 3:O:118:MET:SD | 2.23 | 0.77 |
| 1:S:496:PHE:CD2 | 1:S:514:ASP:HA | 2.19 | 0.77 |
| 1:A:553:MLY:NZ | 4:V:45:VAL:HA | 1.84 | 0.77 |
| 1:A:496:PHE:CD2 | 1:A:514:ASP:HA | 2.19 | 0.77 |
| 3:C:49:ILE:N | 3:C:52:ASN:HD22 | 1.82 | 0.77 |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD13 | 0.91 | 0.77 |
| 1:D:795:ARG:HB3 | 3:F:35:ARG:NH2 | 1.98 | 0.77 |
| 1:G:218:LEU:HA | 1:G:221:GLN:HG2 | 1.62 | 0.77 |
| 1:J:51:THR:O | 1:J:62:VAL:HG13 | 1.84 | 0.77 |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:HD13 | 1.59 | 0.77 |
| 2:K:150:TYR:C | 2:K:151:LYS:CG | 2.48 | 0.77 |
| 1:M:641:LYS:CE | 1:M:647:GLN:HB2 | 2.13 | 0.77 |
| 1:M:732:ILE:CG2 | 1:M:747:LEU:HD13 | 1.34 | 0.77 |
| 1:M:786:ILE:C | 1:M:787:ILE:CA | 2.51 | 0.77 |
| 1:S:538:GLU:OE2 | 4:2:355:MET:HE3 | 1.80 | 0.77 |
| 3:U:49:ILE:N | 3:U:52:ASN:HD22 | 1.82 | 0.77 |
| 4:Y:223:PHE:HD2 | 4:Y:312:ARG:HH21 | 1.33 | 0.77 |
| 4:5:223:PHE:HD2 | 4:5:312:ARG:HH21 | 1.32 | 0.77 |
| 4:9:223:PHE:HD2 | 4:9:312:ARG:HH21 | 1.33 | 0.77 |
| 1:D:635:GLY:HA3 | 4:9:341:ILE:CD1 | 2.14 | 0.77 |
| 1:D:831:TRP:CH2 | 2:E:34:ILE:HG23 | 2.18 | 0.77 |
| 1:D:795:ARG:HD2 | 3:F:35:ARG:HH12 | 1.49 | 0.77 |
| 1:G:407:GLY:HA2 | 1:G:412:ALA:HA | 1.65 | 0.77 |
| 1:J:219:GLU:O | 1:J:223:ILE:HG13 | 1.84 | 0.77 |
| 1:M:496:PHE:CD2 | 1:M:514:ASP:HA | 2.19 | 0.77 |
| 1:M:798:LEU:HD13 | 3:O:126:LEU:HD11 | 1.67 | 0.77 |
| 4:W:223:PHE:HD2 | 4:W:312:ARG:HH21 | 1.33 | 0.77 |
| 1:J:635:GLY:HA3 | 4:W:341:ILE:CD1 | 2.14 | 0.77 |
| 4:1:324:THR:HG23 | 4:3:244:ASP:HA | 1.67 | 0.77 |
| 1:A:642:LYS:CG | 4:8:23:GLY:H | 1.77 | 0.77 |
| 4:8:223:PHE:HD2 | 4:8:312:ARG:HH21 | 1.33 | 0.77 |
| 1:D:557:GLU:N | 4:W:48:GLY:HA2 | 1.90 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:795:ARG:HE | 3:F:116:GLU:HB3 | 1.50 | 0.77 |
| 1:G:51:THR:O | 1:G:62:VAL:HG13 | 1.84 | 0.77 |
| 1:G:725:ARG:HG3 | 1:G:733:PRO:HA | 1.67 | 0.77 |
| 1:G:733:PRO:C | 1:G:737:PHE:HD1 | 1.88 | 0.77 |
| 1:J:407:GLY:HA2 | 1:J:412:ALA:HA | 1.65 | 0.77 |
| 1:J:735:GLY:C | 1:J:743:ALA:HB2 | 1.82 | 0.77 |
| 1:J:84:MLY:CH2 | 1:J:720:PHE:N | 2.48 | 0.77 |
| 1:M:506:GLU:OE2 | 1:M:761:GLY:HA3 | 1.84 | 0.77 |
| 1:M:817:GLN:CB | 2:N:127:ARG:CD | 2.50 | 0.77 |
| 1:S:116:TYR:O | 1:S:153:PRO:HB2 | 1.85 | 0.77 |
| 4:4:287:ILE:HG13 | 4:6:202:THR:CB | 2.12 | 0.77 |
| 1:J:821:ARG:HH21 | 2:K:127:ARG:HG2 | 1.50 | 0.77 |
| 1:M:635:GLY:HA3 | 4:Z:341:ILE:CD1 | 2.14 | 0.77 |
| 1:M:795:ARG:CB | 3:O:35:ARG:NH2 | 2.37 | 0.77 |
| 1:S:218:LEU:HD22 | 1:S:222:ILE:HG12 | 1.67 | 0.77 |
| 1:S:538:GLU:HG3 | 4:2:351:THR:C | 2.03 | 0.77 |
| 1:S:783:LEU:HA | 1:S:786:ILE:HG12 | 1.61 | 0.77 |
| 4:3:223:PHE:HD2 | 4:3:312:ARG:HH21 | 1.33 | 0.77 |
| 1:A:817:GLN:NE2 | 2:B:127:ARG:CD | 2.47 | 0.77 |
| 1:M:646:PHE:HE2 | 1:M:652:LEU:CD2 | 1.97 | 0.77 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:CD1 | 2.63 | 0.77 |
| 3:O:3:SER:O | 3:O:4:LYS:HB2 | 1.85 | 0.77 |
| 4:V:223:PHE:HD2 | 4:V:312:ARG:HH21 | 1.33 | 0.77 |
| 4:X:223:PHE:HD2 | 4:X:312:ARG:HH21 | 1.32 | 0.77 |
| 1:A:116:TYR:O | 1:A:153:PRO:HB2 | 1.85 | 0.77 |
| 1:A:499:GLU:OE2 | 1:A:766:PHE:CE2 | 2.38 | 0.77 |
| 1:A:502:GLU:C | 1:A:761:GLY:CA | 2.53 | 0.77 |
| 1:D:94:MET:CE | 1:D:101:ALA:HB1 | 2.15 | 0.77 |
| 1:D:166:MET:HE3 | 1:D:254:PHE:CD2 | 2.20 | 0.77 |
| 1:D:795:ARG:NE | 3:F:43:ASN:OD1 | 2.18 | 0.77 |
| 1:G:834:LEU:CD1 | 2:H:51:PHE:HE1 | 1.95 | 0.77 |
| 3:L:49:ILE:N | 3:L:52:ASN:HD22 | 1.83 | 0.77 |
| 1:S:641:LYS:CE | 1:S:647:GLN:HB2 | 2.13 | 0.77 |
| 1:S:783:LEU:HA | 1:S:786:ILE:CD1 | 2.14 | 0.77 |
| 1:S:826:VAL:HG21 | 2:T:88:LEU:CD2 | 2.15 | 0.77 |
| 1:S:838:ILE:HD11 | 2:T:54:MET:HE1 | 1.61 | 0.77 |
| 1:A:557:GLU:N | 4:V:48:GLY:HA3 | 1.90 | 0.77 |
| 4:1:201:VAL:O | 4:Y:287:ILE:HD11 | 1.75 | 0.77 |
| 4:7:223:PHE:HD2 | 4:7:312:ARG:HH21 | 1.33 | 0.77 |
| 3:C:50:LEU:C | 3:C:53:PRO:HD2 | 2.03 | 0.77 |
| 1:D:496:PHE:CD2 | 1:D:514:ASP:HA | 2.19 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:822:SER:OG | 2:E:88:LEU:CD2 | 2.33 | 0.77 |
| 1:G:503:TYR:CE1 | 1:G:711:PHE:CD2 | 2.72 | 0.77 |
| 1:J:641:LYS:CE | 1:J:647:GLN:HB2 | 2.13 | 0.77 |
| 1:J:641:LYS:CE | 1:J:647:GLN:CG | 2.60 | 0.77 |
| 1:J:710:GLY:O | 1:J:772:LEU:CB | 2.33 | 0.77 |
| 1:M:116:TYR:O | 1:M:153:PRO:HB2 | 1.85 | 0.77 |
| 1:M:93:MET:HG2 | 1:M:714:ARG:O | 1.84 | 0.77 |
| 1:S:219:GLU:O | 1:S:223:ILE:HG13 | 1.84 | 0.77 |
| 1:S:721:LYS:CA | 1:S:736:GLN:OE1 | 2.33 | 0.77 |
| 4:V:287:ILE:HD11 | 4:X:201:VAL:O | 1.75 | 0.77 |
| 1:S:639:GLY:CA | 4:2:345:ILE:N | 2.47 | 0.77 |
| 1:A:732:ILE:N | 1:A:733:PRO:HD2 | 2.00 | 0.77 |
| 1:D:623:PHE:CA | 1:D:623:PHE:CG | 2.68 | 0.77 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:HD22 | 2.20 | 0.77 |
| 2:E:163:ALA:C | 2:K:21:GLU:HB3 | 2.05 | 0.77 |
| 3:F:3:SER:O | 3:F:4:LYS:HB2 | 1.84 | 0.77 |
| 3:F:49:ILE:N | 3:F:52:ASN:HD22 | 1.82 | 0.77 |
| 1:G:116:TYR:O | 1:G:153:PRO:HB2 | 1.85 | 0.77 |
| 1:J:496:PHE:CD2 | 1:J:514:ASP:HA | 2.19 | 0.77 |
| 1:J:623:PHE:CA | 1:J:623:PHE:CG | 2.68 | 0.77 |
| 1:J:829:TRP:CZ3 | 2:K:84:PHE:CE1 | 2.73 | 0.77 |
| 1:M:819:ASN:OD1 | 2:N:92:ASP:CA | 2.32 | 0.77 |
| 1:S:407:GLY:HA2 | 1:S:412:ALA:HA | 1.65 | 0.77 |
| 1:A:797:PHE:CG | 3:C:146:ILE:HG23 | 2.20 | 0.77 |
| 1:D:116:TYR:O | 1:D:153:PRO:HB2 | 1.85 | 0.77 |
| 1:J:94:MET:CE | 1:J:101:ALA:HB1 | 2.16 | 0.77 |
| 1:J:218:LEU:HB2 | 1:J:221:GLN:CG | 2.09 | 0.77 |
| 2:K:121:LEU:CG | 2:K:128:PHE:HA | 2.14 | 0.77 |
| 1:M:646:PHE:CE2 | 1:M:652:LEU:HD21 | 2.15 | 0.77 |
| 1:M:725:ARG:HG3 | 1:M:733:PRO:HA | 1.67 | 0.77 |
| 1:M:838:ILE:CD1 | 2:N:54:MET:CE | 2.51 | 0.77 |
| 1:S:635:GLY:HA3 | 4:2:341:ILE:CD1 | 2.14 | 0.77 |
| 4:3:287:ILE:HG21 | 4:5:202:THR:C | 2.06 | 0.76 |
| 1:A:218:LEU:HB3 | 1:A:221:GLN:HG3 | 1.61 | 0.76 |
| 1:A:795:ARG:CB | 3:C:35:ARG:NH2 | 2.45 | 0.76 |
| 1:J:721:LYS:CA | 1:J:736:GLN:OE1 | 2.33 | 0.76 |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:CG | 1.98 | 0.76 |
| 1:M:95:THR:CA | 1:M:713:SER:CB | 2.48 | 0.76 |
| 4:Z:223:PHE:HD2 | 4:Z:312:ARG:HH21 | 1.32 | 0.76 |
| 1:A:635:GLY:HA3 | 4:8:341:ILE:CD1 | 2.14 | 0.76 |
| 1:A:481:ASN:N | 1:A:481:ASN:HD22 | 1.82 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:529:PRO:C | 4:8:354:GLN:CB | 2.49 | 0.76 |
| 1:A:725:ARG:HG3 | 1:A:733:PRO:HA | 1.67 | 0.76 |
| 1:A:752:ASP:CG | 1:A:782:MLY:HD3 | 2.05 | 0.76 |
| 1:A:830:PRO:HG2 | 2:B:67:MET:CE | 2.15 | 0.76 |
| 1:D:534:SER:O | 4:9:351:THR:N | 2.19 | 0.76 |
| 1:G:639:GLY:CA | 4:V:345:ILE:N | 2.47 | 0.76 |
| 1:G:599:ASN:CA | 1:G:649:VAL:CB | 2.53 | 0.76 |
| 2:H:121:LEU:CG | 2:H:128:PHE:HA | 2.14 | 0.76 |
| 1:J:836:PHE:CE1 | 2:K:160:GLY:N | 2.53 | 0.76 |
| 1:M:836:PHE:CZ | 2:N:159:HIS:HA | 2.17 | 0.76 |
| 1:S:646:PHE:CE2 | 1:S:652:LEU:HD21 | 2.14 | 0.76 |
| 4:1:287:ILE:CG1 | 4:3:202:THR:CB | 2.63 | 0.76 |
| 1:A:94:MET:CE | 1:A:101:ALA:HB1 | 2.15 | 0.76 |
| 1:A:629:GLU:HA | 1:A:643:GLY:C | 2.05 | 0.76 |
| 1:A:797:PHE:CD1 | 3:C:149:VAL:CG1 | 2.69 | 0.76 |
| 1:G:94:MET:CE | 1:G:101:ALA:HB1 | 2.15 | 0.76 |
| 1:G:97:LEU:HD22 | 1:G:712:PRO:HB3 | 1.65 | 0.76 |
| 1:G:795:ARG:HB2 | 3:I:35:ARG:NH1 | 1.99 | 0.76 |
| 1:J:481:ASN:N | 1:J:481:ASN:HD22 | 1.82 | 0.76 |
| 1:J:642:LYS:HG2 | 4:W:22:ALA:HA | 1.65 | 0.76 |
| 1:J:817:GLN:CG | 2:K:127:ARG:CB | 2.40 | 0.76 |
| 1:M:623:PHE:CG | 1:M:623:PHE:CA | 2.68 | 0.76 |
| 1:M:732:ILE:N | 1:M:733:PRO:HD2 | 2.00 | 0.76 |
| 4:3:324:THR:CB | 4:5:244:ASP:CA | 2.48 | 0.76 |
| 1:D:530:MET:CG | 4:9:354:GLN:CB | 2.30 | 0.76 |
| 1:A:599:ASN:CA | 1:A:649:VAL:CB | 2.54 | 0.76 |
| 1:D:219:GLU:O | 1:D:223:ILE:HG13 | 1.84 | 0.76 |
| 1:D:791:GLN:CD | 3:F:116:GLU:N | 2.25 | 0.76 |
| 1:M:107:MLY:HB3 | 1:M:686:MET:HE2 | 1.67 | 0.76 |
| 4:2:202:THR:CG2 | 4:Z:290:ARG:NH1 | 2.49 | 0.76 |
| 1:A:505:MLY:HG3 | 1:A:741:LYS:HZ3 | 1.48 | 0.76 |
| 1:J:116:TYR:O | 1:J:153:PRO:HB2 | 1.85 | 0.76 |
| 1:J:792:ALA:HA | 3:L:42:THR:HA | 1.65 | 0.76 |
| 1:M:721:LYS:CA | 1:M:736:GLN:OE1 | 2.33 | 0.76 |
| 1:M:816:ILE:HD11 | 2:N:100:ALA:HB1 | 1.66 | 0.76 |
| 1:M:94:MET:CE | 1:M:101:ALA:HB1 | 2.15 | 0.76 |
| 1:S:793:ARG:HH11 | 3:U:40:ASN:CB | 1.98 | 0.76 |
| 4:1:287:ILE:HG21 | 4:3:202:THR:C | 2.06 | 0.76 |
| 4:2:223:PHE:HD2 | 4:2:312:ARG:HH21 | 1.32 | 0.76 |
| 4:4:223:PHE:HD2 | 4:4:312:ARG:HH21 | 1.33 | 0.76 |
| 4:6:223:PHE:HD2 | 4:6:312:ARG:HH21 | 1.33 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:725:ARG:HG3 | 1:D:733:PRO:HA | 1.68 | 0.76 |
| 1:D:724:TYR:CD1 | 1:D:782:MLY:CD | 2.69 | 0.76 |
| 1:G:537:GLU:HG3 | 4:V:350:SER:O | 1.79 | 0.76 |
| 1:G:664:LEU:O | 1:G:667:THR:HB | 1.86 | 0.76 |
| 1:J:817:GLN:CB | 2:K:127:ARG:HH11 | 1.99 | 0.76 |
| 1:M:641:LYS:CE | 1:M:647:GLN:CG | 2.61 | 0.76 |
| 1:M:733:PRO:C | 1:M:737:PHE:HD1 | 1.88 | 0.76 |
| 1:M:805:ALA:O | 1:M:809:ARG:N | 2.18 | 0.76 |
| 1:M:831:TRP:CZ2 | 2:N:47:LEU:HD22 | 2.20 | 0.76 |
| 1:S:725:ARG:HG3 | 1:S:733:PRO:HA | 1.67 | 0.76 |
| 3:U:3:SER:O | 3:U:4:LYS:HB2 | 1.84 | 0.76 |
| 4:1:287:ILE:CD1 | 4:3:203:THR:N | 2.48 | 0.76 |
| 4:9:290:ARG:NH1 | 4:W:202:THR:CG2 | 2.49 | 0.76 |
| 1:A:721:LYS:CA | 1:A:736:GLN:OE1 | 2.33 | 0.76 |
| 1:D:642:LYS:HG2 | 4:9:22:ALA:HA | 1.65 | 0.76 |
| 1:D:712:PRO:CD | 1:D:771:LEU:HD13 | 2.15 | 0.76 |
| 1:G:817:GLN:NE2 | 2:H:127:ARG:HB2 | 2.00 | 0.76 |
| 1:S:831:TRP:HZ3 | 2:T:34:ILE:HD13 | 1.51 | 0.76 |
| 2:T:117:LEU:HB2 | 2:T:147:ASN:HD21 | 1.47 | 0.76 |
| 4:1:288:ASP:N | 4:3:203:THR:CG2 | 2.48 | 0.76 |
| 1:M:649:VAL:CB | 1:M:649:VAL:CG1 | 2.64 | 0.76 |
| 1:M:836:PHE:CD2 | 2:N:160:GLY:N | 2.50 | 0.76 |
| 3:O:49:ILE:N | 3:O:52:ASN:HD22 | 1.82 | 0.76 |
| 1:S:838:ILE:CD1 | 2:T:54:MET:HE3 | 2.11 | 0.76 |
| 4:8:290:ARG:NH1 | 4:V:202:THR:CG2 | 2.49 | 0.76 |
| 4:2:202:THR:HG23 | 4:Z:290:ARG:HH22 | 1.50 | 0.76 |
| 1:A:836:PHE:HZ | 2:B:160:GLY:H | 1.28 | 0.76 |
| 1:D:218:LEU:HB2 | 1:D:221:GLN:CG | 2.09 | 0.76 |
| 1:D:649:VAL:CB | 1:D:649:VAL:CG1 | 2.64 | 0.76 |
| 1:D:721:LYS:CA | 1:D:736:GLN:OE1 | 2.33 | 0.76 |
| 1:G:623:PHE:CG | 1:G:623:PHE:CA | 2.69 | 0.76 |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG12 | 1.67 | 0.76 |
| 1:J:725:ARG:HG3 | 1:J:733:PRO:HA | 1.67 | 0.76 |
| 1:M:534:SER:O | 4:Z:351:THR:N | 2.19 | 0.76 |
| 1:M:636:LYS:O | 1:M:637:LYS:HB2 | 1.86 | 0.76 |
| 1:M:664:LEU:O | 1:M:667:THR:HB | 1.86 | 0.76 |
| 1:S:534:SER:O | 4:2:351:THR:N | 2.19 | 0.76 |
| 1:S:732:ILE:N | 1:S:733:PRO:HD2 | 2.00 | 0.76 |
| 1:S:836:PHE:CE1 | 2:T:160:GLY:H | 1.43 | 0.76 |
| 1:S:797:PHE:CE1 | 3:U:146:ILE:CA | 2.69 | 0.76 |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG12 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:635:GLY:HA3 | 4:V:341:ILE:CD1 | 2.14 | 0.76 |
| 1:A:149:GLN:CB | 1:A:719:ASP:N | 2.49 | 0.75 |
| 1:A:818:TYR:HB2 | 2:B:90:GLY:HA3 | 1.65 | 0.75 |
| 1:G:649:VAL:CB | 1:G:649:VAL:CG1 | 2.64 | 0.75 |
| 1:G:721:LYS:CA | 1:G:736:GLN:OE1 | 2.33 | 0.75 |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CB | 1.85 | 0.75 |
| 1:G:732:ILE:N | 1:G:733:PRO:HD2 | 2.00 | 0.75 |
| 1:G:754:ASP:N | 1:G:779:ARG:HD3 | 2.01 | 0.75 |
| 1:G:757:GLN:CB | 1:G:776:GLU:CG | 2.63 | 0.75 |
| 1:G:795:ARG:HA | 3:I:118:MET:CE | 2.16 | 0.75 |
| 1:J:736:GLN:CA | 1:J:743:ALA:HB2 | 1.95 | 0.75 |
| 1:M:97:LEU:HD23 | 1:M:712:PRO:HB3 | 1.66 | 0.75 |
| 1:M:95:THR:OG1 | 1:M:770:GLY:N | 2.20 | 0.75 |
| 1:S:636:LYS:O | 1:S:637:LYS:HB2 | 1.86 | 0.75 |
| 1:S:649:VAL:CG1 | 1:S:649:VAL:CB | 2.64 | 0.75 |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG12 | 1.67 | 0.75 |
| 1:D:732:ILE:N | 1:D:733:PRO:HD2 | 2.00 | 0.75 |
| 1:G:218:LEU:HB2 | 1:G:221:GLN:CG | 2.09 | 0.75 |
| 1:S:792:ALA:HB2 | 3:U:42:THR:HA | 1.45 | 0.75 |
| 1:A:623:PHE:CG | 1:A:623:PHE:CA | 2.68 | 0.75 |
| 1:D:798:LEU:HD12 | 3:F:126:LEU:HD21 | 1.68 | 0.75 |
| 1:G:636:LYS:O | 1:G:637:LYS:HB2 | 1.86 | 0.75 |
| 1:G:817:GLN:OE1 | 2:H:127:ARG:CD | 2.29 | 0.75 |
| 1:G:832:MET:SD | 2:H:84:PHE:CE2 | 2.74 | 0.75 |
| 2:H:114:LYS:HA | 2:H:146:GLY:C | 2.02 | 0.75 |
| 2:H:111:SER:OG | 2:H:148:VAL:C | 2.15 | 0.75 |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:HG12 | 1.67 | 0.75 |
| 1:S:664:LEU:O | 1:S:667:THR:HB | 1.86 | 0.75 |
| 1:G:534:SER:O | 4:V:351:THR:N | 2.20 | 0.75 |
| 4:X:287:ILE:CG1 | 4:Z:201:VAL:CG2 | 2.63 | 0.75 |
| 1:A:641:LYS:CE | 1:A:647:GLN:CG | 2.60 | 0.75 |
| 1:A:649:VAL:CB | 1:A:649:VAL:CG1 | 2.64 | 0.75 |
| 1:D:732:ILE:CD1 | 1:D:782:MLY:HH21 | 2.16 | 0.75 |
| 1:G:529:PRO:C | 4:V:354:GLN:CB | 2.50 | 0.75 |
| 1:J:664:LEU:O | 1:J:667:THR:HB | 1.86 | 0.75 |
| 1:J:732:ILE:N | 1:J:733:PRO:HD2 | 2.01 | 0.75 |
| 3:L:3:SER:O | 3:L:4:LYS:HB2 | 1.85 | 0.75 |
| 1:M:350:ALA:O | 1:M:354:LEU:HB2 | 1.87 | 0.75 |
| 1:M:641:LYS:HD2 | 1:M:647:GLN:OE1 | 1.81 | 0.75 |
| 1:S:819:ASN:HA | 2:T:90:GLY:C | 2.02 | 0.75 |
| 1:S:831:TRP:CZ2 | 2:T:47:LEU:CD2 | 2.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:94:MET:CE | 1:S:101:ALA:HB1 | 2.15 | 0.75 |
| 1:G:530:MET:HE2 | 4:V:354:GLN:HG3 | 1.67 | 0.75 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:CD2 | 2.69 | 0.75 |
| 1:G:481:ASN:HD22 | 1:G:481:ASN:N | 1.82 | 0.75 |
| 1:J:629:GLU:HA | 1:J:643:GLY:C | 2.05 | 0.75 |
| 1:M:538:GLU:CD | 4:Z:355:MET:HE3 | 2.07 | 0.75 |
| 1:S:350:ALA:O | 1:S:354:LEU:HB2 | 1.87 | 0.75 |
| 1:S:623:PHE:CG | 1:S:623:PHE:CA | 2.68 | 0.75 |
| 1:S:803:TYR:O | 1:S:807:VAL:HG23 | 1.86 | 0.75 |
| 2:T:111:SER:OG | 2:T:148:VAL:C | 2.15 | 0.75 |
| 4:8:288:ASP:H | 4:V:203:THR:HG22 | 1.52 | 0.75 |
| 4:2:287:ILE:CG2 | 4:4:203:THR:H | 2.00 | 0.75 |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CD2 | 2.16 | 0.75 |
| 1:A:838:ILE:CD1 | 2:B:54:MET:SD | 2.74 | 0.75 |
| 2:E:121:LEU:CG | 2:E:128:PHE:HA | 2.14 | 0.75 |
| 1:G:218:LEU:HB3 | 1:G:221:GLN:HG3 | 1.60 | 0.75 |
| 1:G:410:ASN:CG | 4:V:334:GLU:CA | 2.47 | 0.75 |
| 1:G:817:GLN:HB3 | 2:H:127:ARG:HD3 | 1.67 | 0.75 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CG | 2.17 | 0.75 |
| 1:S:481:ASN:N | 1:S:481:ASN:HD22 | 1.82 | 0.75 |
| 1:G:629:GLU:HA | 1:G:643:GLY:C | 2.05 | 0.75 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:CB | 2.64 | 0.75 |
| 1:M:310:TYR:CE2 | 1:M:320:ILE:HD11 | 2.22 | 0.75 |
| 1:M:836:PHE:CE2 | 2:N:160:GLY:CA | 2.70 | 0.75 |
| 1:S:733:PRO:C | 1:S:737:PHE:HD1 | 1.88 | 0.75 |
| 1:S:796:GLY:HA2 | 3:U:35:ARG:HD3 | 0.76 | 0.75 |
| 4:1:287:ILE:CG2 | 4:3:203:THR:N | 2.49 | 0.75 |
| 1:M:556:ASP:HA | 4:2:49:GLN:O | 1.69 | 0.75 |
| 1:A:664:LEU:O | 1:A:667:THR:HB | 1.86 | 0.75 |
| 1:D:541:MET:O | 4:9:143:TYR:CZ | 2.40 | 0.75 |
| 1:D:793:ARG:NH2 | 3:F:147:MET:HE1 | 2.01 | 0.75 |
| 1:J:769:ALA:HB3 | 1:J:770:GLY:CA | 2.15 | 0.75 |
| 1:S:310:TYR:CE2 | 1:S:320:ILE:HD11 | 2.22 | 0.75 |
| 1:S:95:THR:HA | 1:S:713:SER:HB3 | 1.68 | 0.75 |
| 1:S:819:ASN:OD1 | 2:T:92:ASP:CB | 2.34 | 0.75 |
| 4:4:253:GLU:HA | 4:4:256:ARG:HG3 | 1.69 | 0.75 |
| 4:3:287:ILE:CA | 4:5:202:THR:HB | 2.17 | 0.75 |
| 1:A:215:GLN:NE2 | 1:A:336:SER:O | 2.20 | 0.75 |
| 1:A:218:LEU:HB2 | 1:A:221:GLN:CG | 2.09 | 0.75 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CB | 1.85 | 0.75 |
| 1:G:556:ASP:CG | 4:X:47:MET:HE2 | 1.50 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:757:GLN:CD | 1:G:776:GLU:HG2 | 2.05 | 0.75 |
| 1:M:783:LEU:HA | 1:M:786:ILE:CD1 | 2.13 | 0.75 |
| 1:S:541:MET:O | 4:2:143:TYR:CZ | 2.40 | 0.75 |
| 1:S:783:LEU:O | 1:S:786:ILE:CG1 | 2.33 | 0.75 |
| 1:S:797:PHE:HE1 | 3:U:149:VAL:HG12 | 1.52 | 0.75 |
| 1:S:831:TRP:HE1 | 2:T:67:MET:CB | 1.99 | 0.75 |
| 4:2:203:THR:HG22 | 4:Z:288:ASP:H | 1.52 | 0.75 |
| 4:4:287:ILE:HG21 | 4:6:202:THR:C | 2.06 | 0.74 |
| 4:4:322:PRO:CB | 4:6:244:ASP:HB2 | 2.16 | 0.74 |
| 4:7:253:GLU:HA | 4:7:256:ARG:HG3 | 1.69 | 0.74 |
| 1:A:541:MET:O | 4:8:143:TYR:CZ | 2.40 | 0.74 |
| 1:D:215:GLN:NE2 | 1:D:336:SER:O | 2.20 | 0.74 |
| 1:D:350:ALA:O | 1:D:354:LEU:HB2 | 1.87 | 0.74 |
| 1:D:556:ASP:HA | 4:W:49:GLN:O | 1.70 | 0.74 |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CB | 1.84 | 0.74 |
| 1:G:538:GLU:CD | 4:V:355:MET:HE3 | 2.08 | 0.74 |
| 1:J:538:GLU:O | 4:W:349:LEU:HG | 1.86 | 0.74 |
| 1:J:836:PHE:CE2 | 2:K:160:GLY:N | 2.55 | 0.74 |
| 2:N:117:LEU:HB2 | 2:N:147:ASN:HD21 | 1.47 | 0.74 |
| 1:S:641:LYS:CE | 1:S:647:GLN:CG | 2.61 | 0.74 |
| 1:S:783:LEU:HB3 | 1:S:786:ILE:HD12 | 1.69 | 0.74 |
| 4:9:288:ASP:H | 4:W:203:THR:HG22 | 1.52 | 0.74 |
| 1:D:553:MLY:NZ | 4:W:45:VAL:HA | 1.84 | 0.74 |
| 4:6:253:GLU:HA | 4:6:256:ARG:HG3 | 1.69 | 0.74 |
| 1:A:534:SER:O | 4:8:351:THR:N | 2.18 | 0.74 |
| 1:D:664:LEU:O | 1:D:667:THR:HB | 1.86 | 0.74 |
| 1:G:769:ALA:O | 1:G:773:GLY:CA | 2.35 | 0.74 |
| 1:G:791:GLN:NE2 | 3:I:116:GLU:N | 2.35 | 0.74 |
| 1:G:829:TRP:CH2 | 2:H:87:LYS:CE | 2.68 | 0.74 |
| 3:I:49:ILE:N | 3:I:52:ASN:HD22 | 1.82 | 0.74 |
| 1:J:537:GLU:HG3 | 4:W:350:SER:O | 1.78 | 0.74 |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:HD21 | 1.66 | 0.74 |
| 1:M:541:MET:O | 4:Z:143:TYR:CZ | 2.40 | 0.74 |
| 4:2:253:GLU:HA | 4:2:256:ARG:HG3 | 1.69 | 0.74 |
| 1:A:310:TYR:CE2 | 1:A:320:ILE:HD11 | 2.22 | 0.74 |
| 1:A:436:MLY:HE3 | 1:A:626:TYR:CE1 | 2.23 | 0.74 |
| 1:A:830:PRO:HB2 | 2:B:51:PHE:CZ | 2.22 | 0.74 |
| 2:H:117:LEU:HB2 | 2:H:147:ASN:HD21 | 1.47 | 0.74 |
| 1:J:310:TYR:CE2 | 1:J:320:ILE:HD11 | 2.22 | 0.74 |
| 1:J:272:MLY:HH13 | 1:J:435:GLU:OE1 | 1.88 | 0.74 |
| 1:J:792:ALA:HB2 | 3:L:42:THR:HG22 | 0.95 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:537:GLU:HG3 | 4:Z:350:SER:O | 1.78 | 0.74 |
| 4:X:287:ILE:HG23 | 4:Z:201:VAL:HG23 | 1.68 | 0.74 |
| 1:J:93:MET:CE | 1:J:716:LEU:HD12 | 2.17 | 0.74 |
| 1:M:481:ASN:N | 1:M:481:ASN:HD22 | 1.82 | 0.74 |
| 1:S:215:GLN:NE2 | 1:S:336:SER:O | 2.20 | 0.74 |
| 1:S:751:GLY:C | 3:U:86:ASP:OD1 | 2.25 | 0.74 |
| 2:T:121:LEU:CG | 2:T:128:PHE:HA | 2.14 | 0.74 |
| 1:S:793:ARG:HH11 | 3:U:40:ASN:HB2 | 1.49 | 0.74 |
| 4:W:253:GLU:HA | 4:W:256:ARG:HG3 | 1.69 | 0.74 |
| 1:A:636:LYS:O | 1:A:637:LYS:HB2 | 1.86 | 0.74 |
| 1:A:735:GLY:C | 1:A:743:ALA:HB1 | 1.84 | 0.74 |
| 1:D:486:MLY:HH13 | 1:D:527:GLU:OE1 | 1.88 | 0.74 |
| 1:D:708:ARG:O | 1:D:710:GLY:N | 2.20 | 0.74 |
| 1:D:829:TRP:HZ3 | 2:E:84:PHE:HZ | 1.34 | 0.74 |
| 1:D:797:PHE:CZ | 3:F:126:LEU:HD22 | 2.14 | 0.74 |
| 1:G:310:TYR:CE2 | 1:G:320:ILE:HD11 | 2.22 | 0.74 |
| 1:G:783:LEU:O | 1:G:787:ILE:CB | 2.35 | 0.74 |
| 1:M:629:GLU:HA | 1:M:643:GLY:C | 2.05 | 0.74 |
| 1:M:739:ASP:CB | 1:M:742:LYS:HB3 | 2.12 | 0.74 |
| 1:S:629:GLU:HA | 1:S:643:GLY:C | 2.05 | 0.74 |
| 1:S:795:ARG:NH1 | 3:U:43:ASN:CG | 2.08 | 0.74 |
| 4:Y:253:GLU:HA | 4:Y:256:ARG:HG3 | 1.69 | 0.74 |
| 4:X:287:ILE:HG13 | 4:Z:201:VAL:HG23 | 1.69 | 0.74 |
| 1:A:640:LYS:O | 4:8:23:GLY:O | 2.06 | 0.74 |
| 1:A:538:GLU:O | 4:8:349:LEU:HG | 1.86 | 0.74 |
| 1:A:537:GLU:HG3 | 4:8:350:SER:O | 1.79 | 0.74 |
| 1:A:733:PRO:C | 1:A:737:PHE:HD1 | 1.88 | 0.74 |
| 1:A:834:LEU:HD21 | 2:B:54:MET:HE3 | 1.67 | 0.74 |
| 1:D:436:MLY:HE3 | 1:D:626:TYR:CE1 | 2.23 | 0.74 |
| 3:I:3:SER:O | 3:I:4:LYS:HB2 | 1.84 | 0.74 |
| 1:J:534:SER:O | 4:W:351:THR:N | 2.19 | 0.74 |
| 1:J:541:MET:O | 4:W:143:TYR:CZ | 2.40 | 0.74 |
| 1:J:817:GLN:OE1 | 2:K:127:ARG:HD2 | 1.87 | 0.74 |
| 1:S:735:GLY:C | 1:S:743:ALA:HB2 | 1.82 | 0.74 |
| 1:S:786:ILE:O | 1:S:789:ALA:CB | 2.35 | 0.74 |
| 1:S:798:LEU:HD11 | 3:U:126:LEU:HD22 | 1.60 | 0.74 |
| 1:J:556:ASP:CG | 4:Y:47:MET:HE2 | 1.53 | 0.74 |
| 4:4:322:PRO:CB | 4:6:244:ASP:HB3 | 2.12 | 0.74 |
| 1:A:530:MET:HE1 | 4:8:355:MET:SD | 2.27 | 0.74 |
| 1:A:836:PHE:CB | 2:B:161:GLU:OE1 | 2.35 | 0.74 |
| 1:J:636:LYS:O | 1:J:637:LYS:HB2 | 1.86 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:640:LYS:O | 4:W:23:GLY:O | 2.06 | 0.74 |
| 1:S:272:MLY:HH13 | 1:S:435:GLU:OE1 | 1.87 | 0.74 |
| 4:1:244:ASP:OD2 | 4:Y:325:MET:CE | 2.34 | 0.74 |
| 4:1:253:GLU:HA | 4:1:256:ARG:HG3 | 1.69 | 0.74 |
| 4:7:288:ASP:H | 4:9:203:THR:HG22 | 1.52 | 0.74 |
| 4:9:253:GLU:HA | 4:9:256:ARG:HG3 | 1.70 | 0.74 |
| 1:A:557:GLU:N | 4:V:48:GLY:HA2 | 1.90 | 0.74 |
| 1:D:538:GLU:O | 4:9:349:LEU:HG | 1.86 | 0.74 |
| 1:D:640:LYS:O | 4:9:23:GLY:O | 2.06 | 0.74 |
| 1:D:640:LYS:O | 1:D:645:SER:OG | 2.06 | 0.74 |
| 1:D:747:LEU:HD13 | 1:D:782:MLY:CH2 | 2.03 | 0.74 |
| 1:G:350:ALA:O | 1:G:354:LEU:HB2 | 1.87 | 0.74 |
| 1:G:436:MLY:HE3 | 1:G:626:TYR:CE1 | 2.23 | 0.74 |
| 1:G:707:CYS:SG | 1:G:714:ARG:CZ | 2.75 | 0.74 |
| 1:G:819:ASN:CB | 2:H:90:GLY:O | 2.36 | 0.74 |
| 1:J:793:ARG:HH11 | 3:L:40:ASN:HD22 | 1.34 | 0.74 |
| 1:M:410:ASN:CG | 4:Z:334:GLU:CA | 2.47 | 0.74 |
| 1:M:272:MLY:HH13 | 1:M:435:GLU:OE1 | 1.87 | 0.74 |
| 2:N:130:PRO:O | 2:N:132:GLU:N | 2.21 | 0.74 |
| 1:S:732:ILE:N | 1:S:733:PRO:CD | 2.51 | 0.74 |
| 1:S:820:VAL:HG11 | 2:T:136:MET:CE | 2.18 | 0.74 |
| 1:G:541:MET:O | 4:V:143:TYR:CZ | 2.40 | 0.74 |
| 1:G:538:GLU:HA | 4:V:349:LEU:HD12 | 0.74 | 0.74 |
| 4:Z:253:GLU:HA | 4:Z:256:ARG:HG3 | 1.69 | 0.74 |
| 1:S:538:GLU:HA | 4:2:349:LEU:HD12 | 0.75 | 0.74 |
| 1:A:752:ASP:O | 1:A:778:MET:HB3 | 1.87 | 0.74 |
| 1:D:721:LYS:CB | 1:D:736:GLN:CD | 2.56 | 0.74 |
| 1:G:215:GLN:NE2 | 1:G:336:SER:O | 2.21 | 0.74 |
| 1:G:410:ASN:OD1 | 4:V:335:ARG:N | 2.21 | 0.74 |
| 1:G:641:LYS:HD2 | 1:G:647:GLN:OE1 | 1.81 | 0.74 |
| 1:G:732:ILE:N | 1:G:733:PRO:CD | 2.51 | 0.74 |
| 1:G:795:ARG:HA | 3:I:118:MET:HE1 | 1.68 | 0.74 |
| 1:J:350:ALA:O | 1:J:354:LEU:HB2 | 1.87 | 0.74 |
| 1:M:538:GLU:O | 4:Z:349:LEU:HG | 1.86 | 0.74 |
| 1:M:84:MLY:HH12 | 1:M:715:VAL:CG2 | 2.18 | 0.74 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:HD12 | 0.75 | 0.74 |
| 4:1:322:PRO:HB2 | 4:3:244:ASP:HB3 | 1.70 | 0.74 |
| 1:M:557:GLU:N | 4:2:48:GLY:HA3 | 1.90 | 0.74 |
| 1:D:310:TYR:CE2 | 1:D:320:ILE:HD11 | 2.23 | 0.74 |
| 1:J:215:GLN:NE2 | 1:J:336:SER:O | 2.20 | 0.74 |
| 1:J:735:GLY:CA | 1:J:743:ALA:HA | 2.18 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:218:LEU:HB2 | 1:M:221:GLN:CG | 2.09 | 0.74 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:CG | 1.93 | 0.74 |
| 1:J:410:ASN:OD1 | 4:W:335:ARG:N | 2.21 | 0.74 |
| 1:J:538:GLU:HA | 4:W:349:LEU:HD12 | 0.75 | 0.74 |
| 1:A:732:ILE:N | 1:A:733:PRO:CD | 2.51 | 0.73 |
| 1:A:721:LYS:CB | 1:A:736:GLN:CD | 2.56 | 0.73 |
| 1:D:272:MLY:HH13 | 1:D:435:GLU:OE1 | 1.87 | 0.73 |
| 1:D:529:PRO:C | 4:9:354:GLN:CB | 2.49 | 0.73 |
| 1:D:629:GLU:HA | 1:D:643:GLY:C | 2.05 | 0.73 |
| 1:D:636:LYS:O | 1:D:637:LYS:HB2 | 1.86 | 0.73 |
| 1:D:732:ILE:N | 1:D:733:PRO:CD | 2.51 | 0.73 |
| 1:J:410:ASN:CG | 4:W:334:GLU:CA | 2.47 | 0.73 |
| 1:J:486:MLY:HH13 | 1:J:527:GLU:OE1 | 1.88 | 0.73 |
| 2:K:130:PRO:O | 2:K:132:GLU:N | 2.21 | 0.73 |
| 1:M:732:ILE:N | 1:M:733:PRO:CD | 2.51 | 0.73 |
| 1:S:486:MLY:HH13 | 1:S:527:GLU:OE1 | 1.88 | 0.73 |
| 1:S:836:PHE:CD2 | 2:T:160:GLY:HA3 | 2.21 | 0.73 |
| 4:X:253:GLU:HA | 4:X:256:ARG:HG3 | 1.70 | 0.73 |
| 1:D:538:GLU:HA | 4:9:349:LEU:HD12 | 0.74 | 0.73 |
| 1:A:736:GLN:HA | 1:A:743:ALA:HB2 | 1.51 | 0.73 |
| 1:J:409:GLY:HA3 | 4:W:333:PRO:N | 2.03 | 0.73 |
| 1:J:436:MLY:HE3 | 1:J:626:TYR:CE1 | 2.23 | 0.73 |
| 1:J:732:ILE:N | 1:J:733:PRO:CD | 2.51 | 0.73 |
| 1:M:735:GLY:CA | 1:M:743:ALA:HA | 2.18 | 0.73 |
| 1:S:218:LEU:HB2 | 1:S:221:GLN:CG | 2.09 | 0.73 |
| 1:S:786:ILE:CA | 1:S:787:ILE:N | 2.50 | 0.73 |
| 4:V:253:GLU:HA | 4:V:256:ARG:HG3 | 1.69 | 0.73 |
| 1:A:550:PHE:HA | 4:V:46:GLY:HA3 | 1.66 | 0.73 |
| 1:D:487:LEU:O | 1:D:490:PHE:HB3 | 1.88 | 0.73 |
| 1:D:534:SER:CA | 4:9:351:THR:HA | 2.19 | 0.73 |
| 2:E:130:PRO:O | 2:E:132:GLU:N | 2.21 | 0.73 |
| 1:G:735:GLY:CA | 1:G:743:ALA:HA | 2.18 | 0.73 |
| 1:J:487:LEU:O | 1:J:490:PHE:HB3 | 1.89 | 0.73 |
| 1:J:640:LYS:O | 1:J:645:SER:OG | 2.06 | 0.73 |
| 3:L:24:LYS:CA | 3:L:63:ILE:O | 2.37 | 0.73 |
| 1:M:486:MLY:HH13 | 1:M:527:GLU:OE1 | 1.88 | 0.73 |
| 1:M:831:TRP:HE1 | 2:N:67:MET:HB3 | 1.53 | 0.73 |
| 1:S:795:ARG:NH2 | 3:U:116:GLU:CG | 2.51 | 0.73 |
| 1:S:805:ALA:HA | 1:S:808:GLU:N | 2.04 | 0.73 |
| 1:S:92:ALA:CB | 1:S:764:MLY:HH12 | 2.17 | 0.73 |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:HG23 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:130:PRO:O | 2:B:132:GLU:N | 2.21 | 0.73 |
| 3:C:4:LYS:N | 3:C:5:ALA:O | 2.17 | 0.73 |
| 1:D:507:GLY:CA | 1:D:762:HIS:CD2 | 2.71 | 0.73 |
| 1:G:486:MLY:HH13 | 1:G:527:GLU:OE1 | 1.88 | 0.73 |
| 1:J:817:GLN:CG | 2:K:127:ARG:CG | 2.54 | 0.73 |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:HD23 | 1.69 | 0.73 |
| 1:M:190:MLY:HE3 | 1:M:230:GLU:OE2 | 1.89 | 0.73 |
| 1:M:409:GLY:HA3 | 4:Z:333:PRO:N | 2.03 | 0.73 |
| 1:M:436:MLY:HE3 | 1:M:626:TYR:CE1 | 2.23 | 0.73 |
| 1:M:802:GLU:O | 1:M:806:MET:HG3 | 1.89 | 0.73 |
| 1:S:190:MLY:HE3 | 1:S:230:GLU:OE2 | 1.89 | 0.73 |
| 4:3:253:GLU:HA | 4:3:256:ARG:HG3 | 1.70 | 0.73 |
| 4:3:322:PRO:CB | 4:5:244:ASP:HB2 | 2.16 | 0.73 |
| 4:4:287:ILE:HG21 | 4:6:204:ALA:H | 1.54 | 0.73 |
| 4:4:287:ILE:CA | 4:6:202:THR:HB | 2.17 | 0.73 |
| 1:A:538:GLU:HA | 4:8:349:LEU:HD12 | 0.74 | 0.73 |
| 1:A:272:MLY:HH13 | 1:A:435:GLU:OE1 | 1.88 | 0.73 |
| 1:A:409:GLY:HA3 | 4:8:333:PRO:N | 2.03 | 0.73 |
| 1:A:410:ASN:OD1 | 4:8:335:ARG:N | 2.22 | 0.73 |
| 1:A:530:MET:CE | 4:8:355:MET:SD | 2.76 | 0.73 |
| 1:D:726:VAL:O | 1:D:785:GLU:CG | 2.36 | 0.73 |
| 1:D:838:ILE:HD11 | 2:E:54:MET:SD | 2.28 | 0.73 |
| 3:F:24:LYS:CA | 3:F:63:ILE:O | 2.37 | 0.73 |
| 1:G:506:GLU:OE2 | 1:G:760:PHE:O | 2.07 | 0.73 |
| 1:G:643:GLY:N | 4:V:24:ASP:CA | 2.47 | 0.73 |
| 1:G:503:TYR:CE1 | 1:G:711:PHE:HE2 | 2.04 | 0.73 |
| 1:J:721:LYS:CB | 1:J:736:GLN:CD | 2.56 | 0.73 |
| 1:J:733:PRO:C | 1:J:737:PHE:HD1 | 1.88 | 0.73 |
| 1:J:84:MLY:HH22 | 1:J:719:ASP:C | 2.00 | 0.73 |
| 1:M:410:ASN:OD1 | 4:Z:335:ARG:N | 2.21 | 0.73 |
| 1:M:831:TRP:HZ3 | 2:N:34:ILE:HD13 | 1.53 | 0.73 |
| 1:M:838:ILE:CD1 | 2:N:54:MET:HE1 | 2.09 | 0.73 |
| 1:S:802:GLU:O | 1:S:806:MET:HG3 | 1.88 | 0.73 |
| 2:T:130:PRO:O | 2:T:132:GLU:N | 2.21 | 0.73 |
| 1:S:546:THR:CB | 4:4:47:MET:O | 2.37 | 0.73 |
| 4:3:287:ILE:HB | 4:5:203:THR:CG2 | 2.19 | 0.73 |
| 1:A:441:MET:O | 1:A:445:ILE:HG13 | 1.88 | 0.73 |
| 3:C:24:LYS:CA | 3:C:63:ILE:O | 2.37 | 0.73 |
| 1:D:237:THR:HG22 | 1:D:239:ARG:H | 1.54 | 0.73 |
| 1:G:441:MET:O | 1:G:445:ILE:HG13 | 1.88 | 0.73 |
| 1:M:218:LEU:HB3 | 1:M:221:GLN:HG3 | 1.61 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:487:LEU:O | 1:M:490:PHE:HB3 | 1.89 | 0.73 |
| 4:2:287:ILE:HG23 | 4:4:202:THR:HB | 1.71 | 0.73 |
| 1:A:542:PHE:CD2 | 4:8:143:TYR:CE1 | 2.77 | 0.73 |
| 4:7:290:ARG:HH22 | 4:9:202:THR:HG23 | 1.51 | 0.73 |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CZ | 2.24 | 0.73 |
| 1:A:93:MET:HE1 | 1:A:715:VAL:CG1 | 2.16 | 0.73 |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CZ | 2.24 | 0.73 |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CZ | 2.23 | 0.73 |
| 1:J:733:PRO:C | 1:J:737:PHE:CD1 | 2.62 | 0.73 |
| 1:M:215:GLN:NE2 | 1:M:336:SER:O | 2.21 | 0.73 |
| 1:M:95:THR:N | 1:M:713:SER:HB3 | 2.04 | 0.73 |
| 1:S:217:THR:C | 1:S:221:GLN:HE21 | 1.92 | 0.73 |
| 4:8:253:GLU:HA | 4:8:256:ARG:HG3 | 1.69 | 0.73 |
| 1:G:21:GLU:O | 1:G:25:ILE:HG13 | 1.89 | 0.73 |
| 1:G:272:MLY:HH13 | 1:G:435:GLU:OE1 | 1.88 | 0.73 |
| 1:G:84:MLY:CD | 1:G:723:ARG:HD2 | 2.16 | 0.73 |
| 1:G:802:GLU:O | 1:G:806:MET:HG3 | 1.89 | 0.73 |
| 1:G:829:TRP:CZ3 | 2:H:84:PHE:CZ | 2.77 | 0.73 |
| 1:J:21:GLU:O | 1:J:25:ILE:HG13 | 1.89 | 0.73 |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CZ | 2.24 | 0.73 |
| 1:S:735:GLY:CA | 1:S:743:ALA:HA | 2.18 | 0.73 |
| 1:A:21:GLU:O | 1:A:25:ILE:HG13 | 1.88 | 0.73 |
| 1:A:350:ALA:O | 1:A:354:LEU:HB2 | 1.87 | 0.73 |
| 1:A:800:ARG:C | 3:C:149:VAL:HG21 | 2.09 | 0.73 |
| 1:D:21:GLU:O | 1:D:25:ILE:HG13 | 1.89 | 0.73 |
| 1:D:537:GLU:HG3 | 4:9:350:SER:O | 1.79 | 0.73 |
| 1:D:542:PHE:HA | 4:9:143:TYR:HE1 | 1.34 | 0.73 |
| 1:G:753:VAL:N | 1:G:780:ASP:OD1 | 2.21 | 0.73 |
| 1:J:839:MLY:HH13 | 2:K:159:HIS:CD2 | 2.23 | 0.73 |
| 1:M:217:THR:C | 1:M:221:GLN:HE21 | 1.92 | 0.73 |
| 1:M:838:ILE:CD1 | 2:N:54:MET:HE3 | 2.18 | 0.73 |
| 1:S:214:MET:HA | 1:S:340:ILE:HD11 | 1.70 | 0.73 |
| 1:S:21:GLU:O | 1:S:25:ILE:HG13 | 1.88 | 0.73 |
| 1:S:536:LEU:HD13 | 1:S:550:PHE:CZ | 2.24 | 0.73 |
| 1:S:821:ARG:HH22 | 2:T:127:ARG:HE | 1.35 | 0.73 |
| 1:A:190:MLY:HE3 | 1:A:230:GLU:OE2 | 1.89 | 0.73 |
| 1:D:131:TRP:C | 1:D:132:LEU:HD12 | 2.09 | 0.73 |
| 1:D:735:GLY:CA | 1:D:743:ALA:HA | 2.18 | 0.73 |
| 1:D:814:PHE:HD1 | 2:E:127:ARG:HH12 | 1.13 | 0.73 |
| 1:G:237:THR:HG22 | 1:G:239:ARG:H | 1.54 | 0.73 |
| 1:G:721:LYS:CB | 1:G:736:GLN:CD | 2.56 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:24:LYS:CA | 3:I:63:ILE:O | 2.37 | 0.73 |
| 1:J:542:PHE:HA | 4:W:143:TYR:HE1 | 1.34 | 0.73 |
| 1:S:436:MLY:HE3 | 1:S:626:TYR:CE1 | 2.23 | 0.73 |
| 1:S:487:LEU:O | 1:S:490:PHE:HB3 | 1.88 | 0.73 |
| 1:S:538:GLU:O | 4:2:349:LEU:HG | 1.86 | 0.73 |
| 1:M:534:SER:CA | 4:Z:351:THR:HA | 2.19 | 0.73 |
| 4:5:253:GLU:HA | 4:5:256:ARG:HG3 | 1.69 | 0.72 |
| 1:D:542:PHE:CD2 | 4:9:143:TYR:CE1 | 2.77 | 0.72 |
| 1:A:131:TRP:C | 1:A:132:LEU:HD12 | 2.09 | 0.72 |
| 1:A:486:MLY:HH13 | 1:A:527:GLU:OE1 | 1.88 | 0.72 |
| 1:A:802:GLU:O | 1:A:806:MET:HG3 | 1.89 | 0.72 |
| 1:D:190:MLY:HE3 | 1:D:230:GLU:OE2 | 1.89 | 0.72 |
| 1:D:292:MET:HE3 | 1:D:309:PRO:HA | 1.70 | 0.72 |
| 1:D:793:ARG:NH2 | 3:F:147:MET:HE3 | 2.04 | 0.72 |
| 1:G:131:TRP:C | 1:G:132:LEU:HD12 | 2.09 | 0.72 |
| 1:G:217:THR:C | 1:G:221:GLN:HE21 | 1.92 | 0.72 |
| 2:H:130:PRO:O | 2:H:132:GLU:N | 2.21 | 0.72 |
| 2:N:111:SER:OG | 2:N:148:VAL:C | 2.15 | 0.72 |
| 1:S:131:TRP:C | 1:S:132:LEU:HD12 | 2.10 | 0.72 |
| 1:J:534:SER:CA | 4:W:351:THR:HA | 2.19 | 0.72 |
| 1:J:530:MET:CE | 4:W:355:MET:SD | 2.77 | 0.72 |
| 4:3:3:ASP:HA | 4:3:6:THR:CB | 2.18 | 0.72 |
| 4:8:3:ASP:HA | 4:8:6:THR:CB | 2.18 | 0.72 |
| 1:D:409:GLY:HA3 | 4:9:333:PRO:N | 2.03 | 0.72 |
| 1:A:36:SER:O | 1:A:52:ILE:HG12 | 1.90 | 0.72 |
| 1:A:501:GLU:CG | 1:A:762:HIS:ND1 | 2.37 | 0.72 |
| 1:G:487:LEU:O | 1:G:490:PHE:HB3 | 1.89 | 0.72 |
| 1:G:769:ALA:HB3 | 1:G:770:GLY:HA2 | 0.75 | 0.72 |
| 1:J:95:THR:CA | 1:J:713:SER:OG | 2.30 | 0.72 |
| 1:J:93:MET:HE1 | 1:J:716:LEU:HD12 | 1.71 | 0.72 |
| 1:M:214:MET:HA | 1:M:340:ILE:HD11 | 1.70 | 0.72 |
| 1:S:441:MET:O | 1:S:445:ILE:HG13 | 1.88 | 0.72 |
| 1:S:640:LYS:O | 4:2:23:GLY:O | 2.06 | 0.72 |
| 3:U:24:LYS:CA | 3:U:63:ILE:O | 2.37 | 0.72 |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:CG2 | 2.18 | 0.72 |
| 1:S:542:PHE:CD2 | 4:2:143:TYR:CE1 | 2.77 | 0.72 |
| 1:D:530:MET:CE | 4:9:355:MET:SD | 2.76 | 0.72 |
| 1:D:214:MET:HA | 1:D:340:ILE:HD11 | 1.70 | 0.72 |
| 1:G:190:MLY:HE3 | 1:G:230:GLU:OE2 | 1.89 | 0.72 |
| 1:G:519:LEU:N | 1:G:519:LEU:HD12 | 2.05 | 0.72 |
| 1:G:618:THR:O | 1:G:622:LEU:HD13 | 1.89 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:831:TRP:CH2 | 2:H:47:LEU:HD23 | 2.19 | 0.72 |
| 1:G:93:MET:HA | 1:G:714:ARG:N | 2.03 | 0.72 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CA | 2.20 | 0.72 |
| 1:J:290:GLN:C | 1:J:331:LEU:HD12 | 2.09 | 0.72 |
| 1:J:441:MET:O | 1:J:445:ILE:HG13 | 1.88 | 0.72 |
| 1:J:802:GLU:O | 1:J:806:MET:HG3 | 1.89 | 0.72 |
| 1:M:441:MET:O | 1:M:445:ILE:HG13 | 1.88 | 0.72 |
| 1:S:237:THR:HG22 | 1:S:239:ARG:H | 1.54 | 0.72 |
| 1:S:410:ASN:OD1 | 4:2:335:ARG:N | 2.21 | 0.72 |
| 1:S:519:LEU:N | 1:S:519:LEU:HD12 | 2.04 | 0.72 |
| 1:M:542:PHE:CD2 | 4:Z:143:TYR:CE1 | 2.77 | 0.72 |
| 4:7:290:ARG:NH1 | 4:9:202:THR:CG2 | 2.49 | 0.72 |
| 1:A:176:LEU:HD12 | 1:A:176:LEU:N | 2.05 | 0.72 |
| 1:A:534:SER:CA | 4:8:351:THR:HA | 2.18 | 0.72 |
| 1:D:290:GLN:C | 1:D:331:LEU:HD12 | 2.09 | 0.72 |
| 1:D:36:SER:O | 1:D:52:ILE:HG12 | 1.90 | 0.72 |
| 1:D:769:ALA:N | 1:D:771:LEU:HA | 2.05 | 0.72 |
| 1:D:836:PHE:CZ | 2:E:160:GLY:CA | 2.72 | 0.72 |
| 1:D:800:ARG:O | 3:F:149:VAL:CG2 | 2.37 | 0.72 |
| 1:G:534:SER:CA | 4:V:351:THR:HA | 2.19 | 0.72 |
| 1:J:131:TRP:C | 1:J:132:LEU:HD12 | 2.09 | 0.72 |
| 1:J:36:SER:O | 1:J:52:ILE:HG12 | 1.90 | 0.72 |
| 1:J:797:PHE:HE2 | 3:L:126:LEU:CD1 | 2.01 | 0.72 |
| 2:N:121:LEU:CG | 2:N:128:PHE:HA | 2.14 | 0.72 |
| 1:S:409:GLY:HA3 | 4:2:333:PRO:N | 2.03 | 0.72 |
| 1:S:754:ASP:HB3 | 1:S:757:GLN:HG2 | 1.72 | 0.72 |
| 1:S:797:PHE:CE1 | 3:U:146:ILE:C | 2.62 | 0.72 |
| 4:1:287:ILE:HG23 | 4:3:202:THR:HB | 0.80 | 0.72 |
| 1:A:487:LEU:O | 1:A:490:PHE:HB3 | 1.89 | 0.72 |
| 1:D:618:THR:O | 1:D:622:LEU:HD13 | 1.89 | 0.72 |
| 1:D:836:PHE:CZ | 2:E:159:HIS:CA | 2.72 | 0.72 |
| 1:D:800:ARG:HD3 | 3:F:149:VAL:C | 2.10 | 0.72 |
| 1:G:214:MET:HA | 1:G:340:ILE:HD11 | 1.70 | 0.72 |
| 1:G:409:GLY:HA3 | 4:V:333:PRO:N | 2.03 | 0.72 |
| 1:J:214:MET:HA | 1:J:340:ILE:HD11 | 1.70 | 0.72 |
| 1:M:536:LEU:HD13 | 1:M:550:PHE:CZ | 2.24 | 0.72 |
| 1:M:550:PHE:HA | 4:2:46:GLY:HA3 | 1.66 | 0.72 |
| 1:M:618:THR:O | 1:M:622:LEU:HD13 | 1.89 | 0.72 |
| 1:M:84:MLY:CH1 | 1:M:715:VAL:HG22 | 2.19 | 0.72 |
| 1:S:546:THR:OG1 | 4:4:46:GLY:N | 2.22 | 0.72 |
| 1:S:762:HIS:H | 1:S:762:HIS:CD2 | 2.08 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:120:GLY:HA2 | 1:S:764:MLY:HH11 | 1.71 | 0.72 |
| 4:X:324:THR:HB | 4:Z:246:GLN:CA | 2.20 | 0.72 |
| 4:2:166:TYR:OH | 4:4:64:ILE:HD13 | 1.89 | 0.72 |
| 4:4:3:ASP:HA | 4:4:6:THR:CB | 2.17 | 0.72 |
| 1:A:735:GLY:CA | 1:A:743:ALA:HA | 2.18 | 0.72 |
| 2:B:144:VAL:CB | 2:B:153:ILE:HD11 | 2.19 | 0.72 |
| 1:D:819:ASN:O | 2:E:157:ILE:HG23 | 1.90 | 0.72 |
| 1:J:190:MLY:HE3 | 1:J:230:GLU:OE2 | 1.89 | 0.72 |
| 1:J:618:THR:O | 1:J:622:LEU:HD13 | 1.89 | 0.72 |
| 1:M:519:LEU:N | 1:M:519:LEU:HD12 | 2.04 | 0.72 |
| 1:M:783:LEU:CD2 | 1:M:786:ILE:CD1 | 2.66 | 0.72 |
| 2:T:144:VAL:CB | 2:T:153:ILE:HD11 | 2.19 | 0.72 |
| 4:W:287:ILE:HD11 | 4:Y:201:VAL:O | 1.76 | 0.72 |
| 1:M:530:MET:CE | 4:Z:355:MET:SD | 2.77 | 0.72 |
| 1:A:295:MLY:HG3 | 1:A:332:MET:CE | 2.19 | 0.72 |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:CD1 | 2.63 | 0.72 |
| 1:D:727:LEU:CG | 1:D:782:MLY:CH1 | 2.66 | 0.72 |
| 1:D:795:ARG:CD | 3:F:35:ARG:HH12 | 2.02 | 0.72 |
| 1:G:36:SER:O | 1:G:52:ILE:HG12 | 1.90 | 0.72 |
| 1:G:817:GLN:CD | 2:H:127:ARG:HB2 | 2.10 | 0.72 |
| 1:G:829:TRP:CZ3 | 2:H:84:PHE:CE1 | 2.78 | 0.72 |
| 1:J:797:PHE:HE1 | 3:L:146:ILE:HA | 1.54 | 0.72 |
| 1:M:721:LYS:HG2 | 1:M:736:GLN:CD | 1.85 | 0.72 |
| 1:M:35:MLY:HE2 | 1:M:777:GLU:HG3 | 1.70 | 0.72 |
| 3:O:24:LYS:CA | 3:O:63:ILE:O | 2.37 | 0.72 |
| 1:S:534:SER:CA | 4:2:351:THR:HA | 2.19 | 0.72 |
| 4:1:288:ASP:CG | 4:3:203:THR:HG23 | 2.07 | 0.72 |
| 1:A:217:THR:C | 1:A:221:GLN:HE21 | 1.93 | 0.72 |
| 1:A:290:GLN:C | 1:A:331:LEU:HD12 | 2.10 | 0.72 |
| 1:A:530:MET:HE2 | 4:8:354:GLN:HG3 | 1.70 | 0.72 |
| 1:A:618:THR:O | 1:A:622:LEU:HD13 | 1.89 | 0.72 |
| 1:A:640:LYS:O | 1:A:645:SER:OG | 2.06 | 0.72 |
| 1:A:754:ASP:HB3 | 1:A:757:GLN:HG2 | 1.72 | 0.72 |
| 2:B:150:TYR:C | 2:B:151:LYS:CG | 2.49 | 0.72 |
| 1:G:14:ALA:HB3 | 1:G:15:PRO:HD3 | 1.72 | 0.72 |
| 1:M:295:MLY:HG3 | 1:M:332:MET:CE | 2.19 | 0.72 |
| 1:S:176:LEU:N | 1:S:176:LEU:HD12 | 2.05 | 0.72 |
| 1:G:538:GLU:O | 4:V:349:LEU:HG | 1.87 | 0.72 |
| 4:9:290:ARG:HH22 | 4:W:202:THR:HG23 | 1.50 | 0.72 |
| 4:W:325:MET:HE1 | 4:Y:244:ASP:CG | 2.09 | 0.72 |
| 4:X:324:THR:HB | 4:Z:247:VAL:H | 1.55 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:3:ASP:HA | 4:2:6:THR:CB | 2.18 | 0.72 |
| 1:A:538:GLU:CD | 4:8:355:MET:HE3 | 2.10 | 0.72 |
| 1:A:791:GLN:OE1 | 3:C:116:GLU:CG | 2.36 | 0.72 |
| 1:D:519:LEU:N | 1:D:519:LEU:HD12 | 2.05 | 0.72 |
| 2:E:144:VAL:CB | 2:E:153:ILE:HD11 | 2.19 | 0.72 |
| 1:G:295:MLY:HG3 | 1:G:332:MET:CE | 2.20 | 0.72 |
| 1:G:640:LYS:O | 4:V:23:GLY:O | 2.06 | 0.72 |
| 1:G:733:PRO:C | 1:G:737:PHE:CD1 | 2.62 | 0.72 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:CG | 2.68 | 0.72 |
| 2:K:136:MET:O | 2:K:140:PHE:HB2 | 1.90 | 0.72 |
| 1:M:131:TRP:C | 1:M:132:LEU:HD12 | 2.09 | 0.72 |
| 1:S:839:MLY:CH2 | 2:T:158:THR:HG22 | 2.19 | 0.72 |
| 1:J:542:PHE:CD2 | 4:W:143:TYR:CE1 | 2.77 | 0.72 |
| 1:D:550:PHE:HA | 4:W:46:GLY:HA3 | 1.66 | 0.72 |
| 1:S:530:MET:HE3 | 4:2:354:GLN:HG2 | 1.71 | 0.72 |
| 1:D:441:MET:O | 1:D:445:ILE:HG13 | 1.88 | 0.72 |
| 1:D:709:LYS:O | 1:D:710:GLY:HA2 | 1.88 | 0.72 |
| 2:H:144:VAL:CB | 2:H:153:ILE:HD11 | 2.19 | 0.72 |
| 1:J:166:MET:HE1 | 1:J:254:PHE:HB2 | 1.71 | 0.72 |
| 1:J:818:TYR:CG | 2:K:127:ARG:NH1 | 2.58 | 0.72 |
| 1:J:795:ARG:C | 3:L:35:ARG:NH2 | 2.42 | 0.72 |
| 1:S:486:MLY:HH22 | 1:S:527:GLU:OE2 | 1.90 | 0.72 |
| 1:S:836:PHE:CD1 | 2:T:160:GLY:N | 2.58 | 0.72 |
| 1:G:530:MET:CE | 4:V:355:MET:SD | 2.78 | 0.72 |
| 1:S:530:MET:CE | 4:2:355:MET:SD | 2.77 | 0.71 |
| 1:A:237:THR:HG22 | 1:A:239:ARG:H | 1.54 | 0.71 |
| 1:A:753:VAL:CG1 | 1:A:775:LEU:CD2 | 2.68 | 0.71 |
| 1:D:735:GLY:C | 1:D:743:ALA:HB2 | 1.82 | 0.71 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:CB | 2.71 | 0.71 |
| 1:D:802:GLU:O | 1:D:806:MET:HG3 | 1.89 | 0.71 |
| 1:G:640:LYS:O | 1:G:645:SER:OG | 2.06 | 0.71 |
| 1:G:84:MLY:CH1 | 1:G:724:TYR:HE2 | 2.02 | 0.71 |
| 1:G:797:PHE:HE1 | 3:I:146:ILE:HA | 1.55 | 0.71 |
| 1:J:641:LYS:HD2 | 1:J:647:GLN:OE1 | 1.81 | 0.71 |
| 1:J:818:TYR:CD1 | 2:K:127:ARG:CZ | 2.73 | 0.71 |
| 1:M:640:LYS:O | 4:Z:23:GLY:O | 2.06 | 0.71 |
| 2:N:136:MET:O | 2:N:140:PHE:HB2 | 1.90 | 0.71 |
| 2:N:144:VAL:CB | 2:N:153:ILE:HD11 | 2.19 | 0.71 |
| 1:S:14:ALA:HB3 | 1:S:15:PRO:HD3 | 1.72 | 0.71 |
| 1:S:732:ILE:HG23 | 1:S:747:LEU:CB | 1.84 | 0.71 |
| 4:4:287:ILE:HB | 4:6:203:THR:CG2 | 2.19 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:410:ASN:OD1 | 4:9:335:ARG:N | 2.22 | 0.71 |
| 1:A:97:LEU:HD23 | 1:A:712:PRO:CB | 2.14 | 0.71 |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CA | 2.20 | 0.71 |
| 2:E:136:MET:O | 2:E:140:PHE:HB2 | 1.90 | 0.71 |
| 1:J:519:LEU:HD12 | 1:J:519:LEU:N | 2.04 | 0.71 |
| 1:M:36:SER:O | 1:M:52:ILE:HG12 | 1.89 | 0.71 |
| 1:S:798:LEU:HD22 | 3:U:126:LEU:HD11 | 1.65 | 0.71 |
| 4:3:322:PRO:HB2 | 4:5:244:ASP:CB | 2.08 | 0.71 |
| 4:6:3:ASP:HA | 4:6:6:THR:CB | 2.18 | 0.71 |
| 1:D:641:LYS:HD2 | 4:9:348:SER:HA | 1.73 | 0.71 |
| 1:A:754:ASP:OD2 | 1:A:778:MET:HE1 | 1.90 | 0.71 |
| 1:A:817:GLN:CD | 2:B:127:ARG:HE | 1.89 | 0.71 |
| 1:D:800:ARG:CD | 3:F:149:VAL:C | 2.58 | 0.71 |
| 1:J:295:MLY:HG3 | 1:J:332:MET:CE | 2.19 | 0.71 |
| 2:K:144:VAL:CB | 2:K:153:ILE:HD11 | 2.19 | 0.71 |
| 1:J:801:VAL:CG2 | 3:L:126:LEU:HD21 | 2.21 | 0.71 |
| 1:M:176:LEU:HD12 | 1:M:176:LEU:N | 2.05 | 0.71 |
| 1:S:295:MLY:HG3 | 1:S:332:MET:CE | 2.19 | 0.71 |
| 1:S:36:SER:O | 1:S:52:ILE:HG12 | 1.90 | 0.71 |
| 1:S:618:THR:O | 1:S:622:LEU:HD13 | 1.89 | 0.71 |
| 4:8:290:ARG:HH22 | 4:V:202:THR:HG23 | 1.50 | 0.71 |
| 4:V:325:MET:HE1 | 4:X:244:ASP:CG | 2.08 | 0.71 |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:OE2 | 1.90 | 0.71 |
| 1:A:149:GLN:NE2 | 1:A:718:ALA:HB2 | 2.06 | 0.71 |
| 1:D:166:MET:HE3 | 1:D:254:PHE:HD2 | 1.53 | 0.71 |
| 1:D:295:MLY:HG3 | 1:D:332:MET:CE | 2.20 | 0.71 |
| 1:D:56:GLU:CB | 1:D:59:MLY:HB3 | 2.20 | 0.71 |
| 1:D:733:PRO:C | 1:D:737:PHE:HD1 | 1.88 | 0.71 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:NH1 | 2.05 | 0.71 |
| 1:M:14:ALA:HB3 | 1:M:15:PRO:HD3 | 1.73 | 0.71 |
| 1:S:290:GLN:C | 1:S:331:LEU:HD12 | 2.09 | 0.71 |
| 4:Z:3:ASP:HA | 4:Z:6:THR:CB | 2.18 | 0.71 |
| 4:9:3:ASP:HA | 4:9:6:THR:CB | 2.18 | 0.71 |
| 1:A:754:ASP:OD2 | 1:A:774:LEU:CD2 | 2.38 | 0.71 |
| 1:A:93:MET:SD | 1:A:715:VAL:HG22 | 2.31 | 0.71 |
| 1:D:217:THR:O | 1:D:220:ASP:HB2 | 1.90 | 0.71 |
| 2:E:114:LYS:HA | 2:E:146:GLY:C | 2.03 | 0.71 |
| 1:G:217:THR:O | 1:G:220:ASP:HB2 | 1.91 | 0.71 |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:CE1 | 2.24 | 0.71 |
| 2:H:136:MET:O | 2:H:140:PHE:HB2 | 1.90 | 0.71 |
| 1:J:754:ASP:HB3 | 1:J:757:GLN:HG2 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:21:GLU:O | 1:M:25:ILE:HG13 | 1.89 | 0.71 |
| 1:S:245:ARG:HD3 | 1:S:271:GLU:OE1 | 1.90 | 0.71 |
| 1:S:783:LEU:CA | 1:S:786:ILE:CD1 | 2.68 | 0.71 |
| 1:S:831:TRP:HH2 | 2:T:47:LEU:HD23 | 1.48 | 0.71 |
| 3:U:4:LYS:N | 3:U:5:ALA:O | 2.16 | 0.71 |
| 1:A:14:ALA:HB3 | 1:A:15:PRO:HD3 | 1.72 | 0.71 |
| 1:A:217:THR:O | 1:A:220:ASP:HB2 | 1.91 | 0.71 |
| 1:A:831:TRP:CH2 | 2:B:50:THR:CB | 2.70 | 0.71 |
| 1:A:834:LEU:CD2 | 2:B:54:MET:HE2 | 2.16 | 0.71 |
| 1:D:217:THR:C | 1:D:221:GLN:HE21 | 1.92 | 0.71 |
| 3:F:4:LYS:N | 3:F:5:ALA:O | 2.16 | 0.71 |
| 1:G:274:ARG:NH2 | 1:G:282:GLU:OE1 | 2.24 | 0.71 |
| 1:G:290:GLN:C | 1:G:331:LEU:HD12 | 2.10 | 0.71 |
| 1:J:237:THR:HG22 | 1:J:239:ARG:H | 1.54 | 0.71 |
| 1:J:274:ARG:NH2 | 1:J:282:GLU:OE1 | 2.24 | 0.71 |
| 1:M:486:MLY:HH22 | 1:M:527:GLU:OE2 | 1.90 | 0.71 |
| 1:M:641:LYS:HD2 | 4:Z:348:SER:HA | 1.72 | 0.71 |
| 1:M:643:GLY:N | 4:Z:24:ASP:CA | 2.46 | 0.71 |
| 1:M:802:GLU:OE2 | 1:M:809:ARG:NH1 | 2.23 | 0.71 |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CA | 2.19 | 0.71 |
| 1:J:641:LYS:HD2 | 4:W:348:SER:HA | 1.73 | 0.71 |
| 4:X:3:ASP:HA | 4:X:6:THR:CB | 2.17 | 0.71 |
| 1:A:818:TYR:HB2 | 2:B:90:GLY:CA | 2.19 | 0.71 |
| 1:A:831:TRP:CD2 | 2:B:51:PHE:CZ | 2.78 | 0.71 |
| 1:D:508:ILE:HG12 | 1:D:766:PHE:CE1 | 2.26 | 0.71 |
| 1:D:86:ASP:OD2 | 1:D:87:MLY:HH13 | 1.91 | 0.71 |
| 1:D:823:PHE:CZ | 2:E:156:VAL:CG1 | 2.73 | 0.71 |
| 1:G:542:PHE:CD2 | 4:V:143:TYR:CE1 | 2.77 | 0.71 |
| 1:G:762:HIS:H | 1:G:762:HIS:CD2 | 2.07 | 0.71 |
| 1:J:217:THR:O | 1:J:220:ASP:HB2 | 1.91 | 0.71 |
| 1:J:217:THR:C | 1:J:221:GLN:HE21 | 1.92 | 0.71 |
| 1:J:86:ASP:OD2 | 1:J:87:MLY:HH13 | 1.91 | 0.71 |
| 1:M:721:LYS:CB | 1:M:736:GLN:CD | 2.56 | 0.71 |
| 1:M:86:ASP:OD2 | 1:M:87:MLY:HH13 | 1.91 | 0.71 |
| 1:S:546:THR:HG22 | 1:S:548:THR:N | 2.05 | 0.71 |
| 1:S:56:GLU:CB | 1:S:59:MLY:HB3 | 2.19 | 0.71 |
| 1:S:786:ILE:O | 1:S:789:ALA:HB3 | 1.90 | 0.71 |
| 1:S:795:ARG:CB | 3:U:35:ARG:NH1 | 2.53 | 0.71 |
| 4:7:3:ASP:HA | 4:7:6:THR:CB | 2.18 | 0.71 |
| 1:A:641:LYS:HD2 | 4:8:348:SER:HA | 1.73 | 0.71 |
| 1:A:800:ARG:HD2 | 3:C:149:VAL:O | 1.90 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:733:PRO:C | 1:D:737:PHE:CD1 | 2.62 | 0.71 |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CA | 2.20 | 0.71 |
| 1:M:245:ARG:HD3 | 1:M:271:GLU:OE1 | 1.90 | 0.71 |
| 1:M:290:GLN:C | 1:M:331:LEU:HD12 | 2.09 | 0.71 |
| 2:N:163:ALA:C | 2:T:21:GLU:CB | 2.57 | 0.71 |
| 1:S:734:GLU:OE2 | 3:U:94:PHE:CE2 | 2.43 | 0.71 |
| 2:T:117:LEU:HD12 | 2:T:147:ASN:CA | 2.19 | 0.71 |
| 1:A:274:ARG:NH2 | 1:A:282:GLU:OE1 | 2.24 | 0.71 |
| 1:A:214:MET:HA | 1:A:340:ILE:HD11 | 1.71 | 0.71 |
| 1:A:534:SER:C | 4:8:351:THR:CA | 2.47 | 0.71 |
| 2:B:136:MET:O | 2:B:140:PHE:HB2 | 1.90 | 0.71 |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:OE2 | 1.90 | 0.71 |
| 1:J:56:GLU:CB | 1:J:59:MLY:HB3 | 2.19 | 0.71 |
| 1:M:237:THR:HG22 | 1:M:239:ARG:H | 1.54 | 0.71 |
| 1:S:641:LYS:HD2 | 4:2:348:SER:HA | 1.73 | 0.71 |
| 4:2:290:ARG:HH22 | 4:4:202:THR:HG22 | 1.51 | 0.71 |
| 1:A:206:LYS:HD3 | 1:A:217:THR:HG23 | 0.71 | 0.71 |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD11 | 0.73 | 0.71 |
| 1:A:86:ASP:OD2 | 1:A:87:MLY:HH13 | 1.91 | 0.71 |
| 1:D:739:ASP:CB | 1:D:742:LYS:HB3 | 2.12 | 0.71 |
| 1:D:754:ASP:HB3 | 1:D:757:GLN:HG2 | 1.72 | 0.71 |
| 1:J:176:LEU:N | 1:J:176:LEU:HD12 | 2.05 | 0.71 |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:OE2 | 1.90 | 0.71 |
| 1:J:546:THR:HG22 | 1:J:548:THR:N | 2.05 | 0.71 |
| 1:J:72:VAL:HG13 | 1:J:76:GLN:CB | 2.19 | 0.71 |
| 1:M:56:GLU:CB | 1:M:59:MLY:HB3 | 2.19 | 0.71 |
| 1:M:640:LYS:O | 1:M:645:SER:OG | 2.06 | 0.71 |
| 1:M:35:MLY:CH2 | 1:M:777:GLU:CG | 2.50 | 0.71 |
| 1:S:819:ASN:OD1 | 2:T:92:ASP:HB2 | 1.89 | 0.71 |
| 1:S:795:ARG:CB | 3:U:118:MET:HE1 | 2.18 | 0.71 |
| 4:V:286:ASP:OD1 | 4:X:203:THR:N | 2.23 | 0.71 |
| 1:G:530:MET:HE1 | 4:V:355:MET:SD | 2.31 | 0.71 |
| 4:X:291:LYS:HD2 | 4:Z:243:PRO:C | 2.10 | 0.71 |
| 4:2:112:PRO:CB | 4:3:196:ARG:HA | 2.11 | 0.70 |
| 1:A:519:LEU:HD12 | 1:A:519:LEU:N | 2.04 | 0.70 |
| 1:A:768:MLY:CG | 1:A:771:LEU:HD13 | 2.21 | 0.70 |
| 1:A:800:ARG:NH2 | 3:C:40:ASN:OD1 | 2.24 | 0.70 |
| 1:D:727:LEU:HB3 | 1:D:782:MLY:HH13 | 1.64 | 0.70 |
| 1:G:641:LYS:HD2 | 4:V:348:SER:HA | 1.73 | 0.70 |
| 1:M:274:ARG:NH2 | 1:M:282:GLU:OE1 | 2.24 | 0.70 |
| 1:M:796:GLY:HA2 | 3:O:35:ARG:CD | 2.20 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:770:GLY:C | 1:S:771:LEU:N | 2.43 | 0.70 |
| 4:W:286:ASP:OD1 | 4:Y:203:THR:N | 2.23 | 0.70 |
| 1:A:245:ARG:HD3 | 1:A:271:GLU:OE1 | 1.90 | 0.70 |
| 1:A:72:VAL:HG13 | 1:A:76:GLN:CB | 2.19 | 0.70 |
| 1:D:245:ARG:HD3 | 1:D:271:GLU:OE1 | 1.90 | 0.70 |
| 1:D:274:ARG:NH2 | 1:D:282:GLU:OE1 | 2.24 | 0.70 |
| 1:D:798:LEU:CD1 | 3:F:126:LEU:HD13 | 2.14 | 0.70 |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:CA | 2.03 | 0.70 |
| 1:J:14:ALA:HB3 | 1:J:15:PRO:HD3 | 1.73 | 0.70 |
| 1:J:797:PHE:HE2 | 3:L:126:LEU:HD22 | 1.52 | 0.70 |
| 3:L:4:LYS:N | 3:L:5:ALA:O | 2.16 | 0.70 |
| 1:M:821:ARG:NH2 | 2:N:127:ARG:CD | 2.54 | 0.70 |
| 1:S:206:LYS:HD3 | 1:S:217:THR:HG23 | 0.71 | 0.70 |
| 1:D:14:ALA:HB3 | 1:D:15:PRO:HD3 | 1.72 | 0.70 |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:OE2 | 1.90 | 0.70 |
| 1:S:577:ALA:O | 1:S:578:HIS:CG | 2.45 | 0.70 |
| 4:V:3:ASP:HA | 4:V:6:THR:CB | 2.18 | 0.70 |
| 4:1:322:PRO:HB3 | 4:3:244:ASP:CG | 2.10 | 0.70 |
| 1:A:546:THR:HG22 | 1:A:548:THR:N | 2.05 | 0.70 |
| 1:A:762:HIS:CD2 | 1:A:762:HIS:H | 2.08 | 0.70 |
| 1:A:809:ARG:NH1 | 2:B:124:GLY:CA | 2.54 | 0.70 |
| 1:D:176:LEU:HD12 | 1:D:176:LEU:N | 2.05 | 0.70 |
| 1:D:206:LYS:HD3 | 1:D:217:THR:HG23 | 0.71 | 0.70 |
| 1:D:823:PHE:HE1 | 2:E:160:GLY:CA | 2.04 | 0.70 |
| 1:G:176:LEU:N | 1:G:176:LEU:HD12 | 2.05 | 0.70 |
| 1:G:579:PHE:HD2 | 1:G:592:ILE:HD11 | 1.57 | 0.70 |
| 1:J:206:LYS:HD3 | 1:J:217:THR:HG23 | 0.70 | 0.70 |
| 1:J:245:ARG:HD3 | 1:J:271:GLU:OE1 | 1.90 | 0.70 |
| 1:J:739:ASP:CB | 1:J:742:LYS:HB3 | 2.12 | 0.70 |
| 1:J:831:TRP:CZ3 | 2:K:34:ILE:HD13 | 2.25 | 0.70 |
| 1:M:754:ASP:HB3 | 1:M:757:GLN:HG2 | 1.72 | 0.70 |
| 1:M:818:TYR:CD1 | 2:N:127:ARG:CZ | 2.74 | 0.70 |
| 1:S:217:THR:O | 1:S:220:ASP:HB2 | 1.91 | 0.70 |
| 1:S:786:ILE:CG2 | 1:S:787:ILE:N | 2.54 | 0.70 |
| 4:1:203:THR:N | 4:Y:286:ASP:OD1 | 2.23 | 0.70 |
| 4:X:286:ASP:OD1 | 4:Z:203:THR:N | 2.24 | 0.70 |
| 1:D:530:MET:HE3 | 4:9:354:GLN:HG2 | 1.70 | 0.70 |
| 1:A:123:CYS:HB2 | 1:A:158:ILE:HD11 | 1.73 | 0.70 |
| 1:A:579:PHE:HD2 | 1:A:592:ILE:HD11 | 1.57 | 0.70 |
| 1:A:149:GLN:CG | 1:A:718:ALA:HB3 | 2.21 | 0.70 |
| 1:A:733:PRO:C | 1:A:737:PHE:CD1 | 2.62 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:577:ALA:O | 1:D:578:HIS:CG | 2.45 | 0.70 |
| 3:I:25:ILE:O | 3:I:63:ILE:HB | 1.92 | 0.70 |
| 1:J:123:CYS:HB2 | 1:J:158:ILE:HD11 | 1.73 | 0.70 |
| 1:J:579:PHE:HD2 | 1:J:592:ILE:HD11 | 1.57 | 0.70 |
| 1:S:549:SER:CB | 4:4:43:VAL:HG11 | 2.20 | 0.70 |
| 1:S:640:LYS:O | 1:S:645:SER:OG | 2.06 | 0.70 |
| 1:S:793:ARG:NE | 3:U:40:ASN:ND2 | 2.39 | 0.70 |
| 2:T:136:MET:O | 2:T:140:PHE:HB2 | 1.90 | 0.70 |
| 4:Y:3:ASP:HA | 4:Y:6:THR:CB | 2.18 | 0.70 |
| 1:G:546:THR:HG22 | 1:G:548:THR:N | 2.05 | 0.70 |
| 2:N:150:TYR:C | 2:N:151:LYS:CG | 2.48 | 0.70 |
| 1:S:786:ILE:HG22 | 1:S:787:ILE:N | 2.07 | 0.70 |
| 2:T:114:LYS:HA | 2:T:146:GLY:C | 2.03 | 0.70 |
| 1:S:797:PHE:HE2 | 3:U:126:LEU:HD22 | 1.56 | 0.70 |
| 4:4:288:ASP:H | 4:6:203:THR:CG2 | 2.02 | 0.70 |
| 1:A:793:ARG:HE | 3:C:147:MET:HG2 | 1.56 | 0.70 |
| 1:D:727:LEU:H | 1:D:782:MLY:CE | 2.05 | 0.70 |
| 1:D:72:VAL:HG13 | 1:D:76:GLN:CB | 2.19 | 0.70 |
| 1:D:829:TRP:CZ3 | 2:E:84:PHE:HZ | 2.09 | 0.70 |
| 3:F:25:ILE:O | 3:F:63:ILE:HB | 1.92 | 0.70 |
| 1:G:86:ASP:OD2 | 1:G:87:MLY:HH13 | 1.91 | 0.70 |
| 1:J:97:LEU:HD23 | 1:J:712:PRO:HB3 | 1.74 | 0.70 |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:CD | 1.94 | 0.70 |
| 1:M:577:ALA:O | 1:M:578:HIS:CG | 2.45 | 0.70 |
| 1:M:762:HIS:CD2 | 1:M:762:HIS:H | 2.07 | 0.70 |
| 1:S:410:ASN:CG | 4:2:334:GLU:CA | 2.47 | 0.70 |
| 2:T:121:LEU:CG | 2:T:128:PHE:CA | 2.49 | 0.70 |
| 1:J:630:ALA:O | 4:W:25:ASP:HB2 | 1.91 | 0.70 |
| 4:Z:1:ASP:HA | 4:Z:4:GLU:HB3 | 1.74 | 0.70 |
| 4:2:1:ASP:HA | 4:2:4:GLU:HB3 | 1.74 | 0.70 |
| 4:6:1:ASP:HA | 4:6:4:GLU:HB3 | 1.74 | 0.70 |
| 1:D:579:PHE:HD2 | 1:D:592:ILE:HD11 | 1.56 | 0.70 |
| 1:G:56:GLU:CB | 1:G:59:MLY:HB3 | 2.19 | 0.70 |
| 1:G:830:PRO:HB3 | 2:H:67:MET:HE1 | 1.73 | 0.70 |
| 1:G:818:TYR:CD1 | 2:H:127:ARG:NH1 | 2.60 | 0.70 |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD11 | 0.73 | 0.70 |
| 1:M:217:THR:O | 1:M:220:ASP:HB2 | 1.91 | 0.70 |
| 1:S:530:MET:HE2 | 4:2:354:GLN:HG3 | 1.74 | 0.70 |
| 1:S:721:LYS:CB | 1:S:736:GLN:CD | 2.56 | 0.70 |
| 2:T:111:SER:OG | 2:T:148:VAL:HG12 | 1.92 | 0.70 |
| 1:S:818:TYR:HE1 | 2:T:127:ARG:NH2 | 1.88 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:288:ASP:H | 4:5:203:THR:CG2 | 2.02 | 0.70 |
| 2:K:111:SER:OG | 2:K:148:VAL:HG12 | 1.92 | 0.70 |
| 1:M:553:MLY:HG2 | 4:2:47:MET:N | 2.07 | 0.70 |
| 1:S:782:MLY:C | 1:S:783:LEU:HD12 | 2.22 | 0.70 |
| 4:3:287:ILE:HG21 | 4:5:204:ALA:H | 1.54 | 0.70 |
| 1:D:630:ALA:O | 4:9:25:ASP:HB2 | 1.92 | 0.70 |
| 1:A:577:ALA:O | 1:A:578:HIS:CG | 2.45 | 0.70 |
| 2:B:111:SER:OG | 2:B:148:VAL:HG12 | 1.92 | 0.70 |
| 1:D:810:ARG:HG2 | 1:D:810:ARG:HH11 | 1.57 | 0.70 |
| 1:G:123:CYS:HB2 | 1:G:158:ILE:HD11 | 1.73 | 0.70 |
| 1:G:245:ARG:HD3 | 1:G:271:GLU:OE1 | 1.90 | 0.70 |
| 1:G:72:VAL:HG13 | 1:G:76:GLN:CB | 2.19 | 0.70 |
| 1:G:97:LEU:HD22 | 1:G:712:PRO:CB | 2.20 | 0.70 |
| 1:M:166:MET:HE1 | 1:M:254:PHE:HB2 | 1.72 | 0.70 |
| 1:M:579:PHE:HD2 | 1:M:592:ILE:HD11 | 1.57 | 0.70 |
| 1:M:782:MLY:C | 1:M:783:LEU:HD12 | 2.22 | 0.70 |
| 1:S:292:MET:HE3 | 1:S:309:PRO:HA | 1.74 | 0.70 |
| 1:S:733:PRO:C | 1:S:737:PHE:CD1 | 2.62 | 0.70 |
| 1:S:642:LYS:CG | 4:2:23:GLY:H | 1.77 | 0.69 |
| 1:A:215:GLN:CA | 1:A:340:ILE:CG2 | 2.63 | 0.69 |
| 1:D:546:THR:HG22 | 1:D:548:THR:N | 2.05 | 0.69 |
| 1:D:795:ARG:CD | 3:F:43:ASN:CG | 2.59 | 0.69 |
| 2:E:111:SER:OG | 2:E:148:VAL:HG12 | 1.92 | 0.69 |
| 1:G:97:LEU:HD23 | 1:G:712:PRO:CB | 2.20 | 0.69 |
| 1:M:546:THR:HG22 | 1:M:548:THR:N | 2.05 | 0.69 |
| 3:O:4:LYS:N | 3:O:5:ALA:O | 2.16 | 0.69 |
| 1:S:166:MET:HE3 | 1:S:254:PHE:CD2 | 2.27 | 0.69 |
| 1:S:274:ARG:NH2 | 1:S:282:GLU:OE1 | 2.24 | 0.69 |
| 1:D:541:MET:CG | 4:9:345:ILE:O | 2.41 | 0.69 |
| 1:A:752:ASP:O | 1:A:778:MET:SD | 2.49 | 0.69 |
| 1:A:782:MLY:C | 1:A:783:LEU:HD12 | 2.22 | 0.69 |
| 1:A:787:ILE:HG22 | 1:A:788:THR:N | 2.07 | 0.69 |
| 1:D:727:LEU:N | 1:D:782:MLY:HE2 | 2.07 | 0.69 |
| 1:G:577:ALA:O | 1:G:578:HIS:CG | 2.45 | 0.69 |
| 2:H:111:SER:OG | 2:H:148:VAL:HG12 | 1.92 | 0.69 |
| 1:J:577:ALA:O | 1:J:578:HIS:CG | 2.45 | 0.69 |
| 1:J:762:HIS:CD2 | 1:J:762:HIS:H | 2.07 | 0.69 |
| 1:M:206:LYS:HD3 | 1:M:217:THR:HG23 | 0.71 | 0.69 |
| 1:M:787:ILE:HG22 | 1:M:788:THR:N | 2.07 | 0.69 |
| 1:S:148:ARG:HH22 | 1:S:764:MLY:HH21 | 1.54 | 0.69 |
| 1:S:86:ASP:OD2 | 1:S:87:MLY:HH13 | 1.91 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:93:MET:CE | 1:S:716:LEU:HD12 | 2.22 | 0.69 |
| 4:9:1:ASP:HA | 4:9:4:GLU:HB3 | 1.74 | 0.69 |
| 1:D:713:SER:HB3 | 1:D:772:LEU:HD12 | 1.74 | 0.69 |
| 1:G:813:ILE:CG2 | 2:H:128:PHE:CZ | 2.74 | 0.69 |
| 1:J:756:THR:HG21 | 1:J:776:GLU:HA | 1.66 | 0.69 |
| 1:M:123:CYS:HB2 | 1:M:158:ILE:HD11 | 1.73 | 0.69 |
| 1:M:802:GLU:OE1 | 1:M:802:GLU:HA | 1.93 | 0.69 |
| 1:S:731:ALA:HB1 | 3:U:93:VAL:HB | 1.74 | 0.69 |
| 1:S:95:THR:CB | 1:S:713:SER:HB3 | 2.21 | 0.69 |
| 3:U:25:ILE:O | 3:U:63:ILE:HB | 1.92 | 0.69 |
| 4:1:244:ASP:CB | 4:Y:325:MET:CE | 2.70 | 0.69 |
| 1:M:630:ALA:O | 4:Z:25:ASP:CB | 2.41 | 0.69 |
| 4:1:3:ASP:HA | 4:1:6:THR:CB | 2.18 | 0.69 |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:CA | 2.04 | 0.69 |
| 2:B:117:LEU:CB | 2:B:147:ASN:OD1 | 2.39 | 0.69 |
| 3:C:25:ILE:O | 3:C:63:ILE:HB | 1.92 | 0.69 |
| 3:C:48:LYS:HB3 | 3:C:52:ASN:HD21 | 1.57 | 0.69 |
| 2:E:117:LEU:CB | 2:E:147:ASN:OD1 | 2.39 | 0.69 |
| 1:D:822:SER:OG | 2:E:88:LEU:HD22 | 1.91 | 0.69 |
| 1:G:752:ASP:OD2 | 1:G:780:ASP:O | 2.09 | 0.69 |
| 1:J:538:GLU:CD | 4:W:355:MET:HE3 | 2.12 | 0.69 |
| 1:J:798:LEU:CD1 | 3:L:126:LEU:HD13 | 2.17 | 0.69 |
| 1:J:836:PHE:CE2 | 2:K:160:GLY:HA3 | 2.27 | 0.69 |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CA | 2.19 | 0.69 |
| 1:M:806:MET:C | 1:M:807:VAL:CA | 2.60 | 0.69 |
| 1:S:643:GLY:N | 4:2:24:ASP:CA | 2.46 | 0.69 |
| 1:S:820:VAL:CG1 | 2:T:136:MET:CE | 2.70 | 0.69 |
| 4:W:1:ASP:HA | 4:W:4:GLU:HB3 | 1.74 | 0.69 |
| 4:7:1:ASP:HA | 4:7:4:GLU:HB3 | 1.74 | 0.69 |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:C | 1.96 | 0.69 |
| 1:A:800:ARG:NH2 | 3:C:40:ASN:ND2 | 2.38 | 0.69 |
| 1:A:815:CYS:O | 1:A:819:ASN:HB2 | 1.93 | 0.69 |
| 1:D:553:MLY:HG2 | 4:W:47:MET:N | 2.07 | 0.69 |
| 1:G:795:ARG:CB | 3:I:35:ARG:HH12 | 2.04 | 0.69 |
| 1:G:810:ARG:HH11 | 1:G:810:ARG:HG2 | 1.56 | 0.69 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:HA | 1.69 | 0.69 |
| 1:M:797:PHE:CZ | 3:O:146:ILE:HD13 | 2.27 | 0.69 |
| 1:S:123:CYS:HB2 | 1:S:158:ILE:HD11 | 1.73 | 0.69 |
| 1:S:787:ILE:HG22 | 1:S:788:THR:N | 2.07 | 0.69 |
| 4:W:3:ASP:HA | 4:W:6:THR:CB | 2.18 | 0.69 |
| 4:W:325:MET:CE | 4:Y:244:ASP:CB | 2.70 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:287:ILE:HG21 | 4:3:203:THR:N | 2.08 | 0.69 |
| 4:1:1:ASP:HA | 4:1:4:GLU:HB3 | 1.74 | 0.69 |
| 1:D:787:ILE:HG22 | 1:D:788:THR:N | 2.07 | 0.69 |
| 1:G:123:CYS:HB2 | 1:G:158:ILE:CD1 | 2.23 | 0.69 |
| 1:J:505:MLY:HD2 | 1:J:762:HIS:ND1 | 2.05 | 0.69 |
| 1:J:541:MET:CG | 4:W:345:ILE:O | 2.40 | 0.69 |
| 1:J:782:MLY:C | 1:J:783:LEU:HD12 | 2.22 | 0.69 |
| 1:S:120:GLY:O | 1:S:764:MLY:HH22 | 1.92 | 0.69 |
| 1:S:810:ARG:HG2 | 1:S:810:ARG:HH11 | 1.57 | 0.69 |
| 1:S:630:ALA:O | 4:2:25:ASP:HB2 | 1.92 | 0.69 |
| 4:1:287:ILE:HG21 | 4:3:204:ALA:N | 2.06 | 0.69 |
| 1:A:166:MET:HE3 | 1:A:254:PHE:CD2 | 2.28 | 0.69 |
| 1:A:166:MET:HE1 | 1:A:254:PHE:HB2 | 1.73 | 0.69 |
| 1:D:123:CYS:HB2 | 1:D:158:ILE:HD11 | 1.73 | 0.69 |
| 1:J:213:LYS:HA | 1:J:220:ASP:OD1 | 1.92 | 0.69 |
| 1:J:817:GLN:CB | 2:K:127:ARG:HD3 | 2.05 | 0.69 |
| 1:J:815:CYS:O | 1:J:819:ASN:HB2 | 1.93 | 0.69 |
| 1:M:72:VAL:HG13 | 1:M:76:GLN:CB | 2.19 | 0.69 |
| 1:A:630:ALA:O | 4:8:25:ASP:HB2 | 1.92 | 0.69 |
| 1:A:795:ARG:HB2 | 3:C:35:ARG:NH1 | 2.08 | 0.69 |
| 1:D:508:ILE:HD12 | 1:D:766:PHE:CZ | 2.16 | 0.69 |
| 1:D:782:MLY:C | 1:D:783:LEU:HD12 | 2.22 | 0.69 |
| 1:D:815:CYS:O | 1:D:819:ASN:HB2 | 1.93 | 0.69 |
| 1:D:792:ALA:HB2 | 3:F:42:THR:HG22 | 0.76 | 0.69 |
| 1:G:292:MET:HE3 | 1:G:309:PRO:HA | 1.74 | 0.69 |
| 1:G:534:SER:C | 4:V:351:THR:CA | 2.48 | 0.69 |
| 1:G:642:LYS:HB3 | 4:V:21:PHE:O | 1.92 | 0.69 |
| 1:G:787:ILE:HG22 | 1:G:788:THR:N | 2.07 | 0.69 |
| 1:J:93:MET:SD | 1:J:716:LEU:HB2 | 2.31 | 0.69 |
| 1:J:807:VAL:O | 1:J:810:ARG:HB2 | 1.93 | 0.69 |
| 1:J:810:ARG:HH11 | 1:J:810:ARG:HG2 | 1.57 | 0.69 |
| 1:M:783:LEU:O | 1:M:786:ILE:HB | 1.91 | 0.69 |
| 1:J:642:LYS:HB3 | 4:W:21:PHE:O | 1.92 | 0.69 |
| 4:X:1:ASP:HA | 4:X:4:GLU:HB3 | 1.74 | 0.69 |
| 4:4:1:ASP:HA | 4:4:4:GLU:HB3 | 1.74 | 0.69 |
| 1:A:732:ILE:CG2 | 1:A:747:LEU:HD11 | 1.26 | 0.69 |
| 3:I:48:LYS:HB3 | 3:I:52:ASN:HD21 | 1.56 | 0.69 |
| 1:J:643:GLY:N | 4:W:24:ASP:CA | 2.46 | 0.69 |
| 1:J:802:GLU:OE1 | 1:J:802:GLU:HA | 1.93 | 0.69 |
| 1:M:807:VAL:O | 1:M:810:ARG:HB2 | 1.93 | 0.69 |
| 1:S:805:ALA:O | 1:S:809:ARG:CB | 2.40 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:815:CYS:O | 1:S:819:ASN:HB2 | 1.93 | 0.69 |
| 1:M:630:ALA:O | 4:Z:25:ASP:HB2 | 1.91 | 0.69 |
| 4:3:322:PRO:CB | 4:5:244:ASP:HB3 | 2.12 | 0.69 |
| 1:D:807:VAL:O | 1:D:810:ARG:HB2 | 1.93 | 0.69 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:HD13 | 2.28 | 0.69 |
| 1:G:795:ARG:HB3 | 3:I:35:ARG:NH2 | 2.08 | 0.69 |
| 2:K:117:LEU:CB | 2:K:147:ASN:OD1 | 2.39 | 0.69 |
| 1:M:724:TYR:CE2 | 1:M:772:LEU:HD23 | 2.28 | 0.69 |
| 1:M:810:ARG:HH11 | 1:M:810:ARG:HG2 | 1.57 | 0.69 |
| 3:O:3:SER:O | 3:O:4:LYS:CB | 2.41 | 0.69 |
| 1:S:579:PHE:HD2 | 1:S:592:ILE:HD11 | 1.56 | 0.69 |
| 4:X:286:ASP:OD1 | 4:Z:202:THR:C | 2.31 | 0.69 |
| 4:5:3:ASP:HA | 4:5:6:THR:CB | 2.18 | 0.69 |
| 1:A:807:VAL:O | 1:A:810:ARG:HB2 | 1.93 | 0.69 |
| 1:D:213:LYS:HA | 1:D:220:ASP:OD1 | 1.92 | 0.69 |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD11 | 0.73 | 0.69 |
| 3:F:48:LYS:HB3 | 3:F:52:ASN:HD21 | 1.57 | 0.69 |
| 3:F:48:LYS:C | 3:F:52:ASN:HD21 | 1.97 | 0.69 |
| 1:G:533:PHE:O | 1:G:537:GLU:HG2 | 1.93 | 0.69 |
| 1:J:538:GLU:CD | 4:W:355:MET:CE | 2.62 | 0.69 |
| 1:M:123:CYS:HB2 | 1:M:158:ILE:CD1 | 2.23 | 0.69 |
| 1:M:533:PHE:O | 1:M:537:GLU:HG2 | 1.93 | 0.69 |
| 1:M:829:TRP:CZ2 | 2:N:87:LYS:CE | 2.65 | 0.69 |
| 1:S:807:VAL:O | 1:S:810:ARG:HB2 | 1.93 | 0.69 |
| 1:S:826:VAL:HG21 | 2:T:88:LEU:HD21 | 1.74 | 0.69 |
| 1:S:829:TRP:HZ3 | 2:T:84:PHE:CZ | 2.10 | 0.69 |
| 3:U:48:LYS:HB3 | 3:U:52:ASN:HD21 | 1.57 | 0.69 |
| 1:S:630:ALA:O | 4:2:25:ASP:CB | 2.41 | 0.68 |
| 4:5:1:ASP:HA | 4:5:4:GLU:HB3 | 1.74 | 0.68 |
| 1:A:642:LYS:HB3 | 4:8:21:PHE:O | 1.93 | 0.68 |
| 1:A:810:ARG:HG2 | 1:A:810:ARG:HH11 | 1.57 | 0.68 |
| 1:A:92:ALA:O | 1:A:713:SER:HA | 1.93 | 0.68 |
| 1:D:62:VAL:HG12 | 1:D:63:MLY:O | 1.93 | 0.68 |
| 1:D:762:HIS:H | 1:D:762:HIS:CD2 | 2.08 | 0.68 |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:CB | 2.23 | 0.68 |
| 1:J:62:VAL:HG12 | 1:J:63:MLY:O | 1.93 | 0.68 |
| 1:J:839:MLY:CH2 | 2:K:158:THR:HG22 | 2.22 | 0.68 |
| 3:L:48:LYS:HB3 | 3:L:52:ASN:HD21 | 1.57 | 0.68 |
| 1:S:166:MET:HE1 | 1:S:254:PHE:HB2 | 1.75 | 0.68 |
| 1:J:630:ALA:O | 4:W:25:ASP:CB | 2.41 | 0.68 |
| 4:W:325:MET:HE2 | 4:Y:244:ASP:CG | 2.06 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:798:LEU:HG | 3:I:122:GLU:HB3 | 1.74 | 0.68 |
| 1:J:787:ILE:HG22 | 1:J:788:THR:N | 2.07 | 0.68 |
| 1:M:541:MET:CG | 4:Z:345:ILE:O | 2.40 | 0.68 |
| 3:O:25:ILE:O | 3:O:63:ILE:HB | 1.92 | 0.68 |
| 1:M:642:LYS:HB3 | 4:Z:21:PHE:O | 1.92 | 0.68 |
| 1:S:546:THR:CG2 | 4:4:46:GLY:C | 2.62 | 0.68 |
| 1:A:97:LEU:HD22 | 1:A:712:PRO:HB2 | 1.75 | 0.68 |
| 1:G:213:LYS:HA | 1:G:220:ASP:OD1 | 1.92 | 0.68 |
| 1:J:533:PHE:O | 1:J:537:GLU:HG2 | 1.93 | 0.68 |
| 3:L:25:ILE:O | 3:L:63:ILE:HB | 1.92 | 0.68 |
| 1:M:652:LEU:O | 1:M:655:GLU:N | 2.26 | 0.68 |
| 2:N:111:SER:OG | 2:N:148:VAL:HG12 | 1.92 | 0.68 |
| 1:S:652:LEU:O | 1:S:655:GLU:N | 2.27 | 0.68 |
| 1:S:707:CYS:CA | 1:S:714:ARG:HH22 | 2.05 | 0.68 |
| 1:S:731:ALA:CB | 3:U:93:VAL:HB | 2.22 | 0.68 |
| 1:D:557:GLU:N | 4:W:48:GLY:HA3 | 1.90 | 0.68 |
| 1:S:541:MET:CG | 4:2:345:ILE:O | 2.40 | 0.68 |
| 1:A:149:GLN:HE21 | 1:A:718:ALA:CB | 1.91 | 0.68 |
| 1:A:56:GLU:CB | 1:A:59:MLY:HB3 | 2.20 | 0.68 |
| 1:A:652:LEU:O | 1:A:655:GLU:N | 2.27 | 0.68 |
| 1:A:802:GLU:OE1 | 1:A:802:GLU:HA | 1.93 | 0.68 |
| 1:A:822:SER:CB | 2:B:88:LEU:CD2 | 2.66 | 0.68 |
| 1:A:795:ARG:CG | 3:C:35:ARG:NH1 | 2.52 | 0.68 |
| 1:M:733:PRO:C | 1:M:737:PHE:CD1 | 2.62 | 0.68 |
| 1:S:642:LYS:HB3 | 4:2:21:PHE:O | 1.92 | 0.68 |
| 1:A:630:ALA:O | 4:8:25:ASP:CB | 2.41 | 0.68 |
| 1:D:642:LYS:HB3 | 4:9:21:PHE:O | 1.93 | 0.68 |
| 1:A:553:MLY:HG2 | 4:V:47:MET:N | 2.07 | 0.68 |
| 1:G:754:ASP:CG | 1:G:779:ARG:CD | 2.57 | 0.68 |
| 1:G:784:ALA:O | 1:G:788:THR:HB | 1.94 | 0.68 |
| 1:G:807:VAL:O | 1:G:810:ARG:HB2 | 1.93 | 0.68 |
| 1:J:123:CYS:HB2 | 1:J:158:ILE:CD1 | 2.23 | 0.68 |
| 1:M:553:MLY:CG | 4:2:47:MET:N | 2.54 | 0.68 |
| 3:O:48:LYS:HB3 | 3:O:52:ASN:HD21 | 1.57 | 0.68 |
| 1:S:123:CYS:HB2 | 1:S:158:ILE:CD1 | 2.23 | 0.68 |
| 1:S:506:GLU:OE2 | 1:S:760:PHE:CG | 2.43 | 0.68 |
| 1:S:795:ARG:CB | 3:U:35:ARG:HH12 | 2.05 | 0.68 |
| 1:J:530:MET:HE3 | 4:W:354:GLN:HG2 | 1.72 | 0.68 |
| 1:S:544:LYS:HB3 | 4:4:45:VAL:HG22 | 1.76 | 0.68 |
| 1:D:630:ALA:O | 4:9:25:ASP:CB | 2.41 | 0.68 |
| 1:A:123:CYS:HB2 | 1:A:158:ILE:CD1 | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:505:MLY:HB2 | 1:A:762:HIS:N | 2.09 | 0.68 |
| 1:D:643:GLY:N | 4:9:24:ASP:CA | 2.46 | 0.68 |
| 1:D:732:ILE:HD12 | 1:D:782:MLY:HH13 | 1.76 | 0.68 |
| 1:D:836:PHE:HZ | 2:E:160:GLY:H | 0.68 | 0.68 |
| 1:G:782:MLY:C | 1:G:783:LEU:HD12 | 2.22 | 0.68 |
| 1:G:817:GLN:CB | 2:H:127:ARG:HD2 | 2.22 | 0.68 |
| 1:J:557:GLU:HA | 4:Y:48:GLY:CA | 2.18 | 0.68 |
| 1:J:819:ASN:OD1 | 2:K:92:ASP:HB2 | 1.93 | 0.68 |
| 1:M:785:GLU:O | 1:M:787:ILE:N | 2.26 | 0.68 |
| 1:M:836:PHE:CE2 | 2:N:160:GLY:HA3 | 2.29 | 0.68 |
| 1:S:72:VAL:HG13 | 1:S:76:GLN:CB | 2.19 | 0.68 |
| 1:S:732:ILE:HG21 | 1:S:747:LEU:HD11 | 0.73 | 0.68 |
| 4:V:1:ASP:HA | 4:V:4:GLU:HB3 | 1.74 | 0.68 |
| 1:J:530:MET:HE2 | 4:W:354:GLN:HG3 | 1.74 | 0.68 |
| 4:8:1:ASP:HA | 4:8:4:GLU:HB3 | 1.74 | 0.68 |
| 1:G:553:MLY:CD | 4:X:45:VAL:HG12 | 2.23 | 0.68 |
| 1:G:652:LEU:O | 1:G:655:GLU:N | 2.27 | 0.68 |
| 1:G:829:TRP:HZ3 | 2:H:84:PHE:CE1 | 2.12 | 0.68 |
| 3:I:3:SER:O | 3:I:4:LYS:CB | 2.41 | 0.68 |
| 1:J:553:MLY:HH12 | 4:Y:45:VAL:CG2 | 2.21 | 0.68 |
| 1:J:84:MLY:CH2 | 1:J:720:PHE:CA | 2.07 | 0.68 |
| 1:J:819:ASN:OD1 | 2:K:92:ASP:CB | 2.42 | 0.68 |
| 1:S:52:ILE:HD13 | 1:S:52:ILE:N | 2.09 | 0.68 |
| 1:S:786:ILE:C | 1:S:788:THR:N | 2.47 | 0.68 |
| 2:T:117:LEU:CB | 2:T:147:ASN:OD1 | 2.39 | 0.68 |
| 1:J:553:MLY:CD | 4:Y:45:VAL:HG12 | 2.23 | 0.68 |
| 4:1:160:THR:HG21 | 4:1:274:ILE:HD11 | 1.76 | 0.68 |
| 4:1:153:LEU:HD11 | 4:1:274:ILE:HG13 | 1.76 | 0.68 |
| 4:4:160:THR:HG21 | 4:4:274:ILE:HD11 | 1.75 | 0.68 |
| 1:A:541:MET:CG | 4:8:345:ILE:O | 2.40 | 0.68 |
| 2:B:117:LEU:CB | 2:B:147:ASN:ND2 | 2.35 | 0.68 |
| 1:D:123:CYS:HB2 | 1:D:158:ILE:CD1 | 2.23 | 0.68 |
| 1:G:206:LYS:HD3 | 1:G:217:THR:HG23 | 0.70 | 0.68 |
| 1:G:557:GLU:HA | 4:X:48:GLY:CA | 2.18 | 0.68 |
| 1:J:550:PHE:HE2 | 1:J:592:ILE:HG23 | 1.59 | 0.68 |
| 1:M:213:LYS:HA | 1:M:220:ASP:OD1 | 1.92 | 0.68 |
| 1:S:213:LYS:HA | 1:S:220:ASP:OD1 | 1.92 | 0.68 |
| 4:Y:1:ASP:HA | 4:Y:4:GLU:HB3 | 1.74 | 0.68 |
| 4:Y:160:THR:HG21 | 4:Y:274:ILE:HD11 | 1.76 | 0.68 |
| 4:2:160:THR:HG21 | 4:2:274:ILE:HD11 | 1.76 | 0.68 |
| 4:3:153:LEU:HD11 | 4:3:274:ILE:HG13 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:LYS:HA | 1:A:220:ASP:OD1 | 1.92 | 0.68 |
| 1:A:499:GLU:CD | 1:A:766:PHE:CZ | 2.66 | 0.68 |
| 3:C:3:SER:O | 3:C:4:LYS:CB | 2.41 | 0.68 |
| 1:D:823:PHE:CD1 | 2:E:160:GLY:HA2 | 2.28 | 0.68 |
| 1:G:739:ASP:CB | 1:G:742:LYS:HB3 | 2.12 | 0.68 |
| 1:G:797:PHE:CE1 | 3:I:146:ILE:HA | 2.29 | 0.68 |
| 1:G:815:CYS:O | 1:G:819:ASN:HB2 | 1.93 | 0.68 |
| 1:G:831:TRP:HH2 | 2:H:47:LEU:HD21 | 0.63 | 0.68 |
| 1:G:84:MLY:HH21 | 1:G:719:ASP:C | 2.12 | 0.68 |
| 1:J:788:THR:O | 3:L:42:THR:CG2 | 2.37 | 0.68 |
| 2:K:117:LEU:CG | 2:K:147:ASN:HB3 | 2.24 | 0.68 |
| 1:J:795:ARG:C | 3:L:35:ARG:CZ | 2.63 | 0.68 |
| 1:M:52:ILE:N | 1:M:52:ILE:HD13 | 2.09 | 0.68 |
| 1:S:550:PHE:HE2 | 1:S:592:ILE:HG23 | 1.59 | 0.68 |
| 1:S:95:THR:CA | 1:S:713:SER:HB3 | 2.24 | 0.68 |
| 1:S:746:LYS:HZ3 | 3:U:96:LYS:HA | 1.59 | 0.68 |
| 4:2:287:ILE:CG1 | 4:4:203:THR:H | 2.03 | 0.68 |
| 4:6:160:THR:HG21 | 4:6:274:ILE:HD11 | 1.75 | 0.68 |
| 1:A:643:GLY:N | 4:8:24:ASP:CA | 2.46 | 0.68 |
| 1:D:91:MET:HE3 | 1:D:119:SER:HB2 | 1.76 | 0.68 |
| 2:K:117:LEU:HD11 | 2:K:147:ASN:HB3 | 1.76 | 0.68 |
| 3:L:3:SER:O | 3:L:4:LYS:CB | 2.41 | 0.68 |
| 1:M:408:VAL:HG12 | 4:Z:332:PRO:HB3 | 1.75 | 0.68 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:HD21 | 0.72 | 0.68 |
| 1:S:802:GLU:HA | 1:S:802:GLU:OE1 | 1.93 | 0.68 |
| 4:8:153:LEU:HD11 | 4:8:274:ILE:HG13 | 1.76 | 0.67 |
| 1:A:533:PHE:O | 1:A:537:GLU:HG2 | 1.93 | 0.67 |
| 1:A:546:THR:H | 1:A:549:SER:HB3 | 1.60 | 0.67 |
| 1:A:505:MLY:HG2 | 1:A:762:HIS:CD2 | 2.28 | 0.67 |
| 1:D:533:PHE:O | 1:D:537:GLU:HG2 | 1.93 | 0.67 |
| 1:D:814:PHE:CE1 | 2:E:127:ARG:CZ | 2.77 | 0.67 |
| 1:D:820:VAL:HG11 | 2:E:136:MET:HE3 | 1.75 | 0.67 |
| 3:F:3:SER:O | 3:F:4:LYS:CB | 2.41 | 0.67 |
| 1:G:541:MET:CG | 4:V:345:ILE:O | 2.41 | 0.67 |
| 1:J:652:LEU:O | 1:J:655:GLU:N | 2.26 | 0.67 |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:HG2 | 1.57 | 0.67 |
| 1:M:546:THR:H | 1:M:549:SER:HB3 | 1.59 | 0.67 |
| 3:U:3:SER:O | 3:U:4:LYS:CB | 2.41 | 0.67 |
| 1:A:58:GLY:HA2 | 1:A:74:GLU:OE1 | 1.94 | 0.67 |
| 1:A:795:ARG:NE | 3:C:116:GLU:OE2 | 2.26 | 0.67 |
| 1:G:546:THR:H | 1:G:549:SER:HB3 | 1.59 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:753:VAL:C | 1:G:779:ARG:HD3 | 2.13 | 0.67 |
| 1:J:374:GLN:HG3 | 1:J:375:ALA:H | 1.59 | 0.67 |
| 1:J:801:VAL:CG2 | 3:L:126:LEU:CD2 | 2.66 | 0.67 |
| 1:M:550:PHE:HE2 | 1:M:592:ILE:HG23 | 1.59 | 0.67 |
| 1:M:815:CYS:O | 1:M:819:ASN:HB2 | 1.93 | 0.67 |
| 1:S:538:GLU:CD | 4:2:355:MET:CE | 2.62 | 0.67 |
| 1:S:749:GLY:HA3 | 3:U:93:VAL:HG22 | 1.76 | 0.67 |
| 1:S:84:MLY:HD3 | 1:S:723:ARG:HD2 | 1.75 | 0.67 |
| 4:3:1:ASP:HA | 4:3:4:GLU:HB3 | 1.74 | 0.67 |
| 1:G:802:GLU:OE1 | 1:G:802:GLU:HA | 1.93 | 0.67 |
| 1:M:166:MET:HE3 | 1:M:254:PHE:CD2 | 2.29 | 0.67 |
| 1:M:58:GLY:HA2 | 1:M:74:GLU:OE1 | 1.95 | 0.67 |
| 1:M:95:THR:OG1 | 1:M:770:GLY:CA | 2.43 | 0.67 |
| 1:M:817:GLN:HG3 | 2:N:128:PHE:CE1 | 2.30 | 0.67 |
| 1:S:408:VAL:HG12 | 4:2:332:PRO:HB3 | 1.76 | 0.67 |
| 1:S:533:PHE:O | 1:S:537:GLU:HG2 | 1.93 | 0.67 |
| 1:S:795:ARG:HG2 | 3:U:118:MET:HE1 | 0.70 | 0.67 |
| 2:T:117:LEU:CG | 2:T:147:ASN:HB3 | 2.25 | 0.67 |
| 4:Y:153:LEU:HD11 | 4:Y:274:ILE:HG13 | 1.76 | 0.67 |
| 1:A:538:GLU:CD | 4:8:355:MET:CE | 2.62 | 0.67 |
| 2:B:141:PRO:O | 2:B:145:ALA:CB | 2.43 | 0.67 |
| 1:D:131:TRP:O | 1:D:132:LEU:HD12 | 1.95 | 0.67 |
| 1:D:612:GLN:NE2 | 1:D:627:GLY:N | 2.43 | 0.67 |
| 2:E:163:ALA:O | 2:K:21:GLU:CA | 2.43 | 0.67 |
| 1:M:795:ARG:CZ | 3:O:116:GLU:OE2 | 2.42 | 0.67 |
| 2:N:117:LEU:HD11 | 2:N:147:ASN:HB3 | 1.76 | 0.67 |
| 3:O:48:LYS:C | 3:O:52:ASN:HD21 | 1.96 | 0.67 |
| 1:S:290:GLN:O | 1:S:331:LEU:HD12 | 1.95 | 0.67 |
| 1:S:751:GLY:C | 1:S:779:ARG:HH22 | 1.97 | 0.67 |
| 1:S:836:PHE:CD2 | 2:T:160:GLY:CA | 2.77 | 0.67 |
| 2:T:141:PRO:O | 2:T:145:ALA:CB | 2.43 | 0.67 |
| 4:5:153:LEU:HD11 | 4:5:274:ILE:HG13 | 1.76 | 0.67 |
| 1:D:530:MET:HE2 | 4:9:354:GLN:HG3 | 1.75 | 0.67 |
| 1:A:290:GLN:O | 1:A:331:LEU:HD12 | 1.95 | 0.67 |
| 1:D:546:THR:H | 1:D:549:SER:HB3 | 1.59 | 0.67 |
| 1:G:754:ASP:C | 1:G:776:GLU:OE1 | 2.09 | 0.67 |
| 1:J:546:THR:H | 1:J:549:SER:HB3 | 1.59 | 0.67 |
| 2:N:117:LEU:CB | 2:N:147:ASN:OD1 | 2.39 | 0.67 |
| 1:S:537:GLU:C | 4:2:351:THR:H | 1.98 | 0.67 |
| 2:T:117:LEU:HD11 | 2:T:147:ASN:HB3 | 1.76 | 0.67 |
| 1:S:793:ARG:HA | 3:U:40:ASN:HB3 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:325:MET:HE2 | 4:X:244:ASP:CG | 2.08 | 0.67 |
| 4:Z:160:THR:HG21 | 4:Z:274:ILE:HD11 | 1.76 | 0.67 |
| 1:A:52:ILE:HD13 | 1:A:52:ILE:N | 2.08 | 0.67 |
| 1:A:752:ASP:CB | 1:A:782:MLY:HD3 | 2.24 | 0.67 |
| 1:D:652:LEU:O | 1:D:655:GLU:N | 2.27 | 0.67 |
| 1:G:550:PHE:HE2 | 1:G:592:ILE:HG23 | 1.59 | 0.67 |
| 1:J:721:LYS:HG2 | 1:J:736:GLN:CD | 1.86 | 0.67 |
| 1:J:768:MLY:CB | 1:J:773:GLY:HA2 | 1.71 | 0.67 |
| 1:J:757:GLN:HA | 1:J:776:GLU:CB | 2.25 | 0.67 |
| 3:L:48:LYS:C | 3:L:52:ASN:HD21 | 1.97 | 0.67 |
| 1:S:549:SER:HB2 | 4:4:43:VAL:CG2 | 2.24 | 0.67 |
| 1:S:806:MET:C | 1:S:807:VAL:N | 2.47 | 0.67 |
| 4:W:153:LEU:HD11 | 4:W:274:ILE:HG13 | 1.76 | 0.67 |
| 4:3:324:THR:OG1 | 4:5:244:ASP:HB3 | 1.95 | 0.67 |
| 4:9:160:THR:HG21 | 4:9:274:ILE:HD11 | 1.75 | 0.67 |
| 1:A:149:GLN:HG2 | 1:A:719:ASP:H | 1.59 | 0.67 |
| 1:A:829:TRP:HE1 | 2:B:67:MET:HG2 | 1.58 | 0.67 |
| 1:A:830:PRO:HB2 | 2:B:51:PHE:CE1 | 2.30 | 0.67 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:CD | 2.47 | 0.67 |
| 1:J:52:ILE:HD13 | 1:J:52:ILE:N | 2.09 | 0.67 |
| 2:N:141:PRO:O | 2:N:145:ALA:CB | 2.43 | 0.67 |
| 1:S:546:THR:H | 1:S:549:SER:HB3 | 1.59 | 0.67 |
| 4:2:112:PRO:HG2 | 4:3:197:GLY:HA2 | 1.75 | 0.67 |
| 4:3:160:THR:HG21 | 4:3:274:ILE:HD11 | 1.76 | 0.67 |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:HA3 | 1.59 | 0.67 |
| 1:D:712:PRO:HB2 | 1:D:771:LEU:CD2 | 2.25 | 0.67 |
| 1:G:801:VAL:HG21 | 3:I:126:LEU:CD2 | 2.23 | 0.67 |
| 1:J:537:GLU:C | 4:W:351:THR:H | 1.98 | 0.67 |
| 1:J:612:GLN:NE2 | 1:J:627:GLY:N | 2.43 | 0.67 |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:HD1 | 1.59 | 0.67 |
| 1:S:166:MET:HE3 | 1:S:254:PHE:HD2 | 1.59 | 0.67 |
| 1:S:648:THR:CB | 4:2:350:SER:OG | 2.43 | 0.67 |
| 1:S:791:GLN:HE22 | 3:U:115:GLY:C | 1.98 | 0.67 |
| 1:S:795:ARG:HH21 | 3:U:116:GLU:HB3 | 0.99 | 0.67 |
| 4:V:153:LEU:HD11 | 4:V:274:ILE:HG13 | 1.76 | 0.67 |
| 4:2:167:GLU:OE2 | 4:4:43:VAL:O | 2.12 | 0.67 |
| 1:A:61:THR:HG23 | 1:A:71:THR:OG1 | 1.94 | 0.67 |
| 1:A:739:ASP:CB | 1:A:742:LYS:HB3 | 2.12 | 0.67 |
| 1:D:52:ILE:N | 1:D:52:ILE:HD13 | 2.09 | 0.67 |
| 1:D:648:THR:CB | 4:9:350:SER:OG | 2.43 | 0.67 |
| 1:D:727:LEU:HB2 | 1:D:782:MLY:HH13 | 0.68 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:141:PRO:O | 2:E:145:ALA:CB | 2.43 | 0.67 |
| 1:G:797:PHE:HE2 | 3:I:126:LEU:HD22 | 0.87 | 0.67 |
| 1:J:131:TRP:O | 1:J:132:LEU:HD12 | 1.95 | 0.67 |
| 1:J:58:GLY:HA2 | 1:J:74:GLU:OE1 | 1.95 | 0.67 |
| 2:K:141:PRO:O | 2:K:145:ALA:CB | 2.43 | 0.67 |
| 1:S:374:GLN:HG3 | 1:S:375:ALA:H | 1.59 | 0.67 |
| 1:S:739:ASP:CB | 1:S:742:LYS:HB3 | 2.12 | 0.67 |
| 4:W:160:THR:HG21 | 4:W:274:ILE:HD11 | 1.76 | 0.67 |
| 1:G:556:ASP:OD2 | 4:X:47:MET:HE2 | 1.91 | 0.67 |
| 1:A:537:GLU:C | 4:8:351:THR:H | 1.99 | 0.67 |
| 1:A:499:GLU:OE2 | 1:A:766:PHE:HE2 | 1.77 | 0.67 |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:ND2 | 2.10 | 0.67 |
| 1:D:550:PHE:HE2 | 1:D:592:ILE:HG23 | 1.59 | 0.67 |
| 1:D:58:GLY:HA2 | 1:D:74:GLU:OE1 | 1.95 | 0.67 |
| 1:D:727:LEU:CA | 1:D:782:MLY:HE2 | 2.25 | 0.67 |
| 1:G:78:PHE:HB3 | 1:G:98:HIS:CD2 | 2.30 | 0.67 |
| 1:G:829:TRP:CH2 | 2:H:87:LYS:NZ | 2.63 | 0.67 |
| 2:H:117:LEU:CG | 2:H:147:ASN:HB3 | 2.24 | 0.67 |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:ND2 | 2.10 | 0.67 |
| 1:J:792:ALA:H | 3:L:42:THR:CG2 | 2.08 | 0.67 |
| 1:M:292:MET:HE3 | 1:M:309:PRO:HA | 1.77 | 0.67 |
| 1:M:648:THR:CB | 4:Z:350:SER:OG | 2.43 | 0.67 |
| 4:X:153:LEU:HD11 | 4:X:274:ILE:HG13 | 1.76 | 0.67 |
| 4:X:160:THR:HG21 | 4:X:274:ILE:HD11 | 1.76 | 0.67 |
| 4:4:153:LEU:HD11 | 4:4:274:ILE:HG13 | 1.76 | 0.66 |
| 1:S:546:THR:HG21 | 4:4:47:MET:CA | 2.25 | 0.66 |
| 4:7:160:THR:HG21 | 4:7:274:ILE:HD11 | 1.76 | 0.66 |
| 1:D:635:GLY:O | 4:9:341:ILE:HG21 | 1.95 | 0.66 |
| 1:A:78:PHE:HB3 | 1:A:98:HIS:CD2 | 2.30 | 0.66 |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:CG2 | 2.25 | 0.66 |
| 2:E:150:TYR:C | 2:E:151:LYS:CG | 2.48 | 0.66 |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:HD1 | 1.59 | 0.66 |
| 1:G:217:THR:O | 1:G:221:GLN:HG2 | 1.95 | 0.66 |
| 1:G:62:VAL:HG12 | 1:G:63:MLY:O | 1.94 | 0.66 |
| 1:G:503:TYR:HE1 | 1:G:711:PHE:CE2 | 2.11 | 0.66 |
| 1:G:817:GLN:CG | 2:H:127:ARG:CD | 2.73 | 0.66 |
| 1:J:648:THR:CB | 4:W:350:SER:OG | 2.43 | 0.66 |
| 1:J:818:TYR:OH | 2:K:127:ARG:NH2 | 2.27 | 0.66 |
| 1:M:217:THR:O | 1:M:221:GLN:HG2 | 1.95 | 0.66 |
| 1:M:290:GLN:O | 1:M:331:LEU:HD12 | 1.95 | 0.66 |
| 1:M:480:ILE:HG22 | 1:M:481:ASN:ND2 | 2.10 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:803:TYR:O | 1:M:807:VAL:N | 2.28 | 0.66 |
| 3:O:24:LYS:HA | 3:O:63:ILE:O | 1.96 | 0.66 |
| 1:S:534:SER:C | 4:2:351:THR:CA | 2.47 | 0.66 |
| 4:9:153:LEU:HD11 | 4:9:274:ILE:HG13 | 1.76 | 0.66 |
| 3:C:24:LYS:HA | 3:C:63:ILE:O | 1.95 | 0.66 |
| 1:D:418:THR:HG22 | 1:D:419:VAL:N | 2.11 | 0.66 |
| 1:D:802:GLU:HA | 1:D:802:GLU:OE1 | 1.93 | 0.66 |
| 2:E:117:LEU:CG | 2:E:147:ASN:HB3 | 2.24 | 0.66 |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:CG2 | 2.21 | 0.66 |
| 1:J:290:GLN:O | 1:J:331:LEU:HD12 | 1.95 | 0.66 |
| 3:L:24:LYS:HA | 3:L:63:ILE:O | 1.95 | 0.66 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:C | 2.16 | 0.66 |
| 3:O:102:VAL:HG23 | 3:O:139:TYR:HD1 | 1.59 | 0.66 |
| 1:S:90:ASP:OD1 | 1:S:764:MLY:HH11 | 1.95 | 0.66 |
| 4:4:288:ASP:CB | 4:6:203:THR:HG21 | 2.25 | 0.66 |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:ND2 | 2.10 | 0.66 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:HD13 | 2.19 | 0.66 |
| 2:B:117:LEU:CG | 2:B:147:ASN:HB3 | 2.24 | 0.66 |
| 1:A:836:PHE:HB3 | 2:B:161:GLU:OE1 | 1.95 | 0.66 |
| 1:D:290:GLN:O | 1:D:331:LEU:HD12 | 1.95 | 0.66 |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:N | 2.29 | 0.66 |
| 1:G:52:ILE:HD13 | 1:G:52:ILE:N | 2.09 | 0.66 |
| 1:G:503:TYR:CZ | 1:G:711:PHE:CD2 | 2.83 | 0.66 |
| 1:G:757:GLN:HG3 | 1:G:776:GLU:CB | 2.15 | 0.66 |
| 1:G:753:VAL:C | 1:G:779:ARG:HH11 | 1.91 | 0.66 |
| 1:J:166:MET:HE3 | 1:J:254:PHE:CD2 | 2.30 | 0.66 |
| 1:J:408:VAL:HG12 | 4:W:332:PRO:HB3 | 1.76 | 0.66 |
| 1:J:418:THR:HG22 | 1:J:419:VAL:N | 2.11 | 0.66 |
| 1:J:505:MLY:CG | 1:J:762:HIS:HE1 | 2.08 | 0.66 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:C | 2.16 | 0.66 |
| 1:M:537:GLU:C | 4:Z:351:THR:H | 1.98 | 0.66 |
| 1:M:62:VAL:HG12 | 1:M:63:MLY:O | 1.94 | 0.66 |
| 1:M:78:PHE:HB3 | 1:M:98:HIS:CD2 | 2.30 | 0.66 |
| 4:Z:153:LEU:HD11 | 4:Z:274:ILE:HG13 | 1.76 | 0.66 |
| 1:A:707:CYS:CA | 1:A:714:ARG:NH1 | 2.41 | 0.66 |
| 1:A:809:ARG:HH12 | 2:B:124:GLY:HA2 | 1.61 | 0.66 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:HD13 | 2.28 | 0.66 |
| 1:D:322:VAL:HB | 1:D:325:ILE:CD1 | 2.26 | 0.66 |
| 1:D:709:LYS:C | 1:D:710:GLY:CA | 2.63 | 0.66 |
| 1:D:61:THR:HG23 | 1:D:71:THR:OG1 | 1.95 | 0.66 |
| 1:G:612:GLN:NE2 | 1:G:627:GLY:N | 2.43 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:754:ASP:CA | 1:G:779:ARG:HD3 | 2.07 | 0.66 |
| 1:J:78:PHE:HB3 | 1:J:98:HIS:CD2 | 2.30 | 0.66 |
| 1:J:834:LEU:HD12 | 2:K:51:PHE:CE1 | 2.26 | 0.66 |
| 1:M:797:PHE:CE1 | 3:O:146:ILE:HA | 2.31 | 0.66 |
| 1:S:480:ILE:HG22 | 1:S:481:ASN:ND2 | 2.10 | 0.66 |
| 1:S:612:GLN:NE2 | 1:S:627:GLY:N | 2.43 | 0.66 |
| 2:T:150:TYR:C | 2:T:151:LYS:CG | 2.49 | 0.66 |
| 3:U:102:VAL:HG23 | 3:U:139:TYR:HD1 | 1.59 | 0.66 |
| 4:V:325:MET:CE | 4:X:244:ASP:CB | 2.70 | 0.66 |
| 1:J:642:LYS:CD | 4:W:24:ASP:O | 2.43 | 0.66 |
| 1:A:648:THR:CB | 4:8:350:SER:OG | 2.43 | 0.66 |
| 1:A:374:GLN:HG3 | 1:A:375:ALA:H | 1.60 | 0.66 |
| 1:A:550:PHE:HE2 | 1:A:592:ILE:HG23 | 1.59 | 0.66 |
| 1:D:217:THR:O | 1:D:221:GLN:HG2 | 1.94 | 0.66 |
| 1:G:408:VAL:HG12 | 4:V:332:PRO:HB3 | 1.76 | 0.66 |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:ND2 | 2.10 | 0.66 |
| 1:G:537:GLU:C | 4:V:351:THR:H | 1.99 | 0.66 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:N | 2.29 | 0.66 |
| 1:G:149:GLN:CB | 1:G:763:THR:CG2 | 2.73 | 0.66 |
| 3:I:24:LYS:HA | 3:I:63:ILE:O | 1.95 | 0.66 |
| 1:J:97:LEU:CD2 | 1:J:712:PRO:CB | 2.74 | 0.66 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:HD13 | 2.20 | 0.66 |
| 1:M:791:GLN:CD | 3:O:116:GLU:H | 1.96 | 0.66 |
| 1:S:802:GLU:OE2 | 1:S:809:ARG:CZ | 2.44 | 0.66 |
| 1:J:635:GLY:O | 4:W:341:ILE:HG21 | 1.95 | 0.66 |
| 4:1:247:VAL:H | 4:Y:324:THR:HG23 | 1.61 | 0.66 |
| 1:S:530:MET:CA | 4:2:354:GLN:CB | 2.74 | 0.66 |
| 4:6:153:LEU:HD11 | 4:6:274:ILE:HG13 | 1.76 | 0.66 |
| 1:A:408:VAL:HG12 | 4:8:332:PRO:HB3 | 1.76 | 0.66 |
| 1:A:501:GLU:O | 1:A:762:HIS:CG | 2.48 | 0.66 |
| 1:A:538:GLU:HA | 4:8:349:LEU:HB3 | 1.78 | 0.66 |
| 1:A:174:SER:O | 1:A:670:HIS:HB2 | 1.96 | 0.66 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:C | 2.16 | 0.66 |
| 1:D:732:ILE:CG2 | 1:D:747:LEU:HD11 | 1.26 | 0.66 |
| 1:J:339:ASP:OD1 | 1:J:348:MLY:HH13 | 1.95 | 0.66 |
| 2:K:141:PRO:O | 2:K:145:ALA:HB2 | 1.96 | 0.66 |
| 1:M:829:TRP:HZ3 | 2:N:84:PHE:CZ | 2.13 | 0.66 |
| 1:M:798:LEU:HD13 | 3:O:126:LEU:HD21 | 1.58 | 0.66 |
| 1:S:217:THR:O | 1:S:221:GLN:HG2 | 1.95 | 0.66 |
| 1:S:78:PHE:HB3 | 1:S:98:HIS:CD2 | 2.30 | 0.66 |
| 4:1:167:GLU:OE1 | 4:3:44:MET:HA | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:153:LEU:HD11 | 4:7:274:ILE:HG13 | 1.76 | 0.66 |
| 1:A:144:ARG:NH1 | 1:A:160:ASP:OD1 | 2.29 | 0.66 |
| 1:A:418:THR:HG22 | 1:A:419:VAL:N | 2.11 | 0.66 |
| 1:A:612:GLN:NE2 | 1:A:627:GLY:N | 2.43 | 0.66 |
| 1:D:226:ASN:HB2 | 1:D:227:PRO:HD3 | 1.78 | 0.66 |
| 1:D:829:TRP:CZ3 | 2:E:84:PHE:CZ | 2.84 | 0.66 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:HD13 | 2.19 | 0.66 |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:N | 2.11 | 0.66 |
| 1:G:58:GLY:HA2 | 1:G:74:GLU:OE1 | 1.95 | 0.66 |
| 1:G:788:THR:O | 3:I:42:THR:CG2 | 2.43 | 0.66 |
| 1:J:817:GLN:HG3 | 2:K:128:PHE:CE1 | 2.31 | 0.66 |
| 3:L:48:LYS:O | 3:L:52:ASN:CG | 2.34 | 0.66 |
| 1:M:226:ASN:HB2 | 1:M:227:PRO:HD3 | 1.78 | 0.66 |
| 1:M:534:SER:C | 4:Z:351:THR:CA | 2.47 | 0.66 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:N | 2.29 | 0.66 |
| 2:N:141:PRO:O | 2:N:145:ALA:HB2 | 1.96 | 0.66 |
| 1:S:61:THR:HG23 | 1:S:71:THR:OG1 | 1.95 | 0.66 |
| 2:T:141:PRO:O | 2:T:145:ALA:HB2 | 1.96 | 0.66 |
| 1:J:541:MET:O | 4:W:143:TYR:OH | 2.13 | 0.66 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:HB3 | 1.78 | 0.66 |
| 4:2:153:LEU:HD11 | 4:2:274:ILE:HG13 | 1.76 | 0.66 |
| 1:A:217:THR:O | 1:A:221:GLN:HG2 | 1.95 | 0.66 |
| 1:A:296:MLY:HH11 | 1:A:348:MLY:HH21 | 1.78 | 0.66 |
| 1:D:374:GLN:HG3 | 1:D:375:ALA:H | 1.60 | 0.66 |
| 1:D:78:PHE:HB3 | 1:D:98:HIS:CD2 | 2.30 | 0.66 |
| 1:G:202:SER:HA | 1:G:207:LYS:HE3 | 1.72 | 0.66 |
| 1:G:290:GLN:O | 1:G:331:LEU:HD12 | 1.95 | 0.66 |
| 1:G:783:LEU:O | 1:G:787:ILE:CA | 2.43 | 0.66 |
| 2:H:117:LEU:CB | 2:H:147:ASN:OD1 | 2.39 | 0.66 |
| 1:M:553:MLY:CE | 4:2:45:VAL:CA | 2.49 | 0.66 |
| 1:M:612:GLN:NE2 | 1:M:627:GLY:N | 2.43 | 0.66 |
| 1:M:829:TRP:CZ3 | 2:N:84:PHE:CZ | 2.84 | 0.66 |
| 1:S:161:ASN:O | 1:S:165:PHE:HB2 | 1.96 | 0.66 |
| 1:S:339:ASP:OD1 | 1:S:348:MLY:HH13 | 1.95 | 0.66 |
| 1:S:541:MET:HG2 | 4:2:345:ILE:C | 2.16 | 0.66 |
| 1:S:58:GLY:HA2 | 1:S:74:GLU:OE1 | 1.95 | 0.66 |
| 1:G:556:ASP:OD2 | 4:X:47:MET:CE | 2.39 | 0.66 |
| 4:1:288:ASP:OD1 | 4:3:203:THR:HG23 | 1.96 | 0.66 |
| 4:5:160:THR:HG21 | 4:5:274:ILE:HD11 | 1.76 | 0.66 |
| 1:D:537:GLU:C | 4:9:351:THR:H | 1.98 | 0.66 |
| 2:B:141:PRO:O | 2:B:145:ALA:HB2 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:102:VAL:HG23 | 3:C:139:TYR:HD1 | 1.60 | 0.66 |
| 1:D:831:TRP:CZ2 | 2:E:51:PHE:CZ | 2.84 | 0.66 |
| 1:G:817:GLN:NE2 | 2:H:128:PHE:CE1 | 2.64 | 0.66 |
| 1:J:144:ARG:NH1 | 1:J:160:ASP:OD1 | 2.29 | 0.66 |
| 1:J:322:VAL:HB | 1:J:325:ILE:CD1 | 2.26 | 0.66 |
| 1:M:131:TRP:O | 1:M:132:LEU:HD12 | 1.95 | 0.66 |
| 1:M:418:THR:HG22 | 1:M:419:VAL:N | 2.11 | 0.66 |
| 2:N:146:GLY:O | 2:N:147:ASN:HB2 | 1.96 | 0.66 |
| 1:A:226:ASN:HB2 | 1:A:227:PRO:HD3 | 1.78 | 0.66 |
| 1:A:831:TRP:CD2 | 2:B:51:PHE:CE1 | 2.84 | 0.66 |
| 1:D:408:VAL:HG12 | 4:9:332:PRO:HB3 | 1.76 | 0.66 |
| 1:D:466:GLY:HA2 | 1:D:484:ASN:HD21 | 1.61 | 0.66 |
| 1:D:174:SER:O | 1:D:670:HIS:HB2 | 1.96 | 0.66 |
| 2:E:141:PRO:O | 2:E:145:ALA:HB2 | 1.96 | 0.66 |
| 1:G:144:ARG:NH1 | 1:G:160:ASP:OD1 | 2.29 | 0.66 |
| 1:G:226:ASN:HB2 | 1:G:227:PRO:HD3 | 1.78 | 0.66 |
| 2:H:146:GLY:O | 2:H:147:ASN:HB2 | 1.96 | 0.66 |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:HD1 | 1.59 | 0.66 |
| 3:I:48:LYS:C | 3:I:52:ASN:HD21 | 1.97 | 0.66 |
| 1:J:61:THR:HG23 | 1:J:71:THR:OG1 | 1.95 | 0.66 |
| 1:J:505:MLY:HG3 | 1:J:762:HIS:CE1 | 2.31 | 0.66 |
| 1:J:93:MET:HE1 | 1:J:764:MLY:CD | 2.26 | 0.66 |
| 2:K:146:GLY:O | 2:K:147:ASN:HB2 | 1.96 | 0.66 |
| 1:M:161:ASN:O | 1:M:165:PHE:HB2 | 1.96 | 0.66 |
| 1:S:62:VAL:HG12 | 1:S:63:MLY:O | 1.94 | 0.66 |
| 1:S:642:LYS:HA | 4:2:21:PHE:O | 1.96 | 0.66 |
| 1:S:836:PHE:CE1 | 2:T:159:HIS:C | 2.69 | 0.66 |
| 3:U:48:LYS:O | 3:U:52:ASN:CG | 2.34 | 0.66 |
| 1:G:642:LYS:CD | 4:V:24:ASP:O | 2.43 | 0.66 |
| 4:4:324:THR:OG1 | 4:6:244:ASP:HB3 | 1.95 | 0.65 |
| 1:A:131:TRP:O | 1:A:132:LEU:HD12 | 1.95 | 0.65 |
| 1:A:530:MET:CA | 4:8:354:GLN:CB | 2.74 | 0.65 |
| 1:A:62:VAL:HG12 | 1:A:63:MLY:O | 1.94 | 0.65 |
| 1:D:534:SER:C | 4:9:351:THR:CA | 2.47 | 0.65 |
| 1:G:174:SER:O | 1:G:670:HIS:HB2 | 1.96 | 0.65 |
| 1:G:339:ASP:OD1 | 1:G:348:MLY:HH13 | 1.95 | 0.65 |
| 1:G:466:GLY:HA2 | 1:G:484:ASN:HD21 | 1.61 | 0.65 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:C | 2.17 | 0.65 |
| 1:G:93:MET:CA | 1:G:714:ARG:H | 2.04 | 0.65 |
| 1:G:752:ASP:OD1 | 1:G:783:LEU:CB | 2.43 | 0.65 |
| 1:G:795:ARG:HG2 | 3:I:118:MET:SD | 2.33 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:141:PRO:O | 2:H:145:ALA:CB | 2.43 | 0.65 |
| 1:J:217:THR:O | 1:J:221:GLN:HG2 | 1.95 | 0.65 |
| 1:J:466:GLY:HA2 | 1:J:484:ASN:ND2 | 2.11 | 0.65 |
| 1:J:691:VAL:O | 1:J:695:LEU:HD13 | 1.96 | 0.65 |
| 1:M:480:ILE:HG22 | 1:M:481:ASN:N | 2.11 | 0.65 |
| 2:N:117:LEU:CG | 2:N:147:ASN:HB3 | 2.25 | 0.65 |
| 1:S:174:SER:O | 1:S:670:HIS:HB2 | 1.96 | 0.65 |
| 1:S:226:ASN:HB2 | 1:S:227:PRO:HD3 | 1.77 | 0.65 |
| 1:S:466:GLY:HA2 | 1:S:484:ASN:ND2 | 2.12 | 0.65 |
| 1:S:796:GLY:HA2 | 3:U:35:ARG:NE | 2.10 | 0.65 |
| 1:S:747:LEU:HA | 3:U:93:VAL:CG1 | 2.27 | 0.65 |
| 1:G:648:THR:CB | 4:V:350:SER:OG | 2.44 | 0.65 |
| 1:A:642:LYS:CD | 4:8:24:ASP:O | 2.42 | 0.65 |
| 1:D:339:ASP:OD1 | 1:D:348:MLY:HH13 | 1.95 | 0.65 |
| 1:G:296:MLY:HH11 | 1:G:348:MLY:HH21 | 1.79 | 0.65 |
| 1:J:91:MET:HE3 | 1:J:119:SER:HB2 | 1.78 | 0.65 |
| 1:M:174:SER:O | 1:M:670:HIS:HB2 | 1.96 | 0.65 |
| 1:S:322:VAL:HB | 1:S:325:ILE:CD1 | 2.26 | 0.65 |
| 1:S:599:ASN:OD1 | 1:S:649:VAL:N | 2.28 | 0.65 |
| 1:G:635:GLY:O | 4:V:341:ILE:HG21 | 1.95 | 0.65 |
| 4:V:325:MET:CE | 4:X:244:ASP:OD2 | 2.34 | 0.65 |
| 4:2:112:PRO:HG3 | 4:3:197:GLY:H | 1.61 | 0.65 |
| 4:8:160:THR:HG21 | 4:8:274:ILE:HD11 | 1.76 | 0.65 |
| 1:A:107:MLY:HB3 | 1:A:686:MET:CE | 2.27 | 0.65 |
| 1:A:831:TRP:CH2 | 2:B:47:LEU:HA | 2.31 | 0.65 |
| 1:D:466:GLY:HA2 | 1:D:484:ASN:ND2 | 2.11 | 0.65 |
| 1:G:61:THR:HG23 | 1:G:71:THR:OG1 | 1.94 | 0.65 |
| 1:J:599:ASN:OD1 | 1:J:649:VAL:N | 2.29 | 0.65 |
| 1:M:322:VAL:HB | 1:M:325:ILE:CD1 | 2.26 | 0.65 |
| 1:M:374:GLN:HG3 | 1:M:375:ALA:H | 1.59 | 0.65 |
| 1:M:530:MET:CA | 4:Z:354:GLN:CB | 2.74 | 0.65 |
| 1:M:769:ALA:C | 1:M:770:GLY:HA3 | 2.17 | 0.65 |
| 3:U:45:GLU:O | 3:U:49:ILE:HG13 | 1.97 | 0.65 |
| 4:V:160:THR:HG21 | 4:V:274:ILE:HD11 | 1.76 | 0.65 |
| 4:V:288:ASP:H | 4:X:204:ALA:H | 1.43 | 0.65 |
| 1:S:635:GLY:O | 4:2:341:ILE:HG21 | 1.95 | 0.65 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:C | 2.16 | 0.65 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:N | 2.29 | 0.65 |
| 3:F:48:LYS:O | 3:F:52:ASN:CG | 2.34 | 0.65 |
| 3:F:3:SER:HG | 3:F:5:ALA:N | 1.95 | 0.65 |
| 3:F:24:LYS:HA | 3:F:63:ILE:O | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:94:MET:O | 1:G:713:SER:CA | 2.43 | 0.65 |
| 1:G:797:PHE:HE2 | 3:I:126:LEU:CG | 2.08 | 0.65 |
| 1:J:791:GLN:NE2 | 3:L:116:GLU:N | 2.44 | 0.65 |
| 1:M:339:ASP:OD1 | 1:M:348:MLY:HH13 | 1.95 | 0.65 |
| 1:M:538:GLU:CD | 4:Z:355:MET:CE | 2.62 | 0.65 |
| 1:S:131:TRP:O | 1:S:132:LEU:HD12 | 1.95 | 0.65 |
| 1:S:296:MLY:HH11 | 1:S:348:MLY:HH21 | 1.78 | 0.65 |
| 1:S:418:THR:HG22 | 1:S:419:VAL:N | 2.11 | 0.65 |
| 1:S:691:VAL:O | 1:S:695:LEU:HD13 | 1.96 | 0.65 |
| 1:S:805:ALA:O | 1:S:808:GLU:N | 2.29 | 0.65 |
| 1:S:819:ASN:OD1 | 2:T:91:ALA:C | 2.32 | 0.65 |
| 1:J:530:MET:CG | 4:W:354:GLN:CG | 2.72 | 0.65 |
| 4:W:324:THR:HG23 | 4:Y:247:VAL:H | 1.61 | 0.65 |
| 4:3:288:ASP:CB | 4:5:203:THR:HG21 | 2.25 | 0.65 |
| 1:A:149:GLN:HB2 | 1:A:718:ALA:HB1 | 1.76 | 0.65 |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:N | 2.11 | 0.65 |
| 1:A:800:ARG:C | 3:C:149:VAL:CG2 | 2.65 | 0.65 |
| 1:D:161:ASN:O | 1:D:165:PHE:HB2 | 1.96 | 0.65 |
| 1:G:418:THR:HG22 | 1:G:419:VAL:N | 2.11 | 0.65 |
| 2:H:141:PRO:O | 2:H:145:ALA:HB2 | 1.96 | 0.65 |
| 1:M:831:TRP:CZ2 | 2:N:47:LEU:CD2 | 2.76 | 0.65 |
| 1:S:480:ILE:HG22 | 1:S:481:ASN:N | 2.11 | 0.65 |
| 1:S:752:ASP:N | 3:U:86:ASP:CG | 2.49 | 0.65 |
| 4:V:324:THR:HG23 | 4:X:247:VAL:H | 1.61 | 0.65 |
| 4:W:288:ASP:H | 4:Y:204:ALA:H | 1.43 | 0.65 |
| 4:1:287:ILE:HB | 4:3:203:THR:CB | 2.27 | 0.65 |
| 1:A:161:ASN:O | 1:A:165:PHE:HB2 | 1.96 | 0.65 |
| 1:A:322:VAL:HB | 1:A:325:ILE:CD1 | 2.26 | 0.65 |
| 1:A:466:GLY:HA2 | 1:A:484:ASN:ND2 | 2.12 | 0.65 |
| 1:D:144:ARG:NH1 | 1:D:160:ASP:OD1 | 2.29 | 0.65 |
| 1:D:541:MET:O | 4:9:143:TYR:OH | 2.14 | 0.65 |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:CG1 | 2.27 | 0.65 |
| 1:G:131:TRP:O | 1:G:132:LEU:HD12 | 1.95 | 0.65 |
| 1:G:735:GLY:O | 1:G:743:ALA:HA | 1.94 | 0.65 |
| 1:G:818:TYR:HB3 | 2:H:90:GLY:HA3 | 1.78 | 0.65 |
| 1:J:530:MET:CA | 4:W:354:GLN:CB | 2.74 | 0.65 |
| 1:M:296:MLY:HH11 | 1:M:348:MLY:HH21 | 1.78 | 0.65 |
| 1:M:529:PRO:C | 4:Z:354:GLN:CB | 2.49 | 0.65 |
| 1:M:642:LYS:HA | 4:Z:21:PHE:O | 1.96 | 0.65 |
| 1:M:820:VAL:HG11 | 2:N:136:MET:CE | 2.27 | 0.65 |
| 2:N:117:LEU:CB | 2:N:147:ASN:ND2 | 2.35 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:48:LYS:O | 3:O:52:ASN:CG | 2.34 | 0.65 |
| 1:S:541:MET:O | 4:2:143:TYR:OH | 2.13 | 0.65 |
| 1:S:725:ARG:NE | 1:S:737:PHE:HE1 | 1.95 | 0.65 |
| 1:S:793:ARG:HH11 | 3:U:40:ASN:CG | 1.99 | 0.65 |
| 1:S:839:MLY:CD | 2:T:159:HIS:HB3 | 2.26 | 0.65 |
| 1:G:530:MET:CG | 4:V:354:GLN:CG | 2.71 | 0.65 |
| 1:G:557:GLU:HB2 | 4:X:47:MET:C | 2.16 | 0.65 |
| 4:1:204:ALA:H | 4:Y:288:ASP:H | 1.43 | 0.65 |
| 1:M:635:GLY:O | 4:Z:341:ILE:HG21 | 1.95 | 0.65 |
| 1:A:530:MET:HE3 | 4:8:354:GLN:HG2 | 1.77 | 0.65 |
| 1:A:636:LYS:HG3 | 4:8:334:GLU:CD | 2.17 | 0.65 |
| 1:A:642:LYS:HA | 4:8:21:PHE:O | 1.96 | 0.65 |
| 1:A:94:MET:HE1 | 1:A:101:ALA:HB1 | 1.79 | 0.65 |
| 3:C:45:GLU:O | 3:C:49:ILE:HG13 | 1.97 | 0.65 |
| 1:D:530:MET:CA | 4:9:354:GLN:CB | 2.74 | 0.65 |
| 1:G:161:ASN:O | 1:G:165:PHE:HB2 | 1.96 | 0.65 |
| 3:I:48:LYS:O | 3:I:52:ASN:CG | 2.34 | 0.65 |
| 1:J:174:SER:O | 1:J:670:HIS:HB2 | 1.95 | 0.65 |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:N | 1.95 | 0.65 |
| 1:M:144:ARG:NH1 | 1:M:160:ASP:OD1 | 2.29 | 0.65 |
| 1:M:732:ILE:CG2 | 1:M:747:LEU:HD11 | 1.26 | 0.65 |
| 3:O:45:GLU:O | 3:O:49:ILE:HG13 | 1.97 | 0.65 |
| 1:S:799:MET:SD | 3:U:32:ASP:CG | 2.75 | 0.65 |
| 2:T:117:LEU:CB | 2:T:147:ASN:ND2 | 2.35 | 0.65 |
| 1:S:792:ALA:HB1 | 3:U:42:THR:N | 2.11 | 0.65 |
| 4:2:287:ILE:CG1 | 4:4:203:THR:HB | 2.26 | 0.65 |
| 1:A:504:MLY:C | 1:A:762:HIS:NE2 | 2.59 | 0.65 |
| 1:D:636:LYS:HG3 | 4:9:334:GLU:CD | 2.18 | 0.65 |
| 1:D:822:SER:O | 1:D:825:ASN:HB2 | 1.97 | 0.65 |
| 3:F:45:GLU:O | 3:F:49:ILE:HG13 | 1.97 | 0.65 |
| 1:G:466:GLY:HA2 | 1:G:484:ASN:ND2 | 2.12 | 0.65 |
| 1:J:217:THR:HB | 1:J:220:ASP:OD2 | 1.97 | 0.65 |
| 1:M:166:MET:HE3 | 1:M:254:PHE:HD2 | 1.61 | 0.65 |
| 1:M:636:LYS:HG3 | 4:Z:334:GLU:CD | 2.17 | 0.65 |
| 1:S:752:ASP:N | 1:S:779:ARG:HH21 | 1.95 | 0.65 |
| 1:S:530:MET:CG | 4:2:354:GLN:CG | 2.72 | 0.65 |
| 1:S:544:LYS:HD3 | 4:4:45:VAL:CG2 | 2.27 | 0.65 |
| 1:A:717:TYR:HD1 | 1:A:744:SER:HG | 1.45 | 0.65 |
| 3:C:48:LYS:O | 3:C:52:ASN:CG | 2.34 | 0.65 |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:HH21 | 1.78 | 0.65 |
| 1:D:691:VAL:O | 1:D:695:LEU:HD13 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:713:SER:HG | 1:D:771:LEU:HG | 1.57 | 0.65 |
| 2:E:146:GLY:O | 2:E:147:ASN:HB2 | 1.96 | 0.65 |
| 1:G:149:GLN:HG2 | 1:G:763:THR:HG21 | 0.65 | 0.65 |
| 1:J:466:GLY:HA2 | 1:J:484:ASN:HD21 | 1.61 | 0.65 |
| 1:J:97:LEU:CD2 | 1:J:712:PRO:HB3 | 2.26 | 0.65 |
| 1:J:831:TRP:CZ2 | 2:K:47:LEU:HD22 | 2.32 | 0.65 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:CB | 2.71 | 0.65 |
| 3:L:3:SER:HG | 3:L:5:ALA:N | 1.95 | 0.65 |
| 1:M:217:THR:HB | 1:M:220:ASP:OD2 | 1.97 | 0.65 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:CG | 2.56 | 0.65 |
| 1:S:817:GLN:HB3 | 2:T:127:ARG:CZ | 2.25 | 0.65 |
| 1:S:821:ARG:HH22 | 2:T:127:ARG:NE | 1.95 | 0.65 |
| 1:S:820:VAL:CG1 | 2:T:136:MET:HE1 | 2.26 | 0.65 |
| 4:X:291:LYS:HG3 | 4:Z:244:ASP:N | 1.86 | 0.65 |
| 1:D:814:PHE:CD1 | 2:E:127:ARG:CZ | 2.79 | 0.65 |
| 1:G:530:MET:CA | 4:V:354:GLN:CB | 2.75 | 0.65 |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:HH21 | 1.78 | 0.65 |
| 1:J:822:SER:O | 1:J:825:ASN:HB2 | 1.97 | 0.65 |
| 1:J:819:ASN:HD21 | 2:K:92:ASP:HB2 | 1.56 | 0.65 |
| 1:M:466:GLY:HA2 | 1:M:484:ASN:HD21 | 1.61 | 0.65 |
| 1:M:725:ARG:NE | 1:M:737:PHE:HE1 | 1.95 | 0.65 |
| 1:M:803:TYR:CE2 | 3:O:17:PHE:CZ | 2.84 | 0.65 |
| 1:S:642:LYS:CD | 4:2:24:ASP:O | 2.43 | 0.65 |
| 1:S:795:ARG:CZ | 3:U:116:GLU:CB | 2.59 | 0.65 |
| 1:S:94:MET:HE1 | 1:S:101:ALA:HB1 | 1.79 | 0.65 |
| 4:X:287:ILE:CB | 4:Z:201:VAL:HG23 | 2.27 | 0.65 |
| 1:A:635:GLY:O | 4:8:341:ILE:HG21 | 1.96 | 0.64 |
| 1:A:217:THR:HB | 1:A:220:ASP:OD2 | 1.97 | 0.64 |
| 1:A:339:ASP:OD1 | 1:A:348:MLY:HH13 | 1.95 | 0.64 |
| 1:A:504:MLY:HB2 | 1:A:762:HIS:CE1 | 2.33 | 0.64 |
| 1:D:479:CYS:HB3 | 1:D:653:PHE:CE2 | 2.32 | 0.64 |
| 1:D:732:ILE:CG2 | 1:D:782:MLY:CH2 | 2.55 | 0.64 |
| 1:D:799:MET:SD | 3:F:32:ASP:OD2 | 2.54 | 0.64 |
| 1:D:800:ARG:C | 3:F:149:VAL:HG21 | 2.17 | 0.64 |
| 1:J:133:PRO:O | 1:J:136:ASN:HB2 | 1.98 | 0.64 |
| 1:J:725:ARG:NE | 1:J:737:PHE:HE1 | 1.95 | 0.64 |
| 1:M:691:VAL:O | 1:M:695:LEU:HD13 | 1.96 | 0.64 |
| 1:S:821:ARG:NH2 | 2:T:127:ARG:NE | 2.45 | 0.64 |
| 1:M:541:MET:O | 4:Z:143:TYR:OH | 2.14 | 0.64 |
| 1:S:642:LYS:CA | 4:2:21:PHE:O | 2.45 | 0.64 |
| 1:A:133:PRO:O | 1:A:136:ASN:HB2 | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:636:LYS:O | 1:A:637:LYS:CB | 2.45 | 0.64 |
| 1:D:94:MET:HE1 | 1:D:101:ALA:HB1 | 1.79 | 0.64 |
| 1:G:218:LEU:CD2 | 1:G:222:ILE:HG12 | 2.28 | 0.64 |
| 1:G:725:ARG:NE | 1:G:737:PHE:HE1 | 1.95 | 0.64 |
| 1:G:806:MET:O | 1:G:809:ARG:HB2 | 1.98 | 0.64 |
| 1:G:813:ILE:CG2 | 2:H:128:PHE:HE1 | 2.10 | 0.64 |
| 1:G:822:SER:O | 1:G:825:ASN:HB2 | 1.97 | 0.64 |
| 1:J:161:ASN:O | 1:J:165:PHE:HB2 | 1.96 | 0.64 |
| 1:J:505:MLY:CG | 1:J:762:HIS:CE1 | 2.80 | 0.64 |
| 1:M:107:MLY:HB3 | 1:M:686:MET:CE | 2.27 | 0.64 |
| 1:M:61:THR:HG23 | 1:M:71:THR:OG1 | 1.95 | 0.64 |
| 2:N:140:PHE:HB3 | 2:N:144:VAL:CG1 | 2.28 | 0.64 |
| 1:S:502:GLU:OE1 | 1:S:761:GLY:HA2 | 1.95 | 0.64 |
| 2:T:140:PHE:HB3 | 2:T:144:VAL:CG1 | 2.28 | 0.64 |
| 1:G:541:MET:O | 4:V:143:TYR:OH | 2.13 | 0.64 |
| 1:M:642:LYS:CA | 4:Z:21:PHE:O | 2.45 | 0.64 |
| 4:3:288:ASP:CB | 4:5:203:THR:CG2 | 2.75 | 0.64 |
| 1:D:217:THR:HB | 1:D:220:ASP:OD2 | 1.97 | 0.64 |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:N | 1.94 | 0.64 |
| 1:G:133:PRO:O | 1:G:136:ASN:HB2 | 1.98 | 0.64 |
| 1:G:374:GLN:HG3 | 1:G:375:ALA:H | 1.60 | 0.64 |
| 1:G:813:ILE:HG23 | 2:H:128:PHE:CE1 | 2.31 | 0.64 |
| 3:I:3:SER:HG | 3:I:5:ALA:N | 1.95 | 0.64 |
| 1:J:226:ASN:HB2 | 1:J:227:PRO:HD3 | 1.78 | 0.64 |
| 1:J:636:LYS:O | 1:J:637:LYS:CB | 2.45 | 0.64 |
| 1:J:806:MET:O | 1:J:809:ARG:HB2 | 1.98 | 0.64 |
| 2:K:114:LYS:HA | 2:K:146:GLY:C | 2.03 | 0.64 |
| 1:M:215:GLN:CA | 1:M:340:ILE:CG2 | 2.62 | 0.64 |
| 1:S:466:GLY:HA2 | 1:S:484:ASN:HD21 | 1.61 | 0.64 |
| 1:S:636:LYS:HG3 | 4:2:334:GLU:CD | 2.17 | 0.64 |
| 1:S:721:LYS:HG2 | 1:S:736:GLN:CD | 1.86 | 0.64 |
| 1:S:806:MET:CA | 1:S:807:VAL:N | 2.59 | 0.64 |
| 1:S:831:TRP:HE1 | 2:T:67:MET:CG | 2.10 | 0.64 |
| 2:T:146:GLY:O | 2:T:147:ASN:HB2 | 1.96 | 0.64 |
| 1:D:642:LYS:CD | 4:9:24:ASP:O | 2.42 | 0.64 |
| 1:A:149:GLN:HB3 | 1:A:719:ASP:CA | 2.27 | 0.64 |
| 1:A:166:MET:HE3 | 1:A:254:PHE:HD2 | 1.60 | 0.64 |
| 1:A:466:GLY:HA2 | 1:A:484:ASN:HD21 | 1.61 | 0.64 |
| 1:A:806:MET:O | 1:A:809:ARG:HB2 | 1.98 | 0.64 |
| 1:A:822:SER:O | 1:A:825:ASN:HB2 | 1.97 | 0.64 |
| 1:D:636:LYS:O | 1:D:637:LYS:CB | 2.45 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:107:MLY:HB3 | 1:D:686:MET:CE | 2.26 | 0.64 |
| 1:G:322:VAL:HB | 1:G:325:ILE:CD1 | 2.26 | 0.64 |
| 1:G:691:VAL:O | 1:G:695:LEU:HD13 | 1.97 | 0.64 |
| 2:H:140:PHE:HB3 | 2:H:144:VAL:CG1 | 2.28 | 0.64 |
| 1:J:292:MET:HE3 | 1:J:309:PRO:HA | 1.78 | 0.64 |
| 1:S:636:LYS:O | 1:S:637:LYS:CB | 2.45 | 0.64 |
| 3:U:24:LYS:HA | 3:U:63:ILE:O | 1.95 | 0.64 |
| 4:1:287:ILE:HG13 | 4:3:202:THR:HA | 1.78 | 0.64 |
| 1:A:530:MET:CG | 4:8:354:GLN:CG | 2.71 | 0.64 |
| 1:A:831:TRP:CZ2 | 2:B:47:LEU:CA | 2.63 | 0.64 |
| 2:B:140:PHE:HB3 | 2:B:144:VAL:CG1 | 2.28 | 0.64 |
| 1:D:410:ASN:CG | 4:9:334:GLU:CA | 2.47 | 0.64 |
| 1:G:278:GLN:CG | 1:G:317:GLU:HB2 | 2.26 | 0.64 |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:N | 2.13 | 0.64 |
| 1:G:769:ALA:CB | 1:G:770:GLY:N | 2.61 | 0.64 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:O | 1.98 | 0.64 |
| 1:J:756:THR:HG23 | 1:J:779:ARG:HD3 | 1.76 | 0.64 |
| 1:M:218:LEU:CD2 | 1:M:222:ILE:HG12 | 2.28 | 0.64 |
| 1:S:797:PHE:CD1 | 3:U:149:VAL:CG1 | 2.81 | 0.64 |
| 3:U:49:ILE:HA | 3:U:52:ASN:ND2 | 2.06 | 0.64 |
| 1:S:541:MET:HG2 | 4:2:345:ILE:O | 1.98 | 0.64 |
| 1:S:549:SER:HB2 | 4:4:43:VAL:HG11 | 1.80 | 0.64 |
| 1:A:218:LEU:CD2 | 1:A:222:ILE:HG12 | 2.28 | 0.64 |
| 1:A:797:PHE:CD1 | 3:C:149:VAL:HG12 | 2.32 | 0.64 |
| 3:C:3:SER:HG | 3:C:5:ALA:N | 1.95 | 0.64 |
| 1:D:798:LEU:CD1 | 3:F:126:LEU:HD21 | 2.26 | 0.64 |
| 1:G:783:LEU:HD12 | 1:G:783:LEU:N | 2.13 | 0.64 |
| 1:M:133:PRO:O | 1:M:136:ASN:HB2 | 1.98 | 0.64 |
| 1:M:466:GLY:HA2 | 1:M:484:ASN:ND2 | 2.12 | 0.64 |
| 1:S:107:MLY:HB3 | 1:S:686:MET:CE | 2.27 | 0.64 |
| 2:T:144:VAL:HA | 2:T:153:ILE:HD11 | 1.80 | 0.64 |
| 1:G:530:MET:HE3 | 4:V:354:GLN:HG2 | 1.79 | 0.64 |
| 4:X:287:ILE:CG1 | 4:Z:201:VAL:CB | 2.75 | 0.64 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:O | 1.98 | 0.64 |
| 1:A:691:VAL:O | 1:A:695:LEU:HD13 | 1.97 | 0.64 |
| 2:E:117:LEU:CG | 2:E:147:ASN:CB | 2.76 | 0.64 |
| 1:G:210:GLN:O | 1:G:211:SER:OG | 2.15 | 0.64 |
| 1:G:636:LYS:O | 1:G:637:LYS:CB | 2.45 | 0.64 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:HD13 | 2.19 | 0.64 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:O | 1.98 | 0.64 |
| 1:M:783:LEU:C | 1:M:786:ILE:HG13 | 2.16 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:822:SER:O | 1:M:825:ASN:HB2 | 1.97 | 0.64 |
| 2:N:144:VAL:HA | 2:N:153:ILE:HD11 | 1.80 | 0.64 |
| 1:S:643:GLY:H | 4:2:23:GLY:C | 2.01 | 0.64 |
| 1:S:92:ALA:CB | 1:S:764:MLY:CH1 | 2.69 | 0.64 |
| 1:S:783:LEU:N | 1:S:783:LEU:HD12 | 2.13 | 0.64 |
| 1:S:805:ALA:CA | 1:S:808:GLU:N | 2.59 | 0.64 |
| 1:J:543:PRO:HG2 | 4:W:143:TYR:O | 1.98 | 0.64 |
| 1:J:556:ASP:OD2 | 4:Y:47:MET:CE | 2.40 | 0.64 |
| 1:M:530:MET:CG | 4:Z:354:GLN:CG | 2.72 | 0.64 |
| 4:4:324:THR:HG23 | 4:6:244:ASP:C | 2.18 | 0.64 |
| 1:A:541:MET:O | 4:8:143:TYR:OH | 2.14 | 0.64 |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:N | 1.94 | 0.64 |
| 2:B:146:GLY:O | 2:B:147:ASN:HB2 | 1.96 | 0.64 |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:CD | 2.11 | 0.64 |
| 1:D:642:LYS:HA | 4:9:21:PHE:O | 1.96 | 0.64 |
| 1:D:823:PHE:CE1 | 2:E:160:GLY:CA | 2.76 | 0.64 |
| 1:G:642:LYS:HA | 4:V:21:PHE:O | 1.97 | 0.64 |
| 1:J:537:GLU:C | 4:W:351:THR:N | 2.51 | 0.64 |
| 1:J:795:ARG:HE | 3:L:116:GLU:HB3 | 1.63 | 0.64 |
| 3:L:45:GLU:O | 3:L:49:ILE:HG13 | 1.96 | 0.64 |
| 1:M:786:ILE:C | 1:M:787:ILE:C | 2.56 | 0.64 |
| 1:M:803:TYR:HD2 | 3:O:17:PHE:HZ | 1.34 | 0.64 |
| 2:T:117:LEU:CG | 2:T:147:ASN:CB | 2.76 | 0.64 |
| 1:G:538:GLU:HA | 4:V:349:LEU:HB3 | 1.79 | 0.64 |
| 4:Y:190:MET:SD | 4:Y:209:VAL:HG11 | 2.38 | 0.64 |
| 1:M:530:MET:HE3 | 4:Z:354:GLN:CG | 2.23 | 0.64 |
| 1:S:541:MET:CA | 4:2:143:TYR:OH | 2.46 | 0.64 |
| 4:3:190:MET:SD | 4:3:209:VAL:HG11 | 2.38 | 0.64 |
| 4:5:190:MET:SD | 4:5:209:VAL:HG11 | 2.38 | 0.64 |
| 1:A:636:LYS:N | 4:8:334:GLU:OE1 | 2.31 | 0.64 |
| 1:A:752:ASP:OD2 | 1:A:782:MLY:HG2 | 1.98 | 0.64 |
| 2:B:144:VAL:HA | 2:B:153:ILE:HD11 | 1.80 | 0.64 |
| 1:D:218:LEU:CD2 | 1:D:222:ILE:HG12 | 2.28 | 0.64 |
| 1:D:806:MET:O | 1:D:809:ARG:HB2 | 1.98 | 0.64 |
| 3:F:49:ILE:HA | 3:F:52:ASN:ND2 | 2.05 | 0.64 |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:N | 1.94 | 0.64 |
| 1:G:503:TYR:CZ | 1:G:711:PHE:CE2 | 2.85 | 0.64 |
| 2:H:117:LEU:HD11 | 2:H:147:ASN:HB3 | 1.76 | 0.64 |
| 1:J:553:MLY:O | 4:Y:46:GLY:CA | 2.45 | 0.64 |
| 1:J:557:GLU:HB2 | 4:Y:47:MET:C | 2.16 | 0.64 |
| 1:J:577:ALA:O | 1:J:578:HIS:CD2 | 2.51 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:642:LYS:HA | 4:W:21:PHE:O | 1.96 | 0.64 |
| 1:J:710:GLY:O | 1:J:772:LEU:CD2 | 2.45 | 0.64 |
| 1:J:732:ILE:CG2 | 1:J:747:LEU:HD11 | 1.26 | 0.64 |
| 1:J:725:ARG:NE | 1:J:737:PHE:CE1 | 2.66 | 0.64 |
| 1:M:530:MET:HA | 4:Z:354:GLN:CB | 2.28 | 0.64 |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:N | 1.95 | 0.64 |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:HD11 | 0.73 | 0.64 |
| 1:M:783:LEU:N | 1:M:783:LEU:HD12 | 2.13 | 0.64 |
| 1:S:537:GLU:C | 4:2:351:THR:N | 2.51 | 0.64 |
| 1:S:791:GLN:OE1 | 3:U:116:GLU:CG | 2.46 | 0.64 |
| 1:S:731:ALA:CB | 3:U:94:PHE:N | 2.61 | 0.64 |
| 1:G:537:GLU:C | 4:V:351:THR:N | 2.51 | 0.64 |
| 1:J:538:GLU:HA | 4:W:349:LEU:HB3 | 1.78 | 0.64 |
| 1:M:530:MET:HE2 | 4:Z:354:GLN:HG3 | 1.80 | 0.64 |
| 4:4:288:ASP:CB | 4:6:203:THR:CG2 | 2.75 | 0.64 |
| 1:A:725:ARG:NE | 1:A:737:PHE:HE1 | 1.95 | 0.64 |
| 2:B:132:GLU:O | 2:B:136:MET:HG2 | 1.99 | 0.64 |
| 1:A:830:PRO:HG2 | 2:B:67:MET:HE2 | 1.80 | 0.64 |
| 1:D:133:PRO:O | 1:D:136:ASN:HB2 | 1.98 | 0.64 |
| 1:D:537:GLU:C | 4:9:351:THR:N | 2.51 | 0.64 |
| 1:D:577:ALA:O | 1:D:578:HIS:CD2 | 2.51 | 0.64 |
| 1:D:537:GLU:HB3 | 1:D:648:THR:HB | 1.80 | 0.64 |
| 1:G:577:ALA:O | 1:G:578:HIS:CD2 | 2.51 | 0.64 |
| 1:G:642:LYS:CA | 4:V:21:PHE:O | 2.46 | 0.64 |
| 1:G:479:CYS:HB3 | 1:G:653:PHE:CE2 | 2.33 | 0.64 |
| 1:J:94:MET:HE1 | 1:J:101:ALA:HB1 | 1.80 | 0.64 |
| 1:J:479:CYS:HB3 | 1:J:653:PHE:CE2 | 2.33 | 0.64 |
| 2:K:140:PHE:HB3 | 2:K:144:VAL:CG1 | 2.28 | 0.64 |
| 1:M:127:ASN:HD22 | 1:M:128:PRO:CD | 2.11 | 0.64 |
| 1:M:636:LYS:O | 1:M:637:LYS:CB | 2.45 | 0.64 |
| 1:M:479:CYS:HB3 | 1:M:653:PHE:CE2 | 2.33 | 0.64 |
| 1:M:93:MET:CE | 1:M:764:MLY:NZ | 2.61 | 0.64 |
| 1:M:84:MLY:HB3 | 1:M:723:ARG:HD2 | 1.78 | 0.64 |
| 2:N:117:LEU:CG | 2:N:147:ASN:CB | 2.76 | 0.64 |
| 1:M:798:LEU:HD13 | 3:O:126:LEU:CD1 | 2.27 | 0.64 |
| 1:S:538:GLU:HA | 4:2:349:LEU:HB3 | 1.78 | 0.64 |
| 1:S:725:ARG:NE | 1:S:737:PHE:CE1 | 2.66 | 0.64 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:O | 1.98 | 0.64 |
| 1:D:642:LYS:CG | 4:9:22:ALA:C | 2.67 | 0.63 |
| 1:D:541:MET:SD | 4:9:346:LEU:O | 2.48 | 0.63 |
| 1:A:577:ALA:O | 1:A:578:HIS:CD2 | 2.51 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:724:TYR:HB3 | 1:A:727:LEU:HD12 | 1.80 | 0.63 |
| 1:A:783:LEU:N | 1:A:783:LEU:HD12 | 2.13 | 0.63 |
| 2:B:117:LEU:CG | 2:B:147:ASN:CB | 2.76 | 0.63 |
| 1:G:553:MLY:O | 4:X:46:GLY:CA | 2.45 | 0.63 |
| 1:G:817:GLN:HG3 | 2:H:128:PHE:CZ | 2.32 | 0.63 |
| 3:I:45:GLU:O | 3:I:49:ILE:HG13 | 1.97 | 0.63 |
| 1:J:218:LEU:CD2 | 1:J:222:ILE:HG12 | 2.28 | 0.63 |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:N | 2.13 | 0.63 |
| 1:J:636:LYS:HG3 | 4:W:334:GLU:CD | 2.17 | 0.63 |
| 1:S:278:GLN:CG | 1:S:317:GLU:HB2 | 2.27 | 0.63 |
| 1:S:798:LEU:HD11 | 3:U:126:LEU:HD13 | 1.69 | 0.63 |
| 1:S:84:MLY:NZ | 1:S:724:TYR:CE2 | 2.64 | 0.63 |
| 4:1:190:MET:SD | 4:1:209:VAL:HG11 | 2.38 | 0.63 |
| 1:S:642:LYS:CG | 4:2:22:ALA:C | 2.67 | 0.63 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:O | 1.98 | 0.63 |
| 1:A:202:SER:CA | 1:A:207:LYS:HE3 | 2.27 | 0.63 |
| 1:A:537:GLU:HB3 | 1:A:648:THR:HB | 1.80 | 0.63 |
| 1:D:725:ARG:NE | 1:D:737:PHE:HE1 | 1.95 | 0.63 |
| 1:G:107:MLY:HB3 | 1:G:686:MET:CE | 2.27 | 0.63 |
| 1:G:149:GLN:HG2 | 1:G:763:THR:HG22 | 1.69 | 0.63 |
| 1:G:784:ALA:O | 1:G:788:THR:CB | 2.45 | 0.63 |
| 2:H:117:LEU:CG | 2:H:147:ASN:CB | 2.76 | 0.63 |
| 2:H:146:GLY:O | 2:H:147:ASN:CB | 2.46 | 0.63 |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:N | 2.11 | 0.63 |
| 1:J:642:LYS:CG | 4:W:22:ALA:C | 2.67 | 0.63 |
| 1:J:783:LEU:N | 1:J:783:LEU:HD12 | 2.13 | 0.63 |
| 1:M:541:MET:SD | 4:Z:346:LEU:O | 2.48 | 0.63 |
| 1:M:725:ARG:NE | 1:M:737:PHE:CE1 | 2.67 | 0.63 |
| 1:M:805:ALA:O | 1:M:809:ARG:CB | 2.42 | 0.63 |
| 1:S:144:ARG:NH1 | 1:S:160:ASP:OD1 | 2.29 | 0.63 |
| 1:S:505:MLY:CH2 | 1:S:762:HIS:CD2 | 2.80 | 0.63 |
| 4:W:190:MET:SD | 4:W:209:VAL:HG11 | 2.38 | 0.63 |
| 1:S:544:LYS:HB2 | 4:2:147:ARG:HA | 1.80 | 0.63 |
| 1:A:541:MET:CA | 4:8:143:TYR:OH | 2.47 | 0.63 |
| 1:A:818:TYR:HB2 | 2:B:90:GLY:N | 2.13 | 0.63 |
| 1:A:817:GLN:HG3 | 2:B:127:ARG:CG | 2.28 | 0.63 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:CB | 2.46 | 0.63 |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:N | 2.11 | 0.63 |
| 1:J:107:MLY:HB3 | 1:J:686:MET:CE | 2.27 | 0.63 |
| 1:J:544:LYS:HB2 | 4:W:147:ARG:HA | 1.80 | 0.63 |
| 1:J:757:GLN:N | 1:J:776:GLU:HB3 | 2.12 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:132:GLU:O | 2:K:136:MET:HG2 | 1.99 | 0.63 |
| 1:M:210:GLN:O | 1:M:211:SER:OG | 2.15 | 0.63 |
| 1:S:133:PRO:O | 1:S:136:ASN:HB2 | 1.98 | 0.63 |
| 1:S:805:ALA:HA | 1:S:808:GLU:CB | 2.21 | 0.63 |
| 1:S:805:ALA:N | 1:S:807:VAL:N | 2.47 | 0.63 |
| 1:S:91:MET:HE3 | 1:S:119:SER:HB2 | 1.81 | 0.63 |
| 4:V:190:MET:SD | 4:V:209:VAL:HG11 | 2.38 | 0.63 |
| 4:2:287:ILE:HB | 4:4:203:THR:CB | 2.27 | 0.63 |
| 1:S:546:THR:HG23 | 4:4:46:GLY:O | 1.97 | 0.63 |
| 1:D:724:TYR:HB3 | 1:D:727:LEU:HD12 | 1.80 | 0.63 |
| 1:D:724:TYR:HE1 | 1:D:778:MET:C | 2.01 | 0.63 |
| 2:E:140:PHE:HB3 | 2:E:144:VAL:CG1 | 2.28 | 0.63 |
| 2:E:146:GLY:O | 2:E:147:ASN:CB | 2.46 | 0.63 |
| 1:G:217:THR:HB | 1:G:220:ASP:OD2 | 1.97 | 0.63 |
| 1:G:537:GLU:HB3 | 1:G:648:THR:HB | 1.81 | 0.63 |
| 1:G:836:PHE:CE2 | 2:H:160:GLY:N | 2.61 | 0.63 |
| 3:I:4:LYS:N | 3:I:5:ALA:O | 2.16 | 0.63 |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:CD | 2.11 | 0.63 |
| 1:J:724:TYR:HB3 | 1:J:727:LEU:HD12 | 1.80 | 0.63 |
| 1:M:537:GLU:C | 4:Z:351:THR:N | 2.51 | 0.63 |
| 1:M:537:GLU:HB3 | 1:M:648:THR:HB | 1.80 | 0.63 |
| 1:M:642:LYS:CG | 4:Z:22:ALA:C | 2.67 | 0.63 |
| 2:N:146:GLY:O | 2:N:147:ASN:CB | 2.46 | 0.63 |
| 1:M:795:ARG:HH22 | 3:O:116:GLU:CB | 2.00 | 0.63 |
| 1:S:127:ASN:HD22 | 1:S:128:PRO:CD | 2.11 | 0.63 |
| 1:S:546:THR:OG1 | 4:4:47:MET:N | 2.31 | 0.63 |
| 1:G:643:GLY:H | 4:V:23:GLY:C | 2.02 | 0.63 |
| 1:J:642:LYS:CA | 4:W:21:PHE:O | 2.45 | 0.63 |
| 1:M:643:GLY:H | 4:Z:23:GLY:C | 2.02 | 0.63 |
| 4:1:257:CYS:HB3 | 4:1:258:PRO:HD3 | 1.81 | 0.63 |
| 1:D:636:LYS:N | 4:9:334:GLU:OE1 | 2.31 | 0.63 |
| 1:A:831:TRP:CZ3 | 2:B:34:ILE:HG12 | 2.33 | 0.63 |
| 1:G:725:ARG:NE | 1:G:737:PHE:CE1 | 2.67 | 0.63 |
| 1:J:84:MLY:HD2 | 1:J:724:TYR:CE2 | 2.27 | 0.63 |
| 1:J:829:TRP:CH2 | 2:K:84:PHE:CE1 | 2.86 | 0.63 |
| 2:K:144:VAL:CG1 | 2:K:153:ILE:HD13 | 2.20 | 0.63 |
| 1:M:767:PHE:CZ | 1:M:772:LEU:HD13 | 2.32 | 0.63 |
| 1:S:217:THR:HB | 1:S:220:ASP:OD2 | 1.97 | 0.63 |
| 1:S:818:TYR:CE1 | 2:T:127:ARG:CZ | 2.80 | 0.63 |
| 1:S:822:SER:O | 1:S:825:ASN:HB2 | 1.97 | 0.63 |
| 4:Y:257:CYS:HB3 | 4:Y:258:PRO:HD3 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:9:257:CYS:HB3 | 4:9:258:PRO:HD3 | 1.81 | 0.63 |
| 1:A:278:GLN:CG | 1:A:317:GLU:HB2 | 2.27 | 0.63 |
| 1:A:642:LYS:CA | 4:8:21:PHE:O | 2.46 | 0.63 |
| 1:A:725:ARG:NE | 1:A:737:PHE:CE1 | 2.67 | 0.63 |
| 2:E:163:ALA:C | 2:K:22:THR:N | 2.51 | 0.63 |
| 1:D:795:ARG:HB2 | 3:F:35:ARG:NH1 | 2.12 | 0.63 |
| 1:G:202:SER:CA | 1:G:207:LYS:HE3 | 2.28 | 0.63 |
| 1:G:636:LYS:HG3 | 4:V:334:GLU:CD | 2.18 | 0.63 |
| 2:H:121:LEU:HA | 2:H:128:PHE:CG | 2.34 | 0.63 |
| 1:J:567:LYS:HZ1 | 4:Y:92:ASN:ND2 | 1.69 | 0.63 |
| 1:M:202:SER:CA | 1:M:207:LYS:HE3 | 2.27 | 0.63 |
| 1:M:577:ALA:O | 1:M:578:HIS:CD2 | 2.51 | 0.63 |
| 2:N:132:GLU:O | 2:N:136:MET:HG2 | 1.99 | 0.63 |
| 1:S:577:ALA:O | 1:S:578:HIS:CD2 | 2.51 | 0.63 |
| 1:S:612:GLN:HE22 | 1:S:627:GLY:N | 1.95 | 0.63 |
| 1:S:804:ARG:O | 1:S:807:VAL:HB | 1.98 | 0.63 |
| 4:W:257:CYS:HB3 | 4:W:258:PRO:HD3 | 1.81 | 0.63 |
| 4:3:257:CYS:HB3 | 4:3:258:PRO:HD3 | 1.81 | 0.63 |
| 4:7:190:MET:SD | 4:7:209:VAL:HG11 | 2.38 | 0.63 |
| 1:D:642:LYS:CD | 4:9:340:TRP:CZ3 | 2.79 | 0.63 |
| 1:A:149:GLN:CB | 1:A:718:ALA:CB | 2.67 | 0.63 |
| 1:A:642:LYS:CD | 4:8:340:TRP:CZ3 | 2.79 | 0.63 |
| 2:B:146:GLY:O | 2:B:147:ASN:CB | 2.46 | 0.63 |
| 1:D:538:GLU:HA | 4:9:349:LEU:HB3 | 1.78 | 0.63 |
| 1:D:783:LEU:HD12 | 1:D:783:LEU:N | 2.13 | 0.63 |
| 2:E:149:ASP:OD2 | 2:E:150:TYR:C | 2.36 | 0.63 |
| 2:H:111:SER:OG | 2:H:148:VAL:CG1 | 2.47 | 0.63 |
| 2:H:149:ASP:OD2 | 2:H:150:TYR:C | 2.36 | 0.63 |
| 1:J:141:LEU:HD12 | 1:J:141:LEU:H | 1.64 | 0.63 |
| 1:J:251:ARG:HB2 | 1:J:264:ASP:CB | 2.29 | 0.63 |
| 2:K:149:ASP:OD2 | 2:K:150:TYR:C | 2.36 | 0.63 |
| 1:M:278:GLN:CG | 1:M:317:GLU:HB2 | 2.27 | 0.63 |
| 1:M:544:LYS:HB2 | 4:Z:147:ARG:HA | 1.80 | 0.63 |
| 2:N:149:ASP:OD2 | 2:N:150:TYR:C | 2.36 | 0.63 |
| 1:S:406:VAL:HG12 | 1:S:407:GLY:N | 2.13 | 0.63 |
| 1:S:541:MET:C | 4:2:143:TYR:CZ | 2.73 | 0.63 |
| 4:3:287:ILE:CB | 4:5:203:THR:HG22 | 2.29 | 0.63 |
| 4:7:257:CYS:HB3 | 4:7:258:PRO:HD3 | 1.81 | 0.63 |
| 4:8:190:MET:SD | 4:8:209:VAL:HG11 | 2.38 | 0.63 |
| 1:D:541:MET:CA | 4:9:143:TYR:OH | 2.47 | 0.63 |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:N | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:551:MLY:C | 4:V:46:GLY:O | 2.47 | 0.63 |
| 1:A:93:MET:CE | 1:A:716:LEU:H | 2.11 | 0.63 |
| 2:B:121:LEU:HA | 2:B:128:PHE:CG | 2.34 | 0.63 |
| 1:D:202:SER:CA | 1:D:207:LYS:HE3 | 2.27 | 0.63 |
| 1:D:544:LYS:HB2 | 4:9:147:ARG:HA | 1.80 | 0.63 |
| 1:D:642:LYS:CA | 4:9:21:PHE:O | 2.46 | 0.63 |
| 1:D:798:LEU:CD1 | 3:F:126:LEU:CD2 | 2.76 | 0.63 |
| 1:D:831:TRP:CH2 | 2:E:34:ILE:CG2 | 2.82 | 0.63 |
| 1:G:771:LEU:O | 1:G:774:LEU:N | 2.32 | 0.63 |
| 1:J:537:GLU:HB3 | 1:J:648:THR:HB | 1.80 | 0.63 |
| 1:J:813:ILE:HG23 | 2:K:128:PHE:CZ | 2.34 | 0.63 |
| 1:J:831:TRP:CH2 | 2:K:47:LEU:HD22 | 2.32 | 0.63 |
| 1:J:817:GLN:CD | 2:K:127:ARG:CG | 2.66 | 0.63 |
| 2:K:144:VAL:HA | 2:K:153:ILE:HD11 | 1.80 | 0.63 |
| 1:J:795:ARG:CZ | 3:L:116:GLU:OE2 | 2.39 | 0.63 |
| 1:M:724:TYR:HD1 | 1:M:727:LEU:HD11 | 1.64 | 0.63 |
| 1:M:771:LEU:O | 1:M:774:LEU:N | 2.32 | 0.63 |
| 1:M:94:MET:HE1 | 1:M:101:ALA:HB1 | 1.80 | 0.63 |
| 1:S:141:LEU:H | 1:S:141:LEU:HD12 | 1.64 | 0.63 |
| 1:S:202:SER:CA | 1:S:207:LYS:HE3 | 2.27 | 0.63 |
| 1:S:218:LEU:CD2 | 1:S:222:ILE:HG12 | 2.28 | 0.63 |
| 1:G:642:LYS:CD | 4:V:340:TRP:CZ3 | 2.80 | 0.63 |
| 1:J:636:LYS:N | 4:W:334:GLU:OE1 | 2.31 | 0.63 |
| 4:X:190:MET:SD | 4:X:209:VAL:HG11 | 2.38 | 0.63 |
| 4:X:324:THR:O | 4:Z:245:GLY:HA3 | 1.98 | 0.63 |
| 4:Z:190:MET:SD | 4:Z:209:VAL:HG11 | 2.38 | 0.63 |
| 1:A:141:LEU:H | 1:A:141:LEU:HD12 | 1.64 | 0.63 |
| 1:A:479:CYS:HB3 | 1:A:653:PHE:CE2 | 2.33 | 0.63 |
| 1:A:724:TYR:HD1 | 1:A:727:LEU:HD11 | 1.64 | 0.63 |
| 1:D:724:TYR:HD1 | 1:D:782:MLY:CD | 2.10 | 0.63 |
| 2:E:132:GLU:O | 2:E:136:MET:HG2 | 1.99 | 0.63 |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:CD | 2.11 | 0.63 |
| 1:G:830:PRO:CB | 2:H:67:MET:HE1 | 2.29 | 0.63 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:CD1 | 2.29 | 0.63 |
| 1:S:505:MLY:HH21 | 1:S:762:HIS:NE2 | 2.14 | 0.63 |
| 1:S:818:TYR:CZ | 2:T:127:ARG:NH2 | 2.44 | 0.63 |
| 2:T:132:GLU:O | 2:T:136:MET:HG2 | 1.98 | 0.63 |
| 4:X:286:ASP:OD1 | 4:Z:202:THR:CA | 2.44 | 0.63 |
| 4:X:287:ILE:C | 4:Z:205:GLU:OE1 | 2.37 | 0.63 |
| 1:M:642:LYS:CD | 4:Z:340:TRP:CZ3 | 2.79 | 0.63 |
| 1:S:636:LYS:N | 4:2:334:GLU:OE1 | 2.31 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:551:MLY:C | 4:2:46:GLY:O | 2.47 | 0.62 |
| 4:5:257:CYS:HB3 | 4:5:258:PRO:HD3 | 1.81 | 0.62 |
| 4:6:257:CYS:HB3 | 4:6:258:PRO:HD3 | 1.81 | 0.62 |
| 4:8:257:CYS:HB3 | 4:8:258:PRO:HD3 | 1.81 | 0.62 |
| 4:9:190:MET:SD | 4:9:209:VAL:HG11 | 2.38 | 0.62 |
| 1:A:251:ARG:HB2 | 1:A:264:ASP:CB | 2.29 | 0.62 |
| 1:A:542:PHE:CZ | 1:A:553:MLY:HH11 | 2.34 | 0.62 |
| 1:A:752:ASP:OD2 | 1:A:782:MLY:HD3 | 1.99 | 0.62 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:HG23 | 2.33 | 0.62 |
| 1:D:251:ARG:HB2 | 1:D:264:ASP:CB | 2.29 | 0.62 |
| 1:D:725:ARG:NE | 1:D:737:PHE:CE1 | 2.67 | 0.62 |
| 1:D:767:PHE:O | 1:D:771:LEU:HD21 | 1.98 | 0.62 |
| 1:G:724:TYR:HB3 | 1:G:727:LEU:HD12 | 1.80 | 0.62 |
| 1:G:754:ASP:O | 1:G:776:GLU:CD | 2.36 | 0.62 |
| 1:G:791:GLN:CD | 3:I:116:GLU:N | 2.52 | 0.62 |
| 1:G:789:ALA:HB1 | 3:I:81:GLN:NE2 | 2.14 | 0.62 |
| 1:J:166:MET:HE3 | 1:J:254:PHE:HD2 | 1.63 | 0.62 |
| 1:J:735:GLY:O | 1:J:743:ALA:HA | 1.94 | 0.62 |
| 1:M:406:VAL:HG12 | 1:M:407:GLY:N | 2.13 | 0.62 |
| 3:O:24:LYS:HB3 | 3:O:63:ILE:H | 1.64 | 0.62 |
| 1:S:537:GLU:HB3 | 1:S:648:THR:HB | 1.80 | 0.62 |
| 1:S:793:ARG:NH1 | 3:U:40:ASN:HB2 | 2.13 | 0.62 |
| 2:T:144:VAL:CG1 | 2:T:153:ILE:HD13 | 2.20 | 0.62 |
| 4:X:324:THR:OG1 | 4:Z:246:GLN:HA | 1.99 | 0.62 |
| 4:1:324:THR:CG2 | 4:3:244:ASP:HA | 2.29 | 0.62 |
| 4:1:324:THR:OG1 | 4:3:244:ASP:CA | 2.47 | 0.62 |
| 4:4:190:MET:SD | 4:4:209:VAL:HG11 | 2.38 | 0.62 |
| 1:A:302:MET:HG2 | 1:A:303:LEU:CD1 | 2.30 | 0.62 |
| 1:A:541:MET:C | 4:8:143:TYR:CZ | 2.73 | 0.62 |
| 1:D:551:MLY:C | 4:W:46:GLY:O | 2.47 | 0.62 |
| 1:G:94:MET:HE1 | 1:G:101:ALA:HB1 | 1.79 | 0.62 |
| 1:G:557:GLU:HB2 | 4:X:47:MET:N | 2.11 | 0.62 |
| 2:H:132:GLU:O | 2:H:136:MET:HG2 | 1.99 | 0.62 |
| 1:M:251:ARG:HB2 | 1:M:264:ASP:CB | 2.29 | 0.62 |
| 1:M:580:SER:HA | 1:M:588:VAL:O | 2.00 | 0.62 |
| 1:M:724:TYR:HB3 | 1:M:727:LEU:HD12 | 1.80 | 0.62 |
| 1:M:730:SER:C | 1:M:733:PRO:HD2 | 2.20 | 0.62 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:HD3 | 1.78 | 0.62 |
| 2:N:111:SER:OG | 2:N:148:VAL:CG1 | 2.47 | 0.62 |
| 1:M:792:ALA:CB | 3:O:42:THR:HG22 | 2.22 | 0.62 |
| 3:O:49:ILE:HA | 3:O:52:ASN:ND2 | 2.06 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:746:LYS:O | 3:U:93:VAL:CG2 | 2.47 | 0.62 |
| 1:S:795:ARG:CB | 3:U:35:ARG:CZ | 2.77 | 0.62 |
| 2:T:121:LEU:HA | 2:T:128:PHE:CG | 2.34 | 0.62 |
| 1:J:556:ASP:OD2 | 4:Y:47:MET:HE2 | 1.94 | 0.62 |
| 4:4:287:ILE:CG2 | 4:6:202:THR:CA | 2.76 | 0.62 |
| 1:A:530:MET:HA | 4:8:354:GLN:CB | 2.29 | 0.62 |
| 1:A:537:GLU:C | 4:8:351:THR:N | 2.52 | 0.62 |
| 1:A:553:MLY:O | 4:V:48:GLY:HA2 | 1.99 | 0.62 |
| 2:B:114:LYS:HA | 2:B:146:GLY:C | 2.03 | 0.62 |
| 3:C:24:LYS:HB3 | 3:C:63:ILE:H | 1.65 | 0.62 |
| 1:D:530:MET:CG | 4:9:354:GLN:CG | 2.71 | 0.62 |
| 1:D:538:GLU:HA | 4:9:349:LEU:CG | 2.28 | 0.62 |
| 1:D:542:PHE:CZ | 1:D:553:MLY:HH11 | 2.34 | 0.62 |
| 1:D:724:TYR:HD1 | 1:D:727:LEU:HD11 | 1.64 | 0.62 |
| 2:E:121:LEU:HA | 2:E:128:PHE:CG | 2.34 | 0.62 |
| 1:D:834:LEU:CD2 | 2:E:54:MET:HG3 | 2.27 | 0.62 |
| 1:G:752:ASP:OD1 | 1:G:783:LEU:N | 2.32 | 0.62 |
| 1:J:642:LYS:CD | 4:W:340:TRP:CZ3 | 2.79 | 0.62 |
| 1:M:541:MET:C | 4:Z:143:TYR:CZ | 2.73 | 0.62 |
| 1:M:541:MET:CA | 4:Z:143:TYR:OH | 2.47 | 0.62 |
| 1:M:642:LYS:CD | 4:Z:24:ASP:O | 2.43 | 0.62 |
| 1:A:538:GLU:HA | 4:8:349:LEU:CG | 2.27 | 0.62 |
| 1:D:161:ASN:HA | 1:D:164:GLN:HE21 | 1.64 | 0.62 |
| 1:D:278:GLN:HG3 | 1:D:318:GLY:N | 2.15 | 0.62 |
| 1:D:771:LEU:O | 1:D:774:LEU:N | 2.32 | 0.62 |
| 1:D:800:ARG:HG2 | 3:F:149:VAL:HG22 | 1.80 | 0.62 |
| 1:G:141:LEU:H | 1:G:141:LEU:HD12 | 1.64 | 0.62 |
| 1:G:274:ARG:HB2 | 1:G:285:TYR:CE2 | 2.34 | 0.62 |
| 1:G:530:MET:HA | 4:V:354:GLN:CB | 2.30 | 0.62 |
| 1:G:580:SER:HA | 1:G:588:VAL:O | 2.00 | 0.62 |
| 1:G:636:LYS:N | 4:V:334:GLU:OE1 | 2.32 | 0.62 |
| 1:J:278:GLN:HG3 | 1:J:318:GLY:N | 2.15 | 0.62 |
| 1:J:538:GLU:HA | 4:W:349:LEU:CG | 2.28 | 0.62 |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CB | 1.84 | 0.62 |
| 2:K:121:LEU:HA | 2:K:128:PHE:CG | 2.34 | 0.62 |
| 1:M:202:SER:HA | 1:M:207:LYS:HE3 | 1.72 | 0.62 |
| 1:M:803:TYR:O | 1:M:807:VAL:HG23 | 1.99 | 0.62 |
| 1:M:91:MET:HE3 | 1:M:119:SER:HB2 | 1.82 | 0.62 |
| 1:M:95:THR:CB | 1:M:713:SER:CB | 2.77 | 0.62 |
| 1:S:578:HIS:CD2 | 1:S:591:ASN:HA | 2.31 | 0.62 |
| 4:2:190:MET:SD | 4:2:209:VAL:HG11 | 2.38 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:553:MLY:O | 4:2:48:GLY:HA2 | 1.99 | 0.62 |
| 1:A:274:ARG:HB2 | 1:A:285:TYR:CE2 | 2.34 | 0.62 |
| 1:A:278:GLN:HG3 | 1:A:318:GLY:N | 2.15 | 0.62 |
| 1:A:544:LYS:HB2 | 4:8:147:ARG:HA | 1.80 | 0.62 |
| 1:A:578:HIS:CB | 1:A:592:ILE:HD12 | 2.30 | 0.62 |
| 1:A:642:LYS:CG | 4:8:22:ALA:C | 2.67 | 0.62 |
| 1:A:799:MET:SD | 3:C:32:ASP:C | 2.78 | 0.62 |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:C | 2.37 | 0.62 |
| 1:D:730:SER:C | 1:D:733:PRO:HD2 | 2.20 | 0.62 |
| 1:D:839:MLY:CH1 | 2:E:159:HIS:CD2 | 2.82 | 0.62 |
| 1:G:503:TYR:HE1 | 1:G:711:PHE:CD2 | 2.15 | 0.62 |
| 1:G:541:MET:C | 4:V:143:TYR:CZ | 2.73 | 0.62 |
| 1:G:717:TYR:HD1 | 1:G:744:SER:HG | 1.47 | 0.62 |
| 1:G:730:SER:C | 1:G:733:PRO:HD2 | 2.20 | 0.62 |
| 1:J:771:LEU:O | 1:J:774:LEU:N | 2.32 | 0.62 |
| 1:J:830:PRO:HB3 | 2:K:67:MET:HE1 | 1.81 | 0.62 |
| 2:K:146:GLY:O | 2:K:147:ASN:CB | 2.46 | 0.62 |
| 1:M:302:MET:HG2 | 1:M:303:LEU:CD1 | 2.30 | 0.62 |
| 1:M:542:PHE:CZ | 1:M:553:MLY:HH11 | 2.34 | 0.62 |
| 1:M:795:ARG:CB | 3:O:35:ARG:CZ | 2.77 | 0.62 |
| 1:S:479:CYS:HB3 | 1:S:653:PHE:CE2 | 2.33 | 0.62 |
| 1:S:580:SER:HA | 1:S:588:VAL:O | 2.00 | 0.62 |
| 1:S:730:SER:C | 1:S:733:PRO:HD2 | 2.20 | 0.62 |
| 1:S:771:LEU:O | 1:S:774:LEU:N | 2.32 | 0.62 |
| 1:S:829:TRP:CZ3 | 2:T:84:PHE:CZ | 2.87 | 0.62 |
| 1:S:98:HIS:HB3 | 1:S:100:PRO:CD | 2.25 | 0.62 |
| 1:J:541:MET:CA | 4:W:143:TYR:OH | 2.46 | 0.62 |
| 1:M:543:PRO:HG2 | 4:Z:143:TYR:O | 1.98 | 0.62 |
| 4:4:257:CYS:HB3 | 4:4:258:PRO:HD3 | 1.81 | 0.62 |
| 1:A:543:PRO:HG2 | 4:8:143:TYR:O | 1.98 | 0.62 |
| 1:A:580:SER:HA | 1:A:588:VAL:O | 2.00 | 0.62 |
| 1:A:771:LEU:O | 1:A:774:LEU:N | 2.32 | 0.62 |
| 1:A:91:MET:HE3 | 1:A:119:SER:HB2 | 1.82 | 0.62 |
| 1:A:830:PRO:HG2 | 2:B:67:MET:HE1 | 1.81 | 0.62 |
| 1:D:166:MET:HE1 | 1:D:254:PHE:HB2 | 1.82 | 0.62 |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:N | 2.13 | 0.62 |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:CH1 | 2.56 | 0.62 |
| 1:G:544:LYS:HB2 | 4:V:147:ARG:HA | 1.80 | 0.62 |
| 1:J:210:GLN:O | 1:J:211:SER:OG | 2.15 | 0.62 |
| 1:J:730:SER:C | 1:J:733:PRO:HD2 | 2.20 | 0.62 |
| 1:M:154:HIS:CE1 | 1:M:156:PHE:CD2 | 2.88 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:732:ILE:HG22 | 1:M:747:LEU:CD1 | 1.55 | 0.62 |
| 1:M:831:TRP:HE1 | 2:N:67:MET:CB | 2.13 | 0.62 |
| 1:S:538:GLU:CD | 4:2:355:MET:HE3 | 2.19 | 0.62 |
| 1:S:735:GLY:O | 1:S:743:ALA:HA | 1.94 | 0.62 |
| 1:S:798:LEU:CD1 | 3:U:126:LEU:HD13 | 2.22 | 0.62 |
| 2:T:111:SER:OG | 2:T:148:VAL:CG1 | 2.48 | 0.62 |
| 2:T:149:ASP:OD2 | 2:T:150:TYR:C | 2.36 | 0.62 |
| 3:U:24:LYS:HB3 | 3:U:63:ILE:H | 1.64 | 0.62 |
| 4:1:361:GLU:HB3 | 4:1:369:ILE:HG12 | 1.82 | 0.62 |
| 1:D:542:PHE:CB | 4:9:143:TYR:HE1 | 2.13 | 0.62 |
| 1:A:730:SER:C | 1:A:733:PRO:HD2 | 2.20 | 0.62 |
| 1:A:817:GLN:CG | 2:B:127:ARG:CG | 2.76 | 0.62 |
| 1:D:735:GLY:O | 1:D:743:ALA:HA | 1.94 | 0.62 |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HE2 | 1.81 | 0.62 |
| 2:E:114:LYS:HG3 | 2:E:146:GLY:HA2 | 1.82 | 0.62 |
| 1:G:721:LYS:HG2 | 1:G:736:GLN:CD | 1.86 | 0.62 |
| 1:M:717:TYR:HD1 | 1:M:744:SER:HG | 1.46 | 0.62 |
| 1:S:819:ASN:CB | 2:T:90:GLY:O | 2.48 | 0.62 |
| 3:U:48:LYS:C | 3:U:52:ASN:HD21 | 1.96 | 0.62 |
| 1:G:541:MET:CA | 4:V:143:TYR:OH | 2.47 | 0.62 |
| 4:Z:257:CYS:HB3 | 4:Z:258:PRO:HD3 | 1.81 | 0.62 |
| 4:3:324:THR:HG23 | 4:5:244:ASP:C | 2.18 | 0.62 |
| 4:6:190:MET:SD | 4:6:209:VAL:HG11 | 2.38 | 0.62 |
| 1:G:251:ARG:HB2 | 1:G:264:ASP:CB | 2.29 | 0.62 |
| 1:G:302:MET:HG2 | 1:G:303:LEU:CD1 | 2.30 | 0.62 |
| 1:J:542:PHE:CZ | 1:J:553:MLY:HH11 | 2.34 | 0.62 |
| 1:J:580:SER:HA | 1:J:588:VAL:O | 2.00 | 0.62 |
| 1:J:84:MLY:NZ | 1:J:724:TYR:CD2 | 2.68 | 0.62 |
| 1:J:795:ARG:HG3 | 3:L:116:GLU:OE2 | 1.99 | 0.62 |
| 1:M:161:ASN:HA | 1:M:164:GLN:HE21 | 1.63 | 0.62 |
| 1:M:84:MLY:HH12 | 1:M:715:VAL:CG1 | 2.19 | 0.62 |
| 1:S:251:ARG:HB2 | 1:S:264:ASP:CB | 2.29 | 0.62 |
| 1:S:724:TYR:HB3 | 1:S:727:LEU:HD12 | 1.80 | 0.62 |
| 1:S:797:PHE:CE2 | 3:U:146:ILE:HG23 | 2.34 | 0.62 |
| 4:X:257:CYS:HB3 | 4:X:258:PRO:HD3 | 1.81 | 0.62 |
| 4:X:287:ILE:O | 4:Z:205:GLU:CD | 2.38 | 0.62 |
| 1:A:541:MET:HE2 | 4:8:346:LEU:HD12 | 1.82 | 0.62 |
| 1:A:154:HIS:CE1 | 1:A:156:PHE:CD2 | 2.88 | 0.62 |
| 2:B:117:LEU:HD11 | 2:B:147:ASN:HB3 | 1.76 | 0.62 |
| 1:A:815:CYS:O | 2:B:90:GLY:O | 2.16 | 0.62 |
| 3:C:48:LYS:C | 3:C:52:ASN:HD21 | 1.97 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:141:LEU:H | 1:D:141:LEU:HD12 | 1.64 | 0.62 |
| 1:D:541:MET:C | 4:9:143:TYR:CZ | 2.73 | 0.62 |
| 1:G:154:HIS:CE1 | 1:G:156:PHE:CD2 | 2.88 | 0.62 |
| 1:J:829:TRP:HZ3 | 2:K:84:PHE:CE2 | 2.18 | 0.62 |
| 1:S:154:HIS:CE1 | 1:S:156:PHE:CD2 | 2.88 | 0.62 |
| 2:T:146:GLY:O | 2:T:147:ASN:CB | 2.46 | 0.62 |
| 3:U:52:ASN:N | 3:U:53:PRO:HD2 | 2.15 | 0.62 |
| 3:U:50:LEU:O | 3:U:53:PRO:HD2 | 2.00 | 0.62 |
| 4:V:257:CYS:HB3 | 4:V:258:PRO:HD3 | 1.81 | 0.62 |
| 4:X:361:GLU:HB3 | 4:X:369:ILE:HG12 | 1.82 | 0.62 |
| 1:A:542:PHE:N | 4:8:143:TYR:OH | 2.33 | 0.62 |
| 1:D:541:MET:HE1 | 4:9:346:LEU:HD12 | 1.82 | 0.62 |
| 1:D:530:MET:CG | 4:9:354:GLN:HG3 | 2.30 | 0.62 |
| 1:A:98:HIS:HB3 | 1:A:100:PRO:CD | 2.25 | 0.62 |
| 1:D:641:LYS:CE | 1:D:647:GLN:CB | 2.75 | 0.62 |
| 1:D:649:VAL:HA | 1:D:649:VAL:HG22 | 1.80 | 0.62 |
| 1:D:747:LEU:HD22 | 1:D:782:MLY:HH11 | 1.78 | 0.62 |
| 1:G:98:HIS:HB3 | 1:G:100:PRO:CD | 2.25 | 0.62 |
| 2:H:144:VAL:HA | 2:H:153:ILE:HD11 | 1.80 | 0.62 |
| 1:J:161:ASN:HA | 1:J:164:GLN:HE21 | 1.64 | 0.62 |
| 1:J:541:MET:HE2 | 4:W:346:LEU:HD12 | 1.82 | 0.62 |
| 1:J:557:GLU:O | 1:J:557:GLU:HG3 | 2.00 | 0.62 |
| 1:M:636:LYS:N | 4:Z:334:GLU:OE1 | 2.31 | 0.62 |
| 1:M:35:MLY:CE | 1:M:777:GLU:CD | 2.63 | 0.62 |
| 1:S:161:ASN:HA | 1:S:164:GLN:HE21 | 1.64 | 0.62 |
| 1:S:278:GLN:HG3 | 1:S:318:GLY:N | 2.15 | 0.62 |
| 1:S:302:MET:HG2 | 1:S:303:LEU:CD1 | 2.30 | 0.62 |
| 1:S:542:PHE:N | 4:2:143:TYR:OH | 2.33 | 0.62 |
| 1:J:542:PHE:CB | 4:W:143:TYR:HE1 | 2.13 | 0.62 |
| 4:2:257:CYS:HB3 | 4:2:258:PRO:HD3 | 1.81 | 0.61 |
| 1:A:520:ALA:O | 1:A:524:GLU:HG2 | 2.00 | 0.61 |
| 1:A:817:GLN:HE21 | 2:B:127:ARG:HG2 | 0.65 | 0.61 |
| 1:D:274:ARG:HB2 | 1:D:285:TYR:CE2 | 2.34 | 0.61 |
| 1:D:553:MLY:O | 4:W:48:GLY:HA2 | 1.99 | 0.61 |
| 1:D:578:HIS:CB | 1:D:592:ILE:HD12 | 2.30 | 0.61 |
| 1:D:721:LYS:HG2 | 1:D:736:GLN:CD | 1.86 | 0.61 |
| 1:D:724:TYR:CG | 1:D:782:MLY:CD | 2.83 | 0.61 |
| 1:D:798:LEU:HD21 | 3:F:122:GLU:HB3 | 1.82 | 0.61 |
| 1:G:542:PHE:CZ | 1:G:553:MLY:HH11 | 2.34 | 0.61 |
| 1:G:578:HIS:CB | 1:G:592:ILE:HD12 | 2.30 | 0.61 |
| 1:G:579:PHE:CE1 | 1:G:581:LEU:HD13 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:CG | 4:V:22:ALA:C | 2.66 | 0.61 |
| 1:G:643:GLY:O | 1:G:644:SER:CB | 2.48 | 0.61 |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD11 | 0.72 | 0.61 |
| 3:L:52:ASN:N | 3:L:53:PRO:HD2 | 2.15 | 0.61 |
| 1:M:278:GLN:HG3 | 1:M:318:GLY:N | 2.15 | 0.61 |
| 1:M:411:GLU:N | 4:Z:333:PRO:HB2 | 2.11 | 0.61 |
| 1:M:542:PHE:N | 4:Z:143:TYR:OH | 2.33 | 0.61 |
| 1:M:578:HIS:CD2 | 1:M:591:ASN:HA | 2.31 | 0.61 |
| 1:M:98:HIS:HB3 | 1:M:100:PRO:CD | 2.25 | 0.61 |
| 1:S:274:ARG:HB2 | 1:S:285:TYR:CE2 | 2.34 | 0.61 |
| 1:S:505:MLY:CH2 | 1:S:762:HIS:NE2 | 2.63 | 0.61 |
| 1:G:538:GLU:CD | 4:V:355:MET:CE | 2.62 | 0.61 |
| 1:J:634:GLY:N | 4:W:25:ASP:O | 2.31 | 0.61 |
| 4:Y:361:GLU:HB3 | 4:Y:369:ILE:HG12 | 1.82 | 0.61 |
| 1:M:639:GLY:N | 4:Z:344:SER:C | 2.54 | 0.61 |
| 4:3:361:GLU:HB3 | 4:3:369:ILE:HG12 | 1.82 | 0.61 |
| 4:4:361:GLU:HB3 | 4:4:369:ILE:HG12 | 1.82 | 0.61 |
| 3:C:49:ILE:HA | 3:C:52:ASN:ND2 | 2.05 | 0.61 |
| 1:D:520:ALA:O | 1:D:524:GLU:HG2 | 2.00 | 0.61 |
| 1:D:506:GLU:OE2 | 1:D:764:MLY:HE3 | 1.99 | 0.61 |
| 2:E:111:SER:OG | 2:E:148:VAL:CG1 | 2.48 | 0.61 |
| 2:E:144:VAL:HA | 2:E:153:ILE:HD11 | 1.80 | 0.61 |
| 1:G:542:PHE:N | 4:V:143:TYR:OH | 2.33 | 0.61 |
| 2:K:111:SER:OG | 2:K:148:VAL:CG1 | 2.48 | 0.61 |
| 3:L:50:LEU:O | 3:L:53:PRO:HD2 | 2.00 | 0.61 |
| 1:M:274:ARG:HB2 | 1:M:285:TYR:CE2 | 2.34 | 0.61 |
| 2:N:121:LEU:HA | 2:N:128:PHE:CG | 2.34 | 0.61 |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:CD | 2.11 | 0.61 |
| 1:A:93:MET:CE | 1:A:715:VAL:CA | 2.64 | 0.61 |
| 1:D:302:MET:HG2 | 1:D:303:LEU:CD1 | 2.30 | 0.61 |
| 1:D:506:GLU:O | 1:D:762:HIS:HB2 | 2.00 | 0.61 |
| 1:G:506:GLU:CD | 1:G:760:PHE:O | 2.37 | 0.61 |
| 3:I:52:ASN:N | 3:I:53:PRO:HD2 | 2.16 | 0.61 |
| 1:J:302:MET:HG2 | 1:J:303:LEU:CD1 | 2.30 | 0.61 |
| 1:J:541:MET:C | 4:W:143:TYR:CZ | 2.73 | 0.61 |
| 1:J:578:HIS:CB | 1:J:592:ILE:HD12 | 2.30 | 0.61 |
| 1:M:141:LEU:HD12 | 1:M:141:LEU:H | 1.64 | 0.61 |
| 1:S:215:GLN:CA | 1:S:340:ILE:CG2 | 2.63 | 0.61 |
| 1:S:411:GLU:N | 4:2:333:PRO:HB2 | 2.11 | 0.61 |
| 1:S:543:PRO:HG2 | 4:2:143:TYR:O | 1.98 | 0.61 |
| 1:S:623:PHE:CG | 1:S:623:PHE:HA | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:643:GLY:H | 4:W:23:GLY:C | 2.02 | 0.61 |
| 1:A:579:PHE:CE1 | 1:A:581:LEU:HD13 | 2.35 | 0.61 |
| 3:C:50:LEU:O | 3:C:53:PRO:HD2 | 2.00 | 0.61 |
| 3:C:52:ASN:N | 3:C:53:PRO:HD2 | 2.15 | 0.61 |
| 1:D:557:GLU:O | 1:D:557:GLU:HG3 | 2.00 | 0.61 |
| 1:D:732:ILE:HD11 | 1:D:782:MLY:HH11 | 1.79 | 0.61 |
| 2:E:117:LEU:HD11 | 2:E:147:ASN:HB3 | 1.76 | 0.61 |
| 3:F:24:LYS:HB3 | 3:F:63:ILE:H | 1.64 | 0.61 |
| 3:F:63:ILE:HG22 | 3:F:64:THR:O | 2.01 | 0.61 |
| 1:G:724:TYR:HD1 | 1:G:727:LEU:HD11 | 1.64 | 0.61 |
| 3:I:24:LYS:HB3 | 3:I:63:ILE:H | 1.64 | 0.61 |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:HA | 1.80 | 0.61 |
| 1:J:84:MLY:N | 1:J:723:ARG:CZ | 2.64 | 0.61 |
| 3:L:24:LYS:HB3 | 3:L:63:ILE:H | 1.64 | 0.61 |
| 1:J:557:GLU:HB2 | 4:Y:47:MET:N | 2.11 | 0.61 |
| 1:A:639:GLY:N | 4:8:344:SER:C | 2.54 | 0.61 |
| 1:A:524:GLU:O | 1:A:528:MLY:HB3 | 2.01 | 0.61 |
| 2:B:111:SER:OG | 2:B:148:VAL:CG1 | 2.47 | 0.61 |
| 1:D:712:PRO:CB | 1:D:771:LEU:HD22 | 2.19 | 0.61 |
| 1:D:81:ASN:OD1 | 1:D:96:HIS:HB2 | 2.00 | 0.61 |
| 1:G:278:GLN:HG3 | 1:G:318:GLY:N | 2.15 | 0.61 |
| 1:G:752:ASP:OD1 | 1:G:783:LEU:CA | 2.48 | 0.61 |
| 2:H:150:TYR:C | 2:H:151:LYS:CG | 2.48 | 0.61 |
| 1:J:84:MLY:HH12 | 1:J:715:VAL:HG21 | 1.82 | 0.61 |
| 1:M:520:ALA:O | 1:M:524:GLU:HG2 | 2.00 | 0.61 |
| 1:M:643:GLY:O | 1:M:644:SER:CB | 2.49 | 0.61 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:CG | 2.30 | 0.61 |
| 1:S:542:PHE:CZ | 1:S:553:MLY:HH11 | 2.34 | 0.61 |
| 1:S:557:GLU:O | 1:S:557:GLU:HG3 | 2.00 | 0.61 |
| 4:V:361:GLU:HB3 | 4:V:369:ILE:HG12 | 1.82 | 0.61 |
| 1:J:530:MET:CG | 4:W:354:GLN:HG3 | 2.31 | 0.61 |
| 4:8:361:GLU:HB3 | 4:8:369:ILE:HG12 | 1.82 | 0.61 |
| 1:A:686:MET:HG3 | 1:A:691:VAL:HG21 | 1.83 | 0.61 |
| 1:D:580:SER:HA | 1:D:588:VAL:O | 2.00 | 0.61 |
| 3:F:52:ASN:N | 3:F:53:PRO:HD2 | 2.16 | 0.61 |
| 1:G:686:MET:HG3 | 1:G:691:VAL:HG21 | 1.83 | 0.61 |
| 1:G:81:ASN:OD1 | 1:G:96:HIS:HB2 | 2.00 | 0.61 |
| 1:J:524:GLU:O | 1:J:528:MLY:HB3 | 2.01 | 0.61 |
| 1:J:686:MET:HG3 | 1:J:691:VAL:HG21 | 1.83 | 0.61 |
| 1:J:81:ASN:OD1 | 1:J:96:HIS:HB2 | 2.00 | 0.61 |
| 2:K:114:LYS:HG3 | 2:K:146:GLY:HA2 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:524:GLU:O | 1:M:528:MLY:HB3 | 2.01 | 0.61 |
| 1:M:578:HIS:CB | 1:M:592:ILE:HD12 | 2.30 | 0.61 |
| 1:M:84:MLY:HH22 | 1:M:719:ASP:O | 2.01 | 0.61 |
| 1:M:818:TYR:CG | 2:N:127:ARG:NH1 | 2.68 | 0.61 |
| 1:S:578:HIS:CB | 1:S:592:ILE:HD12 | 2.30 | 0.61 |
| 1:S:826:VAL:HG21 | 2:T:88:LEU:HD23 | 1.82 | 0.61 |
| 1:S:793:ARG:NE | 3:U:40:ASN:HD22 | 1.96 | 0.61 |
| 1:S:795:ARG:CZ | 3:U:43:ASN:OD1 | 2.47 | 0.61 |
| 1:J:542:PHE:N | 4:W:143:TYR:OH | 2.33 | 0.61 |
| 4:Z:361:GLU:HB3 | 4:Z:369:ILE:HG12 | 1.82 | 0.61 |
| 4:2:361:GLU:HB3 | 4:2:369:ILE:HG12 | 1.82 | 0.61 |
| 4:6:361:GLU:HB3 | 4:6:369:ILE:HG12 | 1.82 | 0.61 |
| 2:E:34:ILE:O | 2:E:46:ASP:HB3 | 2.01 | 0.61 |
| 1:J:154:HIS:CE1 | 1:J:156:PHE:CD2 | 2.88 | 0.61 |
| 1:J:724:TYR:HD1 | 1:J:727:LEU:HD11 | 1.64 | 0.61 |
| 1:M:557:GLU:HG3 | 1:M:557:GLU:O | 2.00 | 0.61 |
| 1:M:623:PHE:CG | 1:M:623:PHE:HA | 2.35 | 0.61 |
| 2:N:34:ILE:O | 2:N:46:ASP:HB3 | 2.01 | 0.61 |
| 1:S:724:TYR:HD1 | 1:S:727:LEU:HD11 | 1.64 | 0.61 |
| 1:G:530:MET:HE3 | 4:V:355:MET:SD | 2.41 | 0.61 |
| 1:G:553:MLY:HB2 | 4:X:46:GLY:HA3 | 1.83 | 0.61 |
| 1:A:643:GLY:H | 4:8:23:GLY:C | 2.02 | 0.61 |
| 1:D:542:PHE:N | 4:9:143:TYR:OH | 2.33 | 0.61 |
| 1:A:502:GLU:HA | 1:A:762:HIS:H | 1.64 | 0.61 |
| 2:B:114:LYS:HG3 | 2:B:146:GLY:HA2 | 1.82 | 0.61 |
| 1:D:524:GLU:O | 1:D:528:MLY:HB3 | 2.01 | 0.61 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:HD23 | 2.35 | 0.61 |
| 1:G:99:GLU:OE2 | 1:G:696:ARG:NH2 | 2.30 | 0.61 |
| 1:G:829:TRP:CE3 | 2:H:87:LYS:NZ | 2.67 | 0.61 |
| 3:I:63:ILE:HG22 | 3:I:64:THR:O | 2.01 | 0.61 |
| 1:J:643:GLY:O | 1:J:644:SER:CB | 2.48 | 0.61 |
| 1:S:751:GLY:O | 3:U:89:GLU:OE2 | 2.19 | 0.61 |
| 4:V:286:ASP:OD2 | 4:X:203:THR:CG2 | 2.47 | 0.61 |
| 4:5:223:PHE:HD2 | 4:5:312:ARG:NH2 | 1.99 | 0.61 |
| 1:A:643:GLY:O | 1:A:644:SER:CB | 2.48 | 0.61 |
| 2:B:34:ILE:O | 2:B:46:ASP:HB3 | 2.01 | 0.61 |
| 1:D:623:PHE:HA | 1:D:623:PHE:CG | 2.36 | 0.61 |
| 1:D:724:TYR:HB3 | 1:D:782:MLY:CE | 2.29 | 0.61 |
| 1:D:814:PHE:CE1 | 2:E:127:ARG:NH2 | 2.69 | 0.61 |
| 3:F:50:LEU:O | 3:F:53:PRO:HD2 | 2.00 | 0.61 |
| 1:G:217:THR:C | 1:G:221:GLN:HG2 | 2.21 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:520:ALA:O | 1:G:524:GLU:HG2 | 2.00 | 0.61 |
| 1:J:813:ILE:O | 1:J:817:GLN:N | 2.30 | 0.61 |
| 1:M:686:MET:HG3 | 1:M:691:VAL:HG21 | 1.83 | 0.61 |
| 2:N:114:LYS:HA | 2:N:146:GLY:C | 2.03 | 0.61 |
| 3:O:50:LEU:O | 3:O:53:PRO:HD2 | 2.00 | 0.61 |
| 1:S:524:GLU:O | 1:S:528:MLY:HB3 | 2.01 | 0.61 |
| 1:S:795:ARG:HB3 | 3:U:35:ARG:CZ | 2.30 | 0.61 |
| 1:J:38:VAL:HB | 1:J:52:ILE:HD11 | 1.83 | 0.61 |
| 1:J:520:ALA:O | 1:J:524:GLU:HG2 | 2.00 | 0.61 |
| 3:L:63:ILE:HG22 | 3:L:64:THR:O | 2.01 | 0.61 |
| 1:M:579:PHE:CE1 | 1:M:581:LEU:HD13 | 2.35 | 0.61 |
| 1:M:99:GLU:OE2 | 1:M:696:ARG:NH2 | 2.31 | 0.61 |
| 1:S:520:ALA:O | 1:S:524:GLU:HG2 | 2.00 | 0.61 |
| 1:S:579:PHE:CE1 | 1:S:581:LEU:HD13 | 2.35 | 0.61 |
| 1:S:686:MET:HG3 | 1:S:691:VAL:HG21 | 1.83 | 0.61 |
| 1:S:502:GLU:CD | 1:S:761:GLY:HA3 | 2.19 | 0.61 |
| 1:S:797:PHE:CZ | 3:U:146:ILE:CA | 2.80 | 0.61 |
| 1:G:541:MET:HE1 | 4:V:346:LEU:HD12 | 1.82 | 0.61 |
| 1:D:643:GLY:H | 4:9:23:GLY:C | 2.02 | 0.60 |
| 1:A:161:ASN:HA | 1:A:164:GLN:HE21 | 1.63 | 0.60 |
| 1:A:40:VAL:HG22 | 1:A:41:VAL:N | 2.16 | 0.60 |
| 1:A:623:PHE:HA | 1:A:623:PHE:CG | 2.36 | 0.60 |
| 1:D:154:HIS:CE1 | 1:D:156:PHE:CD2 | 2.88 | 0.60 |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CE2 | 2.30 | 0.60 |
| 1:G:506:GLU:OE2 | 1:G:760:PHE:HB2 | 2.01 | 0.60 |
| 1:G:578:HIS:CD2 | 1:G:591:ASN:HA | 2.31 | 0.60 |
| 1:G:734:GLU:OE2 | 3:I:109:HIS:CE1 | 2.54 | 0.60 |
| 1:J:274:ARG:HB2 | 1:J:285:TYR:CE2 | 2.34 | 0.60 |
| 1:J:769:ALA:CB | 1:J:770:GLY:HA3 | 2.31 | 0.60 |
| 2:K:140:PHE:O | 2:K:141:PRO:C | 2.33 | 0.60 |
| 1:J:839:MLY:HD2 | 2:K:159:HIS:HB3 | 1.83 | 0.60 |
| 1:M:786:ILE:N | 1:M:787:ILE:N | 2.48 | 0.60 |
| 1:M:84:MLY:CH2 | 1:M:719:ASP:C | 2.60 | 0.60 |
| 1:S:538:GLU:HA | 4:2:349:LEU:CG | 2.28 | 0.60 |
| 1:G:543:PRO:HG2 | 4:V:143:TYR:O | 1.99 | 0.60 |
| 4:W:223:PHE:HD2 | 4:W:312:ARG:NH2 | 1.99 | 0.60 |
| 4:5:361:GLU:HB3 | 4:5:369:ILE:HG12 | 1.82 | 0.60 |
| 4:6:223:PHE:HD2 | 4:6:312:ARG:NH2 | 1.99 | 0.60 |
| 1:A:542:PHE:CB | 4:8:143:TYR:HE1 | 2.12 | 0.60 |
| 4:8:223:PHE:HD2 | 4:8:312:ARG:NH2 | 1.99 | 0.60 |
| 4:9:361:GLU:HB3 | 4:9:369:ILE:HG12 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:81:ASN:OD1 | 1:A:96:HIS:HB2 | 2.00 | 0.60 |
| 3:C:63:ILE:HG22 | 3:C:64:THR:O | 2.01 | 0.60 |
| 1:D:665:ARG:C | 1:D:667:THR:H | 2.05 | 0.60 |
| 1:G:541:MET:SD | 4:V:346:LEU:O | 2.49 | 0.60 |
| 1:G:557:GLU:O | 1:G:557:GLU:HG3 | 2.01 | 0.60 |
| 1:J:278:GLN:CG | 1:J:317:GLU:HB2 | 2.27 | 0.60 |
| 1:J:541:MET:SD | 4:W:346:LEU:O | 2.48 | 0.60 |
| 2:K:34:ILE:O | 2:K:46:ASP:HB3 | 2.01 | 0.60 |
| 1:M:720:PHE:CZ | 1:M:772:LEU:HD11 | 2.36 | 0.60 |
| 3:O:63:ILE:HG22 | 3:O:64:THR:O | 2.01 | 0.60 |
| 1:S:749:GLY:C | 3:U:89:GLU:HB3 | 2.20 | 0.60 |
| 4:Z:223:PHE:HD2 | 4:Z:312:ARG:NH2 | 1.99 | 0.60 |
| 1:A:156:PHE:CD1 | 1:A:195:TYR:CD1 | 2.89 | 0.60 |
| 1:D:210:GLN:O | 1:D:211:SER:OG | 2.15 | 0.60 |
| 1:D:217:THR:C | 1:D:221:GLN:HG2 | 2.21 | 0.60 |
| 1:D:639:GLY:N | 4:9:344:SER:C | 2.54 | 0.60 |
| 1:D:686:MET:HG3 | 1:D:691:VAL:HG21 | 1.83 | 0.60 |
| 1:D:793:ARG:HH21 | 3:F:147:MET:HE3 | 1.57 | 0.60 |
| 1:G:161:ASN:HA | 1:G:164:GLN:HE21 | 1.64 | 0.60 |
| 1:G:757:GLN:CB | 1:G:776:GLU:HG3 | 2.29 | 0.60 |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:HE1 | 1.60 | 0.60 |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:CD1 | 1.55 | 0.60 |
| 1:J:710:GLY:HA2 | 1:J:772:LEU:HD22 | 1.03 | 0.60 |
| 1:M:217:THR:C | 1:M:221:GLN:HG2 | 2.22 | 0.60 |
| 1:M:124:VAL:CG1 | 1:M:675:ILE:HD13 | 2.31 | 0.60 |
| 1:M:798:LEU:CD2 | 3:O:126:LEU:CD1 | 2.76 | 0.60 |
| 1:S:751:GLY:CA | 1:S:779:ARG:HH22 | 2.14 | 0.60 |
| 1:S:817:GLN:CD | 2:T:127:ARG:CD | 2.58 | 0.60 |
| 3:U:63:ILE:HG22 | 3:U:64:THR:O | 2.01 | 0.60 |
| 4:V:223:PHE:HD2 | 4:V:312:ARG:NH2 | 1.99 | 0.60 |
| 1:M:542:PHE:CB | 4:Z:143:TYR:HE1 | 2.13 | 0.60 |
| 4:7:361:GLU:HB3 | 4:7:369:ILE:HG12 | 1.82 | 0.60 |
| 1:A:149:GLN:CG | 1:A:719:ASP:H | 2.14 | 0.60 |
| 1:A:38:VAL:HB | 1:A:52:ILE:HD11 | 1.84 | 0.60 |
| 1:A:530:MET:CG | 4:8:354:GLN:HG3 | 2.30 | 0.60 |
| 1:A:546:THR:HG22 | 1:A:547:ASP:N | 2.17 | 0.60 |
| 1:A:553:MLY:NZ | 4:V:45:VAL:HG13 | 2.16 | 0.60 |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:CD1 | 1.55 | 0.60 |
| 1:D:530:MET:HA | 4:9:354:GLN:CB | 2.29 | 0.60 |
| 1:D:795:ARG:NE | 3:F:116:GLU:HB3 | 2.16 | 0.60 |
| 1:D:813:ILE:O | 1:D:817:GLN:N | 2.30 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:524:GLU:O | 1:G:528:MLY:HB3 | 2.01 | 0.60 |
| 1:G:754:ASP:CG | 1:G:779:ARG:CB | 2.69 | 0.60 |
| 2:H:114:LYS:HG3 | 2:H:146:GLY:HA2 | 1.82 | 0.60 |
| 3:I:50:LEU:O | 3:I:53:PRO:HD2 | 2.00 | 0.60 |
| 1:J:665:ARG:C | 1:J:667:THR:H | 2.05 | 0.60 |
| 2:K:117:LEU:CG | 2:K:147:ASN:CB | 2.76 | 0.60 |
| 1:S:599:ASN:CB | 1:S:649:VAL:HB | 2.32 | 0.60 |
| 1:S:834:LEU:CD1 | 2:T:51:PHE:CD1 | 2.82 | 0.60 |
| 1:S:84:MLY:CH2 | 1:S:719:ASP:O | 2.49 | 0.60 |
| 2:T:114:LYS:HG3 | 2:T:146:GLY:HA2 | 1.82 | 0.60 |
| 1:S:838:ILE:CD1 | 2:T:54:MET:HE1 | 2.26 | 0.60 |
| 4:1:203:THR:CG2 | 4:Y:286:ASP:OD2 | 2.47 | 0.60 |
| 4:7:287:ILE:HD12 | 4:7:287:ILE:H | 1.67 | 0.60 |
| 4:9:223:PHE:HD2 | 4:9:312:ARG:NH2 | 1.99 | 0.60 |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:HD13 | 1.84 | 0.60 |
| 1:D:579:PHE:CE1 | 1:D:581:LEU:HD13 | 2.35 | 0.60 |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD2 | 2.31 | 0.60 |
| 1:D:820:VAL:HG11 | 2:E:136:MET:HE1 | 1.82 | 0.60 |
| 1:G:156:PHE:CD1 | 1:G:195:TYR:CD1 | 2.90 | 0.60 |
| 1:G:40:VAL:HG22 | 1:G:41:VAL:N | 2.16 | 0.60 |
| 1:G:546:THR:HG22 | 1:G:547:ASP:N | 2.17 | 0.60 |
| 1:G:623:PHE:CG | 1:G:623:PHE:HA | 2.36 | 0.60 |
| 1:G:837:MLY:O | 1:G:840:PRO:HD2 | 2.02 | 0.60 |
| 2:H:34:ILE:O | 2:H:46:ASP:HB3 | 2.01 | 0.60 |
| 1:J:757:GLN:NE2 | 1:J:777:GLU:H | 1.93 | 0.60 |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:HG2 | 1.60 | 0.60 |
| 2:K:130:PRO:HA | 2:K:133:ILE:HD12 | 1.83 | 0.60 |
| 1:M:40:VAL:HG22 | 1:M:41:VAL:N | 2.16 | 0.60 |
| 1:M:599:ASN:CB | 1:M:649:VAL:HB | 2.32 | 0.60 |
| 1:M:753:VAL:CG1 | 1:M:775:LEU:CD1 | 2.75 | 0.60 |
| 1:S:643:GLY:O | 1:S:644:SER:CB | 2.49 | 0.60 |
| 1:S:717:TYR:HD1 | 1:S:744:SER:HG | 1.49 | 0.60 |
| 1:G:530:MET:CG | 4:V:354:GLN:HG3 | 2.30 | 0.60 |
| 4:W:361:GLU:HB3 | 4:W:369:ILE:HG12 | 1.82 | 0.60 |
| 4:X:223:PHE:HD2 | 4:X:312:ARG:NH2 | 1.99 | 0.60 |
| 4:Y:223:PHE:HD2 | 4:Y:312:ARG:NH2 | 1.99 | 0.60 |
| 4:1:287:ILE:HD12 | 4:1:287:ILE:H | 1.67 | 0.60 |
| 1:S:530:MET:CG | 4:2:354:GLN:HG3 | 2.30 | 0.60 |
| 4:9:287:ILE:H | 4:9:287:ILE:HD12 | 1.67 | 0.60 |
| 1:A:837:MLY:O | 1:A:840:PRO:HD2 | 2.02 | 0.60 |
| 1:D:38:VAL:HB | 1:D:52:ILE:HD11 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:643:GLY:O | 1:D:644:SER:CB | 2.48 | 0.60 |
| 1:D:800:ARG:CG | 3:F:149:VAL:HG22 | 2.31 | 0.60 |
| 1:G:550:PHE:CE2 | 1:G:592:ILE:HG23 | 2.37 | 0.60 |
| 1:G:634:GLY:N | 4:V:25:ASP:O | 2.31 | 0.60 |
| 1:G:599:ASN:CB | 1:G:649:VAL:HB | 2.32 | 0.60 |
| 1:G:768:MLY:HH23 | 1:G:772:LEU:HD11 | 1.60 | 0.60 |
| 1:J:557:GLU:CB | 4:Y:47:MET:C | 2.50 | 0.60 |
| 1:J:579:PHE:CE1 | 1:J:581:LEU:HD13 | 2.35 | 0.60 |
| 1:J:95:THR:HG23 | 1:J:96:HIS:ND1 | 2.17 | 0.60 |
| 3:L:52:ASN:HB2 | 3:L:53:PRO:CD | 2.28 | 0.60 |
| 1:M:295:MLY:HG3 | 1:M:332:MET:HE1 | 1.83 | 0.60 |
| 2:N:130:PRO:HA | 2:N:133:ILE:HD12 | 1.84 | 0.60 |
| 1:S:156:PHE:CD1 | 1:S:195:TYR:CD1 | 2.90 | 0.60 |
| 1:S:40:VAL:HG22 | 1:S:41:VAL:N | 2.16 | 0.60 |
| 1:S:124:VAL:CG1 | 1:S:675:ILE:HD13 | 2.32 | 0.60 |
| 1:S:95:THR:HG23 | 1:S:96:HIS:ND1 | 2.17 | 0.60 |
| 2:T:34:ILE:O | 2:T:46:ASP:HB3 | 2.01 | 0.60 |
| 4:2:223:PHE:HD2 | 4:2:312:ARG:NH2 | 1.99 | 0.60 |
| 4:2:287:ILE:HD12 | 4:2:287:ILE:H | 1.67 | 0.60 |
| 4:4:223:PHE:HD2 | 4:4:312:ARG:NH2 | 1.99 | 0.60 |
| 1:D:831:TRP:HZ3 | 2:E:34:ILE:HG12 | 1.65 | 0.60 |
| 1:D:836:PHE:CZ | 2:E:159:HIS:HA | 2.37 | 0.60 |
| 1:D:837:MLY:O | 1:D:840:PRO:HD2 | 2.02 | 0.60 |
| 1:D:95:THR:HG23 | 1:D:96:HIS:ND1 | 2.17 | 0.60 |
| 1:G:124:VAL:CG1 | 1:G:675:ILE:HD13 | 2.31 | 0.60 |
| 1:G:817:GLN:HG2 | 2:H:127:ARG:HB3 | 1.80 | 0.60 |
| 1:J:411:GLU:N | 4:W:333:PRO:HB2 | 2.11 | 0.60 |
| 1:M:541:MET:HE2 | 4:Z:346:LEU:HD12 | 1.81 | 0.60 |
| 1:M:553:MLY:NZ | 4:2:45:VAL:HG13 | 2.17 | 0.60 |
| 1:M:95:THR:OG1 | 1:M:713:SER:OG | 2.20 | 0.60 |
| 1:M:81:ASN:OD1 | 1:M:96:HIS:HB2 | 2.00 | 0.60 |
| 3:O:3:SER:HG | 3:O:5:ALA:N | 1.99 | 0.60 |
| 1:S:38:VAL:HB | 1:S:52:ILE:HD11 | 1.83 | 0.60 |
| 1:S:60:VAL:O | 1:S:71:THR:HA | 2.02 | 0.60 |
| 1:S:81:ASN:OD1 | 1:S:96:HIS:HB2 | 2.00 | 0.60 |
| 1:G:542:PHE:CB | 4:V:143:TYR:HE1 | 2.13 | 0.60 |
| 1:D:411:GLU:N | 4:9:333:PRO:HB2 | 2.11 | 0.60 |
| 1:A:578:HIS:CD2 | 1:A:591:ASN:HA | 2.31 | 0.60 |
| 1:A:831:TRP:CZ3 | 2:B:34:ILE:CG2 | 2.84 | 0.60 |
| 1:D:124:VAL:CG1 | 1:D:675:ILE:HD13 | 2.31 | 0.60 |
| 1:D:278:GLN:CG | 1:D:317:GLU:HB2 | 2.27 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:783:LEU:O | 1:D:787:ILE:N | 2.28 | 0.60 |
| 1:G:38:VAL:HB | 1:G:52:ILE:HD11 | 1.84 | 0.60 |
| 1:G:736:GLN:HA | 1:G:743:ALA:HB1 | 1.27 | 0.60 |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:HB1 | 1.83 | 0.60 |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:HD13 | 1.84 | 0.60 |
| 1:J:127:ASN:ND2 | 1:J:128:PRO:HD2 | 2.16 | 0.60 |
| 1:J:546:THR:HG22 | 1:J:547:ASP:N | 2.17 | 0.60 |
| 1:J:599:ASN:CB | 1:J:649:VAL:HB | 2.32 | 0.60 |
| 1:J:756:THR:CG2 | 1:J:779:ARG:HB3 | 2.31 | 0.60 |
| 1:J:84:MLY:HH11 | 1:J:720:PHE:HD1 | 0.80 | 0.60 |
| 1:M:156:PHE:CD1 | 1:M:195:TYR:CD1 | 2.90 | 0.60 |
| 1:M:665:ARG:C | 1:M:667:THR:H | 2.05 | 0.60 |
| 1:S:7:MET:HE3 | 1:S:14:ALA:HB1 | 1.82 | 0.60 |
| 1:S:217:THR:C | 1:S:221:GLN:HG2 | 2.21 | 0.60 |
| 1:S:550:PHE:CE2 | 1:S:592:ILE:HG23 | 2.37 | 0.60 |
| 2:T:130:PRO:HA | 2:T:133:ILE:HD12 | 1.83 | 0.60 |
| 3:U:3:SER:HG | 3:U:5:ALA:N | 1.99 | 0.60 |
| 1:S:542:PHE:CB | 4:2:143:TYR:HE1 | 2.13 | 0.60 |
| 1:A:124:VAL:CG1 | 1:A:675:ILE:HD13 | 2.31 | 0.60 |
| 1:A:217:THR:C | 1:A:221:GLN:HG2 | 2.21 | 0.60 |
| 1:A:60:VAL:O | 1:A:71:THR:HA | 2.02 | 0.60 |
| 1:A:599:ASN:CB | 1:A:649:VAL:HB | 2.32 | 0.60 |
| 1:A:817:GLN:NE2 | 2:B:127:ARG:NE | 2.47 | 0.60 |
| 1:D:599:ASN:CB | 1:D:649:VAL:HB | 2.32 | 0.60 |
| 1:J:217:THR:C | 1:J:221:GLN:HG2 | 2.21 | 0.60 |
| 1:J:124:VAL:CG1 | 1:J:675:ILE:HD13 | 2.31 | 0.60 |
| 1:M:38:VAL:HB | 1:M:52:ILE:HD11 | 1.83 | 0.60 |
| 1:S:786:ILE:C | 1:S:787:ILE:CA | 2.70 | 0.60 |
| 1:S:839:MLY:HD2 | 2:T:159:HIS:CB | 2.31 | 0.60 |
| 4:W:286:ASP:OD2 | 4:Y:203:THR:CG2 | 2.47 | 0.60 |
| 1:M:530:MET:CG | 4:Z:354:GLN:HG3 | 2.30 | 0.60 |
| 1:A:40:VAL:HG22 | 1:A:41:VAL:H | 1.67 | 0.60 |
| 3:F:52:ASN:N | 3:F:53:PRO:CD | 2.65 | 0.60 |
| 1:G:95:THR:HG23 | 1:G:96:HIS:ND1 | 2.17 | 0.60 |
| 1:J:84:MLY:HD2 | 1:J:724:TYR:CZ | 2.33 | 0.60 |
| 1:S:502:GLU:CD | 1:S:761:GLY:HA2 | 2.22 | 0.60 |
| 1:S:769:ALA:O | 1:S:773:GLY:N | 2.17 | 0.60 |
| 4:V:286:ASP:OD1 | 4:X:202:THR:HB | 2.02 | 0.60 |
| 4:3:287:ILE:H | 4:3:287:ILE:HD12 | 1.67 | 0.59 |
| 1:A:791:GLN:NE2 | 3:C:115:GLY:HA3 | 2.16 | 0.59 |
| 1:D:49:MLY:HH13 | 1:D:108:GLU:OE2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:506:GLU:O | 1:D:762:HIS:CB | 2.49 | 0.59 |
| 1:J:40:VAL:HG22 | 1:J:41:VAL:N | 2.16 | 0.59 |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CE1 | 2.37 | 0.59 |
| 1:J:576:GLU:CG | 1:J:577:ALA:N | 2.44 | 0.59 |
| 1:J:623:PHE:CG | 1:J:623:PHE:HA | 2.35 | 0.59 |
| 1:J:755:HIS:HA | 1:J:758:TYR:HE1 | 1.64 | 0.59 |
| 2:K:117:LEU:CB | 2:K:147:ASN:ND2 | 2.35 | 0.59 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:CG | 2.28 | 0.59 |
| 1:M:60:VAL:O | 1:M:71:THR:HA | 2.02 | 0.59 |
| 1:M:806:MET:C | 1:M:807:VAL:HA | 2.21 | 0.59 |
| 1:M:95:THR:HG23 | 1:M:96:HIS:ND1 | 2.17 | 0.59 |
| 1:S:135:TYR:N | 1:S:135:TYR:CD1 | 2.70 | 0.59 |
| 1:S:503:TYR:HH | 1:S:711:PHE:HD2 | 1.50 | 0.59 |
| 1:S:541:MET:HE2 | 4:2:346:LEU:HD12 | 1.82 | 0.59 |
| 1:S:665:ARG:C | 1:S:667:THR:H | 2.05 | 0.59 |
| 3:U:52:ASN:N | 3:U:53:PRO:CD | 2.65 | 0.59 |
| 4:Z:287:ILE:H | 4:Z:287:ILE:HD12 | 1.67 | 0.59 |
| 1:A:776:GLU:O | 1:A:779:ARG:HB3 | 2.02 | 0.59 |
| 1:A:799:MET:SD | 3:C:32:ASP:O | 2.60 | 0.59 |
| 1:D:578:HIS:CD2 | 1:D:591:ASN:HA | 2.32 | 0.59 |
| 1:D:85:TYR:HH | 1:D:772:LEU:CD2 | 1.75 | 0.59 |
| 1:J:710:GLY:CA | 1:J:772:LEU:HD23 | 2.23 | 0.59 |
| 1:J:787:ILE:O | 1:J:790:THR:N | 2.35 | 0.59 |
| 1:J:836:PHE:CE2 | 2:K:160:GLY:CA | 2.85 | 0.59 |
| 1:J:800:ARG:HD2 | 3:L:149:VAL:HG13 | 1.84 | 0.59 |
| 1:M:795:ARG:HH22 | 3:O:116:GLU:CG | 2.15 | 0.59 |
| 1:S:210:GLN:O | 1:S:211:SER:OG | 2.15 | 0.59 |
| 1:S:506:GLU:CD | 1:S:760:PHE:HD1 | 2.02 | 0.59 |
| 1:S:837:MLY:O | 1:S:840:PRO:HD2 | 2.02 | 0.59 |
| 1:S:94:MET:O | 1:S:713:SER:HA | 2.02 | 0.59 |
| 4:1:202:THR:HB | 4:Y:286:ASP:OD1 | 2.02 | 0.59 |
| 4:1:223:PHE:HD2 | 4:1:312:ARG:NH2 | 1.99 | 0.59 |
| 1:A:665:ARG:C | 1:A:667:THR:H | 2.05 | 0.59 |
| 1:A:752:ASP:O | 1:A:778:MET:CB | 2.51 | 0.59 |
| 1:A:95:THR:HG23 | 1:A:96:HIS:ND1 | 2.16 | 0.59 |
| 1:D:40:VAL:HG22 | 1:D:41:VAL:N | 2.16 | 0.59 |
| 1:G:295:MLY:HG3 | 1:G:332:MET:HE1 | 1.84 | 0.59 |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CE1 | 2.37 | 0.59 |
| 1:G:60:VAL:O | 1:G:71:THR:HA | 2.02 | 0.59 |
| 1:G:776:GLU:O | 1:G:779:ARG:HB3 | 2.03 | 0.59 |
| 1:G:829:TRP:HH2 | 2:H:83:MET:HE3 | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:156:PHE:CD1 | 1:J:195:TYR:CD1 | 2.90 | 0.59 |
| 1:J:550:PHE:CE2 | 1:J:592:ILE:HG23 | 2.37 | 0.59 |
| 1:J:784:ALA:O | 1:J:788:THR:HB | 2.02 | 0.59 |
| 1:M:546:THR:HG22 | 1:M:547:ASP:N | 2.17 | 0.59 |
| 1:S:93:MET:CG | 1:S:715:VAL:CA | 2.80 | 0.59 |
| 1:G:411:GLU:N | 4:V:333:PRO:HB2 | 2.11 | 0.59 |
| 4:8:287:ILE:HD12 | 4:8:287:ILE:H | 1.67 | 0.59 |
| 1:D:798:LEU:CD2 | 3:F:122:GLU:HB3 | 2.33 | 0.59 |
| 1:D:838:ILE:CD1 | 2:E:54:MET:CE | 2.79 | 0.59 |
| 2:E:130:PRO:HA | 2:E:133:ILE:HD12 | 1.84 | 0.59 |
| 1:G:116:TYR:HB2 | 1:G:153:PRO:O | 2.03 | 0.59 |
| 1:G:94:MET:O | 1:G:713:SER:HB3 | 2.02 | 0.59 |
| 1:J:639:GLY:N | 4:W:344:SER:C | 2.54 | 0.59 |
| 1:J:60:VAL:O | 1:J:71:THR:HA | 2.02 | 0.59 |
| 3:L:102:VAL:HG11 | 3:L:107:LEU:HB2 | 1.84 | 0.59 |
| 2:N:114:LYS:HG3 | 2:N:146:GLY:HA2 | 1.82 | 0.59 |
| 2:N:140:PHE:O | 2:N:141:PRO:C | 2.33 | 0.59 |
| 1:S:755:HIS:HA | 1:S:758:TYR:HE1 | 1.64 | 0.59 |
| 1:S:787:ILE:O | 1:S:790:THR:N | 2.35 | 0.59 |
| 1:S:804:ARG:C | 1:S:808:GLU:H | 2.06 | 0.59 |
| 3:U:102:VAL:HG11 | 3:U:107:LEU:HB2 | 1.85 | 0.59 |
| 1:J:552:ASN:C | 4:Y:47:MET:HE1 | 2.22 | 0.59 |
| 4:X:291:LYS:HG3 | 4:Z:243:PRO:C | 2.22 | 0.59 |
| 1:A:411:GLU:N | 4:8:333:PRO:HB2 | 2.11 | 0.59 |
| 1:D:542:PHE:CD1 | 4:9:143:TYR:CE1 | 2.90 | 0.59 |
| 1:A:195:TYR:O | 1:A:199:ILE:HG23 | 2.03 | 0.59 |
| 1:A:210:GLN:O | 1:A:211:SER:OG | 2.15 | 0.59 |
| 1:A:817:GLN:CG | 2:B:127:ARG:HG2 | 2.33 | 0.59 |
| 1:J:135:TYR:N | 1:J:135:TYR:CD1 | 2.69 | 0.59 |
| 1:J:791:GLN:HE22 | 3:L:115:GLY:CA | 2.13 | 0.59 |
| 3:L:52:ASN:N | 3:L:53:PRO:CD | 2.65 | 0.59 |
| 1:M:116:TYR:HB2 | 1:M:153:PRO:O | 2.03 | 0.59 |
| 3:O:102:VAL:HG11 | 3:O:107:LEU:HB2 | 1.85 | 0.59 |
| 1:S:124:VAL:HG13 | 1:S:675:ILE:HD13 | 1.84 | 0.59 |
| 1:S:536:LEU:HD13 | 1:S:550:PHE:CE1 | 2.37 | 0.59 |
| 1:D:553:MLY:NZ | 4:W:45:VAL:HG13 | 2.17 | 0.59 |
| 1:M:542:PHE:CD1 | 4:Z:143:TYR:CE1 | 2.90 | 0.59 |
| 4:7:223:PHE:HD2 | 4:7:312:ARG:NH2 | 1.99 | 0.59 |
| 1:D:538:GLU:CD | 4:9:355:MET:CE | 2.62 | 0.59 |
| 1:A:230:GLU:O | 1:A:234:ASN:HB2 | 2.03 | 0.59 |
| 1:A:649:VAL:HG22 | 1:A:649:VAL:HA | 1.80 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:839:MLY:HH11 | 2:B:159:HIS:CD2 | 2.14 | 0.59 |
| 1:A:831:TRP:CE2 | 2:B:51:PHE:CE2 | 2.89 | 0.59 |
| 1:D:156:PHE:CD1 | 1:D:195:TYR:CD1 | 2.90 | 0.59 |
| 1:D:202:SER:HA | 1:D:207:LYS:HE3 | 1.72 | 0.59 |
| 1:D:265:ILE:HG22 | 1:D:266:GLU:N | 2.18 | 0.59 |
| 1:D:60:VAL:O | 1:D:71:THR:HA | 2.02 | 0.59 |
| 1:D:800:ARG:CB | 3:F:149:VAL:HG22 | 2.33 | 0.59 |
| 1:J:534:SER:C | 4:W:351:THR:CA | 2.47 | 0.59 |
| 1:J:578:HIS:CD2 | 1:J:591:ASN:HA | 2.31 | 0.59 |
| 1:J:793:ARG:NH1 | 3:L:40:ASN:ND2 | 2.50 | 0.59 |
| 1:M:124:VAL:HG13 | 1:M:675:ILE:HD13 | 1.84 | 0.59 |
| 1:M:135:TYR:N | 1:M:135:TYR:CD1 | 2.70 | 0.59 |
| 1:M:94:MET:O | 1:M:713:SER:HA | 2.03 | 0.59 |
| 1:M:95:THR:OG1 | 1:M:770:GLY:HA2 | 2.03 | 0.59 |
| 1:M:836:PHE:CZ | 2:N:160:GLY:H | 1.59 | 0.59 |
| 1:S:49:MLY:HH13 | 1:S:108:GLU:OE2 | 2.02 | 0.59 |
| 1:S:817:GLN:CB | 2:T:127:ARG:NH1 | 2.41 | 0.59 |
| 4:W:286:ASP:OD1 | 4:Y:202:THR:HB | 2.02 | 0.59 |
| 1:A:542:PHE:CD1 | 4:8:143:TYR:CE1 | 2.90 | 0.59 |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CE1 | 2.37 | 0.59 |
| 1:A:800:ARG:CG | 3:C:149:VAL:HG22 | 2.33 | 0.59 |
| 1:D:546:THR:HG22 | 1:D:547:ASP:N | 2.17 | 0.59 |
| 1:G:230:GLU:O | 1:G:234:ASN:HB2 | 2.03 | 0.59 |
| 1:G:549:SER:OG | 1:G:550:PHE:N | 2.36 | 0.59 |
| 1:J:505:MLY:HG3 | 1:J:762:HIS:HE1 | 1.66 | 0.59 |
| 1:J:776:GLU:O | 1:J:779:ARG:HB3 | 2.02 | 0.59 |
| 1:J:832:MET:SD | 2:K:84:PHE:HE2 | 2.26 | 0.59 |
| 1:M:230:GLU:O | 1:M:234:ASN:HB2 | 2.03 | 0.59 |
| 1:M:813:ILE:O | 1:M:817:GLN:N | 2.30 | 0.59 |
| 1:S:542:PHE:CD1 | 4:2:143:TYR:CE1 | 2.91 | 0.59 |
| 1:S:546:THR:HG21 | 4:4:46:GLY:C | 2.21 | 0.59 |
| 1:S:804:ARG:C | 1:S:807:VAL:CB | 2.68 | 0.59 |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:CD1 | 2.33 | 0.59 |
| 1:A:530:MET:HE3 | 4:8:355:MET:SD | 2.42 | 0.59 |
| 1:A:831:TRP:CZ2 | 2:B:47:LEU:HD23 | 2.37 | 0.59 |
| 1:D:543:PRO:HG2 | 4:9:143:TYR:O | 1.98 | 0.59 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:CG2 | 2.72 | 0.59 |
| 1:D:831:TRP:NE1 | 2:E:67:MET:SD | 2.71 | 0.59 |
| 1:D:822:SER:OG | 2:E:88:LEU:HD23 | 2.02 | 0.59 |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:CD1 | 2.33 | 0.59 |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:HD13 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:538:GLU:HA | 4:V:349:LEU:CG | 2.28 | 0.59 |
| 1:G:787:ILE:O | 1:G:790:THR:N | 2.35 | 0.59 |
| 1:M:536:LEU:HD13 | 1:M:550:PHE:CE1 | 2.37 | 0.59 |
| 1:M:787:ILE:O | 1:M:790:THR:N | 2.35 | 0.59 |
| 3:O:52:ASN:N | 3:O:53:PRO:HD2 | 2.15 | 0.59 |
| 1:S:798:LEU:HD23 | 3:U:122:GLU:HB3 | 1.84 | 0.59 |
| 4:X:287:ILE:O | 4:Z:205:GLU:OE1 | 2.21 | 0.59 |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CE1 | 2.37 | 0.59 |
| 1:D:549:SER:OG | 1:D:550:PHE:N | 2.36 | 0.59 |
| 1:D:676:ILE:HG23 | 1:D:676:ILE:O | 2.03 | 0.59 |
| 1:D:727:LEU:HD13 | 1:D:782:MLY:CH1 | 2.26 | 0.59 |
| 1:G:135:TYR:CD1 | 1:G:135:TYR:N | 2.70 | 0.59 |
| 1:G:166:MET:HE3 | 1:G:254:PHE:CD2 | 2.38 | 0.59 |
| 1:G:48:VAL:HG22 | 1:G:49:MLY:N | 2.18 | 0.59 |
| 1:G:649:VAL:HG22 | 1:G:649:VAL:HA | 1.80 | 0.59 |
| 1:G:665:ARG:C | 1:G:667:THR:H | 2.05 | 0.59 |
| 1:G:791:GLN:HE22 | 3:I:115:GLY:C | 2.01 | 0.59 |
| 2:H:130:PRO:HA | 2:H:133:ILE:HD12 | 1.84 | 0.59 |
| 1:J:49:MLY:HH13 | 1:J:108:GLU:OE2 | 2.02 | 0.59 |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:HD1 | 1.68 | 0.59 |
| 1:J:791:GLN:NE2 | 3:L:116:GLU:H | 2.01 | 0.59 |
| 1:M:837:MLY:O | 1:M:840:PRO:HD2 | 2.02 | 0.59 |
| 1:M:819:ASN:CB | 2:N:90:GLY:O | 2.50 | 0.59 |
| 3:O:52:ASN:N | 3:O:53:PRO:CD | 2.65 | 0.59 |
| 1:S:116:TYR:HB2 | 1:S:153:PRO:O | 2.03 | 0.59 |
| 1:S:776:GLU:O | 1:S:779:ARG:HB3 | 2.03 | 0.59 |
| 4:4:287:ILE:H | 4:4:287:ILE:HD12 | 1.67 | 0.59 |
| 1:A:116:TYR:HB2 | 1:A:153:PRO:O | 2.03 | 0.59 |
| 1:A:549:SER:OG | 1:A:550:PHE:N | 2.36 | 0.59 |
| 1:A:787:ILE:O | 1:A:790:THR:N | 2.35 | 0.59 |
| 1:D:529:PRO:HG3 | 4:9:353:GLN:OE1 | 2.03 | 0.59 |
| 1:D:717:TYR:HD1 | 1:D:744:SER:HG | 1.50 | 0.59 |
| 3:F:49:ILE:CA | 3:F:52:ASN:ND2 | 2.53 | 0.59 |
| 1:G:218:LEU:N | 1:G:221:GLN:HE21 | 2.01 | 0.59 |
| 1:G:601:ASP:N | 1:G:602:PRO:HD3 | 2.18 | 0.59 |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:HA | 1.68 | 0.59 |
| 1:G:830:PRO:CB | 2:H:67:MET:CE | 2.81 | 0.59 |
| 1:J:230:GLU:O | 1:J:234:ASN:HB2 | 2.03 | 0.59 |
| 1:J:464:ILE:HG22 | 1:J:465:ALA:N | 2.18 | 0.59 |
| 1:J:839:MLY:CH1 | 2:K:159:HIS:HD2 | 2.14 | 0.59 |
| 3:L:49:ILE:HA | 3:L:52:ASN:ND2 | 2.06 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:40:VAL:HG22 | 1:M:41:VAL:H | 1.67 | 0.59 |
| 1:M:7:MET:HE3 | 1:M:14:ALA:HB1 | 1.84 | 0.59 |
| 1:S:40:VAL:HG22 | 1:S:41:VAL:H | 1.67 | 0.59 |
| 4:5:287:ILE:H | 4:5:287:ILE:HD12 | 1.67 | 0.58 |
| 1:D:530:MET:HE3 | 4:9:354:GLN:CG | 2.29 | 0.58 |
| 1:D:646:PHE:CD2 | 1:D:652:LEU:CD1 | 2.85 | 0.58 |
| 1:D:715:VAL:HG11 | 1:D:720:PHE:HD1 | 1.68 | 0.58 |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:CD1 | 1.55 | 0.58 |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HE3 | 1.84 | 0.58 |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:HA2 | 1.66 | 0.58 |
| 1:G:823:PHE:HE1 | 2:H:160:GLY:HA2 | 1.68 | 0.58 |
| 1:J:549:SER:OG | 1:J:550:PHE:N | 2.35 | 0.58 |
| 1:J:553:MLY:HB2 | 4:Y:46:GLY:HA3 | 1.83 | 0.58 |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:CD1 | 2.33 | 0.58 |
| 1:J:717:TYR:HD1 | 1:J:744:SER:HG | 1.50 | 0.58 |
| 1:J:97:LEU:HD22 | 1:J:712:PRO:CB | 2.33 | 0.58 |
| 1:M:48:VAL:HG22 | 1:M:49:MLY:N | 2.18 | 0.58 |
| 1:M:49:MLY:HH13 | 1:M:108:GLU:OE2 | 2.02 | 0.58 |
| 1:S:629:GLU:HB3 | 1:S:645:SER:N | 2.18 | 0.58 |
| 1:S:676:ILE:O | 1:S:676:ILE:HG23 | 2.03 | 0.58 |
| 1:S:783:LEU:CA | 1:S:786:ILE:HD11 | 2.30 | 0.58 |
| 1:S:797:PHE:CZ | 3:U:146:ILE:HG23 | 2.37 | 0.58 |
| 1:J:542:PHE:CD1 | 4:W:143:TYR:CE1 | 2.91 | 0.58 |
| 1:J:557:GLU:HB2 | 4:Y:47:MET:O | 2.03 | 0.58 |
| 4:6:287:ILE:HD12 | 4:6:287:ILE:H | 1.67 | 0.58 |
| 1:A:135:TYR:N | 1:A:135:TYR:CD1 | 2.70 | 0.58 |
| 1:A:813:ILE:O | 1:A:817:GLN:N | 2.30 | 0.58 |
| 1:D:507:GLY:CA | 1:D:762:HIS:CE1 | 2.82 | 0.58 |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:HG22 | 1.85 | 0.58 |
| 1:G:195:TYR:O | 1:G:199:ILE:HG23 | 2.03 | 0.58 |
| 3:I:52:ASN:N | 3:I:53:PRO:CD | 2.65 | 0.58 |
| 1:J:7:MET:HE3 | 1:J:14:ALA:HB1 | 1.84 | 0.58 |
| 1:J:795:ARG:HE | 3:L:116:GLU:CD | 2.04 | 0.58 |
| 1:S:546:THR:HG22 | 1:S:547:ASP:N | 2.17 | 0.58 |
| 4:1:324:THR:HG23 | 4:3:244:ASP:CA | 2.32 | 0.58 |
| 1:A:550:PHE:CE2 | 1:A:592:ILE:HG23 | 2.37 | 0.58 |
| 1:A:735:GLY:O | 1:A:743:ALA:HA | 1.94 | 0.58 |
| 3:C:52:ASN:N | 3:C:53:PRO:CD | 2.65 | 0.58 |
| 1:D:116:TYR:HB2 | 1:D:153:PRO:O | 2.03 | 0.58 |
| 1:D:195:TYR:O | 1:D:199:ILE:HG23 | 2.03 | 0.58 |
| 1:J:265:ILE:HG22 | 1:J:266:GLU:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:797:PHE:HE2 | 3:L:126:LEU:CD2 | 2.11 | 0.58 |
| 1:J:837:MLY:O | 1:J:840:PRO:HD2 | 2.02 | 0.58 |
| 1:M:124:VAL:HG13 | 1:M:675:ILE:CD1 | 2.33 | 0.58 |
| 1:S:195:TYR:O | 1:S:199:ILE:HG23 | 2.03 | 0.58 |
| 1:S:230:GLU:O | 1:S:234:ASN:HB2 | 2.03 | 0.58 |
| 4:1:288:ASP:H | 4:3:203:THR:CG2 | 2.17 | 0.58 |
| 1:A:7:MET:HE3 | 1:A:14:ALA:HB1 | 1.84 | 0.58 |
| 1:A:464:ILE:HG22 | 1:A:465:ALA:N | 2.18 | 0.58 |
| 1:A:529:PRO:HG3 | 4:8:353:GLN:OE1 | 2.03 | 0.58 |
| 1:A:538:GLU:O | 1:A:541:MET:HB2 | 2.04 | 0.58 |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:HD13 | 1.84 | 0.58 |
| 2:B:130:PRO:HA | 2:B:133:ILE:HD12 | 1.84 | 0.58 |
| 3:C:46:ILE:O | 3:C:50:LEU:CG | 2.47 | 0.58 |
| 1:D:601:ASP:N | 1:D:602:PRO:HD3 | 2.18 | 0.58 |
| 1:D:629:GLU:HB3 | 1:D:645:SER:N | 2.18 | 0.58 |
| 1:D:732:ILE:CD1 | 1:D:782:MLY:HH22 | 2.33 | 0.58 |
| 1:G:819:ASN:CB | 2:H:92:ASP:HB2 | 2.31 | 0.58 |
| 1:J:141:LEU:O | 1:J:144:ARG:HB3 | 2.03 | 0.58 |
| 1:J:195:TYR:O | 1:J:199:ILE:HG23 | 2.03 | 0.58 |
| 1:J:40:VAL:HG22 | 1:J:41:VAL:H | 1.67 | 0.58 |
| 1:J:643:GLY:HA2 | 4:W:24:ASP:OD1 | 2.04 | 0.58 |
| 1:J:676:ILE:O | 1:J:676:ILE:HG23 | 2.03 | 0.58 |
| 1:M:254:PHE:CE2 | 1:M:459:ILE:HD12 | 2.39 | 0.58 |
| 1:M:794:CYS:O | 1:M:798:LEU:N | 2.37 | 0.58 |
| 1:S:124:VAL:HG13 | 1:S:675:ILE:CD1 | 2.33 | 0.58 |
| 1:S:141:LEU:O | 1:S:144:ARG:HB3 | 2.04 | 0.58 |
| 1:M:634:GLY:N | 4:Z:25:ASP:O | 2.31 | 0.58 |
| 1:D:230:GLU:O | 1:D:234:ASN:HB2 | 2.03 | 0.58 |
| 1:D:175:ILE:HA | 1:D:670:HIS:O | 2.04 | 0.58 |
| 3:F:52:ASN:HB2 | 3:F:53:PRO:CD | 2.28 | 0.58 |
| 1:G:40:VAL:HG22 | 1:G:41:VAL:H | 1.67 | 0.58 |
| 1:G:464:ILE:HG22 | 1:G:465:ALA:N | 2.18 | 0.58 |
| 1:G:795:ARG:HA | 3:I:118:MET:SD | 2.43 | 0.58 |
| 1:J:202:SER:HA | 1:J:207:LYS:HE3 | 1.72 | 0.58 |
| 1:J:254:PHE:CE2 | 1:J:459:ILE:HD12 | 2.39 | 0.58 |
| 1:J:93:MET:CE | 1:J:764:MLY:HD2 | 2.31 | 0.58 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:HB3 | 1.72 | 0.58 |
| 1:J:831:TRP:NE1 | 2:K:67:MET:HB3 | 2.14 | 0.58 |
| 1:M:550:PHE:CE2 | 1:M:592:ILE:HG23 | 2.37 | 0.58 |
| 1:M:629:GLU:HB3 | 1:M:645:SER:N | 2.18 | 0.58 |
| 1:M:776:GLU:O | 1:M:779:ARG:HB3 | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:749:GLY:O | 3:U:89:GLU:CB | 2.48 | 0.58 |
| 1:S:796:GLY:N | 3:U:35:ARG:CZ | 2.67 | 0.58 |
| 1:A:265:ILE:HG22 | 1:A:266:GLU:N | 2.18 | 0.58 |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:CD1 | 2.33 | 0.58 |
| 1:D:135:TYR:N | 1:D:135:TYR:CD1 | 2.70 | 0.58 |
| 1:D:713:SER:OG | 1:D:771:LEU:HD23 | 1.25 | 0.58 |
| 1:D:776:GLU:O | 1:D:779:ARG:HB3 | 2.03 | 0.58 |
| 1:D:787:ILE:O | 1:D:790:THR:N | 2.35 | 0.58 |
| 1:D:834:LEU:HD11 | 2:E:54:MET:HG3 | 0.59 | 0.58 |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:CD2 | 2.39 | 0.58 |
| 3:F:102:VAL:HG11 | 3:F:107:LEU:HB2 | 1.85 | 0.58 |
| 3:F:46:ILE:O | 3:F:50:LEU:CG | 2.47 | 0.58 |
| 1:G:265:ILE:HG22 | 1:G:266:GLU:N | 2.18 | 0.58 |
| 1:G:629:GLU:HB3 | 1:G:645:SER:N | 2.18 | 0.58 |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:HD1 | 1.68 | 0.58 |
| 1:G:97:LEU:CD2 | 1:G:712:PRO:CA | 2.82 | 0.58 |
| 1:G:819:ASN:N | 2:H:90:GLY:O | 2.33 | 0.58 |
| 1:J:84:MLY:HH23 | 1:J:719:ASP:C | 2.22 | 0.58 |
| 1:J:819:ASN:OD1 | 2:K:90:GLY:O | 2.21 | 0.58 |
| 1:M:549:SER:OG | 1:M:550:PHE:N | 2.36 | 0.58 |
| 1:M:676:ILE:O | 1:M:676:ILE:HG23 | 2.03 | 0.58 |
| 1:S:175:ILE:HA | 1:S:670:HIS:O | 2.03 | 0.58 |
| 1:S:813:ILE:O | 1:S:817:GLN:N | 2.30 | 0.58 |
| 1:S:819:ASN:OD1 | 2:T:92:ASP:CA | 2.50 | 0.58 |
| 1:J:642:LYS:CG | 4:W:22:ALA:CA | 2.80 | 0.58 |
| 1:M:642:LYS:CG | 4:Z:22:ALA:CA | 2.80 | 0.58 |
| 4:2:167:GLU:OE1 | 4:4:43:VAL:N | 2.36 | 0.58 |
| 1:A:49:MLY:HH13 | 1:A:108:GLU:OE2 | 2.03 | 0.58 |
| 1:A:141:LEU:O | 1:A:144:ARG:HB3 | 2.03 | 0.58 |
| 1:A:254:PHE:CE2 | 1:A:459:ILE:HD12 | 2.39 | 0.58 |
| 1:A:502:GLU:OE2 | 1:A:761:GLY:N | 2.21 | 0.58 |
| 1:A:557:GLU:O | 1:A:557:GLU:HG3 | 2.01 | 0.58 |
| 1:D:40:VAL:HG22 | 1:D:41:VAL:H | 1.67 | 0.58 |
| 1:D:418:THR:HG22 | 1:D:419:VAL:H | 1.69 | 0.58 |
| 1:D:464:ILE:HG22 | 1:D:465:ALA:N | 2.18 | 0.58 |
| 1:D:795:ARG:HE | 3:F:116:GLU:CB | 2.15 | 0.58 |
| 1:D:827:MLY:CH2 | 2:E:139:ALA:HB3 | 2.22 | 0.58 |
| 1:G:175:ILE:HA | 1:G:670:HIS:O | 2.03 | 0.58 |
| 1:J:218:LEU:N | 1:J:221:GLN:HE21 | 2.01 | 0.58 |
| 1:J:93:MET:CE | 1:J:764:MLY:CD | 2.81 | 0.58 |
| 1:M:601:ASP:N | 1:M:602:PRO:HD3 | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:265:ILE:HG22 | 1:S:266:GLU:N | 2.18 | 0.58 |
| 1:S:418:THR:HG22 | 1:S:419:VAL:H | 1.69 | 0.58 |
| 1:S:549:SER:OG | 1:S:550:PHE:N | 2.35 | 0.58 |
| 1:S:796:GLY:CA | 3:U:35:ARG:NE | 2.67 | 0.58 |
| 1:A:794:CYS:O | 1:A:798:LEU:N | 2.37 | 0.58 |
| 2:B:140:PHE:O | 2:B:141:PRO:C | 2.33 | 0.58 |
| 1:A:799:MET:HE1 | 3:C:32:ASP:HB3 | 1.83 | 0.58 |
| 1:D:254:PHE:CE2 | 1:D:459:ILE:HD12 | 2.39 | 0.58 |
| 1:D:279:LEU:HB3 | 1:D:280:PRO:HD2 | 1.86 | 0.58 |
| 1:D:550:PHE:CE2 | 1:D:592:ILE:HG23 | 2.37 | 0.58 |
| 1:D:634:GLY:N | 4:9:25:ASP:O | 2.31 | 0.58 |
| 1:D:726:VAL:C | 1:D:785:GLU:HG2 | 2.23 | 0.58 |
| 1:D:712:PRO:HB2 | 1:D:771:LEU:HD22 | 1.83 | 0.58 |
| 1:D:99:GLU:OE2 | 1:D:696:ARG:NH2 | 2.31 | 0.58 |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:CD1 | 2.39 | 0.58 |
| 1:G:542:PHE:CD1 | 4:V:143:TYR:CE1 | 2.91 | 0.58 |
| 1:G:568:PRO:HG3 | 1:G:578:HIS:H | 1.69 | 0.58 |
| 1:J:48:VAL:HG22 | 1:J:49:MLY:N | 2.18 | 0.58 |
| 1:J:601:ASP:N | 1:J:602:PRO:HD3 | 2.18 | 0.58 |
| 1:J:646:PHE:CD2 | 1:J:652:LEU:CD1 | 2.85 | 0.58 |
| 1:J:92:ALA:O | 1:J:714:ARG:HG3 | 2.02 | 0.58 |
| 1:J:735:GLY:C | 1:J:743:ALA:HB1 | 1.84 | 0.58 |
| 1:M:127:ASN:ND2 | 1:M:128:PRO:HD2 | 2.16 | 0.58 |
| 1:M:529:PRO:HG3 | 4:Z:353:GLN:OE1 | 2.04 | 0.58 |
| 1:S:218:LEU:N | 1:S:221:GLN:HE21 | 2.01 | 0.58 |
| 1:S:538:GLU:O | 1:S:541:MET:HB2 | 2.03 | 0.58 |
| 1:S:642:LYS:CD | 4:2:340:TRP:CZ3 | 2.79 | 0.58 |
| 1:S:64:THR:HG22 | 1:S:65:GLU:N | 2.19 | 0.58 |
| 4:X:287:ILE:HG13 | 4:Z:201:VAL:CB | 2.34 | 0.58 |
| 4:3:322:PRO:HB3 | 4:5:244:ASP:OD2 | 2.03 | 0.58 |
| 1:A:553:MLY:CE | 4:V:45:VAL:CA | 2.49 | 0.58 |
| 1:A:629:GLU:HB3 | 1:A:645:SER:N | 2.18 | 0.58 |
| 3:C:102:VAL:HG11 | 3:C:107:LEU:HB2 | 1.85 | 0.58 |
| 1:D:218:LEU:N | 1:D:221:GLN:HE21 | 2.01 | 0.58 |
| 1:G:49:MLY:HH13 | 1:G:108:GLU:OE2 | 2.03 | 0.58 |
| 1:G:817:GLN:CG | 2:H:127:ARG:CB | 2.74 | 0.58 |
| 1:J:116:TYR:HB2 | 1:J:153:PRO:O | 2.03 | 0.58 |
| 1:J:529:PRO:HG3 | 4:W:353:GLN:OE1 | 2.04 | 0.58 |
| 1:J:64:THR:HG22 | 1:J:65:GLU:N | 2.19 | 0.58 |
| 1:M:464:ILE:HG22 | 1:M:465:ALA:N | 2.18 | 0.58 |
| 3:O:102:VAL:HG23 | 3:O:139:TYR:CD1 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:99:GLU:OE2 | 1:S:696:ARG:NH2 | 2.30 | 0.58 |
| 1:G:642:LYS:CG | 4:V:22:ALA:CA | 2.80 | 0.58 |
| 1:G:529:PRO:HG3 | 4:V:353:GLN:OE1 | 2.04 | 0.58 |
| 4:X:325:MET:CE | 4:Z:244:ASP:OD2 | 2.52 | 0.58 |
| 1:S:529:PRO:HG3 | 4:2:353:GLN:OE1 | 2.04 | 0.58 |
| 4:3:223:PHE:HD2 | 4:3:312:ARG:NH2 | 1.99 | 0.58 |
| 1:A:643:GLY:HA2 | 4:8:24:ASP:OD1 | 2.04 | 0.58 |
| 1:A:676:ILE:O | 1:A:676:ILE:HG23 | 2.03 | 0.58 |
| 1:A:818:TYR:CB | 2:B:90:GLY:N | 2.67 | 0.58 |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CG | 2.38 | 0.58 |
| 1:G:64:THR:HG22 | 1:G:65:GLU:N | 2.19 | 0.58 |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:CD1 | 1.55 | 0.58 |
| 1:M:820:VAL:CG1 | 2:N:136:MET:CE | 2.81 | 0.58 |
| 1:S:279:LEU:HB3 | 1:S:280:PRO:HD2 | 1.86 | 0.58 |
| 4:2:112:PRO:CG | 4:3:196:ARG:CA | 2.80 | 0.57 |
| 4:2:167:GLU:CD | 4:4:43:VAL:O | 2.42 | 0.57 |
| 1:A:601:ASP:N | 1:A:602:PRO:HD3 | 2.18 | 0.57 |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:HA2 | 1.66 | 0.57 |
| 1:A:646:PHE:CD2 | 1:A:652:LEU:CD1 | 2.85 | 0.57 |
| 1:D:141:LEU:O | 1:D:144:ARG:HB3 | 2.03 | 0.57 |
| 1:G:538:GLU:O | 1:G:541:MET:HB2 | 2.04 | 0.57 |
| 1:J:530:MET:HA | 4:W:354:GLN:CB | 2.28 | 0.57 |
| 1:J:175:ILE:HA | 1:J:670:HIS:O | 2.03 | 0.57 |
| 1:M:821:ARG:HH12 | 2:N:127:ARG:NE | 2.02 | 0.57 |
| 1:S:48:VAL:HG22 | 1:S:49:MLY:N | 2.18 | 0.57 |
| 1:S:568:PRO:HG3 | 1:S:578:HIS:H | 1.69 | 0.57 |
| 1:S:730:SER:HB2 | 3:U:94:PHE:CD2 | 2.39 | 0.57 |
| 1:S:749:GLY:CA | 3:U:93:VAL:CG2 | 2.80 | 0.57 |
| 1:S:821:ARG:NH2 | 2:T:127:ARG:CD | 2.66 | 0.57 |
| 2:N:163:ALA:HA | 2:T:21:GLU:OE1 | 2.05 | 0.57 |
| 1:S:530:MET:CA | 4:2:354:GLN:HB3 | 2.35 | 0.57 |
| 4:3:287:ILE:HG21 | 4:5:204:ALA:N | 2.19 | 0.57 |
| 1:G:7:MET:HE3 | 1:G:14:ALA:HB1 | 1.84 | 0.57 |
| 1:G:22:LYS:O | 1:G:26:GLU:N | 2.29 | 0.57 |
| 1:G:279:LEU:HB3 | 1:G:280:PRO:HD2 | 1.86 | 0.57 |
| 1:J:279:LEU:HB3 | 1:J:280:PRO:HD2 | 1.86 | 0.57 |
| 1:M:195:TYR:O | 1:M:199:ILE:HG23 | 2.03 | 0.57 |
| 1:M:265:ILE:HG22 | 1:M:266:GLU:N | 2.18 | 0.57 |
| 1:M:481:ASN:N | 1:M:481:ASN:ND2 | 2.51 | 0.57 |
| 1:M:538:GLU:O | 1:M:541:MET:HB2 | 2.03 | 0.57 |
| 1:M:64:THR:HG22 | 1:M:65:GLU:N | 2.19 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:464:ILE:HG22 | 1:S:465:ALA:N | 2.18 | 0.57 |
| 4:4:322:PRO:HB3 | 4:6:244:ASP:OD2 | 2.04 | 0.57 |
| 4:4:287:ILE:CB | 4:6:203:THR:HG22 | 2.29 | 0.57 |
| 1:D:7:MET:HE3 | 1:D:14:ALA:HB1 | 1.86 | 0.57 |
| 1:D:538:GLU:O | 1:D:541:MET:HB2 | 2.04 | 0.57 |
| 1:D:64:THR:HG22 | 1:D:65:GLU:N | 2.19 | 0.57 |
| 1:D:836:PHE:CE1 | 2:E:159:HIS:HA | 2.40 | 0.57 |
| 1:G:254:PHE:CE2 | 1:G:459:ILE:HD12 | 2.39 | 0.57 |
| 1:G:768:MLY:HH22 | 1:G:772:LEU:HD13 | 1.62 | 0.57 |
| 1:G:91:MET:HE3 | 1:G:119:SER:HB2 | 1.86 | 0.57 |
| 1:J:202:SER:CA | 1:J:207:LYS:HE3 | 2.27 | 0.57 |
| 1:M:797:PHE:HE2 | 3:O:126:LEU:HD22 | 1.50 | 0.57 |
| 1:M:813:ILE:O | 1:M:816:ILE:N | 2.37 | 0.57 |
| 2:T:112:ILE:C | 2:T:147:ASN:O | 2.42 | 0.57 |
| 1:A:175:ILE:HA | 1:A:670:HIS:O | 2.04 | 0.57 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:CG2 | 2.35 | 0.57 |
| 1:D:322:VAL:HG11 | 1:D:325:ILE:HD11 | 1.86 | 0.57 |
| 1:D:579:PHE:CD2 | 1:D:592:ILE:HD11 | 2.40 | 0.57 |
| 1:J:579:PHE:CD2 | 1:J:592:ILE:HD11 | 2.40 | 0.57 |
| 1:J:629:GLU:HB3 | 1:J:645:SER:N | 2.18 | 0.57 |
| 1:J:784:ALA:O | 1:J:788:THR:CB | 2.52 | 0.57 |
| 1:M:530:MET:CA | 4:Z:354:GLN:HB3 | 2.35 | 0.57 |
| 1:S:149:GLN:OE1 | 1:S:762:HIS:O | 2.21 | 0.57 |
| 1:S:731:ALA:CB | 3:U:93:VAL:CB | 2.80 | 0.57 |
| 1:A:322:VAL:HG11 | 1:A:325:ILE:HD11 | 1.86 | 0.57 |
| 1:A:48:VAL:HG22 | 1:A:49:MLY:N | 2.18 | 0.57 |
| 1:A:568:PRO:HG3 | 1:A:578:HIS:H | 1.69 | 0.57 |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:HD1 | 1.68 | 0.57 |
| 1:A:768:MLY:HB3 | 1:A:771:LEU:CD1 | 2.34 | 0.57 |
| 1:G:813:ILE:O | 1:G:816:ILE:N | 2.37 | 0.57 |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:CD1 | 2.39 | 0.57 |
| 1:M:599:ASN:CG | 1:M:649:VAL:HB | 2.25 | 0.57 |
| 1:M:715:VAL:HG11 | 1:M:720:PHE:HD1 | 1.68 | 0.57 |
| 1:S:127:ASN:ND2 | 1:S:128:PRO:HD2 | 2.16 | 0.57 |
| 1:S:601:ASP:N | 1:S:602:PRO:HD3 | 2.18 | 0.57 |
| 1:S:783:LEU:CD2 | 1:S:786:ILE:HD11 | 2.24 | 0.57 |
| 1:S:797:PHE:CD2 | 3:U:146:ILE:HG23 | 2.40 | 0.57 |
| 1:S:731:ALA:HB1 | 3:U:93:VAL:HG12 | 1.87 | 0.57 |
| 1:M:630:ALA:CA | 4:Z:25:ASP:OD2 | 2.53 | 0.57 |
| 1:A:642:LYS:CG | 4:8:22:ALA:CA | 2.81 | 0.57 |
| 1:A:599:ASN:CG | 1:A:649:VAL:HB | 2.25 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:727:LEU:N | 1:D:782:MLY:CE | 2.66 | 0.57 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:CD1 | 2.87 | 0.57 |
| 1:G:141:LEU:O | 1:G:144:ARG:HB3 | 2.03 | 0.57 |
| 1:G:552:ASN:C | 4:X:47:MET:HE1 | 2.24 | 0.57 |
| 1:G:817:GLN:CB | 2:H:127:ARG:CD | 2.79 | 0.57 |
| 1:J:538:GLU:O | 1:J:541:MET:HB2 | 2.03 | 0.57 |
| 1:J:568:PRO:HG3 | 1:J:578:HIS:H | 1.69 | 0.57 |
| 1:J:82:PRO:HD2 | 1:J:85:TYR:CD2 | 2.40 | 0.57 |
| 2:K:112:ILE:C | 2:K:147:ASN:O | 2.42 | 0.57 |
| 1:S:599:ASN:CG | 1:S:649:VAL:HB | 2.25 | 0.57 |
| 1:S:747:LEU:HD23 | 1:S:747:LEU:O | 2.05 | 0.57 |
| 1:S:818:TYR:CD1 | 2:T:127:ARG:NH1 | 2.73 | 0.57 |
| 2:B:112:ILE:C | 2:B:147:ASN:O | 2.42 | 0.57 |
| 1:A:798:LEU:HD21 | 3:C:126:LEU:HD11 | 1.84 | 0.57 |
| 1:D:643:GLY:HA2 | 4:9:24:ASP:OD1 | 2.04 | 0.57 |
| 1:D:813:ILE:O | 1:D:816:ILE:N | 2.37 | 0.57 |
| 1:D:82:PRO:HD2 | 1:D:85:TYR:CD2 | 2.40 | 0.57 |
| 1:D:831:TRP:HH2 | 2:E:34:ILE:HG23 | 1.68 | 0.57 |
| 1:G:747:LEU:HD23 | 1:G:747:LEU:O | 2.05 | 0.57 |
| 3:I:52:ASN:HB2 | 3:I:53:PRO:CD | 2.28 | 0.57 |
| 1:J:322:VAL:HG11 | 1:J:325:ILE:HD11 | 1.86 | 0.57 |
| 1:J:409:GLY:HA3 | 4:W:333:PRO:CD | 2.34 | 0.57 |
| 1:M:141:LEU:O | 1:M:144:ARG:HB3 | 2.04 | 0.57 |
| 1:M:218:LEU:N | 1:M:221:GLN:HE21 | 2.01 | 0.57 |
| 1:M:279:LEU:HB3 | 1:M:280:PRO:HD2 | 1.87 | 0.57 |
| 1:M:409:GLY:HA3 | 4:Z:333:PRO:CD | 2.34 | 0.57 |
| 1:M:747:LEU:O | 1:M:747:LEU:HD23 | 2.04 | 0.57 |
| 1:S:295:MLY:HG3 | 1:S:332:MET:HE1 | 1.86 | 0.57 |
| 1:S:630:ALA:CA | 4:2:25:ASP:OD2 | 2.53 | 0.57 |
| 1:S:642:LYS:CA | 4:2:22:ALA:C | 2.70 | 0.57 |
| 1:G:643:GLY:HA2 | 4:V:24:ASP:OD1 | 2.04 | 0.57 |
| 4:1:204:ALA:H | 4:Y:288:ASP:N | 2.03 | 0.57 |
| 1:S:409:GLY:HA3 | 4:2:333:PRO:CD | 2.35 | 0.57 |
| 1:A:279:LEU:HB3 | 1:A:280:PRO:HD2 | 1.86 | 0.57 |
| 1:A:173:GLN:C | 1:A:667:THR:HG23 | 2.25 | 0.57 |
| 1:A:747:LEU:HD23 | 1:A:747:LEU:O | 2.05 | 0.57 |
| 1:A:813:ILE:O | 1:A:816:ILE:N | 2.37 | 0.57 |
| 1:A:82:PRO:HD2 | 1:A:85:TYR:CD2 | 2.40 | 0.57 |
| 3:C:52:ASN:HB2 | 3:C:53:PRO:CD | 2.28 | 0.57 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:CG2 | 2.35 | 0.57 |
| 1:D:817:GLN:OE1 | 2:E:127:ARG:NH1 | 2.27 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:481:ASN:ND2 | 1:G:481:ASN:N | 2.51 | 0.57 |
| 1:G:599:ASN:CG | 1:G:649:VAL:HB | 2.25 | 0.57 |
| 1:G:173:GLN:C | 1:G:667:THR:HG23 | 2.25 | 0.57 |
| 1:G:676:ILE:O | 1:G:676:ILE:HG23 | 2.03 | 0.57 |
| 1:G:817:GLN:HB3 | 2:H:127:ARG:HH11 | 1.70 | 0.57 |
| 1:J:418:THR:HG22 | 1:J:419:VAL:H | 1.69 | 0.57 |
| 1:J:481:ASN:N | 1:J:481:ASN:ND2 | 2.51 | 0.57 |
| 1:J:747:LEU:HD23 | 1:J:747:LEU:O | 2.05 | 0.57 |
| 1:J:813:ILE:O | 1:J:816:ILE:N | 2.37 | 0.57 |
| 1:M:640:LYS:C | 4:Z:23:GLY:CA | 2.64 | 0.57 |
| 1:M:93:MET:HE2 | 1:M:764:MLY:NZ | 2.20 | 0.57 |
| 1:M:767:PHE:CE1 | 1:M:771:LEU:HB3 | 2.38 | 0.57 |
| 1:S:715:VAL:HG11 | 1:S:720:PHE:HD1 | 1.68 | 0.57 |
| 1:S:795:ARG:C | 3:U:35:ARG:NH2 | 2.58 | 0.57 |
| 1:S:731:ALA:HB1 | 3:U:93:VAL:CG1 | 2.34 | 0.57 |
| 1:A:109:ARG:O | 1:A:114:MET:N | 2.37 | 0.57 |
| 1:A:418:THR:HG22 | 1:A:419:VAL:H | 1.70 | 0.57 |
| 1:A:529:PRO:CG | 4:8:353:GLN:OE1 | 2.53 | 0.57 |
| 1:A:64:THR:HG22 | 1:A:65:GLU:N | 2.19 | 0.57 |
| 1:D:173:GLN:C | 1:D:667:THR:HG23 | 2.25 | 0.57 |
| 1:D:831:TRP:NE1 | 2:E:51:PHE:CZ | 2.60 | 0.57 |
| 2:E:112:ILE:C | 2:E:147:ASN:O | 2.42 | 0.57 |
| 1:G:418:THR:HG22 | 1:G:419:VAL:H | 1.69 | 0.57 |
| 1:G:640:LYS:C | 4:V:23:GLY:CA | 2.64 | 0.57 |
| 1:G:813:ILE:O | 1:G:817:GLN:N | 2.30 | 0.57 |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:CD1 | 2.39 | 0.57 |
| 1:M:175:ILE:HA | 1:M:670:HIS:O | 2.03 | 0.57 |
| 1:S:254:PHE:CE2 | 1:S:459:ILE:HD12 | 2.39 | 0.57 |
| 1:S:642:LYS:CG | 4:2:22:ALA:CA | 2.80 | 0.57 |
| 1:S:805:ALA:O | 1:S:807:VAL:C | 2.43 | 0.57 |
| 1:S:813:ILE:O | 1:S:816:ILE:N | 2.37 | 0.57 |
| 1:S:831:TRP:NE1 | 2:T:67:MET:HB3 | 2.14 | 0.57 |
| 4:X:287:ILE:HG13 | 4:Z:201:VAL:CG2 | 2.32 | 0.57 |
| 1:D:409:GLY:HA3 | 4:9:333:PRO:CD | 2.35 | 0.57 |
| 1:D:530:MET:CA | 4:9:354:GLN:HB3 | 2.35 | 0.57 |
| 1:A:127:ASN:ND2 | 1:A:128:PRO:HD2 | 2.17 | 0.57 |
| 1:A:292:MET:HE3 | 1:A:309:PRO:CA | 2.34 | 0.57 |
| 1:A:338:ILE:HG21 | 1:A:348:MLY:HB3 | 1.87 | 0.57 |
| 1:A:409:GLY:HA3 | 4:8:333:PRO:CD | 2.34 | 0.57 |
| 1:A:707:CYS:SG | 1:A:714:ARG:NH1 | 2.77 | 0.57 |
| 1:D:836:PHE:CE2 | 2:E:160:GLY:O | 2.58 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:166:MET:HE3 | 1:G:254:PHE:HD2 | 1.70 | 0.57 |
| 1:G:557:GLU:HB2 | 4:X:47:MET:O | 2.04 | 0.57 |
| 1:G:791:GLN:NE2 | 3:I:115:GLY:C | 2.56 | 0.57 |
| 1:G:82:PRO:HD2 | 1:G:85:TYR:CD2 | 2.40 | 0.57 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:CG2 | 2.35 | 0.57 |
| 1:J:783:LEU:O | 1:J:787:ILE:CB | 2.52 | 0.57 |
| 1:M:338:ILE:HG21 | 1:M:348:MLY:HB3 | 1.87 | 0.57 |
| 1:M:418:THR:HG22 | 1:M:419:VAL:H | 1.69 | 0.57 |
| 1:M:649:VAL:HG23 | 1:M:649:VAL:HA | 1.83 | 0.57 |
| 1:S:22:LYS:O | 1:S:26:GLU:N | 2.30 | 0.57 |
| 1:S:752:ASP:N | 1:S:779:ARG:HH22 | 1.97 | 0.57 |
| 1:J:530:MET:CA | 4:W:354:GLN:HB3 | 2.35 | 0.57 |
| 1:A:218:LEU:N | 1:A:221:GLN:HE21 | 2.01 | 0.56 |
| 1:A:635:GLY:HA3 | 4:8:334:GLU:CG | 2.30 | 0.56 |
| 1:D:48:VAL:HG22 | 1:D:49:MLY:N | 2.18 | 0.56 |
| 1:D:794:CYS:O | 1:D:798:LEU:N | 2.37 | 0.56 |
| 1:G:646:PHE:CD2 | 1:G:652:LEU:CD1 | 2.85 | 0.56 |
| 3:I:102:VAL:HG11 | 3:I:107:LEU:HB2 | 1.85 | 0.56 |
| 1:J:797:PHE:HE1 | 3:L:146:ILE:CA | 2.18 | 0.56 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:CG2 | 2.35 | 0.56 |
| 1:M:646:PHE:CD2 | 1:M:652:LEU:CD1 | 2.85 | 0.56 |
| 4:3:287:ILE:CG2 | 4:5:202:THR:CA | 2.75 | 0.56 |
| 1:A:530:MET:CA | 4:8:354:GLN:HB3 | 2.35 | 0.56 |
| 1:D:411:GLU:H | 4:9:333:PRO:HG2 | 1.70 | 0.56 |
| 1:D:127:ASN:ND2 | 1:D:128:PRO:HD2 | 2.16 | 0.56 |
| 1:D:568:PRO:HG3 | 1:D:578:HIS:H | 1.69 | 0.56 |
| 1:D:677:PRO:HB2 | 1:D:678:ASN:ND2 | 2.20 | 0.56 |
| 1:D:732:ILE:HD12 | 1:D:782:MLY:HH22 | 1.87 | 0.56 |
| 1:D:831:TRP:CE3 | 2:E:34:ILE:HD13 | 2.40 | 0.56 |
| 1:D:831:TRP:HZ2 | 2:E:47:LEU:HD22 | 1.70 | 0.56 |
| 1:G:409:GLY:HA3 | 4:V:333:PRO:CD | 2.35 | 0.56 |
| 1:G:553:MLY:HH13 | 4:X:45:VAL:CG1 | 2.25 | 0.56 |
| 3:I:49:ILE:HA | 3:I:52:ASN:ND2 | 2.06 | 0.56 |
| 1:J:217:THR:HG22 | 1:J:218:LEU:O | 2.05 | 0.56 |
| 1:J:768:MLY:CH1 | 1:J:772:LEU:CD1 | 2.27 | 0.56 |
| 1:J:792:ALA:HB2 | 3:L:42:THR:CA | 2.35 | 0.56 |
| 1:M:783:LEU:CA | 1:M:786:ILE:CD1 | 2.74 | 0.56 |
| 1:J:638:GLY:CA | 4:W:345:ILE:H | 2.18 | 0.56 |
| 1:D:638:GLY:CA | 4:9:345:ILE:H | 2.19 | 0.56 |
| 1:A:707:CYS:SG | 1:A:714:ARG:HD2 | 2.45 | 0.56 |
| 1:D:116:TYR:CE2 | 1:D:154:HIS:CD2 | 2.94 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:135:TYR:N | 1:D:135:TYR:HD1 | 2.04 | 0.56 |
| 1:D:599:ASN:CG | 1:D:649:VAL:HB | 2.25 | 0.56 |
| 1:J:677:PRO:HB2 | 1:J:678:ASN:ND2 | 2.20 | 0.56 |
| 1:M:818:TYR:OH | 2:N:127:ARG:NH2 | 2.37 | 0.56 |
| 1:S:173:GLN:C | 1:S:667:THR:HG23 | 2.25 | 0.56 |
| 1:S:731:ALA:C | 3:U:93:VAL:CG1 | 2.62 | 0.56 |
| 1:S:731:ALA:HB1 | 3:U:94:PHE:N | 2.17 | 0.56 |
| 1:S:817:GLN:HB3 | 2:T:127:ARG:HD3 | 1.82 | 0.56 |
| 1:G:642:LYS:CA | 4:V:22:ALA:C | 2.70 | 0.56 |
| 4:W:288:ASP:N | 4:Y:204:ALA:H | 2.03 | 0.56 |
| 1:S:639:GLY:N | 4:2:344:SER:C | 2.54 | 0.56 |
| 1:A:630:ALA:CA | 4:8:25:ASP:OD2 | 2.53 | 0.56 |
| 1:A:149:GLN:HB3 | 1:A:718:ALA:C | 2.25 | 0.56 |
| 1:A:302:MET:HG2 | 1:A:303:LEU:HD13 | 1.87 | 0.56 |
| 1:A:755:HIS:HA | 1:A:758:TYR:HE1 | 1.65 | 0.56 |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:CD1 | 2.39 | 0.56 |
| 1:G:322:VAL:HG11 | 1:G:325:ILE:HD11 | 1.86 | 0.56 |
| 1:J:116:TYR:CE2 | 1:J:154:HIS:CD2 | 2.94 | 0.56 |
| 1:J:173:GLN:C | 1:J:667:THR:HG23 | 2.25 | 0.56 |
| 1:J:795:ARG:CD | 3:L:116:GLU:OE2 | 2.53 | 0.56 |
| 1:M:109:ARG:O | 1:M:114:MET:N | 2.37 | 0.56 |
| 1:M:643:GLY:HA2 | 4:Z:24:ASP:OD1 | 2.04 | 0.56 |
| 1:M:173:GLN:C | 1:M:667:THR:HG23 | 2.25 | 0.56 |
| 1:M:677:PRO:HB2 | 1:M:678:ASN:ND2 | 2.20 | 0.56 |
| 1:S:135:TYR:N | 1:S:135:TYR:HD1 | 2.04 | 0.56 |
| 1:S:733:PRO:CA | 1:S:737:PHE:HE1 | 2.19 | 0.56 |
| 4:2:365:ALA:HB3 | 4:2:369:ILE:HB | 1.88 | 0.56 |
| 4:1:287:ILE:HG13 | 4:3:202:THR:CA | 2.31 | 0.56 |
| 4:4:287:ILE:HG21 | 4:6:204:ALA:N | 2.19 | 0.56 |
| 1:A:135:TYR:N | 1:A:135:TYR:HD1 | 2.04 | 0.56 |
| 1:A:677:PRO:HB2 | 1:A:678:ASN:ND2 | 2.20 | 0.56 |
| 1:A:733:PRO:CA | 1:A:737:PHE:HE1 | 2.19 | 0.56 |
| 1:A:795:ARG:CZ | 3:C:116:GLU:CD | 2.43 | 0.56 |
| 1:D:217:THR:HG22 | 1:D:218:LEU:O | 2.06 | 0.56 |
| 1:G:302:MET:HG2 | 1:G:303:LEU:HD13 | 1.88 | 0.56 |
| 1:G:530:MET:CA | 4:V:354:GLN:HB3 | 2.35 | 0.56 |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:HA2 | 1.66 | 0.56 |
| 1:J:599:ASN:CG | 1:J:649:VAL:HB | 2.25 | 0.56 |
| 1:J:819:ASN:ND2 | 2:K:92:ASP:CB | 2.48 | 0.56 |
| 1:M:568:PRO:HG3 | 1:M:578:HIS:H | 1.69 | 0.56 |
| 1:M:819:ASN:ND2 | 2:N:92:ASP:CB | 2.62 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:798:LEU:HD13 | 3:O:126:LEU:CD2 | 2.20 | 0.56 |
| 1:G:639:GLY:N | 4:V:344:SER:C | 2.54 | 0.56 |
| 4:6:365:ALA:HB3 | 4:6:369:ILE:HB | 1.88 | 0.56 |
| 1:A:411:GLU:H | 4:8:333:PRO:HG2 | 1.71 | 0.56 |
| 1:A:733:PRO:CB | 1:A:737:PHE:HE1 | 2.19 | 0.56 |
| 1:D:507:GLY:O | 1:D:761:GLY:HA2 | 2.05 | 0.56 |
| 1:G:217:THR:HG22 | 1:G:218:LEU:O | 2.06 | 0.56 |
| 1:G:768:MLY:CH2 | 1:G:772:LEU:CD1 | 2.06 | 0.56 |
| 1:G:792:ALA:HB1 | 3:I:42:THR:HA | 1.84 | 0.56 |
| 1:J:725:ARG:HG3 | 1:J:733:PRO:CA | 2.36 | 0.56 |
| 1:M:529:PRO:CG | 4:Z:353:GLN:OE1 | 2.54 | 0.56 |
| 1:M:817:GLN:CG | 2:N:127:ARG:HB2 | 2.30 | 0.56 |
| 1:S:302:MET:HG2 | 1:S:303:LEU:HD13 | 1.87 | 0.56 |
| 1:S:541:MET:HG2 | 4:2:345:ILE:CG2 | 2.35 | 0.56 |
| 1:M:411:GLU:H | 4:Z:333:PRO:HG2 | 1.71 | 0.56 |
| 1:S:411:GLU:H | 4:2:333:PRO:HG2 | 1.71 | 0.56 |
| 4:4:287:ILE:HG23 | 4:6:202:THR:CG2 | 2.23 | 0.56 |
| 1:A:217:THR:HG22 | 1:A:218:LEU:O | 2.05 | 0.56 |
| 1:A:295:MLY:HG3 | 1:A:332:MET:HE1 | 1.88 | 0.56 |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:H | 1.71 | 0.56 |
| 1:D:733:PRO:CA | 1:D:737:PHE:HE1 | 2.19 | 0.56 |
| 1:D:800:ARG:HD2 | 3:F:149:VAL:HG13 | 1.86 | 0.56 |
| 1:G:135:TYR:N | 1:G:135:TYR:HD1 | 2.04 | 0.56 |
| 1:J:135:TYR:HD1 | 1:J:135:TYR:N | 2.04 | 0.56 |
| 1:J:22:LYS:HA | 1:J:25:ILE:HB | 1.87 | 0.56 |
| 1:J:733:PRO:CB | 1:J:737:PHE:HE1 | 2.19 | 0.56 |
| 1:J:839:MLY:HH11 | 2:K:158:THR:CG2 | 2.34 | 0.56 |
| 1:M:35:MLY:CE | 1:M:777:GLU:OE2 | 2.51 | 0.56 |
| 1:M:82:PRO:HD2 | 1:M:85:TYR:CD2 | 2.40 | 0.56 |
| 1:S:217:THR:HG22 | 1:S:218:LEU:O | 2.05 | 0.56 |
| 1:S:502:GLU:OE2 | 1:S:761:GLY:CA | 2.48 | 0.56 |
| 1:S:791:GLN:HE22 | 3:U:116:GLU:N | 1.98 | 0.56 |
| 1:J:630:ALA:CA | 4:W:25:ASP:OD2 | 2.53 | 0.56 |
| 1:D:630:ALA:CA | 4:9:25:ASP:OD2 | 2.53 | 0.56 |
| 1:D:530:MET:CB | 4:9:354:GLN:HG3 | 2.36 | 0.56 |
| 1:D:435:GLU:O | 1:D:438:PHE:HB3 | 2.06 | 0.56 |
| 1:D:747:LEU:O | 1:D:747:LEU:HD23 | 2.05 | 0.56 |
| 1:G:411:GLU:H | 4:V:333:PRO:HG2 | 1.70 | 0.56 |
| 1:G:546:THR:HB | 1:G:549:SER:H | 1.71 | 0.56 |
| 1:G:728:ASN:HD21 | 3:I:114:LEU:HA | 1.71 | 0.56 |
| 1:G:733:PRO:CA | 1:G:737:PHE:HE1 | 2.19 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:754:ASP:OD2 | 1:G:776:GLU:CA | 2.49 | 0.56 |
| 1:M:135:TYR:N | 1:M:135:TYR:HD1 | 2.04 | 0.56 |
| 1:M:220:ASP:O | 1:M:224:SER:N | 2.27 | 0.56 |
| 1:M:604:ASN:OD1 | 1:M:607:VAL:HG23 | 2.06 | 0.56 |
| 1:M:95:THR:CB | 1:M:713:SER:OG | 2.54 | 0.56 |
| 1:S:731:ALA:CB | 3:U:93:VAL:HG12 | 2.36 | 0.56 |
| 1:S:794:CYS:O | 1:S:798:LEU:N | 2.37 | 0.56 |
| 1:S:82:PRO:HD2 | 1:S:85:TYR:CD2 | 2.40 | 0.56 |
| 4:V:288:ASP:N | 4:X:204:ALA:H | 2.03 | 0.56 |
| 4:2:287:ILE:CG2 | 4:4:202:THR:HB | 2.35 | 0.56 |
| 4:7:365:ALA:HB3 | 4:7:369:ILE:HB | 1.88 | 0.56 |
| 1:D:529:PRO:CG | 4:9:353:GLN:OE1 | 2.53 | 0.56 |
| 1:A:410:ASN:CG | 4:8:334:GLU:CA | 2.48 | 0.56 |
| 1:A:435:GLU:O | 1:A:438:PHE:HB3 | 2.06 | 0.56 |
| 1:D:733:PRO:CB | 1:D:737:PHE:HE1 | 2.19 | 0.56 |
| 1:D:819:ASN:CA | 2:E:90:GLY:O | 2.53 | 0.56 |
| 1:G:84:MLY:HH21 | 1:G:720:PHE:CA | 2.31 | 0.56 |
| 1:J:99:GLU:OE2 | 1:J:696:ARG:NH2 | 2.30 | 0.56 |
| 1:M:322:VAL:HG11 | 1:M:325:ILE:HD11 | 1.86 | 0.56 |
| 1:M:95:THR:CB | 1:M:713:SER:HB3 | 2.34 | 0.56 |
| 1:M:733:PRO:CB | 1:M:737:PHE:HE1 | 2.19 | 0.56 |
| 1:M:733:PRO:CA | 1:M:737:PHE:HE1 | 2.18 | 0.56 |
| 1:S:546:THR:HG21 | 1:S:548:THR:HB | 1.88 | 0.56 |
| 1:S:604:ASN:OD1 | 1:S:607:VAL:HG23 | 2.06 | 0.56 |
| 1:S:643:GLY:HA2 | 4:2:24:ASP:OD1 | 2.04 | 0.56 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:CG2 | 2.35 | 0.56 |
| 4:Z:365:ALA:HB3 | 4:Z:369:ILE:HB | 1.88 | 0.56 |
| 4:1:365:ALA:HB3 | 4:1:369:ILE:HB | 1.88 | 0.56 |
| 4:2:110:LEU:O | 4:3:195:GLU:HG3 | 2.06 | 0.56 |
| 4:1:322:PRO:CB | 4:3:244:ASP:HB2 | 2.35 | 0.56 |
| 1:A:537:GLU:HB3 | 1:A:648:THR:CB | 2.36 | 0.56 |
| 1:A:546:THR:HG21 | 1:A:548:THR:HB | 1.88 | 0.56 |
| 1:A:634:GLY:N | 4:8:25:ASP:O | 2.31 | 0.56 |
| 1:D:290:GLN:HG2 | 1:D:331:LEU:HA | 1.87 | 0.56 |
| 1:D:629:GLU:O | 1:D:643:GLY:HA3 | 2.06 | 0.56 |
| 1:D:735:GLY:C | 1:D:743:ALA:HB1 | 1.84 | 0.56 |
| 1:D:32:PHE:CG | 1:D:83:PRO:HD3 | 2.41 | 0.56 |
| 1:G:127:ASN:ND2 | 1:G:128:PRO:HD2 | 2.17 | 0.56 |
| 1:G:22:LYS:O | 1:G:26:GLU:HG3 | 2.06 | 0.56 |
| 1:G:435:GLU:O | 1:G:438:PHE:HB3 | 2.06 | 0.56 |
| 1:G:538:GLU:CG | 4:V:351:THR:C | 2.73 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:769:ALA:HB2 | 1:G:770:GLY:N | 2.21 | 0.56 |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:H | 1.71 | 0.56 |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:HA2 | 1.66 | 0.56 |
| 1:M:537:GLU:HB3 | 1:M:648:THR:CB | 2.36 | 0.56 |
| 1:M:649:VAL:CG1 | 1:M:649:VAL:HA | 2.35 | 0.56 |
| 3:O:46:ILE:O | 3:O:50:LEU:CG | 2.47 | 0.56 |
| 1:S:32:PHE:CG | 1:S:83:PRO:HD3 | 2.41 | 0.56 |
| 1:S:410:ASN:CG | 4:2:334:GLU:C | 2.65 | 0.56 |
| 1:S:677:PRO:HB2 | 1:S:678:ASN:ND2 | 2.20 | 0.56 |
| 1:S:795:ARG:HH21 | 3:U:116:GLU:HA | 1.68 | 0.56 |
| 1:A:116:TYR:CE2 | 1:A:154:HIS:CD2 | 2.94 | 0.56 |
| 1:D:725:ARG:HG3 | 1:D:733:PRO:CA | 2.36 | 0.56 |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:HG13 | 1.87 | 0.56 |
| 1:G:338:ILE:HG21 | 1:G:348:MLY:HB3 | 1.87 | 0.56 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:HA | 2.35 | 0.56 |
| 1:G:783:LEU:HA | 1:G:786:ILE:HB | 1.87 | 0.56 |
| 1:G:7:MET:HE3 | 1:G:14:ALA:CB | 2.36 | 0.56 |
| 1:J:206:LYS:HB3 | 1:J:217:THR:OG1 | 2.06 | 0.56 |
| 1:J:640:LYS:C | 1:J:645:SER:OG | 2.44 | 0.56 |
| 1:J:733:PRO:CA | 1:J:737:PHE:HE1 | 2.19 | 0.56 |
| 1:J:794:CYS:O | 1:J:798:LEU:N | 2.37 | 0.56 |
| 1:M:302:MET:HG2 | 1:M:303:LEU:HD13 | 1.88 | 0.56 |
| 1:M:649:VAL:HA | 1:M:649:VAL:HG22 | 1.80 | 0.56 |
| 1:M:725:ARG:HG3 | 1:M:733:PRO:CA | 2.36 | 0.56 |
| 3:O:52:ASN:HB2 | 3:O:53:PRO:CD | 2.28 | 0.56 |
| 4:V:291:LYS:HD2 | 4:X:243:PRO:HB2 | 1.87 | 0.56 |
| 1:J:530:MET:CB | 4:W:354:GLN:HG3 | 2.36 | 0.56 |
| 1:D:643:GLY:N | 4:9:23:GLY:C | 2.55 | 0.55 |
| 4:9:365:ALA:HB3 | 4:9:369:ILE:HB | 1.88 | 0.55 |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:H | 1.71 | 0.55 |
| 1:A:505:MLY:CG | 1:A:762:HIS:CG | 2.89 | 0.55 |
| 1:A:32:PHE:CG | 1:A:83:PRO:HD3 | 2.42 | 0.55 |
| 1:D:640:LYS:C | 1:D:645:SER:OG | 2.44 | 0.55 |
| 1:G:604:ASN:OD1 | 1:G:607:VAL:HG23 | 2.06 | 0.55 |
| 1:G:733:PRO:CB | 1:G:737:PHE:HE1 | 2.19 | 0.55 |
| 1:J:435:GLU:O | 1:J:438:PHE:HB3 | 2.06 | 0.55 |
| 1:M:505:MLY:HG3 | 1:M:762:HIS:HE1 | 1.72 | 0.55 |
| 1:S:109:ARG:O | 1:S:114:MET:N | 2.37 | 0.55 |
| 1:S:116:TYR:CE2 | 1:S:154:HIS:CD2 | 2.94 | 0.55 |
| 1:S:290:GLN:HG2 | 1:S:331:LEU:HA | 1.87 | 0.55 |
| 1:S:546:THR:HG21 | 4:4:47:MET:C | 2.27 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:634:GLY:N | 4:2:25:ASP:O | 2.31 | 0.55 |
| 1:S:649:VAL:HG23 | 1:S:649:VAL:HA | 1.83 | 0.55 |
| 1:S:732:ILE:HG22 | 1:S:747:LEU:CD1 | 1.55 | 0.55 |
| 4:W:365:ALA:HB3 | 4:W:369:ILE:HB | 1.88 | 0.55 |
| 1:A:22:LYS:O | 1:A:26:GLU:HG3 | 2.06 | 0.55 |
| 1:A:345:ALA:O | 1:A:349:THR:N | 2.40 | 0.55 |
| 1:D:22:LYS:HA | 1:D:25:ILE:HB | 1.87 | 0.55 |
| 1:G:206:LYS:HB3 | 1:G:217:THR:OG1 | 2.06 | 0.55 |
| 1:G:546:THR:HG21 | 1:G:548:THR:HB | 1.88 | 0.55 |
| 1:G:635:GLY:HA3 | 4:V:334:GLU:CG | 2.30 | 0.55 |
| 1:G:677:PRO:HB2 | 1:G:678:ASN:ND2 | 2.20 | 0.55 |
| 1:G:725:ARG:HG3 | 1:G:733:PRO:CA | 2.36 | 0.55 |
| 1:J:109:ARG:O | 1:J:114:MET:N | 2.37 | 0.55 |
| 1:J:530:MET:HA | 4:W:354:GLN:CD | 2.11 | 0.55 |
| 1:J:537:GLU:HB3 | 1:J:648:THR:CB | 2.36 | 0.55 |
| 1:S:649:VAL:CG1 | 1:S:649:VAL:HA | 2.35 | 0.55 |
| 4:W:291:LYS:HD2 | 4:Y:243:PRO:HB2 | 1.87 | 0.55 |
| 4:1:243:PRO:HB2 | 4:Y:291:LYS:HD2 | 1.87 | 0.55 |
| 4:5:365:ALA:HB3 | 4:5:369:ILE:HB | 1.88 | 0.55 |
| 1:A:290:GLN:NE2 | 1:A:334:THR:OG1 | 2.40 | 0.55 |
| 1:A:481:ASN:ND2 | 1:A:481:ASN:N | 2.51 | 0.55 |
| 1:A:757:GLN:OE1 | 1:A:771:LEU:CD1 | 2.32 | 0.55 |
| 1:A:783:LEU:O | 1:A:787:ILE:N | 2.28 | 0.55 |
| 1:A:99:GLU:OE2 | 1:A:696:ARG:NH2 | 2.30 | 0.55 |
| 1:D:206:LYS:HB3 | 1:D:217:THR:OG1 | 2.06 | 0.55 |
| 1:D:295:MLY:HG3 | 1:D:332:MET:HE1 | 1.88 | 0.55 |
| 1:D:537:GLU:HB3 | 1:D:648:THR:CB | 2.36 | 0.55 |
| 1:D:85:TYR:OH | 1:D:772:LEU:HD21 | 1.93 | 0.55 |
| 1:J:338:ILE:HG21 | 1:J:348:MLY:HB3 | 1.87 | 0.55 |
| 1:J:529:PRO:CG | 4:W:353:GLN:OE1 | 2.54 | 0.55 |
| 1:M:116:TYR:CE2 | 1:M:154:HIS:CD2 | 2.94 | 0.55 |
| 1:M:206:LYS:HB3 | 1:M:217:THR:OG1 | 2.06 | 0.55 |
| 1:M:22:LYS:HA | 1:M:25:ILE:HB | 1.87 | 0.55 |
| 1:M:290:GLN:HG2 | 1:M:331:LEU:HA | 1.87 | 0.55 |
| 1:M:530:MET:HE3 | 4:Z:354:GLN:CB | 2.36 | 0.55 |
| 1:M:804:ARG:HA | 1:M:807:VAL:HB | 1.89 | 0.55 |
| 1:M:817:GLN:CD | 2:N:127:ARG:CD | 2.69 | 0.55 |
| 1:S:290:GLN:NE2 | 1:S:334:THR:OG1 | 2.40 | 0.55 |
| 1:S:435:GLU:O | 1:S:438:PHE:HB3 | 2.06 | 0.55 |
| 1:S:481:ASN:N | 1:S:481:ASN:ND2 | 2.51 | 0.55 |
| 1:J:411:GLU:H | 4:W:333:PRO:HG2 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:287:ILE:HG22 | 4:6:204:ALA:H | 1.70 | 0.55 |
| 1:D:538:GLU:CG | 4:9:351:THR:C | 2.74 | 0.55 |
| 1:A:290:GLN:HG2 | 1:A:331:LEU:HA | 1.87 | 0.55 |
| 1:A:768:MLY:HB3 | 1:A:771:LEU:HD13 | 1.87 | 0.55 |
| 1:A:831:TRP:CE2 | 2:B:51:PHE:CE1 | 2.94 | 0.55 |
| 1:A:836:PHE:HB2 | 2:B:161:GLU:OE1 | 2.06 | 0.55 |
| 1:D:290:GLN:NE2 | 1:D:334:THR:OG1 | 2.40 | 0.55 |
| 1:J:302:MET:HG2 | 1:J:303:LEU:HD13 | 1.87 | 0.55 |
| 1:J:546:THR:HG21 | 1:J:548:THR:HB | 1.88 | 0.55 |
| 1:J:553:MLY:HH13 | 4:Y:45:VAL:CG1 | 2.26 | 0.55 |
| 1:J:604:ASN:OD1 | 1:J:607:VAL:HG23 | 2.06 | 0.55 |
| 1:J:82:PRO:HD2 | 1:J:85:TYR:HD2 | 1.72 | 0.55 |
| 1:M:32:PHE:CG | 1:M:83:PRO:HD3 | 2.41 | 0.55 |
| 1:M:7:MET:HE3 | 1:M:14:ALA:CB | 2.37 | 0.55 |
| 1:M:839:MLY:HH11 | 2:N:158:THR:CG2 | 2.37 | 0.55 |
| 1:M:800:ARG:HB3 | 3:O:149:VAL:HG21 | 1.83 | 0.55 |
| 2:T:156:VAL:HA | 2:T:159:HIS:O | 2.07 | 0.55 |
| 3:U:123:VAL:O | 3:U:127:MET:HG2 | 2.07 | 0.55 |
| 4:V:365:ALA:HB3 | 4:V:369:ILE:HB | 1.88 | 0.55 |
| 1:J:529:PRO:CB | 4:W:354:GLN:HA | 2.36 | 0.55 |
| 1:S:530:MET:CB | 4:2:354:GLN:HG3 | 2.36 | 0.55 |
| 1:S:538:GLU:CD | 4:2:355:MET:HE1 | 2.22 | 0.55 |
| 1:A:7:MET:HE3 | 1:A:14:ALA:CB | 2.37 | 0.55 |
| 1:A:206:LYS:HB3 | 1:A:217:THR:OG1 | 2.06 | 0.55 |
| 1:A:604:ASN:OD1 | 1:A:607:VAL:HG23 | 2.06 | 0.55 |
| 1:A:739:ASP:CB | 1:A:742:LYS:CB | 2.81 | 0.55 |
| 1:A:97:LEU:CD2 | 1:A:712:PRO:HB2 | 2.31 | 0.55 |
| 1:D:22:LYS:O | 1:D:26:GLU:HG3 | 2.07 | 0.55 |
| 1:G:640:LYS:C | 1:G:645:SER:OG | 2.44 | 0.55 |
| 1:G:84:MLY:CH1 | 1:G:724:TYR:CE2 | 2.89 | 0.55 |
| 1:G:792:ALA:HB1 | 3:I:42:THR:CA | 2.35 | 0.55 |
| 1:J:579:PHE:HE1 | 1:J:581:LEU:HD13 | 1.72 | 0.55 |
| 1:J:797:PHE:CE2 | 3:L:126:LEU:CD1 | 2.83 | 0.55 |
| 1:M:22:LYS:O | 1:M:26:GLU:HG3 | 2.07 | 0.55 |
| 1:M:290:GLN:NE2 | 1:M:334:THR:OG1 | 2.40 | 0.55 |
| 1:M:640:LYS:C | 1:M:645:SER:OG | 2.44 | 0.55 |
| 1:M:629:GLU:O | 1:M:643:GLY:HA3 | 2.06 | 0.55 |
| 3:O:35:ARG:HA | 3:O:39:GLN:O | 2.07 | 0.55 |
| 1:S:579:PHE:CD2 | 1:S:592:ILE:HD11 | 2.39 | 0.55 |
| 1:S:612:GLN:HE22 | 1:S:627:GLY:HA2 | 1.66 | 0.55 |
| 1:S:629:GLU:O | 1:S:643:GLY:HA3 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:35:ARG:HA | 3:C:39:GLN:O | 2.07 | 0.55 |
| 1:G:109:ARG:O | 1:G:114:MET:N | 2.37 | 0.55 |
| 1:G:22:LYS:HA | 1:G:25:ILE:HB | 1.87 | 0.55 |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:H | 1.71 | 0.55 |
| 1:G:537:GLU:HB3 | 1:G:648:THR:CB | 2.36 | 0.55 |
| 3:I:35:ARG:HA | 3:I:39:GLN:O | 2.07 | 0.55 |
| 1:J:220:ASP:O | 1:J:224:SER:N | 2.27 | 0.55 |
| 1:J:290:GLN:HG2 | 1:J:331:LEU:HA | 1.87 | 0.55 |
| 1:M:435:GLU:O | 1:M:438:PHE:HB3 | 2.06 | 0.55 |
| 1:M:630:ALA:HA | 4:Z:25:ASP:OD2 | 2.07 | 0.55 |
| 1:M:646:PHE:CE2 | 1:M:652:LEU:CG | 2.90 | 0.55 |
| 1:M:797:PHE:CD1 | 3:O:146:ILE:O | 2.60 | 0.55 |
| 1:S:206:LYS:HB3 | 1:S:217:THR:OG1 | 2.06 | 0.55 |
| 1:S:322:VAL:HG11 | 1:S:325:ILE:HD11 | 1.86 | 0.55 |
| 1:S:529:PRO:CB | 4:2:354:GLN:HA | 2.36 | 0.55 |
| 1:S:546:THR:HB | 1:S:549:SER:H | 1.71 | 0.55 |
| 4:1:287:ILE:HG22 | 4:3:204:ALA:H | 1.70 | 0.55 |
| 1:D:529:PRO:CB | 4:9:354:GLN:HA | 2.36 | 0.55 |
| 1:A:725:ARG:HG3 | 1:A:733:PRO:CA | 2.36 | 0.55 |
| 1:G:82:PRO:HD2 | 1:G:85:TYR:HD2 | 1.72 | 0.55 |
| 1:J:292:MET:HE1 | 1:J:309:PRO:CD | 2.37 | 0.55 |
| 1:J:84:MLY:CE | 1:J:724:TYR:CE2 | 2.60 | 0.55 |
| 1:M:217:THR:HG22 | 1:M:218:LEU:O | 2.05 | 0.55 |
| 1:M:739:ASP:CB | 1:M:742:LYS:CB | 2.81 | 0.55 |
| 1:M:82:PRO:HD2 | 1:M:85:TYR:HD2 | 1.72 | 0.55 |
| 2:N:112:ILE:C | 2:N:147:ASN:O | 2.42 | 0.55 |
| 1:S:538:GLU:CG | 4:2:351:THR:C | 2.73 | 0.55 |
| 1:S:635:GLY:HA3 | 4:2:334:GLU:CG | 2.30 | 0.55 |
| 1:S:642:LYS:HG2 | 4:2:22:ALA:C | 2.27 | 0.55 |
| 1:S:817:GLN:CB | 2:T:127:ARG:HD3 | 2.37 | 0.55 |
| 1:G:410:ASN:CG | 4:V:334:GLU:C | 2.64 | 0.55 |
| 4:Y:365:ALA:HB3 | 4:Y:369:ILE:HB | 1.88 | 0.55 |
| 1:S:529:PRO:CG | 4:2:353:GLN:OE1 | 2.54 | 0.55 |
| 1:A:638:GLY:CA | 4:8:345:ILE:H | 2.19 | 0.55 |
| 1:D:7:MET:HE3 | 1:D:14:ALA:CB | 2.36 | 0.55 |
| 1:D:135:TYR:HD2 | 1:D:191:ARG:HG2 | 1.72 | 0.55 |
| 1:D:338:ILE:HG21 | 1:D:348:MLY:HB3 | 1.87 | 0.55 |
| 1:D:345:ALA:O | 1:D:349:THR:N | 2.40 | 0.55 |
| 1:D:546:THR:HB | 1:D:549:SER:H | 1.71 | 0.55 |
| 1:D:579:PHE:HE1 | 1:D:581:LEU:HD13 | 1.72 | 0.55 |
| 2:E:156:VAL:HA | 2:E:159:HIS:O | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:123:VAL:O | 3:F:127:MET:HG2 | 2.07 | 0.55 |
| 1:G:290:GLN:NE2 | 1:G:334:THR:OG1 | 2.40 | 0.55 |
| 1:G:529:PRO:CG | 4:V:353:GLN:OE1 | 2.54 | 0.55 |
| 1:G:755:HIS:HA | 1:G:758:TYR:HE1 | 1.64 | 0.55 |
| 1:G:148:ARG:NH2 | 1:G:764:MLY:CH2 | 2.62 | 0.55 |
| 1:J:530:MET:HE3 | 4:W:354:GLN:CG | 2.31 | 0.55 |
| 1:J:546:THR:HB | 1:J:549:SER:H | 1.71 | 0.55 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:CG | 2.90 | 0.55 |
| 1:J:7:MET:HE3 | 1:J:14:ALA:CB | 2.36 | 0.55 |
| 3:L:35:ARG:HA | 3:L:39:GLN:O | 2.07 | 0.55 |
| 1:M:538:GLU:CG | 4:Z:351:THR:C | 2.73 | 0.55 |
| 1:M:546:THR:HG21 | 1:M:548:THR:HB | 1.88 | 0.55 |
| 3:O:123:VAL:O | 3:O:127:MET:HG2 | 2.07 | 0.55 |
| 1:S:22:LYS:HA | 1:S:25:ILE:HB | 1.87 | 0.55 |
| 1:S:338:ILE:HG21 | 1:S:348:MLY:HB3 | 1.87 | 0.55 |
| 1:S:345:ALA:O | 1:S:349:THR:N | 2.40 | 0.55 |
| 1:S:579:PHE:HE1 | 1:S:581:LEU:HD13 | 1.72 | 0.55 |
| 1:S:725:ARG:HG3 | 1:S:733:PRO:CA | 2.36 | 0.55 |
| 1:S:733:PRO:CB | 1:S:737:PHE:HE1 | 2.19 | 0.55 |
| 4:X:285:CYS:O | 4:Z:202:THR:CG2 | 2.48 | 0.55 |
| 1:M:410:ASN:CG | 4:Z:334:GLU:C | 2.65 | 0.55 |
| 4:1:288:ASP:CB | 4:3:203:THR:HG21 | 2.35 | 0.55 |
| 4:3:287:ILE:HG22 | 4:5:204:ALA:H | 1.70 | 0.55 |
| 4:8:365:ALA:HB3 | 4:8:369:ILE:HB | 1.88 | 0.55 |
| 1:A:529:PRO:CB | 4:8:354:GLN:HA | 2.36 | 0.55 |
| 1:A:579:PHE:HE1 | 1:A:581:LEU:HD13 | 1.72 | 0.55 |
| 1:A:629:GLU:CB | 1:A:643:GLY:C | 2.75 | 0.55 |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:CD1 | 0.64 | 0.55 |
| 3:C:123:VAL:O | 3:C:127:MET:HG2 | 2.06 | 0.55 |
| 1:A:800:ARG:O | 3:C:149:VAL:CG2 | 2.55 | 0.55 |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CE2 | 2.42 | 0.55 |
| 2:E:162:ASP:O | 2:K:21:GLU:HB3 | 2.06 | 0.55 |
| 1:G:579:PHE:HE1 | 1:G:581:LEU:HD13 | 1.72 | 0.55 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:CG | 2.90 | 0.55 |
| 2:H:121:LEU:CA | 2:H:128:PHE:CG | 2.89 | 0.55 |
| 1:G:795:ARG:N | 3:I:118:MET:CE | 2.69 | 0.55 |
| 1:J:290:GLN:NE2 | 1:J:334:THR:OG1 | 2.40 | 0.55 |
| 1:J:32:PHE:CG | 1:J:83:PRO:HD3 | 2.41 | 0.55 |
| 1:J:721:LYS:C | 1:J:736:GLN:OE1 | 2.46 | 0.55 |
| 1:J:839:MLY:HH11 | 2:K:158:THR:HG22 | 1.89 | 0.55 |
| 1:M:546:THR:HB | 1:M:549:SER:H | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:793:ARG:NH1 | 3:O:40:ASN:HD21 | 2.04 | 0.55 |
| 1:S:502:GLU:OE2 | 1:S:761:GLY:HA2 | 2.07 | 0.55 |
| 1:S:530:MET:HE3 | 4:2:354:GLN:CG | 2.30 | 0.55 |
| 1:S:638:GLY:CA | 4:2:345:ILE:H | 2.18 | 0.55 |
| 1:S:506:GLU:HG2 | 1:S:759:ALA:HA | 1.88 | 0.55 |
| 1:G:530:MET:CB | 4:V:354:GLN:HG3 | 2.37 | 0.55 |
| 4:4:365:ALA:HB3 | 4:4:369:ILE:HB | 1.88 | 0.55 |
| 1:A:22:LYS:HA | 1:A:25:ILE:HB | 1.88 | 0.55 |
| 1:A:765:VAL:HG12 | 1:A:766:PHE:N | 2.22 | 0.55 |
| 1:A:768:MLY:HB3 | 1:A:771:LEU:CG | 2.36 | 0.55 |
| 1:D:220:ASP:O | 1:D:224:SER:N | 2.27 | 0.55 |
| 1:D:507:GLY:CA | 1:D:762:HIS:ND1 | 2.70 | 0.55 |
| 1:D:82:PRO:HD2 | 1:D:85:TYR:HD2 | 1.72 | 0.55 |
| 1:G:116:TYR:CE2 | 1:G:154:HIS:CD2 | 2.94 | 0.55 |
| 1:G:290:GLN:HG2 | 1:G:331:LEU:HA | 1.87 | 0.55 |
| 1:G:292:MET:HE1 | 1:G:309:PRO:CD | 2.37 | 0.55 |
| 1:G:32:PHE:CG | 1:G:83:PRO:HD3 | 2.41 | 0.55 |
| 1:G:345:ALA:O | 1:G:349:THR:N | 2.40 | 0.55 |
| 1:G:750:GLY:HA3 | 3:I:114:LEU:CD2 | 2.36 | 0.55 |
| 1:J:642:LYS:HG2 | 4:W:22:ALA:C | 2.27 | 0.55 |
| 3:L:123:VAL:O | 3:L:127:MET:HG2 | 2.07 | 0.55 |
| 1:M:579:PHE:HE1 | 1:M:581:LEU:HD13 | 1.72 | 0.55 |
| 1:S:95:THR:HA | 1:S:713:SER:CB | 2.37 | 0.55 |
| 1:S:721:LYS:C | 1:S:736:GLN:OE1 | 2.46 | 0.55 |
| 1:S:84:MLY:CH2 | 1:S:724:TYR:HE2 | 2.19 | 0.55 |
| 1:J:556:ASP:OD2 | 4:Y:44:MET:HG3 | 2.07 | 0.55 |
| 4:2:287:ILE:HD13 | 4:4:203:THR:HB | 1.89 | 0.54 |
| 1:D:630:ALA:HA | 4:9:25:ASP:OD2 | 2.07 | 0.54 |
| 1:D:302:MET:HG2 | 1:D:303:LEU:HD13 | 1.87 | 0.54 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:CG | 2.90 | 0.54 |
| 1:D:723:ARG:HH11 | 1:D:723:ARG:CG | 2.20 | 0.54 |
| 1:G:529:PRO:CB | 4:V:354:GLN:HA | 2.37 | 0.54 |
| 1:G:629:GLU:CB | 1:G:643:GLY:C | 2.76 | 0.54 |
| 1:G:94:MET:C | 1:G:713:SER:HB3 | 2.27 | 0.54 |
| 1:G:723:ARG:CG | 1:G:723:ARG:HH11 | 2.20 | 0.54 |
| 1:G:765:VAL:HG12 | 1:G:766:PHE:N | 2.22 | 0.54 |
| 2:H:156:VAL:HA | 2:H:159:HIS:O | 2.07 | 0.54 |
| 3:I:123:VAL:O | 3:I:127:MET:HG2 | 2.07 | 0.54 |
| 1:J:135:TYR:HD2 | 1:J:191:ARG:HG2 | 1.72 | 0.54 |
| 2:K:156:VAL:HA | 2:K:159:HIS:O | 2.07 | 0.54 |
| 1:M:635:GLY:HA3 | 4:Z:334:GLU:CG | 2.30 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:M:642:LYS:HG2 | 4:Z:22:ALA:C | 2.27 | 0.54 |
| 1:M:735:GLY:O | 1:M:743:ALA:HA | 1.94 | 0.54 |
| 1:S:292:MET:HE1 | 1:S:309:PRO:CD | 2.37 | 0.54 |
| 1:S:82:PRO:HD2 | 1:S:85:TYR:HD2 | 1.72 | 0.54 |
| 3:U:102:VAL:HG23 | 3:U:139:TYR:CD1 | 2.39 | 0.54 |
| 4:3:365:ALA:HB3 | 4:3:369:ILE:HB | 1.88 | 0.54 |
| 1:A:538:GLU:CG | 4:8:351:THR:C | 2.74 | 0.54 |
| 1:A:135:TYR:HD2 | 1:A:191:ARG:HG2 | 1.72 | 0.54 |
| 1:A:546:THR:HB | 1:A:549:SER:H | 1.71 | 0.54 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:CG | 2.90 | 0.54 |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CZ | 2.42 | 0.54 |
| 1:D:629:GLU:CB | 1:D:643:GLY:C | 2.75 | 0.54 |
| 1:D:642:LYS:HG2 | 4:9:22:ALA:C | 2.27 | 0.54 |
| 1:D:649:VAL:HA | 1:D:649:VAL:CG1 | 2.35 | 0.54 |
| 3:F:35:ARG:HA | 3:F:39:GLN:O | 2.07 | 0.54 |
| 1:G:78:PHE:HB3 | 1:G:98:HIS:NE2 | 2.23 | 0.54 |
| 1:G:821:ARG:HH21 | 2:H:127:ARG:HG2 | 1.60 | 0.54 |
| 1:G:830:PRO:CG | 2:H:67:MET:HE2 | 2.37 | 0.54 |
| 1:J:295:MLY:HG3 | 1:J:332:MET:HE1 | 1.89 | 0.54 |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CZ | 2.42 | 0.54 |
| 1:J:630:ALA:HA | 4:W:25:ASP:OD2 | 2.07 | 0.54 |
| 1:J:629:GLU:O | 1:J:643:GLY:HA3 | 2.06 | 0.54 |
| 1:M:10:PHE:O | 1:M:12:GLU:N | 2.40 | 0.54 |
| 1:S:7:MET:HE3 | 1:S:14:ALA:CB | 2.37 | 0.54 |
| 1:S:649:VAL:HG22 | 1:S:649:VAL:HA | 1.81 | 0.54 |
| 1:S:78:PHE:HB3 | 1:S:98:HIS:NE2 | 2.22 | 0.54 |
| 1:G:638:GLY:CA | 4:V:345:ILE:H | 2.18 | 0.54 |
| 1:A:82:PRO:HD2 | 1:A:85:TYR:HD2 | 1.72 | 0.54 |
| 1:D:755:HIS:HA | 1:D:758:TYR:HE1 | 1.64 | 0.54 |
| 1:D:836:PHE:HE2 | 2:E:160:GLY:CA | 2.14 | 0.54 |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CZ | 2.42 | 0.54 |
| 1:G:831:TRP:HE1 | 2:H:67:MET:CG | 2.21 | 0.54 |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CE2 | 2.43 | 0.54 |
| 1:M:292:MET:HE1 | 1:M:309:PRO:CD | 2.37 | 0.54 |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:CZ | 2.42 | 0.54 |
| 1:M:723:ARG:HH11 | 1:M:723:ARG:CG | 2.20 | 0.54 |
| 2:N:156:VAL:HA | 2:N:159:HIS:O | 2.07 | 0.54 |
| 1:S:135:TYR:HD2 | 1:S:191:ARG:HG2 | 1.73 | 0.54 |
| 1:S:537:GLU:HB3 | 1:S:648:THR:CB | 2.36 | 0.54 |
| 1:S:646:PHE:CE2 | 1:S:652:LEU:CG | 2.90 | 0.54 |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CE2 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:604:ASN:OD1 | 1:D:607:VAL:HG23 | 2.06 | 0.54 |
| 1:D:98:HIS:HB3 | 1:D:100:PRO:CD | 2.25 | 0.54 |
| 2:E:121:LEU:CA | 2:E:128:PHE:CG | 2.89 | 0.54 |
| 1:J:757:GLN:CD | 1:J:777:GLU:N | 2.60 | 0.54 |
| 3:L:46:ILE:O | 3:L:50:LEU:CG | 2.47 | 0.54 |
| 1:M:345:ALA:O | 1:M:349:THR:N | 2.40 | 0.54 |
| 1:M:406:VAL:HG12 | 1:M:407:GLY:H | 1.71 | 0.54 |
| 1:M:579:PHE:CD2 | 1:M:592:ILE:HD11 | 2.40 | 0.54 |
| 2:N:146:GLY:O | 2:N:147:ASN:ND2 | 2.41 | 0.54 |
| 1:S:305:ILE:HG22 | 1:S:312:TYR:CZ | 2.42 | 0.54 |
| 1:S:640:LYS:C | 1:S:645:SER:OG | 2.44 | 0.54 |
| 1:S:629:GLU:CB | 1:S:643:GLY:C | 2.76 | 0.54 |
| 1:S:804:ARG:HA | 1:S:807:VAL:CB | 2.29 | 0.54 |
| 4:V:291:LYS:HD2 | 4:X:243:PRO:CB | 2.37 | 0.54 |
| 4:X:365:ALA:HB3 | 4:X:369:ILE:HB | 1.88 | 0.54 |
| 4:X:287:ILE:HG23 | 4:Z:201:VAL:CG2 | 2.38 | 0.54 |
| 1:M:642:LYS:CA | 4:Z:22:ALA:C | 2.70 | 0.54 |
| 1:M:638:GLY:CA | 4:Z:345:ILE:H | 2.18 | 0.54 |
| 1:M:529:PRO:CB | 4:Z:354:GLN:HA | 2.36 | 0.54 |
| 1:M:530:MET:CB | 4:Z:354:GLN:HG3 | 2.37 | 0.54 |
| 4:1:243:PRO:CB | 4:Y:291:LYS:HD2 | 2.38 | 0.54 |
| 1:A:530:MET:CB | 4:8:354:GLN:HG3 | 2.36 | 0.54 |
| 1:A:10:PHE:O | 1:A:12:GLU:N | 2.41 | 0.54 |
| 1:A:629:GLU:O | 1:A:643:GLY:HA3 | 2.06 | 0.54 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:HA | 2.35 | 0.54 |
| 1:D:10:PHE:O | 1:D:12:GLU:N | 2.41 | 0.54 |
| 1:D:292:MET:HE1 | 1:D:309:PRO:CD | 2.37 | 0.54 |
| 1:D:767:PHE:O | 1:D:771:LEU:CD2 | 2.56 | 0.54 |
| 1:G:38:VAL:CB | 1:G:52:ILE:HD11 | 2.38 | 0.54 |
| 1:J:10:PHE:O | 1:J:12:GLU:N | 2.40 | 0.54 |
| 1:J:345:ALA:O | 1:J:349:THR:N | 2.40 | 0.54 |
| 1:J:629:GLU:CB | 1:J:643:GLY:C | 2.76 | 0.54 |
| 1:M:765:VAL:HG12 | 1:M:766:PHE:N | 2.22 | 0.54 |
| 2:N:121:LEU:CA | 2:N:128:PHE:CG | 2.89 | 0.54 |
| 1:S:22:LYS:O | 1:S:26:GLU:HG3 | 2.07 | 0.54 |
| 1:S:406:VAL:HG12 | 1:S:407:GLY:H | 1.71 | 0.54 |
| 1:M:530:MET:CE | 4:Z:354:GLN:HG3 | 2.35 | 0.54 |
| 1:S:552:ASN:N | 4:4:49:GLN:HB2 | 1.91 | 0.54 |
| 1:A:493:HIS:ND1 | 1:A:514:ASP:OD2 | 2.41 | 0.54 |
| 1:A:640:LYS:C | 1:A:645:SER:OG | 2.44 | 0.54 |
| 1:A:126:VAL:HG13 | 1:A:675:ILE:HG22 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:753:VAL:HG11 | 1:A:775:LEU:CD2 | 2.36 | 0.54 |
| 1:A:753:VAL:CG1 | 1:A:775:LEU:CG | 2.25 | 0.54 |
| 1:A:831:TRP:CZ3 | 2:B:50:THR:CB | 2.90 | 0.54 |
| 1:A:94:MET:O | 1:A:713:SER:CB | 2.52 | 0.54 |
| 1:D:546:THR:HG21 | 1:D:548:THR:HB | 1.88 | 0.54 |
| 1:D:78:PHE:HB3 | 1:D:98:HIS:NE2 | 2.22 | 0.54 |
| 2:E:123:THR:HA | 3:F:19:ARG:CZ | 2.37 | 0.54 |
| 1:G:571:ALA:O | 1:G:572:LYS:CB | 2.56 | 0.54 |
| 1:G:638:GLY:HA2 | 4:V:345:ILE:H | 1.72 | 0.54 |
| 1:G:629:GLU:O | 1:G:643:GLY:HA3 | 2.06 | 0.54 |
| 1:G:126:VAL:HG13 | 1:G:675:ILE:HG22 | 1.89 | 0.54 |
| 1:G:769:ALA:HB1 | 1:G:770:GLY:HA2 | 1.74 | 0.54 |
| 1:J:640:LYS:C | 4:W:23:GLY:CA | 2.64 | 0.54 |
| 1:M:538:GLU:HG3 | 4:Z:352:PHE:CA | 2.38 | 0.54 |
| 1:M:721:LYS:C | 1:M:736:GLN:OE1 | 2.46 | 0.54 |
| 1:M:78:PHE:HB3 | 1:M:98:HIS:NE2 | 2.23 | 0.54 |
| 1:M:816:ILE:HD11 | 2:N:100:ALA:CB | 2.36 | 0.54 |
| 1:S:10:PHE:O | 1:S:12:GLU:N | 2.40 | 0.54 |
| 1:S:530:MET:HE3 | 4:2:355:MET:SD | 2.48 | 0.54 |
| 1:S:739:ASP:CB | 1:S:742:LYS:CB | 2.81 | 0.54 |
| 1:S:765:VAL:HG12 | 1:S:766:PHE:N | 2.22 | 0.54 |
| 3:U:35:ARG:HA | 3:U:39:GLN:O | 2.07 | 0.54 |
| 1:S:789:ALA:HA | 3:U:42:THR:HG21 | 1.88 | 0.54 |
| 4:1:287:ILE:HB | 4:3:203:THR:CA | 2.38 | 0.54 |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CZ | 2.43 | 0.54 |
| 1:A:649:VAL:HG23 | 1:A:649:VAL:HA | 1.83 | 0.54 |
| 1:A:723:ARG:HH11 | 1:A:723:ARG:CG | 2.20 | 0.54 |
| 1:A:768:MLY:C | 1:A:771:LEU:HB2 | 2.37 | 0.54 |
| 1:A:78:PHE:HB3 | 1:A:98:HIS:NE2 | 2.23 | 0.54 |
| 1:D:22:LYS:O | 1:D:26:GLU:N | 2.29 | 0.54 |
| 1:D:38:VAL:CB | 1:D:52:ILE:HD11 | 2.38 | 0.54 |
| 1:D:792:ALA:CB | 3:F:42:THR:CG2 | 2.49 | 0.54 |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CE2 | 2.42 | 0.54 |
| 1:G:404:PRO:CG | 1:G:417:GLU:HG3 | 2.38 | 0.54 |
| 1:G:493:HIS:ND1 | 1:G:514:ASP:OD2 | 2.41 | 0.54 |
| 1:G:794:CYS:O | 1:G:798:LEU:N | 2.37 | 0.54 |
| 1:J:218:LEU:CD2 | 1:J:222:ILE:CG1 | 2.86 | 0.54 |
| 1:J:22:LYS:O | 1:J:26:GLU:HG3 | 2.07 | 0.54 |
| 1:J:493:HIS:ND1 | 1:J:514:ASP:OD2 | 2.41 | 0.54 |
| 1:J:126:VAL:HG13 | 1:J:675:ILE:HG22 | 1.90 | 0.54 |
| 1:J:796:GLY:N | 3:L:35:ARG:CZ | 2.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:571:ALA:O | 1:M:572:LYS:CB | 2.56 | 0.54 |
| 1:M:795:ARG:HG3 | 3:O:118:MET:HE1 | 1.70 | 0.54 |
| 1:S:791:GLN:O | 1:S:794:CYS:HB2 | 2.08 | 0.54 |
| 1:S:804:ARG:O | 1:S:807:VAL:CB | 2.55 | 0.54 |
| 1:S:820:VAL:HG13 | 2:T:136:MET:HE1 | 1.89 | 0.54 |
| 1:J:410:ASN:CG | 4:W:334:GLU:C | 2.65 | 0.54 |
| 1:G:556:ASP:OD2 | 4:X:44:MET:HG3 | 2.08 | 0.54 |
| 1:S:538:GLU:HG3 | 4:2:352:PHE:CA | 2.38 | 0.54 |
| 1:A:506:GLU:CD | 1:A:761:GLY:N | 2.61 | 0.54 |
| 1:A:38:VAL:CB | 1:A:52:ILE:HD11 | 2.38 | 0.54 |
| 1:A:813:ILE:HG12 | 2:B:128:PHE:HE1 | 1.71 | 0.54 |
| 1:D:507:GLY:O | 1:D:761:GLY:CA | 2.55 | 0.54 |
| 1:D:765:VAL:HG12 | 1:D:766:PHE:N | 2.22 | 0.54 |
| 2:H:112:ILE:C | 2:H:147:ASN:O | 2.42 | 0.54 |
| 1:J:571:ALA:O | 1:J:572:LYS:CB | 2.56 | 0.54 |
| 1:J:791:GLN:O | 1:J:794:CYS:HB2 | 2.08 | 0.54 |
| 1:M:126:VAL:HG13 | 1:M:675:ILE:HG22 | 1.90 | 0.54 |
| 2:T:146:GLY:O | 2:T:147:ASN:ND2 | 2.41 | 0.54 |
| 3:U:52:ASN:HB2 | 3:U:53:PRO:CD | 2.28 | 0.54 |
| 1:J:530:MET:HE3 | 4:W:355:MET:SD | 2.48 | 0.54 |
| 4:1:287:ILE:CG2 | 4:3:202:THR:C | 2.73 | 0.54 |
| 1:D:642:LYS:CG | 4:9:22:ALA:CA | 2.80 | 0.54 |
| 2:B:156:VAL:HA | 2:B:159:HIS:O | 2.07 | 0.54 |
| 1:D:493:HIS:ND1 | 1:D:514:ASP:OD2 | 2.41 | 0.54 |
| 1:D:126:VAL:HG13 | 1:D:675:ILE:HG22 | 1.90 | 0.54 |
| 1:D:769:ALA:CA | 1:D:771:LEU:CA | 2.21 | 0.54 |
| 1:G:135:TYR:HD2 | 1:G:191:ARG:HG2 | 1.72 | 0.54 |
| 1:G:795:ARG:C | 3:I:35:ARG:NH2 | 2.61 | 0.54 |
| 1:J:723:ARG:HH11 | 1:J:723:ARG:CG | 2.20 | 0.54 |
| 2:K:146:GLY:O | 2:K:147:ASN:ND2 | 2.41 | 0.54 |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:CE2 | 2.43 | 0.54 |
| 1:S:404:PRO:CG | 1:S:417:GLU:HG3 | 2.38 | 0.54 |
| 1:S:630:ALA:HA | 4:2:25:ASP:OD2 | 2.07 | 0.54 |
| 1:S:795:ARG:NE | 3:U:43:ASN:OD1 | 2.39 | 0.54 |
| 1:J:538:GLU:CG | 4:W:351:THR:C | 2.73 | 0.54 |
| 1:A:220:ASP:O | 1:A:224:SER:N | 2.27 | 0.54 |
| 1:A:642:LYS:CA | 4:8:22:ALA:C | 2.71 | 0.54 |
| 1:A:721:LYS:C | 1:A:736:GLN:OE1 | 2.46 | 0.54 |
| 2:B:146:GLY:O | 2:B:147:ASN:ND2 | 2.41 | 0.54 |
| 1:D:553:MLY:O | 4:W:48:GLY:CA | 2.56 | 0.54 |
| 1:D:638:GLY:HA2 | 4:9:345:ILE:H | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:721:LYS:C | 1:D:736:GLN:OE1 | 2.46 | 0.54 |
| 1:D:836:PHE:CE1 | 2:E:159:HIS:C | 2.79 | 0.54 |
| 1:J:757:GLN:CA | 1:J:776:GLU:CG | 2.74 | 0.54 |
| 2:K:114:LYS:O | 2:K:147:ASN:ND2 | 2.41 | 0.54 |
| 1:J:829:TRP:CZ2 | 2:K:83:MET:CE | 2.91 | 0.54 |
| 1:J:829:TRP:HZ2 | 2:K:83:MET:HE1 | 1.73 | 0.54 |
| 1:S:277:PHE:CG | 1:S:278:GLN:N | 2.76 | 0.54 |
| 1:G:642:LYS:CG | 4:V:22:ALA:HA | 2.37 | 0.54 |
| 1:M:642:LYS:CG | 4:Z:22:ALA:HA | 2.37 | 0.54 |
| 4:1:185:LEU:HD23 | 4:1:306:TYR:OH | 2.09 | 0.53 |
| 1:S:541:MET:SD | 4:2:346:LEU:O | 2.48 | 0.53 |
| 4:3:185:LEU:HD23 | 4:3:306:TYR:OH | 2.09 | 0.53 |
| 4:1:148:THR:OG1 | 4:3:45:VAL:CG2 | 2.56 | 0.53 |
| 4:5:185:LEU:HD23 | 4:5:306:TYR:OH | 2.09 | 0.53 |
| 1:A:638:GLY:HA2 | 4:8:345:ILE:H | 1.72 | 0.53 |
| 1:A:831:TRP:CG | 2:B:51:PHE:CE1 | 2.96 | 0.53 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:OE2 | 2.56 | 0.53 |
| 1:J:215:GLN:CA | 1:J:340:ILE:CG2 | 2.63 | 0.53 |
| 1:M:135:TYR:HD2 | 1:M:191:ARG:HG2 | 1.72 | 0.53 |
| 1:M:38:VAL:CB | 1:M:52:ILE:HD11 | 2.38 | 0.53 |
| 1:M:32:PHE:CD1 | 1:M:83:PRO:HD3 | 2.44 | 0.53 |
| 1:S:32:PHE:CD1 | 1:S:83:PRO:HD3 | 2.43 | 0.53 |
| 1:S:802:GLU:OE2 | 1:S:809:ARG:NH1 | 2.41 | 0.53 |
| 1:S:92:ALA:O | 1:S:714:ARG:CD | 2.52 | 0.53 |
| 1:J:643:GLY:N | 4:W:23:GLY:C | 2.55 | 0.53 |
| 4:W:291:LYS:HD2 | 4:Y:243:PRO:CB | 2.38 | 0.53 |
| 1:A:135:TYR:HD2 | 1:A:191:ARG:HD3 | 1.74 | 0.53 |
| 1:D:571:ALA:O | 1:D:572:LYS:CB | 2.56 | 0.53 |
| 1:G:217:THR:C | 1:G:221:GLN:NE2 | 2.62 | 0.53 |
| 1:G:418:THR:CB | 1:G:421:GLU:HG3 | 2.37 | 0.53 |
| 1:J:135:TYR:HD2 | 1:J:191:ARG:HD3 | 1.73 | 0.53 |
| 1:J:38:VAL:CB | 1:J:52:ILE:HD11 | 2.38 | 0.53 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:CB | 2.81 | 0.53 |
| 1:M:493:HIS:ND1 | 1:M:514:ASP:OD2 | 2.41 | 0.53 |
| 1:M:629:GLU:CB | 1:M:643:GLY:C | 2.76 | 0.53 |
| 1:M:791:GLN:O | 1:M:794:CYS:HB2 | 2.08 | 0.53 |
| 1:M:795:ARG:HD2 | 3:O:35:ARG:HH12 | 1.72 | 0.53 |
| 1:S:135:TYR:HD2 | 1:S:191:ARG:HD3 | 1.73 | 0.53 |
| 3:U:92:ARG:HA | 3:U:139:TYR:OH | 2.08 | 0.53 |
| 1:M:539:GLU:OE2 | 4:2:45:VAL:C | 2.47 | 0.53 |
| 4:9:185:LEU:HD23 | 4:9:306:TYR:OH | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:292:MET:HE1 | 1:A:309:PRO:CD | 2.38 | 0.53 |
| 1:A:505:MLY:HB2 | 1:A:761:GLY:HA2 | 1.89 | 0.53 |
| 3:C:92:ARG:HA | 3:C:139:TYR:OH | 2.08 | 0.53 |
| 1:D:154:HIS:CE1 | 1:D:156:PHE:HD2 | 2.26 | 0.53 |
| 1:D:724:TYR:CE1 | 1:D:779:ARG:HA | 2.43 | 0.53 |
| 1:D:791:GLN:OE1 | 3:F:116:GLU:N | 2.41 | 0.53 |
| 2:H:146:GLY:O | 2:H:147:ASN:ND2 | 2.41 | 0.53 |
| 1:J:638:GLY:HA2 | 4:W:345:ILE:H | 1.72 | 0.53 |
| 1:J:739:ASP:CB | 1:J:742:LYS:CB | 2.81 | 0.53 |
| 1:M:135:TYR:HD2 | 1:M:191:ARG:HD3 | 1.73 | 0.53 |
| 1:M:576:GLU:CG | 1:M:577:ALA:N | 2.44 | 0.53 |
| 1:M:759:ALA:O | 1:M:766:PHE:N | 2.32 | 0.53 |
| 1:S:305:ILE:HG22 | 1:S:312:TYR:CE2 | 2.43 | 0.53 |
| 1:S:599:ASN:CG | 1:S:649:VAL:H | 2.12 | 0.53 |
| 1:S:661:MET:O | 1:S:665:ARG:HG3 | 2.09 | 0.53 |
| 4:1:324:THR:OG1 | 4:3:244:ASP:N | 2.41 | 0.53 |
| 1:A:404:PRO:CG | 1:A:417:GLU:HG3 | 2.38 | 0.53 |
| 1:A:541:MET:SD | 4:8:346:LEU:O | 2.49 | 0.53 |
| 1:A:630:ALA:HA | 4:8:25:ASP:OD2 | 2.07 | 0.53 |
| 1:A:661:MET:O | 1:A:665:ARG:HG3 | 2.09 | 0.53 |
| 1:A:795:ARG:HG2 | 3:C:118:MET:HE1 | 1.88 | 0.53 |
| 1:D:800:ARG:HD3 | 3:F:149:VAL:O | 2.08 | 0.53 |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HG3 | 1.90 | 0.53 |
| 1:G:584:TYR:CD1 | 1:G:585:ALA:N | 2.77 | 0.53 |
| 1:G:32:PHE:CD1 | 1:G:83:PRO:HD3 | 2.44 | 0.53 |
| 1:G:84:MLY:HD3 | 1:G:723:ARG:CD | 2.25 | 0.53 |
| 2:H:114:LYS:O | 2:H:147:ASN:ND2 | 2.41 | 0.53 |
| 1:G:831:TRP:HZ3 | 2:H:34:ILE:HG21 | 1.73 | 0.53 |
| 3:I:46:ILE:O | 3:I:50:LEU:CG | 2.47 | 0.53 |
| 1:J:277:PHE:CG | 1:J:278:GLN:N | 2.76 | 0.53 |
| 1:J:404:PRO:CG | 1:J:417:GLU:HG3 | 2.38 | 0.53 |
| 1:J:84:MLY:CH1 | 1:J:724:TYR:CE2 | 2.91 | 0.53 |
| 1:J:98:HIS:HB3 | 1:J:100:PRO:CD | 2.25 | 0.53 |
| 1:M:217:THR:C | 1:M:221:GLN:NE2 | 2.62 | 0.53 |
| 1:M:218:LEU:N | 1:M:221:GLN:HG2 | 2.24 | 0.53 |
| 1:M:277:PHE:CG | 1:M:278:GLN:N | 2.76 | 0.53 |
| 1:M:599:ASN:CG | 1:M:649:VAL:H | 2.12 | 0.53 |
| 1:M:84:MLY:CH1 | 1:M:715:VAL:HG21 | 2.36 | 0.53 |
| 1:S:126:VAL:HG13 | 1:S:675:ILE:HG22 | 1.90 | 0.53 |
| 1:S:493:HIS:ND1 | 1:S:514:ASP:OD2 | 2.41 | 0.53 |
| 1:A:553:MLY:O | 4:V:48:GLY:CA | 2.56 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:642:LYS:CG | 4:2:22:ALA:HA | 2.37 | 0.53 |
| 1:M:553:MLY:O | 4:2:48:GLY:CA | 2.56 | 0.53 |
| 4:3:288:ASP:OD2 | 4:5:203:THR:CB | 2.56 | 0.53 |
| 4:4:288:ASP:OD2 | 4:6:203:THR:CB | 2.56 | 0.53 |
| 1:A:32:PHE:CD1 | 1:A:83:PRO:HD3 | 2.44 | 0.53 |
| 2:B:121:LEU:CA | 2:B:128:PHE:CG | 2.89 | 0.53 |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:HA2 | 1.66 | 0.53 |
| 1:D:661:MET:O | 1:D:665:ARG:HG3 | 2.09 | 0.53 |
| 1:D:791:GLN:O | 1:D:794:CYS:HB2 | 2.08 | 0.53 |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:HD2 | 1.73 | 0.53 |
| 1:G:10:PHE:O | 1:G:12:GLU:N | 2.41 | 0.53 |
| 3:I:92:ARG:HA | 3:I:139:TYR:OH | 2.09 | 0.53 |
| 1:J:661:MET:O | 1:J:665:ARG:HG3 | 2.09 | 0.53 |
| 1:M:584:TYR:CD1 | 1:M:585:ALA:N | 2.77 | 0.53 |
| 1:M:753:VAL:HG11 | 1:M:775:LEU:CD1 | 2.37 | 0.53 |
| 2:N:114:LYS:O | 2:N:147:ASN:ND2 | 2.42 | 0.53 |
| 1:M:796:GLY:CA | 3:O:35:ARG:HD3 | 2.30 | 0.53 |
| 1:S:646:PHE:CD2 | 1:S:652:LEU:CD1 | 2.85 | 0.53 |
| 1:S:723:ARG:HH11 | 1:S:723:ARG:CG | 2.20 | 0.53 |
| 1:S:730:SER:HB2 | 3:U:94:PHE:CE2 | 2.44 | 0.53 |
| 1:G:642:LYS:HG2 | 4:V:22:ALA:C | 2.27 | 0.53 |
| 4:2:166:TYR:CZ | 4:4:64:ILE:CG2 | 2.86 | 0.53 |
| 1:A:576:GLU:CG | 1:A:577:ALA:N | 2.43 | 0.53 |
| 1:D:584:TYR:CD1 | 1:D:585:ALA:N | 2.77 | 0.53 |
| 2:E:114:LYS:O | 2:E:147:ASN:ND2 | 2.41 | 0.53 |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CD1 | 1.05 | 0.53 |
| 1:J:829:TRP:CE2 | 2:K:87:LYS:CE | 2.85 | 0.53 |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:HD11 | 1.75 | 0.53 |
| 1:M:295:MLY:HE2 | 1:M:332:MET:HE1 | 1.91 | 0.53 |
| 1:M:720:PHE:HZ | 1:M:772:LEU:HD11 | 1.70 | 0.53 |
| 2:N:114:LYS:N | 2:N:146:GLY:O | 2.40 | 0.53 |
| 1:S:295:MLY:HE2 | 1:S:332:MET:HE1 | 1.91 | 0.53 |
| 1:S:38:VAL:CB | 1:S:52:ILE:HD11 | 2.38 | 0.53 |
| 1:S:636:LYS:HB2 | 4:2:334:GLU:OE1 | 2.09 | 0.53 |
| 1:S:638:GLY:HA2 | 4:2:345:ILE:H | 1.72 | 0.53 |
| 1:S:805:ALA:C | 1:S:808:GLU:N | 2.62 | 0.53 |
| 1:S:93:MET:HE1 | 1:S:764:MLY:CB | 2.15 | 0.53 |
| 1:S:803:TYR:HE2 | 3:U:17:PHE:CZ | 2.22 | 0.53 |
| 4:W:185:LEU:HD23 | 4:W:306:TYR:OH | 2.09 | 0.53 |
| 1:J:538:GLU:HG3 | 4:W:352:PHE:CA | 2.38 | 0.53 |
| 1:J:529:PRO:HB2 | 4:W:354:GLN:HA | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:324:THR:HB | 4:Z:247:VAL:N | 2.22 | 0.53 |
| 1:A:42:HIS:HB3 | 1:A:45:GLN:O | 2.09 | 0.53 |
| 1:A:571:ALA:O | 1:A:572:LYS:CB | 2.56 | 0.53 |
| 1:A:800:ARG:NH2 | 3:C:40:ASN:CG | 2.62 | 0.53 |
| 1:D:404:PRO:CG | 1:D:417:GLU:HG3 | 2.38 | 0.53 |
| 1:D:404:PRO:HG3 | 1:D:417:GLU:HG3 | 1.91 | 0.53 |
| 1:D:538:GLU:HG3 | 4:9:352:PHE:CA | 2.38 | 0.53 |
| 2:E:146:GLY:O | 2:E:147:ASN:ND2 | 2.41 | 0.53 |
| 1:G:636:LYS:HB2 | 4:V:334:GLU:OE1 | 2.09 | 0.53 |
| 1:G:791:GLN:O | 1:G:794:CYS:HB2 | 2.08 | 0.53 |
| 1:J:599:ASN:CG | 1:J:649:VAL:H | 2.12 | 0.53 |
| 1:J:820:VAL:HG13 | 2:K:136:MET:HE1 | 1.90 | 0.53 |
| 1:M:154:HIS:CE1 | 1:M:156:PHE:HD2 | 2.26 | 0.53 |
| 1:M:783:LEU:CA | 1:M:786:ILE:CG1 | 2.30 | 0.53 |
| 1:S:640:LYS:C | 4:2:23:GLY:CA | 2.64 | 0.53 |
| 1:S:804:ARG:C | 1:S:807:VAL:N | 2.62 | 0.53 |
| 1:M:638:GLY:HA2 | 4:Z:345:ILE:H | 1.72 | 0.53 |
| 1:M:529:PRO:HB2 | 4:Z:354:GLN:HA | 1.91 | 0.53 |
| 1:A:295:MLY:HE2 | 1:A:332:MET:HE1 | 1.91 | 0.53 |
| 1:A:538:GLU:HG3 | 4:8:352:PHE:CA | 2.39 | 0.53 |
| 1:A:584:TYR:CD1 | 1:A:585:ALA:N | 2.77 | 0.53 |
| 1:D:109:ARG:O | 1:D:114:MET:N | 2.37 | 0.53 |
| 1:D:135:TYR:CD2 | 1:D:191:ARG:HG2 | 2.44 | 0.53 |
| 1:D:217:THR:C | 1:D:221:GLN:NE2 | 2.62 | 0.53 |
| 1:D:506:GLU:O | 1:D:762:HIS:CA | 2.57 | 0.53 |
| 1:D:723:ARG:NH2 | 1:D:779:ARG:HH21 | 2.06 | 0.53 |
| 1:D:814:PHE:HE1 | 2:E:127:ARG:CZ | 2.22 | 0.53 |
| 1:G:251:ARG:HB2 | 1:G:264:ASP:HB2 | 1.91 | 0.53 |
| 1:G:295:MLY:HE2 | 1:G:332:MET:HE1 | 1.91 | 0.53 |
| 1:J:135:TYR:CD2 | 1:J:191:ARG:HG2 | 2.44 | 0.53 |
| 1:J:206:LYS:HD2 | 1:J:217:THR:CG2 | 2.17 | 0.53 |
| 1:J:78:PHE:HB3 | 1:J:98:HIS:NE2 | 2.22 | 0.53 |
| 1:J:831:TRP:HZ3 | 2:K:34:ILE:CD1 | 2.20 | 0.53 |
| 2:K:129:THR:O | 2:K:133:ILE:HG13 | 2.09 | 0.53 |
| 3:L:92:ARG:HA | 3:L:139:TYR:OH | 2.08 | 0.53 |
| 1:M:251:ARG:HB2 | 1:M:264:ASP:HB2 | 1.91 | 0.53 |
| 1:M:404:PRO:CG | 1:M:417:GLU:HG3 | 2.38 | 0.53 |
| 1:M:661:MET:O | 1:M:665:ARG:HG3 | 2.09 | 0.53 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:CD | 2.62 | 0.53 |
| 3:O:92:ARG:HA | 3:O:139:TYR:OH | 2.08 | 0.53 |
| 1:S:571:ALA:O | 1:S:572:LYS:CB | 2.56 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:752:ASP:H | 1:S:779:ARG:NH2 | 2.05 | 0.53 |
| 1:S:791:GLN:NE2 | 3:U:115:GLY:CA | 2.38 | 0.53 |
| 2:T:117:LEU:CG | 2:T:147:ASN:OD1 | 2.52 | 0.53 |
| 4:V:324:THR:HG22 | 4:X:247:VAL:HG13 | 1.91 | 0.53 |
| 4:1:288:ASP:H | 4:3:203:THR:HG22 | 1.69 | 0.53 |
| 4:3:287:ILE:HG23 | 4:5:202:THR:HB | 0.99 | 0.53 |
| 4:7:185:LEU:HD23 | 4:7:306:TYR:OH | 2.09 | 0.53 |
| 1:A:642:LYS:CG | 4:8:22:ALA:HA | 2.38 | 0.53 |
| 1:A:418:THR:CB | 1:A:421:GLU:HG3 | 2.37 | 0.53 |
| 1:A:539:GLU:OE2 | 4:V:45:VAL:C | 2.47 | 0.53 |
| 1:A:642:LYS:HG2 | 4:8:22:ALA:C | 2.28 | 0.53 |
| 1:A:759:ALA:O | 1:A:766:PHE:N | 2.32 | 0.53 |
| 1:D:732:ILE:H | 1:D:733:PRO:HD2 | 1.74 | 0.53 |
| 1:D:32:PHE:CD1 | 1:D:83:PRO:HD3 | 2.43 | 0.53 |
| 1:D:795:ARG:CG | 3:F:35:ARG:HH12 | 2.21 | 0.53 |
| 1:G:538:GLU:HG3 | 4:V:352:PHE:CA | 2.38 | 0.53 |
| 1:G:721:LYS:C | 1:G:736:GLN:OE1 | 2.46 | 0.53 |
| 1:J:154:HIS:CE1 | 1:J:156:PHE:HD2 | 2.26 | 0.53 |
| 1:J:584:TYR:CD1 | 1:J:585:ALA:N | 2.77 | 0.53 |
| 1:J:795:ARG:O | 3:L:35:ARG:NH2 | 2.40 | 0.53 |
| 1:M:556:ASP:HB3 | 4:2:43:VAL:HG12 | 1.91 | 0.53 |
| 1:S:218:LEU:N | 1:S:221:GLN:HG2 | 2.24 | 0.53 |
| 1:S:418:THR:CB | 1:S:421:GLU:HG3 | 2.37 | 0.53 |
| 1:S:584:TYR:CD1 | 1:S:585:ALA:N | 2.77 | 0.53 |
| 1:A:553:MLY:HG3 | 4:V:44:MET:O | 2.07 | 0.53 |
| 4:Y:185:LEU:HD23 | 4:Y:306:TYR:OH | 2.09 | 0.53 |
| 4:1:324:THR:CG2 | 4:3:244:ASP:CA | 2.86 | 0.53 |
| 4:2:167:GLU:OE1 | 4:4:43:VAL:O | 2.27 | 0.53 |
| 1:A:154:HIS:CE1 | 1:A:156:PHE:HD2 | 2.26 | 0.53 |
| 1:A:218:LEU:N | 1:A:221:GLN:HG2 | 2.23 | 0.53 |
| 1:A:499:GLU:CD | 1:A:766:PHE:CE2 | 2.82 | 0.53 |
| 1:A:579:PHE:CD2 | 1:A:592:ILE:HD11 | 2.40 | 0.53 |
| 1:A:791:GLN:O | 1:A:794:CYS:HB2 | 2.08 | 0.53 |
| 1:D:529:PRO:HB2 | 4:9:354:GLN:HA | 1.91 | 0.53 |
| 1:D:599:ASN:CG | 1:D:649:VAL:H | 2.12 | 0.53 |
| 3:F:92:ARG:HA | 3:F:139:TYR:OH | 2.08 | 0.53 |
| 1:G:292:MET:CE | 1:G:309:PRO:HA | 2.39 | 0.53 |
| 1:G:42:HIS:HB3 | 1:G:45:GLN:O | 2.09 | 0.53 |
| 1:G:530:MET:HG2 | 4:V:354:GLN:HB2 | 0.57 | 0.53 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:HA | 2.35 | 0.53 |
| 1:J:733:PRO:O | 1:J:737:PHE:CE1 | 2.53 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:32:PHE:CD1 | 1:J:83:PRO:HD3 | 2.43 | 0.53 |
| 3:L:53:PRO:HB2 | 3:L:55:LYS:HG3 | 1.91 | 0.53 |
| 1:M:42:HIS:HB3 | 1:M:45:GLN:O | 2.09 | 0.53 |
| 1:S:491:PHE:HD1 | 1:S:671:PHE:CE2 | 2.27 | 0.53 |
| 1:S:732:ILE:H | 1:S:733:PRO:HD2 | 1.74 | 0.53 |
| 1:S:799:MET:SD | 3:U:32:ASP:HB3 | 2.49 | 0.53 |
| 4:2:185:LEU:HD23 | 4:2:306:TYR:OH | 2.09 | 0.52 |
| 1:S:529:PRO:HB2 | 4:2:354:GLN:HA | 1.91 | 0.52 |
| 1:A:410:ASN:CG | 4:8:334:GLU:C | 2.65 | 0.52 |
| 1:A:529:PRO:HB2 | 4:8:354:GLN:HA | 1.91 | 0.52 |
| 1:A:156:PHE:HD1 | 1:A:195:TYR:CD1 | 2.27 | 0.52 |
| 1:A:599:ASN:CG | 1:A:649:VAL:H | 2.12 | 0.52 |
| 3:C:104:GLY:HA2 | 3:C:137:ILE:HD11 | 1.91 | 0.52 |
| 3:C:49:ILE:CA | 3:C:52:ASN:ND2 | 2.53 | 0.52 |
| 3:C:53:PRO:HB2 | 3:C:55:LYS:HG3 | 1.91 | 0.52 |
| 1:D:135:TYR:HD2 | 1:D:191:ARG:HD3 | 1.73 | 0.52 |
| 2:E:114:LYS:HA | 2:E:147:ASN:HD22 | 1.74 | 0.52 |
| 1:G:404:PRO:HG3 | 1:G:417:GLU:HG3 | 1.91 | 0.52 |
| 3:I:53:PRO:HB2 | 3:I:55:LYS:HG3 | 1.91 | 0.52 |
| 1:J:218:LEU:N | 1:J:221:GLN:HG2 | 2.24 | 0.52 |
| 1:J:817:GLN:OE1 | 2:K:127:ARG:CD | 2.54 | 0.52 |
| 1:M:135:TYR:CD2 | 1:M:191:ARG:HG2 | 2.44 | 0.52 |
| 1:M:292:MET:CE | 1:M:309:PRO:HA | 2.39 | 0.52 |
| 1:M:404:PRO:HG3 | 1:M:417:GLU:HG3 | 1.91 | 0.52 |
| 1:M:95:THR:CA | 1:M:713:SER:OG | 2.49 | 0.52 |
| 1:M:821:ARG:NH1 | 2:N:127:ARG:NE | 2.57 | 0.52 |
| 1:M:836:PHE:CD2 | 2:N:160:GLY:CA | 2.91 | 0.52 |
| 1:S:135:TYR:CD2 | 1:S:191:ARG:HG2 | 2.44 | 0.52 |
| 1:S:251:ARG:HB2 | 1:S:264:ASP:HB2 | 1.91 | 0.52 |
| 1:S:42:HIS:HB3 | 1:S:45:GLN:O | 2.09 | 0.52 |
| 1:S:749:GLY:HA3 | 3:U:93:VAL:HG23 | 1.89 | 0.52 |
| 2:T:114:LYS:O | 2:T:147:ASN:ND2 | 2.41 | 0.52 |
| 1:S:734:GLU:OE2 | 3:U:94:PHE:CD2 | 2.62 | 0.52 |
| 1:A:556:ASP:HB3 | 4:V:43:VAL:HG12 | 1.91 | 0.52 |
| 4:X:287:ILE:CG2 | 4:Z:201:VAL:CG2 | 2.85 | 0.52 |
| 4:6:180:LEU:HD22 | 4:6:267:ILE:HD11 | 1.92 | 0.52 |
| 4:8:180:LEU:HD22 | 4:8:267:ILE:HD11 | 1.92 | 0.52 |
| 3:C:110:VAL:HG13 | 3:C:114:LEU:HD12 | 1.92 | 0.52 |
| 1:D:218:LEU:N | 1:D:221:GLN:HG2 | 2.24 | 0.52 |
| 1:D:42:HIS:HB3 | 1:D:45:GLN:O | 2.09 | 0.52 |
| 1:D:556:ASP:HB3 | 4:W:43:VAL:HG12 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:135:TYR:CD2 | 1:G:191:ARG:HG2 | 2.44 | 0.52 |
| 1:G:63:MLY:HG3 | 1:G:64:THR:H | 1.75 | 0.52 |
| 1:J:156:PHE:HD1 | 1:J:195:TYR:CD1 | 2.27 | 0.52 |
| 1:J:404:PRO:HG3 | 1:J:417:GLU:HG3 | 1.91 | 0.52 |
| 3:L:110:VAL:HG13 | 3:L:114:LEU:HD12 | 1.92 | 0.52 |
| 1:M:819:ASN:OD1 | 2:N:90:GLY:O | 2.26 | 0.52 |
| 1:S:154:HIS:CE1 | 1:S:156:PHE:HD2 | 2.26 | 0.52 |
| 1:S:232:PHE:CE1 | 1:S:287:ILE:HD13 | 2.44 | 0.52 |
| 4:1:285:CYS:O | 4:1:290:ARG:NH1 | 2.43 | 0.52 |
| 4:1:324:THR:OG1 | 4:3:244:ASP:HA | 2.09 | 0.52 |
| 4:4:180:LEU:HD22 | 4:4:267:ILE:HD11 | 1.92 | 0.52 |
| 4:9:180:LEU:HD22 | 4:9:267:ILE:HD11 | 1.92 | 0.52 |
| 1:D:636:LYS:HB2 | 4:9:334:GLU:OE1 | 2.09 | 0.52 |
| 1:A:135:TYR:CD2 | 1:A:191:ARG:HG2 | 2.44 | 0.52 |
| 1:A:251:ARG:HB2 | 1:A:264:ASP:HB2 | 1.91 | 0.52 |
| 1:A:292:MET:HE1 | 1:A:309:PRO:HD3 | 1.91 | 0.52 |
| 1:A:502:GLU:HG3 | 1:A:760:PHE:C | 2.25 | 0.52 |
| 1:A:796:GLY:HA3 | 3:C:40:ASN:OD1 | 2.09 | 0.52 |
| 1:G:154:HIS:CE1 | 1:G:156:PHE:HD2 | 2.27 | 0.52 |
| 1:G:218:LEU:N | 1:G:221:GLN:HG2 | 2.24 | 0.52 |
| 1:G:599:ASN:CG | 1:G:649:VAL:H | 2.12 | 0.52 |
| 1:G:84:MLY:HH12 | 1:G:715:VAL:CG2 | 2.39 | 0.52 |
| 1:J:765:VAL:HG12 | 1:J:766:PHE:N | 2.22 | 0.52 |
| 1:M:109:ARG:HD3 | 1:M:117:THR:HB | 1.92 | 0.52 |
| 1:M:156:PHE:HD1 | 1:M:195:TYR:CD1 | 2.27 | 0.52 |
| 1:M:555:TYR:N | 4:2:48:GLY:N | 2.58 | 0.52 |
| 1:S:404:PRO:HG3 | 1:S:417:GLU:HG3 | 1.91 | 0.52 |
| 4:X:185:LEU:HD23 | 4:X:306:TYR:OH | 2.09 | 0.52 |
| 4:1:247:VAL:HG13 | 4:Y:324:THR:HG22 | 1.91 | 0.52 |
| 4:Z:185:LEU:HD23 | 4:Z:306:TYR:OH | 2.09 | 0.52 |
| 4:5:180:LEU:HD22 | 4:5:267:ILE:HD11 | 1.92 | 0.52 |
| 1:A:218:LEU:CD2 | 1:A:222:ILE:CG1 | 2.85 | 0.52 |
| 1:A:795:ARG:CD | 3:C:43:ASN:CG | 2.77 | 0.52 |
| 1:D:251:ARG:HB2 | 1:D:264:ASP:HB2 | 1.91 | 0.52 |
| 1:D:555:TYR:N | 4:W:48:GLY:N | 2.58 | 0.52 |
| 1:D:712:PRO:CG | 1:D:771:LEU:HD13 | 2.39 | 0.52 |
| 1:G:529:PRO:HB2 | 4:V:354:GLN:HA | 1.92 | 0.52 |
| 1:G:732:ILE:H | 1:G:733:PRO:CD | 2.23 | 0.52 |
| 1:G:818:TYR:CE1 | 2:H:127:ARG:NH1 | 2.48 | 0.52 |
| 2:H:129:THR:O | 2:H:133:ILE:HG13 | 2.09 | 0.52 |
| 1:J:197:ALA:O | 1:J:201:ALA:HB2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:218:LEU:HA | 1:J:221:GLN:HG3 | 1.71 | 0.52 |
| 1:J:530:MET:HG2 | 4:W:354:GLN:HB2 | 0.57 | 0.52 |
| 1:J:84:MLY:HH12 | 1:J:715:VAL:CG2 | 2.39 | 0.52 |
| 2:K:121:LEU:CA | 2:K:128:PHE:CG | 2.89 | 0.52 |
| 3:L:104:GLY:HA2 | 3:L:137:ILE:HD11 | 1.92 | 0.52 |
| 1:M:232:PHE:CE1 | 1:M:287:ILE:HD13 | 2.45 | 0.52 |
| 1:M:491:PHE:HD1 | 1:M:671:PHE:CE2 | 2.27 | 0.52 |
| 1:M:63:MLY:HG3 | 1:M:64:THR:H | 1.75 | 0.52 |
| 2:N:149:ASP:CG | 2:N:150:TYR:N | 2.49 | 0.52 |
| 1:M:832:MET:SD | 2:N:84:PHE:HE2 | 2.31 | 0.52 |
| 1:S:156:PHE:HD1 | 1:S:195:TYR:CD1 | 2.27 | 0.52 |
| 4:V:185:LEU:HD23 | 4:V:306:TYR:OH | 2.09 | 0.52 |
| 4:W:285:CYS:O | 4:W:290:ARG:NH1 | 2.43 | 0.52 |
| 4:X:180:LEU:HD22 | 4:X:267:ILE:HD11 | 1.92 | 0.52 |
| 4:5:285:CYS:O | 4:5:290:ARG:NH1 | 2.43 | 0.52 |
| 4:7:285:CYS:O | 4:7:290:ARG:NH1 | 2.43 | 0.52 |
| 1:D:128:PRO:O | 1:D:129:TYR:HB2 | 2.09 | 0.52 |
| 1:D:277:PHE:CG | 1:D:278:GLN:N | 2.76 | 0.52 |
| 1:D:41:VAL:HG13 | 1:D:42:HIS:N | 2.25 | 0.52 |
| 1:G:135:TYR:HD2 | 1:G:191:ARG:HD3 | 1.73 | 0.52 |
| 1:G:40:VAL:HG13 | 1:G:41:VAL:O | 2.10 | 0.52 |
| 1:G:818:TYR:CG | 2:H:127:ARG:NH1 | 2.77 | 0.52 |
| 1:G:798:LEU:CG | 3:I:122:GLU:HB3 | 2.40 | 0.52 |
| 1:J:292:MET:CE | 1:J:309:PRO:HA | 2.39 | 0.52 |
| 1:J:42:HIS:HB3 | 1:J:45:GLN:O | 2.09 | 0.52 |
| 1:J:553:MLY:HH12 | 4:Y:45:VAL:CG1 | 2.30 | 0.52 |
| 1:J:732:ILE:H | 1:J:733:PRO:CD | 2.23 | 0.52 |
| 2:K:114:LYS:N | 2:K:146:GLY:O | 2.40 | 0.52 |
| 1:M:418:THR:CB | 1:M:421:GLU:HG3 | 2.37 | 0.52 |
| 1:M:831:TRP:NE1 | 2:N:67:MET:HB3 | 2.24 | 0.52 |
| 1:S:753:VAL:HG22 | 1:S:779:ARG:CZ | 2.38 | 0.52 |
| 4:V:180:LEU:HD22 | 4:V:267:ILE:HD11 | 1.92 | 0.52 |
| 4:9:287:ILE:HG22 | 4:W:204:ALA:HB3 | 1.91 | 0.52 |
| 1:J:642:LYS:CA | 4:W:22:ALA:C | 2.70 | 0.52 |
| 4:X:285:CYS:O | 4:X:290:ARG:NH1 | 2.43 | 0.52 |
| 4:Z:180:LEU:HD22 | 4:Z:267:ILE:HD11 | 1.92 | 0.52 |
| 4:2:204:ALA:HB2 | 4:Z:288:ASP:CA | 2.32 | 0.52 |
| 4:2:285:CYS:O | 4:2:290:ARG:NH1 | 2.43 | 0.52 |
| 4:3:285:CYS:O | 4:3:290:ARG:NH1 | 2.43 | 0.52 |
| 4:7:180:LEU:HD22 | 4:7:267:ILE:HD11 | 1.92 | 0.52 |
| 1:D:530:MET:HE3 | 4:9:355:MET:SD | 2.49 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:232:PHE:CE1 | 1:A:287:ILE:HD13 | 2.44 | 0.52 |
| 1:D:63:MLY:HG3 | 1:D:64:THR:H | 1.75 | 0.52 |
| 1:D:795:ARG:HD2 | 3:F:43:ASN:OD1 | 1.95 | 0.52 |
| 3:F:53:PRO:HB2 | 3:F:55:LYS:HG3 | 1.91 | 0.52 |
| 1:G:156:PHE:HD1 | 1:G:195:TYR:CD1 | 2.27 | 0.52 |
| 1:G:232:PHE:CE1 | 1:G:287:ILE:HD13 | 2.45 | 0.52 |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CD1 | 1.04 | 0.52 |
| 1:M:820:VAL:CG1 | 2:N:136:MET:HE1 | 2.40 | 0.52 |
| 1:S:217:THR:C | 1:S:221:GLN:NE2 | 2.62 | 0.52 |
| 1:S:805:ALA:C | 1:S:809:ARG:HB2 | 2.28 | 0.52 |
| 4:W:180:LEU:HD22 | 4:W:267:ILE:HD11 | 1.92 | 0.52 |
| 4:W:324:THR:HG22 | 4:Y:247:VAL:HG13 | 1.91 | 0.52 |
| 4:Z:285:CYS:O | 4:Z:290:ARG:NH1 | 2.43 | 0.52 |
| 4:2:180:LEU:HD22 | 4:2:267:ILE:HD11 | 1.92 | 0.52 |
| 4:4:185:LEU:HD23 | 4:4:306:TYR:OH | 2.09 | 0.52 |
| 4:6:185:LEU:HD23 | 4:6:306:TYR:OH | 2.09 | 0.52 |
| 4:7:287:ILE:HG22 | 4:9:204:ALA:HB3 | 1.91 | 0.52 |
| 4:9:285:CYS:O | 4:9:290:ARG:NH1 | 2.43 | 0.52 |
| 1:A:109:ARG:HD3 | 1:A:117:THR:HB | 1.92 | 0.52 |
| 1:A:128:PRO:O | 1:A:129:TYR:HB2 | 2.10 | 0.52 |
| 1:A:41:VAL:HG13 | 1:A:42:HIS:N | 2.25 | 0.52 |
| 1:D:494:HIS:O | 1:D:498:LEU:HB2 | 2.09 | 0.52 |
| 1:D:538:GLU:HA | 4:9:349:LEU:CB | 2.40 | 0.52 |
| 1:D:642:LYS:HG2 | 4:9:21:PHE:C | 2.30 | 0.52 |
| 3:F:110:VAL:HG13 | 3:F:114:LEU:HD12 | 1.92 | 0.52 |
| 1:G:661:MET:O | 1:G:665:ARG:HG3 | 2.09 | 0.52 |
| 1:G:739:ASP:CB | 1:G:742:LYS:CB | 2.81 | 0.52 |
| 2:H:114:LYS:N | 2:H:146:GLY:O | 2.40 | 0.52 |
| 3:I:104:GLY:HA2 | 3:I:137:ILE:HD11 | 1.92 | 0.52 |
| 1:J:251:ARG:HB2 | 1:J:264:ASP:HB2 | 1.91 | 0.52 |
| 1:J:295:MLY:HG3 | 1:J:332:MET:HE2 | 1.91 | 0.52 |
| 1:J:494:HIS:O | 1:J:498:LEU:HB2 | 2.09 | 0.52 |
| 1:J:63:MLY:HG3 | 1:J:64:THR:H | 1.75 | 0.52 |
| 1:M:494:HIS:O | 1:M:498:LEU:HB2 | 2.09 | 0.52 |
| 1:M:636:LYS:HB2 | 4:Z:334:GLU:OE1 | 2.09 | 0.52 |
| 2:N:114:LYS:HA | 2:N:147:ASN:HD22 | 1.74 | 0.52 |
| 3:O:53:PRO:HB2 | 3:O:55:LYS:HG3 | 1.91 | 0.52 |
| 1:S:805:ALA:O | 1:S:809:ARG:CA | 2.57 | 0.52 |
| 1:S:795:ARG:HE | 3:U:116:GLU:HB3 | 1.74 | 0.52 |
| 4:Y:180:LEU:HD22 | 4:Y:267:ILE:HD11 | 1.92 | 0.52 |
| 4:1:180:LEU:HD22 | 4:1:267:ILE:HD11 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:185:LEU:HD23 | 4:8:306:TYR:OH | 2.09 | 0.52 |
| 1:A:636:LYS:HB2 | 4:8:334:GLU:OE1 | 2.08 | 0.52 |
| 1:A:277:PHE:CG | 1:A:278:GLN:N | 2.76 | 0.52 |
| 1:A:530:MET:HG2 | 4:8:354:GLN:HB2 | 0.57 | 0.52 |
| 1:A:538:GLU:HA | 4:8:349:LEU:CB | 2.39 | 0.52 |
| 1:A:817:GLN:NE2 | 2:B:127:ARG:HE | 2.06 | 0.52 |
| 1:D:156:PHE:HD1 | 1:D:195:TYR:CD1 | 2.27 | 0.52 |
| 1:D:491:PHE:HD1 | 1:D:671:PHE:CE2 | 2.27 | 0.52 |
| 2:E:129:THR:O | 2:E:133:ILE:HG13 | 2.09 | 0.52 |
| 1:G:277:PHE:CG | 1:G:278:GLN:N | 2.76 | 0.52 |
| 1:G:579:PHE:CD2 | 1:G:592:ILE:HD11 | 2.40 | 0.52 |
| 2:B:54:MET:C | 2:H:21:GLU:OE1 | 2.47 | 0.52 |
| 1:J:829:TRP:HZ2 | 2:K:83:MET:CE | 2.21 | 0.52 |
| 1:J:829:TRP:HZ3 | 2:K:84:PHE:CE1 | 2.23 | 0.52 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:CB | 2.40 | 0.52 |
| 1:M:782:MLY:O | 1:M:786:ILE:HG13 | 2.10 | 0.52 |
| 1:M:93:MET:CE | 1:M:764:MLY:CH1 | 2.87 | 0.52 |
| 2:N:137:TRP:CA | 2:N:145:ALA:CB | 2.82 | 0.52 |
| 1:S:63:MLY:HG3 | 1:S:64:THR:H | 1.75 | 0.52 |
| 1:S:831:TRP:NE1 | 2:T:67:MET:CG | 2.73 | 0.52 |
| 1:S:90:ASP:OD1 | 1:S:764:MLY:CH1 | 2.58 | 0.52 |
| 1:S:836:PHE:CD2 | 2:T:160:GLY:N | 2.76 | 0.52 |
| 3:U:110:VAL:HG13 | 3:U:114:LEU:HD12 | 1.92 | 0.52 |
| 1:M:408:VAL:CG1 | 4:Z:332:PRO:HB3 | 2.40 | 0.52 |
| 4:2:204:ALA:HB3 | 4:Z:287:ILE:HG22 | 1.91 | 0.52 |
| 4:3:180:LEU:HD22 | 4:3:267:ILE:HD11 | 1.92 | 0.52 |
| 4:8:285:CYS:O | 4:8:290:ARG:NH1 | 2.43 | 0.52 |
| 1:A:135:TYR:HD2 | 1:A:191:ARG:CD | 2.23 | 0.52 |
| 1:A:491:PHE:HD1 | 1:A:671:PHE:CE2 | 2.27 | 0.52 |
| 1:D:221:GLN:HB2 | 1:D:449:LEU:HD11 | 1.92 | 0.52 |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CD1 | 1.04 | 0.52 |
| 1:G:732:ILE:H | 1:G:733:PRO:HD2 | 1.74 | 0.52 |
| 1:G:796:GLY:N | 3:I:35:ARG:CZ | 2.73 | 0.52 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:HG | 1.81 | 0.52 |
| 1:M:836:PHE:HE1 | 2:N:158:THR:O | 1.93 | 0.52 |
| 1:S:197:ALA:O | 1:S:201:ALA:HB2 | 2.09 | 0.52 |
| 1:S:332:MET:O | 1:S:336:SER:OG | 2.27 | 0.52 |
| 2:T:129:THR:O | 2:T:133:ILE:HG13 | 2.09 | 0.52 |
| 3:U:104:GLY:HA2 | 3:U:137:ILE:HD11 | 1.92 | 0.52 |
| 1:S:552:ASN:H | 4:4:49:GLN:HB2 | 1.75 | 0.52 |
| 4:3:167:GLU:OE1 | 4:5:44:MET:HA | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:221:GLN:HB2 | 1:A:449:LEU:HD11 | 1.92 | 0.52 |
| 1:A:40:VAL:HG13 | 1:A:41:VAL:O | 2.10 | 0.52 |
| 1:A:404:PRO:HG3 | 1:A:417:GLU:HG3 | 1.91 | 0.52 |
| 1:D:109:ARG:HD3 | 1:D:117:THR:HB | 1.92 | 0.52 |
| 1:D:195:TYR:CE2 | 1:D:199:ILE:CD1 | 2.93 | 0.52 |
| 1:G:197:ALA:O | 1:G:201:ALA:HB2 | 2.09 | 0.52 |
| 1:G:494:HIS:O | 1:G:498:LEU:HB2 | 2.09 | 0.52 |
| 1:G:649:VAL:HA | 1:G:649:VAL:HG23 | 1.83 | 0.52 |
| 1:G:813:ILE:HG23 | 2:H:128:PHE:HZ | 1.71 | 0.52 |
| 2:H:114:LYS:HA | 2:H:147:ASN:HD22 | 1.75 | 0.52 |
| 3:I:49:ILE:CA | 3:I:52:ASN:ND2 | 2.53 | 0.52 |
| 1:J:128:PRO:O | 1:J:129:TYR:HB2 | 2.10 | 0.52 |
| 1:J:221:GLN:HB2 | 1:J:449:LEU:HD11 | 1.92 | 0.52 |
| 1:J:829:TRP:CZ2 | 2:K:83:MET:HE1 | 2.45 | 0.52 |
| 1:M:94:MET:C | 1:M:713:SER:HB3 | 2.31 | 0.52 |
| 1:S:218:LEU:CD2 | 1:S:222:ILE:CG1 | 2.86 | 0.52 |
| 1:S:221:GLN:HB2 | 1:S:449:LEU:HD11 | 1.92 | 0.52 |
| 4:V:285:CYS:O | 4:V:290:ARG:NH1 | 2.43 | 0.52 |
| 1:S:408:VAL:CG1 | 4:2:332:PRO:HB3 | 2.40 | 0.51 |
| 4:1:287:ILE:C | 4:3:203:THR:HG22 | 2.30 | 0.51 |
| 1:A:546:THR:CG2 | 1:A:548:THR:HB | 2.41 | 0.51 |
| 1:A:63:MLY:HG3 | 1:A:64:THR:H | 1.75 | 0.51 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:CD2 | 2.87 | 0.51 |
| 1:D:197:ALA:O | 1:D:201:ALA:HB2 | 2.10 | 0.51 |
| 1:D:725:ARG:O | 1:D:729:ALA:HA | 2.10 | 0.51 |
| 1:D:41:VAL:HG21 | 1:D:76:GLN:HG3 | 1.92 | 0.51 |
| 1:G:135:TYR:HD2 | 1:G:191:ARG:CD | 2.23 | 0.51 |
| 1:G:221:GLN:HB2 | 1:G:449:LEU:HD11 | 1.93 | 0.51 |
| 1:J:41:VAL:HG13 | 1:J:42:HIS:N | 2.25 | 0.51 |
| 1:J:798:LEU:HD22 | 3:L:118:MET:SD | 2.50 | 0.51 |
| 1:M:22:LYS:O | 1:M:26:GLU:N | 2.30 | 0.51 |
| 1:M:40:VAL:HG13 | 1:M:41:VAL:O | 2.10 | 0.51 |
| 1:M:592:ILE:O | 1:M:592:ILE:HG22 | 2.10 | 0.51 |
| 1:M:725:ARG:O | 1:M:729:ALA:HA | 2.10 | 0.51 |
| 1:M:798:LEU:CG | 3:O:126:LEU:HD11 | 2.39 | 0.51 |
| 1:S:40:VAL:HG13 | 1:S:41:VAL:O | 2.10 | 0.51 |
| 1:S:797:PHE:HE2 | 3:U:146:ILE:HD12 | 1.60 | 0.51 |
| 4:Y:285:CYS:O | 4:Y:290:ARG:NH1 | 2.43 | 0.51 |
| 1:A:212:GLY:O | 1:A:213:LYS:HB2 | 2.10 | 0.51 |
| 1:A:494:HIS:O | 1:A:498:LEU:HB2 | 2.09 | 0.51 |
| 1:A:831:TRP:CH2 | 2:B:34:ILE:CG2 | 2.81 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:546:THR:CG2 | 1:G:548:THR:HB | 2.41 | 0.51 |
| 1:J:248:MLY:N | 1:J:463:ASP:O | 2.44 | 0.51 |
| 1:J:538:GLU:HA | 4:W:349:LEU:CB | 2.40 | 0.51 |
| 1:J:642:LYS:HG2 | 4:W:21:PHE:C | 2.30 | 0.51 |
| 1:M:135:TYR:HD2 | 1:M:191:ARG:CD | 2.23 | 0.51 |
| 1:M:221:GLN:HB2 | 1:M:449:LEU:HD11 | 1.92 | 0.51 |
| 1:M:578:HIS:O | 1:M:579:PHE:HB3 | 2.11 | 0.51 |
| 1:M:732:ILE:H | 1:M:733:PRO:CD | 2.23 | 0.51 |
| 1:M:742:LYS:O | 1:M:745:GLU:HB2 | 2.10 | 0.51 |
| 3:O:100:GLY:O | 3:O:138:ASN:HA | 2.11 | 0.51 |
| 1:S:725:ARG:O | 1:S:729:ALA:HA | 2.10 | 0.51 |
| 1:A:555:TYR:N | 4:V:48:GLY:N | 2.58 | 0.51 |
| 1:M:553:MLY:HG3 | 4:2:44:MET:O | 2.07 | 0.51 |
| 4:6:285:CYS:O | 4:6:290:ARG:NH1 | 2.43 | 0.51 |
| 4:4:167:GLU:OE1 | 4:6:44:MET:HA | 2.10 | 0.51 |
| 1:A:195:TYR:CE2 | 1:A:199:ILE:CD1 | 2.93 | 0.51 |
| 1:A:499:GLU:OE1 | 1:A:766:PHE:CE2 | 2.60 | 0.51 |
| 1:A:592:ILE:O | 1:A:592:ILE:HG22 | 2.11 | 0.51 |
| 1:A:149:GLN:CG | 1:A:719:ASP:N | 2.73 | 0.51 |
| 1:D:793:ARG:CZ | 3:F:87:PHE:HE1 | 2.24 | 0.51 |
| 1:D:836:PHE:HB2 | 2:E:161:GLU:OE1 | 2.10 | 0.51 |
| 1:D:838:ILE:HD13 | 2:E:54:MET:CE | 2.40 | 0.51 |
| 3:F:104:GLY:HA2 | 3:F:137:ILE:HD11 | 1.92 | 0.51 |
| 1:G:491:PHE:HD1 | 1:G:671:PHE:CE2 | 2.27 | 0.51 |
| 1:G:559:LEU:C | 1:G:559:LEU:HD23 | 2.31 | 0.51 |
| 1:G:834:LEU:CD1 | 2:H:51:PHE:CD1 | 2.93 | 0.51 |
| 1:J:212:GLY:O | 1:J:213:LYS:HB2 | 2.10 | 0.51 |
| 1:J:232:PHE:CE1 | 1:J:287:ILE:HD13 | 2.44 | 0.51 |
| 1:J:40:VAL:HG13 | 1:J:41:VAL:O | 2.10 | 0.51 |
| 1:J:491:PHE:HD1 | 1:J:671:PHE:CE2 | 2.27 | 0.51 |
| 1:M:195:TYR:CE2 | 1:M:199:ILE:CD1 | 2.93 | 0.51 |
| 1:M:248:MLY:N | 1:M:463:ASP:O | 2.44 | 0.51 |
| 1:M:546:THR:CG2 | 1:M:548:THR:HB | 2.41 | 0.51 |
| 1:M:797:PHE:HD1 | 3:O:149:VAL:HG13 | 1.69 | 0.51 |
| 1:S:494:HIS:O | 1:S:498:LEU:HB2 | 2.09 | 0.51 |
| 1:S:538:GLU:HA | 4:2:349:LEU:CB | 2.40 | 0.51 |
| 1:S:733:PRO:O | 1:S:737:PHE:CE1 | 2.53 | 0.51 |
| 1:S:821:ARG:HH12 | 2:T:127:ARG:CZ | 2.23 | 0.51 |
| 1:S:795:ARG:CA | 3:U:118:MET:HE1 | 2.40 | 0.51 |
| 3:U:53:PRO:HB2 | 3:U:55:LYS:HG3 | 1.91 | 0.51 |
| 4:3:287:ILE:HG23 | 4:5:202:THR:CG2 | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:148:THR:OG1 | 4:3:45:VAL:HG23 | 2.09 | 0.51 |
| 4:4:285:CYS:O | 4:4:290:ARG:NH1 | 2.43 | 0.51 |
| 1:A:506:GLU:H | 1:A:761:GLY:HA2 | 1.74 | 0.51 |
| 1:D:530:MET:HG2 | 4:9:354:GLN:HB2 | 0.57 | 0.51 |
| 1:D:107:MLY:CB | 1:D:686:MET:HE2 | 2.38 | 0.51 |
| 1:D:739:ASP:CB | 1:D:742:LYS:CB | 2.81 | 0.51 |
| 2:E:112:ILE:HG23 | 2:E:147:ASN:HB3 | 1.93 | 0.51 |
| 1:G:220:ASP:O | 1:G:224:SER:N | 2.27 | 0.51 |
| 1:G:248:MLY:N | 1:G:463:ASP:O | 2.44 | 0.51 |
| 1:G:508:ILE:CD1 | 1:G:759:ALA:HB2 | 2.09 | 0.51 |
| 1:J:636:LYS:HB2 | 4:W:334:GLU:OE1 | 2.09 | 0.51 |
| 1:M:38:VAL:CG1 | 1:M:39:PHE:N | 2.74 | 0.51 |
| 1:M:559:LEU:C | 1:M:559:LEU:HD23 | 2.31 | 0.51 |
| 4:8:287:ILE:HG22 | 4:V:204:ALA:HB3 | 1.91 | 0.51 |
| 1:G:557:GLU:CB | 4:X:47:MET:C | 2.50 | 0.51 |
| 1:A:578:HIS:O | 1:A:579:PHE:HB3 | 2.11 | 0.51 |
| 2:B:129:THR:O | 2:B:133:ILE:HG13 | 2.10 | 0.51 |
| 1:A:836:PHE:CE1 | 2:B:160:GLY:N | 2.78 | 0.51 |
| 3:C:100:GLY:O | 3:C:138:ASN:HA | 2.11 | 0.51 |
| 1:D:232:PHE:CE1 | 1:D:287:ILE:HD13 | 2.45 | 0.51 |
| 1:D:742:LYS:O | 1:D:745:GLU:HB2 | 2.10 | 0.51 |
| 1:G:109:ARG:HD3 | 1:G:117:THR:HB | 1.92 | 0.51 |
| 1:G:538:GLU:HA | 4:V:349:LEU:CB | 2.40 | 0.51 |
| 1:J:217:THR:C | 1:J:221:GLN:NE2 | 2.62 | 0.51 |
| 1:J:83:PRO:C | 1:J:723:ARG:NH2 | 2.64 | 0.51 |
| 2:K:117:LEU:CG | 2:K:147:ASN:OD1 | 2.52 | 0.51 |
| 1:M:13:ALA:C | 1:M:15:PRO:HD2 | 2.31 | 0.51 |
| 1:M:197:ALA:O | 1:M:201:ALA:HB2 | 2.10 | 0.51 |
| 1:M:418:THR:O | 1:M:422:VAL:HG23 | 2.11 | 0.51 |
| 1:M:41:VAL:HG13 | 1:M:42:HIS:N | 2.25 | 0.51 |
| 3:O:104:GLY:HA2 | 3:O:137:ILE:HD11 | 1.92 | 0.51 |
| 1:S:418:THR:O | 1:S:422:VAL:HG23 | 2.11 | 0.51 |
| 1:S:95:THR:HB | 1:S:713:SER:HB3 | 1.92 | 0.51 |
| 1:S:732:ILE:HG23 | 1:S:747:LEU:CD1 | 1.05 | 0.51 |
| 4:3:287:ILE:CG2 | 4:5:202:THR:C | 2.65 | 0.51 |
| 1:A:13:ALA:C | 1:A:15:PRO:HD2 | 2.31 | 0.51 |
| 1:A:41:VAL:HG21 | 1:A:76:GLN:HG3 | 1.92 | 0.51 |
| 2:B:114:LYS:O | 2:B:147:ASN:ND2 | 2.42 | 0.51 |
| 1:D:218:LEU:N | 1:D:221:GLN:CG | 2.74 | 0.51 |
| 1:D:295:MLY:HE2 | 1:D:332:MET:HE1 | 1.91 | 0.51 |
| 1:D:640:LYS:C | 4:9:23:GLY:CA | 2.64 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:100:GLY:O | 3:F:138:ASN:HA | 2.11 | 0.51 |
| 1:G:13:ALA:C | 1:G:15:PRO:HD2 | 2.31 | 0.51 |
| 1:G:38:VAL:CG1 | 1:G:39:PHE:N | 2.74 | 0.51 |
| 1:G:411:GLU:H | 4:V:333:PRO:CG | 2.24 | 0.51 |
| 1:G:592:ILE:O | 1:G:592:ILE:HG22 | 2.11 | 0.51 |
| 1:G:795:ARG:CB | 3:I:35:ARG:NH1 | 2.67 | 0.51 |
| 1:G:817:GLN:CG | 2:H:128:PHE:CE1 | 2.93 | 0.51 |
| 3:I:110:VAL:HG13 | 3:I:114:LEU:HD12 | 1.91 | 0.51 |
| 1:J:13:ALA:C | 1:J:15:PRO:HD2 | 2.31 | 0.51 |
| 1:J:135:TYR:HD2 | 1:J:191:ARG:CD | 2.23 | 0.51 |
| 1:J:195:TYR:CE2 | 1:J:199:ILE:CD1 | 2.93 | 0.51 |
| 2:K:121:LEU:O | 2:K:128:PHE:CG | 2.61 | 0.51 |
| 1:M:212:GLY:O | 1:M:213:LYS:HB2 | 2.10 | 0.51 |
| 1:M:640:LYS:CA | 1:M:645:SER:OG | 2.58 | 0.51 |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:CD1 | 0.63 | 0.51 |
| 1:M:732:ILE:H | 1:M:733:PRO:HD2 | 1.74 | 0.51 |
| 1:M:41:VAL:HG21 | 1:M:76:GLN:HG3 | 1.93 | 0.51 |
| 2:N:129:THR:O | 2:N:133:ILE:HG13 | 2.09 | 0.51 |
| 1:S:128:PRO:O | 1:S:129:TYR:HB2 | 2.10 | 0.51 |
| 1:S:13:ALA:C | 1:S:15:PRO:HD2 | 2.31 | 0.51 |
| 1:S:38:VAL:CG1 | 1:S:39:PHE:N | 2.74 | 0.51 |
| 1:S:742:LYS:O | 1:S:745:GLU:HB2 | 2.10 | 0.51 |
| 4:3:324:THR:H | 4:5:244:ASP:HA | 1.75 | 0.51 |
| 1:A:400:ALA:HB1 | 1:A:606:THR:HG22 | 1.92 | 0.51 |
| 1:A:725:ARG:O | 1:A:729:ALA:HA | 2.10 | 0.51 |
| 1:D:13:ALA:C | 1:D:15:PRO:HD2 | 2.31 | 0.51 |
| 1:D:202:SER:HB2 | 1:D:207:LYS:NZ | 2.26 | 0.51 |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CD2 | 2.45 | 0.51 |
| 1:D:687:GLU:O | 1:D:691:VAL:HG23 | 2.11 | 0.51 |
| 1:G:195:TYR:CE2 | 1:G:199:ILE:CD1 | 2.93 | 0.51 |
| 1:G:418:THR:O | 1:G:422:VAL:HG23 | 2.11 | 0.51 |
| 1:J:687:GLU:O | 1:J:691:VAL:HG23 | 2.11 | 0.51 |
| 1:M:206:LYS:HD2 | 1:M:217:THR:CG2 | 2.17 | 0.51 |
| 1:M:755:HIS:HA | 1:M:758:TYR:HE1 | 1.64 | 0.51 |
| 1:M:84:MLY:HH23 | 1:M:719:ASP:HB3 | 1.89 | 0.51 |
| 1:S:218:LEU:N | 1:S:221:GLN:CG | 2.74 | 0.51 |
| 1:S:546:THR:CG2 | 1:S:548:THR:HB | 2.41 | 0.51 |
| 2:T:114:LYS:HA | 2:T:147:ASN:HD22 | 1.74 | 0.51 |
| 4:W:322:PRO:HB3 | 4:Y:246:GLN:HG2 | 1.92 | 0.51 |
| 1:A:631:GLU:C | 4:8:25:ASP:HB2 | 2.31 | 0.51 |
| 1:A:38:VAL:CG1 | 1:A:39:PHE:N | 2.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:114:LYS:HA | 2:B:147:ASN:HD22 | 1.75 | 0.51 |
| 1:D:278:GLN:HG3 | 1:D:318:GLY:H | 1.75 | 0.51 |
| 1:D:38:VAL:CG1 | 1:D:39:PHE:N | 2.74 | 0.51 |
| 1:D:538:GLU:OE1 | 4:9:355:MET:HE3 | 2.11 | 0.51 |
| 1:D:559:LEU:C | 1:D:559:LEU:HD23 | 2.31 | 0.51 |
| 1:D:578:HIS:O | 1:D:579:PHE:HB3 | 2.10 | 0.51 |
| 1:D:712:PRO:HG2 | 1:D:771:LEU:HD13 | 1.92 | 0.51 |
| 1:D:829:TRP:HZ3 | 2:E:84:PHE:CZ | 2.20 | 0.51 |
| 1:G:732:ILE:CG2 | 1:G:747:LEU:HD11 | 1.26 | 0.51 |
| 1:J:295:MLY:HE2 | 1:J:332:MET:HE1 | 1.91 | 0.51 |
| 1:J:796:GLY:HA2 | 3:L:35:ARG:NE | 2.24 | 0.51 |
| 1:J:798:LEU:CD2 | 3:L:118:MET:HB3 | 2.41 | 0.51 |
| 1:M:632:GLY:HA3 | 1:M:643:GLY:N | 2.17 | 0.51 |
| 1:S:169:ASP:N | 1:S:169:ASP:OD1 | 2.44 | 0.51 |
| 1:S:135:TYR:HD2 | 1:S:191:ARG:CD | 2.23 | 0.51 |
| 1:S:202:SER:HB2 | 1:S:207:LYS:NZ | 2.26 | 0.51 |
| 1:S:400:ALA:HB1 | 1:S:606:THR:HG22 | 1.93 | 0.51 |
| 1:S:120:GLY:O | 1:S:764:MLY:CH2 | 2.58 | 0.51 |
| 1:G:553:MLY:CB | 4:X:45:VAL:O | 2.57 | 0.51 |
| 1:D:408:VAL:CG1 | 4:9:332:PRO:HB3 | 2.41 | 0.51 |
| 1:A:202:SER:HB2 | 1:A:207:LYS:NZ | 2.26 | 0.51 |
| 1:A:248:MLY:N | 1:A:463:ASP:O | 2.44 | 0.51 |
| 1:A:267:THR:HG21 | 1:A:438:PHE:HE2 | 1.76 | 0.51 |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:HD11 | 1.85 | 0.51 |
| 1:D:212:GLY:O | 1:D:213:LYS:HB2 | 2.11 | 0.51 |
| 1:D:237:THR:O | 1:D:240:ASN:O | 2.29 | 0.51 |
| 1:D:248:MLY:N | 1:D:463:ASP:O | 2.44 | 0.51 |
| 1:D:411:GLU:H | 4:9:333:PRO:CG | 2.24 | 0.51 |
| 1:D:732:ILE:HD11 | 1:D:782:MLY:CH1 | 2.34 | 0.51 |
| 1:G:218:LEU:CD2 | 1:G:222:ILE:CG1 | 2.86 | 0.51 |
| 1:G:795:ARG:CG | 3:I:118:MET:HE2 | 2.07 | 0.51 |
| 3:I:100:GLY:O | 3:I:138:ASN:HA | 2.11 | 0.51 |
| 1:J:169:ASP:N | 1:J:169:ASP:OD1 | 2.44 | 0.51 |
| 1:J:237:THR:O | 1:J:240:ASN:O | 2.29 | 0.51 |
| 1:J:400:ALA:HB1 | 1:J:606:THR:HG22 | 1.93 | 0.51 |
| 1:J:635:GLY:HA3 | 4:W:334:GLU:CG | 2.30 | 0.51 |
| 1:J:795:ARG:CG | 3:L:116:GLU:OE2 | 2.59 | 0.51 |
| 1:J:795:ARG:HD2 | 3:L:43:ASN:N | 2.26 | 0.51 |
| 2:K:114:LYS:HA | 2:K:147:ASN:HD22 | 1.74 | 0.51 |
| 1:J:813:ILE:HG22 | 2:K:128:PHE:HE1 | 1.73 | 0.51 |
| 1:M:128:PRO:O | 1:M:129:TYR:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:202:SER:HB2 | 1:M:207:LYS:NZ | 2.26 | 0.51 |
| 1:S:237:THR:O | 1:S:240:ASN:O | 2.29 | 0.51 |
| 1:S:248:MLY:N | 1:S:463:ASP:O | 2.44 | 0.51 |
| 1:S:311:ASP:HB2 | 1:S:312:TYR:CE1 | 2.46 | 0.51 |
| 1:S:267:THR:HG21 | 1:S:438:PHE:HE2 | 1.76 | 0.51 |
| 1:S:592:ILE:HG22 | 1:S:592:ILE:O | 2.11 | 0.51 |
| 1:S:675:ILE:CG2 | 1:S:676:ILE:N | 2.74 | 0.51 |
| 1:S:753:VAL:HG11 | 1:S:779:ARG:NH1 | 2.24 | 0.51 |
| 1:S:819:ASN:OD1 | 2:T:90:GLY:O | 2.28 | 0.51 |
| 3:U:100:GLY:O | 3:U:138:ASN:HA | 2.11 | 0.51 |
| 1:J:631:GLU:C | 4:W:25:ASP:HB2 | 2.31 | 0.51 |
| 1:M:631:GLU:C | 4:Z:25:ASP:HB2 | 2.32 | 0.51 |
| 1:D:410:ASN:CG | 4:9:334:GLU:C | 2.65 | 0.51 |
| 1:A:311:ASP:HB2 | 1:A:312:TYR:CE1 | 2.46 | 0.51 |
| 1:A:559:LEU:HD23 | 1:A:559:LEU:C | 2.31 | 0.51 |
| 1:A:632:GLY:HA3 | 1:A:643:GLY:N | 2.17 | 0.51 |
| 1:D:640:LYS:CA | 1:D:645:SER:OG | 2.58 | 0.51 |
| 1:G:41:VAL:HG13 | 1:G:42:HIS:N | 2.25 | 0.51 |
| 1:G:640:LYS:CA | 1:G:645:SER:OG | 2.59 | 0.51 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:CD2 | 2.87 | 0.51 |
| 1:G:675:ILE:CG2 | 1:G:676:ILE:N | 2.74 | 0.51 |
| 1:G:742:LYS:O | 1:G:745:GLU:HB2 | 2.10 | 0.51 |
| 1:J:278:GLN:HG3 | 1:J:318:GLY:H | 1.75 | 0.51 |
| 1:J:84:MLY:HH23 | 1:J:719:ASP:O | 1.99 | 0.51 |
| 1:J:725:ARG:O | 1:J:729:ALA:HA | 2.10 | 0.51 |
| 1:J:792:ALA:CB | 3:L:42:THR:CA | 2.89 | 0.51 |
| 2:K:117:LEU:HG | 2:K:147:ASN:HB3 | 1.93 | 0.51 |
| 1:M:218:LEU:N | 1:M:221:GLN:CG | 2.74 | 0.51 |
| 3:O:110:VAL:HG13 | 3:O:114:LEU:HD12 | 1.92 | 0.51 |
| 1:S:41:VAL:HG13 | 1:S:42:HIS:N | 2.25 | 0.51 |
| 1:S:84:MLY:CD | 1:S:723:ARG:HD2 | 2.39 | 0.51 |
| 2:T:117:LEU:HG | 2:T:147:ASN:HB3 | 1.93 | 0.51 |
| 1:J:408:VAL:CG1 | 4:W:332:PRO:HB3 | 2.40 | 0.51 |
| 1:A:411:GLU:H | 4:8:333:PRO:CG | 2.24 | 0.50 |
| 1:A:640:LYS:CA | 1:A:645:SER:OG | 2.58 | 0.50 |
| 1:A:709:LYS:C | 1:A:710:GLY:CA | 2.64 | 0.50 |
| 1:D:135:TYR:HD2 | 1:D:191:ARG:CD | 2.23 | 0.50 |
| 1:D:311:ASP:HB2 | 1:D:312:TYR:CE1 | 2.46 | 0.50 |
| 1:D:631:GLU:C | 4:9:25:ASP:HB2 | 2.31 | 0.50 |
| 1:D:732:ILE:O | 1:D:736:GLN:HG3 | 2.11 | 0.50 |
| 1:G:202:SER:HB2 | 1:G:207:LYS:NZ | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:311:ASP:HB2 | 1:G:312:TYR:CE1 | 2.46 | 0.50 |
| 1:J:202:SER:HB2 | 1:J:207:LYS:NZ | 2.26 | 0.50 |
| 1:J:418:THR:O | 1:J:422:VAL:HG23 | 2.11 | 0.50 |
| 1:J:646:PHE:HE2 | 1:J:652:LEU:CG | 2.25 | 0.50 |
| 1:J:93:MET:HA | 1:J:714:ARG:H | 1.77 | 0.50 |
| 1:M:237:THR:O | 1:M:240:ASN:O | 2.29 | 0.50 |
| 1:M:311:ASP:HB2 | 1:M:312:TYR:CE1 | 2.46 | 0.50 |
| 1:M:400:ALA:HB1 | 1:M:606:THR:HG22 | 1.93 | 0.50 |
| 1:M:675:ILE:CG2 | 1:M:676:ILE:N | 2.74 | 0.50 |
| 1:S:291:ILE:HA | 1:S:331:LEU:CD1 | 2.39 | 0.50 |
| 1:S:470:PHE:O | 1:S:473:ASN:ND2 | 2.40 | 0.50 |
| 1:S:505:MLY:NZ | 1:S:762:HIS:CD2 | 2.79 | 0.50 |
| 1:S:642:LYS:HG2 | 4:2:21:PHE:C | 2.30 | 0.50 |
| 1:S:640:LYS:CA | 1:S:645:SER:OG | 2.58 | 0.50 |
| 1:J:411:GLU:H | 4:W:333:PRO:CG | 2.24 | 0.50 |
| 1:S:546:THR:CB | 4:4:46:GLY:C | 2.80 | 0.50 |
| 1:A:197:ALA:O | 1:A:201:ALA:HB2 | 2.10 | 0.50 |
| 1:A:742:LYS:O | 1:A:745:GLU:HB2 | 2.11 | 0.50 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CD1 | 1.04 | 0.50 |
| 1:D:295:MLY:HG3 | 1:D:332:MET:HE2 | 1.92 | 0.50 |
| 2:E:114:LYS:N | 2:E:146:GLY:O | 2.40 | 0.50 |
| 1:G:128:PRO:O | 1:G:129:TYR:HB2 | 2.09 | 0.50 |
| 1:G:212:GLY:O | 1:G:213:LYS:HB2 | 2.11 | 0.50 |
| 1:G:400:ALA:HB1 | 1:G:606:THR:HG22 | 1.93 | 0.50 |
| 1:G:829:TRP:CH2 | 2:H:83:MET:HE3 | 2.46 | 0.50 |
| 1:G:797:PHE:CD2 | 3:I:126:LEU:CD2 | 2.84 | 0.50 |
| 1:J:553:MLY:O | 4:Y:46:GLY:HA3 | 2.11 | 0.50 |
| 1:J:592:ILE:HG22 | 1:J:592:ILE:O | 2.10 | 0.50 |
| 1:M:795:ARG:CB | 3:O:35:ARG:NH1 | 2.73 | 0.50 |
| 1:S:109:ARG:HD3 | 1:S:117:THR:HB | 1.92 | 0.50 |
| 1:S:214:MET:HA | 1:S:340:ILE:CD1 | 2.41 | 0.50 |
| 1:S:646:PHE:HE2 | 1:S:652:LEU:CG | 2.25 | 0.50 |
| 1:S:84:MLY:HH21 | 1:S:724:TYR:CE2 | 2.46 | 0.50 |
| 1:S:796:GLY:HA2 | 3:U:35:ARG:CG | 2.35 | 0.50 |
| 3:U:46:ILE:O | 3:U:50:LEU:CG | 2.47 | 0.50 |
| 1:J:642:LYS:CG | 4:W:22:ALA:HA | 2.37 | 0.50 |
| 4:2:287:ILE:CB | 4:4:203:THR:CB | 2.87 | 0.50 |
| 1:D:291:ILE:HA | 1:D:331:LEU:CD1 | 2.39 | 0.50 |
| 1:D:215:GLN:CA | 1:D:340:ILE:CG2 | 2.63 | 0.50 |
| 1:D:429:LEU:O | 1:D:433:VAL:HG23 | 2.12 | 0.50 |
| 1:D:546:THR:CG2 | 1:D:548:THR:HB | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:646:PHE:HE2 | 1:D:652:LEU:CG | 2.25 | 0.50 |
| 1:D:732:ILE:H | 1:D:733:PRO:CD | 2.22 | 0.50 |
| 1:D:795:ARG:HD2 | 3:F:43:ASN:CG | 2.32 | 0.50 |
| 1:D:800:ARG:HD2 | 3:F:149:VAL:C | 2.30 | 0.50 |
| 1:G:237:THR:O | 1:G:240:ASN:O | 2.29 | 0.50 |
| 1:G:267:THR:HG21 | 1:G:438:PHE:HE2 | 1.76 | 0.50 |
| 1:G:278:GLN:HG3 | 1:G:318:GLY:H | 1.75 | 0.50 |
| 1:G:429:LEU:O | 1:G:433:VAL:HG23 | 2.12 | 0.50 |
| 1:G:631:GLU:C | 4:V:25:ASP:HB2 | 2.31 | 0.50 |
| 1:G:725:ARG:O | 1:G:729:ALA:HA | 2.10 | 0.50 |
| 1:J:218:LEU:N | 1:J:221:GLN:CG | 2.74 | 0.50 |
| 1:J:470:PHE:O | 1:J:473:ASN:ND2 | 2.40 | 0.50 |
| 1:J:559:LEU:HD23 | 1:J:559:LEU:C | 2.31 | 0.50 |
| 1:J:578:HIS:O | 1:J:579:PHE:HB3 | 2.11 | 0.50 |
| 1:J:829:TRP:CZ3 | 2:K:87:LYS:CE | 2.81 | 0.50 |
| 1:M:429:LEU:O | 1:M:433:VAL:HG23 | 2.12 | 0.50 |
| 1:M:470:PHE:O | 1:M:473:ASN:ND2 | 2.40 | 0.50 |
| 1:M:646:PHE:HE2 | 1:M:652:LEU:CG | 2.25 | 0.50 |
| 1:M:831:TRP:HE1 | 2:N:67:MET:CG | 2.23 | 0.50 |
| 2:N:112:ILE:HG23 | 2:N:147:ASN:HB3 | 1.93 | 0.50 |
| 1:S:530:MET:CE | 4:2:354:GLN:HG3 | 2.35 | 0.50 |
| 1:S:559:LEU:HD23 | 1:S:559:LEU:C | 2.31 | 0.50 |
| 1:S:687:GLU:O | 1:S:691:VAL:HG23 | 2.11 | 0.50 |
| 1:S:93:MET:HG2 | 1:S:715:VAL:HA | 1.90 | 0.50 |
| 2:T:121:LEU:HA | 2:T:128:PHE:CD2 | 2.46 | 0.50 |
| 1:G:408:VAL:CG1 | 4:V:332:PRO:HB3 | 2.41 | 0.50 |
| 4:1:287:ILE:HG13 | 4:3:202:THR:CB | 2.42 | 0.50 |
| 1:S:642:LYS:HB2 | 4:2:24:ASP:O | 1.89 | 0.50 |
| 1:D:642:LYS:CG | 4:9:22:ALA:HA | 2.37 | 0.50 |
| 1:A:418:THR:O | 1:A:422:VAL:HG23 | 2.11 | 0.50 |
| 1:A:629:GLU:CB | 1:A:645:SER:N | 2.74 | 0.50 |
| 1:A:675:ILE:CG2 | 1:A:676:ILE:N | 2.74 | 0.50 |
| 1:A:795:ARG:HD3 | 3:C:35:ARG:HH22 | 1.76 | 0.50 |
| 1:D:169:ASP:OD1 | 1:D:169:ASP:N | 2.44 | 0.50 |
| 1:D:40:VAL:HG13 | 1:D:41:VAL:O | 2.10 | 0.50 |
| 1:D:635:GLY:HA3 | 4:9:334:GLU:CG | 2.30 | 0.50 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:HG12 | 2.45 | 0.50 |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:CG1 | 2.29 | 0.50 |
| 1:G:41:VAL:HG21 | 1:G:76:GLN:HG3 | 1.92 | 0.50 |
| 1:J:154:HIS:CD2 | 1:J:155:ILE:H | 2.30 | 0.50 |
| 1:M:733:PRO:CA | 1:M:737:PHE:CE1 | 2.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:829:TRP:HZ3 | 2:N:84:PHE:CE2 | 2.30 | 0.50 |
| 1:M:836:PHE:CE1 | 2:N:160:GLY:N | 2.75 | 0.50 |
| 1:S:195:TYR:CE2 | 1:S:199:ILE:CD1 | 2.93 | 0.50 |
| 4:9:288:ASP:CA | 4:W:204:ALA:HB2 | 2.31 | 0.50 |
| 1:A:817:GLN:NE2 | 2:B:127:ARG:HG3 | 2.08 | 0.50 |
| 1:D:418:THR:CB | 1:D:421:GLU:HG3 | 2.37 | 0.50 |
| 1:D:795:ARG:HG2 | 3:F:118:MET:HE1 | 0.72 | 0.50 |
| 1:J:109:ARG:HD3 | 1:J:117:THR:HB | 1.92 | 0.50 |
| 1:J:346:ASP:O | 1:J:349:THR:HB | 2.11 | 0.50 |
| 1:J:640:LYS:CA | 1:J:645:SER:OG | 2.58 | 0.50 |
| 1:J:733:PRO:CA | 1:J:737:PHE:CE1 | 2.95 | 0.50 |
| 1:J:742:LYS:O | 1:J:745:GLU:HB2 | 2.10 | 0.50 |
| 1:J:797:PHE:HE2 | 3:L:126:LEU:CG | 2.24 | 0.50 |
| 1:M:642:LYS:HG2 | 4:Z:21:PHE:C | 2.29 | 0.50 |
| 1:M:732:ILE:O | 1:M:736:GLN:HG3 | 2.12 | 0.50 |
| 2:N:121:LEU:O | 2:N:128:PHE:CG | 2.61 | 0.50 |
| 1:S:578:HIS:O | 1:S:579:PHE:HB3 | 2.11 | 0.50 |
| 1:S:732:ILE:HG21 | 1:S:747:LEU:CD1 | 0.63 | 0.50 |
| 1:S:798:LEU:CD1 | 3:U:126:LEU:HD22 | 2.29 | 0.50 |
| 1:D:539:GLU:OE2 | 4:W:45:VAL:C | 2.47 | 0.50 |
| 1:A:218:LEU:N | 1:A:221:GLN:CG | 2.74 | 0.50 |
| 1:A:278:GLN:HG3 | 1:A:318:GLY:H | 1.75 | 0.50 |
| 1:A:346:ASP:O | 1:A:349:THR:HB | 2.11 | 0.50 |
| 1:A:715:VAL:O | 1:A:764:MLY:HB3 | 2.12 | 0.50 |
| 1:D:418:THR:O | 1:D:422:VAL:HG23 | 2.11 | 0.50 |
| 1:D:629:GLU:CB | 1:D:645:SER:N | 2.74 | 0.50 |
| 1:D:712:PRO:HB2 | 1:D:771:LEU:CG | 2.42 | 0.50 |
| 1:D:725:ARG:CA | 1:D:782:MLY:CH2 | 2.89 | 0.50 |
| 1:G:169:ASP:N | 1:G:169:ASP:OD1 | 2.44 | 0.50 |
| 1:G:471:ASP:HB3 | 1:G:573:GLY:O | 2.12 | 0.50 |
| 1:G:578:HIS:O | 1:G:579:PHE:HB3 | 2.10 | 0.50 |
| 1:J:311:ASP:HB2 | 1:J:312:TYR:CE1 | 2.46 | 0.50 |
| 1:J:41:VAL:HG21 | 1:J:76:GLN:HG3 | 1.93 | 0.50 |
| 1:J:800:ARG:HG2 | 3:L:149:VAL:HG22 | 1.93 | 0.50 |
| 1:M:214:MET:HA | 1:M:340:ILE:CD1 | 2.41 | 0.50 |
| 1:A:93:MET:C | 1:A:713:SER:HB3 | 2.32 | 0.50 |
| 1:A:732:ILE:O | 1:A:736:GLN:HG3 | 2.12 | 0.50 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:OE1 | 2.37 | 0.50 |
| 1:D:346:ASP:O | 1:D:349:THR:HB | 2.12 | 0.50 |
| 1:G:553:MLY:O | 4:X:46:GLY:HA3 | 2.12 | 0.50 |
| 1:J:538:GLU:OE1 | 4:W:351:THR:HB | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:546:THR:CG2 | 1:J:548:THR:HB | 2.41 | 0.50 |
| 1:J:715:VAL:O | 1:J:764:MLY:HB3 | 2.12 | 0.50 |
| 1:J:757:GLN:CA | 1:J:776:GLU:CB | 2.90 | 0.50 |
| 1:M:346:ASP:O | 1:M:349:THR:HB | 2.11 | 0.50 |
| 1:M:687:GLU:O | 1:M:691:VAL:HG23 | 2.11 | 0.50 |
| 1:M:782:MLY:O | 1:M:786:ILE:CG1 | 2.60 | 0.50 |
| 1:S:168:THR:HG22 | 1:S:169:ASP:OD1 | 2.12 | 0.50 |
| 1:S:220:ASP:O | 1:S:224:SER:N | 2.27 | 0.50 |
| 1:S:732:ILE:O | 1:S:736:GLN:HG3 | 2.12 | 0.50 |
| 1:M:411:GLU:H | 4:Z:333:PRO:CG | 2.24 | 0.50 |
| 1:D:642:LYS:CA | 4:9:22:ALA:C | 2.71 | 0.50 |
| 1:D:538:GLU:OE1 | 4:9:351:THR:HB | 2.12 | 0.50 |
| 1:A:289:TYR:OH | 1:A:315:VAL:O | 2.27 | 0.50 |
| 1:A:409:GLY:N | 1:A:636:LYS:CD | 2.70 | 0.50 |
| 1:A:687:GLU:O | 1:A:691:VAL:HG23 | 2.11 | 0.50 |
| 1:D:154:HIS:CD2 | 1:D:155:ILE:H | 2.30 | 0.50 |
| 1:J:792:ALA:CA | 3:L:42:THR:CG2 | 2.60 | 0.50 |
| 1:J:839:MLY:N | 1:J:840:PRO:CD | 2.75 | 0.50 |
| 1:J:819:ASN:CB | 2:K:90:GLY:O | 2.60 | 0.50 |
| 3:L:100:GLY:O | 3:L:138:ASN:HA | 2.10 | 0.50 |
| 1:M:128:PRO:O | 1:M:683:PRO:HB3 | 2.12 | 0.50 |
| 1:M:267:THR:HG21 | 1:M:438:PHE:HE2 | 1.76 | 0.50 |
| 1:S:128:PRO:O | 1:S:683:PRO:HB3 | 2.12 | 0.50 |
| 1:S:212:GLY:O | 1:S:213:LYS:HB2 | 2.11 | 0.50 |
| 1:S:346:ASP:O | 1:S:349:THR:HB | 2.11 | 0.50 |
| 1:S:471:ASP:HB3 | 1:S:573:GLY:O | 2.12 | 0.50 |
| 1:S:733:PRO:CA | 1:S:737:PHE:CE1 | 2.95 | 0.50 |
| 4:2:318:THR:HA | 4:2:327:ILE:HG12 | 1.94 | 0.50 |
| 4:4:324:THR:H | 4:6:244:ASP:HA | 1.75 | 0.50 |
| 4:7:70:PRO:HG3 | 4:7:81:ASP:HB3 | 1.94 | 0.50 |
| 1:A:214:MET:HA | 1:A:340:ILE:CD1 | 2.41 | 0.50 |
| 1:A:217:THR:C | 1:A:221:GLN:NE2 | 2.62 | 0.50 |
| 1:D:206:LYS:HD2 | 1:D:217:THR:CG2 | 2.17 | 0.50 |
| 1:D:292:MET:HE1 | 1:D:309:PRO:HD3 | 1.94 | 0.50 |
| 1:D:471:ASP:HB3 | 1:D:573:GLY:O | 2.12 | 0.50 |
| 1:D:400:ALA:HB1 | 1:D:606:THR:HG22 | 1.92 | 0.50 |
| 1:D:649:VAL:HA | 1:D:649:VAL:HG23 | 1.82 | 0.50 |
| 1:D:95:THR:CB | 1:D:772:LEU:HB2 | 2.42 | 0.50 |
| 1:D:732:ILE:HD12 | 1:D:782:MLY:CH2 | 2.39 | 0.50 |
| 1:G:154:HIS:CD2 | 1:G:155:ILE:H | 2.30 | 0.50 |
| 1:G:218:LEU:N | 1:G:221:GLN:CG | 2.74 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:538:GLU:OE1 | 4:V:351:THR:HB | 2.12 | 0.50 |
| 1:G:715:VAL:HG12 | 1:G:716:LEU:O | 2.12 | 0.50 |
| 1:G:733:PRO:CA | 1:G:737:PHE:CE1 | 2.95 | 0.50 |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:HB3 | 1.94 | 0.50 |
| 1:J:595:TRP:CD1 | 1:J:595:TRP:N | 2.80 | 0.50 |
| 1:J:601:ASP:N | 1:J:602:PRO:CD | 2.75 | 0.50 |
| 1:M:291:ILE:HA | 1:M:331:LEU:CD1 | 2.39 | 0.50 |
| 1:M:409:GLY:N | 1:M:636:LYS:CD | 2.70 | 0.50 |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:CD1 | 1.05 | 0.50 |
| 2:N:121:LEU:HA | 2:N:128:PHE:CD2 | 2.46 | 0.50 |
| 2:T:114:LYS:N | 2:T:146:GLY:O | 2.40 | 0.50 |
| 1:S:803:TYR:CD2 | 3:U:17:PHE:CZ | 2.99 | 0.50 |
| 4:X:318:THR:HA | 4:X:327:ILE:HG12 | 1.94 | 0.50 |
| 4:Y:253:GLU:HA | 4:Y:256:ARG:CG | 2.42 | 0.50 |
| 4:X:324:THR:HG21 | 4:Z:247:VAL:HG23 | 1.89 | 0.50 |
| 1:S:411:GLU:H | 4:2:333:PRO:CG | 2.24 | 0.49 |
| 4:6:70:PRO:HG3 | 4:6:81:ASP:HB3 | 1.94 | 0.49 |
| 1:A:154:HIS:CD2 | 1:A:155:ILE:H | 2.30 | 0.49 |
| 1:A:169:ASP:OD1 | 1:A:169:ASP:N | 2.44 | 0.49 |
| 1:A:471:ASP:HB3 | 1:A:573:GLY:O | 2.12 | 0.49 |
| 1:A:498:LEU:HD21 | 1:A:764:MLY:CH2 | 2.40 | 0.49 |
| 1:A:547:ASP:O | 1:A:550:PHE:HB3 | 2.12 | 0.49 |
| 1:A:797:PHE:CE1 | 3:C:149:VAL:HG12 | 2.46 | 0.49 |
| 1:A:815:CYS:SG | 2:B:92:ASP:HB2 | 2.52 | 0.49 |
| 1:D:168:THR:HG22 | 1:D:169:ASP:OD1 | 2.12 | 0.49 |
| 1:D:470:PHE:O | 1:D:473:ASN:ND2 | 2.40 | 0.49 |
| 1:D:601:ASP:N | 1:D:602:PRO:CD | 2.75 | 0.49 |
| 1:D:128:PRO:O | 1:D:683:PRO:HB3 | 2.12 | 0.49 |
| 1:D:739:ASP:OD1 | 1:D:740:SER:N | 2.45 | 0.49 |
| 1:G:510:TRP:CH2 | 1:G:768:MLY:HH11 | 2.47 | 0.49 |
| 1:G:601:ASP:N | 1:G:602:PRO:CD | 2.75 | 0.49 |
| 1:G:732:ILE:O | 1:G:736:GLN:HG3 | 2.12 | 0.49 |
| 1:G:733:PRO:O | 1:G:737:PHE:CE1 | 2.53 | 0.49 |
| 1:J:291:ILE:HA | 1:J:331:LEU:CD1 | 2.39 | 0.49 |
| 1:J:38:VAL:CG1 | 1:J:39:PHE:N | 2.74 | 0.49 |
| 1:J:418:THR:CB | 1:J:421:GLU:HG3 | 2.37 | 0.49 |
| 1:J:429:LEU:O | 1:J:433:VAL:HG23 | 2.12 | 0.49 |
| 1:J:97:LEU:HD23 | 1:J:712:PRO:CB | 2.38 | 0.49 |
| 2:K:112:ILE:HG23 | 2:K:147:ASN:HB3 | 1.93 | 0.49 |
| 1:M:154:HIS:CD2 | 1:M:155:ILE:H | 2.30 | 0.49 |
| 1:M:168:THR:HG22 | 1:M:169:ASP:OD1 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:192:VAL:O | 1:M:195:TYR:HB3 | 2.12 | 0.49 |
| 1:M:642:LYS:HA | 4:Z:22:ALA:C | 2.33 | 0.49 |
| 1:M:715:VAL:O | 1:M:764:MLY:HB3 | 2.12 | 0.49 |
| 1:M:715:VAL:HG12 | 1:M:716:LEU:O | 2.12 | 0.49 |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:HD12 | 0.95 | 0.49 |
| 1:M:831:TRP:CZ3 | 2:N:34:ILE:HD13 | 2.40 | 0.49 |
| 1:S:547:ASP:O | 1:S:550:PHE:HB3 | 2.12 | 0.49 |
| 1:S:642:LYS:HA | 4:2:22:ALA:C | 2.33 | 0.49 |
| 1:S:753:VAL:N | 1:S:779:ARG:NH2 | 2.60 | 0.49 |
| 2:T:121:LEU:CA | 2:T:128:PHE:CG | 2.89 | 0.49 |
| 4:Y:318:THR:HA | 4:Y:327:ILE:HG12 | 1.94 | 0.49 |
| 1:S:631:GLU:C | 4:2:25:ASP:HB2 | 2.32 | 0.49 |
| 4:7:318:THR:HA | 4:7:327:ILE:HG12 | 1.94 | 0.49 |
| 4:9:70:PRO:HG3 | 4:9:81:ASP:HB3 | 1.94 | 0.49 |
| 1:A:51:THR:C | 1:A:62:VAL:HG13 | 2.32 | 0.49 |
| 1:A:768:MLY:CB | 1:A:771:LEU:HD13 | 2.42 | 0.49 |
| 1:D:292:MET:CE | 1:D:309:PRO:HA | 2.39 | 0.49 |
| 1:D:481:ASN:N | 1:D:481:ASN:ND2 | 2.51 | 0.49 |
| 1:D:733:PRO:CA | 1:D:737:PHE:CE1 | 2.94 | 0.49 |
| 1:D:793:ARG:CZ | 3:F:87:PHE:CE1 | 2.95 | 0.49 |
| 1:G:103:LEU:HD12 | 1:G:103:LEU:C | 2.33 | 0.49 |
| 1:G:543:PRO:CD | 4:V:146:GLY:O | 2.61 | 0.49 |
| 2:H:121:LEU:HA | 2:H:128:PHE:CD2 | 2.47 | 0.49 |
| 1:G:789:ALA:HB1 | 3:I:81:GLN:CD | 2.33 | 0.49 |
| 1:J:176:LEU:CD1 | 1:J:176:LEU:N | 2.75 | 0.49 |
| 1:J:543:PRO:CD | 4:W:146:GLY:O | 2.61 | 0.49 |
| 1:M:733:PRO:O | 1:M:737:PHE:CE1 | 2.53 | 0.49 |
| 2:N:93:PRO:O | 2:N:97:ILE:HG13 | 2.12 | 0.49 |
| 1:S:292:MET:CE | 1:S:309:PRO:HA | 2.40 | 0.49 |
| 1:S:739:ASP:OD1 | 1:S:740:SER:N | 2.45 | 0.49 |
| 1:S:41:VAL:HG21 | 1:S:76:GLN:HG3 | 1.93 | 0.49 |
| 2:T:112:ILE:HG23 | 2:T:147:ASN:HB3 | 1.92 | 0.49 |
| 4:5:70:PRO:HG3 | 4:5:81:ASP:HB3 | 1.94 | 0.49 |
| 1:A:538:GLU:OE1 | 4:8:351:THR:HB | 2.12 | 0.49 |
| 4:8:70:PRO:HG3 | 4:8:81:ASP:HB3 | 1.94 | 0.49 |
| 1:D:543:PRO:CD | 4:9:146:GLY:O | 2.61 | 0.49 |
| 1:A:237:THR:O | 1:A:240:ASN:O | 2.29 | 0.49 |
| 1:A:429:LEU:O | 1:A:433:VAL:HG23 | 2.11 | 0.49 |
| 1:A:715:VAL:HG12 | 1:A:716:LEU:O | 2.13 | 0.49 |
| 2:B:140:PHE:HB3 | 2:B:144:VAL:HG12 | 1.94 | 0.49 |
| 1:D:547:ASP:O | 1:D:550:PHE:HB3 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:592:ILE:O | 1:D:592:ILE:HG22 | 2.11 | 0.49 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:HG23 | 2.47 | 0.49 |
| 1:D:839:MLY:HB2 | 1:D:840:PRO:HD3 | 1.95 | 0.49 |
| 1:G:470:PHE:O | 1:G:473:ASN:ND2 | 2.40 | 0.49 |
| 1:G:687:GLU:O | 1:G:691:VAL:HG23 | 2.11 | 0.49 |
| 1:G:792:ALA:HB3 | 3:I:42:THR:CG2 | 2.16 | 0.49 |
| 1:G:820:VAL:CG1 | 2:H:136:MET:CE | 2.87 | 0.49 |
| 2:H:117:LEU:HG | 2:H:147:ASN:HB3 | 1.93 | 0.49 |
| 2:H:93:PRO:O | 2:H:97:ILE:HG13 | 2.12 | 0.49 |
| 1:G:796:GLY:N | 3:I:35:ARG:NH2 | 2.60 | 0.49 |
| 1:J:41:VAL:CG1 | 1:J:42:HIS:N | 2.75 | 0.49 |
| 1:J:128:PRO:O | 1:J:683:PRO:HB3 | 2.12 | 0.49 |
| 1:J:94:MET:C | 1:J:713:SER:CB | 2.61 | 0.49 |
| 1:M:543:PRO:CD | 4:Z:146:GLY:O | 2.61 | 0.49 |
| 1:M:629:GLU:CB | 1:M:645:SER:N | 2.73 | 0.49 |
| 1:S:192:VAL:O | 1:S:195:TYR:HB3 | 2.13 | 0.49 |
| 1:S:595:TRP:N | 1:S:595:TRP:CD1 | 2.80 | 0.49 |
| 1:S:64:THR:CG2 | 1:S:65:GLU:N | 2.75 | 0.49 |
| 1:S:839:MLY:N | 1:S:840:PRO:CD | 2.75 | 0.49 |
| 1:S:795:ARG:NH2 | 3:U:116:GLU:CA | 2.56 | 0.49 |
| 4:V:318:THR:HA | 4:V:327:ILE:HG12 | 1.94 | 0.49 |
| 4:V:70:PRO:HG3 | 4:V:81:ASP:HB3 | 1.94 | 0.49 |
| 4:4:318:THR:HA | 4:4:327:ILE:HG12 | 1.94 | 0.49 |
| 4:6:318:THR:HA | 4:6:327:ILE:HG12 | 1.94 | 0.49 |
| 4:8:318:THR:HA | 4:8:327:ILE:HG12 | 1.95 | 0.49 |
| 1:D:642:LYS:CB | 4:9:24:ASP:O | 2.59 | 0.49 |
| 1:A:128:PRO:O | 1:A:683:PRO:HB3 | 2.12 | 0.49 |
| 1:A:251:ARG:O | 1:A:263:ALA:HA | 2.12 | 0.49 |
| 1:A:756:THR:O | 1:A:758:TYR:N | 2.46 | 0.49 |
| 1:A:836:PHE:CZ | 2:B:160:GLY:CA | 2.95 | 0.49 |
| 1:A:839:MLY:HB2 | 1:A:840:PRO:HD3 | 1.94 | 0.49 |
| 1:A:97:LEU:N | 1:A:97:LEU:HD13 | 2.28 | 0.49 |
| 2:B:117:LEU:CG | 2:B:147:ASN:OD1 | 2.52 | 0.49 |
| 1:G:291:ILE:HA | 1:G:331:LEU:CD1 | 2.40 | 0.49 |
| 1:G:346:ASP:O | 1:G:349:THR:HB | 2.11 | 0.49 |
| 1:G:51:THR:C | 1:G:62:VAL:HG13 | 2.32 | 0.49 |
| 1:G:128:PRO:O | 1:G:683:PRO:HB3 | 2.12 | 0.49 |
| 1:G:725:ARG:NE | 1:G:733:PRO:CB | 1.95 | 0.49 |
| 2:H:121:LEU:O | 2:H:128:PHE:CG | 2.61 | 0.49 |
| 1:G:834:LEU:CD2 | 2:H:34:ILE:HD11 | 2.42 | 0.49 |
| 1:J:168:THR:HG22 | 1:J:169:ASP:OD1 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:215:GLN:H | 1:J:340:ILE:CD1 | 2.20 | 0.49 |
| 1:J:530:MET:CE | 4:W:354:GLN:HG3 | 2.35 | 0.49 |
| 1:J:629:GLU:CA | 1:J:643:GLY:C | 2.73 | 0.49 |
| 1:M:218:LEU:CD2 | 1:M:222:ILE:CG1 | 2.86 | 0.49 |
| 1:M:471:ASP:HB3 | 1:M:573:GLY:O | 2.12 | 0.49 |
| 1:M:839:MLY:HB2 | 1:M:840:PRO:HD3 | 1.94 | 0.49 |
| 2:N:117:LEU:HG | 2:N:147:ASN:HB3 | 1.93 | 0.49 |
| 1:S:715:VAL:HG12 | 1:S:716:LEU:O | 2.12 | 0.49 |
| 1:S:834:LEU:HD11 | 2:T:51:PHE:CD1 | 2.48 | 0.49 |
| 1:S:731:ALA:HB2 | 3:U:94:PHE:N | 2.28 | 0.49 |
| 1:D:556:ASP:CA | 4:W:49:GLN:O | 2.52 | 0.49 |
| 4:W:70:PRO:HG3 | 4:W:81:ASP:HB3 | 1.94 | 0.49 |
| 4:Z:318:THR:HA | 4:Z:327:ILE:HG12 | 1.95 | 0.49 |
| 4:1:124:PHE:CZ | 4:1:132:MET:HG3 | 2.48 | 0.49 |
| 4:1:246:GLN:HG2 | 4:Y:322:PRO:HB3 | 1.93 | 0.49 |
| 4:3:318:THR:HA | 4:3:327:ILE:HG12 | 1.94 | 0.49 |
| 4:3:70:PRO:HG3 | 4:3:81:ASP:HB3 | 1.94 | 0.49 |
| 4:9:318:THR:HA | 4:9:327:ILE:HG12 | 1.95 | 0.49 |
| 1:A:601:ASP:N | 1:A:602:PRO:CD | 2.75 | 0.49 |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CD1 | 2.27 | 0.49 |
| 1:A:834:LEU:CD2 | 2:B:54:MET:HE3 | 2.34 | 0.49 |
| 2:B:121:LEU:HA | 2:B:128:PHE:CD2 | 2.46 | 0.49 |
| 1:D:797:PHE:CG | 3:F:146:ILE:CG2 | 2.77 | 0.49 |
| 1:D:798:LEU:HD12 | 3:F:126:LEU:CD2 | 2.37 | 0.49 |
| 1:G:251:ARG:O | 1:G:263:ALA:HA | 2.12 | 0.49 |
| 2:H:117:LEU:CB | 2:H:147:ASN:ND2 | 2.35 | 0.49 |
| 1:J:192:VAL:O | 1:J:195:TYR:HB3 | 2.13 | 0.49 |
| 1:J:629:GLU:CB | 1:J:645:SER:N | 2.73 | 0.49 |
| 1:J:715:VAL:HG12 | 1:J:716:LEU:O | 2.12 | 0.49 |
| 1:M:290:GLN:HG2 | 1:M:331:LEU:CA | 2.43 | 0.49 |
| 1:S:530:MET:HG2 | 4:2:354:GLN:HB2 | 0.57 | 0.49 |
| 1:S:601:ASP:N | 1:S:602:PRO:CD | 2.75 | 0.49 |
| 4:W:318:THR:HA | 4:W:327:ILE:HG12 | 1.95 | 0.49 |
| 4:X:324:THR:CB | 4:Z:247:VAL:H | 2.23 | 0.49 |
| 4:2:124:PHE:CZ | 4:2:132:MET:HG3 | 2.48 | 0.49 |
| 4:3:124:PHE:CZ | 4:3:132:MET:HG3 | 2.48 | 0.49 |
| 1:A:22:LYS:O | 1:A:26:GLU:N | 2.30 | 0.49 |
| 1:A:640:LYS:C | 4:8:23:GLY:CA | 2.64 | 0.49 |
| 1:A:64:THR:CG2 | 1:A:65:GLU:N | 2.76 | 0.49 |
| 1:A:732:ILE:H | 1:A:733:PRO:CD | 2.23 | 0.49 |
| 2:B:112:ILE:HG23 | 2:B:147:ASN:HB3 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:831:TRP:CZ3 | 2:B:50:THR:HB | 2.39 | 0.49 |
| 1:D:20:SER:HB3 | 1:D:23:GLU:OE1 | 2.13 | 0.49 |
| 1:D:64:THR:CG2 | 1:D:65:GLU:N | 2.75 | 0.49 |
| 1:D:839:MLY:N | 1:D:840:PRO:CD | 2.75 | 0.49 |
| 2:E:121:LEU:HA | 2:E:128:PHE:CD2 | 2.46 | 0.49 |
| 2:E:117:LEU:HG | 2:E:147:ASN:HB3 | 1.93 | 0.49 |
| 1:G:168:THR:HG22 | 1:G:169:ASP:OD1 | 2.12 | 0.49 |
| 1:G:192:VAL:O | 1:G:195:TYR:HB3 | 2.13 | 0.49 |
| 1:G:20:SER:HB3 | 1:G:23:GLU:OE1 | 2.12 | 0.49 |
| 1:G:595:TRP:N | 1:G:595:TRP:CD1 | 2.80 | 0.49 |
| 2:H:112:ILE:HG23 | 2:H:147:ASN:HB3 | 1.93 | 0.49 |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:HG2 | 1.46 | 0.49 |
| 1:J:251:ARG:O | 1:J:263:ALA:HA | 2.12 | 0.49 |
| 1:J:267:THR:HG21 | 1:J:438:PHE:HE2 | 1.76 | 0.49 |
| 1:M:251:ARG:O | 1:M:263:ALA:HA | 2.12 | 0.49 |
| 1:M:538:GLU:OE1 | 4:Z:351:THR:HB | 2.12 | 0.49 |
| 1:M:739:ASP:OD1 | 1:M:740:SER:N | 2.45 | 0.49 |
| 1:M:35:MLY:CE | 1:M:777:GLU:CG | 2.81 | 0.49 |
| 1:M:795:ARG:HB2 | 3:O:35:ARG:NH1 | 2.28 | 0.49 |
| 1:S:103:LEU:C | 1:S:103:LEU:HD12 | 2.33 | 0.49 |
| 1:S:576:GLU:CG | 1:S:577:ALA:N | 2.44 | 0.49 |
| 2:T:114:LYS:HG3 | 2:T:137:TRP:CZ2 | 2.48 | 0.49 |
| 1:J:553:MLY:CB | 4:Y:45:VAL:O | 2.56 | 0.49 |
| 4:1:318:THR:HA | 4:1:327:ILE:HG12 | 1.95 | 0.49 |
| 1:S:543:PRO:CD | 4:2:146:GLY:O | 2.61 | 0.49 |
| 4:5:318:THR:HA | 4:5:327:ILE:HG12 | 1.95 | 0.49 |
| 4:7:288:ASP:CA | 4:9:204:ALA:HB2 | 2.32 | 0.49 |
| 1:A:470:PHE:O | 1:A:473:ASN:ND2 | 2.40 | 0.49 |
| 1:A:839:MLY:N | 1:A:840:PRO:CD | 2.75 | 0.49 |
| 2:B:114:LYS:N | 2:B:146:GLY:O | 2.40 | 0.49 |
| 1:A:795:ARG:CG | 3:C:118:MET:CE | 2.86 | 0.49 |
| 1:D:173:GLN:OE1 | 1:D:668:HIS:HB3 | 2.13 | 0.49 |
| 1:D:405:ARG:HB2 | 1:D:414:THR:OG1 | 2.13 | 0.49 |
| 1:D:713:SER:CB | 1:D:775:LEU:CD2 | 2.51 | 0.49 |
| 1:D:756:THR:O | 1:D:758:TYR:N | 2.45 | 0.49 |
| 1:D:818:TYR:CG | 2:E:90:GLY:CA | 2.78 | 0.49 |
| 2:E:93:PRO:O | 2:E:97:ILE:HG13 | 2.13 | 0.49 |
| 1:G:792:ALA:HB1 | 3:I:42:THR:N | 2.28 | 0.49 |
| 1:J:103:LEU:C | 1:J:103:LEU:HD12 | 2.33 | 0.49 |
| 1:J:732:ILE:O | 1:J:736:GLN:HG3 | 2.12 | 0.49 |
| 1:J:739:ASP:OD1 | 1:J:740:SER:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:595:TRP:CD1 | 1:M:595:TRP:N | 2.80 | 0.49 |
| 1:S:154:HIS:CD2 | 1:S:155:ILE:H | 2.30 | 0.49 |
| 1:S:530:MET:HA | 4:2:354:GLN:CD | 2.11 | 0.49 |
| 1:S:756:THR:O | 1:S:758:TYR:N | 2.46 | 0.49 |
| 2:T:128:PHE:O | 2:T:133:ILE:HD11 | 2.13 | 0.49 |
| 1:J:642:LYS:HA | 4:W:22:ALA:C | 2.33 | 0.49 |
| 4:X:124:PHE:CZ | 4:X:132:MET:HG3 | 2.48 | 0.49 |
| 1:M:538:GLU:HA | 4:Z:351:THR:H | 1.77 | 0.49 |
| 4:2:287:ILE:HB | 4:4:203:THR:HB | 1.95 | 0.49 |
| 4:4:198:TYR:CZ | 4:4:248:ILE:HG13 | 2.48 | 0.49 |
| 4:9:198:TYR:CZ | 4:9:248:ILE:HG13 | 2.48 | 0.49 |
| 1:A:290:GLN:HG2 | 1:A:331:LEU:CA | 2.43 | 0.49 |
| 1:A:733:PRO:CA | 1:A:737:PHE:CE1 | 2.95 | 0.49 |
| 1:A:739:ASP:OD1 | 1:A:740:SER:N | 2.45 | 0.49 |
| 1:A:720:PHE:CD2 | 1:A:744:SER:HB3 | 2.48 | 0.49 |
| 2:B:114:LYS:HG3 | 2:B:137:TRP:CZ2 | 2.48 | 0.49 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:CA | 2.95 | 0.49 |
| 1:D:267:THR:HG21 | 1:D:438:PHE:HE2 | 1.76 | 0.49 |
| 1:D:831:TRP:HZ2 | 2:E:47:LEU:CD2 | 2.21 | 0.49 |
| 2:E:121:LEU:O | 2:E:128:PHE:CG | 2.61 | 0.49 |
| 1:G:547:ASP:O | 1:G:550:PHE:HB3 | 2.12 | 0.49 |
| 1:G:173:GLN:OE1 | 1:G:668:HIS:HB3 | 2.13 | 0.49 |
| 2:H:140:PHE:HB3 | 2:H:144:VAL:HG12 | 1.95 | 0.49 |
| 1:J:20:SER:HB3 | 1:J:23:GLU:OE1 | 2.13 | 0.49 |
| 2:K:93:PRO:O | 2:K:97:ILE:HG13 | 2.12 | 0.49 |
| 1:M:821:ARG:HH12 | 2:N:127:ARG:CZ | 2.26 | 0.49 |
| 2:N:114:LYS:HG3 | 2:N:137:TRP:CZ2 | 2.48 | 0.49 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:NE | 2.09 | 0.49 |
| 1:S:429:LEU:O | 1:S:433:VAL:HG23 | 2.12 | 0.49 |
| 1:S:93:MET:CG | 1:S:715:VAL:HA | 2.43 | 0.49 |
| 4:V:322:PRO:HB3 | 4:X:246:GLN:HG2 | 1.93 | 0.49 |
| 4:Y:124:PHE:CZ | 4:Y:132:MET:HG3 | 2.48 | 0.49 |
| 4:4:124:PHE:CZ | 4:4:132:MET:HG3 | 2.48 | 0.49 |
| 4:5:213:LYS:O | 4:5:217:CYS:HB2 | 2.13 | 0.49 |
| 4:7:198:TYR:CZ | 4:7:248:ILE:HG13 | 2.48 | 0.49 |
| 1:A:103:LEU:HD12 | 1:A:103:LEU:C | 2.33 | 0.49 |
| 1:A:20:SER:HB3 | 1:A:23:GLU:OE1 | 2.13 | 0.49 |
| 1:A:530:MET:HA | 4:8:354:GLN:CD | 2.11 | 0.49 |
| 1:A:543:PRO:CD | 4:8:146:GLY:O | 2.61 | 0.49 |
| 1:A:149:GLN:HG2 | 1:A:719:ASP:N | 2.26 | 0.49 |
| 1:D:251:ARG:O | 1:D:263:ALA:HA | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:114:LYS:HG3 | 2:E:137:TRP:CZ2 | 2.48 | 0.49 |
| 1:G:715:VAL:O | 1:G:764:MLY:HB3 | 2.12 | 0.49 |
| 1:G:720:PHE:CD2 | 1:G:744:SER:HB3 | 2.48 | 0.49 |
| 1:G:757:GLN:HB2 | 1:G:776:GLU:HG3 | 1.95 | 0.49 |
| 1:G:839:MLY:HB2 | 1:G:840:PRO:HD3 | 1.94 | 0.49 |
| 3:I:50:LEU:O | 3:I:55:LYS:HB2 | 2.13 | 0.49 |
| 1:J:214:MET:HA | 1:J:340:ILE:CD1 | 2.41 | 0.49 |
| 1:J:290:GLN:HG2 | 1:J:331:LEU:CA | 2.43 | 0.49 |
| 1:J:312:TYR:N | 1:J:312:TYR:CD1 | 2.81 | 0.49 |
| 1:J:547:ASP:O | 1:J:550:PHE:HB3 | 2.12 | 0.49 |
| 1:J:64:THR:CG2 | 1:J:65:GLU:N | 2.76 | 0.49 |
| 1:J:173:GLN:OE1 | 1:J:668:HIS:HB3 | 2.13 | 0.49 |
| 1:J:756:THR:O | 1:J:758:TYR:N | 2.45 | 0.49 |
| 1:M:839:MLY:N | 1:M:840:PRO:CD | 2.75 | 0.49 |
| 1:S:723:ARG:HH11 | 1:S:723:ARG:HG3 | 1.78 | 0.49 |
| 1:S:120:GLY:CA | 1:S:764:MLY:HH11 | 2.40 | 0.49 |
| 4:X:70:PRO:HG3 | 4:X:81:ASP:HB3 | 1.94 | 0.49 |
| 4:Z:70:PRO:HG3 | 4:Z:81:ASP:HB3 | 1.94 | 0.49 |
| 4:2:198:TYR:CZ | 4:2:248:ILE:HG13 | 2.48 | 0.49 |
| 1:S:642:LYS:CB | 4:2:24:ASP:O | 2.60 | 0.49 |
| 4:4:213:LYS:O | 4:4:217:CYS:HB2 | 2.13 | 0.49 |
| 4:6:124:PHE:CZ | 4:6:132:MET:HG3 | 2.48 | 0.49 |
| 4:6:198:TYR:CZ | 4:6:248:ILE:HG13 | 2.48 | 0.49 |
| 1:A:192:VAL:O | 1:A:195:TYR:HB3 | 2.13 | 0.49 |
| 1:A:312:TYR:N | 1:A:312:TYR:CD1 | 2.80 | 0.49 |
| 1:A:800:ARG:CD | 3:C:149:VAL:O | 2.55 | 0.49 |
| 1:D:506:GLU:CG | 1:D:764:MLY:HE3 | 2.43 | 0.49 |
| 1:D:530:MET:CE | 4:9:354:GLN:HG3 | 2.35 | 0.49 |
| 1:D:642:LYS:HA | 4:9:22:ALA:C | 2.33 | 0.49 |
| 1:D:675:ILE:CG2 | 1:D:676:ILE:N | 2.74 | 0.49 |
| 1:D:715:VAL:O | 1:D:764:MLY:HB3 | 2.12 | 0.49 |
| 2:E:128:PHE:O | 2:E:133:ILE:HD11 | 2.13 | 0.49 |
| 1:G:310:TYR:CE2 | 1:G:320:ILE:CD1 | 2.94 | 0.49 |
| 1:G:290:GLN:HG2 | 1:G:331:LEU:CA | 2.43 | 0.49 |
| 2:H:114:LYS:HG3 | 2:H:137:TRP:CZ2 | 2.48 | 0.49 |
| 1:J:314:TYR:CZ | 1:J:362:GLY:HA2 | 2.48 | 0.49 |
| 2:K:114:LYS:HG3 | 2:K:137:TRP:CZ2 | 2.48 | 0.49 |
| 1:M:278:GLN:HG3 | 1:M:318:GLY:H | 1.75 | 0.49 |
| 1:M:530:MET:HG2 | 4:Z:354:GLN:HB2 | 0.57 | 0.49 |
| 1:M:725:ARG:NE | 1:M:733:PRO:CB | 1.95 | 0.49 |
| 3:U:50:LEU:O | 3:U:55:LYS:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:290:ARG:HH22 | 4:V:202:THR:CG2 | 2.17 | 0.49 |
| 4:W:198:TYR:CZ | 4:W:248:ILE:HG13 | 2.48 | 0.49 |
| 1:J:410:ASN:HD22 | 4:W:336:LYS:HE2 | 1.78 | 0.49 |
| 4:X:198:TYR:CZ | 4:X:248:ILE:HG13 | 2.48 | 0.49 |
| 4:2:70:PRO:HG3 | 4:2:81:ASP:HB3 | 1.94 | 0.48 |
| 4:2:173:HIS:CD2 | 4:3:268:GLY:CA | 2.92 | 0.48 |
| 4:6:120:THR:HG21 | 4:6:370:VAL:HG11 | 1.95 | 0.48 |
| 4:8:124:PHE:CZ | 4:8:132:MET:HG3 | 2.48 | 0.48 |
| 1:A:291:ILE:HA | 1:A:331:LEU:CD1 | 2.39 | 0.48 |
| 1:A:642:LYS:CB | 4:8:24:ASP:O | 2.59 | 0.48 |
| 2:B:130:PRO:O | 2:B:131:GLU:C | 2.52 | 0.48 |
| 2:B:93:PRO:O | 2:B:97:ILE:HG13 | 2.13 | 0.48 |
| 3:C:50:LEU:O | 3:C:55:LYS:HB2 | 2.13 | 0.48 |
| 1:D:192:VAL:O | 1:D:195:TYR:HB3 | 2.13 | 0.48 |
| 1:D:314:TYR:CZ | 1:D:362:GLY:HA2 | 2.48 | 0.48 |
| 1:D:404:PRO:HD2 | 1:D:415:MLY:O | 2.13 | 0.48 |
| 1:D:530:MET:HE3 | 4:9:354:GLN:CB | 2.42 | 0.48 |
| 1:D:629:GLU:CA | 1:D:643:GLY:C | 2.73 | 0.48 |
| 1:D:715:VAL:HG12 | 1:D:716:LEU:O | 2.12 | 0.48 |
| 1:D:97:LEU:N | 1:D:97:LEU:HD13 | 2.27 | 0.48 |
| 1:G:723:ARG:HG3 | 1:G:723:ARG:HH11 | 1.79 | 0.48 |
| 1:G:839:MLY:N | 1:G:840:PRO:CD | 2.75 | 0.48 |
| 2:H:137:TRP:CA | 2:H:145:ALA:CB | 2.82 | 0.48 |
| 1:J:404:PRO:HD2 | 1:J:415:MLY:O | 2.13 | 0.48 |
| 1:J:405:ARG:HB2 | 1:J:414:THR:OG1 | 2.13 | 0.48 |
| 1:J:471:ASP:HB3 | 1:J:573:GLY:O | 2.12 | 0.48 |
| 2:K:140:PHE:HB3 | 2:K:144:VAL:HG12 | 1.94 | 0.48 |
| 1:S:51:THR:C | 1:S:62:VAL:HG13 | 2.32 | 0.48 |
| 2:T:93:PRO:O | 2:T:97:ILE:HG13 | 2.12 | 0.48 |
| 4:V:124:PHE:CZ | 4:V:132:MET:HG3 | 2.48 | 0.48 |
| 1:S:538:GLU:OE1 | 4:2:351:THR:HB | 2.13 | 0.48 |
| 1:S:538:GLU:HA | 4:2:351:THR:H | 1.77 | 0.48 |
| 1:A:168:THR:HG22 | 1:A:169:ASP:OD1 | 2.12 | 0.48 |
| 1:A:173:GLN:OE1 | 1:A:668:HIS:HB3 | 2.13 | 0.48 |
| 1:A:237:THR:HG22 | 1:A:238:VAL:N | 2.28 | 0.48 |
| 1:A:542:PHE:CD2 | 4:8:143:TYR:CD1 | 3.02 | 0.48 |
| 1:A:553:MLY:CG | 4:V:47:MET:N | 2.54 | 0.48 |
| 1:A:752:ASP:OD2 | 1:A:782:MLY:CG | 2.61 | 0.48 |
| 2:B:117:LEU:HG | 2:B:147:ASN:HB3 | 1.93 | 0.48 |
| 1:D:103:LEU:C | 1:D:103:LEU:HD12 | 2.33 | 0.48 |
| 1:D:237:THR:HG22 | 1:D:238:VAL:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:251:ARG:HB2 | 1:D:264:ASP:HB3 | 1.94 | 0.48 |
| 1:D:769:ALA:CA | 1:D:774:LEU:HB2 | 2.43 | 0.48 |
| 2:E:163:ALA:O | 2:K:21:GLU:C | 2.49 | 0.48 |
| 1:G:576:GLU:CG | 1:G:577:ALA:N | 2.44 | 0.48 |
| 1:J:251:ARG:HB2 | 1:J:264:ASP:HB3 | 1.95 | 0.48 |
| 1:M:547:ASP:O | 1:M:550:PHE:HB3 | 2.12 | 0.48 |
| 1:M:601:ASP:N | 1:M:602:PRO:CD | 2.75 | 0.48 |
| 1:M:173:GLN:OE1 | 1:M:668:HIS:HB3 | 2.13 | 0.48 |
| 1:M:84:MLY:HH22 | 1:M:719:ASP:HB3 | 1.95 | 0.48 |
| 1:M:767:PHE:CD1 | 1:M:771:LEU:HB3 | 2.48 | 0.48 |
| 1:S:20:SER:HB3 | 1:S:23:GLU:OE1 | 2.13 | 0.48 |
| 1:S:251:ARG:O | 1:S:263:ALA:HA | 2.12 | 0.48 |
| 1:S:793:ARG:NH1 | 3:U:40:ASN:CG | 2.55 | 0.48 |
| 1:S:839:MLY:HB2 | 1:S:840:PRO:HD3 | 1.94 | 0.48 |
| 4:Y:70:PRO:HG3 | 4:Y:81:ASP:HB3 | 1.94 | 0.48 |
| 4:Z:124:PHE:CZ | 4:Z:132:MET:HG3 | 2.48 | 0.48 |
| 4:1:202:THR:HG22 | 4:Y:285:CYS:O | 2.14 | 0.48 |
| 4:1:253:GLU:HA | 4:1:256:ARG:CG | 2.42 | 0.48 |
| 4:1:70:PRO:HG3 | 4:1:81:ASP:HB3 | 1.94 | 0.48 |
| 4:2:213:LYS:O | 4:2:217:CYS:HB2 | 2.13 | 0.48 |
| 4:7:253:GLU:HA | 4:7:256:ARG:CG | 2.42 | 0.48 |
| 4:8:213:LYS:O | 4:8:217:CYS:HB2 | 2.13 | 0.48 |
| 4:8:120:THR:HG21 | 4:8:370:VAL:HG11 | 1.95 | 0.48 |
| 4:9:120:THR:HG21 | 4:9:370:VAL:HG11 | 1.95 | 0.48 |
| 4:9:213:LYS:O | 4:9:217:CYS:HB2 | 2.13 | 0.48 |
| 1:D:538:GLU:HA | 4:9:351:THR:H | 1.77 | 0.48 |
| 1:A:248:MLY:HE2 | 1:A:250:ILE:HD11 | 1.95 | 0.48 |
| 1:A:310:TYR:CE2 | 1:A:320:ILE:CD1 | 2.94 | 0.48 |
| 1:A:642:LYS:HG2 | 4:8:21:PHE:C | 2.30 | 0.48 |
| 1:D:436:MLY:HE3 | 1:D:626:TYR:HE1 | 1.77 | 0.48 |
| 2:E:140:PHE:HB3 | 2:E:144:VAL:HG12 | 1.94 | 0.48 |
| 1:G:64:THR:CG2 | 1:G:65:GLU:N | 2.76 | 0.48 |
| 2:H:128:PHE:O | 2:H:133:ILE:HD11 | 2.13 | 0.48 |
| 1:J:22:LYS:O | 1:J:26:GLU:N | 2.30 | 0.48 |
| 1:J:97:LEU:HD13 | 1:J:97:LEU:N | 2.27 | 0.48 |
| 1:M:20:SER:HB3 | 1:M:23:GLU:OE1 | 2.13 | 0.48 |
| 1:M:310:TYR:CE2 | 1:M:320:ILE:CD1 | 2.94 | 0.48 |
| 1:M:756:THR:O | 1:M:758:TYR:N | 2.45 | 0.48 |
| 3:O:50:LEU:O | 3:O:55:LYS:HB2 | 2.13 | 0.48 |
| 1:S:817:GLN:CG | 2:T:127:ARG:HB2 | 2.39 | 0.48 |
| 2:T:140:PHE:HB3 | 2:T:144:VAL:HG12 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:287:ILE:HG21 | 4:4:203:THR:CG2 | 2.32 | 0.48 |
| 4:4:70:PRO:HG3 | 4:4:81:ASP:HB3 | 1.94 | 0.48 |
| 4:7:120:THR:HG21 | 4:7:370:VAL:HG11 | 1.95 | 0.48 |
| 4:7:287:ILE:HA | 4:9:202:THR:HG21 | 1.59 | 0.48 |
| 1:A:314:TYR:CZ | 1:A:362:GLY:HA2 | 2.48 | 0.48 |
| 1:A:87:MLY:HH12 | 1:A:87:MLY:HD3 | 1.62 | 0.48 |
| 1:D:312:TYR:CD1 | 1:D:312:TYR:N | 2.81 | 0.48 |
| 1:D:795:ARG:HD2 | 3:F:35:ARG:NH1 | 2.25 | 0.48 |
| 1:D:797:PHE:CD1 | 3:F:146:ILE:CA | 2.96 | 0.48 |
| 3:F:50:LEU:O | 3:F:55:LYS:HB2 | 2.13 | 0.48 |
| 1:G:314:TYR:CZ | 1:G:362:GLY:HA2 | 2.48 | 0.48 |
| 1:G:756:THR:O | 1:G:758:TYR:N | 2.46 | 0.48 |
| 1:G:97:LEU:N | 1:G:97:LEU:HD13 | 2.28 | 0.48 |
| 1:J:237:THR:HG22 | 1:J:238:VAL:N | 2.28 | 0.48 |
| 1:J:550:PHE:CE2 | 1:J:592:ILE:CG2 | 2.97 | 0.48 |
| 1:J:567:LYS:HZ3 | 4:Y:92:ASN:HD21 | 1.59 | 0.48 |
| 1:J:723:ARG:HH11 | 1:J:723:ARG:HG3 | 1.79 | 0.48 |
| 1:J:820:VAL:HG13 | 2:K:136:MET:CE | 2.40 | 0.48 |
| 1:M:103:LEU:C | 1:M:103:LEU:HD12 | 2.33 | 0.48 |
| 1:M:314:TYR:CZ | 1:M:362:GLY:HA2 | 2.48 | 0.48 |
| 1:M:51:THR:C | 1:M:62:VAL:HG13 | 2.33 | 0.48 |
| 1:M:646:PHE:CE2 | 1:M:652:LEU:CD2 | 2.87 | 0.48 |
| 1:M:720:PHE:CD2 | 1:M:744:SER:HB3 | 2.48 | 0.48 |
| 1:M:798:LEU:HD21 | 3:O:122:GLU:HB3 | 1.93 | 0.48 |
| 1:S:312:TYR:CD1 | 1:S:312:TYR:N | 2.81 | 0.48 |
| 1:S:354:LEU:HA | 1:S:354:LEU:HD12 | 1.56 | 0.48 |
| 1:S:499:GLU:HA | 1:S:499:GLU:OE1 | 2.13 | 0.48 |
| 1:S:720:PHE:CD2 | 1:S:744:SER:HB3 | 2.48 | 0.48 |
| 4:V:213:LYS:O | 4:V:217:CYS:HB2 | 2.13 | 0.48 |
| 4:W:120:THR:HG21 | 4:W:370:VAL:HG11 | 1.95 | 0.48 |
| 4:Z:198:TYR:CZ | 4:Z:248:ILE:HG13 | 2.48 | 0.48 |
| 4:5:124:PHE:CZ | 4:5:132:MET:HG3 | 2.48 | 0.48 |
| 4:5:198:TYR:CZ | 4:5:248:ILE:HG13 | 2.48 | 0.48 |
| 1:A:765:VAL:CG1 | 1:A:766:PHE:N | 2.77 | 0.48 |
| 1:D:290:GLN:HG2 | 1:D:331:LEU:CA | 2.43 | 0.48 |
| 1:D:727:LEU:CA | 1:D:782:MLY:HH13 | 2.33 | 0.48 |
| 1:G:554:LEU:HD12 | 1:G:554:LEU:HA | 1.77 | 0.48 |
| 2:K:130:PRO:O | 2:K:131:GLU:C | 2.52 | 0.48 |
| 1:M:64:THR:CG2 | 1:M:65:GLU:N | 2.75 | 0.48 |
| 1:S:278:GLN:HG3 | 1:S:318:GLY:H | 1.75 | 0.48 |
| 1:S:617:MLY:O | 1:S:620:ALA:HB3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:715:VAL:O | 1:S:764:MLY:HB3 | 2.12 | 0.48 |
| 1:S:797:PHE:CE2 | 3:U:126:LEU:HD22 | 2.43 | 0.48 |
| 1:S:800:ARG:HB3 | 3:U:149:VAL:HG22 | 1.95 | 0.48 |
| 4:8:288:ASP:CA | 4:V:204:ALA:HB2 | 2.32 | 0.48 |
| 1:G:642:LYS:HA | 4:V:22:ALA:C | 2.33 | 0.48 |
| 4:W:213:LYS:O | 4:W:217:CYS:HB2 | 2.13 | 0.48 |
| 4:W:285:CYS:O | 4:Y:202:THR:HG22 | 2.14 | 0.48 |
| 4:Y:198:TYR:CZ | 4:Y:248:ILE:HG13 | 2.48 | 0.48 |
| 4:Z:213:LYS:O | 4:Z:217:CYS:HB2 | 2.13 | 0.48 |
| 4:1:213:LYS:O | 4:1:217:CYS:HB2 | 2.13 | 0.48 |
| 1:A:642:LYS:HA | 4:8:22:ALA:C | 2.33 | 0.48 |
| 1:A:251:ARG:HB2 | 1:A:264:ASP:HB3 | 1.95 | 0.48 |
| 1:A:406:VAL:CG1 | 1:A:407:GLY:N | 2.77 | 0.48 |
| 1:A:505:MLY:CG | 1:A:741:LYS:NZ | 2.59 | 0.48 |
| 1:A:831:TRP:CZ2 | 2:B:47:LEU:CD2 | 2.97 | 0.48 |
| 1:D:617:MLY:O | 1:D:620:ALA:HB3 | 2.14 | 0.48 |
| 1:D:733:PRO:O | 1:D:737:PHE:CE1 | 2.53 | 0.48 |
| 1:D:765:VAL:CG1 | 1:D:766:PHE:N | 2.77 | 0.48 |
| 1:D:838:ILE:C | 1:D:840:PRO:HD2 | 2.34 | 0.48 |
| 1:D:814:PHE:CE1 | 2:E:127:ARG:NH1 | 2.71 | 0.48 |
| 1:G:248:MLY:HE2 | 1:G:250:ILE:HD11 | 1.95 | 0.48 |
| 1:G:292:MET:HE1 | 1:G:309:PRO:HD3 | 1.96 | 0.48 |
| 1:G:689:GLU:HG2 | 1:G:689:GLU:O | 2.14 | 0.48 |
| 1:G:739:ASP:OD1 | 1:G:740:SER:N | 2.45 | 0.48 |
| 1:G:815:CYS:SG | 2:H:92:ASP:OD1 | 2.72 | 0.48 |
| 1:J:689:GLU:O | 1:J:689:GLU:HG2 | 2.14 | 0.48 |
| 1:J:93:MET:HE3 | 1:J:716:LEU:HD12 | 1.93 | 0.48 |
| 1:M:248:MLY:HE2 | 1:M:250:ILE:HD11 | 1.95 | 0.48 |
| 1:M:804:ARG:CA | 1:M:807:VAL:HB | 2.43 | 0.48 |
| 1:M:829:TRP:CZ3 | 2:N:84:PHE:CE1 | 3.02 | 0.48 |
| 1:S:237:THR:HG22 | 1:S:238:VAL:N | 2.28 | 0.48 |
| 1:S:292:MET:HE1 | 1:S:309:PRO:HD3 | 1.96 | 0.48 |
| 1:S:290:GLN:HG2 | 1:S:331:LEU:CA | 2.43 | 0.48 |
| 1:S:405:ARG:HB2 | 1:S:414:THR:OG1 | 2.13 | 0.48 |
| 1:S:173:GLN:OE1 | 1:S:668:HIS:HB3 | 2.13 | 0.48 |
| 1:S:759:ALA:O | 1:S:766:PHE:N | 2.32 | 0.48 |
| 1:S:831:TRP:HE1 | 2:T:67:MET:HG2 | 1.79 | 0.48 |
| 4:Y:213:LYS:O | 4:Y:217:CYS:HB2 | 2.13 | 0.48 |
| 4:3:250:ILE:HG23 | 4:3:253:GLU:HG2 | 1.96 | 0.48 |
| 4:8:250:ILE:HG23 | 4:8:253:GLU:HG2 | 1.96 | 0.48 |
| 2:B:128:PHE:O | 2:B:133:ILE:HD11 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:550:PHE:CE2 | 1:D:592:ILE:CG2 | 2.97 | 0.48 |
| 1:G:10:PHE:CD2 | 1:G:17:LEU:HD23 | 2.49 | 0.48 |
| 1:G:405:ARG:HB2 | 1:G:414:THR:OG1 | 2.13 | 0.48 |
| 1:G:503:TYR:CZ | 1:G:711:PHE:HE2 | 2.29 | 0.48 |
| 1:G:787:ILE:CG2 | 1:G:788:THR:N | 2.77 | 0.48 |
| 1:G:789:ALA:CB | 3:I:81:GLN:CD | 2.82 | 0.48 |
| 1:M:10:PHE:CD2 | 1:M:17:LEU:HD23 | 2.49 | 0.48 |
| 1:M:237:THR:HG22 | 1:M:238:VAL:N | 2.28 | 0.48 |
| 1:M:251:ARG:HB2 | 1:M:264:ASP:HB3 | 1.95 | 0.48 |
| 1:M:312:TYR:CD1 | 1:M:312:TYR:N | 2.81 | 0.48 |
| 1:M:410:ASN:HA | 4:Z:334:GLU:HB3 | 1.29 | 0.48 |
| 1:M:499:GLU:OE1 | 1:M:499:GLU:HA | 2.13 | 0.48 |
| 1:S:314:TYR:CZ | 1:S:362:GLY:HA2 | 2.48 | 0.48 |
| 1:S:149:GLN:CG | 1:S:763:THR:HG23 | 2.44 | 0.48 |
| 1:S:797:PHE:CE1 | 3:U:146:ILE:HG23 | 2.48 | 0.48 |
| 4:V:120:THR:HG21 | 4:V:370:VAL:HG11 | 1.95 | 0.48 |
| 4:W:124:PHE:CZ | 4:W:132:MET:HG3 | 2.48 | 0.48 |
| 4:W:250:ILE:HG23 | 4:W:253:GLU:HG2 | 1.96 | 0.48 |
| 1:D:553:MLY:HG3 | 4:W:44:MET:O | 2.07 | 0.48 |
| 4:2:299:MET:HE2 | 4:2:331:ALA:HB2 | 1.95 | 0.48 |
| 4:1:287:ILE:HG21 | 4:3:202:THR:OG1 | 2.04 | 0.48 |
| 4:9:250:ILE:HG23 | 4:9:253:GLU:HG2 | 1.96 | 0.48 |
| 1:D:410:ASN:HD22 | 4:9:336:LYS:HE2 | 1.78 | 0.48 |
| 1:A:202:SER:HA | 1:A:207:LYS:NZ | 2.22 | 0.48 |
| 1:A:295:MLY:HG3 | 1:A:332:MET:HE2 | 1.92 | 0.48 |
| 1:D:595:TRP:CD1 | 1:D:595:TRP:N | 2.80 | 0.48 |
| 1:D:712:PRO:HG2 | 1:D:771:LEU:CD1 | 2.43 | 0.48 |
| 2:E:130:PRO:O | 2:E:131:GLU:C | 2.52 | 0.48 |
| 1:G:530:MET:HA | 4:V:354:GLN:CD | 2.11 | 0.48 |
| 1:J:720:PHE:CD2 | 1:J:744:SER:HB3 | 2.48 | 0.48 |
| 1:J:732:ILE:H | 1:J:733:PRO:HD2 | 1.74 | 0.48 |
| 1:J:819:ASN:OD1 | 2:K:91:ALA:C | 2.51 | 0.48 |
| 1:M:406:VAL:CG1 | 1:M:407:GLY:N | 2.77 | 0.48 |
| 2:N:140:PHE:HB3 | 2:N:144:VAL:HG12 | 1.94 | 0.48 |
| 1:S:689:GLU:O | 1:S:689:GLU:HG2 | 2.14 | 0.48 |
| 1:S:797:PHE:CE1 | 3:U:149:VAL:HG11 | 2.45 | 0.48 |
| 4:X:213:LYS:O | 4:X:217:CYS:HB2 | 2.13 | 0.48 |
| 1:S:410:ASN:HD22 | 4:2:336:LYS:HE2 | 1.78 | 0.48 |
| 1:S:530:MET:HE3 | 4:2:354:GLN:CB | 2.43 | 0.48 |
| 4:4:250:ILE:HG23 | 4:4:253:GLU:HG2 | 1.96 | 0.48 |
| 4:7:250:ILE:HG23 | 4:7:253:GLU:HG2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:410:ASN:HD22 | 4:8:336:LYS:HE2 | 1.78 | 0.48 |
| 1:A:214:MET:C | 1:A:340:ILE:CD1 | 2.82 | 0.48 |
| 1:A:404:PRO:HD2 | 1:A:415:MLY:O | 2.13 | 0.48 |
| 1:A:499:GLU:HA | 1:A:499:GLU:OE1 | 2.13 | 0.48 |
| 1:A:546:THR:CG2 | 1:A:547:ASP:N | 2.77 | 0.48 |
| 1:A:723:ARG:HH11 | 1:A:723:ARG:HG3 | 1.79 | 0.48 |
| 2:B:112:ILE:CG2 | 2:B:147:ASN:O | 2.62 | 0.48 |
| 1:D:214:MET:HA | 1:D:340:ILE:CD1 | 2.41 | 0.48 |
| 1:D:712:PRO:HG2 | 1:D:771:LEU:CG | 2.40 | 0.48 |
| 2:E:112:ILE:CG2 | 2:E:147:ASN:O | 2.62 | 0.48 |
| 2:E:123:THR:CA | 3:F:19:ARG:HH22 | 2.07 | 0.48 |
| 1:G:202:SER:HA | 1:G:207:LYS:NZ | 2.22 | 0.48 |
| 1:G:215:GLN:H | 1:G:340:ILE:CD1 | 2.20 | 0.48 |
| 1:G:251:ARG:HB2 | 1:G:264:ASP:HB3 | 1.95 | 0.48 |
| 1:G:409:GLY:N | 1:G:636:LYS:CD | 2.71 | 0.48 |
| 1:G:564:ASN:HD22 | 1:G:582:VAL:HB | 1.79 | 0.48 |
| 1:G:642:LYS:HG2 | 4:V:21:PHE:C | 2.30 | 0.48 |
| 1:G:789:ALA:CB | 3:I:81:GLN:NE2 | 2.76 | 0.48 |
| 1:J:10:PHE:CD2 | 1:J:17:LEU:HD23 | 2.49 | 0.48 |
| 1:J:725:ARG:NE | 1:J:733:PRO:CB | 1.95 | 0.48 |
| 1:M:602:PRO:O | 1:M:603:LEU:HD12 | 2.14 | 0.48 |
| 1:M:800:ARG:HH22 | 3:O:40:ASN:CG | 2.17 | 0.48 |
| 1:M:838:ILE:C | 1:M:840:PRO:HD2 | 2.35 | 0.48 |
| 1:S:404:PRO:HD2 | 1:S:415:MLY:O | 2.13 | 0.48 |
| 1:S:41:VAL:CG1 | 1:S:42:HIS:N | 2.76 | 0.48 |
| 1:S:546:THR:CG2 | 1:S:547:ASP:N | 2.77 | 0.48 |
| 1:S:838:ILE:C | 1:S:840:PRO:HD2 | 2.34 | 0.48 |
| 4:V:250:ILE:HG23 | 4:V:253:GLU:HG2 | 1.96 | 0.48 |
| 4:Y:250:ILE:HG23 | 4:Y:253:GLU:HG2 | 1.96 | 0.48 |
| 4:Z:120:THR:HG21 | 4:Z:370:VAL:HG11 | 1.95 | 0.48 |
| 4:1:198:TYR:CZ | 4:1:248:ILE:HG13 | 2.48 | 0.48 |
| 4:1:250:ILE:HG23 | 4:1:253:GLU:HG2 | 1.96 | 0.48 |
| 4:2:253:GLU:HA | 4:2:256:ARG:CG | 2.42 | 0.48 |
| 4:5:120:THR:HG21 | 4:5:370:VAL:HG11 | 1.95 | 0.48 |
| 4:4:287:ILE:HG23 | 4:6:202:THR:HB | 0.99 | 0.48 |
| 1:A:504:MLY:HB2 | 1:A:762:HIS:NE2 | 2.29 | 0.48 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:HA | 2.37 | 0.48 |
| 1:D:546:THR:CG2 | 1:D:547:ASP:N | 2.77 | 0.48 |
| 1:G:795:ARG:N | 3:I:118:MET:HE3 | 2.29 | 0.48 |
| 1:J:839:MLY:HB2 | 1:J:840:PRO:HD3 | 1.94 | 0.48 |
| 2:K:128:PHE:O | 2:K:133:ILE:HD11 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:295:MLY:HG3 | 1:S:332:MET:HE2 | 1.94 | 0.48 |
| 1:S:97:LEU:N | 1:S:97:LEU:HD13 | 2.28 | 0.48 |
| 4:V:198:TYR:CZ | 4:V:248:ILE:HG13 | 2.48 | 0.48 |
| 4:X:120:THR:HG21 | 4:X:370:VAL:HG11 | 1.95 | 0.48 |
| 4:X:291:LYS:CG | 4:Z:243:PRO:C | 2.74 | 0.48 |
| 4:1:202:THR:CG2 | 4:Y:285:CYS:O | 2.62 | 0.47 |
| 4:2:250:ILE:HG23 | 4:2:253:GLU:HG2 | 1.96 | 0.47 |
| 4:5:250:ILE:HG23 | 4:5:253:GLU:HG2 | 1.96 | 0.47 |
| 4:6:213:LYS:O | 4:6:217:CYS:HB2 | 2.13 | 0.47 |
| 4:7:124:PHE:CZ | 4:7:132:MET:HG3 | 2.48 | 0.47 |
| 4:9:124:PHE:CZ | 4:9:132:MET:HG3 | 2.48 | 0.47 |
| 1:A:10:PHE:CD2 | 1:A:17:LEU:HD23 | 2.49 | 0.47 |
| 1:A:405:ARG:HB2 | 1:A:414:THR:OG1 | 2.13 | 0.47 |
| 1:A:564:ASN:HD22 | 1:A:582:VAL:HB | 1.79 | 0.47 |
| 1:A:617:MLY:O | 1:A:620:ALA:HB3 | 2.14 | 0.47 |
| 1:D:578:HIS:HB3 | 1:D:592:ILE:CD1 | 2.38 | 0.47 |
| 1:G:218:LEU:HA | 1:G:221:GLN:H | 1.79 | 0.47 |
| 1:G:499:GLU:HA | 1:G:499:GLU:OE1 | 2.13 | 0.47 |
| 1:G:640:LYS:HD2 | 1:G:646:PHE:O | 2.15 | 0.47 |
| 1:G:838:ILE:C | 1:G:840:PRO:HD2 | 2.34 | 0.47 |
| 1:J:51:THR:C | 1:J:62:VAL:HG13 | 2.32 | 0.47 |
| 1:J:530:MET:HE3 | 4:W:354:GLN:CB | 2.43 | 0.47 |
| 1:J:546:THR:CG2 | 1:J:547:ASP:N | 2.77 | 0.47 |
| 1:J:617:MLY:O | 1:J:620:ALA:HB3 | 2.14 | 0.47 |
| 1:J:830:PRO:HB3 | 2:K:67:MET:CE | 2.42 | 0.47 |
| 1:J:838:ILE:C | 1:J:840:PRO:HD2 | 2.35 | 0.47 |
| 1:M:405:ARG:HB2 | 1:M:414:THR:OG1 | 2.13 | 0.47 |
| 1:M:640:LYS:HB3 | 1:M:645:SER:CB | 2.42 | 0.47 |
| 1:M:84:MLY:HB3 | 1:M:723:ARG:CD | 2.44 | 0.47 |
| 1:M:765:VAL:CG1 | 1:M:766:PHE:N | 2.77 | 0.47 |
| 1:S:10:PHE:CD2 | 1:S:17:LEU:HD23 | 2.49 | 0.47 |
| 1:S:568:PRO:HD3 | 1:S:579:PHE:HA | 1.96 | 0.47 |
| 1:S:732:ILE:H | 1:S:733:PRO:CD | 2.23 | 0.47 |
| 1:S:770:GLY:O | 1:S:771:LEU:C | 2.44 | 0.47 |
| 2:T:130:PRO:O | 2:T:131:GLU:C | 2.52 | 0.47 |
| 4:V:285:CYS:O | 4:X:202:THR:HG22 | 2.14 | 0.47 |
| 4:X:324:THR:CG2 | 4:Z:247:VAL:H | 2.27 | 0.47 |
| 1:M:410:ASN:HD22 | 4:Z:336:LYS:HE2 | 1.78 | 0.47 |
| 1:M:538:GLU:OE1 | 4:Z:355:MET:HE3 | 2.14 | 0.47 |
| 1:A:642:LYS:HB2 | 4:8:24:ASP:O | 1.88 | 0.47 |
| 1:A:122:PHE:CE2 | 1:A:700:VAL:HA | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:708:ARG:HA | 1:A:712:PRO:HA | 1.96 | 0.47 |
| 1:A:783:LEU:HA | 1:A:786:ILE:HB | 1.97 | 0.47 |
| 1:D:106:LEU:HD12 | 1:D:117:THR:HG21 | 1.96 | 0.47 |
| 1:D:542:PHE:CD2 | 4:9:143:TYR:CD1 | 3.02 | 0.47 |
| 1:D:759:ALA:O | 1:D:766:PHE:N | 2.32 | 0.47 |
| 3:F:53:PRO:O | 3:F:55:LYS:HG3 | 2.14 | 0.47 |
| 1:G:122:PHE:CE2 | 1:G:700:VAL:HA | 2.50 | 0.47 |
| 1:G:278:GLN:HB3 | 1:G:278:GLN:HE21 | 1.42 | 0.47 |
| 1:G:312:TYR:N | 1:G:312:TYR:CD1 | 2.81 | 0.47 |
| 1:G:214:MET:C | 1:G:340:ILE:CD1 | 2.82 | 0.47 |
| 1:G:404:PRO:HD2 | 1:G:415:MLY:O | 2.13 | 0.47 |
| 1:G:546:THR:CG2 | 1:G:547:ASP:N | 2.77 | 0.47 |
| 1:G:94:MET:O | 1:G:713:SER:CB | 2.61 | 0.47 |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:CD1 | 2.49 | 0.47 |
| 1:J:799:MET:CE | 3:L:32:ASP:HB3 | 2.44 | 0.47 |
| 1:M:332:MET:O | 1:M:336:SER:OG | 2.27 | 0.47 |
| 1:M:214:MET:C | 1:M:340:ILE:CD1 | 2.82 | 0.47 |
| 1:M:436:MLY:HE3 | 1:M:626:TYR:HE1 | 1.77 | 0.47 |
| 1:M:617:MLY:O | 1:M:620:ALA:HB3 | 2.14 | 0.47 |
| 1:M:689:GLU:HG2 | 1:M:689:GLU:O | 2.14 | 0.47 |
| 2:N:128:PHE:O | 2:N:133:ILE:HD11 | 2.13 | 0.47 |
| 2:N:144:VAL:HG12 | 2:N:153:ILE:HD11 | 1.75 | 0.47 |
| 1:S:206:LYS:HD2 | 1:S:217:THR:CG2 | 2.17 | 0.47 |
| 1:S:218:LEU:HA | 1:S:221:GLN:H | 1.79 | 0.47 |
| 1:S:731:ALA:HB2 | 3:U:94:PHE:HB2 | 1.96 | 0.47 |
| 3:U:49:ILE:CA | 3:U:52:ASN:ND2 | 2.54 | 0.47 |
| 1:G:410:ASN:HD22 | 4:V:336:LYS:HE2 | 1.79 | 0.47 |
| 4:Z:250:ILE:HG23 | 4:Z:253:GLU:HG2 | 1.96 | 0.47 |
| 4:6:250:ILE:HG23 | 4:6:253:GLU:HG2 | 1.96 | 0.47 |
| 4:7:213:LYS:O | 4:7:217:CYS:HB2 | 2.13 | 0.47 |
| 1:A:106:LEU:HD12 | 1:A:117:THR:HG21 | 1.96 | 0.47 |
| 1:A:41:VAL:CG1 | 1:A:42:HIS:N | 2.76 | 0.47 |
| 1:A:640:LYS:HD2 | 1:A:646:PHE:O | 2.14 | 0.47 |
| 1:A:838:ILE:C | 1:A:840:PRO:HD2 | 2.35 | 0.47 |
| 1:A:97:LEU:HD23 | 1:A:712:PRO:CA | 2.44 | 0.47 |
| 1:D:218:LEU:HA | 1:D:221:GLN:H | 1.79 | 0.47 |
| 1:D:41:VAL:CG1 | 1:D:42:HIS:N | 2.75 | 0.47 |
| 1:D:499:GLU:OE1 | 1:D:499:GLU:HA | 2.13 | 0.47 |
| 1:D:51:THR:C | 1:D:62:VAL:HG13 | 2.32 | 0.47 |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HD12 | 0.95 | 0.47 |
| 1:G:237:THR:HG22 | 1:G:238:VAL:N | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:765:VAL:CG1 | 1:G:766:PHE:N | 2.77 | 0.47 |
| 1:G:818:TYR:HB3 | 2:H:90:GLY:CA | 2.44 | 0.47 |
| 1:J:406:VAL:CG1 | 1:J:407:GLY:N | 2.77 | 0.47 |
| 1:J:542:PHE:CD2 | 4:W:143:TYR:CD1 | 3.02 | 0.47 |
| 1:J:568:PRO:HD3 | 1:J:579:PHE:HA | 1.96 | 0.47 |
| 1:J:632:GLY:HA3 | 1:J:643:GLY:N | 2.17 | 0.47 |
| 1:J:765:VAL:CG1 | 1:J:766:PHE:N | 2.77 | 0.47 |
| 1:J:769:ALA:HB3 | 1:J:770:GLY:HA3 | 1.94 | 0.47 |
| 1:M:218:LEU:HA | 1:M:221:GLN:H | 1.79 | 0.47 |
| 1:M:404:PRO:HD2 | 1:M:415:MLY:O | 2.13 | 0.47 |
| 1:M:797:PHE:HE2 | 3:O:126:LEU:HD23 | 1.70 | 0.47 |
| 1:S:310:TYR:CE2 | 1:S:320:ILE:CD1 | 2.94 | 0.47 |
| 1:S:550:PHE:CE2 | 1:S:592:ILE:CG2 | 2.97 | 0.47 |
| 1:S:643:GLY:CA | 4:2:24:ASP:OD1 | 2.61 | 0.47 |
| 1:S:725:ARG:NE | 1:S:733:PRO:CB | 1.95 | 0.47 |
| 4:V:285:CYS:O | 4:X:202:THR:CG2 | 2.62 | 0.47 |
| 4:2:120:THR:HG21 | 4:2:370:VAL:HG11 | 1.95 | 0.47 |
| 4:2:287:ILE:CB | 4:4:203:THR:H | 2.26 | 0.47 |
| 4:8:198:TYR:CZ | 4:8:248:ILE:HG13 | 2.48 | 0.47 |
| 1:A:798:LEU:HA | 1:A:798:LEU:HD12 | 1.37 | 0.47 |
| 2:B:160:GLY:O | 2:B:161:GLU:HG2 | 2.14 | 0.47 |
| 1:A:798:LEU:CG | 3:C:126:LEU:HD11 | 2.43 | 0.47 |
| 1:D:136:ASN:O | 1:D:139:VAL:N | 2.47 | 0.47 |
| 1:D:524:GLU:HB3 | 1:D:528:MLY:HG2 | 1.96 | 0.47 |
| 1:D:568:PRO:HD3 | 1:D:579:PHE:HA | 1.96 | 0.47 |
| 1:D:564:ASN:HD22 | 1:D:582:VAL:HB | 1.79 | 0.47 |
| 1:D:400:ALA:HB1 | 1:D:606:THR:CG2 | 2.45 | 0.47 |
| 1:D:720:PHE:CD2 | 1:D:744:SER:HB3 | 2.48 | 0.47 |
| 1:D:795:ARG:CZ | 3:F:43:ASN:OD1 | 2.61 | 0.47 |
| 1:G:406:VAL:CG1 | 1:G:407:GLY:N | 2.77 | 0.47 |
| 1:G:820:VAL:CG1 | 2:H:136:MET:HE1 | 2.45 | 0.47 |
| 1:J:436:MLY:HE3 | 1:J:626:TYR:HE1 | 1.77 | 0.47 |
| 1:J:499:GLU:OE1 | 1:J:499:GLU:HA | 2.13 | 0.47 |
| 2:K:112:ILE:CG2 | 2:K:147:ASN:O | 2.62 | 0.47 |
| 3:L:50:LEU:O | 3:L:55:LYS:HB2 | 2.13 | 0.47 |
| 1:M:169:ASP:OD1 | 1:M:169:ASP:N | 2.44 | 0.47 |
| 1:M:636:LYS:O | 4:Z:144:ALA:HB1 | 2.14 | 0.47 |
| 1:M:93:MET:HE2 | 1:M:764:MLY:CH1 | 2.45 | 0.47 |
| 1:M:821:ARG:NH2 | 2:N:127:ARG:NE | 2.63 | 0.47 |
| 3:O:53:PRO:O | 3:O:55:LYS:HG3 | 2.15 | 0.47 |
| 1:S:248:MLY:HE2 | 1:S:250:ILE:HD11 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:636:LYS:O | 4:V:144:ALA:HB1 | 2.14 | 0.47 |
| 4:X:250:ILE:HG23 | 4:X:253:GLU:HG2 | 1.96 | 0.47 |
| 4:1:120:THR:HG21 | 4:1:370:VAL:HG11 | 1.95 | 0.47 |
| 4:1:162:ASN:OD1 | 4:1:277:THR:HG22 | 2.15 | 0.47 |
| 4:2:162:ASN:OD1 | 4:2:277:THR:HG22 | 2.15 | 0.47 |
| 1:S:410:ASN:HA | 4:2:334:GLU:HB3 | 1.29 | 0.47 |
| 4:4:253:GLU:HA | 4:4:256:ARG:CG | 2.42 | 0.47 |
| 4:4:120:THR:HG21 | 4:4:370:VAL:HG11 | 1.95 | 0.47 |
| 4:9:162:ASN:OD1 | 4:9:277:THR:HG22 | 2.15 | 0.47 |
| 1:A:449:LEU:HD12 | 1:A:449:LEU:HA | 1.60 | 0.47 |
| 1:A:797:PHE:CD1 | 3:C:149:VAL:HG11 | 2.50 | 0.47 |
| 1:D:602:PRO:O | 1:D:603:LEU:HD12 | 2.14 | 0.47 |
| 1:D:640:LYS:HD2 | 1:D:646:PHE:O | 2.14 | 0.47 |
| 1:D:664:LEU:HD12 | 1:D:664:LEU:HA | 1.53 | 0.47 |
| 1:G:602:PRO:O | 1:G:603:LEU:HD12 | 2.14 | 0.47 |
| 1:G:617:MLY:O | 1:G:620:ALA:HB3 | 2.14 | 0.47 |
| 2:H:112:ILE:CG2 | 2:H:147:ASN:O | 2.62 | 0.47 |
| 1:J:602:PRO:O | 1:J:603:LEU:HD12 | 2.14 | 0.47 |
| 1:J:636:LYS:O | 4:W:144:ALA:HB1 | 2.14 | 0.47 |
| 1:J:795:ARG:HD2 | 3:L:43:ASN:H | 1.80 | 0.47 |
| 2:K:139:ALA:C | 2:K:141:PRO:HD3 | 2.33 | 0.47 |
| 1:J:829:TRP:CH2 | 2:K:83:MET:HE3 | 2.49 | 0.47 |
| 1:M:568:PRO:HD3 | 1:M:579:PHE:HA | 1.96 | 0.47 |
| 1:M:640:LYS:HD2 | 1:M:646:PHE:O | 2.15 | 0.47 |
| 1:M:122:PHE:CE2 | 1:M:700:VAL:HA | 2.50 | 0.47 |
| 1:M:97:LEU:N | 1:M:97:LEU:HD13 | 2.28 | 0.47 |
| 2:N:112:ILE:CG2 | 2:N:147:ASN:O | 2.62 | 0.47 |
| 1:S:251:ARG:HB2 | 1:S:264:ASP:HB3 | 1.95 | 0.47 |
| 1:S:409:GLY:N | 1:S:636:LYS:CD | 2.70 | 0.47 |
| 1:S:636:LYS:O | 4:2:144:ALA:HB1 | 2.14 | 0.47 |
| 1:S:640:LYS:HB3 | 1:S:645:SER:CB | 2.42 | 0.47 |
| 2:T:137:TRP:CA | 2:T:145:ALA:HB2 | 2.37 | 0.47 |
| 1:S:797:PHE:CZ | 3:U:146:ILE:HD12 | 2.23 | 0.47 |
| 1:J:642:LYS:CB | 4:W:24:ASP:O | 2.60 | 0.47 |
| 4:Y:120:THR:HG21 | 4:Y:370:VAL:HG11 | 1.95 | 0.47 |
| 4:W:325:MET:CE | 4:Y:244:ASP:OD2 | 2.34 | 0.47 |
| 4:3:213:LYS:O | 4:3:217:CYS:HB2 | 2.13 | 0.47 |
| 4:3:162:ASN:OD1 | 4:3:277:THR:HG22 | 2.15 | 0.47 |
| 4:4:162:ASN:OD1 | 4:4:277:THR:HG22 | 2.15 | 0.47 |
| 4:4:299:MET:HE2 | 4:4:331:ALA:HB2 | 1.95 | 0.47 |
| 4:8:162:ASN:OD1 | 4:8:277:THR:HG22 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:LEU:HA | 1:A:221:GLN:H | 1.79 | 0.47 |
| 1:A:278:GLN:HB3 | 1:A:278:GLN:HE21 | 1.42 | 0.47 |
| 1:A:530:MET:CE | 4:8:354:GLN:HG3 | 2.35 | 0.47 |
| 1:A:602:PRO:O | 1:A:603:LEU:HD12 | 2.14 | 0.47 |
| 1:A:831:TRP:HZ3 | 2:B:34:ILE:HG12 | 1.77 | 0.47 |
| 1:A:834:LEU:CD2 | 2:B:54:MET:SD | 2.94 | 0.47 |
| 3:C:53:PRO:O | 3:C:55:LYS:HG3 | 2.15 | 0.47 |
| 1:D:144:ARG:HD2 | 1:D:144:ARG:HA | 1.78 | 0.47 |
| 1:D:689:GLU:O | 1:D:689:GLU:HG2 | 2.14 | 0.47 |
| 1:D:814:PHE:HE1 | 2:E:127:ARG:NH2 | 2.12 | 0.47 |
| 1:G:176:LEU:N | 1:G:176:LEU:CD1 | 2.75 | 0.47 |
| 1:G:550:PHE:CE2 | 1:G:592:ILE:CG2 | 2.97 | 0.47 |
| 1:G:629:GLU:CB | 1:G:645:SER:N | 2.74 | 0.47 |
| 1:J:122:PHE:CE2 | 1:J:700:VAL:HA | 2.50 | 0.47 |
| 1:J:214:MET:C | 1:J:340:ILE:CD1 | 2.82 | 0.47 |
| 1:J:400:ALA:HB1 | 1:J:606:THR:CG2 | 2.45 | 0.47 |
| 1:J:818:TYR:CE1 | 2:K:127:ARG:NH1 | 2.74 | 0.47 |
| 1:M:546:THR:CG2 | 1:M:547:ASP:N | 2.77 | 0.47 |
| 1:S:406:VAL:CG1 | 1:S:407:GLY:N | 2.77 | 0.47 |
| 1:S:542:PHE:CD2 | 4:2:143:TYR:CD1 | 3.02 | 0.47 |
| 1:S:602:PRO:O | 1:S:603:LEU:HD12 | 2.14 | 0.47 |
| 2:T:112:ILE:CG2 | 2:T:147:ASN:O | 2.62 | 0.47 |
| 4:V:162:ASN:OD1 | 4:V:277:THR:HG22 | 2.15 | 0.47 |
| 4:W:286:ASP:HA | 4:Y:202:THR:HG22 | 1.63 | 0.47 |
| 4:Y:162:ASN:OD1 | 4:Y:277:THR:HG22 | 2.15 | 0.47 |
| 4:3:198:TYR:CZ | 4:3:248:ILE:HG13 | 2.48 | 0.47 |
| 4:3:120:THR:HG21 | 4:3:370:VAL:HG11 | 1.95 | 0.47 |
| 1:A:411:GLU:H | 4:8:333:PRO:HB2 | 1.80 | 0.47 |
| 1:A:636:LYS:O | 4:8:144:ALA:HB1 | 2.15 | 0.47 |
| 1:D:10:PHE:CD2 | 1:D:17:LEU:HD23 | 2.49 | 0.47 |
| 1:D:188:ASN:ND2 | 1:D:674:CYS:SG | 2.88 | 0.47 |
| 1:D:202:SER:HA | 1:D:207:LYS:NZ | 2.23 | 0.47 |
| 1:D:506:GLU:HG3 | 1:D:764:MLY:HE3 | 1.96 | 0.47 |
| 1:D:783:LEU:HA | 1:D:786:ILE:HB | 1.97 | 0.47 |
| 1:D:800:ARG:CD | 3:F:149:VAL:O | 2.63 | 0.47 |
| 1:G:599:ASN:CG | 1:G:649:VAL:CB | 2.80 | 0.47 |
| 1:G:817:GLN:CD | 2:H:127:ARG:CB | 2.81 | 0.47 |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:HD13 | 1.92 | 0.47 |
| 1:J:106:LEU:HD12 | 1:J:117:THR:HG21 | 1.96 | 0.47 |
| 1:J:640:LYS:HD2 | 1:J:646:PHE:O | 2.15 | 0.47 |
| 2:K:137:TRP:CZ3 | 2:K:145:ALA:N | 2.81 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:723:ARG:HH11 | 1:M:723:ARG:HG3 | 1.78 | 0.47 |
| 1:S:727:LEU:HD22 | 1:S:783:LEU:HD22 | 1.96 | 0.47 |
| 1:S:87:MLY:HD3 | 1:S:87:MLY:HH12 | 1.61 | 0.47 |
| 4:Z:162:ASN:OD1 | 4:Z:277:THR:HG22 | 2.15 | 0.47 |
| 4:2:244:ASP:HA | 4:Z:324:THR:O | 2.09 | 0.47 |
| 4:Z:299:MET:HE2 | 4:Z:331:ALA:HB2 | 1.96 | 0.47 |
| 4:8:299:MET:HE2 | 4:8:331:ALA:HB2 | 1.96 | 0.47 |
| 1:A:188:ASN:ND2 | 1:A:674:CYS:SG | 2.88 | 0.47 |
| 1:A:559:LEU:HD23 | 1:A:560:GLY:N | 2.30 | 0.47 |
| 1:A:595:TRP:CD1 | 1:A:595:TRP:N | 2.80 | 0.47 |
| 1:A:695:LEU:HB3 | 1:A:701:LEU:HD22 | 1.97 | 0.47 |
| 1:D:154:HIS:CE1 | 1:D:156:PHE:CE2 | 3.02 | 0.47 |
| 1:D:723:ARG:HE | 1:D:779:ARG:HG3 | 1.80 | 0.47 |
| 1:G:154:HIS:CE1 | 1:G:156:PHE:CE2 | 3.02 | 0.47 |
| 1:G:646:PHE:HE2 | 1:G:652:LEU:CG | 2.24 | 0.47 |
| 1:G:506:GLU:HG2 | 1:G:759:ALA:HB1 | 1.97 | 0.47 |
| 2:H:160:GLY:O | 2:H:161:GLU:HG2 | 2.15 | 0.47 |
| 1:J:154:HIS:CE1 | 1:J:156:PHE:CE2 | 3.02 | 0.47 |
| 1:J:248:MLY:HE2 | 1:J:250:ILE:HD11 | 1.95 | 0.47 |
| 1:J:524:GLU:HB3 | 1:J:528:MLY:HG2 | 1.97 | 0.47 |
| 1:J:578:HIS:HB3 | 1:J:592:ILE:CD1 | 2.38 | 0.47 |
| 1:J:675:ILE:CG2 | 1:J:676:ILE:N | 2.74 | 0.47 |
| 1:M:629:GLU:CA | 1:M:643:GLY:C | 2.73 | 0.47 |
| 1:S:176:LEU:N | 1:S:176:LEU:CD1 | 2.75 | 0.47 |
| 1:S:214:MET:C | 1:S:340:ILE:CD1 | 2.82 | 0.47 |
| 1:G:542:PHE:CD2 | 4:V:143:TYR:CD1 | 3.03 | 0.47 |
| 1:G:411:GLU:H | 4:V:333:PRO:HB2 | 1.80 | 0.47 |
| 4:X:162:ASN:OD1 | 4:X:277:THR:HG22 | 2.15 | 0.47 |
| 4:2:287:ILE:CD1 | 4:4:203:THR:HB | 2.44 | 0.47 |
| 4:7:299:MET:HE2 | 4:7:331:ALA:HB2 | 1.96 | 0.47 |
| 4:9:253:GLU:HA | 4:9:256:ARG:CG | 2.42 | 0.47 |
| 1:A:332:MET:O | 1:A:336:SER:OG | 2.27 | 0.47 |
| 1:A:554:LEU:HD12 | 1:A:554:LEU:HA | 1.76 | 0.47 |
| 1:A:646:PHE:HE2 | 1:A:652:LEU:CG | 2.24 | 0.47 |
| 1:D:507:GLY:HA2 | 1:D:762:HIS:ND1 | 2.30 | 0.47 |
| 1:D:723:ARG:HG3 | 1:D:723:ARG:HH11 | 1.79 | 0.47 |
| 2:E:137:TRP:CA | 2:E:145:ALA:HB2 | 2.38 | 0.47 |
| 1:G:106:LEU:HD12 | 1:G:117:THR:HG21 | 1.96 | 0.47 |
| 1:G:136:ASN:O | 1:G:139:VAL:N | 2.47 | 0.47 |
| 1:G:640:LYS:HB3 | 1:G:645:SER:CB | 2.42 | 0.47 |
| 1:G:762:HIS:N | 1:G:762:HIS:CD2 | 2.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:130:PRO:O | 2:H:131:GLU:C | 2.52 | 0.47 |
| 1:J:218:LEU:HA | 1:J:221:GLN:H | 1.80 | 0.47 |
| 1:J:406:VAL:CG1 | 1:J:407:GLY:H | 2.28 | 0.47 |
| 1:J:84:MLY:CH1 | 1:J:715:VAL:HG21 | 2.44 | 0.47 |
| 2:K:160:GLY:O | 2:K:161:GLU:HG2 | 2.14 | 0.47 |
| 1:M:106:LEU:HD12 | 1:M:117:THR:HG21 | 1.96 | 0.47 |
| 1:M:278:GLN:HB3 | 1:M:278:GLN:HE21 | 1.42 | 0.47 |
| 1:M:292:MET:HE1 | 1:M:309:PRO:HD3 | 1.97 | 0.47 |
| 1:M:542:PHE:CD2 | 4:Z:143:TYR:CD1 | 3.02 | 0.47 |
| 1:M:695:LEU:HB3 | 1:M:701:LEU:HD22 | 1.97 | 0.47 |
| 1:M:804:ARG:C | 1:M:808:GLU:H | 2.09 | 0.47 |
| 1:S:107:MLY:CB | 1:S:686:MET:HE2 | 2.39 | 0.47 |
| 4:V:299:MET:HE2 | 4:V:331:ALA:HB2 | 1.96 | 0.47 |
| 1:G:538:GLU:HA | 4:V:351:THR:H | 1.77 | 0.47 |
| 4:X:253:GLU:HA | 4:X:256:ARG:CG | 2.42 | 0.47 |
| 4:X:299:MET:HE2 | 4:X:331:ALA:HB2 | 1.95 | 0.47 |
| 4:2:287:ILE:HG21 | 4:4:203:THR:CA | 2.44 | 0.47 |
| 4:5:162:ASN:OD1 | 4:5:277:THR:HG22 | 2.15 | 0.47 |
| 4:6:253:GLU:HA | 4:6:256:ARG:CG | 2.42 | 0.47 |
| 4:6:162:ASN:OD1 | 4:6:277:THR:HG22 | 2.15 | 0.47 |
| 1:A:538:GLU:HA | 4:8:351:THR:H | 1.78 | 0.47 |
| 1:A:154:HIS:CE1 | 1:A:156:PHE:CE2 | 3.02 | 0.47 |
| 1:A:543:PRO:HD2 | 4:8:146:GLY:O | 2.15 | 0.47 |
| 1:A:550:PHE:CE2 | 1:A:592:ILE:CG2 | 2.97 | 0.47 |
| 1:A:689:GLU:O | 1:A:689:GLU:HG2 | 2.14 | 0.47 |
| 2:B:139:ALA:C | 2:B:141:PRO:HD3 | 2.33 | 0.47 |
| 1:D:248:MLY:HE2 | 1:D:250:ILE:HD11 | 1.96 | 0.47 |
| 1:D:311:ASP:CB | 1:D:312:TYR:CE1 | 2.98 | 0.47 |
| 1:D:714:ARG:HD3 | 1:D:766:PHE:CE2 | 2.50 | 0.47 |
| 2:E:160:GLY:O | 2:E:161:GLU:HG2 | 2.14 | 0.47 |
| 1:G:41:VAL:CG1 | 1:G:42:HIS:N | 2.75 | 0.47 |
| 1:G:559:LEU:HD23 | 1:G:560:GLY:N | 2.30 | 0.47 |
| 3:I:53:PRO:O | 3:I:55:LYS:HG3 | 2.14 | 0.47 |
| 1:J:640:LYS:C | 4:W:23:GLY:C | 2.74 | 0.47 |
| 1:J:795:ARG:HE | 3:L:116:GLU:CB | 2.28 | 0.47 |
| 1:M:154:HIS:CE1 | 1:M:156:PHE:CE2 | 3.02 | 0.47 |
| 1:S:564:ASN:HD22 | 1:S:582:VAL:HB | 1.79 | 0.47 |
| 1:S:640:LYS:HD2 | 1:S:646:PHE:O | 2.15 | 0.47 |
| 1:S:762:HIS:CD2 | 1:S:762:HIS:N | 2.78 | 0.47 |
| 1:S:765:VAL:CG1 | 1:S:766:PHE:N | 2.77 | 0.47 |
| 1:S:795:ARG:HB2 | 3:U:35:ARG:CZ | 2.40 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:543:PRO:HD2 | 4:W:146:GLY:O | 2.15 | 0.47 |
| 4:W:285:CYS:O | 4:Y:202:THR:CG2 | 2.62 | 0.47 |
| 4:4:322:PRO:CA | 4:6:244:ASP:HB2 | 2.45 | 0.47 |
| 1:A:732:ILE:H | 1:A:733:PRO:HD2 | 1.74 | 0.47 |
| 1:A:793:ARG:O | 1:A:797:PHE:N | 2.40 | 0.47 |
| 2:B:88:LEU:HB3 | 2:B:91:ALA:HB2 | 1.97 | 0.47 |
| 1:D:406:VAL:CG1 | 1:D:407:GLY:H | 2.28 | 0.47 |
| 1:D:543:PRO:HD2 | 4:9:146:GLY:O | 2.15 | 0.47 |
| 1:D:559:LEU:HD23 | 1:D:560:GLY:N | 2.30 | 0.47 |
| 1:G:556:ASP:OD1 | 4:X:47:MET:CE | 2.27 | 0.47 |
| 1:G:510:TRP:CZ2 | 1:G:768:MLY:HH11 | 2.50 | 0.47 |
| 1:G:97:LEU:HD12 | 1:G:97:LEU:HA | 1.67 | 0.47 |
| 1:J:188:ASN:ND2 | 1:J:674:CYS:SG | 2.88 | 0.47 |
| 1:J:311:ASP:CB | 1:J:312:TYR:CE1 | 2.98 | 0.47 |
| 1:J:42:HIS:O | 1:J:45:GLN:O | 2.33 | 0.47 |
| 1:J:559:LEU:HD23 | 1:J:560:GLY:N | 2.30 | 0.47 |
| 1:J:715:VAL:CG1 | 1:J:720:PHE:HB2 | 2.45 | 0.47 |
| 1:J:732:ILE:CG2 | 1:J:747:LEU:HD12 | 0.35 | 0.47 |
| 1:M:550:PHE:CE2 | 1:M:592:ILE:CG2 | 2.97 | 0.47 |
| 1:M:783:LEU:CD1 | 1:M:783:LEU:N | 2.78 | 0.47 |
| 2:N:130:PRO:O | 2:N:131:GLU:C | 2.52 | 0.47 |
| 2:N:160:GLY:O | 2:N:161:GLU:HG2 | 2.14 | 0.47 |
| 1:S:154:HIS:CE1 | 1:S:156:PHE:CE2 | 3.02 | 0.47 |
| 1:S:122:PHE:CE2 | 1:S:700:VAL:HA | 2.50 | 0.47 |
| 1:J:538:GLU:HA | 4:W:351:THR:H | 1.77 | 0.47 |
| 1:M:530:MET:HE3 | 4:Z:355:MET:SD | 2.54 | 0.47 |
| 4:3:253:GLU:HA | 4:3:256:ARG:CG | 2.42 | 0.46 |
| 4:6:299:MET:HE2 | 4:6:331:ALA:HB2 | 1.96 | 0.46 |
| 1:A:406:VAL:CG1 | 1:A:407:GLY:H | 2.28 | 0.46 |
| 1:A:524:GLU:HB3 | 1:A:528:MLY:HG2 | 1.96 | 0.46 |
| 1:A:724:TYR:HD1 | 1:A:727:LEU:CD1 | 2.27 | 0.46 |
| 1:D:332:MET:O | 1:D:336:SER:OG | 2.27 | 0.46 |
| 1:D:214:MET:C | 1:D:340:ILE:CD1 | 2.82 | 0.46 |
| 1:D:406:VAL:CG1 | 1:D:407:GLY:N | 2.77 | 0.46 |
| 1:D:640:LYS:C | 4:9:23:GLY:C | 2.74 | 0.46 |
| 1:D:793:ARG:O | 1:D:797:PHE:N | 2.39 | 0.46 |
| 3:F:50:LEU:O | 3:F:53:PRO:CD | 2.63 | 0.46 |
| 1:G:695:LEU:HB3 | 1:G:701:LEU:HD22 | 1.97 | 0.46 |
| 1:G:715:VAL:CG1 | 1:G:720:PHE:HB2 | 2.46 | 0.46 |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG13 | 1.95 | 0.46 |
| 1:J:496:PHE:CE2 | 1:J:514:ASP:HA | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:540:CYS:N | 4:W:349:LEU:HD11 | 2.31 | 0.46 |
| 1:J:84:MLY:CH1 | 1:J:720:PHE:CE1 | 2.82 | 0.46 |
| 1:J:84:MLY:N | 1:J:723:ARG:NE | 2.34 | 0.46 |
| 1:M:712:PRO:HB2 | 1:M:713:SER:H | 1.61 | 0.46 |
| 1:M:505:MLY:HG3 | 1:M:762:HIS:CE1 | 2.49 | 0.46 |
| 2:N:117:LEU:CG | 2:N:147:ASN:OD1 | 2.52 | 0.46 |
| 1:M:797:PHE:CD2 | 3:O:126:LEU:HD22 | 2.49 | 0.46 |
| 1:S:136:ASN:HA | 1:S:137:PRO:HD3 | 1.50 | 0.46 |
| 3:U:50:LEU:O | 3:U:53:PRO:CD | 2.63 | 0.46 |
| 3:U:53:PRO:O | 3:U:55:LYS:HG3 | 2.15 | 0.46 |
| 1:S:543:PRO:HD2 | 4:2:146:GLY:O | 2.15 | 0.46 |
| 1:A:543:PRO:CD | 4:8:143:TYR:O | 2.64 | 0.46 |
| 1:D:529:PRO:HB2 | 4:9:354:GLN:HB3 | 1.98 | 0.46 |
| 1:A:374:GLN:NE2 | 1:A:403:TYR:CE1 | 2.84 | 0.46 |
| 1:A:568:PRO:HD3 | 1:A:579:PHE:HA | 1.96 | 0.46 |
| 1:A:715:VAL:CG1 | 1:A:720:PHE:HB2 | 2.45 | 0.46 |
| 1:A:769:ALA:C | 1:A:772:LEU:H | 2.19 | 0.46 |
| 1:D:218:LEU:CD2 | 1:D:222:ILE:CG1 | 2.86 | 0.46 |
| 1:D:30:MLY:HB3 | 1:D:31:PRO:HD2 | 1.97 | 0.46 |
| 1:D:322:VAL:HB | 1:D:325:ILE:HG13 | 1.98 | 0.46 |
| 1:D:374:GLN:NE2 | 1:D:403:TYR:CE1 | 2.84 | 0.46 |
| 1:D:695:LEU:HB3 | 1:D:701:LEU:HD22 | 1.97 | 0.46 |
| 1:G:795:ARG:N | 3:I:118:MET:HE1 | 2.28 | 0.46 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:CA | 2.99 | 0.46 |
| 1:M:768:MLY:O | 1:M:770:GLY:CA | 2.63 | 0.46 |
| 1:S:188:ASN:ND2 | 1:S:674:CYS:SG | 2.88 | 0.46 |
| 1:S:265:ILE:CG2 | 1:S:266:GLU:N | 2.78 | 0.46 |
| 1:S:400:ALA:HB1 | 1:S:606:THR:CG2 | 2.45 | 0.46 |
| 1:S:810:ARG:NH1 | 1:S:810:ARG:HG2 | 2.29 | 0.46 |
| 2:T:140:PHE:O | 2:T:141:PRO:C | 2.33 | 0.46 |
| 1:G:543:PRO:HD2 | 4:V:146:GLY:O | 2.15 | 0.46 |
| 4:V:253:GLU:HA | 4:V:256:ARG:CG | 2.42 | 0.46 |
| 1:J:642:LYS:HA | 4:W:21:PHE:C | 2.36 | 0.46 |
| 1:M:411:GLU:H | 4:Z:333:PRO:HB2 | 1.81 | 0.46 |
| 4:7:162:ASN:OD1 | 4:7:277:THR:HG22 | 2.15 | 0.46 |
| 1:D:534:SER:HB2 | 4:9:354:GLN:HE22 | 1.56 | 0.46 |
| 1:A:496:PHE:CE2 | 1:A:514:ASP:HA | 2.50 | 0.46 |
| 1:A:810:ARG:HG2 | 1:A:810:ARG:NH1 | 2.29 | 0.46 |
| 1:A:82:PRO:HG2 | 1:A:85:TYR:CE2 | 2.50 | 0.46 |
| 2:B:121:LEU:O | 2:B:128:PHE:CG | 2.61 | 0.46 |
| 1:D:540:CYS:N | 4:9:349:LEU:HD11 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:715:VAL:HG11 | 1:D:720:PHE:CD1 | 2.49 | 0.46 |
| 1:D:783:LEU:CD1 | 1:D:783:LEU:N | 2.78 | 0.46 |
| 1:D:831:TRP:CE3 | 2:E:34:ILE:CD1 | 2.97 | 0.46 |
| 1:G:265:ILE:CG2 | 1:G:266:GLU:N | 2.79 | 0.46 |
| 1:G:322:VAL:HB | 1:G:325:ILE:HG13 | 1.98 | 0.46 |
| 1:G:406:VAL:CG1 | 1:G:407:GLY:H | 2.28 | 0.46 |
| 1:G:643:GLY:CA | 4:V:24:ASP:OD1 | 2.62 | 0.46 |
| 1:G:90:ASP:OD2 | 1:G:764:MLY:HH12 | 2.00 | 0.46 |
| 3:I:52:ASN:CB | 3:I:53:PRO:HD3 | 2.28 | 0.46 |
| 1:J:649:VAL:HG23 | 1:J:649:VAL:HA | 1.83 | 0.46 |
| 1:J:82:PRO:HG2 | 1:J:85:TYR:CE2 | 2.50 | 0.46 |
| 1:M:136:ASN:O | 1:M:139:VAL:N | 2.47 | 0.46 |
| 1:M:496:PHE:CE2 | 1:M:514:ASP:HA | 2.50 | 0.46 |
| 1:M:400:ALA:HB1 | 1:M:606:THR:CG2 | 2.45 | 0.46 |
| 1:M:84:MLY:CH2 | 1:M:715:VAL:HG13 | 2.46 | 0.46 |
| 1:M:839:MLY:HH11 | 2:N:158:THR:HG21 | 1.97 | 0.46 |
| 1:S:508:ILE:CD1 | 1:S:759:ALA:CB | 2.71 | 0.46 |
| 1:S:559:LEU:HD23 | 1:S:560:GLY:N | 2.30 | 0.46 |
| 2:T:88:LEU:HB3 | 2:T:91:ALA:HB2 | 1.98 | 0.46 |
| 4:3:299:MET:HE2 | 4:3:331:ALA:HB2 | 1.97 | 0.46 |
| 4:3:6:THR:HG22 | 4:3:101:HIS:HA | 1.97 | 0.46 |
| 4:5:299:MET:HE2 | 4:5:331:ALA:HB2 | 1.97 | 0.46 |
| 1:D:642:LYS:HA | 4:9:21:PHE:C | 2.36 | 0.46 |
| 1:A:144:ARG:HA | 1:A:144:ARG:HD2 | 1.79 | 0.46 |
| 1:A:311:ASP:CB | 1:A:312:TYR:CE1 | 2.98 | 0.46 |
| 1:D:122:PHE:CE2 | 1:D:700:VAL:HA | 2.50 | 0.46 |
| 1:D:134:VAL:C | 1:D:136:ASN:H | 2.16 | 0.46 |
| 1:D:519:LEU:N | 1:D:519:LEU:CD1 | 2.77 | 0.46 |
| 1:D:834:LEU:CD1 | 2:E:54:MET:HB2 | 2.44 | 0.46 |
| 1:G:436:MLY:HE3 | 1:G:626:TYR:HE1 | 1.77 | 0.46 |
| 1:G:149:GLN:CB | 1:G:763:THR:HG23 | 2.43 | 0.46 |
| 1:G:714:ARG:HD3 | 1:G:766:PHE:CE2 | 2.50 | 0.46 |
| 2:H:137:TRP:CA | 2:H:145:ALA:HB2 | 2.37 | 0.46 |
| 1:J:30:MLY:HB3 | 1:J:31:PRO:HD2 | 1.97 | 0.46 |
| 1:J:374:GLN:NE2 | 1:J:403:TYR:CE1 | 2.84 | 0.46 |
| 1:J:519:LEU:CD1 | 1:J:519:LEU:N | 2.77 | 0.46 |
| 1:J:149:GLN:OE1 | 1:J:763:THR:HG21 | 2.15 | 0.46 |
| 1:J:757:GLN:CA | 1:J:776:GLU:HB3 | 2.44 | 0.46 |
| 1:J:798:LEU:HD22 | 3:L:118:MET:CG | 2.45 | 0.46 |
| 1:M:374:GLN:NE2 | 1:M:403:TYR:CE1 | 2.84 | 0.46 |
| 1:M:418:THR:CG2 | 1:M:419:VAL:N | 2.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:41:VAL:CG1 | 1:M:42:HIS:N | 2.75 | 0.46 |
| 1:M:797:PHE:CE2 | 3:O:146:ILE:CD1 | 2.98 | 0.46 |
| 1:S:406:VAL:CG1 | 1:S:407:GLY:H | 2.28 | 0.46 |
| 1:S:418:THR:CG2 | 1:S:419:VAL:N | 2.79 | 0.46 |
| 1:S:770:GLY:O | 1:S:771:LEU:CA | 2.63 | 0.46 |
| 1:S:818:TYR:C | 2:T:90:GLY:HA3 | 2.35 | 0.46 |
| 1:J:529:PRO:HB2 | 4:W:354:GLN:HB3 | 1.98 | 0.46 |
| 4:Y:6:THR:HG22 | 4:Y:101:HIS:HA | 1.98 | 0.46 |
| 1:A:322:VAL:HB | 1:A:325:ILE:HG13 | 1.98 | 0.46 |
| 1:A:42:HIS:O | 1:A:45:GLN:O | 2.33 | 0.46 |
| 1:A:544:LYS:HD2 | 4:8:147:ARG:CB | 2.36 | 0.46 |
| 1:A:400:ALA:HB1 | 1:A:606:THR:CG2 | 2.45 | 0.46 |
| 1:D:553:MLY:CE | 4:W:45:VAL:CA | 2.49 | 0.46 |
| 1:D:820:VAL:HG11 | 2:E:136:MET:SD | 2.55 | 0.46 |
| 1:G:42:HIS:O | 1:G:45:GLN:O | 2.33 | 0.46 |
| 1:G:496:PHE:CE2 | 1:G:514:ASP:HA | 2.50 | 0.46 |
| 1:G:524:GLU:HB3 | 1:G:528:MLY:HG2 | 1.97 | 0.46 |
| 1:G:568:PRO:HD3 | 1:G:579:PHE:HA | 1.97 | 0.46 |
| 3:I:50:LEU:O | 3:I:53:PRO:CD | 2.63 | 0.46 |
| 1:J:292:MET:HE1 | 1:J:309:PRO:CG | 2.46 | 0.46 |
| 1:J:322:VAL:HB | 1:J:325:ILE:HG13 | 1.98 | 0.46 |
| 1:J:448:GLN:C | 1:J:450:ASP:H | 2.19 | 0.46 |
| 3:L:53:PRO:O | 3:L:55:LYS:HG3 | 2.15 | 0.46 |
| 1:M:188:ASN:ND2 | 1:M:674:CYS:SG | 2.88 | 0.46 |
| 1:M:361:TYR:O | 1:M:364:LEU:HB2 | 2.16 | 0.46 |
| 1:M:406:VAL:CG1 | 1:M:407:GLY:H | 2.28 | 0.46 |
| 1:M:715:VAL:CG1 | 1:M:720:PHE:HB2 | 2.45 | 0.46 |
| 1:M:805:ALA:O | 1:M:807:VAL:N | 2.44 | 0.46 |
| 1:M:821:ARG:CZ | 2:N:127:ARG:CD | 2.94 | 0.46 |
| 1:S:524:GLU:HB3 | 1:S:528:MLY:HG2 | 1.97 | 0.46 |
| 1:S:770:GLY:C | 1:S:771:LEU:HA | 2.32 | 0.46 |
| 3:U:52:ASN:CB | 3:U:53:PRO:HD3 | 2.28 | 0.46 |
| 4:9:6:THR:HG22 | 4:9:101:HIS:HA | 1.98 | 0.46 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HD12 | 0.94 | 0.46 |
| 1:D:508:ILE:HA | 1:D:761:GLY:HA3 | 1.97 | 0.46 |
| 1:D:723:ARG:NH2 | 1:D:779:ARG:CZ | 2.79 | 0.46 |
| 1:D:82:PRO:HG2 | 1:D:85:TYR:CE2 | 2.50 | 0.46 |
| 2:E:114:LYS:CG | 2:E:146:GLY:HA2 | 2.46 | 0.46 |
| 1:G:139:VAL:HG12 | 1:G:143:TYR:HD2 | 1.81 | 0.46 |
| 1:G:84:MLY:CG | 1:G:723:ARG:HD2 | 2.45 | 0.46 |
| 2:H:88:LEU:HB3 | 2:H:91:ALA:HB2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:52:ASN:CB | 3:I:53:PRO:CD | 2.92 | 0.46 |
| 1:J:310:TYR:CE2 | 1:J:320:ILE:CD1 | 2.94 | 0.46 |
| 1:J:564:ASN:HD22 | 1:J:582:VAL:HB | 1.79 | 0.46 |
| 2:K:121:LEU:HA | 2:K:128:PHE:CD2 | 2.47 | 0.46 |
| 1:M:139:VAL:HG12 | 1:M:143:TYR:HD2 | 1.81 | 0.46 |
| 1:M:564:ASN:HD22 | 1:M:582:VAL:HB | 1.79 | 0.46 |
| 1:M:714:ARG:HD3 | 1:M:766:PHE:CE2 | 2.50 | 0.46 |
| 1:S:139:VAL:HG12 | 1:S:143:TYR:HD2 | 1.81 | 0.46 |
| 1:S:326:ASP:O | 1:S:330:GLU:HG2 | 2.16 | 0.46 |
| 1:S:496:PHE:CE2 | 1:S:514:ASP:HA | 2.50 | 0.46 |
| 1:S:746:LYS:HZ1 | 3:U:96:LYS:CA | 2.13 | 0.46 |
| 1:S:805:ALA:CA | 1:S:807:VAL:N | 2.78 | 0.46 |
| 1:S:820:VAL:CG1 | 2:T:136:MET:HE3 | 2.30 | 0.46 |
| 1:M:642:LYS:HA | 4:Z:21:PHE:C | 2.36 | 0.46 |
| 1:S:543:PRO:CD | 4:2:143:TYR:O | 2.64 | 0.46 |
| 4:2:204:ALA:H | 4:Z:287:ILE:CB | 2.13 | 0.46 |
| 4:3:322:PRO:CA | 4:5:244:ASP:HB2 | 2.45 | 0.46 |
| 1:A:139:VAL:HG12 | 1:A:143:TYR:HD2 | 1.81 | 0.46 |
| 1:A:725:ARG:NE | 1:A:733:PRO:CB | 1.95 | 0.46 |
| 1:A:797:PHE:CD2 | 3:C:146:ILE:HD12 | 2.49 | 0.46 |
| 1:D:42:HIS:O | 1:D:45:GLN:O | 2.33 | 0.46 |
| 1:D:636:LYS:O | 4:9:144:ALA:HB1 | 2.15 | 0.46 |
| 1:D:732:ILE:CG2 | 1:D:747:LEU:CD1 | 0.65 | 0.46 |
| 1:D:836:PHE:CD2 | 2:E:161:GLU:HG2 | 2.51 | 0.46 |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:HD11 | 1.75 | 0.46 |
| 1:G:725:ARG:CG | 1:G:733:PRO:HA | 2.43 | 0.46 |
| 1:G:725:ARG:HH21 | 1:G:733:PRO:HB2 | 1.81 | 0.46 |
| 1:G:784:ALA:O | 1:G:788:THR:CA | 2.61 | 0.46 |
| 1:G:834:LEU:HD21 | 2:H:34:ILE:HG12 | 1.98 | 0.46 |
| 1:G:817:GLN:CD | 2:H:127:ARG:CG | 2.84 | 0.46 |
| 1:J:202:SER:HA | 1:J:207:LYS:NZ | 2.22 | 0.46 |
| 1:J:265:ILE:CG2 | 1:J:266:GLU:N | 2.79 | 0.46 |
| 1:J:361:TYR:O | 1:J:364:LEU:HB2 | 2.16 | 0.46 |
| 1:J:714:ARG:HD3 | 1:J:766:PHE:CE2 | 2.50 | 0.46 |
| 1:J:783:LEU:N | 1:J:783:LEU:CD1 | 2.78 | 0.46 |
| 1:J:792:ALA:CB | 3:L:42:THR:N | 2.78 | 0.46 |
| 2:K:88:LEU:HB3 | 2:K:91:ALA:HB2 | 1.98 | 0.46 |
| 1:M:322:VAL:HB | 1:M:325:ILE:HG13 | 1.98 | 0.46 |
| 1:M:449:LEU:HA | 1:M:449:LEU:HD12 | 1.60 | 0.46 |
| 1:M:524:GLU:HB3 | 1:M:528:MLY:HG2 | 1.97 | 0.46 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:HE | 1.61 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:817:GLN:OE1 | 2:N:127:ARG:HD2 | 2.16 | 0.46 |
| 2:N:114:LYS:CG | 2:N:146:GLY:HA2 | 2.46 | 0.46 |
| 2:N:88:LEU:HB3 | 2:N:91:ALA:HB2 | 1.98 | 0.46 |
| 1:M:800:ARG:CB | 3:O:149:VAL:HG22 | 2.31 | 0.46 |
| 1:S:311:ASP:CB | 1:S:312:TYR:CE1 | 2.98 | 0.46 |
| 1:S:361:TYR:O | 1:S:364:LEU:HB2 | 2.16 | 0.46 |
| 1:S:642:LYS:HA | 4:2:21:PHE:C | 2.35 | 0.46 |
| 1:S:783:LEU:N | 1:S:783:LEU:CD1 | 2.78 | 0.46 |
| 4:W:162:ASN:OD1 | 4:W:277:THR:HG22 | 2.15 | 0.46 |
| 4:W:6:THR:HG22 | 4:W:101:HIS:HA | 1.98 | 0.46 |
| 1:M:543:PRO:CD | 4:Z:143:TYR:O | 2.64 | 0.46 |
| 4:6:190:MET:O | 4:6:194:THR:HG23 | 2.16 | 0.46 |
| 4:9:299:MET:HE2 | 4:9:331:ALA:HB2 | 1.97 | 0.46 |
| 1:A:206:LYS:CE | 1:A:217:THR:HG23 | 2.30 | 0.46 |
| 1:A:292:MET:CE | 1:A:309:PRO:HA | 2.39 | 0.46 |
| 1:A:335:ASP:OD1 | 1:A:348:MLY:NZ | 2.49 | 0.46 |
| 1:A:629:GLU:HG2 | 1:A:643:GLY:C | 2.35 | 0.46 |
| 1:D:265:ILE:CG2 | 1:D:266:GLU:N | 2.78 | 0.46 |
| 1:D:292:MET:HE3 | 1:D:309:PRO:CA | 2.43 | 0.46 |
| 1:D:289:TYR:OH | 1:D:315:VAL:O | 2.27 | 0.46 |
| 2:E:139:ALA:C | 2:E:141:PRO:HD3 | 2.33 | 0.46 |
| 1:G:188:ASN:ND2 | 1:G:674:CYS:SG | 2.88 | 0.46 |
| 1:G:311:ASP:CB | 1:G:312:TYR:CE1 | 2.98 | 0.46 |
| 1:G:795:ARG:CB | 3:I:35:ARG:HH22 | 2.18 | 0.46 |
| 1:J:732:ILE:CG2 | 1:J:747:LEU:CD1 | 0.65 | 0.46 |
| 1:M:326:ASP:O | 1:M:330:GLU:HG2 | 2.16 | 0.46 |
| 1:S:374:GLN:NE2 | 1:S:403:TYR:CE1 | 2.84 | 0.46 |
| 1:S:664:LEU:HD12 | 1:S:664:LEU:HA | 1.52 | 0.46 |
| 1:S:715:VAL:CG1 | 1:S:720:PHE:HB2 | 2.45 | 0.46 |
| 4:W:190:MET:O | 4:W:194:THR:HG23 | 2.16 | 0.46 |
| 1:M:529:PRO:HB2 | 4:Z:354:GLN:HB3 | 1.98 | 0.46 |
| 4:1:190:MET:O | 4:1:194:THR:HG23 | 2.16 | 0.46 |
| 4:1:6:THR:HG22 | 4:1:101:HIS:HA | 1.98 | 0.46 |
| 1:S:529:PRO:HB2 | 4:2:354:GLN:HB3 | 1.98 | 0.46 |
| 4:7:6:THR:HG22 | 4:7:101:HIS:HA | 1.98 | 0.46 |
| 4:9:366:GLY:O | 4:9:369:ILE:HG22 | 2.16 | 0.46 |
| 1:A:732:ILE:CG2 | 1:A:747:LEU:CD1 | 0.65 | 0.46 |
| 1:D:206:LYS:HD3 | 1:D:217:THR:OG1 | 2.16 | 0.46 |
| 1:D:640:LYS:HB3 | 1:D:645:SER:CB | 2.42 | 0.46 |
| 1:G:544:LYS:HD2 | 4:V:147:ARG:CB | 2.36 | 0.46 |
| 1:G:754:ASP:N | 1:G:779:ARG:CD | 2.65 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:82:PRO:HG2 | 1:G:85:TYR:CE2 | 2.51 | 0.46 |
| 1:J:544:LYS:HD2 | 4:W:147:ARG:CB | 2.36 | 0.46 |
| 1:M:311:ASP:CB | 1:M:312:TYR:CE1 | 2.98 | 0.46 |
| 1:M:354:LEU:HA | 1:M:354:LEU:HD12 | 1.55 | 0.46 |
| 1:M:725:ARG:CG | 1:M:733:PRO:HA | 2.43 | 0.46 |
| 1:S:106:LEU:HD12 | 1:S:117:THR:HG21 | 1.96 | 0.46 |
| 1:S:218:LEU:HD22 | 1:S:222:ILE:HG13 | 1.95 | 0.46 |
| 1:S:322:VAL:HB | 1:S:325:ILE:HG13 | 1.98 | 0.46 |
| 1:S:544:LYS:HD2 | 4:2:147:ARG:CB | 2.36 | 0.46 |
| 1:S:714:ARG:HD3 | 1:S:766:PHE:CE2 | 2.50 | 0.46 |
| 2:T:121:LEU:O | 2:T:128:PHE:CG | 2.61 | 0.46 |
| 1:S:836:PHE:CD1 | 2:T:159:HIS:HA | 2.37 | 0.46 |
| 1:G:538:GLU:OE1 | 4:V:355:MET:HE3 | 2.15 | 0.46 |
| 1:M:642:LYS:CB | 4:Z:24:ASP:O | 2.60 | 0.46 |
| 4:Z:253:GLU:HA | 4:Z:256:ARG:CG | 2.42 | 0.46 |
| 4:1:366:GLY:O | 4:1:369:ILE:HG22 | 2.16 | 0.46 |
| 1:S:540:CYS:N | 4:2:349:LEU:HD11 | 2.30 | 0.46 |
| 4:3:190:MET:O | 4:3:194:THR:HG23 | 2.16 | 0.46 |
| 4:3:366:GLY:O | 4:3:369:ILE:HG22 | 2.16 | 0.46 |
| 4:4:322:PRO:C | 4:6:244:ASP:HB2 | 2.37 | 0.46 |
| 4:5:6:THR:HG22 | 4:5:101:HIS:HA | 1.97 | 0.46 |
| 4:6:366:GLY:O | 4:6:369:ILE:HG22 | 2.16 | 0.46 |
| 1:A:136:ASN:HA | 1:A:137:PRO:HD3 | 1.49 | 0.46 |
| 1:A:418:THR:CG2 | 1:A:419:VAL:N | 2.79 | 0.46 |
| 1:A:485:GLU:OE1 | 1:A:583:HIS:ND1 | 2.49 | 0.46 |
| 1:A:519:LEU:CD1 | 1:A:519:LEU:N | 2.77 | 0.46 |
| 1:A:768:MLY:C | 1:A:771:LEU:CB | 2.94 | 0.46 |
| 1:A:831:TRP:HH2 | 2:B:50:THR:CB | 2.15 | 0.46 |
| 3:C:50:LEU:O | 3:C:53:PRO:CD | 2.63 | 0.46 |
| 1:D:335:ASP:OD1 | 1:D:348:MLY:NZ | 2.49 | 0.46 |
| 1:G:326:ASP:O | 1:G:330:GLU:HG2 | 2.16 | 0.46 |
| 1:G:418:THR:CG2 | 1:G:419:VAL:N | 2.79 | 0.46 |
| 1:G:540:CYS:N | 4:V:349:LEU:HD11 | 2.31 | 0.46 |
| 1:G:95:THR:N | 1:G:713:SER:HB3 | 2.30 | 0.46 |
| 1:G:87:MLY:HH12 | 1:G:87:MLY:HD3 | 1.62 | 0.46 |
| 1:J:629:GLU:HG2 | 1:J:643:GLY:C | 2.35 | 0.46 |
| 1:J:641:LYS:CD | 1:J:647:GLN:CG | 2.72 | 0.46 |
| 1:J:89:GLU:CD | 1:J:153:PRO:HD2 | 2.36 | 0.46 |
| 2:K:112:ILE:O | 2:K:148:VAL:HA | 2.16 | 0.46 |
| 1:M:667:THR:O | 1:M:669:PRO:HD3 | 2.17 | 0.46 |
| 1:S:89:GLU:CD | 1:S:153:PRO:HD2 | 2.36 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:695:LEU:HB3 | 1:S:701:LEU:HD22 | 1.97 | 0.46 |
| 1:S:803:TYR:CE2 | 3:U:17:PHE:CE2 | 3.03 | 0.46 |
| 1:S:835:PHE:O | 1:S:839:MLY:N | 2.49 | 0.46 |
| 2:T:137:TRP:CZ3 | 2:T:145:ALA:N | 2.81 | 0.46 |
| 1:G:642:LYS:CB | 4:V:24:ASP:O | 2.60 | 0.46 |
| 4:Y:366:GLY:O | 4:Y:369:ILE:HG22 | 2.16 | 0.46 |
| 1:M:543:PRO:HD2 | 4:Z:146:GLY:O | 2.15 | 0.46 |
| 4:Z:223:PHE:CD2 | 4:Z:259:GLU:HG3 | 2.51 | 0.46 |
| 4:2:223:PHE:CD2 | 4:2:259:GLU:HG3 | 2.52 | 0.45 |
| 4:4:32:PRO:HB2 | 4:4:34:ILE:HD11 | 1.98 | 0.45 |
| 4:5:190:MET:O | 4:5:194:THR:HG23 | 2.16 | 0.45 |
| 4:6:223:PHE:CD2 | 4:6:259:GLU:HG3 | 2.52 | 0.45 |
| 4:8:223:PHE:CD2 | 4:8:259:GLU:HG3 | 2.51 | 0.45 |
| 1:A:506:GLU:OE2 | 1:A:717:TYR:OH | 2.33 | 0.45 |
| 1:A:795:ARG:CG | 3:C:118:MET:HE1 | 2.46 | 0.45 |
| 1:D:715:VAL:CG1 | 1:D:720:PHE:HB2 | 2.46 | 0.45 |
| 2:E:163:ALA:HA | 2:K:21:GLU:CB | 2.26 | 0.45 |
| 1:G:144:ARG:HA | 1:G:144:ARG:HD2 | 1.78 | 0.45 |
| 1:G:335:ASP:OD1 | 1:G:348:MLY:NZ | 2.49 | 0.45 |
| 1:G:476:GLU:OE2 | 1:G:598:MLY:HH13 | 2.16 | 0.45 |
| 1:G:732:ILE:CG2 | 1:G:747:LEU:HD12 | 0.35 | 0.45 |
| 1:G:835:PHE:O | 1:G:839:MLY:N | 2.49 | 0.45 |
| 1:J:292:MET:HE1 | 1:J:309:PRO:HD3 | 1.97 | 0.45 |
| 1:J:695:LEU:HB3 | 1:J:701:LEU:HD22 | 1.97 | 0.45 |
| 1:J:87:MLY:HD3 | 1:J:87:MLY:HH12 | 1.61 | 0.45 |
| 1:M:265:ILE:CG2 | 1:M:266:GLU:N | 2.79 | 0.45 |
| 1:M:292:MET:HE1 | 1:M:309:PRO:CG | 2.46 | 0.45 |
| 1:M:476:GLU:OE2 | 1:M:598:MLY:HH13 | 2.16 | 0.45 |
| 1:M:94:MET:O | 1:M:713:SER:CA | 2.64 | 0.45 |
| 1:M:786:ILE:CB | 1:M:787:ILE:N | 2.79 | 0.45 |
| 1:M:839:MLY:HH11 | 2:N:158:THR:HG22 | 1.98 | 0.45 |
| 2:N:112:ILE:O | 2:N:148:VAL:HA | 2.17 | 0.45 |
| 1:S:42:HIS:O | 1:S:45:GLN:O | 2.33 | 0.45 |
| 1:S:732:ILE:CG2 | 1:S:747:LEU:CD1 | 0.65 | 0.45 |
| 2:T:139:ALA:C | 2:T:141:PRO:HD3 | 2.33 | 0.45 |
| 1:S:831:TRP:CZ3 | 2:T:34:ILE:HD13 | 2.41 | 0.45 |
| 1:S:795:ARG:HG3 | 3:U:118:MET:HE2 | 1.82 | 0.45 |
| 4:V:223:PHE:CD2 | 4:V:259:GLU:HG3 | 2.51 | 0.45 |
| 1:J:543:PRO:CD | 4:W:143:TYR:O | 2.64 | 0.45 |
| 4:4:190:MET:O | 4:4:194:THR:HG23 | 2.16 | 0.45 |
| 4:5:223:PHE:CD2 | 4:5:259:GLU:HG3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:5:366:GLY:O | 4:5:369:ILE:HG22 | 2.16 | 0.45 |
| 4:6:6:THR:HG22 | 4:6:101:HIS:HA | 1.98 | 0.45 |
| 1:A:206:LYS:HD3 | 1:A:217:THR:OG1 | 2.16 | 0.45 |
| 1:A:265:ILE:CG2 | 1:A:266:GLU:N | 2.79 | 0.45 |
| 1:A:30:MLY:HB3 | 1:A:31:PRO:HD2 | 1.97 | 0.45 |
| 1:A:346:ASP:O | 1:A:350:ALA:N | 2.46 | 0.45 |
| 1:A:464:ILE:CG2 | 1:A:465:ALA:N | 2.79 | 0.45 |
| 1:A:640:LYS:C | 4:8:23:GLY:C | 2.74 | 0.45 |
| 1:A:642:LYS:HA | 4:8:21:PHE:C | 2.36 | 0.45 |
| 1:A:714:ARG:HD3 | 1:A:766:PHE:CE2 | 2.51 | 0.45 |
| 1:A:794:CYS:O | 1:A:797:PHE:HB3 | 2.17 | 0.45 |
| 1:A:800:ARG:CB | 3:C:149:VAL:CG2 | 2.54 | 0.45 |
| 1:D:221:GLN:H | 1:D:221:GLN:HG2 | 1.47 | 0.45 |
| 1:D:326:ASP:O | 1:D:330:GLU:HG2 | 2.16 | 0.45 |
| 1:D:724:TYR:HD1 | 1:D:727:LEU:CD1 | 2.27 | 0.45 |
| 1:D:836:PHE:CB | 2:E:161:GLU:OE1 | 2.65 | 0.45 |
| 1:G:374:GLN:NE2 | 1:G:403:TYR:CE1 | 2.84 | 0.45 |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:CD1 | 2.50 | 0.45 |
| 1:J:206:LYS:HD3 | 1:J:217:THR:OG1 | 2.16 | 0.45 |
| 1:J:326:ASP:O | 1:J:330:GLU:HG2 | 2.16 | 0.45 |
| 1:J:725:ARG:HH21 | 1:J:733:PRO:HB2 | 1.82 | 0.45 |
| 3:L:49:ILE:CA | 3:L:52:ASN:ND2 | 2.54 | 0.45 |
| 3:L:50:LEU:O | 3:L:53:PRO:CD | 2.63 | 0.45 |
| 1:M:179:GLY:O | 1:M:185:LYS:HE2 | 2.17 | 0.45 |
| 1:M:42:HIS:O | 1:M:45:GLN:O | 2.33 | 0.45 |
| 1:S:578:HIS:HB3 | 1:S:592:ILE:CD1 | 2.38 | 0.45 |
| 1:S:82:PRO:HG2 | 1:S:85:TYR:CE2 | 2.50 | 0.45 |
| 2:T:112:ILE:O | 2:T:148:VAL:HA | 2.16 | 0.45 |
| 4:X:324:THR:O | 4:Z:245:GLY:CA | 2.64 | 0.45 |
| 4:4:366:GLY:O | 4:4:369:ILE:HG22 | 2.16 | 0.45 |
| 1:A:326:ASP:O | 1:A:330:GLU:HG2 | 2.16 | 0.45 |
| 1:A:640:LYS:HB3 | 1:A:645:SER:CB | 2.42 | 0.45 |
| 1:A:642:LYS:NZ | 4:8:340:TRP:O | 2.50 | 0.45 |
| 1:A:505:MLY:HB2 | 1:A:761:GLY:C | 2.36 | 0.45 |
| 1:A:809:ARG:CZ | 2:B:124:GLY:CA | 2.94 | 0.45 |
| 2:B:149:ASP:CG | 2:B:150:TYR:N | 2.49 | 0.45 |
| 1:D:14:ALA:N | 1:D:15:PRO:HD2 | 2.32 | 0.45 |
| 1:D:186:THR:O | 1:D:190:MLY:HG2 | 2.17 | 0.45 |
| 1:D:346:ASP:O | 1:D:350:ALA:N | 2.46 | 0.45 |
| 1:D:448:GLN:C | 1:D:450:ASP:H | 2.19 | 0.45 |
| 1:D:507:GLY:HA2 | 1:D:762:HIS:NE2 | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:794:CYS:O | 1:D:797:PHE:HB3 | 2.17 | 0.45 |
| 1:G:400:ALA:HB1 | 1:G:606:THR:CG2 | 2.45 | 0.45 |
| 1:G:723:ARG:CG | 1:G:723:ARG:NH1 | 2.80 | 0.45 |
| 1:G:89:GLU:CD | 1:G:153:PRO:HD2 | 2.36 | 0.45 |
| 1:J:136:ASN:O | 1:J:139:VAL:N | 2.47 | 0.45 |
| 1:J:136:ASN:HA | 1:J:137:PRO:HD3 | 1.50 | 0.45 |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:HG13 | 1.95 | 0.45 |
| 1:M:559:LEU:HD23 | 1:M:560:GLY:N | 2.30 | 0.45 |
| 1:M:408:VAL:HG22 | 1:M:636:LYS:HG2 | 1.52 | 0.45 |
| 1:M:723:ARG:NH1 | 1:M:723:ARG:CG | 2.79 | 0.45 |
| 1:S:103:LEU:HD22 | 1:S:692:LEU:HG | 1.98 | 0.45 |
| 1:S:448:GLN:C | 1:S:450:ASP:H | 2.19 | 0.45 |
| 1:S:449:LEU:HA | 1:S:449:LEU:HD12 | 1.60 | 0.45 |
| 1:S:792:ALA:CB | 3:U:42:THR:N | 2.75 | 0.45 |
| 1:S:791:GLN:CD | 3:U:115:GLY:HA3 | 2.32 | 0.45 |
| 4:W:299:MET:HE2 | 4:W:331:ALA:HB2 | 1.99 | 0.45 |
| 4:X:190:MET:O | 4:X:194:THR:HG23 | 2.16 | 0.45 |
| 4:1:223:PHE:CD2 | 4:1:259:GLU:HG3 | 2.52 | 0.45 |
| 4:3:322:PRO:C | 4:5:244:ASP:HB2 | 2.37 | 0.45 |
| 1:A:639:GLY:CA | 4:8:344:SER:O | 2.40 | 0.45 |
| 1:A:529:PRO:HB2 | 4:8:354:GLN:HB3 | 1.98 | 0.45 |
| 1:A:134:VAL:C | 1:A:136:ASN:H | 2.16 | 0.45 |
| 1:A:448:GLN:C | 1:A:450:ASP:H | 2.19 | 0.45 |
| 1:A:667:THR:O | 1:A:669:PRO:HD3 | 2.17 | 0.45 |
| 1:A:783:LEU:N | 1:A:783:LEU:CD1 | 2.79 | 0.45 |
| 1:A:831:TRP:CD1 | 2:B:67:MET:SD | 3.09 | 0.45 |
| 1:D:99:GLU:N | 1:D:100:PRO:CD | 2.79 | 0.45 |
| 1:D:310:TYR:CE2 | 1:D:320:ILE:CD1 | 2.95 | 0.45 |
| 1:D:361:TYR:O | 1:D:364:LEU:HB2 | 2.16 | 0.45 |
| 1:D:418:THR:CG2 | 1:D:419:VAL:N | 2.79 | 0.45 |
| 1:D:818:TYR:HB3 | 2:E:90:GLY:HA3 | 0.45 | 0.45 |
| 1:D:795:ARG:CG | 3:F:118:MET:CE | 2.55 | 0.45 |
| 1:G:206:LYS:HD2 | 1:G:217:THR:CG2 | 2.17 | 0.45 |
| 1:G:30:MLY:HB3 | 1:G:31:PRO:HD2 | 1.97 | 0.45 |
| 1:G:384:ASP:OD1 | 1:G:394:SER:OG | 2.28 | 0.45 |
| 1:G:464:ILE:CG2 | 1:G:465:ALA:N | 2.80 | 0.45 |
| 1:G:84:MLY:NZ | 1:G:724:TYR:HE2 | 2.14 | 0.45 |
| 1:G:795:ARG:CB | 3:I:35:ARG:NH2 | 2.78 | 0.45 |
| 1:J:810:ARG:NH1 | 1:J:810:ARG:HG2 | 2.29 | 0.45 |
| 1:M:186:THR:O | 1:M:190:MLY:HG2 | 2.17 | 0.45 |
| 1:M:296:MLY:O | 1:M:299:LEU:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:701:LEU:HD12 | 1:M:701:LEU:HA | 1.55 | 0.45 |
| 1:M:783:LEU:O | 1:M:786:ILE:CB | 2.63 | 0.45 |
| 3:O:62:ALA:O | 3:O:63:ILE:HG13 | 2.14 | 0.45 |
| 1:S:179:GLY:O | 1:S:185:LYS:HE2 | 2.17 | 0.45 |
| 1:S:335:ASP:OD1 | 1:S:348:MLY:NZ | 2.49 | 0.45 |
| 1:S:798:LEU:HD12 | 1:S:798:LEU:HA | 1.36 | 0.45 |
| 2:T:160:GLY:O | 2:T:161:GLU:HG2 | 2.14 | 0.45 |
| 1:G:529:PRO:HB2 | 4:V:354:GLN:HB3 | 1.98 | 0.45 |
| 4:W:366:GLY:O | 4:W:369:ILE:HG22 | 2.16 | 0.45 |
| 4:8:366:GLY:O | 4:8:369:ILE:HG22 | 2.16 | 0.45 |
| 1:A:176:LEU:CD1 | 1:A:176:LEU:N | 2.74 | 0.45 |
| 1:A:322:VAL:CG1 | 1:A:325:ILE:HD11 | 2.47 | 0.45 |
| 1:D:89:GLU:CD | 1:D:153:PRO:HD2 | 2.36 | 0.45 |
| 1:D:692:LEU:HD23 | 1:D:692:LEU:HA | 1.84 | 0.45 |
| 1:D:726:VAL:CG1 | 1:D:785:GLU:HG3 | 2.34 | 0.45 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:CG1 | 2.99 | 0.45 |
| 1:D:835:PHE:O | 1:D:839:MLY:N | 2.49 | 0.45 |
| 1:G:206:LYS:HD3 | 1:G:217:THR:OG1 | 2.16 | 0.45 |
| 1:G:332:MET:O | 1:G:336:SER:OG | 2.27 | 0.45 |
| 1:G:361:TYR:O | 1:G:364:LEU:HB2 | 2.16 | 0.45 |
| 1:G:783:LEU:CD1 | 1:G:783:LEU:N | 2.78 | 0.45 |
| 1:G:831:TRP:NE1 | 2:H:67:MET:CB | 2.60 | 0.45 |
| 1:J:99:GLU:N | 1:J:100:PRO:CD | 2.80 | 0.45 |
| 1:J:612:GLN:NE2 | 1:J:627:GLY:H | 2.15 | 0.45 |
| 1:M:640:LYS:C | 4:Z:23:GLY:C | 2.74 | 0.45 |
| 1:M:836:PHE:CD1 | 2:N:159:HIS:CA | 2.83 | 0.45 |
| 3:O:50:LEU:O | 3:O:53:PRO:CD | 2.63 | 0.45 |
| 1:S:486:MLY:HH22 | 1:S:527:GLU:CD | 2.37 | 0.45 |
| 1:S:488:GLN:O | 1:S:491:PHE:HB3 | 2.17 | 0.45 |
| 1:S:612:GLN:NE2 | 1:S:627:GLY:H | 2.15 | 0.45 |
| 1:M:642:LYS:NZ | 4:Z:340:TRP:O | 2.50 | 0.45 |
| 4:2:366:GLY:O | 4:2:369:ILE:HG22 | 2.16 | 0.45 |
| 4:3:223:PHE:CD2 | 4:3:259:GLU:HG3 | 2.52 | 0.45 |
| 1:A:99:GLU:N | 1:A:100:PRO:CD | 2.80 | 0.45 |
| 1:A:163:TYR:O | 1:A:166:MET:HB3 | 2.17 | 0.45 |
| 1:A:194:GLN:HB3 | 1:A:194:GLN:HE21 | 1.43 | 0.45 |
| 1:A:753:VAL:HA | 1:A:778:MET:SD | 2.57 | 0.45 |
| 1:A:501:GLU:CB | 1:A:762:HIS:ND1 | 2.80 | 0.45 |
| 1:A:835:PHE:O | 1:A:839:MLY:N | 2.49 | 0.45 |
| 1:D:179:GLY:O | 1:D:185:LYS:HE2 | 2.17 | 0.45 |
| 1:D:568:PRO:CG | 1:D:578:HIS:H | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:629:GLU:HG2 | 1:D:643:GLY:C | 2.35 | 0.45 |
| 1:D:725:ARG:C | 1:D:782:MLY:HH22 | 2.37 | 0.45 |
| 1:D:724:TYR:CB | 1:D:782:MLY:HD2 | 2.12 | 0.45 |
| 1:D:747:LEU:CG | 1:D:782:MLY:HH21 | 2.34 | 0.45 |
| 1:D:836:PHE:HE2 | 2:E:160:GLY:HA3 | 1.81 | 0.45 |
| 2:E:137:TRP:CZ3 | 2:E:145:ALA:N | 2.81 | 0.45 |
| 1:G:14:ALA:HB3 | 1:G:15:PRO:CD | 2.46 | 0.45 |
| 1:G:186:THR:O | 1:G:190:MLY:HG2 | 2.17 | 0.45 |
| 1:G:173:GLN:HG3 | 1:G:670:HIS:HD2 | 1.82 | 0.45 |
| 2:H:139:ALA:C | 2:H:141:PRO:HD3 | 2.33 | 0.45 |
| 1:J:186:THR:O | 1:J:190:MLY:HG2 | 2.17 | 0.45 |
| 1:J:330:GLU:O | 1:J:333:ALA:HB3 | 2.16 | 0.45 |
| 1:J:173:GLN:HG3 | 1:J:670:HIS:HD2 | 1.82 | 0.45 |
| 1:J:92:ALA:O | 1:J:714:ARG:CG | 2.64 | 0.45 |
| 1:J:836:PHE:CD1 | 2:K:159:HIS:HA | 2.36 | 0.45 |
| 1:M:103:LEU:HD22 | 1:M:692:LEU:HG | 1.98 | 0.45 |
| 1:M:30:MLY:HB3 | 1:M:31:PRO:HD2 | 1.97 | 0.45 |
| 1:M:335:ASP:OD1 | 1:M:348:MLY:NZ | 2.49 | 0.45 |
| 1:M:488:GLN:O | 1:M:491:PHE:HB3 | 2.17 | 0.45 |
| 1:M:793:ARG:O | 1:M:797:PHE:N | 2.39 | 0.45 |
| 1:M:835:PHE:O | 1:M:839:MLY:N | 2.49 | 0.45 |
| 1:M:82:PRO:HG2 | 1:M:85:TYR:CE2 | 2.50 | 0.45 |
| 1:S:296:MLY:O | 1:S:299:LEU:HB2 | 2.17 | 0.45 |
| 1:S:330:GLU:O | 1:S:333:ALA:HB3 | 2.16 | 0.45 |
| 1:S:546:THR:HG21 | 4:4:47:MET:HA | 1.96 | 0.45 |
| 1:S:629:GLU:CB | 1:S:645:SER:N | 2.74 | 0.45 |
| 4:X:223:PHE:CD2 | 4:X:259:GLU:HG3 | 2.51 | 0.45 |
| 4:X:32:PRO:HB2 | 4:X:34:ILE:HD11 | 1.98 | 0.45 |
| 4:7:223:PHE:CD2 | 4:7:259:GLU:HG3 | 2.52 | 0.45 |
| 4:8:6:THR:HG22 | 4:8:101:HIS:HA | 1.97 | 0.45 |
| 4:9:190:MET:O | 4:9:194:THR:HG23 | 2.16 | 0.45 |
| 1:A:179:GLY:O | 1:A:185:LYS:HE2 | 2.17 | 0.45 |
| 1:A:186:THR:O | 1:A:190:MLY:HG2 | 2.17 | 0.45 |
| 1:A:476:GLU:OE2 | 1:A:598:MLY:HH13 | 2.17 | 0.45 |
| 1:A:791:GLN:OE1 | 3:C:116:GLU:N | 2.47 | 0.45 |
| 2:B:137:TRP:CA | 2:B:145:ALA:HB2 | 2.38 | 0.45 |
| 1:D:476:GLU:OE2 | 1:D:598:MLY:HH13 | 2.16 | 0.45 |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:CD | 2.37 | 0.45 |
| 1:D:642:LYS:NZ | 4:9:340:TRP:O | 2.50 | 0.45 |
| 1:D:95:THR:HB | 1:D:772:LEU:HD22 | 1.98 | 0.45 |
| 1:G:448:GLN:C | 1:G:450:ASP:H | 2.19 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:488:GLN:O | 1:G:491:PHE:HB3 | 2.17 | 0.45 |
| 1:G:629:GLU:HG2 | 1:G:643:GLY:C | 2.35 | 0.45 |
| 1:G:724:TYR:HD1 | 1:G:727:LEU:CD1 | 2.27 | 0.45 |
| 1:G:759:ALA:O | 1:G:766:PHE:N | 2.32 | 0.45 |
| 1:G:792:ALA:CB | 3:I:42:THR:N | 2.80 | 0.45 |
| 1:J:179:GLY:O | 1:J:185:LYS:HE2 | 2.17 | 0.45 |
| 1:J:335:ASP:OD1 | 1:J:348:MLY:NZ | 2.49 | 0.45 |
| 1:J:793:ARG:HH11 | 3:L:40:ASN:ND2 | 2.08 | 0.45 |
| 1:J:84:MLY:CD | 1:J:724:TYR:OH | 2.53 | 0.45 |
| 1:J:792:ALA:HB3 | 3:L:42:THR:CG2 | 2.19 | 0.45 |
| 1:M:37:SER:O | 1:M:38:VAL:HG23 | 2.17 | 0.45 |
| 1:M:554:LEU:HD12 | 1:M:554:LEU:HA | 1.77 | 0.45 |
| 1:S:163:TYR:O | 1:S:166:MET:HB3 | 2.17 | 0.45 |
| 1:S:554:LEU:HD12 | 1:S:554:LEU:HA | 1.77 | 0.45 |
| 1:S:791:GLN:HE22 | 3:U:114:LEU:C | 2.20 | 0.45 |
| 4:V:366:GLY:O | 4:V:369:ILE:HG22 | 2.16 | 0.45 |
| 4:W:223:PHE:CD2 | 4:W:259:GLU:HG3 | 2.51 | 0.45 |
| 1:J:556:ASP:OD1 | 4:Y:47:MET:CE | 2.27 | 0.45 |
| 4:Z:6:THR:HG22 | 4:Z:101:HIS:HA | 1.97 | 0.45 |
| 4:2:190:MET:O | 4:2:194:THR:HG23 | 2.16 | 0.45 |
| 1:S:642:LYS:NZ | 4:2:340:TRP:O | 2.50 | 0.45 |
| 1:A:540:CYS:C | 4:8:349:LEU:HD21 | 2.36 | 0.45 |
| 4:9:223:PHE:CD2 | 4:9:259:GLU:HG3 | 2.52 | 0.45 |
| 1:A:14:ALA:N | 1:A:15:PRO:HD2 | 2.32 | 0.45 |
| 1:A:89:GLU:CD | 1:A:153:PRO:HD2 | 2.37 | 0.45 |
| 1:A:195:TYR:CE2 | 1:A:199:ILE:HD12 | 2.52 | 0.45 |
| 1:A:296:MLY:O | 1:A:299:LEU:HB2 | 2.17 | 0.45 |
| 1:A:361:TYR:O | 1:A:364:LEU:HB2 | 2.16 | 0.45 |
| 1:A:488:GLN:O | 1:A:491:PHE:HB3 | 2.17 | 0.45 |
| 1:A:675:ILE:HG23 | 1:A:676:ILE:N | 2.32 | 0.45 |
| 1:A:829:TRP:O | 1:A:832:MET:N | 2.50 | 0.45 |
| 2:B:112:ILE:O | 2:B:148:VAL:HA | 2.17 | 0.45 |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG13 | 1.95 | 0.45 |
| 1:D:775:LEU:HD12 | 1:D:775:LEU:HA | 1.70 | 0.45 |
| 1:G:55:MLY:HH23 | 1:G:60:VAL:HG22 | 1.99 | 0.45 |
| 1:J:206:LYS:CE | 1:J:217:THR:HG23 | 2.29 | 0.45 |
| 1:J:226:ASN:N | 1:J:227:PRO:HD2 | 2.32 | 0.45 |
| 1:J:476:GLU:OE2 | 1:J:598:MLY:HH13 | 2.17 | 0.45 |
| 1:M:163:TYR:O | 1:M:166:MET:HB3 | 2.17 | 0.45 |
| 1:M:486:MLY:HH22 | 1:M:527:GLU:CD | 2.37 | 0.45 |
| 1:S:278:GLN:HB3 | 1:S:278:GLN:HE21 | 1.42 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:794:CYS:O | 1:S:797:PHE:HB3 | 2.17 | 0.45 |
| 1:G:642:LYS:HA | 4:V:21:PHE:C | 2.36 | 0.45 |
| 4:W:253:GLU:HA | 4:W:256:ARG:CG | 2.42 | 0.45 |
| 4:X:6:THR:HG22 | 4:X:101:HIS:HA | 1.98 | 0.45 |
| 4:Y:190:MET:O | 4:Y:194:THR:HG23 | 2.16 | 0.45 |
| 4:1:32:PRO:HB2 | 4:1:34:ILE:HD11 | 1.98 | 0.45 |
| 4:2:6:THR:HG22 | 4:2:101:HIS:HA | 1.98 | 0.45 |
| 1:S:549:SER:N | 4:4:47:MET:O | 2.50 | 0.45 |
| 4:4:6:THR:HG22 | 4:4:101:HIS:HA | 1.98 | 0.45 |
| 1:D:206:LYS:CE | 1:D:217:THR:HG23 | 2.29 | 0.45 |
| 1:D:226:ASN:N | 1:D:227:PRO:HD2 | 2.32 | 0.45 |
| 1:D:544:LYS:HD2 | 4:9:147:ARG:CB | 2.37 | 0.45 |
| 1:D:576:GLU:CG | 1:D:577:ALA:N | 2.44 | 0.45 |
| 1:D:712:PRO:CB | 1:D:771:LEU:HB3 | 2.32 | 0.45 |
| 1:D:798:LEU:CD2 | 3:F:126:LEU:HD11 | 2.45 | 0.45 |
| 1:G:296:MLY:O | 1:G:299:LEU:HB2 | 2.17 | 0.45 |
| 1:J:296:MLY:O | 1:J:299:LEU:HB2 | 2.17 | 0.45 |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:CD | 2.37 | 0.45 |
| 1:J:83:PRO:HB2 | 1:J:723:ARG:HH21 | 1.82 | 0.45 |
| 1:J:725:ARG:CG | 1:J:733:PRO:CA | 2.95 | 0.45 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:C | 2.70 | 0.45 |
| 1:M:106:LEU:HA | 1:M:106:LEU:HD12 | 1.80 | 0.45 |
| 1:M:540:CYS:N | 4:Z:349:LEU:HD11 | 2.31 | 0.45 |
| 1:M:643:GLY:CA | 4:Z:24:ASP:OD1 | 2.62 | 0.45 |
| 1:M:725:ARG:HH21 | 1:M:733:PRO:HB2 | 1.82 | 0.45 |
| 1:M:747:LEU:C | 1:M:749:GLY:H | 2.20 | 0.45 |
| 2:N:139:ALA:C | 2:N:141:PRO:HD3 | 2.33 | 0.45 |
| 1:S:99:GLU:N | 1:S:100:PRO:CD | 2.80 | 0.45 |
| 1:S:173:GLN:HG3 | 1:S:670:HIS:HD2 | 1.82 | 0.45 |
| 1:S:746:LYS:NZ | 3:U:96:LYS:CA | 2.61 | 0.45 |
| 1:S:804:ARG:C | 1:S:807:VAL:CA | 2.85 | 0.45 |
| 1:S:734:GLU:OE1 | 3:U:94:PHE:O | 2.34 | 0.45 |
| 4:Y:32:PRO:HB2 | 4:Y:34:ILE:HD11 | 1.98 | 0.45 |
| 4:Y:299:MET:HE2 | 4:Y:331:ALA:HB2 | 1.99 | 0.45 |
| 4:Z:366:GLY:O | 4:Z:369:ILE:HG22 | 2.16 | 0.45 |
| 4:7:32:PRO:HB2 | 4:7:34:ILE:HD11 | 1.98 | 0.45 |
| 4:7:366:GLY:O | 4:7:369:ILE:HG22 | 2.16 | 0.45 |
| 1:A:538:GLU:OE1 | 4:8:355:MET:HE3 | 2.16 | 0.45 |
| 1:A:48:VAL:HA | 1:A:104:TYR:OH | 2.17 | 0.45 |
| 1:A:136:ASN:O | 1:A:139:VAL:N | 2.47 | 0.45 |
| 1:A:599:ASN:CG | 1:A:649:VAL:CB | 2.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:278:GLN:HB3 | 1:D:278:GLN:HE21 | 1.42 | 0.45 |
| 1:D:37:SER:O | 1:D:38:VAL:HG23 | 2.17 | 0.45 |
| 1:D:725:ARG:NE | 1:D:733:PRO:CB | 1.95 | 0.45 |
| 1:D:791:GLN:NE2 | 3:F:114:LEU:O | 2.42 | 0.45 |
| 2:E:123:THR:HB | 3:F:19:ARG:HH12 | 1.82 | 0.45 |
| 3:F:69:LEU:HB3 | 3:F:70:PRO:HD3 | 1.99 | 0.45 |
| 1:G:449:LEU:HD12 | 1:G:449:LEU:HA | 1.60 | 0.45 |
| 1:G:675:ILE:HG23 | 1:G:676:ILE:N | 2.32 | 0.45 |
| 1:G:725:ARG:CG | 1:G:733:PRO:CA | 2.95 | 0.45 |
| 1:G:747:LEU:C | 1:G:749:GLY:H | 2.20 | 0.45 |
| 1:G:769:ALA:O | 1:G:773:GLY:HA2 | 2.13 | 0.45 |
| 1:G:798:LEU:CD2 | 3:I:122:GLU:HB3 | 2.47 | 0.45 |
| 1:G:99:GLU:N | 1:G:100:PRO:CD | 2.80 | 0.45 |
| 1:G:838:ILE:CG1 | 2:H:54:MET:CE | 2.92 | 0.45 |
| 1:J:667:THR:O | 1:J:669:PRO:HD3 | 2.17 | 0.45 |
| 1:J:794:CYS:O | 1:J:797:PHE:HB3 | 2.17 | 0.45 |
| 1:M:173:GLN:HG3 | 1:M:670:HIS:HD2 | 1.82 | 0.45 |
| 1:M:330:GLU:O | 1:M:333:ALA:HB3 | 2.16 | 0.45 |
| 1:M:629:GLU:HG2 | 1:M:643:GLY:C | 2.35 | 0.45 |
| 1:S:14:ALA:N | 1:S:15:PRO:HD2 | 2.32 | 0.45 |
| 3:U:69:LEU:HB3 | 3:U:70:PRO:HD3 | 1.99 | 0.45 |
| 1:S:747:LEU:O | 3:U:93:VAL:HG21 | 2.17 | 0.45 |
| 1:J:642:LYS:NZ | 4:W:340:TRP:O | 2.50 | 0.45 |
| 4:Z:190:MET:O | 4:Z:194:THR:HG23 | 2.16 | 0.45 |
| 1:M:642:LYS:HB2 | 4:Z:24:ASP:O | 1.88 | 0.45 |
| 4:4:223:PHE:CD2 | 4:4:259:GLU:HG3 | 2.51 | 0.44 |
| 4:5:253:GLU:HA | 4:5:256:ARG:CG | 2.42 | 0.44 |
| 4:5:32:PRO:HB2 | 4:5:34:ILE:HD11 | 1.98 | 0.44 |
| 1:A:639:GLY:H | 4:8:344:SER:HB3 | 1.82 | 0.44 |
| 1:A:129:TYR:HD1 | 1:A:129:TYR:HA | 1.65 | 0.44 |
| 1:A:540:CYS:N | 4:8:349:LEU:HD11 | 2.31 | 0.44 |
| 1:A:505:MLY:CG | 1:A:741:LYS:HZ2 | 2.17 | 0.44 |
| 1:A:797:PHE:CE1 | 3:C:149:VAL:CG1 | 3.00 | 0.44 |
| 1:D:296:MLY:O | 1:D:299:LEU:HB2 | 2.17 | 0.44 |
| 1:D:330:GLU:O | 1:D:333:ALA:HB3 | 2.17 | 0.44 |
| 1:D:675:ILE:HG23 | 1:D:676:ILE:N | 2.32 | 0.44 |
| 2:E:112:ILE:O | 2:E:148:VAL:HA | 2.17 | 0.44 |
| 1:G:14:ALA:N | 1:G:15:PRO:HD2 | 2.32 | 0.44 |
| 1:J:163:TYR:O | 1:J:166:MET:HB3 | 2.17 | 0.44 |
| 1:J:640:LYS:HB3 | 1:J:645:SER:CB | 2.42 | 0.44 |
| 1:J:64:THR:HB | 1:J:68:GLU:N | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:725:ARG:HA | 1:J:732:ILE:HG22 | 1.99 | 0.44 |
| 1:M:155:ILE:HG22 | 1:M:156:PHE:N | 2.33 | 0.44 |
| 1:M:195:TYR:CE2 | 1:M:199:ILE:HD12 | 2.52 | 0.44 |
| 1:M:224:SER:O | 1:M:227:PRO:HD2 | 2.17 | 0.44 |
| 1:M:448:GLN:C | 1:M:450:ASP:H | 2.19 | 0.44 |
| 1:M:829:TRP:O | 1:M:832:MET:N | 2.50 | 0.44 |
| 1:S:322:VAL:CG1 | 1:S:325:ILE:HD11 | 2.47 | 0.44 |
| 1:S:485:GLU:OE1 | 1:S:583:HIS:ND1 | 2.49 | 0.44 |
| 1:S:597:GLU:O | 1:S:600:MLY:N | 2.50 | 0.44 |
| 1:S:791:GLN:HB3 | 3:U:116:GLU:HB2 | 1.98 | 0.44 |
| 2:T:129:THR:HG23 | 2:T:132:GLU:OE1 | 2.17 | 0.44 |
| 4:V:32:PRO:HB2 | 4:V:34:ILE:HD11 | 1.98 | 0.44 |
| 1:G:411:GLU:H | 4:V:333:PRO:CB | 2.29 | 0.44 |
| 1:M:540:CYS:C | 4:Z:349:LEU:HD21 | 2.36 | 0.44 |
| 1:M:530:MET:HA | 4:Z:354:GLN:CD | 2.11 | 0.44 |
| 4:1:287:ILE:CG2 | 4:3:202:THR:CA | 2.89 | 0.44 |
| 4:3:32:PRO:HB2 | 4:3:34:ILE:HD11 | 1.98 | 0.44 |
| 4:3:324:THR:N | 4:5:244:ASP:HA | 2.33 | 0.44 |
| 4:8:253:GLU:HA | 4:8:256:ARG:CG | 2.42 | 0.44 |
| 1:A:411:GLU:H | 4:8:333:PRO:CB | 2.30 | 0.44 |
| 1:A:436:MLY:HE3 | 1:A:626:TYR:HE1 | 1.77 | 0.44 |
| 1:A:55:MLY:HH23 | 1:A:60:VAL:HG22 | 1.99 | 0.44 |
| 1:A:701:LEU:HA | 1:A:701:LEU:HD12 | 1.55 | 0.44 |
| 1:A:791:GLN:NE2 | 3:C:114:LEU:O | 2.51 | 0.44 |
| 1:D:139:VAL:HG12 | 1:D:143:TYR:HD2 | 1.81 | 0.44 |
| 1:D:64:THR:HB | 1:D:68:GLU:N | 2.33 | 0.44 |
| 1:D:689:GLU:HA | 1:D:692:LEU:HB2 | 2.00 | 0.44 |
| 1:D:103:LEU:HD22 | 1:D:692:LEU:HG | 1.98 | 0.44 |
| 1:D:692:LEU:O | 1:D:696:ARG:HG3 | 2.18 | 0.44 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:CG2 | 3.00 | 0.44 |
| 1:G:163:TYR:O | 1:G:166:MET:HB3 | 2.17 | 0.44 |
| 1:G:292:MET:HE1 | 1:G:309:PRO:CG | 2.47 | 0.44 |
| 1:G:485:GLU:HA | 1:G:584:TYR:HE2 | 1.83 | 0.44 |
| 1:J:195:TYR:CE2 | 1:J:199:ILE:HD12 | 2.52 | 0.44 |
| 1:J:493:HIS:O | 1:J:496:PHE:HB3 | 2.18 | 0.44 |
| 1:J:597:GLU:O | 1:J:600:MLY:N | 2.50 | 0.44 |
| 1:J:768:MLY:CB | 1:J:773:GLY:HA3 | 2.08 | 0.44 |
| 1:J:97:LEU:HD22 | 1:J:712:PRO:HB2 | 1.98 | 0.44 |
| 1:M:226:ASN:HB2 | 1:M:227:PRO:CD | 2.47 | 0.44 |
| 1:M:544:LYS:HD2 | 4:Z:147:ARG:CB | 2.36 | 0.44 |
| 1:M:578:HIS:HB3 | 1:M:592:ILE:CD1 | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:818:TYR:CE1 | 2:N:127:ARG:NH1 | 2.76 | 0.44 |
| 2:N:129:THR:HG23 | 2:N:132:GLU:OE1 | 2.17 | 0.44 |
| 1:S:506:GLU:HG2 | 1:S:760:PHE:H | 1.81 | 0.44 |
| 1:S:84:MLY:CH2 | 1:S:724:TYR:CE2 | 3.00 | 0.44 |
| 4:1:202:THR:CG2 | 4:Y:290:ARG:NH1 | 2.81 | 0.44 |
| 4:7:190:MET:O | 4:7:194:THR:HG23 | 2.16 | 0.44 |
| 4:8:190:MET:O | 4:8:194:THR:HG23 | 2.16 | 0.44 |
| 1:A:485:GLU:OE2 | 1:A:584:TYR:N | 2.50 | 0.44 |
| 1:A:173:GLN:HG3 | 1:A:670:HIS:HD2 | 1.82 | 0.44 |
| 1:A:103:LEU:HD22 | 1:A:692:LEU:HG | 1.98 | 0.44 |
| 1:A:723:ARG:CG | 1:A:723:ARG:NH1 | 2.80 | 0.44 |
| 3:C:69:LEU:HB3 | 3:C:70:PRO:HD3 | 2.00 | 0.44 |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:CD1 | 2.48 | 0.44 |
| 1:D:725:ARG:HA | 1:D:732:ILE:HG22 | 1.99 | 0.44 |
| 1:D:725:ARG:HH21 | 1:D:733:PRO:HB2 | 1.81 | 0.44 |
| 2:E:129:THR:HG23 | 2:E:132:GLU:OE1 | 2.17 | 0.44 |
| 3:F:122:GLU:HA | 3:F:125:GLU:OE1 | 2.18 | 0.44 |
| 1:G:195:TYR:CE2 | 1:G:199:ILE:HD12 | 2.52 | 0.44 |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG13 | 1.95 | 0.44 |
| 1:G:519:LEU:CD1 | 1:G:519:LEU:N | 2.77 | 0.44 |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:CD | 2.37 | 0.44 |
| 1:G:597:GLU:O | 1:G:600:MLY:N | 2.50 | 0.44 |
| 1:G:642:LYS:NZ | 4:V:340:TRP:O | 2.50 | 0.44 |
| 1:G:829:TRP:CH2 | 2:H:83:MET:CE | 3.01 | 0.44 |
| 1:J:139:VAL:HG12 | 1:J:143:TYR:HD2 | 1.81 | 0.44 |
| 1:J:14:ALA:N | 1:J:15:PRO:HD2 | 2.32 | 0.44 |
| 1:J:194:GLN:HE21 | 1:J:194:GLN:HB3 | 1.44 | 0.44 |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:CD1 | 0.63 | 0.44 |
| 1:J:762:HIS:N | 1:J:762:HIS:CD2 | 2.78 | 0.44 |
| 1:M:14:ALA:N | 1:M:15:PRO:HD2 | 2.32 | 0.44 |
| 1:M:493:HIS:O | 1:M:496:PHE:HB3 | 2.18 | 0.44 |
| 1:M:639:GLY:H | 4:Z:344:SER:HB3 | 1.82 | 0.44 |
| 1:M:89:GLU:CD | 1:M:153:PRO:HD2 | 2.37 | 0.44 |
| 1:S:224:SER:O | 1:S:227:PRO:HD2 | 2.17 | 0.44 |
| 1:S:30:MLY:HB3 | 1:S:31:PRO:HD2 | 1.97 | 0.44 |
| 1:S:320:ILE:HG22 | 1:S:320:ILE:O | 2.18 | 0.44 |
| 1:S:332:MET:HG2 | 1:S:332:MET:H | 1.52 | 0.44 |
| 1:S:476:GLU:OE2 | 1:S:598:MLY:HH13 | 2.16 | 0.44 |
| 1:S:629:GLU:HG2 | 1:S:643:GLY:C | 2.35 | 0.44 |
| 1:S:640:LYS:C | 4:2:23:GLY:C | 2.74 | 0.44 |
| 1:S:701:LEU:HA | 1:S:701:LEU:HD12 | 1.55 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:724:TYR:HD1 | 1:S:727:LEU:CD1 | 2.27 | 0.44 |
| 1:S:725:ARG:CG | 1:S:733:PRO:CA | 2.95 | 0.44 |
| 1:S:747:LEU:C | 1:S:749:GLY:H | 2.20 | 0.44 |
| 1:S:793:ARG:HD3 | 3:U:40:ASN:CG | 2.37 | 0.44 |
| 4:W:32:PRO:HB2 | 4:W:34:ILE:HD11 | 1.98 | 0.44 |
| 4:Y:223:PHE:HB3 | 4:Y:259:GLU:OE2 | 2.18 | 0.44 |
| 4:1:223:PHE:HB3 | 4:1:259:GLU:OE2 | 2.18 | 0.44 |
| 4:3:223:PHE:HB3 | 4:3:259:GLU:OE2 | 2.18 | 0.44 |
| 4:4:324:THR:N | 4:6:244:ASP:HA | 2.33 | 0.44 |
| 1:A:408:VAL:CG1 | 4:8:332:PRO:HB3 | 2.40 | 0.44 |
| 1:A:410:ASN:HA | 4:8:334:GLU:HB3 | 1.29 | 0.44 |
| 4:9:223:PHE:HB3 | 4:9:259:GLU:OE2 | 2.18 | 0.44 |
| 1:D:411:GLU:H | 4:9:333:PRO:CB | 2.30 | 0.44 |
| 1:D:541:MET:HB3 | 4:9:345:ILE:HG22 | 2.00 | 0.44 |
| 1:D:540:CYS:C | 4:9:349:LEU:HD21 | 2.36 | 0.44 |
| 1:A:206:LYS:HD2 | 1:A:217:THR:CG2 | 2.17 | 0.44 |
| 1:A:224:SER:O | 1:A:227:PRO:HD2 | 2.17 | 0.44 |
| 1:A:725:ARG:CG | 1:A:733:PRO:CA | 2.95 | 0.44 |
| 1:A:711:PHE:HB3 | 1:A:766:PHE:HB3 | 1.99 | 0.44 |
| 1:D:439:LEU:CD1 | 1:D:439:LEU:N | 2.81 | 0.44 |
| 1:D:488:GLN:O | 1:D:491:PHE:HB3 | 2.17 | 0.44 |
| 1:D:639:GLY:H | 4:9:344:SER:HB3 | 1.83 | 0.44 |
| 1:D:701:LEU:HD12 | 1:D:701:LEU:HA | 1.55 | 0.44 |
| 2:E:88:LEU:HB3 | 2:E:91:ALA:HB2 | 1.98 | 0.44 |
| 1:G:48:VAL:HA | 1:G:104:TYR:OH | 2.18 | 0.44 |
| 1:G:64:THR:HB | 1:G:68:GLU:N | 2.32 | 0.44 |
| 1:G:103:LEU:HD22 | 1:G:692:LEU:HG | 1.98 | 0.44 |
| 1:G:84:MLY:HB3 | 1:G:723:ARG:CZ | 2.46 | 0.44 |
| 2:H:140:PHE:HA | 2:H:141:PRO:HD2 | 1.57 | 0.44 |
| 2:H:112:ILE:O | 2:H:148:VAL:HA | 2.16 | 0.44 |
| 1:J:692:LEU:O | 1:J:696:ARG:HG3 | 2.18 | 0.44 |
| 1:J:724:TYR:HD1 | 1:J:727:LEU:CD1 | 2.27 | 0.44 |
| 1:J:757:GLN:N | 1:J:776:GLU:CG | 2.80 | 0.44 |
| 1:M:485:GLU:HA | 1:M:584:TYR:HE2 | 1.83 | 0.44 |
| 1:M:519:LEU:N | 1:M:519:LEU:CD1 | 2.77 | 0.44 |
| 1:M:675:ILE:HG23 | 1:M:676:ILE:N | 2.33 | 0.44 |
| 1:M:794:CYS:O | 1:M:797:PHE:HB3 | 2.17 | 0.44 |
| 1:S:206:LYS:HD3 | 1:S:217:THR:OG1 | 2.16 | 0.44 |
| 1:S:37:SER:O | 1:S:38:VAL:HG23 | 2.17 | 0.44 |
| 1:S:667:THR:O | 1:S:669:PRO:HD3 | 2.16 | 0.44 |
| 1:S:715:VAL:HG11 | 1:S:720:PHE:CD1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:48:LYS:HA | 3:U:48:LYS:HD3 | 1.17 | 0.44 |
| 1:J:411:GLU:H | 4:W:333:PRO:CB | 2.30 | 0.44 |
| 4:Y:223:PHE:CD2 | 4:Y:259:GLU:HG3 | 2.52 | 0.44 |
| 1:M:411:GLU:H | 4:Z:333:PRO:CB | 2.30 | 0.44 |
| 4:Z:32:PRO:HB2 | 4:Z:34:ILE:HD11 | 1.98 | 0.44 |
| 4:1:299:MET:HE2 | 4:1:331:ALA:HB2 | 2.00 | 0.44 |
| 4:2:32:PRO:HB2 | 4:2:34:ILE:HD11 | 1.98 | 0.44 |
| 4:4:223:PHE:HB3 | 4:4:259:GLU:OE2 | 2.18 | 0.44 |
| 4:7:223:PHE:HB3 | 4:7:259:GLU:OE2 | 2.18 | 0.44 |
| 4:9:32:PRO:HB2 | 4:9:34:ILE:HD11 | 1.98 | 0.44 |
| 1:A:155:ILE:HG22 | 1:A:156:PHE:N | 2.33 | 0.44 |
| 1:A:320:ILE:O | 1:A:320:ILE:HG22 | 2.18 | 0.44 |
| 1:A:354:LEU:HA | 1:A:354:LEU:HD12 | 1.55 | 0.44 |
| 1:A:725:ARG:HH21 | 1:A:733:PRO:HB2 | 1.81 | 0.44 |
| 1:A:93:MET:CE | 1:A:716:LEU:N | 2.81 | 0.44 |
| 1:D:195:TYR:CE2 | 1:D:199:ILE:HD12 | 2.52 | 0.44 |
| 1:D:554:LEU:HA | 1:D:554:LEU:HD12 | 1.77 | 0.44 |
| 1:D:597:GLU:O | 1:D:600:MLY:N | 2.50 | 0.44 |
| 1:D:724:TYR:HD1 | 1:D:782:MLY:CG | 2.30 | 0.44 |
| 1:D:711:PHE:HB3 | 1:D:766:PHE:HB3 | 2.00 | 0.44 |
| 1:G:640:LYS:C | 4:V:23:GLY:C | 2.75 | 0.44 |
| 1:G:810:ARG:HG2 | 1:G:810:ARG:NH1 | 2.28 | 0.44 |
| 1:J:278:GLN:HE21 | 1:J:278:GLN:HB3 | 1.42 | 0.44 |
| 1:J:332:MET:O | 1:J:336:SER:OG | 2.27 | 0.44 |
| 1:J:439:LEU:CD1 | 1:J:439:LEU:N | 2.81 | 0.44 |
| 1:J:464:ILE:CG2 | 1:J:465:ALA:N | 2.80 | 0.44 |
| 1:J:516:GLY:O | 1:J:518:ASP:N | 2.51 | 0.44 |
| 1:J:689:GLU:HA | 1:J:692:LEU:HB2 | 2.00 | 0.44 |
| 1:J:103:LEU:HD22 | 1:J:692:LEU:HG | 1.98 | 0.44 |
| 1:J:725:ARG:CZ | 1:J:733:PRO:CB | 2.83 | 0.44 |
| 1:J:791:GLN:NE2 | 3:L:115:GLY:C | 2.69 | 0.44 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:CZ | 2.48 | 0.44 |
| 3:L:48:LYS:HA | 3:L:48:LYS:HD3 | 1.17 | 0.44 |
| 1:M:99:GLU:N | 1:M:100:PRO:CD | 2.80 | 0.44 |
| 1:M:464:ILE:CG2 | 1:M:465:ALA:N | 2.80 | 0.44 |
| 1:M:725:ARG:CZ | 1:M:737:PHE:CZ | 3.01 | 0.44 |
| 1:S:186:THR:O | 1:S:190:MLY:HG2 | 2.17 | 0.44 |
| 1:S:464:ILE:CG2 | 1:S:465:ALA:N | 2.80 | 0.44 |
| 1:S:516:GLY:O | 1:S:518:ASP:N | 2.51 | 0.44 |
| 1:S:834:LEU:HD11 | 2:T:51:PHE:CE1 | 2.42 | 0.44 |
| 3:U:119:THR:O | 3:U:123:VAL:HG23 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:190:MET:O | 4:V:194:THR:HG23 | 2.16 | 0.44 |
| 1:G:530:MET:CB | 4:V:354:GLN:CB | 2.96 | 0.44 |
| 4:V:6:THR:HG22 | 4:V:101:HIS:HA | 1.98 | 0.44 |
| 4:V:287:ILE:HG13 | 4:X:202:THR:HG23 | 1.65 | 0.44 |
| 4:6:32:PRO:HB2 | 4:6:34:ILE:HD11 | 1.98 | 0.44 |
| 1:A:330:GLU:O | 1:A:333:ALA:HB3 | 2.17 | 0.44 |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:CD | 2.37 | 0.44 |
| 1:A:64:THR:HB | 1:A:68:GLU:N | 2.33 | 0.44 |
| 1:A:505:MLY:CG | 1:A:741:LYS:HZ3 | 2.25 | 0.44 |
| 1:A:752:ASP:OD2 | 1:A:782:MLY:CD | 2.66 | 0.44 |
| 1:A:502:GLU:OE2 | 1:A:764:MLY:O | 2.35 | 0.44 |
| 1:A:768:MLY:CA | 1:A:771:LEU:HB2 | 2.41 | 0.44 |
| 1:A:776:GLU:O | 1:A:780:ASP:N | 2.45 | 0.44 |
| 1:A:798:LEU:HD21 | 3:C:122:GLU:HB3 | 1.99 | 0.44 |
| 3:C:48:LYS:HA | 3:C:48:LYS:HD3 | 1.17 | 0.44 |
| 1:D:667:THR:O | 1:D:669:PRO:HD3 | 2.16 | 0.44 |
| 1:G:667:THR:O | 1:G:669:PRO:HD3 | 2.17 | 0.44 |
| 1:G:750:GLY:HA2 | 3:I:114:LEU:HD13 | 2.00 | 0.44 |
| 1:G:829:TRP:O | 1:G:832:MET:N | 2.50 | 0.44 |
| 1:J:214:MET:CA | 1:J:340:ILE:HD11 | 2.45 | 0.44 |
| 1:J:354:LEU:HA | 1:J:354:LEU:HD12 | 1.55 | 0.44 |
| 1:J:485:GLU:OE1 | 1:J:583:HIS:ND1 | 2.49 | 0.44 |
| 1:J:568:PRO:CG | 1:J:578:HIS:H | 2.30 | 0.44 |
| 1:J:664:LEU:HD12 | 1:J:664:LEU:HA | 1.52 | 0.44 |
| 1:J:839:MLY:CH1 | 2:K:158:THR:HG22 | 2.48 | 0.44 |
| 2:K:114:LYS:CG | 2:K:146:GLY:HA2 | 2.46 | 0.44 |
| 3:L:122:GLU:HA | 3:L:125:GLU:OE1 | 2.18 | 0.44 |
| 1:M:206:LYS:HD3 | 1:M:217:THR:OG1 | 2.16 | 0.44 |
| 1:M:193:ILE:HD11 | 1:M:250:ILE:CD1 | 2.48 | 0.44 |
| 1:M:715:VAL:HG11 | 1:M:720:PHE:CD1 | 2.50 | 0.44 |
| 3:O:101:THR:HA | 3:O:137:ILE:O | 2.18 | 0.44 |
| 1:S:725:ARG:HH21 | 1:S:733:PRO:HB2 | 1.81 | 0.44 |
| 4:X:223:PHE:HB3 | 4:X:259:GLU:OE2 | 2.18 | 0.44 |
| 4:X:366:GLY:O | 4:X:369:ILE:HG22 | 2.16 | 0.44 |
| 1:A:123:CYS:CB | 1:A:158:ILE:HD13 | 2.48 | 0.44 |
| 1:A:505:MLY:HB2 | 1:A:761:GLY:CA | 2.48 | 0.44 |
| 1:A:725:ARG:HA | 1:A:732:ILE:HG22 | 1.99 | 0.44 |
| 1:D:48:VAL:HA | 1:D:104:TYR:OH | 2.18 | 0.44 |
| 1:D:266:GLU:OE1 | 1:D:659:MLY:NZ | 2.51 | 0.44 |
| 1:D:464:ILE:CG2 | 1:D:465:ALA:N | 2.79 | 0.44 |
| 1:D:485:GLU:HA | 1:D:584:TYR:HE2 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:496:PHE:CE2 | 1:D:514:ASP:HA | 2.50 | 0.44 |
| 1:D:725:ARG:CG | 1:D:733:PRO:CA | 2.95 | 0.44 |
| 1:D:810:ARG:HG2 | 1:D:810:ARG:NH1 | 2.29 | 0.44 |
| 1:D:87:MLY:HD3 | 1:D:87:MLY:HH12 | 1.61 | 0.44 |
| 2:E:140:PHE:O | 2:E:141:PRO:C | 2.33 | 0.44 |
| 1:G:179:GLY:O | 1:G:185:LYS:HE2 | 2.17 | 0.44 |
| 1:G:308:ASN:HA | 1:G:309:PRO:HD2 | 1.88 | 0.44 |
| 1:G:322:VAL:CG1 | 1:G:325:ILE:HD11 | 2.47 | 0.44 |
| 1:G:516:GLY:O | 1:G:518:ASP:N | 2.51 | 0.44 |
| 1:G:530:MET:CE | 4:V:354:GLN:CB | 2.95 | 0.44 |
| 1:G:568:PRO:CG | 1:G:578:HIS:H | 2.30 | 0.44 |
| 1:G:831:TRP:NE1 | 2:H:67:MET:CG | 2.81 | 0.44 |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:CD1 | 2.48 | 0.44 |
| 1:J:322:VAL:CG1 | 1:J:325:ILE:HD11 | 2.47 | 0.44 |
| 1:J:418:THR:CG2 | 1:J:419:VAL:N | 2.79 | 0.44 |
| 1:J:747:LEU:C | 1:J:749:GLY:H | 2.20 | 0.44 |
| 1:J:835:PHE:O | 1:J:839:MLY:N | 2.49 | 0.44 |
| 3:L:69:LEU:HB3 | 3:L:70:PRO:HD3 | 2.00 | 0.44 |
| 1:M:144:ARG:HD2 | 1:M:144:ARG:HA | 1.78 | 0.44 |
| 1:M:176:LEU:CD1 | 1:M:176:LEU:N | 2.75 | 0.44 |
| 1:M:295:MLY:HG3 | 1:M:332:MET:HE2 | 1.97 | 0.44 |
| 1:M:48:VAL:HA | 1:M:104:TYR:OH | 2.18 | 0.44 |
| 1:M:597:GLU:O | 1:M:600:MLY:N | 2.50 | 0.44 |
| 1:M:174:SER:OG | 1:M:669:PRO:HA | 2.18 | 0.44 |
| 1:S:195:TYR:CE2 | 1:S:199:ILE:HD12 | 2.52 | 0.44 |
| 1:S:292:MET:HE1 | 1:S:309:PRO:CG | 2.47 | 0.44 |
| 1:S:541:MET:HG2 | 4:2:345:ILE:HG22 | 2.00 | 0.44 |
| 1:S:639:GLY:H | 4:2:344:SER:HB3 | 1.82 | 0.44 |
| 1:S:747:LEU:C | 1:S:749:GLY:N | 2.71 | 0.44 |
| 1:S:829:TRP:O | 1:S:832:MET:N | 2.50 | 0.44 |
| 3:U:101:THR:HA | 3:U:137:ILE:O | 2.18 | 0.44 |
| 4:V:290:ARG:NH1 | 4:X:202:THR:CG2 | 2.81 | 0.44 |
| 4:W:223:PHE:HB3 | 4:W:259:GLU:OE2 | 2.18 | 0.44 |
| 4:W:290:ARG:NH1 | 4:Y:202:THR:CG2 | 2.81 | 0.44 |
| 4:7:193:LEU:O | 4:7:198:TYR:HD2 | 2.01 | 0.44 |
| 1:A:530:MET:HE3 | 4:8:354:GLN:CG | 2.37 | 0.44 |
| 1:A:715:VAL:HG12 | 1:A:720:PHE:HB2 | 2.00 | 0.44 |
| 1:A:725:ARG:CZ | 1:A:737:PHE:CZ | 3.01 | 0.44 |
| 1:A:747:LEU:C | 1:A:749:GLY:N | 2.71 | 0.44 |
| 1:D:163:TYR:O | 1:D:166:MET:HB3 | 2.17 | 0.44 |
| 1:D:174:SER:OG | 1:D:669:PRO:HA | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:516:GLY:O | 1:D:518:ASP:N | 2.51 | 0.44 |
| 1:D:768:MLY:C | 1:D:771:LEU:HA | 2.47 | 0.44 |
| 1:D:797:PHE:HD1 | 3:F:146:ILE:O | 2.00 | 0.44 |
| 3:F:50:LEU:O | 3:F:53:PRO:HG2 | 2.18 | 0.44 |
| 1:G:206:LYS:CE | 1:G:217:THR:HG23 | 2.30 | 0.44 |
| 1:G:330:GLU:O | 1:G:333:ALA:HB3 | 2.17 | 0.44 |
| 1:G:214:MET:HA | 1:G:340:ILE:CD1 | 2.41 | 0.44 |
| 1:G:346:ASP:O | 1:G:350:ALA:N | 2.46 | 0.44 |
| 1:G:836:PHE:CZ | 2:H:160:GLY:N | 2.75 | 0.44 |
| 3:I:122:GLU:HA | 3:I:125:GLU:OE1 | 2.18 | 0.44 |
| 1:J:266:GLU:OE1 | 1:J:659:MLY:NZ | 2.51 | 0.44 |
| 1:J:476:GLU:CD | 1:J:476:GLU:H | 2.21 | 0.44 |
| 1:J:541:MET:HB3 | 4:W:345:ILE:HG22 | 2.00 | 0.44 |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:HD13 | 1.92 | 0.44 |
| 3:L:50:LEU:O | 3:L:53:PRO:HG2 | 2.18 | 0.44 |
| 1:M:55:MLY:HH23 | 1:M:60:VAL:HG22 | 1.99 | 0.44 |
| 1:S:91:MET:CE | 1:S:119:SER:HB2 | 2.48 | 0.44 |
| 1:S:123:CYS:HB2 | 1:S:158:ILE:HD13 | 2.00 | 0.44 |
| 1:S:529:PRO:HB3 | 4:2:354:GLN:HA | 2.00 | 0.44 |
| 1:S:174:SER:OG | 1:S:669:PRO:HA | 2.18 | 0.44 |
| 1:S:725:ARG:CZ | 1:S:737:PHE:CZ | 3.01 | 0.44 |
| 4:2:287:ILE:CB | 4:4:203:THR:HB | 2.47 | 0.44 |
| 4:3:205:GLU:O | 4:3:208:ILE:HG22 | 2.18 | 0.44 |
| 4:8:32:PRO:HB2 | 4:8:34:ILE:HD11 | 1.98 | 0.44 |
| 1:A:37:SER:O | 1:A:38:VAL:HG23 | 2.17 | 0.44 |
| 1:A:391:GLY:HA3 | 1:A:616:VAL:HG23 | 2.00 | 0.44 |
| 1:A:538:GLU:CA | 4:8:351:THR:N | 2.69 | 0.44 |
| 1:A:597:GLU:O | 1:A:600:MLY:N | 2.50 | 0.44 |
| 1:A:692:LEU:O | 1:A:696:ARG:HG3 | 2.18 | 0.44 |
| 3:C:101:THR:HA | 3:C:137:ILE:O | 2.18 | 0.44 |
| 1:D:476:GLU:H | 1:D:476:GLU:CD | 2.22 | 0.44 |
| 1:D:485:GLU:OE2 | 1:D:584:TYR:N | 2.50 | 0.44 |
| 1:D:799:MET:HE1 | 3:F:32:ASP:CB | 2.28 | 0.44 |
| 1:G:14:ALA:N | 1:G:15:PRO:CD | 2.81 | 0.44 |
| 1:G:224:SER:O | 1:G:227:PRO:HD2 | 2.17 | 0.44 |
| 1:G:37:SER:O | 1:G:38:VAL:HG23 | 2.17 | 0.44 |
| 1:G:659:MLY:HD2 | 1:G:659:MLY:HH22 | 1.42 | 0.44 |
| 1:G:725:ARG:HA | 1:G:732:ILE:HG22 | 1.99 | 0.44 |
| 1:G:795:ARG:NE | 3:I:116:GLU:OE2 | 2.51 | 0.44 |
| 3:I:50:LEU:O | 3:I:53:PRO:HG2 | 2.18 | 0.44 |
| 1:J:55:MLY:HH23 | 1:J:60:VAL:HG22 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:701:LEU:HA | 1:J:701:LEU:HD12 | 1.55 | 0.44 |
| 1:J:783:LEU:HA | 1:J:786:ILE:HB | 1.99 | 0.44 |
| 1:M:711:PHE:HB3 | 1:M:766:PHE:HB3 | 2.00 | 0.44 |
| 1:M:785:GLU:C | 1:M:787:ILE:N | 2.71 | 0.44 |
| 3:O:50:LEU:O | 3:O:53:PRO:HG2 | 2.18 | 0.44 |
| 1:S:123:CYS:CB | 1:S:158:ILE:HD13 | 2.48 | 0.44 |
| 1:S:193:ILE:HD11 | 1:S:250:ILE:CD1 | 2.48 | 0.44 |
| 1:S:55:MLY:HH23 | 1:S:60:VAL:HG22 | 1.99 | 0.44 |
| 1:S:746:LYS:C | 3:U:93:VAL:HG13 | 2.37 | 0.44 |
| 3:U:50:LEU:O | 3:U:53:PRO:HG2 | 2.18 | 0.44 |
| 1:J:541:MET:CE | 4:W:346:LEU:HD12 | 2.47 | 0.44 |
| 4:Y:205:GLU:O | 4:Y:208:ILE:HG22 | 2.18 | 0.44 |
| 4:X:286:ASP:OD2 | 4:Z:203:THR:HG22 | 2.18 | 0.44 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:HG22 | 2.00 | 0.44 |
| 4:2:193:LEU:O | 4:2:198:TYR:HD2 | 2.01 | 0.43 |
| 4:5:193:LEU:O | 4:5:198:TYR:HD2 | 2.01 | 0.43 |
| 4:5:223:PHE:HB3 | 4:5:259:GLU:OE2 | 2.18 | 0.43 |
| 4:6:223:PHE:HB3 | 4:6:259:GLU:OE2 | 2.18 | 0.43 |
| 4:8:324:THR:O | 4:V:244:ASP:HA | 2.08 | 0.43 |
| 1:A:295:MLY:CE | 1:A:332:MET:CE | 2.96 | 0.43 |
| 1:A:439:LEU:CD1 | 1:A:439:LEU:N | 2.81 | 0.43 |
| 1:A:568:PRO:CG | 1:A:578:HIS:H | 2.30 | 0.43 |
| 1:A:774:LEU:HD23 | 1:A:778:MET:HE3 | 2.00 | 0.43 |
| 1:A:806:MET:SD | 3:C:17:PHE:HE2 | 2.41 | 0.43 |
| 3:C:11:LYS:HE2 | 3:C:11:LYS:HB3 | 1.83 | 0.43 |
| 3:C:119:THR:O | 3:C:123:VAL:HG23 | 2.18 | 0.43 |
| 1:D:123:CYS:CB | 1:D:158:ILE:HD13 | 2.48 | 0.43 |
| 1:D:292:MET:HE1 | 1:D:309:PRO:CG | 2.48 | 0.43 |
| 1:D:322:VAL:CG1 | 1:D:325:ILE:HG13 | 2.48 | 0.43 |
| 1:D:747:LEU:C | 1:D:749:GLY:N | 2.71 | 0.43 |
| 2:E:149:ASP:OD2 | 2:E:150:TYR:CA | 2.64 | 0.43 |
| 1:G:91:MET:CE | 1:G:119:SER:HB2 | 2.48 | 0.43 |
| 1:G:391:GLY:HA3 | 1:G:616:VAL:HG23 | 2.00 | 0.43 |
| 1:J:166:MET:CE | 1:J:254:PHE:CD2 | 3.01 | 0.43 |
| 1:J:37:SER:O | 1:J:38:VAL:HG23 | 2.17 | 0.43 |
| 1:J:725:ARG:CG | 1:J:733:PRO:HA | 2.43 | 0.43 |
| 1:J:839:MLY:NZ | 2:K:158:THR:HG22 | 2.33 | 0.43 |
| 1:M:123:CYS:CB | 1:M:158:ILE:HD13 | 2.48 | 0.43 |
| 1:M:612:GLN:NE2 | 1:M:627:GLY:H | 2.15 | 0.43 |
| 1:M:724:TYR:HD1 | 1:M:727:LEU:CD1 | 2.27 | 0.43 |
| 1:M:732:ILE:CG2 | 1:M:747:LEU:CD1 | 0.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:95:THR:HB | 1:M:713:SER:CB | 2.47 | 0.43 |
| 3:O:119:THR:O | 3:O:123:VAL:HG23 | 2.18 | 0.43 |
| 1:S:485:GLU:HA | 1:S:584:TYR:HE2 | 1.83 | 0.43 |
| 1:S:493:HIS:O | 1:S:496:PHE:HB3 | 2.18 | 0.43 |
| 1:S:64:THR:HB | 1:S:68:GLU:N | 2.33 | 0.43 |
| 1:S:266:GLU:OE1 | 1:S:659:MLY:NZ | 2.51 | 0.43 |
| 1:S:64:THR:CG2 | 1:S:65:GLU:H | 2.31 | 0.43 |
| 1:S:675:ILE:HG23 | 1:S:676:ILE:N | 2.32 | 0.43 |
| 1:S:725:ARG:HA | 1:S:732:ILE:HG22 | 1.99 | 0.43 |
| 1:S:787:ILE:HD13 | 1:S:787:ILE:HG21 | 1.67 | 0.43 |
| 4:V:220:ALA:HB3 | 4:V:223:PHE:CD1 | 2.53 | 0.43 |
| 4:9:287:ILE:CB | 4:W:204:ALA:H | 2.13 | 0.43 |
| 4:X:220:ALA:HB3 | 4:X:223:PHE:CD1 | 2.53 | 0.43 |
| 4:X:290:ARG:NH2 | 4:Z:201:VAL:HG21 | 2.33 | 0.43 |
| 1:M:529:PRO:HB3 | 4:Z:354:GLN:HA | 2.00 | 0.43 |
| 4:2:315:LYS:HD2 | 4:2:315:LYS:HA | 1.92 | 0.43 |
| 4:8:223:PHE:HB3 | 4:8:259:GLU:OE2 | 2.18 | 0.43 |
| 1:A:530:MET:CB | 4:8:354:GLN:CB | 2.95 | 0.43 |
| 4:9:171:LEU:HA | 4:9:172:PRO:HD2 | 1.84 | 0.43 |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:CD1 | 2.48 | 0.43 |
| 1:A:226:ASN:N | 1:A:227:PRO:HD2 | 2.32 | 0.43 |
| 1:A:229:LEU:HA | 1:A:229:LEU:HD12 | 1.75 | 0.43 |
| 1:A:493:HIS:O | 1:A:496:PHE:HB3 | 2.18 | 0.43 |
| 1:A:436:MLY:CE | 1:A:626:TYR:CE1 | 2.99 | 0.43 |
| 2:B:129:THR:HG23 | 2:B:132:GLU:OE1 | 2.18 | 0.43 |
| 1:D:224:SER:O | 1:D:227:PRO:HD2 | 2.17 | 0.43 |
| 1:D:493:HIS:O | 1:D:496:PHE:HB3 | 2.18 | 0.43 |
| 1:D:400:ALA:CB | 1:D:606:THR:HG22 | 2.48 | 0.43 |
| 1:D:88:ILE:HG21 | 1:D:88:ILE:HD12 | 1.78 | 0.43 |
| 1:D:800:ARG:HH22 | 3:F:40:ASN:HD21 | 1.31 | 0.43 |
| 3:F:52:ASN:CB | 3:F:53:PRO:HD3 | 2.28 | 0.43 |
| 2:H:129:THR:HG23 | 2:H:132:GLU:OE1 | 2.17 | 0.43 |
| 1:G:831:TRP:CZ3 | 2:H:34:ILE:HG21 | 2.52 | 0.43 |
| 1:J:224:SER:O | 1:J:227:PRO:HD2 | 2.17 | 0.43 |
| 1:J:496:PHE:HB2 | 1:J:515:PHE:CD2 | 2.53 | 0.43 |
| 1:J:93:MET:HE2 | 1:J:764:MLY:HD3 | 2.00 | 0.43 |
| 2:K:129:THR:HG23 | 2:K:132:GLU:OE1 | 2.17 | 0.43 |
| 2:K:140:PHE:HA | 2:K:141:PRO:HD2 | 1.56 | 0.43 |
| 1:M:35:MLY:HG3 | 1:M:777:GLU:OE2 | 2.17 | 0.43 |
| 1:M:659:MLY:HD2 | 1:M:659:MLY:HH22 | 1.42 | 0.43 |
| 1:M:725:ARG:HA | 1:M:732:ILE:HG22 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:122:GLU:HA | 3:O:125:GLU:OE1 | 2.18 | 0.43 |
| 1:S:439:LEU:N | 1:S:439:LEU:CD1 | 2.81 | 0.43 |
| 3:U:122:GLU:HA | 3:U:125:GLU:OE1 | 2.18 | 0.43 |
| 4:V:223:PHE:HB3 | 4:V:259:GLU:OE2 | 2.18 | 0.43 |
| 4:X:287:ILE:O | 4:Z:205:GLU:OE2 | 2.36 | 0.43 |
| 4:Z:171:LEU:HA | 4:Z:172:PRO:HD2 | 1.84 | 0.43 |
| 4:1:205:GLU:O | 4:1:208:ILE:HG22 | 2.18 | 0.43 |
| 4:9:193:LEU:O | 4:9:198:TYR:HD2 | 2.01 | 0.43 |
| 1:D:530:MET:CB | 4:9:354:GLN:CB | 2.95 | 0.43 |
| 1:A:109:ARG:CD | 1:A:117:THR:HB | 2.49 | 0.43 |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG13 | 1.95 | 0.43 |
| 1:A:485:GLU:HA | 1:A:584:TYR:HE2 | 1.83 | 0.43 |
| 1:A:643:GLY:CA | 4:8:24:ASP:OD1 | 2.62 | 0.43 |
| 1:A:266:GLU:OE1 | 1:A:659:MLY:NZ | 2.51 | 0.43 |
| 1:D:55:MLY:HH23 | 1:D:60:VAL:HG22 | 1.99 | 0.43 |
| 1:G:109:ARG:CD | 1:G:117:THR:HB | 2.48 | 0.43 |
| 1:G:123:CYS:CB | 1:G:158:ILE:HD13 | 2.48 | 0.43 |
| 1:G:493:HIS:O | 1:G:496:PHE:HB3 | 2.18 | 0.43 |
| 1:G:768:MLY:HG3 | 1:G:772:LEU:HD23 | 1.78 | 0.43 |
| 1:G:787:ILE:HG23 | 1:G:791:GLN:HG3 | 2.00 | 0.43 |
| 1:G:817:GLN:HE21 | 2:H:127:ARG:HB2 | 1.82 | 0.43 |
| 1:J:226:ASN:HB2 | 1:J:227:PRO:CD | 2.47 | 0.43 |
| 1:J:488:GLN:O | 1:J:491:PHE:HB3 | 2.17 | 0.43 |
| 1:J:798:LEU:CD2 | 3:L:118:MET:SD | 3.06 | 0.43 |
| 1:M:309:PRO:C | 1:M:311:ASP:H | 2.22 | 0.43 |
| 1:M:346:ASP:O | 1:M:350:ALA:N | 2.45 | 0.43 |
| 1:M:516:GLY:O | 1:M:518:ASP:N | 2.51 | 0.43 |
| 1:M:549:SER:C | 4:2:45:VAL:O | 2.56 | 0.43 |
| 1:M:725:ARG:CG | 1:M:733:PRO:CA | 2.95 | 0.43 |
| 3:O:69:LEU:HB3 | 3:O:70:PRO:HD3 | 2.00 | 0.43 |
| 1:S:48:VAL:HA | 1:S:104:TYR:OH | 2.18 | 0.43 |
| 1:S:519:LEU:N | 1:S:519:LEU:CD1 | 2.77 | 0.43 |
| 1:S:541:MET:HB3 | 4:2:345:ILE:HG22 | 2.00 | 0.43 |
| 1:S:732:ILE:CG2 | 1:S:747:LEU:HD11 | 1.26 | 0.43 |
| 1:S:787:ILE:HG23 | 1:S:791:GLN:HG3 | 2.00 | 0.43 |
| 1:S:829:TRP:HZ3 | 2:T:84:PHE:CE2 | 2.35 | 0.43 |
| 4:V:193:LEU:O | 4:V:198:TYR:HD2 | 2.01 | 0.43 |
| 1:A:549:SER:C | 4:V:45:VAL:O | 2.56 | 0.43 |
| 4:Y:149:THR:HA | 4:Y:165:ILE:O | 2.19 | 0.43 |
| 4:Z:193:LEU:O | 4:Z:198:TYR:HD2 | 2.01 | 0.43 |
| 4:X:324:THR:O | 4:Z:245:GLY:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:149:THR:HA | 4:3:165:ILE:O | 2.19 | 0.43 |
| 4:4:220:ALA:HB3 | 4:4:223:PHE:CD1 | 2.53 | 0.43 |
| 4:5:149:THR:HA | 4:5:165:ILE:O | 2.19 | 0.43 |
| 4:5:205:GLU:O | 4:5:208:ILE:HG22 | 2.18 | 0.43 |
| 4:6:149:THR:HA | 4:6:165:ILE:O | 2.19 | 0.43 |
| 4:8:220:ALA:HB3 | 4:8:223:PHE:CD1 | 2.53 | 0.43 |
| 1:D:543:PRO:CD | 4:9:143:TYR:O | 2.64 | 0.43 |
| 1:A:217:THR:HG22 | 1:A:218:LEU:N | 2.34 | 0.43 |
| 1:A:322:VAL:CG1 | 1:A:325:ILE:HG13 | 2.49 | 0.43 |
| 1:A:516:GLY:O | 1:A:518:ASP:N | 2.51 | 0.43 |
| 3:C:52:ASN:CB | 3:C:53:PRO:HD3 | 2.28 | 0.43 |
| 1:D:14:ALA:N | 1:D:15:PRO:CD | 2.81 | 0.43 |
| 1:D:155:ILE:HG22 | 1:D:156:PHE:N | 2.33 | 0.43 |
| 1:D:166:MET:CE | 1:D:254:PHE:HB2 | 2.46 | 0.43 |
| 1:D:292:MET:CE | 1:D:309:PRO:CA | 2.97 | 0.43 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:HG22 | 2.00 | 0.43 |
| 1:D:391:GLY:HA3 | 1:D:616:VAL:HG23 | 2.00 | 0.43 |
| 1:D:723:ARG:NH1 | 1:D:723:ARG:CG | 2.80 | 0.43 |
| 1:D:727:LEU:HB3 | 1:D:782:MLY:HH12 | 1.82 | 0.43 |
| 1:D:797:PHE:CD1 | 3:F:146:ILE:CB | 2.93 | 0.43 |
| 2:E:112:ILE:O | 2:E:148:VAL:N | 2.50 | 0.43 |
| 3:F:101:THR:HA | 3:F:137:ILE:O | 2.18 | 0.43 |
| 1:G:175:ILE:C | 1:G:176:LEU:HD12 | 2.38 | 0.43 |
| 1:G:226:ASN:N | 1:G:227:PRO:HD2 | 2.32 | 0.43 |
| 1:G:322:VAL:CG1 | 1:G:325:ILE:HG13 | 2.49 | 0.43 |
| 1:G:578:HIS:HB3 | 1:G:592:ILE:CD1 | 2.38 | 0.43 |
| 1:G:408:VAL:HG22 | 1:G:636:LYS:HG2 | 1.51 | 0.43 |
| 3:I:101:THR:HA | 3:I:137:ILE:O | 2.18 | 0.43 |
| 1:J:123:CYS:CB | 1:J:158:ILE:HD13 | 2.48 | 0.43 |
| 1:J:174:SER:OG | 1:J:669:PRO:HA | 2.18 | 0.43 |
| 1:J:292:MET:CE | 1:J:309:PRO:CA | 2.97 | 0.43 |
| 1:J:322:VAL:CG1 | 1:J:325:ILE:HG13 | 2.49 | 0.43 |
| 1:J:391:GLY:HA3 | 1:J:616:VAL:HG23 | 2.01 | 0.43 |
| 1:J:64:THR:CG2 | 1:J:65:GLU:H | 2.32 | 0.43 |
| 1:J:88:ILE:HG21 | 1:J:88:ILE:HD12 | 1.78 | 0.43 |
| 1:M:134:VAL:C | 1:M:136:ASN:H | 2.16 | 0.43 |
| 1:M:14:ALA:N | 1:M:15:PRO:CD | 2.82 | 0.43 |
| 1:M:226:ASN:N | 1:M:227:PRO:HD2 | 2.32 | 0.43 |
| 1:M:28:GLN:CB | 1:M:723:ARG:HH12 | 2.31 | 0.43 |
| 1:M:322:VAL:CG1 | 1:M:325:ILE:HD11 | 2.47 | 0.43 |
| 1:M:541:MET:HB3 | 4:Z:345:ILE:HG22 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:391:GLY:HA3 | 1:M:616:VAL:HG23 | 2.01 | 0.43 |
| 1:M:64:THR:HB | 1:M:68:GLU:N | 2.33 | 0.43 |
| 1:M:86:ASP:OD2 | 1:M:87:MLY:HH22 | 2.19 | 0.43 |
| 1:S:226:ASN:N | 1:S:227:PRO:HD2 | 2.32 | 0.43 |
| 1:S:443:ILE:HG22 | 1:S:444:ARG:N | 2.29 | 0.43 |
| 1:S:711:PHE:HB3 | 1:S:766:PHE:HB3 | 2.00 | 0.43 |
| 1:S:725:ARG:CZ | 1:S:737:PHE:CE1 | 3.02 | 0.43 |
| 1:S:798:LEU:CG | 3:U:126:LEU:CD1 | 2.44 | 0.43 |
| 1:S:86:ASP:OD2 | 1:S:87:MLY:HH22 | 2.19 | 0.43 |
| 1:J:642:LYS:HB2 | 4:W:24:ASP:O | 1.89 | 0.43 |
| 1:J:639:GLY:H | 4:W:344:SER:HB3 | 1.82 | 0.43 |
| 4:X:193:LEU:O | 4:X:198:TYR:HD2 | 2.01 | 0.43 |
| 4:1:193:LEU:O | 4:1:198:TYR:HD2 | 2.01 | 0.43 |
| 4:1:220:ALA:HB3 | 4:1:223:PHE:CD1 | 2.53 | 0.43 |
| 4:7:149:THR:HA | 4:7:165:ILE:O | 2.19 | 0.43 |
| 4:9:149:THR:HA | 4:9:165:ILE:O | 2.19 | 0.43 |
| 4:9:205:GLU:O | 4:9:208:ILE:HG22 | 2.18 | 0.43 |
| 1:A:787:ILE:HG23 | 1:A:791:GLN:HG3 | 2.00 | 0.43 |
| 1:D:322:VAL:CG1 | 1:D:325:ILE:HD11 | 2.47 | 0.43 |
| 1:D:354:LEU:HA | 1:D:354:LEU:HD12 | 1.56 | 0.43 |
| 1:D:637:LYS:HD2 | 4:9:144:ALA:HB3 | 1.20 | 0.43 |
| 1:D:40:VAL:HG23 | 1:D:76:GLN:O | 2.19 | 0.43 |
| 1:D:798:LEU:HA | 1:D:798:LEU:HD12 | 1.37 | 0.43 |
| 1:D:819:ASN:HB3 | 2:E:157:ILE:HG21 | 1.99 | 0.43 |
| 1:G:155:ILE:HG22 | 1:G:156:PHE:N | 2.33 | 0.43 |
| 1:G:201:ALA:O | 1:G:202:SER:OG | 2.36 | 0.43 |
| 1:G:639:GLY:H | 4:V:344:SER:HB3 | 1.83 | 0.43 |
| 1:G:725:ARG:CZ | 1:G:737:PHE:CZ | 3.01 | 0.43 |
| 1:G:750:GLY:HA3 | 3:I:114:LEU:HD22 | 2.00 | 0.43 |
| 1:G:793:ARG:O | 1:G:797:PHE:N | 2.39 | 0.43 |
| 1:G:794:CYS:O | 1:G:797:PHE:HB3 | 2.17 | 0.43 |
| 1:J:346:ASP:O | 1:J:350:ALA:N | 2.46 | 0.43 |
| 1:J:485:GLU:HA | 1:J:584:TYR:HE2 | 1.83 | 0.43 |
| 1:J:84:MLY:HH23 | 1:J:715:VAL:CG1 | 2.48 | 0.43 |
| 1:J:747:LEU:C | 1:J:749:GLY:N | 2.71 | 0.43 |
| 2:K:137:TRP:CA | 2:K:145:ALA:CB | 2.82 | 0.43 |
| 1:M:292:MET:CE | 1:M:309:PRO:CA | 2.97 | 0.43 |
| 1:M:295:MLY:CE | 1:M:332:MET:CE | 2.97 | 0.43 |
| 1:M:485:GLU:OE1 | 1:M:583:HIS:ND1 | 2.49 | 0.43 |
| 1:M:64:THR:CG2 | 1:M:65:GLU:H | 2.31 | 0.43 |
| 1:M:805:ALA:O | 1:M:808:GLU:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:40:VAL:HG23 | 1:S:76:GLN:O | 2.19 | 0.43 |
| 1:S:798:LEU:HD22 | 3:U:126:LEU:CD1 | 2.27 | 0.43 |
| 4:Y:220:ALA:HB3 | 4:Y:223:PHE:CD1 | 2.53 | 0.43 |
| 4:X:291:LYS:CE | 4:Z:243:PRO:HB3 | 2.09 | 0.43 |
| 4:4:171:LEU:HA | 4:4:172:PRO:HD2 | 1.84 | 0.43 |
| 4:4:193:LEU:O | 4:4:198:TYR:HD2 | 2.01 | 0.43 |
| 4:5:220:ALA:HB3 | 4:5:223:PHE:CD1 | 2.53 | 0.43 |
| 4:8:149:THR:HA | 4:8:165:ILE:O | 2.19 | 0.43 |
| 1:A:309:PRO:C | 1:A:311:ASP:H | 2.22 | 0.43 |
| 1:A:747:LEU:C | 1:A:749:GLY:H | 2.20 | 0.43 |
| 3:C:122:GLU:HA | 3:C:125:GLU:OE1 | 2.18 | 0.43 |
| 1:D:195:TYR:CD2 | 1:D:199:ILE:HD13 | 2.54 | 0.43 |
| 1:D:217:THR:HG22 | 1:D:218:LEU:N | 2.34 | 0.43 |
| 1:D:442:VAL:O | 1:D:445:ILE:HB | 2.19 | 0.43 |
| 1:D:436:MLY:CE | 1:D:626:TYR:CE1 | 2.99 | 0.43 |
| 1:D:173:GLN:HG3 | 1:D:670:HIS:HD2 | 1.82 | 0.43 |
| 1:D:732:ILE:CG2 | 1:D:747:LEU:HD12 | 0.35 | 0.43 |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:CD1 | 2.48 | 0.43 |
| 1:G:266:GLU:OE1 | 1:G:659:MLY:NZ | 2.51 | 0.43 |
| 1:G:295:MLY:HG3 | 1:G:332:MET:HE2 | 1.97 | 0.43 |
| 1:G:292:MET:CE | 1:G:309:PRO:CA | 2.97 | 0.43 |
| 1:G:309:PRO:C | 1:G:311:ASP:H | 2.22 | 0.43 |
| 1:G:701:LEU:HD12 | 1:G:701:LEU:HA | 1.55 | 0.43 |
| 1:G:797:PHE:CE1 | 3:I:146:ILE:CG2 | 2.93 | 0.43 |
| 1:J:246:PHE:HB3 | 1:J:270:LEU:HD12 | 2.01 | 0.43 |
| 1:J:409:GLY:N | 1:J:636:LYS:CD | 2.70 | 0.43 |
| 1:J:554:LEU:HA | 1:J:554:LEU:HD12 | 1.77 | 0.43 |
| 1:J:711:PHE:HB3 | 1:J:766:PHE:HB3 | 2.00 | 0.43 |
| 1:J:725:ARG:CZ | 1:J:737:PHE:CE1 | 3.02 | 0.43 |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:HD11 | 0.83 | 0.43 |
| 1:M:151:ALA:HB1 | 1:M:152:PRO:HD2 | 2.01 | 0.43 |
| 1:M:217:THR:HG22 | 1:M:218:LEU:N | 2.34 | 0.43 |
| 1:M:266:GLU:OE1 | 1:M:659:MLY:NZ | 2.51 | 0.43 |
| 1:S:151:ALA:HB1 | 1:S:152:PRO:HD2 | 2.01 | 0.43 |
| 1:S:246:PHE:HB3 | 1:S:270:LEU:HD12 | 2.01 | 0.43 |
| 1:S:391:GLY:HA3 | 1:S:616:VAL:HG23 | 2.01 | 0.43 |
| 1:G:543:PRO:CD | 4:V:143:TYR:O | 2.64 | 0.43 |
| 4:3:193:LEU:O | 4:3:198:TYR:HD2 | 2.01 | 0.43 |
| 4:7:205:GLU:O | 4:7:208:ILE:HG22 | 2.18 | 0.43 |
| 4:8:193:LEU:O | 4:8:198:TYR:HD2 | 2.01 | 0.43 |
| 1:A:123:CYS:HB2 | 1:A:158:ILE:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:151:ALA:HB1 | 1:A:152:PRO:HD2 | 2.01 | 0.43 |
| 1:A:175:ILE:C | 1:A:176:LEU:HD12 | 2.38 | 0.43 |
| 1:A:308:ASN:HA | 1:A:309:PRO:HD2 | 1.88 | 0.43 |
| 1:A:500:GLN:HB2 | 1:A:512:PHE:CZ | 2.54 | 0.43 |
| 1:A:86:ASP:OD2 | 1:A:87:MLY:HH22 | 2.19 | 0.43 |
| 1:A:97:LEU:CD2 | 1:A:712:PRO:CA | 2.96 | 0.43 |
| 1:D:496:PHE:HB2 | 1:D:515:PHE:CD2 | 2.54 | 0.43 |
| 1:D:831:TRP:CD1 | 2:E:51:PHE:HZ | 2.34 | 0.43 |
| 1:G:439:LEU:N | 1:G:439:LEU:CD1 | 2.81 | 0.43 |
| 1:G:612:GLN:NE2 | 1:G:627:GLY:H | 2.14 | 0.43 |
| 1:J:134:VAL:C | 1:J:136:ASN:H | 2.16 | 0.43 |
| 1:J:201:ALA:O | 1:J:202:SER:OG | 2.36 | 0.43 |
| 1:J:48:VAL:HA | 1:J:104:TYR:OH | 2.18 | 0.43 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:HG22 | 2.00 | 0.43 |
| 3:L:119:THR:O | 3:L:123:VAL:HG23 | 2.18 | 0.43 |
| 1:M:109:ARG:CD | 1:M:117:THR:HB | 2.49 | 0.43 |
| 1:M:201:ALA:O | 1:M:202:SER:OG | 2.36 | 0.43 |
| 1:M:215:GLN:H | 1:M:340:ILE:CD1 | 2.20 | 0.43 |
| 1:M:439:LEU:N | 1:M:439:LEU:CD1 | 2.81 | 0.43 |
| 1:M:568:PRO:CG | 1:M:578:HIS:H | 2.30 | 0.43 |
| 1:M:689:GLU:HA | 1:M:692:LEU:HB2 | 2.00 | 0.43 |
| 1:M:725:ARG:CZ | 1:M:737:PHE:CE1 | 3.02 | 0.43 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:CZ | 2.48 | 0.43 |
| 1:M:798:LEU:HD21 | 3:O:126:LEU:CD1 | 2.48 | 0.43 |
| 1:S:292:MET:CE | 1:S:309:PRO:CA | 2.97 | 0.43 |
| 1:S:500:GLN:HB2 | 1:S:512:PHE:CZ | 2.54 | 0.43 |
| 1:S:689:GLU:HA | 1:S:692:LEU:HB2 | 2.00 | 0.43 |
| 1:S:692:LEU:O | 1:S:696:ARG:HG3 | 2.18 | 0.43 |
| 1:S:84:MLY:HH21 | 1:S:724:TYR:HE2 | 1.80 | 0.43 |
| 1:S:731:ALA:HA | 3:U:94:PHE:HA | 2.01 | 0.43 |
| 2:T:140:PHE:HA | 2:T:141:PRO:HD2 | 1.56 | 0.43 |
| 1:G:639:GLY:CA | 4:V:344:SER:O | 2.40 | 0.43 |
| 1:G:530:MET:CE | 4:V:354:GLN:HG3 | 2.34 | 0.43 |
| 4:W:205:GLU:O | 4:W:208:ILE:HG22 | 2.18 | 0.43 |
| 4:Z:220:ALA:HB3 | 4:Z:223:PHE:CD1 | 2.53 | 0.43 |
| 4:1:149:THR:HA | 4:1:165:ILE:O | 2.19 | 0.43 |
| 4:2:220:ALA:HB3 | 4:2:223:PHE:CD1 | 2.53 | 0.43 |
| 4:6:205:GLU:O | 4:6:208:ILE:HG22 | 2.18 | 0.43 |
| 4:6:220:ALA:HB3 | 4:6:223:PHE:CD1 | 2.53 | 0.43 |
| 4:8:287:ILE:HA | 4:V:202:THR:HG21 | 1.59 | 0.43 |
| 1:A:292:MET:CE | 1:A:309:PRO:CA | 2.97 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:529:PRO:HB3 | 4:8:354:GLN:HA | 1.99 | 0.43 |
| 1:A:537:GLU:OE1 | 4:8:350:SER:HA | 2.19 | 0.43 |
| 1:A:757:GLN:HB2 | 1:A:771:LEU:HD21 | 1.29 | 0.43 |
| 1:D:123:CYS:HB2 | 1:D:158:ILE:HD13 | 2.00 | 0.43 |
| 1:D:246:PHE:HB3 | 1:D:270:LEU:HD12 | 2.01 | 0.43 |
| 1:D:537:GLU:OE1 | 4:9:350:SER:HA | 2.19 | 0.43 |
| 1:D:549:SER:C | 4:W:45:VAL:O | 2.57 | 0.43 |
| 1:D:725:ARG:CZ | 1:D:737:PHE:CZ | 3.01 | 0.43 |
| 1:G:40:VAL:HG23 | 1:G:76:GLN:O | 2.19 | 0.43 |
| 1:G:747:LEU:C | 1:G:749:GLY:N | 2.71 | 0.43 |
| 3:I:119:THR:O | 3:I:123:VAL:HG23 | 2.18 | 0.43 |
| 3:I:63:ILE:CG2 | 3:I:64:THR:H | 2.32 | 0.43 |
| 1:J:169:ASP:O | 1:J:170:ARG:HB2 | 2.19 | 0.43 |
| 1:J:175:ILE:C | 1:J:176:LEU:HD12 | 2.39 | 0.43 |
| 1:J:715:VAL:HG12 | 1:J:720:PHE:HB2 | 2.00 | 0.43 |
| 1:M:246:PHE:HB3 | 1:M:270:LEU:HD12 | 2.01 | 0.43 |
| 1:M:87:MLY:HD3 | 1:M:87:MLY:HH12 | 1.62 | 0.43 |
| 1:S:214:MET:CA | 1:S:340:ILE:HD11 | 2.45 | 0.43 |
| 1:S:411:GLU:H | 4:2:333:PRO:CB | 2.30 | 0.43 |
| 1:S:476:GLU:H | 1:S:476:GLU:CD | 2.21 | 0.43 |
| 1:S:799:MET:SD | 3:U:32:ASP:CB | 3.07 | 0.43 |
| 4:W:220:ALA:HB3 | 4:W:223:PHE:CD1 | 2.53 | 0.43 |
| 4:X:149:THR:HA | 4:X:165:ILE:O | 2.19 | 0.43 |
| 4:Y:193:LEU:O | 4:Y:198:TYR:HD2 | 2.01 | 0.43 |
| 4:2:110:LEU:O | 4:3:195:GLU:CA | 2.58 | 0.43 |
| 4:6:217:CYS:C | 4:6:218:TYR:HD1 | 2.23 | 0.43 |
| 4:8:205:GLU:O | 4:8:208:ILE:HG22 | 2.18 | 0.43 |
| 4:7:324:THR:N | 4:9:245:GLY:CA | 2.69 | 0.43 |
| 1:A:40:VAL:HG23 | 1:A:76:GLN:O | 2.19 | 0.43 |
| 1:A:442:VAL:O | 1:A:445:ILE:HB | 2.19 | 0.43 |
| 1:A:689:GLU:HA | 1:A:692:LEU:HB2 | 2.00 | 0.43 |
| 1:A:725:ARG:CZ | 1:A:737:PHE:CE1 | 3.02 | 0.43 |
| 2:B:140:PHE:HA | 2:B:141:PRO:HD2 | 1.56 | 0.43 |
| 3:C:50:LEU:O | 3:C:53:PRO:HG2 | 2.18 | 0.43 |
| 1:D:229:LEU:HD12 | 1:D:229:LEU:HA | 1.75 | 0.43 |
| 1:D:402:CYS:C | 1:D:404:PRO:HD3 | 2.40 | 0.43 |
| 1:D:530:MET:HA | 4:9:354:GLN:CD | 2.11 | 0.43 |
| 1:D:64:THR:CG2 | 1:D:65:GLU:H | 2.32 | 0.43 |
| 1:D:724:TYR:HE1 | 1:D:779:ARG:N | 2.16 | 0.43 |
| 1:D:727:LEU:HG | 1:D:782:MLY:HG3 | 1.24 | 0.43 |
| 1:D:725:ARG:O | 1:D:782:MLY:HH22 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:63:ILE:CG2 | 3:F:64:THR:H | 2.32 | 0.43 |
| 1:G:129:TYR:HD1 | 1:G:129:TYR:HA | 1.65 | 0.43 |
| 1:G:217:THR:HG22 | 1:G:218:LEU:N | 2.34 | 0.43 |
| 1:G:406:VAL:O | 1:G:412:ALA:HA | 2.19 | 0.43 |
| 1:G:689:GLU:HA | 1:G:692:LEU:HB2 | 2.00 | 0.43 |
| 1:G:692:LEU:O | 1:G:696:ARG:HG3 | 2.18 | 0.43 |
| 1:G:732:ILE:CG2 | 1:G:747:LEU:CD1 | 0.65 | 0.43 |
| 1:G:834:LEU:CD2 | 2:H:34:ILE:CD1 | 2.96 | 0.43 |
| 1:G:86:ASP:OD2 | 1:G:87:MLY:HH22 | 2.19 | 0.43 |
| 3:I:69:LEU:HB3 | 3:I:70:PRO:HD3 | 1.99 | 0.43 |
| 1:J:217:THR:HG22 | 1:J:218:LEU:N | 2.34 | 0.43 |
| 1:J:485:GLU:OE2 | 1:J:584:TYR:N | 2.50 | 0.43 |
| 1:J:63:MLY:HH23 | 1:J:63:MLY:HD3 | 1.76 | 0.43 |
| 1:J:84:MLY:HG2 | 1:J:723:ARG:CB | 2.33 | 0.43 |
| 1:J:725:ARG:CZ | 1:J:737:PHE:CZ | 3.01 | 0.43 |
| 1:J:93:MET:CE | 1:J:764:MLY:HD3 | 2.48 | 0.43 |
| 1:M:400:ALA:CB | 1:M:606:THR:HG22 | 2.49 | 0.43 |
| 1:M:692:LEU:O | 1:M:696:ARG:HG3 | 2.18 | 0.43 |
| 1:M:97:LEU:HD12 | 1:M:97:LEU:HA | 1.67 | 0.43 |
| 1:S:134:VAL:C | 1:S:136:ASN:H | 2.16 | 0.43 |
| 1:S:17:LEU:HA | 1:S:17:LEU:HD12 | 1.67 | 0.43 |
| 1:S:406:VAL:O | 1:S:412:ALA:HA | 2.19 | 0.43 |
| 1:S:400:ALA:CB | 1:S:606:THR:HG22 | 2.49 | 0.43 |
| 1:S:715:VAL:HG12 | 1:S:720:PHE:HB2 | 2.00 | 0.43 |
| 1:S:732:ILE:HG23 | 1:S:747:LEU:HD12 | 0.95 | 0.43 |
| 1:S:803:TYR:CE2 | 3:U:17:PHE:HZ | 2.30 | 0.43 |
| 4:2:110:LEU:C | 4:3:195:GLU:HG3 | 2.37 | 0.43 |
| 1:S:639:GLY:CA | 4:2:344:SER:O | 2.39 | 0.43 |
| 4:3:220:ALA:HB3 | 4:3:223:PHE:CD1 | 2.53 | 0.43 |
| 4:9:220:ALA:HB3 | 4:9:223:PHE:CD1 | 2.53 | 0.43 |
| 4:9:180:LEU:HD11 | 4:9:261:LEU:HD23 | 2.01 | 0.43 |
| 1:A:294:ASN:OD1 | 1:A:307:THR:HG21 | 2.19 | 0.43 |
| 1:A:496:PHE:HB2 | 1:A:515:PHE:CD2 | 2.53 | 0.43 |
| 1:A:637:LYS:HD2 | 4:8:144:ALA:HB3 | 1.21 | 0.43 |
| 1:A:712:PRO:HB2 | 1:A:713:SER:H | 1.61 | 0.43 |
| 1:A:93:MET:CE | 1:A:715:VAL:CG1 | 2.84 | 0.43 |
| 2:B:140:PHE:CD2 | 2:B:144:VAL:HG11 | 2.54 | 0.43 |
| 2:B:137:TRP:CZ3 | 2:B:145:ALA:N | 2.81 | 0.43 |
| 1:D:169:ASP:O | 1:D:170:ARG:HB2 | 2.19 | 0.43 |
| 1:D:175:ILE:C | 1:D:176:LEU:HD12 | 2.39 | 0.43 |
| 1:D:279:LEU:CB | 1:D:280:PRO:HD2 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:294:ASN:OD1 | 1:D:307:THR:HG21 | 2.19 | 0.43 |
| 1:D:485:GLU:OE1 | 1:D:583:HIS:ND1 | 2.49 | 0.43 |
| 1:D:533:PHE:HA | 1:D:533:PHE:HD1 | 1.79 | 0.43 |
| 1:D:612:GLN:NE2 | 1:D:627:GLY:H | 2.14 | 0.43 |
| 1:D:747:LEU:C | 1:D:749:GLY:H | 2.21 | 0.43 |
| 1:G:166:MET:CE | 1:G:254:PHE:CD2 | 3.01 | 0.43 |
| 1:G:485:GLU:OE1 | 1:G:583:HIS:ND1 | 2.49 | 0.43 |
| 1:G:496:PHE:HB2 | 1:G:515:PHE:CD2 | 2.53 | 0.43 |
| 1:G:799:MET:SD | 3:I:32:ASP:CG | 2.97 | 0.43 |
| 1:J:91:MET:CE | 1:J:119:SER:HB2 | 2.48 | 0.43 |
| 1:J:129:TYR:HD1 | 1:J:129:TYR:HA | 1.65 | 0.43 |
| 1:J:294:ASN:OD1 | 1:J:307:THR:HG21 | 2.19 | 0.43 |
| 1:J:402:CYS:C | 1:J:404:PRO:HD3 | 2.40 | 0.43 |
| 1:J:40:VAL:HG23 | 1:J:76:GLN:O | 2.19 | 0.43 |
| 1:J:675:ILE:HG23 | 1:J:676:ILE:N | 2.33 | 0.43 |
| 1:M:40:VAL:HG23 | 1:M:76:GLN:O | 2.19 | 0.43 |
| 1:M:476:GLU:CD | 1:M:476:GLU:H | 2.22 | 0.43 |
| 1:M:506:GLU:HG3 | 1:M:760:PHE:O | 2.19 | 0.43 |
| 1:M:537:GLU:OE1 | 4:Z:350:SER:HA | 2.19 | 0.43 |
| 1:M:747:LEU:C | 1:M:749:GLY:N | 2.71 | 0.43 |
| 1:M:797:PHE:CD2 | 3:O:126:LEU:CD2 | 3.02 | 0.43 |
| 1:S:169:ASP:O | 1:S:170:ARG:HB2 | 2.19 | 0.43 |
| 1:S:536:LEU:HA | 1:S:536:LEU:HD12 | 1.69 | 0.43 |
| 1:G:642:LYS:HB2 | 4:V:24:ASP:O | 1.89 | 0.43 |
| 1:A:550:PHE:C | 4:V:46:GLY:CA | 2.87 | 0.43 |
| 4:W:149:THR:HA | 4:W:165:ILE:O | 2.19 | 0.43 |
| 4:W:193:LEU:O | 4:W:198:TYR:HD2 | 2.01 | 0.43 |
| 4:Z:223:PHE:HB3 | 4:Z:259:GLU:OE2 | 2.18 | 0.43 |
| 1:S:530:MET:CB | 4:2:354:GLN:CB | 2.95 | 0.42 |
| 4:4:217:CYS:C | 4:4:218:TYR:HD1 | 2.22 | 0.42 |
| 4:5:180:LEU:HD11 | 4:5:261:LEU:HD23 | 2.01 | 0.42 |
| 4:5:315:LYS:HA | 4:5:315:LYS:HD2 | 1.92 | 0.42 |
| 4:7:220:ALA:HB3 | 4:7:223:PHE:CD1 | 2.53 | 0.42 |
| 1:A:530:MET:HE3 | 4:8:354:GLN:CB | 2.49 | 0.42 |
| 1:A:322:VAL:HA | 1:A:323:PRO:HD3 | 1.87 | 0.42 |
| 1:A:578:HIS:HB3 | 1:A:592:ILE:CD1 | 2.38 | 0.42 |
| 1:A:60:VAL:O | 1:A:72:VAL:N | 2.51 | 0.42 |
| 1:A:408:VAL:HG22 | 1:A:636:LYS:HG2 | 1.51 | 0.42 |
| 1:D:204:GLU:N | 1:D:207:LYS:HE3 | 2.23 | 0.42 |
| 1:D:215:GLN:H | 1:D:340:ILE:CD1 | 2.21 | 0.42 |
| 1:D:449:LEU:HD12 | 1:D:449:LEU:HA | 1.60 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:642:LYS:HB3 | 4:9:24:ASP:HB2 | 1.37 | 0.42 |
| 1:D:713:SER:O | 1:D:771:LEU:HD21 | 2.19 | 0.42 |
| 1:G:151:ALA:HB1 | 1:G:152:PRO:HD2 | 2.01 | 0.42 |
| 1:G:442:VAL:O | 1:G:445:ILE:HB | 2.19 | 0.42 |
| 1:G:400:ALA:CB | 1:G:606:THR:HG22 | 2.49 | 0.42 |
| 1:G:796:GLY:HA2 | 3:I:35:ARG:NE | 2.31 | 0.42 |
| 2:H:112:ILE:O | 2:H:148:VAL:N | 2.50 | 0.42 |
| 2:H:114:LYS:CG | 2:H:146:GLY:HA2 | 2.46 | 0.42 |
| 1:J:14:ALA:N | 1:J:15:PRO:CD | 2.82 | 0.42 |
| 1:J:155:ILE:HG22 | 1:J:156:PHE:N | 2.33 | 0.42 |
| 1:J:195:TYR:CD2 | 1:J:199:ILE:HD13 | 2.54 | 0.42 |
| 1:J:400:ALA:CB | 1:J:606:THR:HG22 | 2.49 | 0.42 |
| 1:J:449:LEU:HA | 1:J:449:LEU:HD12 | 1.60 | 0.42 |
| 1:J:538:GLU:OE1 | 4:W:355:MET:HE3 | 2.18 | 0.42 |
| 1:J:829:TRP:O | 1:J:832:MET:N | 2.50 | 0.42 |
| 1:J:839:MLY:N | 1:J:840:PRO:HD2 | 2.34 | 0.42 |
| 3:L:101:THR:HA | 3:L:137:ILE:O | 2.18 | 0.42 |
| 1:M:322:VAL:CG1 | 1:M:325:ILE:HG13 | 2.49 | 0.42 |
| 1:S:136:ASN:O | 1:S:139:VAL:N | 2.47 | 0.42 |
| 1:S:144:ARG:HD2 | 1:S:144:ARG:HA | 1.78 | 0.42 |
| 1:S:294:ASN:OD1 | 1:S:307:THR:HG21 | 2.19 | 0.42 |
| 1:S:568:PRO:O | 1:S:570:PRO:HD3 | 2.19 | 0.42 |
| 1:S:568:PRO:CG | 1:S:578:HIS:H | 2.30 | 0.42 |
| 1:S:62:VAL:HG12 | 1:S:63:MLY:N | 2.34 | 0.42 |
| 1:S:839:MLY:N | 1:S:840:PRO:HD2 | 2.34 | 0.42 |
| 1:S:842:LEU:N | 1:S:842:LEU:CD1 | 2.82 | 0.42 |
| 1:S:795:ARG:HE | 3:U:118:MET:HE2 | 1.83 | 0.42 |
| 4:V:149:THR:HA | 4:V:165:ILE:O | 2.19 | 0.42 |
| 4:V:222:ASP:OD1 | 4:V:224:GLU:HB3 | 2.19 | 0.42 |
| 4:1:322:PRO:HB3 | 4:3:244:ASP:HB2 | 1.88 | 0.42 |
| 4:2:223:PHE:HB3 | 4:2:259:GLU:OE2 | 2.18 | 0.42 |
| 4:3:217:CYS:C | 4:3:218:TYR:HD1 | 2.22 | 0.42 |
| 4:4:149:THR:HA | 4:4:165:ILE:O | 2.19 | 0.42 |
| 1:A:636:LYS:CB | 4:8:334:GLU:OE1 | 2.67 | 0.42 |
| 1:A:541:MET:CE | 4:8:346:LEU:HD12 | 2.48 | 0.42 |
| 1:A:14:ALA:N | 1:A:15:PRO:CD | 2.81 | 0.42 |
| 1:A:185:LYS:HG3 | 1:A:185:LYS:H | 1.63 | 0.42 |
| 1:A:530:MET:CE | 4:8:354:GLN:CB | 2.96 | 0.42 |
| 1:A:62:VAL:O | 1:A:69:THR:HA | 2.19 | 0.42 |
| 1:A:659:MLY:HH22 | 1:A:659:MLY:HD2 | 1.42 | 0.42 |
| 2:B:54:MET:O | 2:H:21:GLU:OE1 | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:409:GLY:N | 1:D:636:LYS:CD | 2.71 | 0.42 |
| 1:D:480:ILE:CG2 | 1:D:481:ASN:N | 2.74 | 0.42 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:HG23 | 2.01 | 0.42 |
| 1:D:62:VAL:HG12 | 1:D:63:MLY:N | 2.35 | 0.42 |
| 1:D:724:TYR:HB3 | 1:D:727:LEU:CD1 | 2.48 | 0.42 |
| 1:D:817:GLN:HG2 | 2:E:127:ARG:HB3 | 1.64 | 0.42 |
| 1:G:134:VAL:C | 1:G:136:ASN:H | 2.16 | 0.42 |
| 1:G:174:SER:OG | 1:G:669:PRO:HA | 2.18 | 0.42 |
| 1:G:226:ASN:HB2 | 1:G:227:PRO:CD | 2.48 | 0.42 |
| 1:G:229:LEU:HA | 1:G:229:LEU:HD12 | 1.75 | 0.42 |
| 1:G:246:PHE:HB3 | 1:G:270:LEU:HD12 | 2.00 | 0.42 |
| 1:G:320:ILE:O | 1:G:320:ILE:HG22 | 2.18 | 0.42 |
| 1:G:443:ILE:HG22 | 1:G:444:ARG:N | 2.29 | 0.42 |
| 1:G:476:GLU:H | 1:G:476:GLU:CD | 2.22 | 0.42 |
| 1:G:568:PRO:O | 1:G:570:PRO:HD3 | 2.19 | 0.42 |
| 1:G:692:LEU:HA | 1:G:692:LEU:HD23 | 1.85 | 0.42 |
| 1:G:84:MLY:HH23 | 1:G:715:VAL:HG13 | 2.01 | 0.42 |
| 1:J:62:VAL:O | 1:J:69:THR:HA | 2.20 | 0.42 |
| 1:M:406:VAL:O | 1:M:412:ALA:HA | 2.19 | 0.42 |
| 1:S:148:ARG:HE | 1:S:763:THR:HG21 | 1.84 | 0.42 |
| 1:S:14:ALA:N | 1:S:15:PRO:CD | 2.81 | 0.42 |
| 1:S:175:ILE:C | 1:S:176:LEU:HD12 | 2.39 | 0.42 |
| 1:S:496:PHE:HB2 | 1:S:515:PHE:CD2 | 2.53 | 0.42 |
| 1:S:659:MLY:HH22 | 1:S:659:MLY:HD2 | 1.42 | 0.42 |
| 1:S:797:PHE:CD1 | 3:U:149:VAL:HG13 | 2.54 | 0.42 |
| 1:S:831:TRP:NE1 | 2:T:67:MET:HG2 | 2.33 | 0.42 |
| 4:Y:217:CYS:C | 4:Y:218:TYR:HD1 | 2.22 | 0.42 |
| 4:Z:222:ASP:OD1 | 4:Z:224:GLU:HB3 | 2.20 | 0.42 |
| 4:1:180:LEU:HD11 | 4:1:261:LEU:HD23 | 2.01 | 0.42 |
| 4:2:171:LEU:HA | 4:2:172:PRO:HD2 | 1.84 | 0.42 |
| 4:6:180:LEU:HD11 | 4:6:261:LEU:HD23 | 2.02 | 0.42 |
| 4:8:217:CYS:C | 4:8:218:TYR:HD1 | 2.23 | 0.42 |
| 1:A:534:SER:CB | 4:8:351:THR:HA | 2.48 | 0.42 |
| 1:A:174:SER:OG | 1:A:669:PRO:HA | 2.18 | 0.42 |
| 1:A:195:TYR:CD2 | 1:A:199:ILE:HD13 | 2.54 | 0.42 |
| 1:A:166:MET:CE | 1:A:254:PHE:HB2 | 2.46 | 0.42 |
| 1:A:406:VAL:O | 1:A:412:ALA:HA | 2.19 | 0.42 |
| 1:A:400:ALA:CB | 1:A:606:THR:HG22 | 2.48 | 0.42 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:C | 2.87 | 0.42 |
| 1:D:136:ASN:HA | 1:D:137:PRO:HD3 | 1.50 | 0.42 |
| 1:D:226:ASN:HB2 | 1:D:227:PRO:CD | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:406:VAL:O | 1:D:412:ALA:HA | 2.20 | 0.42 |
| 1:D:568:PRO:O | 1:D:570:PRO:HD3 | 2.19 | 0.42 |
| 1:D:715:VAL:HG12 | 1:D:720:PHE:HB2 | 2.00 | 0.42 |
| 1:D:725:ARG:CZ | 1:D:737:PHE:CE1 | 3.01 | 0.42 |
| 1:G:213:LYS:HA | 1:G:220:ASP:OD2 | 2.19 | 0.42 |
| 1:G:402:CYS:C | 1:G:404:PRO:HD3 | 2.40 | 0.42 |
| 1:G:64:THR:CG2 | 1:G:65:GLU:H | 2.32 | 0.42 |
| 2:H:140:PHE:CD2 | 2:H:144:VAL:HG11 | 2.55 | 0.42 |
| 1:J:295:MLY:CE | 1:J:332:MET:CE | 2.97 | 0.42 |
| 1:J:408:VAL:HG22 | 1:J:636:LYS:HG2 | 1.52 | 0.42 |
| 1:J:759:ALA:O | 1:J:766:PHE:N | 2.32 | 0.42 |
| 1:J:86:ASP:OD2 | 1:J:87:MLY:HH22 | 2.19 | 0.42 |
| 2:K:140:PHE:CD2 | 2:K:144:VAL:HG11 | 2.54 | 0.42 |
| 1:M:213:LYS:HA | 1:M:220:ASP:OD2 | 2.19 | 0.42 |
| 1:M:294:ASN:OD1 | 1:M:307:THR:HG21 | 2.19 | 0.42 |
| 1:M:496:PHE:HB2 | 1:M:515:PHE:CD2 | 2.53 | 0.42 |
| 1:M:500:GLN:HB2 | 1:M:512:PHE:CZ | 2.54 | 0.42 |
| 1:M:568:PRO:O | 1:M:570:PRO:HD3 | 2.19 | 0.42 |
| 1:M:62:VAL:HG12 | 1:M:63:MLY:N | 2.35 | 0.42 |
| 1:M:804:ARG:C | 1:M:807:VAL:HB | 2.40 | 0.42 |
| 2:N:137:TRP:CZ3 | 2:N:145:ALA:N | 2.81 | 0.42 |
| 1:S:195:TYR:CD2 | 1:S:199:ILE:HD13 | 2.54 | 0.42 |
| 1:S:201:ALA:O | 1:S:202:SER:OG | 2.36 | 0.42 |
| 1:S:213:LYS:HA | 1:S:220:ASP:OD2 | 2.19 | 0.42 |
| 1:S:38:VAL:HG13 | 1:S:39:PHE:N | 2.35 | 0.42 |
| 1:S:120:GLY:CA | 1:S:764:MLY:CH1 | 2.82 | 0.42 |
| 1:S:818:TYR:CD1 | 2:T:127:ARG:CZ | 3.02 | 0.42 |
| 1:S:792:ALA:CA | 3:U:42:THR:HA | 2.45 | 0.42 |
| 1:S:731:ALA:HB3 | 3:U:93:VAL:HB | 1.97 | 0.42 |
| 1:G:642:LYS:HB3 | 4:V:24:ASP:HB2 | 1.38 | 0.42 |
| 1:G:633:GLY:HA2 | 4:V:25:ASP:HA | 1.26 | 0.42 |
| 4:2:202:THR:HG21 | 4:Z:287:ILE:HA | 1.59 | 0.42 |
| 4:Z:315:LYS:HA | 4:Z:315:LYS:HD2 | 1.92 | 0.42 |
| 1:M:639:GLY:CA | 4:Z:344:SER:O | 2.39 | 0.42 |
| 1:M:534:SER:CB | 4:Z:351:THR:HA | 2.49 | 0.42 |
| 4:1:206:ARG:O | 4:1:209:VAL:HG12 | 2.20 | 0.42 |
| 4:1:217:CYS:C | 4:1:218:TYR:HD1 | 2.23 | 0.42 |
| 4:2:149:THR:HA | 4:2:165:ILE:O | 2.19 | 0.42 |
| 4:2:245:GLY:CA | 4:Z:324:THR:N | 2.69 | 0.42 |
| 4:3:206:ARG:O | 4:3:209:VAL:HG12 | 2.20 | 0.42 |
| 4:6:193:LEU:O | 4:6:198:TYR:HD2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:180:LEU:HD11 | 4:7:261:LEU:HD23 | 2.01 | 0.42 |
| 4:8:222:ASP:OD1 | 4:8:224:GLU:HB3 | 2.20 | 0.42 |
| 1:A:169:ASP:O | 1:A:170:ARG:HB2 | 2.19 | 0.42 |
| 1:A:246:PHE:HB3 | 1:A:270:LEU:HD12 | 2.01 | 0.42 |
| 1:A:38:VAL:HG13 | 1:A:39:PHE:N | 2.35 | 0.42 |
| 1:A:612:GLN:NE2 | 1:A:627:GLY:H | 2.14 | 0.42 |
| 1:A:733:PRO:O | 1:A:737:PHE:CE1 | 2.53 | 0.42 |
| 1:D:109:ARG:CD | 1:D:117:THR:HB | 2.49 | 0.42 |
| 1:D:320:ILE:O | 1:D:320:ILE:HG22 | 2.18 | 0.42 |
| 1:D:174:SER:HA | 1:D:460:GLY:O | 2.20 | 0.42 |
| 1:D:529:PRO:HB3 | 4:9:354:GLN:HA | 2.00 | 0.42 |
| 1:D:713:SER:HG | 1:D:771:LEU:CG | 2.17 | 0.42 |
| 1:D:829:TRP:O | 1:D:832:MET:N | 2.50 | 0.42 |
| 1:D:839:MLY:N | 1:D:840:PRO:HD2 | 2.35 | 0.42 |
| 2:E:140:PHE:CD2 | 2:E:144:VAL:HG11 | 2.54 | 0.42 |
| 3:F:119:THR:O | 3:F:123:VAL:HG23 | 2.18 | 0.42 |
| 1:G:195:TYR:CD2 | 1:G:199:ILE:HD13 | 2.54 | 0.42 |
| 1:G:295:MLY:CE | 1:G:332:MET:CE | 2.97 | 0.42 |
| 1:G:500:GLN:HB2 | 1:G:512:PHE:CZ | 2.54 | 0.42 |
| 1:G:578:HIS:CD2 | 1:G:592:ILE:H | 2.38 | 0.42 |
| 1:G:62:VAL:HG12 | 1:G:63:MLY:N | 2.34 | 0.42 |
| 1:G:173:GLN:HG3 | 1:G:670:HIS:CD2 | 2.55 | 0.42 |
| 1:G:715:VAL:HG12 | 1:G:720:PHE:HB2 | 2.00 | 0.42 |
| 1:J:406:VAL:O | 1:J:412:ALA:HA | 2.19 | 0.42 |
| 1:M:206:LYS:CE | 1:M:217:THR:HG23 | 2.29 | 0.42 |
| 1:M:348:MLY:HH12 | 1:M:348:MLY:HD2 | 1.81 | 0.42 |
| 1:M:823:PHE:CE1 | 2:N:156:VAL:O | 2.73 | 0.42 |
| 1:M:826:VAL:O | 1:M:828:HIS:N | 2.53 | 0.42 |
| 1:S:309:PRO:C | 1:S:311:ASP:H | 2.22 | 0.42 |
| 1:S:322:VAL:CG1 | 1:S:325:ILE:HG13 | 2.49 | 0.42 |
| 1:S:295:MLY:CE | 1:S:332:MET:CE | 2.97 | 0.42 |
| 1:S:723:ARG:NH1 | 1:S:723:ARG:CG | 2.79 | 0.42 |
| 1:S:93:MET:HE2 | 1:S:764:MLY:HD3 | 1.91 | 0.42 |
| 1:S:750:GLY:N | 3:U:89:GLU:HB3 | 2.33 | 0.42 |
| 4:V:206:ARG:O | 4:V:209:VAL:HG12 | 2.20 | 0.42 |
| 4:V:180:LEU:HD11 | 4:V:261:LEU:HD23 | 2.01 | 0.42 |
| 4:W:180:LEU:HD11 | 4:W:261:LEU:HD23 | 2.02 | 0.42 |
| 1:J:530:MET:CB | 4:W:354:GLN:CB | 2.95 | 0.42 |
| 1:J:529:PRO:HB3 | 4:W:354:GLN:HA | 2.00 | 0.42 |
| 4:X:206:ARG:O | 4:X:209:VAL:HG12 | 2.20 | 0.42 |
| 4:Y:180:LEU:HD11 | 4:Y:261:LEU:HD23 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Z:217:CYS:C | 4:Z:218:TYR:HD1 | 2.23 | 0.42 |
| 4:2:206:ARG:O | 4:2:209:VAL:HG12 | 2.20 | 0.42 |
| 4:3:180:LEU:HD11 | 4:3:261:LEU:HD23 | 2.02 | 0.42 |
| 4:4:222:ASP:OD1 | 4:4:224:GLU:HB3 | 2.19 | 0.42 |
| 1:S:546:THR:HG1 | 4:4:47:MET:N | 2.18 | 0.42 |
| 4:8:180:LEU:HD11 | 4:8:261:LEU:HD23 | 2.02 | 0.42 |
| 4:7:287:ILE:CB | 4:9:204:ALA:H | 2.13 | 0.42 |
| 1:D:541:MET:CE | 4:9:346:LEU:HD12 | 2.48 | 0.42 |
| 1:A:402:CYS:C | 1:A:404:PRO:HD3 | 2.40 | 0.42 |
| 1:A:541:MET:HB3 | 4:8:345:ILE:HG22 | 2.00 | 0.42 |
| 1:A:568:PRO:O | 1:A:570:PRO:HD3 | 2.19 | 0.42 |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:CD1 | 2.50 | 0.42 |
| 1:A:800:ARG:HD3 | 3:C:149:VAL:C | 2.30 | 0.42 |
| 1:D:309:PRO:C | 1:D:311:ASP:H | 2.22 | 0.42 |
| 1:D:322:VAL:HA | 1:D:323:PRO:HD3 | 1.87 | 0.42 |
| 1:G:294:ASN:OD1 | 1:G:307:THR:HG21 | 2.19 | 0.42 |
| 1:G:62:VAL:O | 1:G:69:THR:HA | 2.20 | 0.42 |
| 1:G:725:ARG:HA | 1:G:732:ILE:CG2 | 2.50 | 0.42 |
| 1:G:711:PHE:HB3 | 1:G:766:PHE:HB3 | 2.00 | 0.42 |
| 1:G:823:PHE:CZ | 2:H:156:VAL:HG12 | 2.54 | 0.42 |
| 1:J:123:CYS:HB2 | 1:J:158:ILE:HD13 | 2.00 | 0.42 |
| 1:J:144:ARG:HD2 | 1:J:144:ARG:HA | 1.78 | 0.42 |
| 1:J:320:ILE:O | 1:J:320:ILE:HG22 | 2.18 | 0.42 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:HG23 | 2.01 | 0.42 |
| 1:J:568:PRO:O | 1:J:570:PRO:HD3 | 2.19 | 0.42 |
| 1:J:173:GLN:HG3 | 1:J:670:HIS:CD2 | 2.54 | 0.42 |
| 1:J:793:ARG:O | 1:J:797:PHE:N | 2.39 | 0.42 |
| 2:K:137:TRP:CA | 2:K:145:ALA:HB2 | 2.37 | 0.42 |
| 1:M:175:ILE:C | 1:M:176:LEU:HD12 | 2.39 | 0.42 |
| 1:M:195:TYR:CD2 | 1:M:199:ILE:HD13 | 2.54 | 0.42 |
| 1:M:295:MLY:CG | 1:M:332:MET:HE1 | 2.49 | 0.42 |
| 1:S:109:ARG:CD | 1:S:117:THR:HB | 2.49 | 0.42 |
| 1:S:155:ILE:HG22 | 1:S:156:PHE:N | 2.33 | 0.42 |
| 1:S:25:ILE:HG23 | 1:S:29:ASN:HD22 | 1.85 | 0.42 |
| 1:S:348:MLY:HH12 | 1:S:348:MLY:HD2 | 1.81 | 0.42 |
| 1:S:534:SER:CB | 4:2:351:THR:HA | 2.49 | 0.42 |
| 1:S:751:GLY:HA3 | 1:S:779:ARG:HH22 | 1.85 | 0.42 |
| 1:S:839:MLY:HH11 | 2:T:158:THR:HG22 | 2.00 | 0.42 |
| 3:U:11:LYS:HE2 | 3:U:11:LYS:HB3 | 1.83 | 0.42 |
| 4:X:180:LEU:HD11 | 4:X:261:LEU:HD23 | 2.01 | 0.42 |
| 4:Y:222:ASP:OD1 | 4:Y:224:GLU:HB3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:222:ASP:OD1 | 4:1:224:GLU:HB3 | 2.19 | 0.42 |
| 4:2:196:ARG:HH21 | 4:2:249:THR:HG23 | 1.85 | 0.42 |
| 4:2:205:GLU:O | 4:2:208:ILE:HG22 | 2.19 | 0.42 |
| 4:2:217:CYS:C | 4:2:218:TYR:HD1 | 2.23 | 0.42 |
| 4:4:180:LEU:HD11 | 4:4:261:LEU:HD23 | 2.02 | 0.42 |
| 4:2:287:ILE:HG12 | 4:4:203:THR:HB | 2.00 | 0.42 |
| 4:4:206:ARG:O | 4:4:209:VAL:HG12 | 2.20 | 0.42 |
| 4:4:205:GLU:O | 4:4:208:ILE:HG22 | 2.18 | 0.42 |
| 4:8:206:ARG:O | 4:8:209:VAL:HG12 | 2.20 | 0.42 |
| 4:8:196:ARG:HH21 | 4:8:249:THR:HG23 | 1.85 | 0.42 |
| 4:8:315:LYS:HA | 4:8:315:LYS:HD2 | 1.92 | 0.42 |
| 1:A:218:LEU:HA | 1:A:221:GLN:HG3 | 1.71 | 0.42 |
| 1:A:578:HIS:CD2 | 1:A:592:ILE:H | 2.38 | 0.42 |
| 1:A:690:LEU:O | 1:A:694:GLN:HG3 | 2.20 | 0.42 |
| 2:B:113:LYS:O | 2:B:147:ASN:HB2 | 2.20 | 0.42 |
| 1:D:62:VAL:O | 1:D:69:THR:HA | 2.20 | 0.42 |
| 1:D:642:LYS:HB2 | 4:9:24:ASP:O | 1.88 | 0.42 |
| 1:D:834:LEU:HD12 | 2:E:54:MET:CB | 2.44 | 0.42 |
| 1:G:38:VAL:HG13 | 1:G:39:PHE:N | 2.35 | 0.42 |
| 1:G:93:MET:HG3 | 1:G:714:ARG:HG3 | 2.01 | 0.42 |
| 1:J:109:ARG:CD | 1:J:117:THR:HB | 2.49 | 0.42 |
| 1:J:309:PRO:C | 1:J:311:ASP:H | 2.22 | 0.42 |
| 1:J:642:LYS:HB3 | 4:W:24:ASP:HB2 | 1.37 | 0.42 |
| 1:J:690:LEU:O | 1:J:694:GLN:HG3 | 2.20 | 0.42 |
| 1:J:735:GLY:HA3 | 1:J:743:ALA:HA | 2.01 | 0.42 |
| 1:J:817:GLN:CD | 2:K:127:ARG:HG3 | 2.40 | 0.42 |
| 2:K:139:ALA:O | 2:K:141:PRO:CD | 2.51 | 0.42 |
| 1:M:169:ASP:O | 1:M:170:ARG:HB2 | 2.19 | 0.42 |
| 1:M:229:LEU:HD12 | 1:M:229:LEU:HA | 1.75 | 0.42 |
| 1:M:332:MET:H | 1:M:332:MET:HG2 | 1.52 | 0.42 |
| 1:M:715:VAL:HG12 | 1:M:720:PHE:HB2 | 2.00 | 0.42 |
| 1:M:787:ILE:HG23 | 1:M:791:GLN:HG3 | 2.00 | 0.42 |
| 1:M:797:PHE:CZ | 3:O:146:ILE:CD1 | 3.01 | 0.42 |
| 1:S:217:THR:HG22 | 1:S:218:LEU:N | 2.34 | 0.42 |
| 1:S:442:VAL:O | 1:S:445:ILE:HB | 2.19 | 0.42 |
| 2:T:114:LYS:CG | 2:T:146:GLY:HA2 | 2.46 | 0.42 |
| 4:V:217:CYS:C | 4:V:218:TYR:HD1 | 2.22 | 0.42 |
| 4:X:205:GLU:O | 4:X:208:ILE:HG22 | 2.19 | 0.42 |
| 4:X:291:LYS:HE2 | 4:Z:243:PRO:CA | 2.41 | 0.42 |
| 4:Z:180:LEU:HD11 | 4:Z:261:LEU:HD23 | 2.01 | 0.42 |
| 1:S:643:GLY:N | 4:2:23:GLY:C | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:6:196:ARG:HH21 | 4:6:249:THR:HG23 | 1.85 | 0.42 |
| 4:7:206:ARG:O | 4:7:209:VAL:HG12 | 2.20 | 0.42 |
| 4:9:217:CYS:C | 4:9:218:TYR:HD1 | 2.23 | 0.42 |
| 1:D:410:ASN:HA | 4:9:334:GLU:HB3 | 1.29 | 0.42 |
| 1:A:476:GLU:H | 1:A:476:GLU:CD | 2.22 | 0.42 |
| 1:A:744:SER:O | 1:A:748:LEU:HD12 | 2.20 | 0.42 |
| 1:A:819:ASN:H | 2:B:90:GLY:HA3 | 1.84 | 0.42 |
| 1:D:295:MLY:CE | 1:D:332:MET:CE | 2.97 | 0.42 |
| 1:D:38:VAL:HG13 | 1:D:39:PHE:N | 2.34 | 0.42 |
| 1:D:578:HIS:CD2 | 1:D:592:ILE:H | 2.38 | 0.42 |
| 1:D:725:ARG:HA | 1:D:732:ILE:CG2 | 2.50 | 0.42 |
| 1:G:149:GLN:HB2 | 1:G:149:GLN:HE21 | 1.71 | 0.42 |
| 1:G:529:PRO:HB3 | 4:V:354:GLN:HA | 2.00 | 0.42 |
| 1:G:725:ARG:CZ | 1:G:737:PHE:CE1 | 3.02 | 0.42 |
| 1:J:17:LEU:HA | 1:J:17:LEU:HD12 | 1.67 | 0.42 |
| 1:J:537:GLU:OE1 | 4:W:350:SER:HA | 2.19 | 0.42 |
| 1:J:578:HIS:CD2 | 1:J:592:ILE:H | 2.38 | 0.42 |
| 1:J:723:ARG:CG | 1:J:723:ARG:NH1 | 2.79 | 0.42 |
| 1:J:791:GLN:OE1 | 3:L:116:GLU:CG | 2.59 | 0.42 |
| 1:M:462:LEU:HD11 | 1:M:464:ILE:CD1 | 2.50 | 0.42 |
| 1:M:747:LEU:O | 1:M:749:GLY:N | 2.53 | 0.42 |
| 1:M:805:ALA:O | 1:M:807:VAL:C | 2.58 | 0.42 |
| 1:M:818:TYR:N | 2:N:127:ARG:HH11 | 2.18 | 0.42 |
| 1:S:537:GLU:OE1 | 4:2:350:SER:HA | 2.19 | 0.42 |
| 1:S:553:MLY:N | 4:4:49:GLN:HG3 | 2.27 | 0.42 |
| 1:S:747:LEU:O | 1:S:749:GLY:N | 2.53 | 0.42 |
| 2:T:113:LYS:O | 2:T:147:ASN:HB2 | 2.20 | 0.42 |
| 4:V:196:ARG:HH21 | 4:V:249:THR:HG23 | 1.85 | 0.42 |
| 4:W:217:CYS:C | 4:W:218:TYR:HD1 | 2.23 | 0.42 |
| 1:M:643:GLY:N | 4:Z:23:GLY:C | 2.55 | 0.42 |
| 4:2:180:LEU:HD11 | 4:2:261:LEU:HD23 | 2.01 | 0.42 |
| 4:2:222:ASP:OD1 | 4:2:224:GLU:HB3 | 2.20 | 0.42 |
| 4:3:222:ASP:OD1 | 4:3:224:GLU:HB3 | 2.20 | 0.42 |
| 4:6:222:ASP:OD1 | 4:6:224:GLU:HB3 | 2.20 | 0.42 |
| 1:D:636:LYS:CB | 4:9:334:GLU:OE1 | 2.68 | 0.42 |
| 1:A:110:TYR:O | 1:A:113:TRP:N | 2.42 | 0.42 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:HG22 | 2.00 | 0.42 |
| 1:A:775:LEU:HD12 | 1:A:775:LEU:HA | 1.71 | 0.42 |
| 1:D:332:MET:H | 1:D:332:MET:HG2 | 1.52 | 0.42 |
| 1:D:818:TYR:HB3 | 2:E:90:GLY:C | 2.26 | 0.42 |
| 1:D:804:ARG:NH2 | 3:F:149:VAL:HA | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:537:GLU:OE1 | 4:V:350:SER:HA | 2.20 | 0.42 |
| 1:G:673:ARG:HA | 1:G:673:ARG:HD2 | 1.79 | 0.42 |
| 1:G:747:LEU:O | 1:G:749:GLY:N | 2.52 | 0.42 |
| 1:G:819:ASN:ND2 | 2:H:92:ASP:CA | 2.82 | 0.42 |
| 1:G:839:MLY:N | 1:G:840:PRO:HD2 | 2.35 | 0.42 |
| 1:J:174:SER:HA | 1:J:460:GLY:O | 2.20 | 0.42 |
| 1:J:500:GLN:HB2 | 1:J:512:PHE:CZ | 2.54 | 0.42 |
| 1:J:643:GLY:CA | 4:W:24:ASP:OD1 | 2.61 | 0.42 |
| 1:J:741:LYS:HG2 | 1:J:742:LYS:N | 2.35 | 0.42 |
| 1:J:744:SER:O | 1:J:748:LEU:HD12 | 2.20 | 0.42 |
| 1:J:842:LEU:N | 1:J:842:LEU:CD1 | 2.83 | 0.42 |
| 3:L:25:ILE:O | 3:L:63:ILE:CB | 2.66 | 0.42 |
| 1:J:792:ALA:CA | 3:L:42:THR:HA | 2.42 | 0.42 |
| 1:M:320:ILE:HG22 | 1:M:320:ILE:O | 2.18 | 0.42 |
| 1:M:402:CYS:C | 1:M:404:PRO:HD3 | 2.40 | 0.42 |
| 1:M:744:SER:O | 1:M:748:LEU:HD12 | 2.20 | 0.42 |
| 1:M:35:MLY:CH1 | 1:M:781:ASP:OD2 | 2.67 | 0.42 |
| 1:M:800:ARG:HD2 | 3:O:149:VAL:C | 2.40 | 0.42 |
| 1:S:62:VAL:O | 1:S:69:THR:HA | 2.20 | 0.42 |
| 1:S:676:ILE:HA | 1:S:677:PRO:HD3 | 1.82 | 0.42 |
| 1:S:839:MLY:HH11 | 2:T:158:THR:CG2 | 2.49 | 0.42 |
| 4:V:205:GLU:O | 4:V:208:ILE:HG22 | 2.18 | 0.42 |
| 4:V:315:LYS:HD2 | 4:V:315:LYS:HA | 1.92 | 0.42 |
| 1:G:541:MET:HB3 | 4:V:345:ILE:HG22 | 2.01 | 0.42 |
| 4:W:222:ASP:OD1 | 4:W:224:GLU:HB3 | 2.19 | 0.42 |
| 4:X:222:ASP:OD1 | 4:X:224:GLU:HB3 | 2.20 | 0.42 |
| 1:G:553:MLY:C | 4:X:46:GLY:HA3 | 2.50 | 0.42 |
| 1:J:553:MLY:CB | 4:Y:46:GLY:HA3 | 2.49 | 0.42 |
| 4:1:369:ILE:HG23 | 4:1:370:VAL:N | 2.35 | 0.42 |
| 4:4:193:LEU:HD11 | 4:4:250:ILE:HG13 | 2.02 | 0.42 |
| 1:A:62:VAL:HG12 | 1:A:63:MLY:N | 2.35 | 0.42 |
| 1:A:735:GLY:HA3 | 1:A:743:ALA:HA | 2.01 | 0.42 |
| 1:A:732:ILE:CG2 | 1:A:747:LEU:HD12 | 0.35 | 0.42 |
| 1:A:797:PHE:CD2 | 1:A:798:LEU:HD12 | 2.55 | 0.42 |
| 2:B:114:LYS:CG | 2:B:146:GLY:HA2 | 2.46 | 0.42 |
| 1:D:11:GLY:O | 1:D:14:ALA:HB3 | 2.20 | 0.42 |
| 1:D:151:ALA:HB1 | 1:D:152:PRO:HD2 | 2.01 | 0.42 |
| 1:D:813:ILE:HG23 | 2:E:128:PHE:HZ | 0.66 | 0.42 |
| 1:G:11:GLY:O | 1:G:14:ALA:HB3 | 2.20 | 0.42 |
| 1:G:169:ASP:O | 1:G:170:ARG:HB2 | 2.19 | 0.42 |
| 1:G:60:VAL:O | 1:G:72:VAL:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:724:TYR:HB3 | 1:G:727:LEU:CD1 | 2.48 | 0.42 |
| 1:J:553:MLY:C | 4:Y:46:GLY:HA3 | 2.50 | 0.42 |
| 1:M:91:MET:CE | 1:M:119:SER:HB2 | 2.48 | 0.42 |
| 1:M:442:VAL:O | 1:M:445:ILE:HB | 2.19 | 0.42 |
| 1:M:536:LEU:HA | 1:M:536:LEU:HD12 | 1.69 | 0.42 |
| 1:M:578:HIS:CD2 | 1:M:592:ILE:H | 2.38 | 0.42 |
| 1:M:692:LEU:HA | 1:M:692:LEU:HD23 | 1.85 | 0.42 |
| 2:N:140:PHE:CD2 | 2:N:144:VAL:HG11 | 2.54 | 0.42 |
| 1:S:195:TYR:CE2 | 1:S:199:ILE:HD13 | 2.55 | 0.42 |
| 1:S:539:GLU:OE2 | 1:S:553:MLY:HD3 | 2.20 | 0.42 |
| 1:S:829:TRP:CE2 | 2:T:87:LYS:HE2 | 2.50 | 0.42 |
| 3:U:25:ILE:O | 3:U:63:ILE:CB | 2.66 | 0.42 |
| 1:S:793:ARG:CD | 3:U:40:ASN:HD22 | 2.17 | 0.42 |
| 1:J:636:LYS:CB | 4:W:334:GLU:OE1 | 2.68 | 0.42 |
| 4:X:369:ILE:HG23 | 4:X:370:VAL:N | 2.35 | 0.42 |
| 4:Y:206:ARG:O | 4:Y:209:VAL:HG12 | 2.20 | 0.42 |
| 1:M:541:MET:CE | 4:Z:346:LEU:HD12 | 2.47 | 0.42 |
| 1:S:636:LYS:CB | 4:2:334:GLU:OE1 | 2.68 | 0.42 |
| 1:S:540:CYS:C | 4:2:349:LEU:HD21 | 2.36 | 0.42 |
| 4:4:287:ILE:HG21 | 4:6:202:THR:CA | 2.49 | 0.42 |
| 4:5:217:CYS:C | 4:5:218:TYR:HD1 | 2.23 | 0.42 |
| 4:5:193:LEU:HD11 | 4:5:250:ILE:HG13 | 2.02 | 0.42 |
| 4:8:193:LEU:HD11 | 4:8:250:ILE:HG13 | 2.02 | 0.42 |
| 1:A:195:TYR:CE2 | 1:A:199:ILE:HD13 | 2.55 | 0.42 |
| 1:A:335:ASP:O | 1:A:338:ILE:HB | 2.20 | 0.42 |
| 1:A:64:THR:CG2 | 1:A:65:GLU:H | 2.32 | 0.42 |
| 1:A:673:ARG:HD2 | 1:A:673:ARG:HA | 1.79 | 0.42 |
| 1:A:752:ASP:HB3 | 1:A:782:MLY:HD3 | 2.00 | 0.42 |
| 1:D:214:MET:CA | 1:D:340:ILE:HD11 | 2.45 | 0.42 |
| 1:D:356:GLY:HA2 | 1:D:359:MET:HG3 | 2.02 | 0.42 |
| 1:D:500:GLN:HB2 | 1:D:512:PHE:CZ | 2.54 | 0.42 |
| 1:D:507:GLY:CA | 1:D:762:HIS:NE2 | 2.83 | 0.42 |
| 1:D:795:ARG:NE | 3:F:116:GLU:CB | 2.80 | 0.42 |
| 1:D:826:VAL:O | 1:D:828:HIS:N | 2.53 | 0.42 |
| 1:D:86:ASP:OD2 | 1:D:87:MLY:HH22 | 2.19 | 0.42 |
| 1:G:93:MET:HA | 1:G:714:ARG:CG | 2.50 | 0.42 |
| 1:J:151:ALA:HB1 | 1:J:152:PRO:HD2 | 2.01 | 0.42 |
| 1:J:195:TYR:CE2 | 1:J:199:ILE:HD13 | 2.55 | 0.42 |
| 1:J:295:MLY:CG | 1:J:332:MET:CE | 2.96 | 0.42 |
| 1:J:408:VAL:HA | 1:J:636:LYS:HG3 | 1.03 | 0.42 |
| 1:J:442:VAL:O | 1:J:445:ILE:HB | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:747:LEU:O | 1:J:749:GLY:N | 2.53 | 0.42 |
| 1:J:787:ILE:HG23 | 1:J:791:GLN:HG3 | 2.00 | 0.42 |
| 2:K:149:ASP:CG | 2:K:150:TYR:N | 2.49 | 0.42 |
| 1:M:141:LEU:N | 1:M:141:LEU:HD12 | 2.32 | 0.42 |
| 1:M:17:LEU:HA | 1:M:17:LEU:HD12 | 1.68 | 0.42 |
| 1:M:330:GLU:OE1 | 1:M:330:GLU:HA | 2.20 | 0.42 |
| 1:M:445:ILE:HG22 | 1:M:449:LEU:HD22 | 2.02 | 0.42 |
| 1:S:11:GLY:O | 1:S:14:ALA:HB3 | 2.20 | 0.42 |
| 1:S:226:ASN:HB2 | 1:S:227:PRO:CD | 2.47 | 0.42 |
| 1:S:445:ILE:HG22 | 1:S:449:LEU:HD22 | 2.02 | 0.42 |
| 1:S:173:GLN:HG3 | 1:S:670:HIS:CD2 | 2.54 | 0.42 |
| 1:S:770:GLY:O | 1:S:771:LEU:HA | 2.19 | 0.42 |
| 1:S:826:VAL:O | 1:S:828:HIS:N | 2.53 | 0.42 |
| 2:T:144:VAL:HG12 | 2:T:153:ILE:HD11 | 1.75 | 0.42 |
| 4:W:171:LEU:HA | 4:W:172:PRO:HD2 | 1.84 | 0.42 |
| 4:X:315:LYS:HD2 | 4:X:315:LYS:HA | 1.92 | 0.42 |
| 4:Z:149:THR:HA | 4:Z:165:ILE:O | 2.19 | 0.42 |
| 4:1:196:ARG:HH21 | 4:1:249:THR:HG23 | 1.85 | 0.41 |
| 4:1:193:LEU:HD11 | 4:1:250:ILE:HG13 | 2.02 | 0.41 |
| 4:1:221:LEU:HA | 4:1:312:ARG:HG2 | 2.02 | 0.41 |
| 4:2:226:GLU:HG3 | 4:2:255:PHE:CE2 | 2.55 | 0.41 |
| 4:3:193:LEU:HD11 | 4:3:250:ILE:HG13 | 2.02 | 0.41 |
| 4:4:369:ILE:HG23 | 4:4:370:VAL:N | 2.35 | 0.41 |
| 4:5:171:LEU:HA | 4:5:172:PRO:HD2 | 1.84 | 0.41 |
| 4:9:222:ASP:OD1 | 4:9:224:GLU:HB3 | 2.19 | 0.41 |
| 1:D:534:SER:CB | 4:9:351:THR:HA | 2.49 | 0.41 |
| 1:A:330:GLU:OE1 | 1:A:330:GLU:HA | 2.20 | 0.41 |
| 1:A:332:MET:HG2 | 1:A:332:MET:H | 1.52 | 0.41 |
| 1:A:445:ILE:HG22 | 1:A:449:LEU:HD22 | 2.01 | 0.41 |
| 1:A:449:LEU:N | 1:A:449:LEU:CD1 | 2.82 | 0.41 |
| 1:A:173:GLN:HG3 | 1:A:670:HIS:CD2 | 2.54 | 0.41 |
| 1:A:724:TYR:HB3 | 1:A:727:LEU:CD1 | 2.48 | 0.41 |
| 1:A:795:ARG:HE | 3:C:118:MET:HE1 | 1.85 | 0.41 |
| 3:C:63:ILE:CG2 | 3:C:64:THR:H | 2.33 | 0.41 |
| 1:D:129:TYR:HA | 1:D:129:TYR:HD1 | 1.66 | 0.41 |
| 1:D:471:ASP:CB | 1:D:573:GLY:O | 2.68 | 0.41 |
| 1:D:838:ILE:HD13 | 2:E:54:MET:HE3 | 2.01 | 0.41 |
| 1:G:141:LEU:HD12 | 1:G:141:LEU:N | 2.32 | 0.41 |
| 1:G:445:ILE:HG22 | 1:G:449:LEU:HD22 | 2.01 | 0.41 |
| 3:I:48:LYS:HD3 | 3:I:48:LYS:HA | 1.17 | 0.41 |
| 1:J:38:VAL:HG13 | 1:J:39:PHE:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:471:ASP:CB | 1:J:573:GLY:O | 2.68 | 0.41 |
| 1:J:797:PHE:CD2 | 1:J:798:LEU:HD12 | 2.55 | 0.41 |
| 1:J:826:VAL:O | 1:J:828:HIS:N | 2.53 | 0.41 |
| 1:M:107:MLY:N | 1:M:686:MET:HE1 | 2.35 | 0.41 |
| 1:M:202:SER:HA | 1:M:207:LYS:NZ | 2.22 | 0.41 |
| 1:M:636:LYS:CB | 4:Z:334:GLU:OE1 | 2.68 | 0.41 |
| 1:M:84:MLY:HD3 | 1:M:723:ARG:HD2 | 2.02 | 0.41 |
| 3:O:63:ILE:CG2 | 3:O:64:THR:H | 2.33 | 0.41 |
| 1:S:217:THR:CA | 1:S:221:GLN:HE21 | 2.33 | 0.41 |
| 1:S:725:ARG:HA | 1:S:732:ILE:CG2 | 2.50 | 0.41 |
| 1:S:798:LEU:CG | 3:U:126:LEU:HD21 | 2.42 | 0.41 |
| 1:G:636:LYS:CB | 4:V:334:GLU:OE1 | 2.68 | 0.41 |
| 4:X:193:LEU:HD11 | 4:X:250:ILE:HG13 | 2.02 | 0.41 |
| 4:Y:221:LEU:HA | 4:Y:312:ARG:HG2 | 2.02 | 0.41 |
| 4:Z:206:ARG:O | 4:Z:209:VAL:HG12 | 2.20 | 0.41 |
| 1:M:550:PHE:C | 4:2:46:GLY:CA | 2.88 | 0.41 |
| 4:3:196:ARG:HH21 | 4:3:249:THR:HG23 | 1.85 | 0.41 |
| 4:5:196:ARG:HH21 | 4:5:249:THR:HG23 | 1.85 | 0.41 |
| 4:5:206:ARG:O | 4:5:209:VAL:HG12 | 2.20 | 0.41 |
| 4:8:226:GLU:HG3 | 4:8:255:PHE:CE2 | 2.55 | 0.41 |
| 4:9:206:ARG:O | 4:9:209:VAL:HG12 | 2.20 | 0.41 |
| 1:A:136:ASN:O | 1:A:138:MLY:N | 2.54 | 0.41 |
| 1:D:271:GLU:OE1 | 1:D:274:ARG:NH1 | 2.53 | 0.41 |
| 1:D:335:ASP:O | 1:D:338:ILE:HB | 2.20 | 0.41 |
| 1:D:462:LEU:HD11 | 1:D:464:ILE:CD1 | 2.50 | 0.41 |
| 1:D:507:GLY:HA3 | 1:D:762:HIS:H | 1.85 | 0.41 |
| 1:D:568:PRO:CG | 1:D:578:HIS:N | 2.83 | 0.41 |
| 1:D:173:GLN:HG3 | 1:D:670:HIS:CD2 | 2.54 | 0.41 |
| 1:D:747:LEU:O | 1:D:749:GLY:N | 2.52 | 0.41 |
| 1:D:834:LEU:HD21 | 2:E:54:MET:CG | 2.50 | 0.41 |
| 2:E:137:TRP:CA | 2:E:145:ALA:CB | 2.82 | 0.41 |
| 3:F:62:ALA:O | 3:F:63:ILE:HG13 | 2.14 | 0.41 |
| 1:G:123:CYS:HB2 | 1:G:158:ILE:HD13 | 2.00 | 0.41 |
| 1:G:195:TYR:CE2 | 1:G:199:ILE:HD13 | 2.55 | 0.41 |
| 1:G:335:ASP:O | 1:G:338:ILE:HB | 2.20 | 0.41 |
| 1:G:741:LYS:HG2 | 1:G:742:LYS:N | 2.35 | 0.41 |
| 1:G:772:LEU:HA | 1:G:772:LEU:HD12 | 1.82 | 0.41 |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:CD | 2.30 | 0.41 |
| 2:H:113:LYS:O | 2:H:147:ASN:HB2 | 2.20 | 0.41 |
| 1:J:11:GLY:O | 1:J:14:ALA:HB3 | 2.20 | 0.41 |
| 1:J:107:MLY:CB | 1:J:686:MET:HE2 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:725:ARG:HA | 1:J:732:ILE:CG2 | 2.50 | 0.41 |
| 1:J:830:PRO:CB | 2:K:67:MET:CE | 2.98 | 0.41 |
| 1:M:166:MET:CE | 1:M:254:PHE:CD2 | 3.01 | 0.41 |
| 1:M:533:PHE:HA | 1:M:533:PHE:HD1 | 1.79 | 0.41 |
| 1:M:739:ASP:C | 1:M:739:ASP:OD1 | 2.58 | 0.41 |
| 1:S:330:GLU:HG2 | 1:S:330:GLU:H | 1.54 | 0.41 |
| 1:S:369:MLY:HH22 | 1:S:369:MLY:HD3 | 1.78 | 0.41 |
| 1:S:436:MLY:HE3 | 1:S:626:TYR:HE1 | 1.77 | 0.41 |
| 1:S:629:GLU:CA | 1:S:643:GLY:C | 2.73 | 0.41 |
| 1:S:791:GLN:OE1 | 3:U:116:GLU:CB | 2.69 | 0.41 |
| 1:S:836:PHE:CG | 2:T:160:GLY:N | 2.88 | 0.41 |
| 4:V:193:LEU:HD11 | 4:V:250:ILE:HG13 | 2.02 | 0.41 |
| 1:G:541:MET:CE | 4:V:346:LEU:HD12 | 2.48 | 0.41 |
| 1:J:541:MET:CG | 4:W:345:ILE:C | 2.87 | 0.41 |
| 1:J:534:SER:CB | 4:W:351:THR:HA | 2.49 | 0.41 |
| 4:X:217:CYS:C | 4:X:218:TYR:HD1 | 2.23 | 0.41 |
| 4:Y:369:ILE:HG23 | 4:Y:370:VAL:N | 2.35 | 0.41 |
| 4:Z:193:LEU:HD11 | 4:Z:250:ILE:HG13 | 2.02 | 0.41 |
| 1:M:556:ASP:OD1 | 4:2:50:LYS:CG | 2.69 | 0.41 |
| 4:3:287:ILE:CB | 4:5:204:ALA:H | 2.33 | 0.41 |
| 4:5:226:GLU:HG3 | 4:5:255:PHE:CE2 | 2.55 | 0.41 |
| 4:7:217:CYS:C | 4:7:218:TYR:HD1 | 2.23 | 0.41 |
| 4:7:369:ILE:HG23 | 4:7:370:VAL:N | 2.35 | 0.41 |
| 4:9:196:ARG:HH21 | 4:9:249:THR:HG23 | 1.85 | 0.41 |
| 4:9:193:LEU:HD11 | 4:9:250:ILE:HG13 | 2.02 | 0.41 |
| 1:A:11:GLY:O | 1:A:14:ALA:HB3 | 2.20 | 0.41 |
| 1:A:443:ILE:HG22 | 1:A:444:ARG:N | 2.29 | 0.41 |
| 1:A:541:MET:N | 4:8:349:LEU:CD2 | 2.69 | 0.41 |
| 1:A:692:LEU:HA | 1:A:692:LEU:HD23 | 1.85 | 0.41 |
| 1:A:826:VAL:O | 1:A:828:HIS:N | 2.53 | 0.41 |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:CA | 2.64 | 0.41 |
| 1:D:320:ILE:CG2 | 1:D:320:ILE:O | 2.68 | 0.41 |
| 1:D:713:SER:HG | 1:D:771:LEU:HD21 | 1.80 | 0.41 |
| 1:D:787:ILE:HG23 | 1:D:791:GLN:HG3 | 2.01 | 0.41 |
| 1:D:797:PHE:CD2 | 1:D:798:LEU:HD12 | 2.55 | 0.41 |
| 2:E:113:LYS:O | 2:E:147:ASN:HB2 | 2.20 | 0.41 |
| 1:G:25:ILE:HG23 | 1:G:29:ASN:HD22 | 1.85 | 0.41 |
| 1:G:757:GLN:OE1 | 1:G:772:LEU:CB | 2.59 | 0.41 |
| 1:G:787:ILE:HD13 | 1:G:787:ILE:HG21 | 1.67 | 0.41 |
| 3:I:11:LYS:HE2 | 3:I:11:LYS:HB3 | 1.83 | 0.41 |
| 1:J:295:MLY:CD | 1:J:332:MET:HE2 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:464:ILE:HD13 | 1:J:464:ILE:HG21 | 1.69 | 0.41 |
| 1:M:136:ASN:O | 1:M:138:MLY:N | 2.54 | 0.41 |
| 1:M:471:ASP:CB | 1:M:573:GLY:O | 2.68 | 0.41 |
| 1:M:63:MLY:HH23 | 1:M:63:MLY:HD3 | 1.76 | 0.41 |
| 1:M:725:ARG:HA | 1:M:732:ILE:CG2 | 2.50 | 0.41 |
| 1:M:733:PRO:CB | 1:M:737:PHE:CE1 | 3.02 | 0.41 |
| 1:M:839:MLY:N | 1:M:840:PRO:HD2 | 2.35 | 0.41 |
| 2:N:113:LYS:O | 2:N:147:ASN:HB2 | 2.20 | 0.41 |
| 1:M:797:PHE:HE1 | 3:O:149:VAL:HG12 | 1.79 | 0.41 |
| 1:S:141:LEU:HD12 | 1:S:141:LEU:N | 2.32 | 0.41 |
| 1:S:202:SER:HA | 1:S:207:LYS:NZ | 2.22 | 0.41 |
| 1:S:356:GLY:HA2 | 1:S:359:MET:HG3 | 2.02 | 0.41 |
| 1:S:462:LEU:HD11 | 1:S:464:ILE:CD1 | 2.50 | 0.41 |
| 1:S:690:LEU:O | 1:S:694:GLN:HG3 | 2.20 | 0.41 |
| 1:S:797:PHE:CG | 3:U:146:ILE:HG23 | 2.53 | 0.41 |
| 3:U:63:ILE:CG2 | 3:U:64:THR:H | 2.32 | 0.41 |
| 1:D:551:MLY:C | 4:W:47:MET:HA | 2.48 | 0.41 |
| 4:2:202:THR:CG2 | 4:Z:287:ILE:N | 2.77 | 0.41 |
| 4:2:288:ASP:OD2 | 4:4:62:ARG:HG3 | 2.20 | 0.41 |
| 4:3:369:ILE:HG23 | 4:3:370:VAL:N | 2.35 | 0.41 |
| 4:4:221:LEU:HA | 4:4:312:ARG:HG2 | 2.02 | 0.41 |
| 4:6:171:LEU:HA | 4:6:172:PRO:HD2 | 1.84 | 0.41 |
| 4:6:193:LEU:HD11 | 4:6:250:ILE:HG13 | 2.02 | 0.41 |
| 4:7:196:ARG:HH21 | 4:7:249:THR:HG23 | 1.85 | 0.41 |
| 1:A:135:TYR:HD2 | 1:A:191:ARG:CG | 2.33 | 0.41 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HD13 | 1.37 | 0.41 |
| 1:A:504:MLY:HG3 | 1:A:762:HIS:CE1 | 2.55 | 0.41 |
| 1:D:798:LEU:HD13 | 3:F:126:LEU:HD13 | 1.91 | 0.41 |
| 1:D:819:ASN:HA | 2:E:90:GLY:O | 2.19 | 0.41 |
| 1:G:462:LEU:HD11 | 1:G:464:ILE:CD1 | 2.50 | 0.41 |
| 1:G:568:PRO:CG | 1:G:578:HIS:N | 2.83 | 0.41 |
| 1:G:63:MLY:HD3 | 1:G:63:MLY:HH23 | 1.76 | 0.41 |
| 1:G:640:LYS:C | 1:G:645:SER:HG | 2.14 | 0.41 |
| 1:G:744:SER:O | 1:G:748:LEU:HD12 | 2.20 | 0.41 |
| 1:G:834:LEU:HD22 | 2:H:34:ILE:CD1 | 2.50 | 0.41 |
| 1:J:539:GLU:OE2 | 1:J:553:MLY:HD3 | 2.20 | 0.41 |
| 1:J:568:PRO:CG | 1:J:578:HIS:N | 2.84 | 0.41 |
| 1:J:637:LYS:HD2 | 4:W:144:ALA:HB3 | 1.20 | 0.41 |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HD12 | 0.95 | 0.41 |
| 1:M:11:GLY:O | 1:M:14:ALA:HB3 | 2.20 | 0.41 |
| 1:M:296:MLY:HH11 | 1:M:348:MLY:CH2 | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:335:ASP:O | 1:M:338:ILE:HB | 2.20 | 0.41 |
| 1:M:384:ASP:HA | 1:M:394:SER:OG | 2.21 | 0.41 |
| 1:M:38:VAL:HG13 | 1:M:39:PHE:N | 2.35 | 0.41 |
| 1:M:528:MLY:HB2 | 1:M:529:PRO:HD2 | 2.03 | 0.41 |
| 1:M:637:LYS:HD2 | 4:Z:144:ALA:HB3 | 1.20 | 0.41 |
| 1:M:173:GLN:HG3 | 1:M:670:HIS:CD2 | 2.54 | 0.41 |
| 2:N:112:ILE:O | 2:N:148:VAL:N | 2.50 | 0.41 |
| 3:O:52:ASN:CB | 3:O:53:PRO:CD | 2.92 | 0.41 |
| 3:O:56:GLU:OE1 | 3:O:59:ASN:ND2 | 2.54 | 0.41 |
| 1:S:204:GLU:N | 1:S:207:LYS:HE3 | 2.23 | 0.41 |
| 1:S:210:GLN:C | 1:S:211:SER:HG | 2.16 | 0.41 |
| 1:S:471:ASP:CB | 1:S:573:GLY:O | 2.68 | 0.41 |
| 1:S:568:PRO:CG | 1:S:578:HIS:N | 2.84 | 0.41 |
| 1:S:408:VAL:HG22 | 1:S:636:LYS:HG2 | 1.51 | 0.41 |
| 1:S:717:TYR:OH | 1:S:760:PHE:HB3 | 2.21 | 0.41 |
| 1:S:84:MLY:HH22 | 1:S:719:ASP:O | 2.18 | 0.41 |
| 1:S:756:THR:HB | 1:S:757:GLN:H | 1.63 | 0.41 |
| 1:S:797:PHE:CD2 | 1:S:798:LEU:HD12 | 2.56 | 0.41 |
| 1:S:817:GLN:HB3 | 2:T:127:ARG:NE | 2.34 | 0.41 |
| 1:S:829:TRP:CZ3 | 2:T:84:PHE:CE1 | 3.07 | 0.41 |
| 1:S:93:MET:CE | 1:S:764:MLY:CG | 2.85 | 0.41 |
| 4:X:226:GLU:HG3 | 4:X:255:PHE:CE2 | 2.55 | 0.41 |
| 4:2:193:LEU:HD11 | 4:2:250:ILE:HG13 | 2.02 | 0.41 |
| 4:4:226:GLU:HG3 | 4:4:255:PHE:CE2 | 2.56 | 0.41 |
| 4:5:369:ILE:HG23 | 4:5:370:VAL:N | 2.35 | 0.41 |
| 4:7:222:ASP:OD1 | 4:7:224:GLU:HB3 | 2.20 | 0.41 |
| 4:7:193:LEU:HD11 | 4:7:250:ILE:HG13 | 2.02 | 0.41 |
| 1:A:91:MET:CE | 1:A:119:SER:HB2 | 2.48 | 0.41 |
| 1:A:17:LEU:HA | 1:A:17:LEU:HD12 | 1.68 | 0.41 |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:HD12 | 2.03 | 0.41 |
| 1:A:747:LEU:O | 1:A:749:GLY:N | 2.52 | 0.41 |
| 1:D:449:LEU:CD1 | 1:D:449:LEU:N | 2.82 | 0.41 |
| 1:D:787:ILE:HG21 | 1:D:787:ILE:HD13 | 1.67 | 0.41 |
| 1:D:800:ARG:CB | 3:F:149:VAL:CG2 | 2.95 | 0.41 |
| 1:G:471:ASP:CB | 1:G:573:GLY:O | 2.68 | 0.41 |
| 1:G:750:GLY:HA3 | 3:I:114:LEU:HD21 | 2.03 | 0.41 |
| 1:G:148:ARG:NH2 | 1:G:764:MLY:HH11 | 2.35 | 0.41 |
| 1:G:826:VAL:O | 1:G:828:HIS:N | 2.53 | 0.41 |
| 1:G:95:THR:HA | 1:G:713:SER:OG | 2.20 | 0.41 |
| 3:I:25:ILE:O | 3:I:63:ILE:CB | 2.66 | 0.41 |
| 1:G:796:GLY:CA | 3:I:35:ARG:CD | 2.77 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:95:ASP:OD1 | 3:I:139:TYR:HE1 | 2.04 | 0.41 |
| 1:J:135:TYR:CD2 | 1:J:191:ARG:HD3 | 2.55 | 0.41 |
| 1:J:62:VAL:HG12 | 1:J:63:MLY:N | 2.35 | 0.41 |
| 1:J:812:SER:O | 1:J:816:ILE:HG13 | 2.21 | 0.41 |
| 1:J:819:ASN:HA | 2:K:90:GLY:C | 2.20 | 0.41 |
| 3:L:52:ASN:CB | 3:L:53:PRO:CD | 2.92 | 0.41 |
| 3:L:63:ILE:CG2 | 3:L:64:THR:H | 2.33 | 0.41 |
| 1:M:214:MET:CA | 1:M:340:ILE:HD11 | 2.45 | 0.41 |
| 1:M:762:HIS:N | 1:M:762:HIS:CD2 | 2.78 | 0.41 |
| 3:O:48:LYS:HA | 3:O:48:LYS:HD3 | 1.17 | 0.41 |
| 1:S:384:ASP:HA | 1:S:394:SER:OG | 2.21 | 0.41 |
| 1:S:449:LEU:CD1 | 1:S:449:LEU:N | 2.82 | 0.41 |
| 1:S:485:GLU:OE2 | 1:S:584:TYR:N | 2.50 | 0.41 |
| 1:S:528:MLY:HB2 | 1:S:529:PRO:HD2 | 2.03 | 0.41 |
| 1:S:578:HIS:CD2 | 1:S:592:ILE:H | 2.38 | 0.41 |
| 1:S:731:ALA:CB | 3:U:93:VAL:CG1 | 2.95 | 0.41 |
| 2:T:141:PRO:HB3 | 2:T:142:PRO:CD | 2.49 | 0.41 |
| 4:V:171:LEU:HA | 4:V:172:PRO:HD2 | 1.84 | 0.41 |
| 4:V:227:MET:O | 4:V:230:ALA:HB3 | 2.21 | 0.41 |
| 1:G:534:SER:CB | 4:V:351:THR:HA | 2.50 | 0.41 |
| 1:J:540:CYS:C | 4:W:349:LEU:HD21 | 2.36 | 0.41 |
| 1:D:550:PHE:C | 4:W:46:GLY:CA | 2.88 | 0.41 |
| 4:Y:193:LEU:HD11 | 4:Y:250:ILE:HG13 | 2.02 | 0.41 |
| 4:Z:226:GLU:HG3 | 4:Z:255:PHE:CE2 | 2.55 | 0.41 |
| 4:2:110:LEU:O | 4:3:195:GLU:CG | 2.69 | 0.41 |
| 4:2:290:ARG:NH2 | 4:4:202:THR:HG21 | 1.99 | 0.41 |
| 4:6:206:ARG:O | 4:6:209:VAL:HG12 | 2.20 | 0.41 |
| 4:8:171:LEU:HA | 4:8:172:PRO:HD2 | 1.84 | 0.41 |
| 1:A:193:ILE:CD1 | 1:A:250:ILE:HD13 | 2.51 | 0.41 |
| 1:A:642:LYS:HB3 | 4:8:24:ASP:HB2 | 1.37 | 0.41 |
| 1:A:725:ARG:HA | 1:A:732:ILE:CG2 | 2.50 | 0.41 |
| 1:A:717:TYR:OH | 1:A:760:PHE:HB3 | 2.20 | 0.41 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:CG2 | 3.03 | 0.41 |
| 1:A:839:MLY:N | 1:A:840:PRO:HD2 | 2.35 | 0.41 |
| 3:C:25:ILE:O | 3:C:63:ILE:CB | 2.66 | 0.41 |
| 1:D:135:TYR:HD2 | 1:D:191:ARG:CG | 2.33 | 0.41 |
| 1:D:322:VAL:HB | 1:D:325:ILE:HD12 | 2.03 | 0.41 |
| 1:D:330:GLU:HA | 1:D:330:GLU:OE1 | 2.21 | 0.41 |
| 1:D:63:MLY:HH23 | 1:D:63:MLY:HD3 | 1.76 | 0.41 |
| 1:D:657:LEU:HD12 | 1:D:657:LEU:O | 2.21 | 0.41 |
| 1:D:741:LYS:HG2 | 1:D:742:LYS:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:812:SER:O | 1:D:816:ILE:HG13 | 2.21 | 0.41 |
| 1:D:795:ARG:CB | 3:F:35:ARG:CZ | 2.75 | 0.41 |
| 1:G:136:ASN:O | 1:G:138:MLY:N | 2.54 | 0.41 |
| 1:G:369:MLY:HD3 | 1:G:369:MLY:HH22 | 1.79 | 0.41 |
| 1:G:690:LEU:O | 1:G:694:GLN:HG3 | 2.20 | 0.41 |
| 1:G:827:MLY:HH21 | 2:H:139:ALA:HB3 | 2.01 | 0.41 |
| 1:G:817:GLN:NE2 | 2:H:128:PHE:HE1 | 2.12 | 0.41 |
| 2:H:137:TRP:CZ3 | 2:H:145:ALA:N | 2.81 | 0.41 |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:HD12 | 2.03 | 0.41 |
| 1:J:271:GLU:OE1 | 1:J:274:ARG:NH1 | 2.53 | 0.41 |
| 1:J:330:GLU:OE1 | 1:J:330:GLU:HA | 2.20 | 0.41 |
| 1:J:335:ASP:O | 1:J:338:ILE:HB | 2.20 | 0.41 |
| 1:J:462:LEU:HD11 | 1:J:464:ILE:CD1 | 2.50 | 0.41 |
| 2:K:112:ILE:O | 2:K:148:VAL:N | 2.50 | 0.41 |
| 3:L:56:GLU:OE1 | 3:L:59:ASN:ND2 | 2.54 | 0.41 |
| 1:M:369:MLY:HD3 | 1:M:369:MLY:HH22 | 1.79 | 0.41 |
| 1:M:741:LYS:HG2 | 1:M:742:LYS:N | 2.35 | 0.41 |
| 2:N:140:PHE:HB3 | 2:N:144:VAL:HG11 | 2.03 | 0.41 |
| 1:S:193:ILE:CD1 | 1:S:250:ILE:HD13 | 2.51 | 0.41 |
| 1:S:335:ASP:O | 1:S:338:ILE:HB | 2.21 | 0.41 |
| 1:S:174:SER:HA | 1:S:460:GLY:O | 2.20 | 0.41 |
| 1:S:707:CYS:CA | 1:S:714:ARG:NH2 | 2.76 | 0.41 |
| 1:S:744:SER:O | 1:S:748:LEU:HD12 | 2.20 | 0.41 |
| 1:S:812:SER:O | 1:S:816:ILE:HG13 | 2.21 | 0.41 |
| 3:U:95:ASP:OD1 | 3:U:139:TYR:HE1 | 2.03 | 0.41 |
| 4:V:144:ALA:HB2 | 4:V:342:GLY:CA | 2.51 | 0.41 |
| 4:Y:32:PRO:HB2 | 4:Y:34:ILE:CD1 | 2.51 | 0.41 |
| 4:Z:205:GLU:O | 4:Z:208:ILE:HG22 | 2.18 | 0.41 |
| 4:1:226:GLU:HG3 | 4:1:255:PHE:CE2 | 2.55 | 0.41 |
| 4:1:144:ALA:HB2 | 4:1:342:GLY:CA | 2.51 | 0.41 |
| 4:2:144:ALA:HB2 | 4:2:342:GLY:CA | 2.51 | 0.41 |
| 1:S:541:MET:CE | 4:2:346:LEU:HD12 | 2.47 | 0.41 |
| 4:3:221:LEU:HA | 4:3:312:ARG:HG2 | 2.02 | 0.41 |
| 4:3:227:MET:O | 4:3:230:ALA:HB3 | 2.21 | 0.41 |
| 4:3:144:ALA:HB2 | 4:3:342:GLY:CA | 2.51 | 0.41 |
| 4:4:227:MET:O | 4:4:230:ALA:HB3 | 2.21 | 0.41 |
| 4:5:222:ASP:OD1 | 4:5:224:GLU:HB3 | 2.19 | 0.41 |
| 4:5:227:MET:O | 4:5:230:ALA:HB3 | 2.21 | 0.41 |
| 4:6:227:MET:O | 4:6:230:ALA:HB3 | 2.21 | 0.41 |
| 4:8:144:ALA:HB2 | 4:8:342:GLY:CA | 2.51 | 0.41 |
| 1:D:643:GLY:CA | 4:9:24:ASP:OD1 | 2.62 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:217:THR:CA | 1:A:221:GLN:HE21 | 2.33 | 0.41 |
| 1:A:25:ILE:HG23 | 1:A:29:ASN:HD22 | 1.85 | 0.41 |
| 1:A:842:LEU:N | 1:A:842:LEU:CD1 | 2.83 | 0.41 |
| 2:B:140:PHE:HB3 | 2:B:144:VAL:HG11 | 2.03 | 0.41 |
| 1:D:536:LEU:HD12 | 1:D:536:LEU:HA | 1.69 | 0.41 |
| 1:D:690:LEU:O | 1:D:694:GLN:HG3 | 2.20 | 0.41 |
| 1:G:217:THR:CA | 1:G:221:GLN:HE21 | 2.34 | 0.41 |
| 1:G:528:MLY:HB2 | 1:G:529:PRO:HD2 | 2.03 | 0.41 |
| 1:G:797:PHE:CD2 | 1:G:798:LEU:HD12 | 2.55 | 0.41 |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:CD1 | 2.54 | 0.41 |
| 3:I:56:GLU:OE1 | 3:I:59:ASN:ND2 | 2.54 | 0.41 |
| 1:J:106:LEU:HD12 | 1:J:106:LEU:HA | 1.79 | 0.41 |
| 1:J:445:ILE:HG22 | 1:J:449:LEU:HD22 | 2.01 | 0.41 |
| 1:J:657:LEU:HD12 | 1:J:657:LEU:O | 2.21 | 0.41 |
| 1:M:14:ALA:HB3 | 1:M:15:PRO:CD | 2.46 | 0.41 |
| 1:M:28:GLN:HB3 | 1:M:723:ARG:NH1 | 2.35 | 0.41 |
| 1:M:356:GLY:HA2 | 1:M:359:MET:HG3 | 2.02 | 0.41 |
| 1:M:60:VAL:O | 1:M:72:VAL:N | 2.51 | 0.41 |
| 1:M:62:VAL:O | 1:M:69:THR:HA | 2.20 | 0.41 |
| 1:S:402:CYS:C | 1:S:404:PRO:HD3 | 2.40 | 0.41 |
| 1:S:741:LYS:HG2 | 1:S:742:LYS:N | 2.35 | 0.41 |
| 1:S:802:GLU:OE2 | 1:S:809:ARG:NH2 | 2.54 | 0.41 |
| 1:S:821:ARG:NH1 | 2:T:127:ARG:NE | 2.69 | 0.41 |
| 2:T:140:PHE:CD2 | 2:T:144:VAL:HG11 | 2.55 | 0.41 |
| 1:S:798:LEU:HD13 | 3:U:126:LEU:CD1 | 2.32 | 0.41 |
| 3:U:62:ALA:O | 3:U:63:ILE:HG13 | 2.14 | 0.41 |
| 4:8:324:THR:N | 4:V:245:GLY:CA | 2.69 | 0.41 |
| 4:V:369:ILE:HG23 | 4:V:370:VAL:N | 2.35 | 0.41 |
| 4:W:206:ARG:O | 4:W:209:VAL:HG12 | 2.20 | 0.41 |
| 1:J:534:SER:HB2 | 4:W:354:GLN:HE22 | 1.56 | 0.41 |
| 4:Y:196:ARG:HH21 | 4:Y:249:THR:HG23 | 1.85 | 0.41 |
| 4:Y:226:GLU:HG3 | 4:Y:255:PHE:CE2 | 2.55 | 0.41 |
| 4:Z:227:MET:O | 4:Z:230:ALA:HB3 | 2.21 | 0.41 |
| 4:X:291:LYS:HD2 | 4:Z:243:PRO:HB2 | 1.93 | 0.41 |
| 4:Z:144:ALA:HB2 | 4:Z:342:GLY:CA | 2.51 | 0.41 |
| 4:2:369:ILE:HG23 | 4:2:370:VAL:N | 2.35 | 0.41 |
| 4:1:324:THR:CB | 4:3:244:ASP:HA | 2.51 | 0.41 |
| 4:4:32:PRO:HB2 | 4:4:34:ILE:CD1 | 2.51 | 0.41 |
| 4:5:32:PRO:HB2 | 4:5:34:ILE:CD1 | 2.51 | 0.41 |
| 4:7:227:MET:O | 4:7:230:ALA:HB3 | 2.21 | 0.41 |
| 4:8:227:MET:O | 4:8:230:ALA:HB3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:541:MET:HG2 | 4:8:345:ILE:HG23 | 2.01 | 0.41 |
| 4:9:221:LEU:HA | 4:9:312:ARG:HG2 | 2.02 | 0.41 |
| 1:A:141:LEU:HD12 | 1:A:141:LEU:N | 2.33 | 0.41 |
| 1:A:213:LYS:HA | 1:A:220:ASP:OD2 | 2.19 | 0.41 |
| 1:A:295:MLY:CD | 1:A:332:MET:HE2 | 2.51 | 0.41 |
| 1:A:369:MLY:HD3 | 1:A:369:MLY:HH22 | 1.79 | 0.41 |
| 1:A:49:MLY:HH23 | 1:A:80:MET:CE | 2.51 | 0.41 |
| 1:A:665:ARG:C | 1:A:667:THR:N | 2.74 | 0.41 |
| 2:B:150:TYR:HB3 | 2:B:151:LYS:HG3 | 2.03 | 0.41 |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:HD11 | 1.75 | 0.41 |
| 2:B:54:MET:O | 2:H:21:GLU:HB2 | 2.21 | 0.41 |
| 1:D:135:TYR:CD2 | 1:D:191:ARG:HD3 | 2.55 | 0.41 |
| 1:D:25:ILE:HG23 | 1:D:29:ASN:HD22 | 1.85 | 0.41 |
| 1:D:322:VAL:HG12 | 1:D:325:ILE:HG13 | 2.03 | 0.41 |
| 1:D:445:ILE:HG22 | 1:D:449:LEU:HD22 | 2.02 | 0.41 |
| 3:F:56:GLU:OE1 | 3:F:59:ASN:ND2 | 2.54 | 0.41 |
| 1:G:322:VAL:HA | 1:G:323:PRO:HD3 | 1.87 | 0.41 |
| 1:G:536:LEU:HA | 1:G:536:LEU:HD12 | 1.69 | 0.41 |
| 1:J:322:VAL:HB | 1:J:325:ILE:HD12 | 2.03 | 0.41 |
| 1:J:408:VAL:HA | 1:J:636:LYS:HG2 | 1.14 | 0.41 |
| 1:J:449:LEU:CD1 | 1:J:449:LEU:N | 2.81 | 0.41 |
| 1:J:60:VAL:O | 1:J:72:VAL:N | 2.51 | 0.41 |
| 2:K:113:LYS:O | 2:K:147:ASN:HB2 | 2.20 | 0.41 |
| 2:E:163:ALA:O | 2:K:21:GLU:HB3 | 2.20 | 0.41 |
| 1:M:193:ILE:CD1 | 1:M:250:ILE:HD13 | 2.51 | 0.41 |
| 1:M:568:PRO:CG | 1:M:578:HIS:N | 2.84 | 0.41 |
| 1:S:136:ASN:O | 1:S:138:MLY:N | 2.54 | 0.41 |
| 1:S:166:MET:CE | 1:S:254:PHE:CD2 | 3.01 | 0.41 |
| 1:S:346:ASP:O | 1:S:350:ALA:N | 2.46 | 0.41 |
| 1:S:657:LEU:HD12 | 1:S:657:LEU:O | 2.21 | 0.41 |
| 1:G:637:LYS:HD2 | 4:V:144:ALA:HB3 | 1.20 | 0.41 |
| 4:W:196:ARG:HH21 | 4:W:249:THR:HG23 | 1.85 | 0.41 |
| 4:W:193:LEU:HD11 | 4:W:250:ILE:HG13 | 2.02 | 0.41 |
| 4:W:221:LEU:HA | 4:W:312:ARG:HG2 | 2.02 | 0.41 |
| 4:X:196:ARG:HH21 | 4:X:249:THR:HG23 | 1.85 | 0.41 |
| 4:X:227:MET:O | 4:X:230:ALA:HB3 | 2.21 | 0.41 |
| 4:W:287:ILE:HG13 | 4:Y:202:THR:HG23 | 1.65 | 0.41 |
| 4:Z:32:PRO:HB2 | 4:Z:34:ILE:CD1 | 2.51 | 0.41 |
| 1:S:637:LYS:HD2 | 4:2:144:ALA:HB3 | 1.20 | 0.41 |
| 4:3:32:PRO:HB2 | 4:3:34:ILE:CD1 | 2.51 | 0.41 |
| 4:4:144:ALA:HB2 | 4:4:342:GLY:CA | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:369:ILE:HG23 | 4:8:370:VAL:N | 2.35 | 0.41 |
| 4:9:287:ILE:N | 4:W:202:THR:CG2 | 2.77 | 0.41 |
| 4:9:32:PRO:HB2 | 4:9:34:ILE:CD1 | 2.51 | 0.41 |
| 1:A:356:GLY:HA2 | 1:A:359:MET:HG3 | 2.02 | 0.41 |
| 1:A:174:SER:HA | 1:A:460:GLY:O | 2.20 | 0.41 |
| 1:A:462:LEU:HD11 | 1:A:464:ILE:CD1 | 2.50 | 0.41 |
| 1:A:711:PHE:O | 1:A:714:ARG:NH2 | 2.54 | 0.41 |
| 1:A:72:VAL:O | 1:A:73:LYS:O | 2.39 | 0.41 |
| 1:D:136:ASN:O | 1:D:138:MLY:N | 2.54 | 0.41 |
| 1:D:295:MLY:CD | 1:D:332:MET:HE2 | 2.51 | 0.41 |
| 1:D:533:PHE:O | 1:D:537:GLU:N | 2.49 | 0.41 |
| 1:D:556:ASP:OD1 | 4:W:50:LYS:CG | 2.69 | 0.41 |
| 1:D:673:ARG:HA | 1:D:673:ARG:HD2 | 1.79 | 0.41 |
| 1:D:744:SER:O | 1:D:748:LEU:HD12 | 2.20 | 0.41 |
| 1:D:762:HIS:N | 1:D:762:HIS:CD2 | 2.79 | 0.41 |
| 1:G:135:TYR:HD2 | 1:G:191:ARG:CG | 2.33 | 0.41 |
| 1:G:295:MLY:CG | 1:G:332:MET:HE1 | 2.49 | 0.41 |
| 1:G:530:MET:HE3 | 4:V:354:GLN:CB | 2.51 | 0.41 |
| 1:G:539:GLU:OE2 | 1:G:553:MLY:HD3 | 2.20 | 0.41 |
| 1:J:136:ASN:O | 1:J:138:MLY:N | 2.54 | 0.41 |
| 1:J:322:VAL:HG12 | 1:J:325:ILE:HG13 | 2.03 | 0.41 |
| 1:J:493:HIS:O | 1:J:496:PHE:N | 2.54 | 0.41 |
| 1:J:739:ASP:C | 1:J:739:ASP:OD1 | 2.58 | 0.41 |
| 1:J:753:VAL:O | 1:J:755:HIS:ND1 | 2.54 | 0.41 |
| 1:J:775:LEU:HD12 | 1:J:775:LEU:HA | 1.71 | 0.41 |
| 1:J:830:PRO:CB | 2:K:67:MET:HE1 | 2.51 | 0.41 |
| 1:M:303:LEU:O | 1:M:304:LEU:HB2 | 2.21 | 0.41 |
| 1:M:493:HIS:O | 1:M:496:PHE:N | 2.54 | 0.41 |
| 1:M:817:GLN:HG3 | 2:N:128:PHE:HE1 | 1.80 | 0.41 |
| 1:M:842:LEU:N | 1:M:842:LEU:CD1 | 2.83 | 0.41 |
| 3:O:95:ASP:OD1 | 3:O:139:TYR:HE1 | 2.03 | 0.41 |
| 1:S:193:ILE:HD11 | 1:S:250:ILE:HD12 | 2.03 | 0.41 |
| 1:S:303:LEU:O | 1:S:304:LEU:HB2 | 2.21 | 0.41 |
| 4:W:227:MET:O | 4:W:230:ALA:HB3 | 2.21 | 0.41 |
| 4:5:144:ALA:HB2 | 4:5:342:GLY:CA | 2.51 | 0.41 |
| 4:6:221:LEU:HA | 4:6:312:ARG:HG2 | 2.02 | 0.41 |
| 4:6:144:ALA:HB2 | 4:6:342:GLY:CA | 2.51 | 0.41 |
| 4:6:369:ILE:HG23 | 4:6:370:VAL:N | 2.35 | 0.41 |
| 4:7:288:ASP:OD1 | 4:9:204:ALA:HA | 2.21 | 0.41 |
| 4:7:221:LEU:HA | 4:7:312:ARG:HG2 | 2.02 | 0.41 |
| 4:7:32:PRO:HB2 | 4:7:34:ILE:CD1 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:741:LYS:HG2 | 1:A:742:LYS:N | 2.35 | 0.41 |
| 1:D:195:TYR:CE2 | 1:D:199:ILE:HD13 | 2.55 | 0.41 |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:HD12 | 2.03 | 0.41 |
| 1:D:193:ILE:CD1 | 1:D:250:ILE:HD13 | 2.51 | 0.41 |
| 1:D:528:MLY:HB2 | 1:D:529:PRO:HD2 | 2.03 | 0.41 |
| 1:D:610:LEU:N | 1:D:610:LEU:CD1 | 2.84 | 0.41 |
| 1:D:818:TYR:CB | 2:E:90:GLY:C | 2.80 | 0.41 |
| 1:D:842:LEU:CD1 | 1:D:842:LEU:N | 2.83 | 0.41 |
| 1:G:17:LEU:HA | 1:G:17:LEU:HD12 | 1.67 | 0.41 |
| 1:G:356:GLY:HA2 | 1:G:359:MET:HG3 | 2.02 | 0.41 |
| 1:G:384:ASP:HA | 1:G:394:SER:OG | 2.21 | 0.41 |
| 1:G:449:LEU:CD1 | 1:G:449:LEU:N | 2.82 | 0.41 |
| 1:G:657:LEU:O | 1:G:657:LEU:HD12 | 2.21 | 0.41 |
| 1:G:717:TYR:OH | 1:G:760:PHE:HB3 | 2.21 | 0.41 |
| 2:H:150:TYR:HB3 | 2:H:151:LYS:HG3 | 2.03 | 0.41 |
| 1:G:831:TRP:CZ3 | 2:H:34:ILE:HD13 | 2.56 | 0.41 |
| 1:J:166:MET:CE | 1:J:254:PHE:HB2 | 2.47 | 0.41 |
| 1:J:25:ILE:HG23 | 1:J:29:ASN:HD22 | 1.85 | 0.41 |
| 1:J:48:VAL:CG2 | 1:J:49:MLY:N | 2.84 | 0.41 |
| 1:J:692:LEU:HD23 | 1:J:692:LEU:HA | 1.85 | 0.41 |
| 1:J:757:GLN:N | 1:J:776:GLU:CB | 2.82 | 0.41 |
| 1:M:129:TYR:HD1 | 1:M:129:TYR:HA | 1.65 | 0.41 |
| 1:M:195:TYR:CE2 | 1:M:199:ILE:HD13 | 2.55 | 0.41 |
| 1:M:217:THR:CA | 1:M:221:GLN:HE21 | 2.33 | 0.41 |
| 1:M:193:ILE:HD11 | 1:M:250:ILE:HD12 | 2.03 | 0.41 |
| 1:M:724:TYR:HB3 | 1:M:727:LEU:CD1 | 2.48 | 0.41 |
| 1:M:797:PHE:CD2 | 1:M:798:LEU:HD12 | 2.55 | 0.41 |
| 2:T:112:ILE:O | 2:T:148:VAL:N | 2.50 | 0.41 |
| 1:S:797:PHE:CD1 | 3:U:146:ILE:HG23 | 2.56 | 0.41 |
| 4:V:226:GLU:HG3 | 4:V:255:PHE:CE2 | 2.56 | 0.41 |
| 1:G:410:ASN:HA | 4:V:334:GLU:HB3 | 1.29 | 0.41 |
| 1:A:551:MLY:C | 4:V:47:MET:HA | 2.48 | 0.41 |
| 4:W:32:PRO:HB2 | 4:W:34:ILE:CD1 | 2.51 | 0.41 |
| 4:X:144:ALA:HB2 | 4:X:342:GLY:CA | 2.51 | 0.41 |
| 4:Z:369:ILE:HG23 | 4:Z:370:VAL:N | 2.35 | 0.41 |
| 4:1:32:PRO:HB2 | 4:1:34:ILE:CD1 | 2.51 | 0.41 |
| 4:2:32:PRO:HB2 | 4:2:34:ILE:CD1 | 2.51 | 0.41 |
| 4:3:287:ILE:HB | 4:5:203:THR:CB | 2.45 | 0.41 |
| 4:8:32:PRO:HB2 | 4:8:34:ILE:CD1 | 2.51 | 0.41 |
| 4:9:226:GLU:HG3 | 4:9:255:PHE:CE2 | 2.55 | 0.41 |
| 4:9:369:ILE:HG23 | 4:9:370:VAL:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:303:LEU:O | 1:A:304:LEU:HB2 | 2.21 | 0.41 |
| 1:A:629:GLU:CA | 1:A:643:GLY:C | 2.73 | 0.41 |
| 2:B:111:SER:OG | 2:B:148:VAL:CA | 2.69 | 0.41 |
| 2:B:63:GLU:O | 2:B:67:MET:HG3 | 2.21 | 0.41 |
| 1:D:724:TYR:CB | 1:D:782:MLY:NZ | 2.79 | 0.41 |
| 1:D:49:MLY:HH23 | 1:D:80:MET:CE | 2.51 | 0.41 |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:HD12 | 2.03 | 0.41 |
| 1:G:303:LEU:O | 1:G:304:LEU:HB2 | 2.21 | 0.41 |
| 1:G:629:GLU:HB3 | 1:G:643:GLY:C | 2.41 | 0.41 |
| 1:J:204:GLU:N | 1:J:207:LYS:HE3 | 2.23 | 0.41 |
| 1:J:193:ILE:CD1 | 1:J:250:ILE:HD13 | 2.51 | 0.41 |
| 1:J:356:GLY:HA2 | 1:J:359:MET:HG3 | 2.02 | 0.41 |
| 1:J:536:LEU:HA | 1:J:536:LEU:HD12 | 1.69 | 0.41 |
| 1:J:553:MLY:HA | 4:Y:45:VAL:O | 2.20 | 0.41 |
| 1:J:629:GLU:HB3 | 1:J:643:GLY:C | 2.42 | 0.41 |
| 1:J:710:GLY:O | 1:J:772:LEU:HD22 | 2.14 | 0.41 |
| 1:M:221:GLN:H | 1:M:221:GLN:HG2 | 1.47 | 0.41 |
| 1:M:166:MET:CE | 1:M:254:PHE:HB2 | 2.47 | 0.41 |
| 1:M:25:ILE:HG23 | 1:M:29:ASN:HD22 | 1.85 | 0.41 |
| 1:M:172:ASN:OD1 | 1:M:457:TYR:HA | 2.21 | 0.41 |
| 1:M:724:TYR:CE2 | 1:M:772:LEU:CD2 | 3.02 | 0.41 |
| 1:M:726:VAL:HG13 | 3:O:89:GLU:OE1 | 2.21 | 0.41 |
| 1:M:812:SER:O | 1:M:816:ILE:HG13 | 2.21 | 0.41 |
| 1:M:836:PHE:CD2 | 2:N:160:GLY:HA3 | 2.55 | 0.41 |
| 1:S:296:MLY:HH11 | 1:S:348:MLY:CH2 | 2.48 | 0.41 |
| 1:S:60:VAL:O | 1:S:72:VAL:N | 2.51 | 0.41 |
| 1:S:72:VAL:O | 1:S:73:LYS:O | 2.39 | 0.41 |
| 1:S:753:VAL:O | 1:S:755:HIS:ND1 | 2.54 | 0.41 |
| 1:S:821:ARG:CZ | 2:T:127:ARG:NE | 2.84 | 0.41 |
| 3:U:56:GLU:OE1 | 3:U:59:ASN:ND2 | 2.54 | 0.41 |
| 4:V:219:VAL:HG22 | 4:V:258:PRO:CB | 2.51 | 0.41 |
| 1:G:643:GLY:N | 4:V:23:GLY:C | 2.55 | 0.41 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:HG23 | 2.02 | 0.41 |
| 1:J:642:LYS:HE2 | 4:W:344:SER:HA | 1.56 | 0.41 |
| 4:X:219:VAL:HG22 | 4:X:258:PRO:CB | 2.51 | 0.41 |
| 4:Z:196:ARG:HH21 | 4:Z:249:THR:HG23 | 1.85 | 0.41 |
| 4:1:315:LYS:HD2 | 4:1:315:LYS:HA | 1.92 | 0.40 |
| 4:2:219:VAL:HG22 | 4:2:258:PRO:CB | 2.52 | 0.40 |
| 4:2:287:ILE:CD1 | 4:2:287:ILE:H | 2.31 | 0.40 |
| 4:4:196:ARG:HH21 | 4:4:249:THR:HG23 | 1.85 | 0.40 |
| 4:5:287:ILE:H | 4:5:287:ILE:CD1 | 2.31 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:226:GLU:HG3 | 4:7:255:PHE:CE2 | 2.56 | 0.40 |
| 4:8:219:VAL:HG22 | 4:8:258:PRO:CB | 2.51 | 0.40 |
| 1:A:296:MLY:HH11 | 1:A:348:MLY:CH2 | 2.48 | 0.40 |
| 1:A:407:GLY:HA2 | 1:A:411:GLU:O | 2.21 | 0.40 |
| 2:B:112:ILE:O | 2:B:148:VAL:N | 2.50 | 0.40 |
| 2:B:139:ALA:O | 2:B:141:PRO:CD | 2.51 | 0.40 |
| 3:C:95:ASP:OD1 | 3:C:139:TYR:HE1 | 2.04 | 0.40 |
| 1:D:201:ALA:O | 1:D:202:SER:OG | 2.36 | 0.40 |
| 2:E:150:TYR:HB3 | 2:E:151:LYS:HG3 | 2.03 | 0.40 |
| 1:G:193:ILE:CD1 | 1:G:250:ILE:HD13 | 2.51 | 0.40 |
| 1:G:493:HIS:O | 1:G:496:PHE:N | 2.54 | 0.40 |
| 1:G:707:CYS:CB | 1:G:714:ARG:NH2 | 2.84 | 0.40 |
| 1:J:135:TYR:HD2 | 1:J:191:ARG:CG | 2.33 | 0.40 |
| 1:J:217:THR:CA | 1:J:221:GLN:HE21 | 2.33 | 0.40 |
| 1:J:659:MLY:HH22 | 1:J:659:MLY:HD2 | 1.42 | 0.40 |
| 1:J:717:TYR:OH | 1:J:760:PHE:HB3 | 2.21 | 0.40 |
| 1:M:485:GLU:OE1 | 1:M:583:HIS:HB3 | 2.21 | 0.40 |
| 1:M:496:PHE:CG | 1:M:514:ASP:HA | 2.57 | 0.40 |
| 1:M:720:PHE:CE1 | 1:M:772:LEU:CD1 | 3.04 | 0.40 |
| 1:M:753:VAL:O | 1:M:755:HIS:ND1 | 2.54 | 0.40 |
| 2:N:111:SER:OG | 2:N:148:VAL:CA | 2.69 | 0.40 |
| 1:S:172:ASN:OD1 | 1:S:457:TYR:HA | 2.21 | 0.40 |
| 1:S:49:MLY:HH23 | 1:S:80:MET:CE | 2.51 | 0.40 |
| 1:S:496:PHE:CG | 1:S:514:ASP:HA | 2.57 | 0.40 |
| 1:S:485:GLU:OE1 | 1:S:583:HIS:HB3 | 2.21 | 0.40 |
| 1:S:724:TYR:HB3 | 1:S:727:LEU:CD1 | 2.49 | 0.40 |
| 1:S:792:ALA:CB | 3:U:42:THR:CB | 2.53 | 0.40 |
| 2:T:149:ASP:OD2 | 2:T:150:TYR:CA | 2.65 | 0.40 |
| 2:T:150:TYR:HB3 | 2:T:151:LYS:HG3 | 2.03 | 0.40 |
| 1:A:556:ASP:OD1 | 4:V:50:LYS:CG | 2.69 | 0.40 |
| 4:W:369:ILE:HG23 | 4:W:370:VAL:N | 2.35 | 0.40 |
| 4:Y:144:ALA:HB2 | 4:Y:342:GLY:CA | 2.51 | 0.40 |
| 4:1:227:MET:O | 4:1:230:ALA:HB3 | 2.21 | 0.40 |
| 4:2:250:ILE:HG22 | 4:2:254:ARG:HB2 | 2.04 | 0.40 |
| 4:2:221:LEU:HA | 4:2:312:ARG:HG2 | 2.02 | 0.40 |
| 1:M:554:LEU:N | 4:2:46:GLY:O | 2.52 | 0.40 |
| 4:3:287:ILE:HG22 | 4:5:204:ALA:HB3 | 2.03 | 0.40 |
| 1:A:471:ASP:CB | 1:A:573:GLY:O | 2.68 | 0.40 |
| 1:A:528:MLY:HB2 | 1:A:529:PRO:HD2 | 2.03 | 0.40 |
| 1:A:568:PRO:CG | 1:A:578:HIS:N | 2.84 | 0.40 |
| 1:D:172:ASN:OD1 | 1:D:457:TYR:HA | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:17:LEU:HD12 | 1:D:17:LEU:HA | 1.67 | 0.40 |
| 1:D:47:PHE:HE1 | 1:D:78:PHE:CE1 | 2.39 | 0.40 |
| 1:D:466:GLY:CA | 1:D:484:ASN:HD21 | 2.32 | 0.40 |
| 1:D:485:GLU:OE1 | 1:D:583:HIS:HB3 | 2.21 | 0.40 |
| 1:D:712:PRO:CB | 1:D:771:LEU:CD2 | 2.88 | 0.40 |
| 1:D:747:LEU:CD2 | 1:D:782:MLY:HH21 | 2.47 | 0.40 |
| 1:D:89:GLU:HB3 | 1:D:153:PRO:HG3 | 2.03 | 0.40 |
| 1:G:110:TYR:O | 1:G:113:TRP:N | 2.42 | 0.40 |
| 1:G:174:SER:HA | 1:G:460:GLY:O | 2.20 | 0.40 |
| 1:G:193:ILE:HD13 | 1:G:252:ILE:HD11 | 2.04 | 0.40 |
| 1:G:172:ASN:OD1 | 1:G:457:TYR:HA | 2.22 | 0.40 |
| 1:G:791:GLN:HE22 | 3:I:115:GLY:HA3 | 0.45 | 0.40 |
| 1:G:813:ILE:HG21 | 2:H:128:PHE:CE1 | 2.51 | 0.40 |
| 2:H:139:ALA:O | 2:H:141:PRO:CD | 2.51 | 0.40 |
| 1:J:237:THR:CG2 | 1:J:238:VAL:N | 2.84 | 0.40 |
| 1:J:49:MLY:HH23 | 1:J:80:MET:CE | 2.51 | 0.40 |
| 1:M:136:ASN:HA | 1:M:137:PRO:HD3 | 1.50 | 0.40 |
| 1:M:485:GLU:OE2 | 1:M:584:TYR:N | 2.50 | 0.40 |
| 1:M:665:ARG:C | 1:M:667:THR:N | 2.74 | 0.40 |
| 1:S:295:MLY:CD | 1:S:332:MET:HE2 | 2.51 | 0.40 |
| 1:S:320:ILE:CG2 | 1:S:320:ILE:O | 2.68 | 0.40 |
| 1:S:330:GLU:OE1 | 1:S:330:GLU:HA | 2.21 | 0.40 |
| 1:S:541:MET:HG2 | 4:2:345:ILE:HG23 | 2.02 | 0.40 |
| 1:S:821:ARG:NH1 | 2:T:127:ARG:CZ | 2.84 | 0.40 |
| 4:8:288:ASP:OD1 | 4:V:204:ALA:HA | 2.21 | 0.40 |
| 4:V:256:ARG:HH11 | 4:V:256:ARG:HD2 | 1.78 | 0.40 |
| 1:G:530:MET:HE3 | 4:V:354:GLN:CG | 2.39 | 0.40 |
| 4:9:288:ASP:OD1 | 4:W:204:ALA:HA | 2.20 | 0.40 |
| 4:W:226:GLU:HG3 | 4:W:255:PHE:CE2 | 2.55 | 0.40 |
| 4:3:226:GLU:HG3 | 4:3:255:PHE:CE2 | 2.55 | 0.40 |
| 4:5:219:VAL:HG22 | 4:5:258:PRO:CB | 2.52 | 0.40 |
| 4:4:288:ASP:CA | 4:6:203:THR:CG2 | 3.00 | 0.40 |
| 4:7:219:VAL:HG22 | 4:7:258:PRO:CB | 2.52 | 0.40 |
| 4:9:120:THR:HG21 | 4:9:370:VAL:CG1 | 2.52 | 0.40 |
| 1:A:166:MET:CE | 1:A:254:PHE:CD2 | 3.01 | 0.40 |
| 3:C:62:ALA:O | 3:C:63:ILE:HG13 | 2.13 | 0.40 |
| 3:C:96:LYS:H | 3:C:96:LYS:HG3 | 1.66 | 0.40 |
| 1:D:213:LYS:HA | 1:D:220:ASP:OD2 | 2.19 | 0.40 |
| 1:D:493:HIS:O | 1:D:496:PHE:N | 2.54 | 0.40 |
| 1:D:629:GLU:HB3 | 1:D:643:GLY:C | 2.41 | 0.40 |
| 1:D:659:MLY:HH22 | 1:D:659:MLY:HD2 | 1.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:271:GLU:OE1 | 1:G:274:ARG:NH1 | 2.53 | 0.40 |
| 1:G:330:GLU:HA | 1:G:330:GLU:OE1 | 2.20 | 0.40 |
| 1:G:553:MLY:HA | 4:X:45:VAL:O | 2.21 | 0.40 |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:CH2 | 2.48 | 0.40 |
| 1:J:320:ILE:O | 1:J:320:ILE:CG2 | 2.68 | 0.40 |
| 1:J:818:TYR:N | 2:K:127:ARG:HH11 | 2.20 | 0.40 |
| 1:J:829:TRP:HH2 | 2:K:83:MET:HE3 | 1.86 | 0.40 |
| 1:M:135:TYR:HD2 | 1:M:191:ARG:CG | 2.33 | 0.40 |
| 1:M:271:GLU:OE1 | 1:M:274:ARG:NH1 | 2.53 | 0.40 |
| 1:M:580:SER:O | 1:M:581:LEU:HD12 | 2.22 | 0.40 |
| 1:M:610:LEU:CD1 | 1:M:610:LEU:N | 2.84 | 0.40 |
| 1:M:690:LEU:O | 1:M:694:GLN:HG3 | 2.20 | 0.40 |
| 1:M:717:TYR:OH | 1:M:760:PHE:HB3 | 2.21 | 0.40 |
| 2:N:144:VAL:HG12 | 2:N:153:ILE:HD13 | 1.92 | 0.40 |
| 1:S:135:TYR:CD2 | 1:S:191:ARG:HD3 | 2.55 | 0.40 |
| 1:S:322:VAL:HB | 1:S:325:ILE:HD12 | 2.02 | 0.40 |
| 1:S:610:LEU:CD1 | 1:S:610:LEU:N | 2.84 | 0.40 |
| 1:S:88:ILE:HG22 | 1:S:90:ASP:C | 2.42 | 0.40 |
| 2:T:144:VAL:HG12 | 2:T:153:ILE:HD13 | 1.92 | 0.40 |
| 4:V:32:PRO:HB2 | 4:V:34:ILE:CD1 | 2.51 | 0.40 |
| 1:J:410:ASN:HA | 4:W:334:GLU:HB3 | 1.28 | 0.40 |
| 4:X:256:ARG:HD2 | 4:X:256:ARG:HH11 | 1.78 | 0.40 |
| 4:X:221:LEU:HA | 4:X:312:ARG:HG2 | 2.02 | 0.40 |
| 4:Z:219:VAL:HG22 | 4:Z:258:PRO:CB | 2.51 | 0.40 |
| 4:2:204:ALA:HA | 4:Z:288:ASP:OD1 | 2.21 | 0.40 |
| 4:2:256:ARG:HD2 | 4:2:256:ARG:HH11 | 1.78 | 0.40 |
| 4:4:287:ILE:H | 4:4:287:ILE:CD1 | 2.31 | 0.40 |
| 4:4:287:ILE:HG22 | 4:6:204:ALA:HB3 | 2.03 | 0.40 |
| 4:7:171:LEU:HA | 4:7:172:PRO:HD2 | 1.84 | 0.40 |
| 4:7:287:ILE:N | 4:9:202:THR:CG2 | 2.77 | 0.40 |
| 4:8:287:ILE:H | 4:8:287:ILE:CD1 | 2.31 | 0.40 |
| 4:9:227:MET:O | 4:9:230:ALA:HB3 | 2.21 | 0.40 |
| 1:A:172:ASN:OD1 | 1:A:457:TYR:HA | 2.21 | 0.40 |
| 1:A:657:LEU:HD12 | 1:A:657:LEU:O | 2.21 | 0.40 |
| 1:A:28:GLN:NE2 | 1:A:723:ARG:NH2 | 2.47 | 0.40 |
| 1:A:809:ARG:CZ | 2:B:124:GLY:HA3 | 2.51 | 0.40 |
| 3:C:56:GLU:OE1 | 3:C:59:ASN:ND2 | 2.54 | 0.40 |
| 1:D:237:THR:CG2 | 1:D:238:VAL:N | 2.85 | 0.40 |
| 1:D:348:MLY:HD2 | 1:D:348:MLY:HH12 | 1.82 | 0.40 |
| 1:D:739:ASP:C | 1:D:739:ASP:OD1 | 2.58 | 0.40 |
| 1:D:88:ILE:HG22 | 1:D:90:ASP:C | 2.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:95:ASP:OD1 | 3:F:139:TYR:HE1 | 2.04 | 0.40 |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:OH | 2.22 | 0.40 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:C | 2.60 | 0.40 |
| 1:G:72:VAL:O | 1:G:73:LYS:O | 2.39 | 0.40 |
| 1:G:812:SER:O | 1:G:816:ILE:HG13 | 2.21 | 0.40 |
| 1:J:172:ASN:OD1 | 1:J:457:TYR:HA | 2.21 | 0.40 |
| 1:J:528:MLY:HB2 | 1:J:529:PRO:HD2 | 2.03 | 0.40 |
| 1:J:789:ALA:CB | 3:L:81:GLN:CD | 2.90 | 0.40 |
| 3:L:95:ASP:OD1 | 3:L:139:TYR:HE1 | 2.03 | 0.40 |
| 1:M:292:MET:HE3 | 1:M:309:PRO:CA | 2.50 | 0.40 |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:OH | 2.21 | 0.40 |
| 1:M:408:VAL:HA | 1:M:636:LYS:HG2 | 1.14 | 0.40 |
| 1:M:174:SER:HA | 1:M:460:GLY:O | 2.20 | 0.40 |
| 1:M:544:LYS:N | 4:Z:146:GLY:O | 2.55 | 0.40 |
| 1:M:641:LYS:CE | 1:M:647:GLN:CB | 2.75 | 0.40 |
| 1:M:107:MLY:CA | 1:M:686:MET:HE1 | 2.52 | 0.40 |
| 1:S:407:GLY:HA2 | 1:S:411:GLU:O | 2.21 | 0.40 |
| 1:S:692:LEU:HD23 | 1:S:692:LEU:HA | 1.85 | 0.40 |
| 1:S:783:LEU:O | 1:S:786:ILE:CB | 2.70 | 0.40 |
| 1:S:786:ILE:C | 1:S:789:ALA:N | 2.47 | 0.40 |
| 1:S:93:MET:HA | 1:S:714:ARG:CA | 2.52 | 0.40 |
| 2:T:140:PHE:HB3 | 2:T:144:VAL:HG11 | 2.03 | 0.40 |
| 4:9:324:THR:N | 4:W:245:GLY:CA | 2.69 | 0.40 |
| 4:Y:219:VAL:HG22 | 4:Y:258:PRO:CB | 2.51 | 0.40 |
| 4:Z:120:THR:HG21 | 4:Z:370:VAL:CG1 | 2.52 | 0.40 |
| 1:M:530:MET:CB | 4:Z:354:GLN:CB | 2.95 | 0.40 |
| 4:2:166:TYR:OH | 4:4:64:ILE:CD1 | 2.62 | 0.40 |
| 4:2:227:MET:O | 4:2:230:ALA:HB3 | 2.21 | 0.40 |
| 4:4:219:VAL:HG22 | 4:4:258:PRO:CB | 2.52 | 0.40 |
| 4:3:324:THR:CA | 4:5:244:ASP:HA | 2.49 | 0.40 |
| 1:A:633:GLY:HA2 | 4:8:25:ASP:HA | 1.25 | 0.40 |
| 1:A:215:GLN:H | 1:A:340:ILE:CD1 | 2.21 | 0.40 |
| 1:A:271:GLU:OE1 | 1:A:274:ARG:NH1 | 2.53 | 0.40 |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:OH | 2.22 | 0.40 |
| 1:A:812:SER:O | 1:A:816:ILE:HG13 | 2.21 | 0.40 |
| 1:A:818:TYR:HB3 | 2:B:90:GLY:N | 2.35 | 0.40 |
| 1:D:261:ALA:O | 1:D:451:THR:OG1 | 2.40 | 0.40 |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:CH2 | 2.48 | 0.40 |
| 1:D:303:LEU:O | 1:D:389:LEU:HD21 | 2.22 | 0.40 |
| 1:D:384:ASP:HA | 1:D:394:SER:OG | 2.21 | 0.40 |
| 1:D:407:GLY:HA2 | 1:D:411:GLU:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:519:LEU:HD12 | 1:D:519:LEU:H | 1.83 | 0.40 |
| 1:D:400:ALA:CB | 1:D:606:THR:CG2 | 3.00 | 0.40 |
| 2:E:48:ARG:HH11 | 2:E:48:ARG:HD2 | 1.78 | 0.40 |
| 3:F:25:ILE:O | 3:F:63:ILE:CB | 2.66 | 0.40 |
| 1:G:295:MLY:CG | 1:G:332:MET:CE | 2.97 | 0.40 |
| 1:G:49:MLY:HH23 | 1:G:80:MET:CE | 2.51 | 0.40 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:HG22 | 2.01 | 0.40 |
| 1:J:279:LEU:CB | 1:J:280:PRO:HD2 | 2.49 | 0.40 |
| 1:J:303:LEU:O | 1:J:304:LEU:HB2 | 2.21 | 0.40 |
| 1:J:610:LEU:CD1 | 1:J:610:LEU:N | 2.84 | 0.40 |
| 1:J:64:THR:OG1 | 1:J:68:GLU:HB3 | 2.22 | 0.40 |
| 1:M:322:VAL:HB | 1:M:325:ILE:CG1 | 2.52 | 0.40 |
| 1:M:49:MLY:HH23 | 1:M:80:MET:CE | 2.51 | 0.40 |
| 1:M:506:GLU:OE2 | 1:M:762:HIS:N | 2.54 | 0.40 |
| 1:M:657:LEU:HD12 | 1:M:657:LEU:O | 2.21 | 0.40 |
| 1:M:64:THR:OG1 | 1:M:68:GLU:HB3 | 2.22 | 0.40 |
| 1:M:795:ARG:HH12 | 3:O:43:ASN:HB2 | 0.55 | 0.40 |
| 1:M:810:ARG:NH1 | 1:M:810:ARG:HG2 | 2.29 | 0.40 |
| 1:S:493:HIS:O | 1:S:496:PHE:N | 2.54 | 0.40 |
| 1:S:64:THR:OG1 | 1:S:68:GLU:HB3 | 2.22 | 0.40 |
| 1:S:94:MET:HE1 | 1:S:101:ALA:CB | 2.51 | 0.40 |
| 2:T:111:SER:OG | 2:T:148:VAL:CA | 2.69 | 0.40 |
| 1:G:642:LYS:HE2 | 4:V:344:SER:HA | 1.56 | 0.40 |
| 4:W:250:ILE:HG22 | 4:W:254:ARG:HB2 | 2.04 | 0.40 |
| 4:X:32:PRO:HB2 | 4:X:34:ILE:CD1 | 2.51 | 0.40 |
| 4:Y:227:MET:O | 4:Y:230:ALA:HB3 | 2.21 | 0.40 |

All (10487) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:196:ARG:O | 4:9:212:ILE:CG1[1_554] | 0.10 | 2.10 |
| 4:4:192:ILE:CG1 | 4:7:213:LYS:NZ[1_554] | 0.11 | 2.09 |
| 4:6:191:LYS:CA | 4:9:186:THR:C[1_554] | 0.15 | 2.05 |
| 4:5:196:ARG:O | 4:8:212:ILE:CG1[1_554] | 0.19 | 2.01 |
| 4:4:243:PRO:CB | 4:7:61:LYS:N[1_554] | 0.19 | 2.01 |
| 4:5:194:THR:C | 4:8:209:VAL:CG2[1_554] | 0.20 | 2.00 |
| 4:5:112:PRO:C | 4:9:253:GLU:CD[1_554] | 0.20 | 2.00 |
| 4:6:304:THR:N | 4:9:137:GLN:OE1[1_554] | 0.21 | 1.99 |
| 4:4:213:LYS:CE | 4:7:14:SER:C[1_554] | 0.22 | 1.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:188:TYR:CZ | 4:9:185:LEU:CD2[1_554] | 0.24 | 1.96 |
| 4:4:281:SER:OG | 4:7:173:HIS:N[1_554] | 0.24 | 1.96 |
| 4:5:346:LEU:CG | 4:8:368:SER:CB[1_554] | 0.25 | 1.95 |
| 4:3:75:ILE:N | 4:7:198:TYR:N[1_554] | 0.25 | 1.95 |
| 4:5:191:LYS:CA | 4:8:186:THR:C[1_554] | 0.25 | 1.95 |
| 4:4:75:ILE:N | 4:8:198:TYR:N[1_554] | 0.25 | 1.95 |
| 4:5:141:SER:O | 4:8:116:ARG:NH1[1_554] | 0.25 | 1.95 |
| 4:5:166:TYR:CD1 | 4:V:40:HIS:ND1[1_554] | 0.26 | 1.94 |
| 4:3:74:GLY:O | 4:7:197:GLY:CA[1_554] | 0.26 | 1.94 |
| 4:4:116:ARG:CG | 4:8:252:ASN:OD1[1_554] | 0.26 | 1.94 |
| 4:6:194:THR:C | 4:9:209:VAL:CG2[1_554] | 0.27 | 1.93 |
| 4:3:291:LYS:CG | 4:8:64:ILE:CD1[1_554] | 0.28 | 1.92 |
| 4:5:221:LEU:CB | 4:8:332:PRO:CD[1_554] | 0.28 | 1.92 |
| 4:4:274:ILE:N | 4:7:162:ASN:N[1_554] | 0.29 | 1.91 |
| 4:5:188:TYR:CZ | 4:8:185:LEU:CD2[1_554] | 0.30 | 1.90 |
| 1:D:637:LYS:NZ | 4:6:311:ASP:CA[1_556] | 0.31 | 1.89 |
| 4:4:259:GLU:OE1 | 4:7:304:THR:C[1_554] | 0.31 | 1.89 |
| 4:4:329:ILE:CG2 | 4:7:139:VAL:CB[1_554] | 0.33 | 1.87 |
| 4:3:116:ARG:CG | 4:7:252:ASN:OD1[1_554] | 0.33 | 1.87 |
| 4:4:277:THR:CG2 | 4:7:175:ILE:C[1_554] | 0.33 | 1.87 |
| 4:5:335:ARG:N | 4:8:105:LEU:C[1_554] | 0.33 | 1.87 |
| 4:5:369:ILE:CG2 | 4:9:232:SER:CA[1_554] | 0.33 | 1.87 |
| 4:5:304:THR:N | 4:8:137:GLN:OE1[1_554] | 0.33 | 1.87 |
| 4:6:188:TYR:CE1 | 4:9:185:LEU:CG[1_554] | 0.33 | 1.87 |
| 4:6:193:LEU:O | 4:9:209:VAL:C[1_554] | 0.33 | 1.87 |
| 4:6:221:LEU:CB | 4:9:332:PRO:CD[1_554] | 0.34 | 1.86 |
| 4:5:284:LYS:O | 4:9:268:GLY:O[1_554] | 0.34 | 1.86 |
| 4:5:162:ASN:ND2 | 4:8:175:ILE:CG1[1_554] | 0.34 | 1.86 |
| 4:5:257:CYS:CA | 4:8:303:THR:OG1[1_554] | 0.34 | 1.86 |
| 4:4:186:THR:OG1 | 4:7:183:ARG:NH2[1_554] | 0.34 | 1.86 |
| 4:6:343:GLY:O | 4:9:367:PRO:CA[1_554] | 0.34 | 1.86 |
| 4:4:336:LYS:CE | 4:7:86:TRP:CE2[1_554] | 0.34 | 1.86 |
| 4:4:287:ILE:O | 4:9:63:GLY:CA[1_554] | 0.35 | 1.85 |
| 4:4:74:GLY:O | 4:8:197:GLY:CA[1_554] | 0.35 | 1.85 |
| 4:4:226:GLU:CD | 4:7:333:PRO:O[1_554] | 0.35 | 1.85 |
| 4:4:291:LYS:CG | 4:9:64:ILE:CD1[1_554] | 0.35 | 1.85 |
| 4:6:335:ARG:N | 4:9:105:LEU:C[1_554] | 0.36 | 1.84 |
| 4:6:337:TYR:CE1 | 4:9:86:TRP:CZ2[1_554] | 0.36 | 1.84 |
| 4:6:325:MET:SD | 4:9:166:TYR:OH[1_554] | 0.36 | 1.84 |
| 4:3:169:TYR:OH | 4:7:266:PHE:CE1[1_554] | 0.36 | 1.84 |
| 4:4:333:PRO:CA | 4:7:105:LEU:N[1_554] | 0.36 | 1.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:346:LEU:CG | 4:9:368:SER:CB[1_554] | 0.36 | 1.84 |
| 4:4:299:MET:CE | 4:7:136:ILE:O[1_554] | 0.37 | 1.83 |
| 4:6:221:LEU:C | 4:9:331:ALA:C[1_554] | 0.37 | 1.83 |
| 4:4:220:ALA:N | 4:7:335:ARG:O[1_554] | 0.37 | 1.83 |
| 4:5:210:ARG:CZ | 4:8:33:SER:O[1_554] | 0.37 | 1.83 |
| 4:6:151:ILE:CD1 | 4:9:171:LEU:CA[1_554] | 0.38 | 1.82 |
| 4:6:112:PRO:C | 4:V:253:GLU:CD[1_554] | 0.38 | 1.82 |
| 4:4:260:THR:CA | 4:7:155:SER:OG[1_554] | 0.38 | 1.82 |
| 4:6:166:TYR:CD1 | 4:W:40:HIS:ND1[1_554] | 0.38 | 1.82 |
| 4:5:193:LEU:O | 4:8:209:VAL:C[1_554] | 0.39 | 1.81 |
| 4:4:340:TRP:CB | 4:7:118:LYS:CA[1_554] | 0.39 | 1.81 |
| 4:5:255:PHE:CG | 4:8:305:MET:CB[1_554] | 0.39 | 1.81 |
| 4:5:211:ASP:CB | 4:8:32:PRO:CB[1_554] | 0.40 | 1.80 |
| 4:4:26:ALA:CB | 4:7:122:ILE:C[1_554] | 0.40 | 1.80 |
| 4:5:258:PRO:CA | 4:8:155:SER:O[1_554] | 0.40 | 1.80 |
| 4:5:25:ASP:OD2 | 4:8:129:VAL:O[1_554] | 0.40 | 1.80 |
| 4:4:243:PRO:N | 4:7:60:SER:CA[1_554] | 0.40 | 1.80 |
| 4:4:213:LYS:C | 4:7:16:LEU:N[1_554] | 0.40 | 1.80 |
| 4:5:185:LEU:C | 4:8:157:ASP:O[1_554] | 0.41 | 1.79 |
| 4:6:267:ILE:CG1 | 4:9:180:LEU:CG[1_554] | 0.41 | 1.79 |
| 4:4:305:MET:C | 4:7:11:ASP:OD1[1_554] | 0.41 | 1.79 |
| 4:6:283:MET:CB | 4:9:285:CYS:C[1_554] | 0.41 | 1.79 |
| 4:5:189:LEU:O | 4:8:186:THR:OG1[1_554] | 0.41 | 1.79 |
| 4:6:25:ASP:OD2 | 4:9:129:VAL:O[1_554] | 0.41 | 1.79 |
| 1:A:637:LYS:NZ | 4:5:311:ASP:CA[1_556] | 0.41 | 1.79 |
| 4:6:200:PHE:CA | 4:9:206:ARG:CG[1_554] | 0.42 | 1.78 |
| 4:5:267:ILE:CG1 | 4:8:180:LEU:CG[1_554] | 0.42 | 1.78 |
| 4:6:167:GLU:OE2 | 4:W:41:GLN:N[1_554] | 0.42 | 1.78 |
| 4:6:141:SER:O | 4:9:116:ARG:NH1[1_554] | 0.42 | 1.78 |
| 4:5:200:PHE:CA | 4:8:206:ARG:CG[1_554] | 0.42 | 1.78 |
| 4:4:357:ILE:CG2 | 4:8:232:SER:C[1_554] | 0.42 | 1.78 |
| 4:5:286:ASP:CB | 4:9:270:GLU:OE1[1_554] | 0.42 | 1.78 |
| 4:4:27:PRO:CG | 4:7:122:ILE:CD1[1_554] | 0.42 | 1.78 |
| 4:6:273:GLY:C | 4:9:162:ASN:CG[1_554] | 0.43 | 1.77 |
| 4:6:340:TRP:CD1 | 4:9:118:LYS:C[1_554] | 0.43 | 1.77 |
| 4:6:286:ASP:CB | 4:V:270:GLU:OE1[1_554] | 0.43 | 1.77 |
| 4:6:315:LYS:CD | 4:9:147:ARG:NH1[1_554] | 0.43 | 1.77 |
| 4:6:185:LEU:C | 4:9:157:ASP:O[1_554] | 0.43 | 1.77 |
| 4:6:223:PHE:CZ | 4:9:304:THR:OG1[1_554] | 0.44 | 1.76 |
| 4:5:222:ASP:N | 4:8:331:ALA:CA[1_554] | 0.44 | 1.76 |
| 4:6:369:ILE:CG2 | 4:V:232:SER:CA[1_554] | 0.44 | 1.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:340:TRP:CD1 | 4:8:118:LYS:C[1_554] | 0.44 | 1.76 |
| 4:5:113:LYS:CB | 4:9:252:ASN:C[1_554] | 0.44 | 1.76 |
| 4:6:299:MET:C | 4:9:136:ILE:CA[1_554] | 0.44 | 1.76 |
| 4:6:113:LYS:CB | 4:V:252:ASN:C[1_554] | 0.45 | 1.75 |
| 4:4:161:HIS:C | 4:7:110:LEU:CG[1_554] | 0.45 | 1.75 |
| 4:5:204:ALA:C | 4:8:62:ARG:CD[1_554] | 0.45 | 1.75 |
| 4:5:333:PRO:N | 4:8:104:LEU:CD2[1_554] | 0.45 | 1.75 |
| 4:4:255:PHE:CD1 | 4:7:305:MET:CG[1_554] | 0.45 | 1.75 |
| 4:4:286:ASP:CA | 4:8:270:GLU:CD[1_554] | 0.45 | 1.75 |
| 4:3:108:ALA:CB | 4:7:195:GLU:C[1_554] | 0.45 | 1.75 |
| 4:5:266:PHE:CG | 4:8:261:LEU:CG[1_554] | 0.46 | 1.74 |
| 4:5:262:PHE:CD1 | 4:8:153:LEU:CA[1_554] | 0.46 | 1.74 |
| 4:4:315:LYS:CE | 4:7:147:ARG:NE[1_554] | 0.46 | 1.74 |
| 4:6:24:ASP:OD2 | 4:9:125:GLU:CA[1_554] | 0.46 | 1.74 |
| 4:5:114:ALA:CB | 4:9:250:ILE:C[1_554] | 0.46 | 1.74 |
| 4:5:263:GLN:CA | 4:8:274:ILE:CG1[1_554] | 0.46 | 1.74 |
| 4:6:289:ILE:N | 4:W:63:GLY:C[1_554] | 0.46 | 1.74 |
| 4:4:15:GLY:CA | 4:7:77:THR:CG2[1_554] | 0.46 | 1.74 |
| 4:6:189:LEU:O | 4:9:186:THR:OG1[1_554] | 0.46 | 1.74 |
| 4:4:169:TYR:OH | 4:8:266:PHE:CE1[1_554] | 0.46 | 1.74 |
| 4:5:109:PRO:C | 4:9:195:GLU:CD[1_554] | 0.47 | 1.73 |
| 4:5:211:ASP:OD1 | 4:8:32:PRO:CD[1_554] | 0.47 | 1.73 |
| 4:3:284:LYS:O | 4:7:268:GLY:C[1_554] | 0.47 | 1.73 |
| 4:4:319:ALA:CB | 4:7:296:ASN:CB[1_554] | 0.47 | 1.73 |
| 4:5:337:TYR:CE1 | 4:8:86:TRP:CZ2[1_554] | 0.48 | 1.72 |
| 4:5:188:TYR:CE1 | 4:8:185:LEU:CG[1_554] | 0.48 | 1.72 |
| 4:5:223:PHE:CZ | 4:8:304:THR:OG1[1_554] | 0.48 | 1.72 |
| 4:5:326:LYS:CA | 4:8:167:GLU:OE2[1_554] | 0.48 | 1.72 |
| 4:6:279:TYR:O | 4:9:285:CYS:SG[1_554] | 0.48 | 1.72 |
| 4:4:369:ILE:O | 4:8:229:THR:C[1_554] | 0.48 | 1.72 |
| 4:4:137:GLN:O | 4:7:113:LYS:CA[1_554] | 0.48 | 1.72 |
| 4:5:283:MET:CB | 4:8:285:CYS:C[1_554] | 0.49 | 1.71 |
| 4:5:314:GLN:NE2 | 4:8:147:ARG:O[1_554] | 0.49 | 1.71 |
| 4:6:258:PRO:CA | 4:9:155:SER:O[1_554] | 0.49 | 1.71 |
| 4:5:28:ARG:CB | 4:8:126:THR:CG2[1_554] | 0.49 | 1.71 |
| 4:4:144:ALA:C | 4:7:370:VAL:C[1_554] | 0.49 | 1.71 |
| 4:4:262:PHE:CG | 4:7:153:LEU:C[1_554] | 0.50 | 1.70 |
| 4:6:24:ASP:CB | 4:9:124:PHE:C[1_554] | 0.50 | 1.70 |
| 4:6:205:GLU:OE2 | 4:7:288:ASP:OD2[1_554] | 0.50 | 1.70 |
| 4:6:162:ASN:ND2 | 4:9:175:ILE:CG1[1_554] | 0.50 | 1.70 |
| 4:6:312:ARG:NE | 4:9:299:MET:CB[1_554] | 0.50 | 1.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:284:LYS:O | 4:V:268:GLY:O[1_554] | 0.50 | 1.70 |
| 4:6:145:SER:N | 4:9:372:ARG:NH2[1_554] | 0.50 | 1.70 |
| 4:6:278:THR:CB | 4:9:164:PRO:N[1_554] | 0.50 | 1.70 |
| 4:5:151:ILE:CD1 | 4:8:171:LEU:CA[1_554] | 0.50 | 1.70 |
| 4:5:368:SER:O | 4:9:230:ALA:N[1_554] | 0.50 | 1.70 |
| 4:4:357:ILE:CG1 | 4:8:232:SER:N[1_554] | 0.51 | 1.69 |
| 4:5:315:LYS:CD | 4:8:147:ARG:NH1[1_554] | 0.51 | 1.69 |
| 4:3:287:ILE:O | 4:8:63:GLY:CA[1_554] | 0.51 | 1.69 |
| 4:4:200:PHE:N | 4:7:206:ARG:CG[1_554] | 0.51 | 1.69 |
| 4:5:23:GLY:N | 4:8:362:TYR:CE2[1_554] | 0.51 | 1.69 |
| 4:4:109:PRO:CA | 4:8:195:GLU:CD[1_554] | 0.51 | 1.69 |
| 4:6:339:VAL:CG1 | 4:9:116:ARG:N[1_554] | 0.51 | 1.69 |
| 4:5:270:GLU:O | 4:8:272:ALA:CB[1_554] | 0.51 | 1.69 |
| 4:4:24:ASP:N | 4:7:125:GLU:OE2[1_554] | 0.52 | 1.68 |
| 4:4:340:TRP:CH2 | 4:7:121:GLN:CG[1_554] | 0.52 | 1.68 |
| 4:5:173:HIS:CE1 | 4:9:265:SER:C[1_554] | 0.52 | 1.68 |
| 4:5:343:GLY:O | 4:8:367:PRO:CA[1_554] | 0.52 | 1.68 |
| 4:6:255:PHE:CG | 4:9:305:MET:CB[1_554] | 0.52 | 1.68 |
| 4:5:255:PHE:CD1 | 4:8:305:MET:CA[1_554] | 0.52 | 1.68 |
| 4:3:357:ILE:CG1 | 4:7:232:SER:N[1_554] | 0.52 | 1.68 |
| 4:5:15:GLY:N | 4:8:77:THR:OG1[1_554] | 0.53 | 1.67 |
| 4:6:272:ALA:C | 4:9:277:THR:CG2[1_554] | 0.53 | 1.67 |
| 4:6:257:CYS:CA | 4:9:303:THR:OG1[1_554] | 0.53 | 1.67 |
| 4:6:204:ALA:C | 4:9:62:ARG:CD[1_554] | 0.53 | 1.67 |
| 4:6:162:ASN:OD1 | 4:9:175:ILE:CB[1_554] | 0.53 | 1.67 |
| 4:5:310:ALA:C | 4:8:141:SER:C[1_554] | 0.53 | 1.67 |
| 4:4:338:SER:C | 4:7:116:ARG:C[1_554] | 0.53 | 1.67 |
| 4:5:262:PHE:CB | 4:8:153:LEU:CG[1_554] | 0.53 | 1.67 |
| 4:5:325:MET:SD | 4:8:166:TYR:OH[1_554] | 0.53 | 1.67 |
| 4:5:277:THR:N | 4:8:281:SER:OG[1_554] | 0.53 | 1.67 |
| 4:5:255:PHE:CE1 | 4:8:305:MET:C[1_554] | 0.53 | 1.67 |
| 4:4:77:THR:O | 4:8:246:GLN:NE2[1_554] | 0.54 | 1.66 |
| 4:4:283:MET:CG | 4:7:286:ASP:N[1_554] | 0.54 | 1.66 |
| 4:4:273:GLY:CA | 4:7:162:ASN:OD1[1_554] | 0.54 | 1.66 |
| 4:2:291:LYS:CG | 4:7:40:HIS:N[1_554] | 0.54 | 1.66 |
| 4:6:255:PHE:CE1 | 4:9:305:MET:O[1_554] | 0.54 | 1.66 |
| 4:5:157:ASP:OD2 | 4:8:72:GLU:CB[1_554] | 0.54 | 1.66 |
| 4:5:272:ALA:C | 4:8:277:THR:CG2[1_554] | 0.55 | 1.65 |
| 4:4:256:ARG:O | 4:7:303:THR:CB[1_554] | 0.55 | 1.65 |
| 4:4:204:ALA:CB | 4:7:62:ARG:C[1_554] | 0.55 | 1.65 |
| 4:6:109:PRO:C | 4:V:195:GLU:CD[1_554] | 0.55 | 1.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:137:GLN:CB | 4:8:112:PRO:C[1_554] | 0.55 | 1.65 |
| 4:5:221:LEU:C | 4:8:331:ALA:C[1_554] | 0.55 | 1.65 |
| 4:6:270:GLU:CA | 4:9:272:ALA:CA[1_554] | 0.55 | 1.65 |
| 4:3:286:ASP:N | 4:7:270:GLU:OE2[1_554] | 0.55 | 1.65 |
| 4:5:276:GLU:CG | 4:8:278:THR:O[1_554] | 0.55 | 1.65 |
| 4:5:167:GLU:OE2 | 4:V:41:GLN:N[1_554] | 0.55 | 1.65 |
| 4:6:210:ARG:CZ | 4:9:33:SER:O[1_554] | 0.56 | 1.64 |
| 4:5:193:LEU:CG | 4:8:210:ARG:CB[1_554] | 0.56 | 1.64 |
| 4:5:24:ASP:OD2 | 4:8:125:GLU:CA[1_554] | 0.56 | 1.64 |
| 4:4:108:ALA:CB | 4:8:195:GLU:C[1_554] | 0.56 | 1.64 |
| 4:6:368:SER:O | 4:V:230:ALA:N[1_554] | 0.56 | 1.64 |
| 4:3:357:ILE:CG2 | 4:7:232:SER:C[1_554] | 0.56 | 1.64 |
| 4:3:286:ASP:CA | 4:7:270:GLU:CD[1_554] | 0.56 | 1.64 |
| 4:5:18:LYS:N | 4:8:79:TRP:CD2[1_554] | 0.56 | 1.64 |
| 4:3:77:THR:CG2 | 4:7:246:GLN:OE1[1_554] | 0.56 | 1.64 |
| 4:6:210:ARG:NH2 | 4:9:33:SER:C[1_554] | 0.56 | 1.64 |
| 4:4:345:ILE:N | 4:7:367:PRO:CD[1_554] | 0.56 | 1.64 |
| 4:5:273:GLY:C | 4:8:162:ASN:CG[1_554] | 0.56 | 1.64 |
| 4:4:185:LEU:CB | 4:7:158:GLY:N[1_554] | 0.57 | 1.63 |
| 4:6:338:SER:CB | 4:9:134:VAL:CG1[1_554] | 0.57 | 1.63 |
| 4:6:211:ASP:CB | 4:9:32:PRO:CB[1_554] | 0.57 | 1.63 |
| 4:6:173:HIS:CE1 | 4:V:265:SER:C[1_554] | 0.57 | 1.63 |
| 4:6:28:ARG:CB | 4:9:126:THR:CG2[1_554] | 0.57 | 1.63 |
| 4:5:367:PRO:N | 4:9:234:SER:N[1_554] | 0.57 | 1.63 |
| 4:6:198:TYR:CD1 | 4:9:208:ILE:CB[1_554] | 0.57 | 1.63 |
| 4:4:337:TYR:CB | 4:7:119:MET:CA[1_554] | 0.57 | 1.63 |
| 4:6:310:ALA:C | 4:9:141:SER:C[1_554] | 0.57 | 1.63 |
| 4:6:222:ASP:N | 4:9:331:ALA:CA[1_554] | 0.57 | 1.63 |
| 4:5:219:VAL:CG1 | 4:8:300:SER:CA[1_554] | 0.57 | 1.63 |
| 4:5:172:PRO:C | 4:9:266:PHE:O[1_554] | 0.57 | 1.63 |
| 4:4:314:GLN:C | 4:7:142:LEU:CG[1_554] | 0.57 | 1.63 |
| 4:6:255:PHE:CD1 | 4:9:305:MET:CA[1_554] | 0.57 | 1.63 |
| 4:5:227:MET:CB | 4:8:307:PRO:CA[1_554] | 0.57 | 1.63 |
| 4:6:326:LYS:CA | 4:9:167:GLU:OE2[1_554] | 0.58 | 1.62 |
| 4:4:270:GLU:CB | 4:7:272:ALA:CA[1_554] | 0.58 | 1.62 |
| 4:4:115:ASN:C | 4:8:196:ARG:NH2[1_554] | 0.58 | 1.62 |
| 4:5:371:HIS:CB | 4:9:230:ALA:CB[1_554] | 0.58 | 1.62 |
| 4:6:312:ARG:O | 4:9:298:VAL:CB[1_554] | 0.58 | 1.62 |
| 4:6:334:GLU:C | 4:9:105:LEU:CA[1_554] | 0.58 | 1.62 |
| 1:A:637:LYS:CD | 4:5:311:ASP:OD1[1_556] | 0.58 | 1.62 |
| 4:5:305:MET:CB | 4:8:11:ASP:OD1[1_554] | 0.58 | 1.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:227:MET:CB | 4:9:307:PRO:CA[1_554] | 0.59 | 1.61 |
| 4:4:162:ASN:N | 4:7:110:LEU:CD2[1_554] | 0.59 | 1.61 |
| 4:6:276:GLU:CG | 4:9:278:THR:O[1_554] | 0.59 | 1.61 |
| 4:5:198:TYR:CD1 | 4:8:208:ILE:CB[1_554] | 0.59 | 1.61 |
| 4:6:255:PHE:CB | 4:9:305:MET:CG[1_554] | 0.59 | 1.61 |
| 4:5:312:ARG:NE | 4:8:299:MET:CB[1_554] | 0.59 | 1.61 |
| 4:6:295:ALA:CA | 4:9:167:GLU:C[1_554] | 0.59 | 1.61 |
| 4:5:335:ARG:CG | 4:8:106:THR:CB[1_554] | 0.59 | 1.61 |
| 4:5:114:ALA:CA | 4:9:251:GLY:N[1_554] | 0.59 | 1.61 |
| 4:5:299:MET:C | 4:8:136:ILE:CA[1_554] | 0.59 | 1.61 |
| 4:5:339:VAL:CG1 | 4:8:116:ARG:N[1_554] | 0.60 | 1.60 |
| 4:6:337:TYR:CZ | 4:9:86:TRP:CE2[1_554] | 0.60 | 1.60 |
| 4:4:211:ASP:C | 4:7:32:PRO:CA[1_554] | 0.60 | 1.60 |
| 4:6:172:PRO:C | 4:V:266:PHE:O[1_554] | 0.60 | 1.60 |
| 4:5:157:ASP:CG | 4:8:72:GLU:CA[1_554] | 0.60 | 1.60 |
| 4:3:117:GLU:CB | 4:7:237:GLU:CA[1_554] | 0.60 | 1.60 |
| 4:6:173:HIS:CA | 4:V:267:ILE:CA[1_554] | 0.60 | 1.60 |
| 4:6:23:GLY:N | 4:9:362:TYR:CE2[1_554] | 0.60 | 1.60 |
| 4:6:219:VAL:CG1 | 4:9:300:SER:CA[1_554] | 0.60 | 1.60 |
| 4:6:18:LYS:N | 4:9:79:TRP:CD2[1_554] | 0.60 | 1.60 |
| 4:5:313:MET:CB | 4:8:152:VAL:CG2[1_554] | 0.61 | 1.59 |
| 4:6:114:ALA:CB | 4:V:250:ILE:C[1_554] | 0.61 | 1.59 |
| 4:5:289:ILE:N | 4:V:63:GLY:C[1_554] | 0.61 | 1.59 |
| 4:6:270:GLU:O | 4:9:272:ALA:CB[1_554] | 0.61 | 1.59 |
| 4:6:263:GLN:CA | 4:9:274:ILE:CG1[1_554] | 0.61 | 1.59 |
| 4:6:305:MET:CB | 4:9:11:ASP:OD1[1_554] | 0.61 | 1.59 |
| 4:6:313:MET:CB | 4:9:152:VAL:CG2[1_554] | 0.61 | 1.59 |
| 4:6:278:THR:CA | 4:9:164:PRO:CD[1_554] | 0.62 | 1.58 |
| 4:4:30:VAL:CB | 4:7:79:TRP:O[1_554] | 0.62 | 1.58 |
| 4:6:314:GLN:NE2 | 4:9:147:ARG:O[1_554] | 0.62 | 1.58 |
| 4:4:286:ASP:N | 4:8:270:GLU:OE2[1_554] | 0.62 | 1.58 |
| 4:5:279:TYR:O | 4:8:285:CYS:SG[1_554] | 0.62 | 1.58 |
| 4:6:308:GLY:N | 4:9:338:SER:CA[1_554] | 0.62 | 1.58 |
| 4:6:262:PHE:CD1 | 4:9:153:LEU:CA[1_554] | 0.62 | 1.58 |
| 4:4:75:ILE:CD1 | 4:8:193:LEU:O[1_554] | 0.62 | 1.58 |
| 4:6:340:TRP:NE1 | 4:9:118:LYS:O[1_554] | 0.62 | 1.58 |
| 4:4:367:PRO:O | 4:8:236:LEU:CD2[1_554] | 0.63 | 1.57 |
| 4:6:334:GLU:CA | 4:9:105:LEU:N[1_554] | 0.63 | 1.57 |
| 4:6:371:HIS:CB | 4:V:230:ALA:CB[1_554] | 0.63 | 1.57 |
| 4:3:75:ILE:CD1 | 4:7:193:LEU:O[1_554] | 0.63 | 1.57 |
| 4:5:270:GLU:CA | 4:8:272:ALA:CA[1_554] | 0.63 | 1.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:337:TYR:CZ | 4:8:86:TRP:CE2[1_554] | 0.63 | 1.57 |
| 4:6:333:PRO:N | 4:9:104:LEU:CD2[1_554] | 0.63 | 1.57 |
| 4:6:211:ASP:OD1 | 4:9:32:PRO:CD[1_554] | 0.63 | 1.57 |
| 4:4:154:ASP:OD2 | 4:7:111:ASN:C[1_554] | 0.63 | 1.57 |
| 4:4:284:LYS:O | 4:8:268:GLY:C[1_554] | 0.63 | 1.57 |
| 4:5:24:ASP:CB | 4:8:124:PHE:C[1_554] | 0.63 | 1.57 |
| 4:6:266:PHE:CG | 4:9:261:LEU:CG[1_554] | 0.63 | 1.57 |
| 4:5:311:ASP:N | 4:8:141:SER:O[1_554] | 0.63 | 1.57 |
| 4:5:199:SER:CA | 4:8:206:ARG:CA[1_554] | 0.63 | 1.57 |
| 4:4:340:TRP:CZ3 | 4:7:121:GLN:CB[1_554] | 0.63 | 1.57 |
| 4:5:278:THR:CB | 4:8:164:PRO:N[1_554] | 0.63 | 1.57 |
| 4:4:144:ALA:CA | 4:7:371:HIS:N[1_554] | 0.64 | 1.56 |
| 4:4:275:HIS:N | 4:7:163:VAL:N[1_554] | 0.64 | 1.56 |
| 4:4:109:PRO:N | 4:8:195:GLU:CG[1_554] | 0.64 | 1.56 |
| 4:5:332:PRO:CD | 4:8:135:ALA:CB[1_554] | 0.64 | 1.56 |
| 4:5:289:ILE:N | 4:V:63:GLY:O[1_554] | 0.64 | 1.56 |
| 4:6:277:THR:N | 4:9:281:SER:OG[1_554] | 0.64 | 1.56 |
| 4:6:322:PRO:CA | 4:9:291:LYS:NZ[1_554] | 0.64 | 1.56 |
| 4:3:369:ILE:O | 4:7:229:THR:C[1_554] | 0.64 | 1.56 |
| 4:5:295:ALA:CA | 4:8:167:GLU:C[1_554] | 0.64 | 1.56 |
| 4:6:161:HIS:CB | 4:9:110:LEU:CB[1_554] | 0.64 | 1.56 |
| 4:6:177:ARG:NH1 | 4:V:194:THR:OG1[1_554] | 0.64 | 1.56 |
| 4:5:210:ARG:NH2 | 4:8:33:SER:C[1_554] | 0.64 | 1.56 |
| 4:5:115:ASN:CA | 4:9:196:ARG:CZ[1_554] | 0.64 | 1.56 |
| 4:6:334:GLU:O | 4:9:105:LEU:CB[1_554] | 0.64 | 1.56 |
| 4:3:372:ARG:CG | 4:7:227:MET:CA[1_554] | 0.65 | 1.55 |
| 4:4:311:ASP:C | 4:7:141:SER:C[1_554] | 0.65 | 1.55 |
| 4:6:195:GLU:CB | 4:9:189:LEU:CG[1_554] | 0.65 | 1.55 |
| 4:6:218:TYR:CG | 4:9:336:LYS:CG[1_554] | 0.65 | 1.55 |
| 4:4:273:GLY:O | 4:7:162:ASN:CB[1_554] | 0.65 | 1.55 |
| 4:6:214:GLU:CA | 4:9:16:LEU:CB[1_554] | 0.65 | 1.55 |
| 4:4:154:ASP:CB | 4:7:111:ASN:N[1_554] | 0.65 | 1.55 |
| 4:4:194:THR:O | 4:7:209:VAL:CB[1_554] | 0.65 | 1.55 |
| 4:5:145:SER:N | 4:8:372:ARG:NH2[1_554] | 0.66 | 1.54 |
| 4:5:308:GLY:CA | 4:8:338:SER:CB[1_554] | 0.66 | 1.54 |
| 4:4:207:GLU:CD | 4:7:67:LEU:CA[1_554] | 0.66 | 1.54 |
| 4:6:311:ASP:N | 4:9:141:SER:O[1_554] | 0.66 | 1.54 |
| 4:6:309:ILE:C | 4:9:141:SER:CB[1_554] | 0.66 | 1.54 |
| 4:4:312:ARG:NE | 4:7:299:MET:C[1_554] | 0.66 | 1.54 |
| 4:6:335:ARG:CG | 4:9:106:THR:CB[1_554] | 0.66 | 1.54 |
| 4:4:227:MET:CE | 4:7:306:TYR:N[1_554] | 0.66 | 1.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:214:GLU:C | 4:7:17:VAL:N[1_554] | 0.66 | 1.54 |
| 4:6:341:ILE:CG1 | 4:9:132:MET:CE[1_554] | 0.66 | 1.54 |
| 4:6:15:GLY:N | 4:9:77:THR:OG1[1_554] | 0.66 | 1.54 |
| 4:5:177:ARG:NH1 | 4:9:194:THR:OG1[1_554] | 0.66 | 1.54 |
| 4:4:318:THR:CA | 4:7:149:THR:C[1_554] | 0.66 | 1.54 |
| 4:3:116:ARG:C | 4:7:237:GLU:OE2[1_554] | 0.66 | 1.54 |
| 4:6:367:PRO:O | 4:V:230:ALA:O[1_554] | 0.66 | 1.54 |
| 4:4:304:THR:CA | 4:7:137:GLN:NE2[1_554] | 0.66 | 1.54 |
| 4:5:337:TYR:CA | 4:8:119:MET:CE[1_554] | 0.67 | 1.53 |
| 4:4:284:LYS:O | 4:8:268:GLY:O[1_554] | 0.67 | 1.53 |
| 4:4:196:ARG:N | 4:7:209:VAL:O[1_554] | 0.67 | 1.53 |
| 4:6:205:GLU:N | 4:9:62:ARG:NE[1_554] | 0.67 | 1.53 |
| 4:4:188:TYR:CD2 | 4:7:182:GLY:N[1_554] | 0.67 | 1.53 |
| 4:3:114:ALA:CA | 4:7:250:ILE:O[1_554] | 0.67 | 1.53 |
| 4:4:223:PHE:O | 4:7:335:ARG:NH2[1_554] | 0.67 | 1.53 |
| 4:6:115:ASN:CA | 4:V:196:ARG:CZ[1_554] | 0.67 | 1.53 |
| 4:4:214:GLU:CG | 4:7:33:SER:OG[1_554] | 0.67 | 1.53 |
| 4:4:30:VAL:CB | 4:7:79:TRP:C[1_554] | 0.67 | 1.53 |
| 4:3:109:PRO:CA | 4:7:195:GLU:CD[1_554] | 0.67 | 1.53 |
| 4:4:110:LEU:CA | 4:8:192:ILE:CA[1_554] | 0.67 | 1.53 |
| 4:4:111:ASN:N | 4:8:192:ILE:O[1_554] | 0.67 | 1.53 |
| 4:4:280:ASN:ND2 | 4:7:281:SER:O[1_554] | 0.68 | 1.52 |
| 4:4:332:PRO:CB | 4:7:134:VAL:N[1_554] | 0.68 | 1.52 |
| 4:6:157:ASP:CG | 4:9:72:GLU:CA[1_554] | 0.68 | 1.52 |
| 4:5:274:ILE:CA | 4:8:162:ASN:N[1_554] | 0.68 | 1.52 |
| 4:5:218:TYR:CG | 4:8:336:LYS:CG[1_554] | 0.68 | 1.52 |
| 4:4:262:PHE:O | 4:7:153:LEU:CD1[1_554] | 0.68 | 1.52 |
| 4:6:367:PRO:N | 4:V:234:SER:N[1_554] | 0.68 | 1.52 |
| 4:5:263:GLN:C | 4:8:274:ILE:CD1[1_554] | 0.68 | 1.52 |
| 4:5:338:SER:CB | 4:8:134:VAL:CG1[1_554] | 0.68 | 1.52 |
| 4:4:317:ILE:C | 4:7:150:GLY:N[1_554] | 0.68 | 1.52 |
| 4:5:334:GLU:CA | 4:8:105:LEU:N[1_554] | 0.68 | 1.52 |
| 4:5:300:SER:CB | 4:8:107:GLU:CG[1_554] | 0.68 | 1.52 |
| 4:4:211:ASP:O | 4:7:32:PRO:CA[1_554] | 0.68 | 1.52 |
| 4:5:309:ILE:C | 4:8:141:SER:CB[1_554] | 0.68 | 1.52 |
| 4:6:367:PRO:CA | 4:V:233:SER:CA[1_554] | 0.69 | 1.51 |
| 4:4:213:LYS:CB | 4:7:15:GLY:CA[1_554] | 0.69 | 1.51 |
| 4:4:332:PRO:CD | 4:7:134:VAL:C[1_554] | 0.69 | 1.51 |
| 4:6:297:ASN:N | 4:9:168:GLY:O[1_554] | 0.69 | 1.51 |
| 4:4:270:GLU:CA | 4:7:272:ALA:C[1_554] | 0.69 | 1.51 |
| 4:4:259:GLU:CG | 4:7:304:THR:CB[1_554] | 0.69 | 1.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:276:GLU:CD | 4:9:278:THR:C[1_554] | 0.69 | 1.51 |
| 4:4:186:THR:CB | 4:7:183:ARG:CZ[1_554] | 0.69 | 1.51 |
| 4:5:159:VAL:C | 4:8:177:ARG:NH1[1_554] | 0.69 | 1.51 |
| 4:6:137:GLN:CB | 4:9:112:PRO:C[1_554] | 0.69 | 1.51 |
| 4:6:141:SER:CA | 4:9:116:ARG:NE[1_554] | 0.69 | 1.51 |
| 4:6:327:ILE:O | 4:9:148:THR:CB[1_554] | 0.69 | 1.51 |
| 4:4:154:ASP:CG | 4:7:111:ASN:CA[1_554] | 0.69 | 1.51 |
| 4:5:322:PRO:CA | 4:8:291:LYS:NZ[1_554] | 0.69 | 1.51 |
| 4:6:332:PRO:CD | 4:9:135:ALA:CB[1_554] | 0.69 | 1.51 |
| 4:5:291:LYS:NZ | 4:V:64:ILE:CG1[1_554] | 0.69 | 1.51 |
| 4:5:20:GLY:C | 4:8:121:GLN:NE2[1_554] | 0.69 | 1.51 |
| 4:6:341:ILE:N | 4:9:120:THR:OG1[1_554] | 0.69 | 1.51 |
| 4:5:173:HIS:CA | 4:9:267:ILE:CA[1_554] | 0.70 | 1.50 |
| 4:4:220:ALA:CB | 4:7:335:ARG:CA[1_554] | 0.70 | 1.50 |
| 4:5:327:ILE:O | 4:8:148:THR:CB[1_554] | 0.70 | 1.50 |
| 4:6:346:LEU:O | 4:9:365:ALA:O[1_554] | 0.70 | 1.50 |
| 4:4:300:SER:CB | 4:7:107:GLU:OE1[1_554] | 0.70 | 1.50 |
| 4:5:341:ILE:N | 4:8:120:THR:OG1[1_554] | 0.70 | 1.50 |
| 4:6:261:LEU:CB | 4:9:154:ASP:O[1_554] | 0.70 | 1.50 |
| 4:2:287:ILE:O | 4:7:39:ARG:NH1[1_554] | 0.70 | 1.50 |
| 4:6:14:SER:C | 4:9:77:THR:OG1[1_554] | 0.70 | 1.50 |
| 4:5:334:GLU:C | 4:8:105:LEU:CA[1_554] | 0.70 | 1.50 |
| 4:6:199:SER:CA | 4:9:206:ARG:CA[1_554] | 0.71 | 1.49 |
| 4:6:157:ASP:OD2 | 4:9:72:GLU:CB[1_554] | 0.71 | 1.49 |
| 4:6:262:PHE:CB | 4:9:153:LEU:CG[1_554] | 0.71 | 1.49 |
| 4:5:162:ASN:OD1 | 4:8:175:ILE:CB[1_554] | 0.71 | 1.49 |
| 4:5:143:TYR:CB | 4:8:372:ARG:N[1_554] | 0.71 | 1.49 |
| 4:5:334:GLU:O | 4:8:105:LEU:CB[1_554] | 0.71 | 1.49 |
| 4:5:346:LEU:O | 4:8:365:ALA:O[1_554] | 0.71 | 1.49 |
| 4:4:222:ASP:N | 4:7:332:PRO:CD[1_554] | 0.71 | 1.49 |
| 4:4:187:ASP:N | 4:7:183:ARG:CD[1_554] | 0.71 | 1.49 |
| 4:4:370:VAL:C | 4:8:230:ALA:CA[1_554] | 0.71 | 1.49 |
| 4:5:218:TYR:OH | 4:8:337:TYR:CE2[1_554] | 0.71 | 1.49 |
| 4:3:77:THR:O | 4:7:246:GLN:NE2[1_554] | 0.71 | 1.49 |
| 4:6:198:TYR:CE1 | 4:9:208:ILE:CG1[1_554] | 0.71 | 1.49 |
| 4:4:18:LYS:CG | 4:7:79:TRP:CD2[1_554] | 0.71 | 1.49 |
| 4:5:221:LEU:CG | 4:8:332:PRO:CG[1_554] | 0.71 | 1.49 |
| 4:5:255:PHE:CE1 | 4:8:305:MET:O[1_554] | 0.71 | 1.49 |
| 4:4:77:THR:CG2 | 4:8:246:GLN:OE1[1_554] | 0.72 | 1.48 |
| 4:6:255:PHE:CE1 | 4:9:305:MET:C[1_554] | 0.72 | 1.48 |
| 4:5:261:LEU:CB | 4:8:154:ASP:O[1_554] | 0.72 | 1.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:151:ILE:CB | 4:9:170:ALA:O[1_554] | 0.72 | 1.48 |
| 4:6:304:THR:OG1 | 4:9:137:GLN:CG[1_554] | 0.72 | 1.48 |
| 4:5:106:THR:CB | 4:8:114:ALA:CB[1_554] | 0.72 | 1.48 |
| 4:5:161:HIS:CB | 4:8:110:LEU:CB[1_554] | 0.72 | 1.48 |
| 4:4:222:ASP:CA | 4:7:332:PRO:N[1_554] | 0.72 | 1.48 |
| 4:5:294:TYR:C | 4:8:166:TYR:C[1_554] | 0.72 | 1.48 |
| 4:4:331:ALA:CA | 4:7:135:ALA:CA[1_554] | 0.72 | 1.48 |
| 4:3:177:ARG:NH1 | 4:7:194:THR:CG2[1_554] | 0.72 | 1.48 |
| 4:5:255:PHE:CB | 4:8:305:MET:CG[1_554] | 0.72 | 1.48 |
| 4:3:370:VAL:C | 4:7:230:ALA:CA[1_554] | 0.72 | 1.48 |
| 4:5:278:THR:CA | 4:8:164:PRO:CD[1_554] | 0.72 | 1.48 |
| 4:6:159:VAL:CA | 4:9:177:ARG:NH1[1_554] | 0.72 | 1.48 |
| 4:5:308:GLY:N | 4:8:338:SER:CA[1_554] | 0.73 | 1.47 |
| 4:5:372:ARG:C | 4:9:227:MET:CA[1_554] | 0.73 | 1.47 |
| 4:6:372:ARG:C | 4:V:227:MET:CB[1_554] | 0.73 | 1.47 |
| 4:6:114:ALA:CA | 4:V:251:GLY:N[1_554] | 0.73 | 1.47 |
| 4:6:198:TYR:CG | 4:9:208:ILE:CA[1_554] | 0.73 | 1.47 |
| 4:6:337:TYR:CA | 4:9:119:MET:CE[1_554] | 0.73 | 1.47 |
| 4:5:151:ILE:CB | 4:8:170:ALA:O[1_554] | 0.73 | 1.47 |
| 4:6:314:GLN:NE2 | 4:9:147:ARG:C[1_554] | 0.73 | 1.47 |
| 4:5:205:GLU:CA | 4:8:62:ARG:NE[1_554] | 0.73 | 1.47 |
| 4:4:198:TYR:CB | 4:7:207:GLU:C[1_554] | 0.73 | 1.47 |
| 4:4:116:ARG:C | 4:8:237:GLU:OE2[1_554] | 0.73 | 1.47 |
| 4:4:166:TYR:CD1 | 4:9:40:HIS:NE2[1_554] | 0.73 | 1.47 |
| 4:6:319:ALA:CB | 4:9:295:ALA:C[1_554] | 0.73 | 1.47 |
| 4:3:110:LEU:CA | 4:7:192:ILE:CA[1_554] | 0.73 | 1.47 |
| 4:5:262:PHE:CE2 | 4:8:153:LEU:O[1_554] | 0.73 | 1.47 |
| 4:3:115:ASN:C | 4:7:196:ARG:NH2[1_554] | 0.73 | 1.47 |
| 4:4:144:ALA:O | 4:7:370:VAL:CA[1_554] | 0.73 | 1.47 |
| 4:4:293:LEU:O | 4:7:169:TYR:CG[1_554] | 0.73 | 1.47 |
| 4:5:195:GLU:CB | 4:8:189:LEU:CG[1_554] | 0.74 | 1.46 |
| 4:6:367:PRO:N | 4:V:233:SER:C[1_554] | 0.74 | 1.46 |
| 4:4:30:VAL:O | 4:7:80:ASP:CA[1_554] | 0.74 | 1.46 |
| 4:4:212:ILE:O | 4:7:16:LEU:CD1[1_554] | 0.74 | 1.46 |
| 4:5:166:TYR:CG | 4:V:40:HIS:CE1[1_554] | 0.74 | 1.46 |
| 4:4:154:ASP:OD1 | 4:7:111:ASN:CA[1_554] | 0.74 | 1.46 |
| 4:6:193:LEU:CG | 4:9:210:ARG:CB[1_554] | 0.74 | 1.46 |
| 4:4:207:GLU:CB | 4:7:67:LEU:CB[1_554] | 0.74 | 1.46 |
| 4:6:254:ARG:CZ | 4:9:336:LYS:NZ[1_554] | 0.74 | 1.46 |
| 4:5:327:ILE:CG1 | 4:8:149:THR:CB[1_554] | 0.74 | 1.46 |
| 4:6:307:PRO:C | 4:9:338:SER:N[1_554] | 0.74 | 1.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:188:TYR:N | 4:8:184:ASP:N[1_554] | 0.74 | 1.46 |
| 4:6:294:TYR:C | 4:9:166:TYR:C[1_554] | 0.74 | 1.46 |
| 4:4:193:LEU:CA | 4:7:210:ARG:CB[1_554] | 0.75 | 1.45 |
| 4:5:30:VAL:CG1 | 4:8:82:MET:CB[1_554] | 0.75 | 1.45 |
| 4:6:274:ILE:O | 4:9:162:ASN:C[1_554] | 0.75 | 1.45 |
| 4:5:24:ASP:CG | 4:8:125:GLU:CA[1_554] | 0.75 | 1.45 |
| 4:6:142:LEU:O | 4:9:372:ARG:NE[1_554] | 0.75 | 1.45 |
| 4:4:177:ARG:NH1 | 4:8:194:THR:CG2[1_554] | 0.75 | 1.45 |
| 4:6:150:GLY:O | 4:9:169:TYR:CE1[1_554] | 0.75 | 1.45 |
| 4:2:292:ASP:N | 4:7:40:HIS:CD2[1_554] | 0.75 | 1.45 |
| 4:3:111:ASN:CG | 4:7:196:ARG:CG[1_554] | 0.75 | 1.45 |
| 4:4:145:SER:OG | 4:7:372:ARG:NE[1_554] | 0.75 | 1.45 |
| 4:5:312:ARG:O | 4:8:298:VAL:CB[1_554] | 0.75 | 1.45 |
| 4:3:75:ILE:CG2 | 4:7:198:TYR:CD2[1_554] | 0.75 | 1.45 |
| 4:4:16:LEU:CA | 4:7:77:THR:O[1_554] | 0.75 | 1.45 |
| 4:5:274:ILE:O | 4:8:162:ASN:C[1_554] | 0.75 | 1.45 |
| 4:5:198:TYR:CE1 | 4:8:208:ILE:CG1[1_554] | 0.75 | 1.45 |
| 4:5:137:GLN:CA | 4:8:113:LYS:N[1_554] | 0.75 | 1.45 |
| 4:5:282:ILE:CD1 | 4:8:171:LEU:CD1[1_554] | 0.75 | 1.45 |
| 4:4:196:ARG:CG | 4:7:211:ASP:CA[1_554] | 0.76 | 1.44 |
| 4:5:218:TYR:CB | 4:8:336:LYS:CB[1_554] | 0.76 | 1.44 |
| 4:6:221:LEU:CG | 4:9:332:PRO:CG[1_554] | 0.76 | 1.44 |
| 4:4:311:ASP:C | 4:7:141:SER:O[1_554] | 0.76 | 1.44 |
| 4:5:340:TRP:NE1 | 4:8:118:LYS:O[1_554] | 0.76 | 1.44 |
| 4:5:110:LEU:CD1 | 4:9:191:LYS:CG[1_554] | 0.76 | 1.44 |
| 4:5:310:ALA:N | 4:8:141:SER:CB[1_554] | 0.76 | 1.44 |
| 4:4:24:ASP:CA | 4:7:125:GLU:CG[1_554] | 0.76 | 1.44 |
| 4:4:223:PHE:O | 4:7:335:ARG:CZ[1_554] | 0.76 | 1.44 |
| 4:5:288:ASP:O | 4:V:64:ILE:N[1_554] | 0.76 | 1.44 |
| 4:4:291:LYS:CD | 4:9:64:ILE:CG1[1_554] | 0.76 | 1.44 |
| 4:5:367:PRO:CA | 4:9:233:SER:CA[1_554] | 0.76 | 1.44 |
| 4:6:30:VAL:CG1 | 4:9:82:MET:CB[1_554] | 0.76 | 1.44 |
| 4:3:111:ASN:N | 4:7:192:ILE:O[1_554] | 0.76 | 1.44 |
| 4:4:329:ILE:CB | 4:7:139:VAL:CG1[1_554] | 0.76 | 1.44 |
| 4:4:117:GLU:CB | 4:8:237:GLU:CA[1_554] | 0.76 | 1.44 |
| 4:4:341:ILE:N | 4:7:117:GLU:O[1_554] | 0.76 | 1.44 |
| 4:6:266:PHE:CD2 | 4:9:261:LEU:CD1[1_554] | 0.76 | 1.44 |
| 4:6:274:ILE:CA | 4:9:162:ASN:CA[1_554] | 0.76 | 1.44 |
| 1:D:637:LYS:CD | 4:6:311:ASP:OD1[1_556] | 0.76 | 1.44 |
| 4:5:314:GLN:NE2 | 4:8:147:ARG:C[1_554] | 0.77 | 1.43 |
| 4:5:141:SER:CA | 4:8:116:ARG:NE[1_554] | 0.77 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:349:LEU:CA | 4:8:365:ALA:CA[1_554] | 0.77 | 1.43 |
| 4:5:334:GLU:OE1 | 4:8:133:TYR:O[1_554] | 0.77 | 1.43 |
| 4:6:327:ILE:CG1 | 4:9:149:THR:CB[1_554] | 0.77 | 1.43 |
| 4:6:301:GLY:N | 4:9:107:GLU:CA[1_554] | 0.77 | 1.43 |
| 4:6:310:ALA:N | 4:9:141:SER:CA[1_554] | 0.77 | 1.43 |
| 4:6:349:LEU:CA | 4:9:365:ALA:CA[1_554] | 0.77 | 1.43 |
| 4:4:341:ILE:CG2 | 4:7:120:THR:CG2[1_554] | 0.77 | 1.43 |
| 4:6:106:THR:CB | 4:9:114:ALA:CA[1_554] | 0.77 | 1.43 |
| 4:5:24:ASP:CB | 4:8:125:GLU:N[1_554] | 0.77 | 1.43 |
| 4:5:367:PRO:N | 4:9:233:SER:C[1_554] | 0.77 | 1.43 |
| 4:6:276:GLU:OE2 | 4:9:279:TYR:N[1_554] | 0.77 | 1.43 |
| 4:6:368:SER:C | 4:V:229:THR:C[1_554] | 0.77 | 1.43 |
| 4:4:25:ASP:O | 4:7:120:THR:O[1_554] | 0.77 | 1.43 |
| 4:4:316:GLU:O | 4:7:151:ILE:N[1_554] | 0.77 | 1.43 |
| 4:5:368:SER:C | 4:9:229:THR:C[1_554] | 0.77 | 1.43 |
| 4:5:198:TYR:CG | 4:8:208:ILE:CA[1_554] | 0.78 | 1.42 |
| 4:3:115:ASN:CG | 4:7:249:THR:O[1_554] | 0.78 | 1.42 |
| 4:6:187:ASP:O | 4:9:183:ARG:O[1_554] | 0.78 | 1.42 |
| 4:4:30:VAL:C | 4:7:80:ASP:N[1_554] | 0.78 | 1.42 |
| 4:5:255:PHE:CZ | 4:8:305:MET:O[1_554] | 0.78 | 1.42 |
| 4:6:166:TYR:CG | 4:W:40:HIS:CE1[1_554] | 0.78 | 1.42 |
| 4:5:253:GLU:CD | 4:8:214:GLU:N[1_554] | 0.78 | 1.42 |
| 4:5:317:ILE:CB | 4:8:150:GLY:O[1_554] | 0.78 | 1.42 |
| 4:5:277:THR:CG2 | 4:8:175:ILE:C[1_554] | 0.78 | 1.42 |
| 4:5:21:PHE:CA | 4:8:125:GLU:OE1[1_554] | 0.78 | 1.42 |
| 4:2:287:ILE:O | 4:7:39:ARG:CZ[1_554] | 0.78 | 1.42 |
| 4:4:145:SER:N | 4:7:370:VAL:O[1_554] | 0.78 | 1.42 |
| 4:4:340:TRP:CA | 4:7:118:LYS:N[1_554] | 0.78 | 1.42 |
| 4:4:24:ASP:CA | 4:7:125:GLU:CD[1_554] | 0.78 | 1.42 |
| 4:3:367:PRO:CD | 4:7:235:SER:CA[1_554] | 0.78 | 1.42 |
| 4:5:266:PHE:CD2 | 4:8:261:LEU:CD1[1_554] | 0.78 | 1.42 |
| 4:6:291:LYS:NZ | 4:W:64:ILE:CG1[1_554] | 0.78 | 1.42 |
| 4:4:114:ALA:CA | 4:8:250:ILE:O[1_554] | 0.78 | 1.42 |
| 4:4:332:PRO:O | 4:7:105:LEU:O[1_554] | 0.78 | 1.42 |
| 4:4:191:LYS:CD | 4:7:185:LEU:C[1_554] | 0.78 | 1.42 |
| 4:3:367:PRO:O | 4:7:236:LEU:CD2[1_554] | 0.79 | 1.41 |
| 4:5:276:GLU:OE2 | 4:8:279:TYR:N[1_554] | 0.79 | 1.41 |
| 4:5:24:ASP:C | 4:8:124:PHE:CA[1_554] | 0.79 | 1.41 |
| 4:2:324:THR:CG2 | 4:7:61:LYS:CD[1_554] | 0.79 | 1.41 |
| 4:6:281:SER:O | 4:9:173:HIS:NE2[1_554] | 0.79 | 1.41 |
| 4:5:200:PHE:N | 4:8:206:ARG:CB[1_554] | 0.79 | 1.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:207:GLU:OE2 | 4:7:67:LEU:C[1_554] | 0.79 | 1.41 |
| 4:3:166:TYR:CD1 | 4:8:40:HIS:NE2[1_554] | 0.79 | 1.41 |
| 4:4:31:PHE:C | 4:7:78:ASN:OD1[1_554] | 0.79 | 1.41 |
| 4:4:308:GLY:CA | 4:7:339:VAL:N[1_554] | 0.79 | 1.41 |
| 4:4:367:PRO:CD | 4:8:235:SER:CA[1_554] | 0.79 | 1.41 |
| 4:6:311:ASP:OD1 | 4:9:144:ALA:C[1_554] | 0.79 | 1.41 |
| 4:5:368:SER:C | 4:9:229:THR:O[1_554] | 0.79 | 1.41 |
| 4:5:304:THR:OG1 | 4:8:137:GLN:CG[1_554] | 0.79 | 1.41 |
| 4:4:24:ASP:N | 4:7:125:GLU:CD[1_554] | 0.79 | 1.41 |
| 4:4:293:LEU:O | 4:7:169:TYR:CB[1_554] | 0.80 | 1.40 |
| 4:4:178:LEU:CG | 4:7:177:ARG:CA[1_554] | 0.80 | 1.40 |
| 4:5:301:GLY:N | 4:8:107:GLU:CA[1_554] | 0.80 | 1.40 |
| 4:6:136:ILE:C | 4:9:113:LYS:CB[1_554] | 0.80 | 1.40 |
| 4:6:214:GLU:CB | 4:9:16:LEU:CA[1_554] | 0.80 | 1.40 |
| 4:4:372:ARG:CG | 4:8:227:MET:CA[1_554] | 0.80 | 1.40 |
| 4:5:297:ASN:N | 4:8:168:GLY:O[1_554] | 0.80 | 1.40 |
| 4:3:357:ILE:CG2 | 4:7:232:SER:O[1_554] | 0.80 | 1.40 |
| 4:3:291:LYS:CD | 4:8:64:ILE:CG1[1_554] | 0.80 | 1.40 |
| 4:5:339:VAL:C | 4:8:116:ARG:C[1_554] | 0.80 | 1.40 |
| 4:6:308:GLY:CA | 4:9:338:SER:CB[1_554] | 0.80 | 1.40 |
| 4:6:264:PRO:N | 4:9:274:ILE:CD1[1_554] | 0.80 | 1.40 |
| 4:4:299:MET:CB | 4:7:136:ILE:CA[1_554] | 0.80 | 1.40 |
| 4:6:190:MET:O | 4:9:186:THR:CG2[1_554] | 0.80 | 1.40 |
| 4:4:370:VAL:CB | 4:8:230:ALA:O[1_554] | 0.80 | 1.40 |
| 4:4:297:ASN:OD1 | 4:7:170:ALA:CA[1_554] | 0.80 | 1.40 |
| 4:4:325:MET:O | 4:7:167:GLU:OE2[1_554] | 0.80 | 1.40 |
| 4:6:205:GLU:CA | 4:9:62:ARG:NE[1_554] | 0.80 | 1.40 |
| 4:6:274:ILE:CA | 4:9:162:ASN:N[1_554] | 0.80 | 1.40 |
| 4:6:310:ALA:CA | 4:9:141:SER:CA[1_554] | 0.80 | 1.40 |
| 4:4:154:ASP:OD2 | 4:7:112:PRO:N[1_554] | 0.80 | 1.40 |
| 4:5:154:ASP:N | 4:8:109:PRO:C[1_554] | 0.80 | 1.40 |
| 4:2:292:ASP:N | 4:7:40:HIS:CG[1_554] | 0.80 | 1.40 |
| 4:6:157:ASP:CG | 4:9:72:GLU:N[1_554] | 0.81 | 1.39 |
| 4:6:304:THR:CB | 4:9:137:GLN:CB[1_554] | 0.81 | 1.39 |
| 4:6:301:GLY:N | 4:9:107:GLU:C[1_554] | 0.81 | 1.39 |
| 4:4:332:PRO:CD | 4:7:134:VAL:O[1_554] | 0.81 | 1.39 |
| 4:5:281:SER:O | 4:8:173:HIS:CD2[1_554] | 0.81 | 1.39 |
| 4:6:331:ALA:CB | 4:9:140:LEU:CG[1_554] | 0.81 | 1.39 |
| 4:6:150:GLY:C | 4:9:169:TYR:CD1[1_554] | 0.81 | 1.39 |
| 4:6:211:ASP:CG | 4:9:32:PRO:CD[1_554] | 0.81 | 1.39 |
| 4:5:161:HIS:CA | 4:8:110:LEU:CD1[1_554] | 0.81 | 1.39 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:340:TRP:CD1 | 4:9:118:LYS:O[1_554] | 0.81 | 1.39 |
| 4:6:337:TYR:OH | 4:9:86:TRP:CE2[1_554] | 0.81 | 1.39 |
| 4:6:300:SER:CB | 4:9:107:GLU:CG[1_554] | 0.81 | 1.39 |
| 4:5:300:SER:C | 4:8:107:GLU:C[1_554] | 0.81 | 1.39 |
| 4:6:370:VAL:CA | 4:V:231:ALA:CB[1_554] | 0.81 | 1.39 |
| 4:5:156:GLY:O | 4:8:74:GLY:N[1_554] | 0.81 | 1.39 |
| 4:6:372:ARG:O | 4:V:227:MET:CG[1_554] | 0.81 | 1.39 |
| 4:6:300:SER:C | 4:9:107:GLU:C[1_554] | 0.81 | 1.39 |
| 4:3:108:ALA:CA | 4:7:195:GLU:O[1_554] | 0.81 | 1.39 |
| 4:6:279:TYR:CD1 | 4:9:293:LEU:CD2[1_554] | 0.81 | 1.39 |
| 4:5:337:TYR:OH | 4:8:86:TRP:CE2[1_554] | 0.81 | 1.39 |
| 4:5:75:ILE:C | 4:9:197:GLY:O[1_554] | 0.81 | 1.39 |
| 4:6:110:LEU:CD1 | 4:V:191:LYS:CG[1_554] | 0.81 | 1.39 |
| 4:5:331:ALA:CB | 4:8:140:LEU:CG[1_554] | 0.82 | 1.38 |
| 4:6:110:LEU:CD2 | 4:V:191:LYS:CE[1_554] | 0.82 | 1.38 |
| 4:5:341:ILE:CG1 | 4:8:132:MET:CE[1_554] | 0.82 | 1.38 |
| 4:4:162:ASN:ND2 | 4:7:175:ILE:CD1[1_554] | 0.82 | 1.38 |
| 4:2:325:MET:CE | 4:7:64:ILE:CG2[1_554] | 0.82 | 1.38 |
| 4:5:214:GLU:CA | 4:8:16:LEU:CB[1_554] | 0.82 | 1.38 |
| 4:3:109:PRO:N | 4:7:195:GLU:CG[1_554] | 0.82 | 1.38 |
| 4:4:344:SER:C | 4:7:367:PRO:CD[1_554] | 0.82 | 1.38 |
| 4:6:289:ILE:N | 4:W:63:GLY:O[1_554] | 0.82 | 1.38 |
| 4:4:218:TYR:CD2 | 4:7:337:TYR:CG[1_554] | 0.82 | 1.38 |
| 4:5:312:ARG:CD | 4:8:299:MET:CA[1_554] | 0.82 | 1.38 |
| 4:6:106:THR:CA | 4:9:114:ALA:CB[1_554] | 0.82 | 1.38 |
| 4:4:317:ILE:CA | 4:7:150:GLY:O[1_554] | 0.82 | 1.38 |
| 4:5:173:HIS:N | 4:9:266:PHE:C[1_554] | 0.82 | 1.38 |
| 4:4:26:ALA:N | 4:7:121:GLN:O[1_554] | 0.82 | 1.38 |
| 4:5:274:ILE:C | 4:8:162:ASN:C[1_554] | 0.82 | 1.38 |
| 4:6:312:ARG:CZ | 4:9:299:MET:CG[1_554] | 0.82 | 1.38 |
| 4:5:207:GLU:CB | 4:8:67:LEU:CD1[1_554] | 0.82 | 1.38 |
| 4:5:136:ILE:C | 4:8:113:LYS:CB[1_554] | 0.82 | 1.38 |
| 4:5:254:ARG:CZ | 4:8:336:LYS:NZ[1_554] | 0.82 | 1.38 |
| 4:6:221:LEU:CG | 4:9:332:PRO:CB[1_554] | 0.82 | 1.38 |
| 4:5:336:LYS:CG | 4:8:12:ASN:ND2[1_554] | 0.82 | 1.38 |
| 4:4:157:ASP:CG | 4:7:72:GLU:CB[1_554] | 0.82 | 1.38 |
| 4:6:159:VAL:C | 4:9:177:ARG:NH1[1_554] | 0.82 | 1.38 |
| 4:4:108:ALA:CA | 4:8:195:GLU:O[1_554] | 0.82 | 1.38 |
| 4:4:318:THR:N | 4:7:149:THR:C[1_554] | 0.83 | 1.37 |
| 4:4:256:ARG:N | 4:7:302:GLY:O[1_554] | 0.83 | 1.37 |
| 4:6:262:PHE:CE2 | 4:9:153:LEU:O[1_554] | 0.83 | 1.37 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:328:LYS:N | 4:7:168:GLY:CA[1_554] | 0.83 | 1.37 |
| 4:5:339:VAL:O | 4:8:116:ARG:C[1_554] | 0.83 | 1.37 |
| 4:6:263:GLN:C | 4:9:274:ILE:CD1[1_554] | 0.83 | 1.37 |
| 4:5:150:GLY:O | 4:8:169:TYR:CE1[1_554] | 0.83 | 1.37 |
| 4:5:205:GLU:N | 4:8:62:ARG:NE[1_554] | 0.83 | 1.37 |
| 4:4:345:ILE:CA | 4:7:366:GLY:C[1_554] | 0.83 | 1.37 |
| 4:6:347:ALA:C | 4:9:366:GLY:CA[1_554] | 0.83 | 1.37 |
| 4:6:110:LEU:CD1 | 4:V:191:LYS:CD[1_554] | 0.83 | 1.37 |
| 4:3:173:HIS:C | 4:7:267:ILE:CA[1_554] | 0.83 | 1.37 |
| 4:5:137:GLN:CD | 4:8:112:PRO:CB[1_554] | 0.83 | 1.37 |
| 4:4:341:ILE:CG1 | 4:7:120:THR:CA[1_554] | 0.83 | 1.37 |
| 4:4:311:ASP:N | 4:7:140:LEU:O[1_554] | 0.83 | 1.37 |
| 4:5:26:ALA:CA | 4:8:123:MET:CA[1_554] | 0.83 | 1.37 |
| 4:4:18:LYS:CD | 4:7:79:TRP:CE2[1_554] | 0.83 | 1.37 |
| 4:4:111:ASN:CG | 4:8:196:ARG:CG[1_554] | 0.83 | 1.37 |
| 4:5:312:ARG:CZ | 4:8:299:MET:CG[1_554] | 0.83 | 1.37 |
| 4:5:214:GLU:CB | 4:8:16:LEU:CA[1_554] | 0.83 | 1.37 |
| 4:5:369:ILE:N | 4:9:229:THR:O[1_554] | 0.83 | 1.37 |
| 4:6:200:PHE:N | 4:9:206:ARG:CB[1_554] | 0.83 | 1.37 |
| 4:5:372:ARG:O | 4:9:227:MET:CG[1_554] | 0.83 | 1.37 |
| 4:5:367:PRO:O | 4:9:230:ALA:O[1_554] | 0.83 | 1.37 |
| 4:6:188:TYR:CB | 4:9:181:ALA:O[1_554] | 0.83 | 1.37 |
| 4:3:173:HIS:CE1 | 4:7:266:PHE:N[1_554] | 0.83 | 1.37 |
| 4:5:310:ALA:CA | 4:8:141:SER:CA[1_554] | 0.83 | 1.37 |
| 4:4:157:ASP:CA | 4:7:72:GLU:O[1_554] | 0.83 | 1.37 |
| 4:6:20:GLY:C | 4:9:121:GLN:NE2[1_554] | 0.84 | 1.36 |
| 4:4:139:VAL:O | 4:7:371:HIS:NE2[1_554] | 0.84 | 1.36 |
| 4:3:284:LYS:O | 4:7:268:GLY:O[1_554] | 0.84 | 1.36 |
| 4:4:326:LYS:O | 4:7:167:GLU:CB[1_554] | 0.84 | 1.36 |
| 4:5:316:GLU:CB | 4:8:151:ILE:O[1_554] | 0.84 | 1.36 |
| 4:5:301:GLY:N | 4:8:107:GLU:C[1_554] | 0.84 | 1.36 |
| 4:5:145:SER:CA | 4:8:372:ARG:NH2[1_554] | 0.84 | 1.36 |
| 4:6:143:TYR:CB | 4:9:372:ARG:N[1_554] | 0.84 | 1.36 |
| 4:6:334:GLU:OE1 | 4:9:133:TYR:O[1_554] | 0.84 | 1.36 |
| 4:5:327:ILE:CG2 | 4:8:149:THR:N[1_554] | 0.84 | 1.36 |
| 4:5:194:THR:CA | 4:8:209:VAL:CG1[1_554] | 0.84 | 1.36 |
| 4:6:207:GLU:CB | 4:9:67:LEU:CD1[1_554] | 0.84 | 1.36 |
| 4:6:188:TYR:N | 4:9:184:ASP:N[1_554] | 0.84 | 1.36 |
| 4:5:370:VAL:CA | 4:9:231:ALA:CA[1_554] | 0.84 | 1.36 |
| 4:4:183:ARG:NE | 4:7:72:GLU:OE1[1_554] | 0.84 | 1.36 |
| 4:5:198:TYR:CG | 4:8:208:ILE:C[1_554] | 0.84 | 1.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:266:PHE:CB | 4:7:261:LEU:CD2[1_554] | 0.84 | 1.36 |
| 4:5:276:GLU:CD | 4:8:278:THR:C[1_554] | 0.84 | 1.36 |
| 4:4:191:LYS:C | 4:7:186:THR:CB[1_554] | 0.85 | 1.35 |
| 4:5:157:ASP:CG | 4:8:72:GLU:N[1_554] | 0.85 | 1.35 |
| 4:6:24:ASP:C | 4:9:124:PHE:CA[1_554] | 0.85 | 1.35 |
| 4:4:372:ARG:CG | 4:8:227:MET:CB[1_554] | 0.85 | 1.35 |
| 4:5:340:TRP:CD1 | 4:8:118:LYS:O[1_554] | 0.85 | 1.35 |
| 4:6:156:GLY:O | 4:9:74:GLY:N[1_554] | 0.85 | 1.35 |
| 4:5:274:ILE:CA | 4:8:162:ASN:CA[1_554] | 0.85 | 1.35 |
| 4:6:262:PHE:CA | 4:9:153:LEU:CG[1_554] | 0.85 | 1.35 |
| 4:6:327:ILE:CG2 | 4:9:149:THR:N[1_554] | 0.85 | 1.35 |
| 4:6:174:ALA:O | 4:9:173:HIS:CB[1_554] | 0.85 | 1.35 |
| 4:4:255:PHE:CE1 | 4:7:305:MET:CB[1_554] | 0.85 | 1.35 |
| 4:6:198:TYR:CG | 4:9:208:ILE:C[1_554] | 0.85 | 1.35 |
| 4:6:301:GLY:O | 4:9:137:GLN:NE2[1_554] | 0.85 | 1.35 |
| 4:4:208:ILE:CG2 | 4:7:59:GLN:CD[1_554] | 0.85 | 1.35 |
| 4:4:341:ILE:N | 4:7:117:GLU:C[1_554] | 0.85 | 1.35 |
| 4:5:334:GLU:OE1 | 4:8:133:TYR:C[1_554] | 0.85 | 1.35 |
| 4:6:187:ASP:C | 4:9:183:ARG:C[1_554] | 0.85 | 1.35 |
| 4:6:317:ILE:CB | 4:9:150:GLY:O[1_554] | 0.85 | 1.35 |
| 4:6:218:TYR:CB | 4:9:336:LYS:CB[1_554] | 0.85 | 1.35 |
| 4:6:243:PRO:CB | 4:9:60:SER:CA[1_554] | 0.85 | 1.35 |
| 4:6:141:SER:C | 4:9:116:ARG:NH1[1_554] | 0.85 | 1.35 |
| 4:6:75:ILE:C | 4:V:197:GLY:C[1_554] | 0.85 | 1.35 |
| 4:4:339:VAL:CG1 | 4:7:114:ALA:C[1_554] | 0.85 | 1.35 |
| 4:4:227:MET:SD | 4:7:305:MET:O[1_554] | 0.85 | 1.35 |
| 4:5:310:ALA:N | 4:8:141:SER:CA[1_554] | 0.85 | 1.35 |
| 4:5:281:SER:O | 4:8:173:HIS:NE2[1_554] | 0.85 | 1.35 |
| 4:6:336:LYS:CB | 4:9:12:ASN:ND2[1_554] | 0.86 | 1.34 |
| 4:4:218:TYR:OH | 4:7:27:PRO:CG[1_554] | 0.86 | 1.34 |
| 4:4:214:GLU:O | 4:7:17:VAL:N[1_554] | 0.86 | 1.34 |
| 4:3:284:LYS:C | 4:7:268:GLY:O[1_554] | 0.86 | 1.34 |
| 4:4:274:ILE:C | 4:7:162:ASN:C[1_554] | 0.86 | 1.34 |
| 4:6:242:LEU:CD2 | 4:9:207:GLU:OE1[1_554] | 0.86 | 1.34 |
| 4:5:370:VAL:CA | 4:9:231:ALA:CB[1_554] | 0.86 | 1.34 |
| 4:4:173:HIS:C | 4:8:267:ILE:CA[1_554] | 0.86 | 1.34 |
| 4:4:276:GLU:OE2 | 4:7:278:THR:C[1_554] | 0.86 | 1.34 |
| 4:5:173:HIS:N | 4:9:266:PHE:O[1_554] | 0.86 | 1.34 |
| 4:4:310:ALA:CB | 4:7:140:LEU:CB[1_554] | 0.86 | 1.34 |
| 4:4:318:THR:N | 4:7:150:GLY:N[1_554] | 0.86 | 1.34 |
| 4:5:142:LEU:O | 4:8:372:ARG:NE[1_554] | 0.86 | 1.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:243:PRO:CB | 4:8:60:SER:CA[1_554] | 0.86 | 1.34 |
| 4:5:17:VAL:C | 4:8:79:TRP:CG[1_554] | 0.86 | 1.34 |
| 4:4:117:GLU:C | 4:8:237:GLU:CG[1_554] | 0.86 | 1.34 |
| 4:5:140:LEU:N | 4:8:371:HIS:CE1[1_554] | 0.86 | 1.34 |
| 4:5:288:ASP:C | 4:V:63:GLY:C[1_554] | 0.86 | 1.34 |
| 4:6:274:ILE:CD1 | 4:9:161:HIS:CA[1_554] | 0.86 | 1.34 |
| 4:4:335:ARG:NH2 | 4:7:106:THR:CG2[1_554] | 0.86 | 1.34 |
| 4:6:208:ILE:CB | 4:9:59:GLN:CG[1_554] | 0.86 | 1.34 |
| 4:5:346:LEU:CB | 4:8:368:SER:CA[1_554] | 0.86 | 1.34 |
| 4:5:253:GLU:OE1 | 4:8:214:GLU:N[1_554] | 0.86 | 1.34 |
| 4:5:322:PRO:CG | 4:8:288:ASP:O[1_554] | 0.86 | 1.34 |
| 4:5:214:GLU:C | 4:8:16:LEU:CB[1_554] | 0.86 | 1.34 |
| 4:5:311:ASP:OD1 | 4:8:144:ALA:C[1_554] | 0.87 | 1.33 |
| 4:4:255:PHE:C | 4:7:302:GLY:CA[1_554] | 0.87 | 1.33 |
| 4:6:210:ARG:NH2 | 4:9:34:ILE:N[1_554] | 0.87 | 1.33 |
| 4:5:327:ILE:CD1 | 4:8:149:THR:CG2[1_554] | 0.87 | 1.33 |
| 4:5:327:ILE:CB | 4:8:149:THR:N[1_554] | 0.87 | 1.33 |
| 4:6:307:PRO:CB | 4:9:337:TYR:CA[1_554] | 0.87 | 1.33 |
| 4:4:198:TYR:CB | 4:7:208:ILE:N[1_554] | 0.87 | 1.33 |
| 4:6:288:ASP:CB | 4:W:62:ARG:O[1_554] | 0.87 | 1.33 |
| 4:5:340:TRP:CH2 | 4:8:121:GLN:C[1_554] | 0.87 | 1.33 |
| 4:5:186:THR:CB | 4:8:183:ARG:NE[1_554] | 0.87 | 1.33 |
| 4:4:267:ILE:CA | 4:7:180:LEU:CD1[1_554] | 0.87 | 1.33 |
| 4:5:372:ARG:C | 4:9:227:MET:CB[1_554] | 0.87 | 1.33 |
| 4:6:161:HIS:CA | 4:9:110:LEU:CG[1_554] | 0.87 | 1.33 |
| 4:6:268:GLY:C | 4:9:264:PRO:CB[1_554] | 0.87 | 1.33 |
| 4:5:299:MET:CA | 4:8:136:ILE:CB[1_554] | 0.87 | 1.33 |
| 4:4:276:GLU:CD | 4:7:278:THR:O[1_554] | 0.87 | 1.33 |
| 4:4:192:ILE:CB | 4:7:213:LYS:CE[1_554] | 0.88 | 1.32 |
| 4:4:227:MET:CE | 4:7:306:TYR:CA[1_554] | 0.88 | 1.32 |
| 4:4:197:GLY:O | 4:7:208:ILE:CG2[1_554] | 0.88 | 1.32 |
| 4:6:75:ILE:CA | 4:V:197:GLY:CA[1_554] | 0.88 | 1.32 |
| 4:5:174:ALA:O | 4:8:173:HIS:CB[1_554] | 0.88 | 1.32 |
| 4:5:75:ILE:C | 4:9:197:GLY:C[1_554] | 0.88 | 1.32 |
| 4:6:282:ILE:CD1 | 4:9:171:LEU:CD1[1_554] | 0.88 | 1.32 |
| 4:6:196:ARG:CA | 4:9:212:ILE:CB[1_554] | 0.88 | 1.32 |
| 4:5:341:ILE:CA | 4:8:120:THR:OG1[1_554] | 0.88 | 1.32 |
| 4:6:204:ALA:CA | 4:9:62:ARG:CB[1_554] | 0.88 | 1.32 |
| 4:5:14:SER:C | 4:8:77:THR:OG1[1_554] | 0.88 | 1.32 |
| 4:4:144:ALA:N | 4:7:371:HIS:N[1_554] | 0.88 | 1.32 |
| 4:5:259:GLU:OE2 | 4:8:309:ILE:CG1[1_554] | 0.88 | 1.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:339:VAL:O | 4:9:116:ARG:C[1_554] | 0.88 | 1.32 |
| 4:4:75:ILE:CG2 | 4:8:198:TYR:CD2[1_554] | 0.88 | 1.32 |
| 4:6:340:TRP:CZ2 | 4:9:121:GLN:C[1_554] | 0.88 | 1.32 |
| 4:6:253:GLU:CD | 4:9:214:GLU:CA[1_554] | 0.88 | 1.32 |
| 4:4:16:LEU:CA | 4:7:77:THR:C[1_554] | 0.88 | 1.32 |
| 4:6:173:HIS:N | 4:V:266:PHE:C[1_554] | 0.88 | 1.32 |
| 4:4:282:ILE:CD1 | 4:7:171:LEU:CG[1_554] | 0.88 | 1.32 |
| 4:5:294:TYR:C | 4:8:166:TYR:O[1_554] | 0.88 | 1.32 |
| 4:5:142:LEU:O | 4:8:372:ARG:CD[1_554] | 0.88 | 1.32 |
| 4:5:59:GLN:CG | 4:8:68:LYS:CG[1_554] | 0.88 | 1.32 |
| 4:5:204:ALA:CA | 4:8:62:ARG:CB[1_554] | 0.88 | 1.32 |
| 4:6:310:ALA:N | 4:9:141:SER:CB[1_554] | 0.88 | 1.32 |
| 4:5:273:GLY:CA | 4:8:162:ASN:OD1[1_554] | 0.88 | 1.32 |
| 4:5:162:ASN:CG | 4:8:175:ILE:CB[1_554] | 0.88 | 1.32 |
| 4:6:335:ARG:N | 4:9:105:LEU:O[1_554] | 0.89 | 1.31 |
| 4:6:327:ILE:CD1 | 4:9:149:THR:CB[1_554] | 0.89 | 1.31 |
| 4:5:110:LEU:O | 4:9:192:ILE:C[1_554] | 0.89 | 1.31 |
| 4:4:253:GLU:OE1 | 4:7:214:GLU:CB[1_554] | 0.89 | 1.31 |
| 4:4:276:GLU:OE2 | 4:7:278:THR:CA[1_554] | 0.89 | 1.31 |
| 4:6:370:VAL:N | 4:V:231:ALA:CA[1_554] | 0.89 | 1.31 |
| 4:6:218:TYR:OH | 4:9:337:TYR:CE2[1_554] | 0.89 | 1.31 |
| 4:6:334:GLU:N | 4:9:104:LEU:C[1_554] | 0.89 | 1.31 |
| 4:5:301:GLY:O | 4:8:137:GLN:NE2[1_554] | 0.89 | 1.31 |
| 4:3:117:GLU:C | 4:7:237:GLU:CG[1_554] | 0.89 | 1.31 |
| 4:4:253:GLU:CD | 4:7:214:GLU:CG[1_554] | 0.89 | 1.31 |
| 4:6:327:ILE:CB | 4:9:149:THR:N[1_554] | 0.89 | 1.31 |
| 4:6:312:ARG:CD | 4:9:299:MET:CA[1_554] | 0.89 | 1.31 |
| 4:4:186:THR:CA | 4:7:183:ARG:NE[1_554] | 0.89 | 1.31 |
| 4:4:16:LEU:N | 4:7:77:THR:C[1_554] | 0.89 | 1.31 |
| 4:6:259:GLU:OE2 | 4:9:309:ILE:CB[1_554] | 0.89 | 1.31 |
| 4:4:339:VAL:N | 4:7:116:ARG:CA[1_554] | 0.89 | 1.31 |
| 4:6:194:THR:CA | 4:9:209:VAL:CG1[1_554] | 0.89 | 1.31 |
| 4:4:75:ILE:CB | 4:8:198:TYR:CB[1_554] | 0.89 | 1.31 |
| 4:6:137:GLN:CG | 4:9:112:PRO:C[1_554] | 0.89 | 1.31 |
| 4:6:308:GLY:C | 4:9:338:SER:CB[1_554] | 0.89 | 1.31 |
| 4:4:281:SER:C | 4:7:173:HIS:CD2[1_554] | 0.89 | 1.31 |
| 4:4:223:PHE:C | 4:7:335:ARG:CZ[1_554] | 0.89 | 1.31 |
| 4:5:161:HIS:CA | 4:8:110:LEU:CG[1_554] | 0.90 | 1.30 |
| 4:6:218:TYR:CA | 4:9:336:LYS:CA[1_554] | 0.90 | 1.30 |
| 4:6:221:LEU:O | 4:9:331:ALA:O[1_554] | 0.90 | 1.30 |
| 4:5:307:PRO:CB | 4:8:337:TYR:CA[1_554] | 0.90 | 1.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:174:ALA:O | 4:9:173:HIS:CA[1_554] | 0.90 | 1.30 |
| 4:4:311:ASP:N | 4:7:140:LEU:C[1_554] | 0.90 | 1.30 |
| 4:4:191:LYS:CB | 4:7:187:ASP:N[1_554] | 0.90 | 1.30 |
| 4:5:214:GLU:CA | 4:8:16:LEU:CA[1_554] | 0.90 | 1.30 |
| 4:5:26:ALA:C | 4:8:123:MET:N[1_554] | 0.90 | 1.30 |
| 4:4:226:GLU:OE1 | 4:7:333:PRO:C[1_554] | 0.90 | 1.30 |
| 4:6:313:MET:CG | 4:9:152:VAL:CB[1_554] | 0.90 | 1.30 |
| 4:4:331:ALA:CA | 4:7:135:ALA:CB[1_554] | 0.90 | 1.30 |
| 4:4:305:MET:O | 4:7:11:ASP:CG[1_554] | 0.90 | 1.30 |
| 4:5:337:TYR:CZ | 4:8:86:TRP:CZ2[1_554] | 0.90 | 1.30 |
| 4:4:173:HIS:CE1 | 4:8:266:PHE:N[1_554] | 0.90 | 1.30 |
| 4:5:157:ASP:C | 4:8:72:GLU:O[1_554] | 0.90 | 1.30 |
| 4:6:156:GLY:O | 4:9:74:GLY:CA[1_554] | 0.90 | 1.30 |
| 4:4:191:LYS:C | 4:7:186:THR:CA[1_554] | 0.90 | 1.30 |
| 4:6:278:THR:CG2 | 4:9:164:PRO:C[1_554] | 0.90 | 1.30 |
| 4:5:75:ILE:CA | 4:9:197:GLY:CA[1_554] | 0.90 | 1.30 |
| 4:5:208:ILE:CB | 4:8:59:GLN:CD[1_554] | 0.90 | 1.30 |
| 4:6:266:PHE:N | 4:9:261:LEU:CA[1_554] | 0.90 | 1.30 |
| 4:6:255:PHE:CZ | 4:9:305:MET:O[1_554] | 0.90 | 1.30 |
| 4:6:210:ARG:CZ | 4:9:33:SER:C[1_554] | 0.90 | 1.30 |
| 4:6:106:THR:CB | 4:9:114:ALA:CB[1_554] | 0.90 | 1.30 |
| 4:4:325:MET:CG | 4:7:166:TYR:CE2[1_554] | 0.90 | 1.30 |
| 4:6:112:PRO:C | 4:V:253:GLU:OE1[1_554] | 0.90 | 1.30 |
| 4:6:372:ARG:C | 4:V:227:MET:CA[1_554] | 0.90 | 1.30 |
| 4:6:204:ALA:CA | 4:9:62:ARG:CG[1_554] | 0.90 | 1.30 |
| 4:6:162:ASN:CG | 4:9:175:ILE:CB[1_554] | 0.90 | 1.30 |
| 4:6:288:ASP:O | 4:W:64:ILE:N[1_554] | 0.90 | 1.30 |
| 4:4:341:ILE:O | 4:7:367:PRO:CB[1_554] | 0.90 | 1.30 |
| 4:5:27:PRO:C | 4:8:122:ILE:CG2[1_554] | 0.90 | 1.30 |
| 4:6:277:THR:CG2 | 4:9:175:ILE:C[1_554] | 0.90 | 1.30 |
| 4:4:266:PHE:CD1 | 4:7:261:LEU:CD1[1_554] | 0.90 | 1.30 |
| 4:5:249:THR:C | 4:8:211:ASP:OD2[1_554] | 0.90 | 1.30 |
| 4:4:333:PRO:O | 4:7:105:LEU:CB[1_554] | 0.90 | 1.30 |
| 4:3:75:ILE:CB | 4:7:198:TYR:CB[1_554] | 0.90 | 1.30 |
| 4:5:159:VAL:CA | 4:8:177:ARG:NH1[1_554] | 0.91 | 1.29 |
| 4:5:190:MET:SD | 4:8:206:ARG:NH2[1_554] | 0.91 | 1.29 |
| 4:3:110:LEU:CA | 4:7:192:ILE:CB[1_554] | 0.91 | 1.29 |
| 4:5:143:TYR:N | 4:8:372:ARG:CB[1_554] | 0.91 | 1.29 |
| 4:6:279:TYR:C | 4:9:285:CYS:SG[1_554] | 0.91 | 1.29 |
| 4:4:110:LEU:CB | 4:8:192:ILE:N[1_554] | 0.91 | 1.29 |
| 4:6:162:ASN:CG | 4:9:175:ILE:CG1[1_554] | 0.91 | 1.29 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:28:ARG:NE | 4:9:126:THR:CA[1_554] | 0.91 | 1.29 |
| 4:5:106:THR:CB | 4:8:114:ALA:CA[1_554] | 0.91 | 1.29 |
| 4:5:336:LYS:CB | 4:8:12:ASN:ND2[1_554] | 0.91 | 1.29 |
| 4:4:306:TYR:C | 4:7:11:ASP:OD2[1_554] | 0.91 | 1.29 |
| 4:5:273:GLY:C | 4:8:162:ASN:OD1[1_554] | 0.91 | 1.29 |
| 4:4:178:LEU:CD2 | 4:7:177:ARG:CA[1_554] | 0.91 | 1.29 |
| 4:6:187:ASP:N | 4:9:183:ARG:CB[1_554] | 0.91 | 1.29 |
| 4:4:195:GLU:CG | 4:7:189:LEU:CD2[1_554] | 0.91 | 1.29 |
| 4:5:188:TYR:CB | 4:8:181:ALA:O[1_554] | 0.91 | 1.29 |
| 4:4:194:THR:CA | 4:7:209:VAL:CG1[1_554] | 0.91 | 1.29 |
| 4:4:310:ALA:CB | 4:7:140:LEU:CA[1_554] | 0.91 | 1.29 |
| 4:6:142:LEU:O | 4:9:372:ARG:CD[1_554] | 0.91 | 1.29 |
| 4:4:270:GLU:N | 4:7:272:ALA:O[1_554] | 0.91 | 1.29 |
| 4:4:115:ASN:N | 4:8:250:ILE:CA[1_554] | 0.91 | 1.29 |
| 4:4:267:ILE:N | 4:7:180:LEU:CD1[1_554] | 0.91 | 1.29 |
| 4:4:154:ASP:CG | 4:7:111:ASN:C[1_554] | 0.91 | 1.29 |
| 4:6:348:SER:CB | 4:9:362:TYR:O[1_554] | 0.91 | 1.29 |
| 4:5:227:MET:SD | 4:8:306:TYR:C[1_554] | 0.91 | 1.29 |
| 4:6:312:ARG:CD | 4:9:299:MET:N[1_554] | 0.91 | 1.29 |
| 4:6:219:VAL:CG2 | 4:9:301:GLY:N[1_554] | 0.91 | 1.29 |
| 4:6:29:ALA:CA | 4:9:83:GLU:OE1[1_554] | 0.91 | 1.29 |
| 4:6:192:ILE:CG1 | 4:9:213:LYS:CD[1_554] | 0.91 | 1.29 |
| 4:6:282:ILE:CG1 | 4:9:171:LEU:CG[1_554] | 0.91 | 1.29 |
| 4:4:345:ILE:N | 4:7:367:PRO:N[1_554] | 0.91 | 1.29 |
| 4:6:308:GLY:N | 4:9:338:SER:N[1_554] | 0.91 | 1.29 |
| 4:4:191:LYS:CD | 4:7:185:LEU:O[1_554] | 0.91 | 1.29 |
| 4:5:319:ALA:CB | 4:8:295:ALA:C[1_554] | 0.91 | 1.29 |
| 4:5:150:GLY:C | 4:8:169:TYR:CD1[1_554] | 0.91 | 1.29 |
| 4:6:137:GLN:CD | 4:9:112:PRO:CB[1_554] | 0.92 | 1.28 |
| 4:4:299:MET:CE | 4:7:136:ILE:C[1_554] | 0.92 | 1.28 |
| 4:5:307:PRO:C | 4:8:338:SER:N[1_554] | 0.92 | 1.28 |
| 4:6:299:MET:O | 4:9:136:ILE:N[1_554] | 0.92 | 1.28 |
| 4:6:322:PRO:CG | 4:9:288:ASP:O[1_554] | 0.92 | 1.28 |
| 4:6:249:THR:O | 4:9:211:ASP:CG[1_554] | 0.92 | 1.28 |
| 4:4:357:ILE:CG2 | 4:8:232:SER:O[1_554] | 0.92 | 1.28 |
| 4:6:173:HIS:N | 4:V:266:PHE:O[1_554] | 0.92 | 1.28 |
| 4:4:214:GLU:CD | 4:7:33:SER:OG[1_554] | 0.92 | 1.28 |
| 4:4:281:SER:O | 4:7:173:HIS:CD2[1_554] | 0.92 | 1.28 |
| 4:4:23:GLY:C | 4:7:125:GLU:OE2[1_554] | 0.92 | 1.28 |
| 4:5:214:GLU:OE2 | 4:8:33:SER:OG[1_554] | 0.92 | 1.28 |
| 4:4:335:ARG:CZ | 4:7:106:THR:CG2[1_554] | 0.92 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:314:GLN:OE1 | 4:7:147:ARG:O[1_554] | 0.92 | 1.28 |
| 4:6:157:ASP:OD2 | 4:9:72:GLU:CA[1_554] | 0.92 | 1.28 |
| 4:4:151:ILE:CD1 | 4:7:172:PRO:N[1_554] | 0.92 | 1.28 |
| 4:5:299:MET:CB | 4:8:136:ILE:C[1_554] | 0.92 | 1.28 |
| 4:4:151:ILE:CD1 | 4:7:172:PRO:CD[1_554] | 0.92 | 1.28 |
| 4:5:319:ALA:CB | 4:8:296:ASN:N[1_554] | 0.92 | 1.28 |
| 4:4:273:GLY:N | 4:7:162:ASN:OD1[1_554] | 0.92 | 1.28 |
| 4:6:369:ILE:N | 4:V:229:THR:O[1_554] | 0.92 | 1.28 |
| 4:4:153:LEU:CA | 4:7:109:PRO:O[1_554] | 0.92 | 1.28 |
| 4:6:266:PHE:CB | 4:9:261:LEU:CG[1_554] | 0.93 | 1.27 |
| 4:6:368:SER:C | 4:V:229:THR:O[1_554] | 0.93 | 1.27 |
| 4:4:314:GLN:N | 4:7:142:LEU:CB[1_554] | 0.93 | 1.27 |
| 4:4:304:THR:CA | 4:7:137:GLN:CD[1_554] | 0.93 | 1.27 |
| 4:5:274:ILE:C | 4:8:162:ASN:CA[1_554] | 0.93 | 1.27 |
| 4:6:253:GLU:CD | 4:9:214:GLU:N[1_554] | 0.93 | 1.27 |
| 4:5:313:MET:CG | 4:8:152:VAL:CB[1_554] | 0.93 | 1.27 |
| 4:5:334:GLU:N | 4:8:104:LEU:C[1_554] | 0.93 | 1.27 |
| 4:4:340:TRP:C | 4:7:117:GLU:C[1_554] | 0.93 | 1.27 |
| 4:6:274:ILE:C | 4:9:162:ASN:C[1_554] | 0.93 | 1.27 |
| 4:6:60:SER:CB | 4:9:37:ARG:CB[1_554] | 0.93 | 1.27 |
| 4:6:158:GLY:O | 4:9:177:ARG:NH2[1_554] | 0.93 | 1.27 |
| 4:4:345:ILE:CB | 4:7:366:GLY:O[1_554] | 0.93 | 1.27 |
| 4:4:116:ARG:O | 4:8:237:GLU:OE2[1_554] | 0.93 | 1.27 |
| 4:6:321:ALA:N | 4:9:293:LEU:N[1_554] | 0.93 | 1.27 |
| 4:5:115:ASN:N | 4:9:196:ARG:NH2[1_554] | 0.93 | 1.27 |
| 4:6:24:ASP:CG | 4:9:125:GLU:CA[1_554] | 0.93 | 1.27 |
| 4:4:294:TYR:CD1 | 4:7:166:TYR:CB[1_554] | 0.93 | 1.27 |
| 4:5:210:ARG:NH2 | 4:8:34:ILE:N[1_554] | 0.93 | 1.27 |
| 4:6:137:GLN:CA | 4:9:113:LYS:N[1_554] | 0.93 | 1.27 |
| 4:4:260:THR:N | 4:7:155:SER:CB[1_554] | 0.93 | 1.27 |
| 4:6:336:LYS:CG | 4:9:12:ASN:ND2[1_554] | 0.93 | 1.27 |
| 4:6:115:ASN:N | 4:V:196:ARG:CZ[1_554] | 0.93 | 1.27 |
| 4:6:227:MET:SD | 4:9:306:TYR:C[1_554] | 0.93 | 1.27 |
| 4:5:242:LEU:CD2 | 4:8:207:GLU:OE1[1_554] | 0.93 | 1.27 |
| 4:5:264:PRO:N | 4:8:274:ILE:CD1[1_554] | 0.93 | 1.27 |
| 4:5:339:VAL:CA | 4:8:116:ARG:CA[1_554] | 0.94 | 1.26 |
| 4:4:339:VAL:CG1 | 4:7:115:ASN:N[1_554] | 0.94 | 1.26 |
| 4:6:161:HIS:CA | 4:9:110:LEU:CD1[1_554] | 0.94 | 1.26 |
| 4:4:115:ASN:CG | 4:8:249:THR:O[1_554] | 0.94 | 1.26 |
| 4:5:348:SER:OG | 4:8:362:TYR:O[1_554] | 0.94 | 1.26 |
| 4:6:207:GLU:OE1 | 4:9:67:LEU:CD2[1_554] | 0.94 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:310:ALA:C | 4:7:140:LEU:C[1_554] | 0.94 | 1.26 |
| 4:6:178:LEU:CB | 4:9:177:ARG:N[1_554] | 0.94 | 1.26 |
| 4:5:316:GLU:OE1 | 4:8:297:ASN:CG[1_554] | 0.94 | 1.26 |
| 4:4:339:VAL:N | 4:7:116:ARG:N[1_554] | 0.94 | 1.26 |
| 4:6:254:ARG:NH2 | 4:9:336:LYS:NZ[1_554] | 0.94 | 1.26 |
| 4:5:154:ASP:OD2 | 4:8:111:ASN:CA[1_554] | 0.94 | 1.26 |
| 4:5:279:TYR:CD1 | 4:8:293:LEU:CD2[1_554] | 0.94 | 1.26 |
| 4:5:221:LEU:CG | 4:8:332:PRO:CB[1_554] | 0.94 | 1.26 |
| 4:4:110:LEU:C | 4:8:192:ILE:C[1_554] | 0.94 | 1.26 |
| 4:6:273:GLY:O | 4:9:162:ASN:CB[1_554] | 0.94 | 1.26 |
| 4:6:273:GLY:CA | 4:9:162:ASN:OD1[1_554] | 0.94 | 1.26 |
| 4:6:190:MET:SD | 4:9:206:ARG:NH2[1_554] | 0.94 | 1.26 |
| 4:6:299:MET:CB | 4:9:136:ILE:O[1_554] | 0.94 | 1.26 |
| 4:4:340:TRP:CZ3 | 4:7:121:GLN:CG[1_554] | 0.94 | 1.26 |
| 4:6:110:LEU:O | 4:V:192:ILE:CA[1_554] | 0.94 | 1.26 |
| 4:6:249:THR:C | 4:9:211:ASP:OD2[1_554] | 0.94 | 1.26 |
| 4:5:256:ARG:CD | 4:8:306:TYR:CD1[1_554] | 0.94 | 1.26 |
| 4:5:282:ILE:CG1 | 4:8:171:LEU:CG[1_554] | 0.94 | 1.26 |
| 4:5:335:ARG:N | 4:8:105:LEU:O[1_554] | 0.94 | 1.26 |
| 4:4:284:LYS:C | 4:8:268:GLY:O[1_554] | 0.94 | 1.26 |
| 4:5:24:ASP:C | 4:8:124:PHE:CB[1_554] | 0.94 | 1.26 |
| 4:6:21:PHE:CA | 4:9:125:GLU:OE1[1_554] | 0.94 | 1.26 |
| 4:5:210:ARG:O | 4:8:15:GLY:O[1_554] | 0.94 | 1.26 |
| 4:6:196:ARG:NH2 | 4:9:215:LYS:CG[1_554] | 0.94 | 1.26 |
| 4:5:143:TYR:CB | 4:8:372:ARG:CA[1_554] | 0.95 | 1.25 |
| 4:6:26:ALA:CA | 4:9:123:MET:CA[1_554] | 0.95 | 1.25 |
| 4:6:220:ALA:N | 4:9:335:ARG:CG[1_554] | 0.95 | 1.25 |
| 4:4:161:HIS:O | 4:7:110:LEU:CG[1_554] | 0.95 | 1.25 |
| 4:4:111:ASN:ND2 | 4:8:196:ARG:CG[1_554] | 0.95 | 1.25 |
| 4:6:340:TRP:CZ3 | 4:9:120:THR:O[1_554] | 0.95 | 1.25 |
| 4:6:223:PHE:CE2 | 4:9:304:THR:OG1[1_554] | 0.95 | 1.25 |
| 4:4:166:TYR:OH | 4:9:39:ARG:O[1_554] | 0.95 | 1.25 |
| 4:4:332:PRO:N | 4:7:135:ALA:N[1_554] | 0.95 | 1.25 |
| 4:5:140:LEU:CA | 4:8:371:HIS:ND1[1_554] | 0.95 | 1.25 |
| 4:6:281:SER:O | 4:9:173:HIS:CD2[1_554] | 0.95 | 1.25 |
| 4:4:218:TYR:CB | 4:7:336:LYS:O[1_554] | 0.95 | 1.25 |
| 4:5:310:ALA:CB | 4:8:140:LEU:C[1_554] | 0.95 | 1.25 |
| 4:6:183:ARG:NE | 4:9:72:GLU:CD[1_554] | 0.95 | 1.25 |
| 4:5:29:ALA:CA | 4:8:83:GLU:OE1[1_554] | 0.95 | 1.25 |
| 4:5:196:ARG:NE | 4:8:211:ASP:O[1_554] | 0.95 | 1.25 |
| 4:5:115:ASN:CB | 4:9:196:ARG:NE[1_554] | 0.95 | 1.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:56:ASP:CB | 4:9:37:ARG:NH1[1_554] | 0.95 | 1.25 |
| 4:5:110:LEU:CD1 | 4:9:191:LYS:CD[1_554] | 0.95 | 1.25 |
| 4:6:262:PHE:C | 4:9:153:LEU:CD1[1_554] | 0.95 | 1.25 |
| 4:6:208:ILE:N | 4:9:59:GLN:NE2[1_554] | 0.95 | 1.25 |
| 4:6:157:ASP:C | 4:9:72:GLU:O[1_554] | 0.95 | 1.25 |
| 4:5:220:ALA:CA | 4:8:335:ARG:CG[1_554] | 0.95 | 1.25 |
| 4:6:143:TYR:N | 4:9:372:ARG:CB[1_554] | 0.95 | 1.25 |
| 4:5:106:THR:CA | 4:8:114:ALA:CB[1_554] | 0.95 | 1.25 |
| 4:6:294:TYR:CA | 4:9:166:TYR:C[1_554] | 0.95 | 1.25 |
| 4:5:249:THR:O | 4:8:211:ASP:CG[1_554] | 0.95 | 1.25 |
| 4:6:339:VAL:C | 4:9:116:ARG:C[1_554] | 0.95 | 1.25 |
| 4:4:320:LEU:CG | 4:7:293:LEU:CB[1_554] | 0.95 | 1.25 |
| 4:5:308:GLY:N | 4:8:338:SER:N[1_554] | 0.95 | 1.25 |
| 4:3:112:PRO:CD | 4:7:193:LEU:CD1[1_554] | 0.95 | 1.25 |
| 4:4:308:GLY:C | 4:7:339:VAL:N[1_554] | 0.95 | 1.25 |
| 4:6:154:ASP:N | 4:9:109:PRO:CA[1_554] | 0.95 | 1.25 |
| 4:5:41:GLN:CG | 4:7:224:GLU:OE2[1_554] | 0.95 | 1.25 |
| 4:5:279:TYR:C | 4:8:285:CYS:SG[1_554] | 0.95 | 1.25 |
| 4:4:30:VAL:CG1 | 4:7:79:TRP:CA[1_554] | 0.96 | 1.24 |
| 4:4:218:TYR:CE2 | 4:7:337:TYR:CG[1_554] | 0.96 | 1.24 |
| 4:5:187:ASP:O | 4:8:183:ARG:O[1_554] | 0.96 | 1.24 |
| 4:6:24:ASP:CB | 4:9:125:GLU:N[1_554] | 0.96 | 1.24 |
| 4:5:180:LEU:CG | 4:8:178:LEU:O[1_554] | 0.96 | 1.24 |
| 4:5:211:ASP:CG | 4:8:32:PRO:CD[1_554] | 0.96 | 1.24 |
| 4:6:263:GLN:C | 4:9:274:ILE:CG1[1_554] | 0.96 | 1.24 |
| 4:4:300:SER:CA | 4:7:107:GLU:CG[1_554] | 0.96 | 1.24 |
| 4:3:175:ILE:CD1 | 4:7:191:LYS:NZ[1_554] | 0.96 | 1.24 |
| 4:6:288:ASP:C | 4:W:63:GLY:C[1_554] | 0.96 | 1.24 |
| 4:4:334:GLU:CG | 4:7:132:MET:CE[1_554] | 0.96 | 1.24 |
| 4:5:166:TYR:CB | 4:V:40:HIS:NE2[1_554] | 0.96 | 1.24 |
| 4:6:210:ARG:O | 4:9:15:GLY:O[1_554] | 0.96 | 1.24 |
| 4:5:208:ILE:CB | 4:8:59:GLN:CG[1_554] | 0.96 | 1.24 |
| 4:4:25:ASP:CB | 4:7:124:PHE:CA[1_554] | 0.96 | 1.24 |
| 4:6:271:SER:O | 4:9:277:THR:OG1[1_554] | 0.96 | 1.24 |
| 4:5:136:ILE:O | 4:8:113:LYS:CB[1_554] | 0.96 | 1.24 |
| 4:4:153:LEU:C | 4:7:109:PRO:O[1_554] | 0.96 | 1.24 |
| 4:4:188:TYR:O | 4:7:182:GLY:O[1_554] | 0.96 | 1.24 |
| 4:5:274:ILE:CD1 | 4:8:161:HIS:CA[1_554] | 0.96 | 1.24 |
| 4:6:143:TYR:CB | 4:9:372:ARG:CA[1_554] | 0.96 | 1.24 |
| 4:5:262:PHE:CA | 4:8:153:LEU:CD1[1_554] | 0.96 | 1.24 |
| 4:4:110:LEU:CD1 | 4:8:191:LYS:CG[1_554] | 0.96 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:327:ILE:CD1 | 4:8:149:THR:CB[1_554] | 0.96 | 1.24 |
| 4:5:59:GLN:CB | 4:8:68:LYS:CD[1_554] | 0.96 | 1.24 |
| 4:5:177:ARG:NH1 | 4:9:194:THR:CB[1_554] | 0.96 | 1.24 |
| 4:4:341:ILE:CB | 4:7:120:THR:CB[1_554] | 0.96 | 1.24 |
| 4:4:256:ARG:N | 4:7:302:GLY:C[1_554] | 0.96 | 1.24 |
| 4:5:340:TRP:CZ2 | 4:8:121:GLN:C[1_554] | 0.96 | 1.24 |
| 4:5:215:LYS:CG | 4:8:31:PHE:N[1_554] | 0.96 | 1.24 |
| 4:4:26:ALA:CA | 4:7:122:ILE:N[1_554] | 0.96 | 1.24 |
| 4:4:298:VAL:C | 4:7:136:ILE:CD1[1_554] | 0.96 | 1.24 |
| 4:5:183:ARG:NE | 4:8:72:GLU:CD[1_554] | 0.96 | 1.24 |
| 4:4:185:LEU:CD1 | 4:7:159:VAL:N[1_554] | 0.96 | 1.24 |
| 4:2:323:SER:O | 4:7:44:MET:SD[1_554] | 0.97 | 1.23 |
| 4:6:75:ILE:C | 4:V:197:GLY:O[1_554] | 0.97 | 1.23 |
| 4:5:253:GLU:CD | 4:8:214:GLU:CA[1_554] | 0.97 | 1.23 |
| 4:5:288:ASP:CA | 4:V:62:ARG:O[1_554] | 0.97 | 1.23 |
| 4:6:346:LEU:CB | 4:9:368:SER:CA[1_554] | 0.97 | 1.23 |
| 4:5:190:MET:O | 4:8:186:THR:CG2[1_554] | 0.97 | 1.23 |
| 4:5:321:ALA:N | 4:8:293:LEU:N[1_554] | 0.97 | 1.23 |
| 4:3:117:GLU:CD | 4:7:236:LEU:O[1_554] | 0.97 | 1.23 |
| 4:6:31:PHE:O | 4:9:78:ASN:C[1_554] | 0.97 | 1.23 |
| 4:6:110:LEU:N | 4:V:195:GLU:CD[1_554] | 0.97 | 1.23 |
| 4:4:215:LYS:CD | 4:7:31:PHE:CB[1_554] | 0.97 | 1.23 |
| 4:4:303:THR:OG1 | 4:7:74:GLY:CA[1_554] | 0.97 | 1.23 |
| 4:5:342:GLY:O | 4:8:367:PRO:O[1_554] | 0.97 | 1.23 |
| 4:5:24:ASP:O | 4:8:124:PHE:CB[1_554] | 0.97 | 1.23 |
| 4:3:367:PRO:N | 4:7:235:SER:N[1_554] | 0.97 | 1.23 |
| 4:3:370:VAL:CB | 4:7:230:ALA:O[1_554] | 0.97 | 1.23 |
| 4:6:344:SER:O | 4:9:362:TYR:CD1[1_554] | 0.97 | 1.23 |
| 4:5:347:ALA:C | 4:8:366:GLY:CA[1_554] | 0.97 | 1.23 |
| 4:6:312:ARG:CA | 4:9:298:VAL:CG1[1_554] | 0.97 | 1.23 |
| 4:5:166:TYR:CG | 4:V:40:HIS:NE2[1_554] | 0.97 | 1.23 |
| 4:6:316:GLU:OE1 | 4:9:297:ASN:CG[1_554] | 0.97 | 1.23 |
| 4:5:268:GLY:C | 4:8:264:PRO:CB[1_554] | 0.97 | 1.23 |
| 4:6:20:GLY:O | 4:9:121:GLN:NE2[1_554] | 0.97 | 1.23 |
| 4:5:75:ILE:CA | 4:9:197:GLY:C[1_554] | 0.97 | 1.23 |
| 4:6:109:PRO:C | 4:V:195:GLU:OE2[1_554] | 0.97 | 1.23 |
| 4:5:294:TYR:CG | 4:8:166:TYR:CG[1_554] | 0.97 | 1.23 |
| 4:4:259:GLU:C | 4:7:155:SER:CB[1_554] | 0.97 | 1.23 |
| 4:3:110:LEU:CB | 4:7:192:ILE:N[1_554] | 0.97 | 1.23 |
| 4:6:253:GLU:OE1 | 4:9:214:GLU:N[1_554] | 0.97 | 1.23 |
| 4:4:242:LEU:C | 4:7:60:SER:CB[1_554] | 0.98 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:192:ILE:CB | 4:9:213:LYS:CD[1_554] | 0.98 | 1.22 |
| 4:6:180:LEU:CG | 4:9:178:LEU:O[1_554] | 0.98 | 1.22 |
| 4:6:294:TYR:CG | 4:9:166:TYR:CG[1_554] | 0.98 | 1.22 |
| 4:5:221:LEU:O | 4:8:331:ALA:O[1_554] | 0.98 | 1.22 |
| 4:2:291:LYS:NZ | 4:7:39:ARG:O[1_554] | 0.98 | 1.22 |
| 4:5:310:ALA:O | 4:8:142:LEU:N[1_554] | 0.98 | 1.22 |
| 4:4:326:LYS:CE | 4:9:45:VAL:N[1_554] | 0.98 | 1.22 |
| 4:5:304:THR:CB | 4:8:137:GLN:CB[1_554] | 0.98 | 1.22 |
| 4:6:110:LEU:O | 4:V:192:ILE:C[1_554] | 0.98 | 1.22 |
| 4:6:299:MET:CB | 4:9:136:ILE:C[1_554] | 0.98 | 1.22 |
| 4:5:221:LEU:O | 4:8:331:ALA:C[1_554] | 0.98 | 1.22 |
| 4:5:273:GLY:O | 4:8:162:ASN:CB[1_554] | 0.98 | 1.22 |
| 4:4:337:TYR:CB | 4:7:119:MET:CB[1_554] | 0.98 | 1.22 |
| 4:5:312:ARG:CA | 4:8:298:VAL:CG1[1_554] | 0.98 | 1.22 |
| 4:6:181:ALA:O | 4:9:158:GLY:C[1_554] | 0.98 | 1.22 |
| 4:6:114:ALA:CB | 4:V:251:GLY:N[1_554] | 0.98 | 1.22 |
| 4:4:175:ILE:CD1 | 4:8:191:LYS:NZ[1_554] | 0.98 | 1.22 |
| 4:5:110:LEU:CD2 | 4:9:191:LYS:CE[1_554] | 0.98 | 1.22 |
| 4:6:319:ALA:CB | 4:9:296:ASN:N[1_554] | 0.98 | 1.22 |
| 4:5:370:VAL:N | 4:9:231:ALA:CA[1_554] | 0.98 | 1.22 |
| 4:5:28:ARG:NE | 4:8:126:THR:CA[1_554] | 0.98 | 1.22 |
| 4:3:115:ASN:N | 4:7:250:ILE:CA[1_554] | 0.98 | 1.22 |
| 4:3:116:ARG:O | 4:7:237:GLU:OE2[1_554] | 0.98 | 1.22 |
| 4:4:196:ARG:CB | 4:7:211:ASP:N[1_554] | 0.99 | 1.21 |
| 4:6:295:ALA:CA | 4:9:167:GLU:O[1_554] | 0.99 | 1.21 |
| 4:6:199:SER:CB | 4:9:206:ARG:N[1_554] | 0.99 | 1.21 |
| 4:4:188:TYR:CG | 4:7:181:ALA:O[1_554] | 0.99 | 1.21 |
| 4:6:316:GLU:CB | 4:9:151:ILE:O[1_554] | 0.99 | 1.21 |
| 4:5:115:ASN:CG | 4:9:196:ARG:NE[1_554] | 0.99 | 1.21 |
| 4:5:327:ILE:CG1 | 4:8:149:THR:CA[1_554] | 0.99 | 1.21 |
| 4:4:281:SER:C | 4:7:173:HIS:NE2[1_554] | 0.99 | 1.21 |
| 4:6:189:LEU:N | 4:9:182:GLY:C[1_554] | 0.99 | 1.21 |
| 4:5:113:LYS:CG | 4:9:252:ASN:O[1_554] | 0.99 | 1.21 |
| 4:4:313:MET:CG | 4:7:138:ALA:CB[1_554] | 0.99 | 1.21 |
| 4:5:336:LYS:CD | 4:8:12:ASN:OD1[1_554] | 0.99 | 1.21 |
| 4:4:192:ILE:N | 4:7:186:THR:OG1[1_554] | 0.99 | 1.21 |
| 4:6:154:ASP:N | 4:9:109:PRO:C[1_554] | 0.99 | 1.21 |
| 4:6:166:TYR:CB | 4:W:40:HIS:NE2[1_554] | 0.99 | 1.21 |
| 4:4:180:LEU:CD2 | 4:7:178:LEU:O[1_554] | 0.99 | 1.21 |
| 4:6:262:PHE:CA | 4:9:153:LEU:CD1[1_554] | 0.99 | 1.21 |
| 4:4:326:LYS:C | 4:7:167:GLU:CB[1_554] | 0.99 | 1.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:205:GLU:CA | 4:7:62:ARG:CD[1_554] | 0.99 | 1.21 |
| 4:5:312:ARG:CD | 4:8:299:MET:N[1_554] | 0.99 | 1.21 |
| 4:4:335:ARG:CG | 4:7:106:THR:C[1_554] | 0.99 | 1.21 |
| 4:6:199:SER:CA | 4:9:206:ARG:N[1_554] | 0.99 | 1.21 |
| 4:4:371:HIS:ND1 | 4:8:252:ASN:CA[1_554] | 0.99 | 1.21 |
| 4:5:192:ILE:CG1 | 4:8:213:LYS:CD[1_554] | 0.99 | 1.21 |
| 4:5:193:LEU:CD2 | 4:8:210:ARG:CD[1_554] | 0.99 | 1.21 |
| 4:5:264:PRO:CB | 4:8:178:LEU:CD2[1_554] | 0.99 | 1.21 |
| 4:3:172:PRO:CG | 4:7:266:PHE:CG[1_554] | 0.99 | 1.21 |
| 4:5:288:ASP:CB | 4:V:62:ARG:O[1_554] | 0.99 | 1.21 |
| 4:5:196:ARG:CG | 4:8:212:ILE:CA[1_554] | 0.99 | 1.21 |
| 4:6:288:ASP:CA | 4:W:62:ARG:O[1_554] | 0.99 | 1.21 |
| 4:4:154:ASP:CA | 4:7:111:ASN:N[1_554] | 1.00 | 1.20 |
| 4:5:348:SER:N | 4:8:366:GLY:CA[1_554] | 1.00 | 1.20 |
| 4:6:312:ARG:C | 4:9:298:VAL:CG1[1_554] | 1.00 | 1.20 |
| 4:5:223:PHE:CD1 | 4:8:304:THR:O[1_554] | 1.00 | 1.20 |
| 4:4:194:THR:C | 4:7:209:VAL:CB[1_554] | 1.00 | 1.20 |
| 4:5:295:ALA:CA | 4:8:167:GLU:O[1_554] | 1.00 | 1.20 |
| 4:5:259:GLU:OE2 | 4:8:309:ILE:CB[1_554] | 1.00 | 1.20 |
| 4:6:137:GLN:N | 4:9:113:LYS:N[1_554] | 1.00 | 1.20 |
| 4:4:308:GLY:CA | 4:7:338:SER:C[1_554] | 1.00 | 1.20 |
| 4:4:109:PRO:CB | 4:8:195:GLU:OE2[1_554] | 1.00 | 1.20 |
| 4:6:178:LEU:CG | 4:9:177:ARG:CA[1_554] | 1.00 | 1.20 |
| 4:5:141:SER:C | 4:8:116:ARG:NH1[1_554] | 1.00 | 1.20 |
| 4:5:334:GLU:CA | 4:8:105:LEU:CA[1_554] | 1.00 | 1.20 |
| 4:5:186:THR:C | 4:8:183:ARG:CB[1_554] | 1.00 | 1.20 |
| 4:6:317:ILE:CB | 4:9:150:GLY:C[1_554] | 1.00 | 1.20 |
| 4:6:274:ILE:C | 4:9:162:ASN:CA[1_554] | 1.00 | 1.20 |
| 4:5:158:GLY:O | 4:8:177:ARG:NH2[1_554] | 1.00 | 1.20 |
| 4:5:308:GLY:C | 4:8:338:SER:CB[1_554] | 1.00 | 1.20 |
| 4:5:140:LEU:N | 4:8:371:HIS:ND1[1_554] | 1.00 | 1.20 |
| 4:4:255:PHE:C | 4:7:302:GLY:C[1_554] | 1.00 | 1.20 |
| 4:6:215:LYS:CG | 4:9:31:PHE:N[1_554] | 1.00 | 1.20 |
| 4:5:198:TYR:CD2 | 4:8:208:ILE:C[1_554] | 1.00 | 1.20 |
| 4:3:372:ARG:CG | 4:7:227:MET:CB[1_554] | 1.00 | 1.20 |
| 4:4:180:LEU:CA | 4:7:179:ASP:OD1[1_554] | 1.00 | 1.20 |
| 4:4:312:ARG:N | 4:7:141:SER:C[1_554] | 1.00 | 1.20 |
| 4:5:270:GLU:CA | 4:8:272:ALA:N[1_554] | 1.00 | 1.20 |
| 4:6:327:ILE:O | 4:9:148:THR:OG1[1_554] | 1.00 | 1.20 |
| 4:6:334:GLU:OE1 | 4:9:133:TYR:C[1_554] | 1.00 | 1.20 |
| 4:4:26:ALA:CA | 4:7:122:ILE:CA[1_554] | 1.00 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:256:ARG:NH1 | 4:7:306:TYR:CE1[1_554] | 1.00 | 1.20 |
| 4:6:113:LYS:CD | 4:V:252:ASN:O[1_554] | 1.00 | 1.20 |
| 4:5:271:SER:O | 4:8:277:THR:OG1[1_554] | 1.01 | 1.19 |
| 4:5:113:LYS:CD | 4:9:252:ASN:O[1_554] | 1.01 | 1.19 |
| 4:4:367:PRO:CD | 4:8:235:SER:C[1_554] | 1.01 | 1.19 |
| 4:6:299:MET:SD | 4:9:139:VAL:N[1_554] | 1.01 | 1.19 |
| 4:6:305:MET:CB | 4:9:11:ASP:CG[1_554] | 1.01 | 1.19 |
| 4:5:346:LEU:CD2 | 4:8:368:SER:OG[1_554] | 1.01 | 1.19 |
| 4:5:278:THR:CG2 | 4:8:164:PRO:O[1_554] | 1.01 | 1.19 |
| 4:6:115:ASN:CG | 4:V:196:ARG:CD[1_554] | 1.01 | 1.19 |
| 4:5:137:GLN:CG | 4:8:112:PRO:C[1_554] | 1.01 | 1.19 |
| 4:6:347:ALA:N | 4:9:366:GLY:C[1_554] | 1.01 | 1.19 |
| 4:6:268:GLY:CA | 4:9:264:PRO:CA[1_554] | 1.01 | 1.19 |
| 4:4:369:ILE:C | 4:8:229:THR:O[1_554] | 1.01 | 1.19 |
| 4:6:348:SER:OG | 4:9:362:TYR:O[1_554] | 1.01 | 1.19 |
| 4:5:210:ARG:CZ | 4:8:33:SER:C[1_554] | 1.01 | 1.19 |
| 4:4:218:TYR:CG | 4:7:337:TYR:CD1[1_554] | 1.01 | 1.19 |
| 4:4:188:TYR:C | 4:7:183:ARG:N[1_554] | 1.01 | 1.19 |
| 4:3:286:ASP:CA | 4:7:270:GLU:OE2[1_554] | 1.01 | 1.19 |
| 4:3:372:ARG:CA | 4:7:226:GLU:O[1_554] | 1.01 | 1.19 |
| 4:5:56:ASP:CB | 4:8:37:ARG:NH1[1_554] | 1.01 | 1.19 |
| 4:5:26:ALA:O | 4:8:122:ILE:O[1_554] | 1.01 | 1.19 |
| 4:5:28:ARG:NH2 | 4:8:125:GLU:O[1_554] | 1.01 | 1.19 |
| 4:5:195:GLU:CB | 4:8:189:LEU:CB[1_554] | 1.01 | 1.19 |
| 4:4:159:VAL:C | 4:7:177:ARG:NH1[1_554] | 1.01 | 1.19 |
| 4:5:338:SER:OG | 4:8:134:VAL:CG1[1_554] | 1.01 | 1.19 |
| 4:6:28:ARG:NH2 | 4:9:125:GLU:O[1_554] | 1.01 | 1.19 |
| 4:5:262:PHE:C | 4:8:153:LEU:CD1[1_554] | 1.01 | 1.19 |
| 4:6:156:GLY:CA | 4:9:74:GLY:C[1_554] | 1.01 | 1.19 |
| 4:6:214:GLU:OE2 | 4:9:33:SER:OG[1_554] | 1.01 | 1.19 |
| 4:6:153:LEU:CD1 | 4:9:163:VAL:CG2[1_554] | 1.01 | 1.19 |
| 4:5:340:TRP:CZ3 | 4:8:120:THR:O[1_554] | 1.01 | 1.19 |
| 4:6:255:PHE:CD1 | 4:9:305:MET:C[1_554] | 1.01 | 1.19 |
| 4:4:192:ILE:CB | 4:7:213:LYS:CD[1_554] | 1.01 | 1.19 |
| 4:4:327:ILE:CG2 | 4:7:148:THR:O[1_554] | 1.01 | 1.19 |
| 4:6:194:THR:CA | 4:9:209:VAL:CB[1_554] | 1.01 | 1.19 |
| 4:6:186:THR:C | 4:9:183:ARG:CB[1_554] | 1.01 | 1.19 |
| 4:4:256:ARG:O | 4:7:303:THR:CA[1_554] | 1.01 | 1.19 |
| 4:5:223:PHE:CE2 | 4:8:304:THR:OG1[1_554] | 1.01 | 1.19 |
| 4:6:327:ILE:CD1 | 4:9:149:THR:CG2[1_554] | 1.01 | 1.19 |
| 4:5:372:ARG:N | 4:9:227:MET:O[1_554] | 1.02 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:110:LEU:C | 4:7:192:ILE:C[1_554] | 1.02 | 1.18 |
| 4:6:227:MET:CA | 4:9:307:PRO:CB[1_554] | 1.02 | 1.18 |
| 4:6:310:ALA:CA | 4:9:141:SER:C[1_554] | 1.02 | 1.18 |
| 4:6:205:GLU:CA | 4:9:62:ARG:CZ[1_554] | 1.02 | 1.18 |
| 4:5:227:MET:CA | 4:8:307:PRO:CB[1_554] | 1.02 | 1.18 |
| 4:5:281:SER:OG | 4:8:173:HIS:N[1_554] | 1.02 | 1.18 |
| 4:4:265:SER:O | 4:7:261:LEU:CA[1_554] | 1.02 | 1.18 |
| 4:6:27:PRO:C | 4:9:122:ILE:CG2[1_554] | 1.02 | 1.18 |
| 4:6:24:ASP:O | 4:9:124:PHE:CB[1_554] | 1.02 | 1.18 |
| 4:5:314:GLN:CA | 4:8:142:LEU:CD1[1_554] | 1.02 | 1.18 |
| 4:6:199:SER:N | 4:9:205:GLU:O[1_554] | 1.02 | 1.18 |
| 4:4:327:ILE:CB | 4:7:148:THR:O[1_554] | 1.02 | 1.18 |
| 4:5:156:GLY:O | 4:8:74:GLY:CA[1_554] | 1.02 | 1.18 |
| 4:6:370:VAL:CA | 4:V:231:ALA:CA[1_554] | 1.02 | 1.18 |
| 4:6:166:TYR:CG | 4:W:40:HIS:ND1[1_554] | 1.02 | 1.18 |
| 4:4:139:VAL:N | 4:7:113:LYS:CG[1_554] | 1.02 | 1.18 |
| 4:6:26:ALA:C | 4:9:123:MET:N[1_554] | 1.02 | 1.18 |
| 4:5:276:GLU:C | 4:8:281:SER:CB[1_554] | 1.02 | 1.18 |
| 4:4:110:LEU:CA | 4:8:192:ILE:CB[1_554] | 1.02 | 1.18 |
| 4:4:242:LEU:O | 4:7:60:SER:CB[1_554] | 1.02 | 1.18 |
| 4:5:254:ARG:NH2 | 4:8:336:LYS:NZ[1_554] | 1.02 | 1.18 |
| 4:5:219:VAL:CG2 | 4:8:301:GLY:N[1_554] | 1.02 | 1.18 |
| 4:3:113:LYS:CB | 4:7:254:ARG:CB[1_554] | 1.02 | 1.18 |
| 4:6:327:ILE:CG1 | 4:9:149:THR:CA[1_554] | 1.02 | 1.18 |
| 4:5:154:ASP:N | 4:8:109:PRO:CA[1_554] | 1.02 | 1.18 |
| 4:4:172:PRO:CG | 4:8:266:PHE:CG[1_554] | 1.02 | 1.18 |
| 4:3:177:ARG:CZ | 4:7:194:THR:CG2[1_554] | 1.02 | 1.18 |
| 4:5:283:MET:CB | 4:8:285:CYS:O[1_554] | 1.02 | 1.18 |
| 4:5:305:MET:O | 4:8:11:ASP:OD2[1_554] | 1.02 | 1.18 |
| 4:5:196:ARG:CA | 4:8:212:ILE:CB[1_554] | 1.02 | 1.18 |
| 4:5:162:ASN:N | 4:8:110:LEU:CD2[1_554] | 1.02 | 1.18 |
| 4:6:145:SER:CA | 4:9:372:ARG:NH2[1_554] | 1.02 | 1.18 |
| 4:6:282:ILE:CG1 | 4:9:171:LEU:CD1[1_554] | 1.02 | 1.18 |
| 4:4:183:ARG:CG | 4:7:72:GLU:OE2[1_554] | 1.02 | 1.18 |
| 4:6:273:GLY:C | 4:9:162:ASN:OD1[1_554] | 1.02 | 1.18 |
| 4:5:174:ALA:O | 4:8:173:HIS:CA[1_554] | 1.02 | 1.18 |
| 4:6:340:TRP:CH2 | 4:9:121:GLN:C[1_554] | 1.02 | 1.18 |
| 4:5:31:PHE:O | 4:8:78:ASN:C[1_554] | 1.02 | 1.18 |
| 4:4:204:ALA:O | 4:7:62:ARG:CB[1_554] | 1.02 | 1.18 |
| 4:4:265:SER:CA | 4:7:261:LEU:O[1_554] | 1.02 | 1.18 |
| 4:5:208:ILE:N | 4:8:59:GLN:NE2[1_554] | 1.03 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:299:MET:CA | 4:9:136:ILE:CB[1_554] | 1.03 | 1.17 |
| 4:6:17:VAL:C | 4:9:79:TRP:CG[1_554] | 1.03 | 1.17 |
| 4:6:157:ASP:N | 4:9:75:ILE:N[1_554] | 1.03 | 1.17 |
| 4:4:319:ALA:O | 4:7:292:ASP:O[1_554] | 1.03 | 1.17 |
| 4:4:113:LYS:CG | 4:8:254:ARG:CA[1_554] | 1.03 | 1.17 |
| 4:3:115:ASN:CB | 4:7:249:THR:O[1_554] | 1.03 | 1.17 |
| 4:5:191:LYS:C | 4:8:186:THR:CA[1_554] | 1.03 | 1.17 |
| 4:6:180:LEU:CB | 4:9:178:LEU:C[1_554] | 1.03 | 1.17 |
| 4:6:319:ALA:O | 4:9:294:TYR:C[1_554] | 1.03 | 1.17 |
| 4:4:204:ALA:C | 4:7:62:ARG:CB[1_554] | 1.03 | 1.17 |
| 4:6:115:ASN:CB | 4:V:196:ARG:CD[1_554] | 1.03 | 1.17 |
| 4:4:297:ASN:OD1 | 4:7:170:ALA:N[1_554] | 1.03 | 1.17 |
| 4:4:267:ILE:CD1 | 4:7:180:LEU:N[1_554] | 1.03 | 1.17 |
| 4:4:264:PRO:N | 4:7:274:ILE:CD1[1_554] | 1.03 | 1.17 |
| 4:3:113:LYS:CG | 4:7:254:ARG:CA[1_554] | 1.03 | 1.17 |
| 4:4:222:ASP:CB | 4:7:332:PRO:N[1_554] | 1.03 | 1.17 |
| 4:5:192:ILE:CB | 4:8:213:LYS:CD[1_554] | 1.03 | 1.17 |
| 4:4:214:GLU:C | 4:7:16:LEU:C[1_554] | 1.03 | 1.17 |
| 4:5:262:PHE:CA | 4:8:153:LEU:CG[1_554] | 1.03 | 1.17 |
| 4:4:226:GLU:OE1 | 4:7:333:PRO:O[1_554] | 1.03 | 1.17 |
| 4:4:333:PRO:O | 4:7:105:LEU:CG[1_554] | 1.03 | 1.17 |
| 4:6:227:MET:SD | 4:9:307:PRO:N[1_554] | 1.03 | 1.17 |
| 4:4:297:ASN:ND2 | 4:7:170:ALA:CB[1_554] | 1.03 | 1.17 |
| 4:6:214:GLU:C | 4:9:16:LEU:CB[1_554] | 1.03 | 1.17 |
| 1:D:637:LYS:CG | 4:6:311:ASP:OD1[1_556] | 1.03 | 1.17 |
| 4:6:26:ALA:CA | 4:9:123:MET:CB[1_554] | 1.03 | 1.17 |
| 4:3:115:ASN:N | 4:7:250:ILE:N[1_554] | 1.03 | 1.17 |
| 4:5:348:SER:CB | 4:8:362:TYR:O[1_554] | 1.03 | 1.17 |
| 4:6:345:ILE:CA | 4:9:369:ILE:CG2[1_554] | 1.03 | 1.17 |
| 4:4:185:LEU:CA | 4:7:158:GLY:CA[1_554] | 1.03 | 1.17 |
| 4:5:187:ASP:C | 4:8:183:ARG:C[1_554] | 1.03 | 1.17 |
| 4:6:189:LEU:N | 4:9:182:GLY:O[1_554] | 1.03 | 1.17 |
| 4:6:59:GLN:CG | 4:9:68:LYS:CG[1_554] | 1.03 | 1.17 |
| 4:4:370:VAL:O | 4:8:230:ALA:CB[1_554] | 1.03 | 1.17 |
| 4:5:207:GLU:OE1 | 4:8:67:LEU:CD2[1_554] | 1.03 | 1.17 |
| 4:4:182:GLY:N | 4:7:73:HIS:CA[1_554] | 1.03 | 1.17 |
| 4:6:259:GLU:OE2 | 4:9:309:ILE:CG1[1_554] | 1.03 | 1.17 |
| 4:6:196:ARG:CG | 4:9:212:ILE:CA[1_554] | 1.03 | 1.17 |
| 4:6:295:ALA:C | 4:9:167:GLU:O[1_554] | 1.03 | 1.17 |
| 4:4:188:TYR:CD2 | 4:7:182:GLY:CA[1_554] | 1.04 | 1.16 |
| 4:4:298:VAL:O | 4:7:136:ILE:CD1[1_554] | 1.04 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:312:ARG:CZ | 4:7:299:MET:CA[1_554] | 1.04 | 1.16 |
| 4:3:109:PRO:CB | 4:7:195:GLU:OE2[1_554] | 1.04 | 1.16 |
| 4:6:187:ASP:N | 4:9:183:ARG:CG[1_554] | 1.04 | 1.16 |
| 4:3:111:ASN:O | 4:7:253:GLU:CG[1_554] | 1.04 | 1.16 |
| 4:6:214:GLU:CA | 4:9:16:LEU:CA[1_554] | 1.04 | 1.16 |
| 4:5:255:PHE:CD1 | 4:8:305:MET:C[1_554] | 1.04 | 1.16 |
| 4:5:299:MET:O | 4:8:136:ILE:N[1_554] | 1.04 | 1.16 |
| 4:6:220:ALA:CA | 4:9:335:ARG:CG[1_554] | 1.04 | 1.16 |
| 4:5:110:LEU:O | 4:9:192:ILE:CA[1_554] | 1.04 | 1.16 |
| 4:5:317:ILE:N | 4:8:151:ILE:N[1_554] | 1.04 | 1.16 |
| 4:6:271:SER:C | 4:9:277:THR:OG1[1_554] | 1.04 | 1.16 |
| 4:6:341:ILE:CA | 4:9:120:THR:OG1[1_554] | 1.04 | 1.16 |
| 4:5:114:ALA:CB | 4:9:251:GLY:N[1_554] | 1.04 | 1.16 |
| 4:4:254:ARG:CZ | 4:7:337:TYR:OH[1_554] | 1.04 | 1.16 |
| 4:6:199:SER:C | 4:9:206:ARG:CA[1_554] | 1.04 | 1.16 |
| 4:6:337:TYR:CZ | 4:9:86:TRP:CZ2[1_554] | 1.04 | 1.16 |
| 4:5:218:TYR:CA | 4:8:336:LYS:CA[1_554] | 1.04 | 1.16 |
| 4:4:340:TRP:CE3 | 4:7:121:GLN:CB[1_554] | 1.04 | 1.16 |
| 4:5:178:LEU:CG | 4:8:177:ARG:CA[1_554] | 1.04 | 1.16 |
| 4:4:341:ILE:CD1 | 4:7:120:THR:CA[1_554] | 1.04 | 1.16 |
| 4:4:335:ARG:CZ | 4:7:106:THR:CB[1_554] | 1.04 | 1.16 |
| 4:2:291:LYS:CD | 4:7:39:ARG:C[1_554] | 1.04 | 1.16 |
| 4:6:290:ARG:NE | 4:9:286:ASP:CG[1_554] | 1.04 | 1.16 |
| 4:5:16:LEU:N | 4:8:77:THR:N[1_554] | 1.04 | 1.16 |
| 4:6:310:ALA:CB | 4:9:140:LEU:C[1_554] | 1.04 | 1.16 |
| 4:5:199:SER:C | 4:8:206:ARG:CB[1_554] | 1.04 | 1.16 |
| 4:6:186:THR:CB | 4:9:183:ARG:NE[1_554] | 1.04 | 1.16 |
| 4:4:227:MET:CG | 4:7:305:MET:O[1_554] | 1.04 | 1.16 |
| 4:3:166:TYR:OH | 4:8:39:ARG:O[1_554] | 1.04 | 1.16 |
| 4:4:194:THR:O | 4:7:209:VAL:CA[1_554] | 1.04 | 1.16 |
| 4:6:278:THR:CG2 | 4:9:164:PRO:O[1_554] | 1.04 | 1.16 |
| 4:5:115:ASN:N | 4:9:196:ARG:CZ[1_554] | 1.04 | 1.16 |
| 4:4:18:LYS:CD | 4:7:79:TRP:CD2[1_554] | 1.04 | 1.16 |
| 4:5:187:ASP:N | 4:8:183:ARG:CG[1_554] | 1.04 | 1.16 |
| 4:6:283:MET:CB | 4:9:285:CYS:O[1_554] | 1.04 | 1.16 |
| 4:6:316:GLU:C | 4:9:296:ASN:O[1_554] | 1.04 | 1.16 |
| 4:5:325:MET:SD | 4:8:166:TYR:CZ[1_554] | 1.04 | 1.16 |
| 4:5:266:PHE:N | 4:8:261:LEU:CA[1_554] | 1.04 | 1.16 |
| 4:6:288:ASP:C | 4:W:64:ILE:N[1_554] | 1.04 | 1.16 |
| 4:5:294:TYR:OH | 4:8:289:ILE:CD1[1_554] | 1.04 | 1.16 |
| 4:5:278:THR:CG2 | 4:8:164:PRO:C[1_554] | 1.04 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:258:PRO:O | 4:7:155:SER:N[1_554] | 1.04 | 1.16 |
| 4:6:140:LEU:N | 4:9:371:HIS:CE1[1_554] | 1.04 | 1.16 |
| 4:5:199:SER:CA | 4:8:206:ARG:N[1_554] | 1.05 | 1.15 |
| 4:4:193:LEU:O | 4:7:210:ARG:N[1_554] | 1.05 | 1.15 |
| 4:4:31:PHE:CA | 4:7:78:ASN:OD1[1_554] | 1.05 | 1.15 |
| 4:2:291:LYS:N | 4:7:40:HIS:ND1[1_554] | 1.05 | 1.15 |
| 4:6:369:ILE:CG2 | 4:V:232:SER:N[1_554] | 1.05 | 1.15 |
| 4:4:142:LEU:O | 4:7:372:ARG:CB[1_554] | 1.05 | 1.15 |
| 4:5:117:GLU:OE2 | 4:9:236:LEU:CD1[1_554] | 1.05 | 1.15 |
| 4:6:257:CYS:C | 4:9:303:THR:CB[1_554] | 1.05 | 1.15 |
| 4:5:198:TYR:CD1 | 4:8:208:ILE:CA[1_554] | 1.05 | 1.15 |
| 4:4:137:GLN:C | 4:7:113:LYS:N[1_554] | 1.05 | 1.15 |
| 4:5:27:PRO:CA | 4:8:122:ILE:CB[1_554] | 1.05 | 1.15 |
| 4:5:189:LEU:N | 4:8:182:GLY:C[1_554] | 1.05 | 1.15 |
| 4:3:108:ALA:CB | 4:7:195:GLU:O[1_554] | 1.05 | 1.15 |
| 4:3:111:ASN:ND2 | 4:7:196:ARG:CG[1_554] | 1.05 | 1.15 |
| 4:4:154:ASP:CB | 4:7:110:LEU:C[1_554] | 1.05 | 1.15 |
| 4:3:367:PRO:N | 4:7:235:SER:CA[1_554] | 1.05 | 1.15 |
| 4:4:267:ILE:C | 4:7:180:LEU:CD2[1_554] | 1.05 | 1.15 |
| 4:4:340:TRP:CD1 | 4:7:118:LYS:CD[1_554] | 1.05 | 1.15 |
| 4:6:113:LYS:CB | 4:V:253:GLU:N[1_554] | 1.05 | 1.15 |
| 4:6:196:ARG:NE | 4:9:211:ASP:O[1_554] | 1.05 | 1.15 |
| 4:5:180:LEU:CB | 4:8:178:LEU:C[1_554] | 1.05 | 1.15 |
| 4:5:156:GLY:CA | 4:8:74:GLY:C[1_554] | 1.05 | 1.15 |
| 4:6:164:PRO:N | 4:9:172:PRO:CG[1_554] | 1.05 | 1.15 |
| 4:6:160:THR:CG2 | 4:9:161:HIS:CD2[1_554] | 1.05 | 1.15 |
| 4:5:112:PRO:C | 4:9:253:GLU:OE1[1_554] | 1.05 | 1.15 |
| 4:6:59:GLN:CB | 4:9:68:LYS:CD[1_554] | 1.05 | 1.15 |
| 4:5:372:ARG:O | 4:9:227:MET:CB[1_554] | 1.05 | 1.15 |
| 4:4:218:TYR:CD2 | 4:7:337:TYR:CD1[1_554] | 1.05 | 1.15 |
| 4:4:193:LEU:CD1 | 4:7:210:ARG:NE[1_554] | 1.05 | 1.15 |
| 4:6:214:GLU:CB | 4:9:16:LEU:C[1_554] | 1.05 | 1.15 |
| 4:4:288:ASP:O | 4:9:64:ILE:CA[1_554] | 1.05 | 1.15 |
| 4:4:112:PRO:CD | 4:8:193:LEU:CD1[1_554] | 1.05 | 1.15 |
| 4:6:294:TYR:C | 4:9:166:TYR:O[1_554] | 1.05 | 1.15 |
| 4:6:310:ALA:O | 4:9:142:LEU:N[1_554] | 1.05 | 1.15 |
| 4:6:331:ALA:CB | 4:9:140:LEU:CB[1_554] | 1.05 | 1.15 |
| 4:4:334:GLU:CA | 4:7:105:LEU:CD1[1_554] | 1.05 | 1.15 |
| 4:5:204:ALA:CA | 4:8:62:ARG:CG[1_554] | 1.06 | 1.14 |
| 4:4:318:THR:CA | 4:7:149:THR:O[1_554] | 1.06 | 1.14 |
| 4:6:188:TYR:N | 4:9:183:ARG:C[1_554] | 1.06 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:20:GLY:O | 4:8:121:GLN:NE2[1_554] | 1.06 | 1.14 |
| 4:6:266:PHE:CG | 4:9:261:LEU:CD1[1_554] | 1.06 | 1.14 |
| 4:4:339:VAL:CB | 4:7:115:ASN:N[1_554] | 1.06 | 1.14 |
| 4:4:337:TYR:CE2 | 4:7:86:TRP:CZ3[1_554] | 1.06 | 1.14 |
| 4:5:315:LYS:O | 4:8:296:ASN:C[1_554] | 1.06 | 1.14 |
| 4:3:109:PRO:CB | 4:7:195:GLU:CD[1_554] | 1.06 | 1.14 |
| 4:2:291:LYS:C | 4:7:40:HIS:CG[1_554] | 1.06 | 1.14 |
| 4:6:154:ASP:OD2 | 4:9:111:ASN:CA[1_554] | 1.06 | 1.14 |
| 4:6:41:GLN:CG | 4:8:224:GLU:OE2[1_554] | 1.06 | 1.14 |
| 4:4:304:THR:OG1 | 4:7:107:GLU:C[1_554] | 1.06 | 1.14 |
| 4:4:288:ASP:O | 4:9:64:ILE:C[1_554] | 1.06 | 1.14 |
| 4:6:294:TYR:CD2 | 4:9:166:TYR:CD1[1_554] | 1.06 | 1.14 |
| 4:6:24:ASP:C | 4:9:124:PHE:CB[1_554] | 1.06 | 1.14 |
| 4:4:338:SER:O | 4:7:116:ARG:C[1_554] | 1.06 | 1.14 |
| 4:6:193:LEU:CD2 | 4:9:210:ARG:CD[1_554] | 1.06 | 1.14 |
| 4:6:266:PHE:CA | 4:9:261:LEU:CA[1_554] | 1.06 | 1.14 |
| 4:4:199:SER:CA | 4:7:206:ARG:CA[1_554] | 1.06 | 1.14 |
| 4:6:140:LEU:N | 4:9:371:HIS:ND1[1_554] | 1.06 | 1.14 |
| 4:6:22:ALA:CA | 4:9:362:TYR:OH[1_554] | 1.06 | 1.14 |
| 4:6:25:ASP:CB | 4:9:129:VAL:CG2[1_554] | 1.06 | 1.14 |
| 4:5:24:ASP:CA | 4:8:124:PHE:C[1_554] | 1.06 | 1.14 |
| 4:5:227:MET:CB | 4:8:307:PRO:C[1_554] | 1.06 | 1.14 |
| 4:6:252:ASN:OD1 | 4:9:215:LYS:O[1_554] | 1.06 | 1.14 |
| 4:5:253:GLU:OE1 | 4:8:213:LYS:C[1_554] | 1.06 | 1.14 |
| 4:5:75:ILE:O | 4:9:197:GLY:O[1_554] | 1.06 | 1.14 |
| 4:5:199:SER:C | 4:8:206:ARG:CA[1_554] | 1.06 | 1.14 |
| 4:4:367:PRO:N | 4:8:235:SER:N[1_554] | 1.06 | 1.14 |
| 4:6:208:ILE:CB | 4:9:59:GLN:CD[1_554] | 1.06 | 1.14 |
| 4:6:314:GLN:OE1 | 4:9:147:ARG:CG[1_554] | 1.06 | 1.14 |
| 4:4:372:ARG:CB | 4:8:227:MET:CA[1_554] | 1.06 | 1.14 |
| 4:6:221:LEU:O | 4:9:331:ALA:C[1_554] | 1.06 | 1.14 |
| 4:5:188:TYR:CE1 | 4:8:185:LEU:CD1[1_554] | 1.07 | 1.13 |
| 4:5:194:THR:O | 4:8:209:VAL:CG2[1_554] | 1.07 | 1.13 |
| 4:4:156:GLY:CA | 4:7:75:ILE:CA[1_554] | 1.07 | 1.13 |
| 4:6:16:LEU:N | 4:9:77:THR:N[1_554] | 1.07 | 1.13 |
| 4:4:256:ARG:C | 4:7:303:THR:CA[1_554] | 1.07 | 1.13 |
| 4:4:115:ASN:CB | 4:8:249:THR:O[1_554] | 1.07 | 1.13 |
| 4:4:18:LYS:CE | 4:7:79:TRP:CE2[1_554] | 1.07 | 1.13 |
| 4:5:345:ILE:CA | 4:8:369:ILE:CG2[1_554] | 1.07 | 1.13 |
| 4:6:191:LYS:C | 4:9:186:THR:CA[1_554] | 1.07 | 1.13 |
| 4:4:18:LYS:CE | 4:7:79:TRP:NE1[1_554] | 1.07 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:22:ALA:CA | 4:8:362:TYR:OH[1_554] | 1.07 | 1.13 |
| 4:6:223:PHE:CD1 | 4:9:304:THR:O[1_554] | 1.07 | 1.13 |
| 4:4:337:TYR:CA | 4:7:119:MET:CB[1_554] | 1.07 | 1.13 |
| 4:3:177:ARG:NH1 | 4:7:194:THR:CB[1_554] | 1.07 | 1.13 |
| 4:5:60:SER:CB | 4:8:37:ARG:CB[1_554] | 1.07 | 1.13 |
| 4:5:250:ILE:CB | 4:8:214:GLU:OE1[1_554] | 1.07 | 1.13 |
| 4:6:192:ILE:O | 4:9:213:LYS:CB[1_554] | 1.07 | 1.13 |
| 4:5:161:HIS:C | 4:8:110:LEU:CG[1_554] | 1.07 | 1.13 |
| 4:5:106:THR:CG2 | 4:8:114:ALA:CA[1_554] | 1.07 | 1.13 |
| 4:5:314:GLN:OE1 | 4:8:147:ARG:CG[1_554] | 1.07 | 1.13 |
| 4:5:339:VAL:C | 4:8:116:ARG:CA[1_554] | 1.07 | 1.13 |
| 4:5:137:GLN:N | 4:8:113:LYS:N[1_554] | 1.07 | 1.13 |
| 4:5:26:ALA:CA | 4:8:123:MET:CB[1_554] | 1.07 | 1.13 |
| 4:3:288:ASP:O | 4:8:64:ILE:C[1_554] | 1.07 | 1.13 |
| 4:4:283:MET:CB | 4:7:286:ASP:N[1_554] | 1.07 | 1.13 |
| 4:6:115:ASN:N | 4:V:196:ARG:NH2[1_554] | 1.07 | 1.13 |
| 4:5:268:GLY:CA | 4:8:264:PRO:CA[1_554] | 1.07 | 1.13 |
| 4:4:223:PHE:CA | 4:7:335:ARG:NE[1_554] | 1.07 | 1.13 |
| 4:3:369:ILE:C | 4:7:229:THR:O[1_554] | 1.07 | 1.13 |
| 4:5:200:PHE:N | 4:8:206:ARG:CG[1_554] | 1.07 | 1.13 |
| 4:4:223:PHE:CA | 4:7:335:ARG:CD[1_554] | 1.07 | 1.13 |
| 4:4:308:GLY:N | 4:7:340:TRP:N[1_554] | 1.08 | 1.12 |
| 4:6:372:ARG:O | 4:V:227:MET:CB[1_554] | 1.08 | 1.12 |
| 4:4:286:ASP:CA | 4:8:270:GLU:OE1[1_554] | 1.08 | 1.12 |
| 4:6:26:ALA:C | 4:9:123:MET:CA[1_554] | 1.08 | 1.12 |
| 4:6:205:GLU:N | 4:9:62:ARG:CD[1_554] | 1.08 | 1.12 |
| 4:5:259:GLU:CD | 4:8:309:ILE:CD1[1_554] | 1.08 | 1.12 |
| 4:5:257:CYS:C | 4:8:303:THR:CB[1_554] | 1.08 | 1.12 |
| 4:5:277:THR:O | 4:8:174:ALA:C[1_554] | 1.08 | 1.12 |
| 4:6:278:THR:OG1 | 4:9:163:VAL:C[1_554] | 1.08 | 1.12 |
| 4:6:264:PRO:CB | 4:9:178:LEU:CD2[1_554] | 1.08 | 1.12 |
| 4:6:256:ARG:CD | 4:9:306:TYR:CD1[1_554] | 1.08 | 1.12 |
| 4:6:309:ILE:CA | 4:9:141:SER:OG[1_554] | 1.08 | 1.12 |
| 4:6:75:ILE:CB | 4:V:198:TYR:N[1_554] | 1.08 | 1.12 |
| 4:5:265:SER:O | 4:8:260:THR:O[1_554] | 1.08 | 1.12 |
| 4:5:339:VAL:CA | 4:8:116:ARG:CB[1_554] | 1.08 | 1.12 |
| 4:6:60:SER:C | 4:9:66:THR:OG1[1_554] | 1.08 | 1.12 |
| 4:3:173:HIS:CA | 4:7:267:ILE:CG2[1_554] | 1.08 | 1.12 |
| 4:5:110:LEU:N | 4:9:195:GLU:CD[1_554] | 1.08 | 1.12 |
| 4:5:309:ILE:CD1 | 4:8:154:ASP:OD2[1_554] | 1.08 | 1.12 |
| 4:4:115:ASN:N | 4:8:250:ILE:N[1_554] | 1.08 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:334:GLU:N | 4:8:105:LEU:N[1_554] | 1.08 | 1.12 |
| 4:6:157:ASP:OD1 | 4:9:71:ILE:O[1_554] | 1.08 | 1.12 |
| 4:6:196:ARG:C | 4:9:212:ILE:CB[1_554] | 1.08 | 1.12 |
| 4:5:181:ALA:O | 4:8:158:GLY:C[1_554] | 1.08 | 1.12 |
| 4:6:115:ASN:CG | 4:V:196:ARG:NE[1_554] | 1.08 | 1.12 |
| 4:5:286:ASP:CA | 4:9:270:GLU:CD[1_554] | 1.08 | 1.12 |
| 4:6:336:LYS:CD | 4:9:12:ASN:OD1[1_554] | 1.08 | 1.12 |
| 4:6:23:GLY:N | 4:9:362:TYR:CD2[1_554] | 1.08 | 1.12 |
| 4:5:326:LYS:CG | 4:8:167:GLU:OE1[1_554] | 1.09 | 1.11 |
| 4:5:162:ASN:CG | 4:8:175:ILE:CG1[1_554] | 1.09 | 1.11 |
| 4:5:309:ILE:CA | 4:8:141:SER:OG[1_554] | 1.09 | 1.11 |
| 4:6:141:SER:C | 4:9:116:ARG:CZ[1_554] | 1.09 | 1.11 |
| 4:5:166:TYR:OH | 4:V:39:ARG:CA[1_554] | 1.09 | 1.11 |
| 4:4:116:ARG:N | 4:8:196:ARG:NH2[1_554] | 1.09 | 1.11 |
| 4:6:349:LEU:CB | 4:9:365:ALA:CB[1_554] | 1.09 | 1.11 |
| 4:5:205:GLU:N | 4:8:62:ARG:CD[1_554] | 1.09 | 1.11 |
| 4:5:274:ILE:CG1 | 4:8:161:HIS:CB[1_554] | 1.09 | 1.11 |
| 4:6:110:LEU:CG | 4:V:191:LYS:CD[1_554] | 1.09 | 1.11 |
| 4:4:320:LEU:CB | 4:7:293:LEU:CB[1_554] | 1.09 | 1.11 |
| 4:4:142:LEU:O | 4:7:372:ARG:CA[1_554] | 1.09 | 1.11 |
| 4:4:177:ARG:NH1 | 4:8:194:THR:CB[1_554] | 1.09 | 1.11 |
| 4:5:157:ASP:OD2 | 4:8:72:GLU:CA[1_554] | 1.09 | 1.11 |
| 4:3:370:VAL:O | 4:7:230:ALA:CB[1_554] | 1.09 | 1.11 |
| 4:3:372:ARG:CB | 4:7:227:MET:CA[1_554] | 1.09 | 1.11 |
| 4:5:320:LEU:N | 4:8:293:LEU:C[1_554] | 1.09 | 1.11 |
| 4:5:166:TYR:OH | 4:V:39:ARG:C[1_554] | 1.09 | 1.11 |
| 4:4:320:LEU:CA | 4:7:293:LEU:CA[1_554] | 1.09 | 1.11 |
| 4:5:214:GLU:CB | 4:8:16:LEU:C[1_554] | 1.09 | 1.11 |
| 4:5:187:ASP:N | 4:8:183:ARG:CB[1_554] | 1.09 | 1.11 |
| 4:5:188:TYR:N | 4:8:183:ARG:C[1_554] | 1.09 | 1.11 |
| 4:5:220:ALA:N | 4:8:335:ARG:CG[1_554] | 1.09 | 1.11 |
| 4:5:157:ASP:N | 4:8:75:ILE:N[1_554] | 1.09 | 1.11 |
| 4:5:319:ALA:O | 4:8:294:TYR:C[1_554] | 1.09 | 1.11 |
| 4:6:339:VAL:CA | 4:9:116:ARG:CA[1_554] | 1.09 | 1.11 |
| 4:5:178:LEU:CB | 4:8:177:ARG:N[1_554] | 1.09 | 1.11 |
| 4:5:299:MET:CB | 4:8:136:ILE:O[1_554] | 1.09 | 1.11 |
| 4:5:274:ILE:O | 4:8:162:ASN:O[1_554] | 1.09 | 1.11 |
| 4:5:333:PRO:CG | 4:8:104:LEU:CB[1_554] | 1.09 | 1.11 |
| 4:5:136:ILE:N | 4:8:113:LYS:CE[1_554] | 1.09 | 1.11 |
| 4:4:196:ARG:NE | 4:7:211:ASP:CG[1_554] | 1.10 | 1.10 |
| 4:4:253:GLU:CG | 4:7:214:GLU:CG[1_554] | 1.10 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:196:ARG:NH2 | 4:8:215:LYS:CG[1_554] | 1.10 | 1.10 |
| 4:4:173:HIS:CB | 4:8:267:ILE:CG1[1_554] | 1.10 | 1.10 |
| 4:6:115:ASN:CB | 4:V:196:ARG:NE[1_554] | 1.10 | 1.10 |
| 4:6:346:LEU:CD2 | 4:9:368:SER:OG[1_554] | 1.10 | 1.10 |
| 4:6:164:PRO:CD | 4:9:172:PRO:CG[1_554] | 1.10 | 1.10 |
| 4:4:371:HIS:CE1 | 4:8:252:ASN:O[1_554] | 1.10 | 1.10 |
| 4:4:118:LYS:CB | 4:8:249:THR:OG1[1_554] | 1.10 | 1.10 |
| 4:4:196:ARG:CA | 4:7:212:ILE:N[1_554] | 1.10 | 1.10 |
| 4:5:193:LEU:CD2 | 4:8:210:ARG:CG[1_554] | 1.10 | 1.10 |
| 4:3:109:PRO:CA | 4:7:195:GLU:OE1[1_554] | 1.10 | 1.10 |
| 4:6:310:ALA:CB | 4:9:140:LEU:O[1_554] | 1.10 | 1.10 |
| 4:4:274:ILE:CD1 | 4:7:161:HIS:CG[1_554] | 1.10 | 1.10 |
| 4:5:26:ALA:O | 4:8:122:ILE:C[1_554] | 1.10 | 1.10 |
| 4:5:299:MET:CA | 4:8:136:ILE:CA[1_554] | 1.10 | 1.10 |
| 4:6:111:ASN:OD1 | 4:V:196:ARG:CA[1_554] | 1.10 | 1.10 |
| 4:4:193:LEU:CB | 4:7:210:ARG:CG[1_554] | 1.10 | 1.10 |
| 4:6:211:ASP:CB | 4:9:32:PRO:CG[1_554] | 1.10 | 1.10 |
| 4:4:260:THR:N | 4:7:155:SER:OG[1_554] | 1.10 | 1.10 |
| 4:5:199:SER:CB | 4:8:206:ARG:N[1_554] | 1.10 | 1.10 |
| 4:4:258:PRO:C | 4:7:155:SER:O[1_554] | 1.10 | 1.10 |
| 4:5:191:LYS:CA | 4:8:187:ASP:N[1_554] | 1.10 | 1.10 |
| 4:6:276:GLU:CD | 4:9:279:TYR:N[1_554] | 1.10 | 1.10 |
| 4:6:24:ASP:O | 4:9:124:PHE:CG[1_554] | 1.10 | 1.10 |
| 4:3:371:HIS:CB | 4:7:236:LEU:CD1[1_554] | 1.10 | 1.10 |
| 4:3:116:ARG:CD | 4:7:252:ASN:CG[1_554] | 1.10 | 1.10 |
| 4:5:335:ARG:CB | 4:8:106:THR:CA[1_554] | 1.10 | 1.10 |
| 4:6:348:SER:N | 4:9:366:GLY:CA[1_554] | 1.10 | 1.10 |
| 4:5:75:ILE:CB | 4:9:198:TYR:N[1_554] | 1.10 | 1.10 |
| 4:5:277:THR:OG1 | 4:8:176:MET:CG[1_554] | 1.10 | 1.10 |
| 4:5:109:PRO:O | 4:9:195:GLU:OE1[1_554] | 1.10 | 1.10 |
| 4:6:205:GLU:CG | 4:9:203:THR:OG1[1_554] | 1.10 | 1.10 |
| 4:6:75:ILE:CA | 4:V:197:GLY:C[1_554] | 1.10 | 1.10 |
| 4:4:326:LYS:N | 4:7:167:GLU:CG[1_554] | 1.10 | 1.10 |
| 4:4:336:LYS:NZ | 4:7:86:TRP:CD2[1_554] | 1.10 | 1.10 |
| 4:4:266:PHE:CA | 4:7:261:LEU:CD2[1_554] | 1.11 | 1.09 |
| 4:6:342:GLY:O | 4:9:367:PRO:O[1_554] | 1.11 | 1.09 |
| 4:3:75:ILE:N | 4:7:197:GLY:C[1_554] | 1.11 | 1.09 |
| 4:5:186:THR:C | 4:8:183:ARG:CG[1_554] | 1.11 | 1.09 |
| 4:5:263:GLN:C | 4:8:274:ILE:CG1[1_554] | 1.11 | 1.09 |
| 4:6:325:MET:SD | 4:9:166:TYR:CZ[1_554] | 1.11 | 1.09 |
| 4:3:116:ARG:N | 4:7:196:ARG:NH2[1_554] | 1.11 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:136:ILE:O | 4:9:113:LYS:CB[1_554] | 1.11 | 1.09 |
| 4:3:77:THR:C | 4:7:246:GLN:NE2[1_554] | 1.11 | 1.09 |
| 4:5:288:ASP:C | 4:V:64:ILE:N[1_554] | 1.11 | 1.09 |
| 4:5:344:SER:O | 4:8:362:TYR:CD1[1_554] | 1.11 | 1.09 |
| 4:6:198:TYR:CD2 | 4:9:208:ILE:C[1_554] | 1.11 | 1.09 |
| 4:5:266:PHE:CB | 4:8:261:LEU:CG[1_554] | 1.11 | 1.09 |
| 4:6:288:ASP:CA | 4:W:62:ARG:C[1_554] | 1.11 | 1.09 |
| 4:4:196:ARG:CG | 4:7:211:ASP:C[1_554] | 1.11 | 1.09 |
| 4:4:265:SER:CB | 4:7:261:LEU:O[1_554] | 1.11 | 1.09 |
| 4:6:160:THR:CG2 | 4:9:161:HIS:NE2[1_554] | 1.11 | 1.09 |
| 4:6:281:SER:N | 4:9:174:ALA:CB[1_554] | 1.11 | 1.09 |
| 4:6:213:LYS:CD | 4:9:157:ASP:CB[1_554] | 1.11 | 1.09 |
| 4:5:109:PRO:C | 4:9:195:GLU:OE2[1_554] | 1.11 | 1.09 |
| 4:6:193:LEU:CD1 | 4:9:210:ARG:C[1_554] | 1.11 | 1.09 |
| 4:6:193:LEU:C | 4:9:209:VAL:C[1_554] | 1.11 | 1.09 |
| 4:4:304:THR:CG2 | 4:7:108:ALA:CA[1_554] | 1.11 | 1.09 |
| 4:5:317:ILE:CB | 4:8:150:GLY:C[1_554] | 1.11 | 1.09 |
| 4:4:357:ILE:CG1 | 4:8:231:ALA:C[1_554] | 1.11 | 1.09 |
| 4:4:314:GLN:O | 4:7:142:LEU:CD2[1_554] | 1.11 | 1.09 |
| 4:4:293:LEU:CB | 4:7:169:TYR:CE2[1_554] | 1.11 | 1.09 |
| 4:6:215:LYS:CA | 4:9:30:VAL:CG1[1_554] | 1.11 | 1.09 |
| 4:4:154:ASP:OD1 | 4:7:111:ASN:CB[1_554] | 1.11 | 1.09 |
| 4:5:345:ILE:CB | 4:8:369:ILE:CG2[1_554] | 1.11 | 1.09 |
| 4:4:222:ASP:O | 4:7:332:PRO:O[1_554] | 1.11 | 1.09 |
| 4:4:139:VAL:CB | 4:7:113:LYS:CD[1_554] | 1.11 | 1.09 |
| 4:6:318:THR:OG1 | 4:9:296:ASN:CG[1_554] | 1.11 | 1.09 |
| 4:4:368:SER:CA | 4:8:236:LEU:CB[1_554] | 1.11 | 1.09 |
| 4:6:270:GLU:C | 4:9:272:ALA:CB[1_554] | 1.11 | 1.09 |
| 4:4:108:ALA:CB | 4:8:195:GLU:O[1_554] | 1.11 | 1.09 |
| 4:4:210:ARG:CG | 4:7:69:TYR:CD2[1_554] | 1.11 | 1.09 |
| 4:5:196:ARG:CG | 4:8:212:ILE:N[1_554] | 1.11 | 1.09 |
| 4:5:15:GLY:N | 4:8:77:THR:CB[1_554] | 1.11 | 1.09 |
| 4:6:334:GLU:CA | 4:9:105:LEU:CA[1_554] | 1.11 | 1.09 |
| 4:6:317:ILE:CG2 | 4:9:150:GLY:O[1_554] | 1.11 | 1.09 |
| 4:4:286:ASP:CA | 4:8:270:GLU:OE2[1_554] | 1.11 | 1.09 |
| 4:5:164:PRO:N | 4:8:172:PRO:CG[1_554] | 1.11 | 1.09 |
| 4:3:75:ILE:CG2 | 4:7:198:TYR:CG[1_554] | 1.11 | 1.09 |
| 4:6:178:LEU:O | 4:9:177:ARG:CG[1_554] | 1.11 | 1.09 |
| 4:4:156:GLY:C | 4:7:75:ILE:N[1_554] | 1.11 | 1.09 |
| 4:5:250:ILE:CG2 | 4:8:214:GLU:OE1[1_554] | 1.11 | 1.09 |
| 4:4:366:GLY:O | 4:8:234:SER:CB[1_554] | 1.12 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:310:ALA:C | 4:9:141:SER:O[1_554] | 1.12 | 1.08 |
| 4:6:24:ASP:CA | 4:9:124:PHE:C[1_554] | 1.12 | 1.08 |
| 4:6:299:MET:O | 4:9:135:ALA:C[1_554] | 1.12 | 1.08 |
| 4:5:262:PHE:CZ | 4:8:153:LEU:O[1_554] | 1.12 | 1.08 |
| 4:4:262:PHE:CG | 4:7:154:ASP:N[1_554] | 1.12 | 1.08 |
| 4:6:332:PRO:C | 4:9:104:LEU:CD2[1_554] | 1.12 | 1.08 |
| 4:5:223:PHE:CE2 | 4:8:304:THR:CB[1_554] | 1.12 | 1.08 |
| 4:5:213:LYS:CD | 4:8:157:ASP:CB[1_554] | 1.12 | 1.08 |
| 4:4:283:MET:CG | 4:7:286:ASP:CA[1_554] | 1.12 | 1.08 |
| 4:6:26:ALA:O | 4:9:122:ILE:O[1_554] | 1.12 | 1.08 |
| 4:5:237:GLU:OE1 | 4:8:215:LYS:CE[1_554] | 1.12 | 1.08 |
| 4:5:193:LEU:CD1 | 4:8:210:ARG:C[1_554] | 1.12 | 1.08 |
| 4:6:262:PHE:CB | 4:9:153:LEU:CD2[1_554] | 1.12 | 1.08 |
| 4:6:106:THR:CG2 | 4:9:114:ALA:CA[1_554] | 1.12 | 1.08 |
| 4:5:294:TYR:CA | 4:8:166:TYR:C[1_554] | 1.12 | 1.08 |
| 4:5:294:TYR:CG | 4:8:166:TYR:CB[1_554] | 1.12 | 1.08 |
| 4:6:140:LEU:CA | 4:9:371:HIS:ND1[1_554] | 1.12 | 1.08 |
| 4:4:162:ASN:ND2 | 4:7:175:ILE:CG1[1_554] | 1.12 | 1.08 |
| 4:5:266:PHE:CA | 4:8:261:LEU:CA[1_554] | 1.12 | 1.08 |
| 4:4:274:ILE:O | 4:7:162:ASN:O[1_554] | 1.12 | 1.08 |
| 4:6:177:ARG:NH1 | 4:V:194:THR:CB[1_554] | 1.12 | 1.08 |
| 4:4:113:LYS:CB | 4:8:254:ARG:CB[1_554] | 1.12 | 1.08 |
| 4:2:291:LYS:CE | 4:7:39:ARG:C[1_554] | 1.12 | 1.08 |
| 4:4:315:LYS:CE | 4:7:147:ARG:CZ[1_554] | 1.12 | 1.08 |
| 4:4:282:ILE:CG1 | 4:7:171:LEU:CD2[1_554] | 1.12 | 1.08 |
| 4:4:75:ILE:CG2 | 4:8:198:TYR:CG[1_554] | 1.12 | 1.08 |
| 4:4:314:GLN:CA | 4:7:142:LEU:CB[1_554] | 1.12 | 1.08 |
| 4:4:304:THR:OG1 | 4:7:107:GLU:O[1_554] | 1.12 | 1.08 |
| 4:6:273:GLY:O | 4:9:162:ASN:CG[1_554] | 1.12 | 1.08 |
| 4:5:205:GLU:CG | 4:8:203:THR:OG1[1_554] | 1.12 | 1.08 |
| 4:6:18:LYS:CA | 4:9:79:TRP:CE3[1_554] | 1.12 | 1.08 |
| 4:5:204:ALA:C | 4:8:62:ARG:CG[1_554] | 1.12 | 1.08 |
| 4:4:320:LEU:CA | 4:7:293:LEU:N[1_554] | 1.12 | 1.08 |
| 4:5:151:ILE:CD1 | 4:8:171:LEU:C[1_554] | 1.13 | 1.07 |
| 4:4:293:LEU:C | 4:7:169:TYR:CG[1_554] | 1.13 | 1.07 |
| 4:4:280:ASN:CG | 4:7:281:SER:O[1_554] | 1.13 | 1.07 |
| 4:5:331:ALA:O | 4:8:140:LEU:CD2[1_554] | 1.13 | 1.07 |
| 4:5:160:THR:CG2 | 4:8:161:HIS:NE2[1_554] | 1.13 | 1.07 |
| 4:5:314:GLN:N | 4:8:142:LEU:CD1[1_554] | 1.13 | 1.07 |
| 4:5:266:PHE:CD1 | 4:8:261:LEU:CB[1_554] | 1.13 | 1.07 |
| 4:4:195:GLU:C | 4:7:209:VAL:O[1_554] | 1.13 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:312:ARG:CG | 4:8:299:MET:CA[1_554] | 1.13 | 1.07 |
| 4:4:370:VAL:CA | 4:8:230:ALA:C[1_554] | 1.13 | 1.07 |
| 4:6:308:GLY:CA | 4:9:338:SER:OG[1_554] | 1.13 | 1.07 |
| 4:6:265:SER:O | 4:9:260:THR:O[1_554] | 1.13 | 1.07 |
| 4:4:186:THR:C | 4:7:183:ARG:CD[1_554] | 1.13 | 1.07 |
| 4:4:262:PHE:CB | 4:7:153:LEU:C[1_554] | 1.13 | 1.07 |
| 4:2:323:SER:C | 4:7:44:MET:SD[1_554] | 1.13 | 1.07 |
| 4:6:166:TYR:CG | 4:W:40:HIS:NE2[1_554] | 1.13 | 1.07 |
| 4:3:110:LEU:CD1 | 4:7:191:LYS:CG[1_554] | 1.13 | 1.07 |
| 4:5:347:ALA:N | 4:8:366:GLY:C[1_554] | 1.13 | 1.07 |
| 4:5:157:ASP:CA | 4:8:72:GLU:O[1_554] | 1.13 | 1.07 |
| 4:4:77:THR:C | 4:8:246:GLN:NE2[1_554] | 1.13 | 1.07 |
| 4:4:366:GLY:C | 4:8:235:SER:N[1_554] | 1.13 | 1.07 |
| 4:4:253:GLU:CG | 4:7:214:GLU:CD[1_554] | 1.13 | 1.07 |
| 4:5:313:MET:CA | 4:8:152:VAL:CG2[1_554] | 1.13 | 1.07 |
| 4:5:252:ASN:OD1 | 4:8:215:LYS:O[1_554] | 1.13 | 1.07 |
| 4:3:367:PRO:CD | 4:7:235:SER:C[1_554] | 1.13 | 1.07 |
| 4:5:191:LYS:CB | 4:8:187:ASP:N[1_554] | 1.13 | 1.07 |
| 4:6:26:ALA:CB | 4:9:123:MET:SD[1_554] | 1.13 | 1.07 |
| 4:2:288:ASP:CA | 4:7:39:ARG:CD[1_554] | 1.13 | 1.07 |
| 4:6:193:LEU:CD2 | 4:9:210:ARG:CG[1_554] | 1.13 | 1.07 |
| 4:3:371:HIS:ND1 | 4:7:252:ASN:CA[1_554] | 1.13 | 1.07 |
| 4:4:275:HIS:N | 4:7:162:ASN:C[1_554] | 1.13 | 1.07 |
| 4:5:32:PRO:CA | 4:8:78:ASN:CB[1_554] | 1.13 | 1.07 |
| 4:6:331:ALA:O | 4:9:140:LEU:CD2[1_554] | 1.13 | 1.07 |
| 4:4:300:SER:CB | 4:7:107:GLU:CD[1_554] | 1.13 | 1.07 |
| 4:3:372:ARG:O | 4:7:255:PHE:CZ[1_554] | 1.13 | 1.07 |
| 4:5:279:TYR:N | 4:8:164:PRO:CG[1_554] | 1.13 | 1.07 |
| 4:5:115:ASN:CB | 4:9:196:ARG:CD[1_554] | 1.13 | 1.07 |
| 4:5:368:SER:O | 4:9:229:THR:C[1_554] | 1.13 | 1.07 |
| 4:5:227:MET:CA | 4:8:307:PRO:CA[1_554] | 1.13 | 1.07 |
| 4:6:279:TYR:N | 4:9:164:PRO:CB[1_554] | 1.13 | 1.07 |
| 4:5:194:THR:CA | 4:8:209:VAL:CB[1_554] | 1.13 | 1.07 |
| 4:4:336:LYS:CE | 4:7:86:TRP:NE1[1_554] | 1.13 | 1.07 |
| 4:4:139:VAL:C | 4:7:371:HIS:NE2[1_554] | 1.13 | 1.07 |
| 4:4:320:LEU:CB | 4:7:293:LEU:CG[1_554] | 1.13 | 1.07 |
| 4:5:109:PRO:C | 4:9:195:GLU:OE1[1_554] | 1.13 | 1.07 |
| 4:3:113:LYS:O | 4:7:251:GLY:C[1_554] | 1.13 | 1.07 |
| 4:4:270:GLU:CA | 4:7:272:ALA:CA[1_554] | 1.13 | 1.07 |
| 4:4:338:SER:C | 4:7:116:ARG:CA[1_554] | 1.13 | 1.07 |
| 4:4:157:ASP:OD1 | 4:7:72:GLU:CA[1_554] | 1.14 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:19:ALA:O | 4:9:122:ILE:CG1[1_554] | 1.14 | 1.06 |
| 4:6:326:LYS:C | 4:9:167:GLU:OE2[1_554] | 1.14 | 1.06 |
| 4:6:299:MET:CA | 4:9:136:ILE:CA[1_554] | 1.14 | 1.06 |
| 4:6:159:VAL:CA | 4:9:177:ARG:CZ[1_554] | 1.14 | 1.06 |
| 4:4:220:ALA:CA | 4:7:335:ARG:CA[1_554] | 1.14 | 1.06 |
| 4:5:178:LEU:CG | 4:8:177:ARG:C[1_554] | 1.14 | 1.06 |
| 4:4:308:GLY:N | 4:7:339:VAL:C[1_554] | 1.14 | 1.06 |
| 4:5:249:THR:CA | 4:8:211:ASP:OD2[1_554] | 1.14 | 1.06 |
| 4:5:270:GLU:C | 4:8:272:ALA:CB[1_554] | 1.14 | 1.06 |
| 4:6:18:LYS:N | 4:9:79:TRP:CE3[1_554] | 1.14 | 1.06 |
| 4:5:250:ILE:CG2 | 4:8:214:GLU:CD[1_554] | 1.14 | 1.06 |
| 4:3:286:ASP:C | 4:7:270:GLU:OE1[1_554] | 1.14 | 1.06 |
| 4:6:276:GLU:C | 4:9:281:SER:CB[1_554] | 1.14 | 1.06 |
| 4:5:60:SER:C | 4:8:66:THR:OG1[1_554] | 1.14 | 1.06 |
| 4:5:255:PHE:C | 4:8:302:GLY:O[1_554] | 1.14 | 1.06 |
| 4:6:319:ALA:O | 4:9:295:ALA:N[1_554] | 1.14 | 1.06 |
| 4:4:197:GLY:O | 4:7:208:ILE:CB[1_554] | 1.14 | 1.06 |
| 4:4:191:LYS:CG | 4:7:186:THR:N[1_554] | 1.14 | 1.06 |
| 4:6:166:TYR:CE2 | 4:W:39:ARG:O[1_554] | 1.14 | 1.06 |
| 4:5:343:GLY:C | 4:8:367:PRO:CA[1_554] | 1.14 | 1.06 |
| 4:6:194:THR:O | 4:9:209:VAL:CG2[1_554] | 1.14 | 1.06 |
| 4:4:140:LEU:C | 4:7:371:HIS:ND1[1_554] | 1.14 | 1.06 |
| 4:5:299:MET:SD | 4:8:139:VAL:N[1_554] | 1.14 | 1.06 |
| 4:5:332:PRO:C | 4:8:104:LEU:CD2[1_554] | 1.14 | 1.06 |
| 4:4:205:GLU:CA | 4:7:62:ARG:NE[1_554] | 1.14 | 1.06 |
| 4:4:367:PRO:N | 4:8:235:SER:CA[1_554] | 1.14 | 1.06 |
| 4:6:262:PHE:CZ | 4:9:153:LEU:O[1_554] | 1.14 | 1.06 |
| 4:3:117:GLU:C | 4:7:237:GLU:CB[1_554] | 1.14 | 1.06 |
| 4:5:25:ASP:CB | 4:8:129:VAL:CG2[1_554] | 1.14 | 1.06 |
| 4:3:326:LYS:CE | 4:8:45:VAL:N[1_554] | 1.14 | 1.06 |
| 4:6:314:GLN:OE1 | 4:9:147:ARG:CB[1_554] | 1.14 | 1.06 |
| 4:6:272:ALA:O | 4:9:277:THR:CG2[1_554] | 1.14 | 1.06 |
| 4:4:207:GLU:CD | 4:7:67:LEU:C[1_554] | 1.14 | 1.06 |
| 4:2:291:LYS:CD | 4:7:39:ARG:CA[1_554] | 1.14 | 1.06 |
| 4:5:318:THR:OG1 | 4:8:296:ASN:CG[1_554] | 1.14 | 1.06 |
| 4:6:173:HIS:CB | 4:V:267:ILE:CA[1_554] | 1.14 | 1.06 |
| 4:4:227:MET:SD | 4:7:305:MET:C[1_554] | 1.14 | 1.06 |
| 4:5:278:THR:CB | 4:8:164:PRO:CD[1_554] | 1.14 | 1.06 |
| 4:4:271:SER:O | 4:7:277:THR:OG1[1_554] | 1.14 | 1.06 |
| 4:4:271:SER:C | 4:7:277:THR:OG1[1_554] | 1.14 | 1.06 |
| 4:5:276:GLU:C | 4:8:281:SER:OG[1_554] | 1.14 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:18:LYS:CA | 4:8:79:TRP:CE3[1_554] | 1.14 | 1.06 |
| 4:6:193:LEU:CB | 4:9:210:ARG:CB[1_554] | 1.14 | 1.06 |
| 4:6:156:GLY:C | 4:9:74:GLY:C[1_554] | 1.14 | 1.06 |
| 4:6:112:PRO:O | 4:V:253:GLU:OE1[1_554] | 1.15 | 1.05 |
| 4:3:113:LYS:O | 4:7:251:GLY:CA[1_554] | 1.15 | 1.05 |
| 4:5:166:TYR:CE2 | 4:V:39:ARG:O[1_554] | 1.15 | 1.05 |
| 4:5:312:ARG:CG | 4:8:299:MET:C[1_554] | 1.15 | 1.05 |
| 4:4:259:GLU:CD | 4:7:304:THR:CA[1_554] | 1.15 | 1.05 |
| 4:4:215:LYS:CB | 4:7:31:PHE:N[1_554] | 1.15 | 1.05 |
| 4:5:15:GLY:CA | 4:8:77:THR:CB[1_554] | 1.15 | 1.05 |
| 4:6:279:TYR:N | 4:9:164:PRO:CG[1_554] | 1.15 | 1.05 |
| 4:6:117:GLU:OE2 | 4:V:236:LEU:CD1[1_554] | 1.15 | 1.05 |
| 4:5:219:VAL:CB | 4:8:301:GLY:N[1_554] | 1.15 | 1.05 |
| 4:5:304:THR:CA | 4:8:137:GLN:OE1[1_554] | 1.15 | 1.05 |
| 4:4:258:PRO:C | 4:7:155:SER:C[1_554] | 1.15 | 1.05 |
| 4:6:339:VAL:C | 4:9:116:ARG:CA[1_554] | 1.15 | 1.05 |
| 4:6:334:GLU:C | 4:9:105:LEU:C[1_554] | 1.15 | 1.05 |
| 4:6:318:THR:OG1 | 4:9:296:ASN:OD1[1_554] | 1.15 | 1.05 |
| 4:6:198:TYR:CD1 | 4:9:208:ILE:CA[1_554] | 1.15 | 1.05 |
| 4:4:304:THR:N | 4:7:137:GLN:NE2[1_554] | 1.15 | 1.05 |
| 4:5:144:ALA:N | 4:8:370:VAL:O[1_554] | 1.15 | 1.05 |
| 4:4:299:MET:CA | 4:7:136:ILE:CG1[1_554] | 1.15 | 1.05 |
| 4:6:300:SER:C | 4:9:107:GLU:O[1_554] | 1.15 | 1.05 |
| 4:5:199:SER:N | 4:8:205:GLU:O[1_554] | 1.15 | 1.05 |
| 4:4:211:ASP:O | 4:7:32:PRO:N[1_554] | 1.15 | 1.05 |
| 4:6:173:HIS:O | 4:V:267:ILE:O[1_554] | 1.15 | 1.05 |
| 4:5:221:LEU:CD1 | 4:8:332:PRO:CG[1_554] | 1.15 | 1.05 |
| 4:4:218:TYR:CA | 4:7:336:LYS:O[1_554] | 1.15 | 1.05 |
| 4:4:117:GLU:CD | 4:8:236:LEU:O[1_554] | 1.15 | 1.05 |
| 4:4:313:MET:CB | 4:7:138:ALA:O[1_554] | 1.15 | 1.05 |
| 4:5:294:TYR:OH | 4:8:289:ILE:CG1[1_554] | 1.15 | 1.05 |
| 4:6:185:LEU:CA | 4:9:157:ASP:O[1_554] | 1.15 | 1.05 |
| 1:A:637:LYS:CG | 4:5:311:ASP:OD1[1_556] | 1.15 | 1.05 |
| 4:6:297:ASN:CG | 4:9:165:ILE:CG1[1_554] | 1.15 | 1.05 |
| 4:6:161:HIS:CB | 4:9:110:LEU:CG[1_554] | 1.15 | 1.05 |
| 4:3:117:GLU:CA | 4:7:237:GLU:CG[1_554] | 1.15 | 1.05 |
| 4:6:160:THR:CB | 4:9:161:HIS:NE2[1_554] | 1.15 | 1.05 |
| 4:5:295:ALA:C | 4:8:167:GLU:O[1_554] | 1.15 | 1.05 |
| 4:4:76:ILE:O | 4:8:198:TYR:CE1[1_554] | 1.15 | 1.05 |
| 4:4:186:THR:CB | 4:7:183:ARG:NH2[1_554] | 1.15 | 1.05 |
| 4:5:211:ASP:CG | 4:8:32:PRO:CG[1_554] | 1.15 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:199:SER:N | 4:7:207:GLU:N[1_554] | 1.15 | 1.05 |
| 4:6:198:TYR:CD2 | 4:9:208:ILE:O[1_554] | 1.15 | 1.05 |
| 4:4:259:GLU:N | 4:7:155:SER:O[1_554] | 1.15 | 1.05 |
| 4:4:114:ALA:C | 4:8:250:ILE:C[1_554] | 1.15 | 1.05 |
| 4:5:189:LEU:N | 4:8:182:GLY:O[1_554] | 1.15 | 1.05 |
| 4:5:273:GLY:O | 4:8:162:ASN:CG[1_554] | 1.15 | 1.05 |
| 4:6:339:VAL:CA | 4:9:116:ARG:CB[1_554] | 1.15 | 1.05 |
| 4:3:72:GLU:O | 4:7:198:TYR:C[1_554] | 1.15 | 1.05 |
| 4:4:335:ARG:NE | 4:7:106:THR:CB[1_554] | 1.15 | 1.05 |
| 4:4:144:ALA:N | 4:7:371:HIS:CA[1_554] | 1.16 | 1.04 |
| 4:6:195:GLU:CB | 4:9:189:LEU:CB[1_554] | 1.16 | 1.04 |
| 4:6:314:GLN:N | 4:9:142:LEU:CD1[1_554] | 1.16 | 1.04 |
| 4:4:30:VAL:O | 4:7:80:ASP:CB[1_554] | 1.16 | 1.04 |
| 4:5:310:ALA:CB | 4:8:141:SER:N[1_554] | 1.16 | 1.04 |
| 4:2:292:ASP:CA | 4:7:40:HIS:CD2[1_554] | 1.16 | 1.04 |
| 4:5:255:PHE:CA | 4:8:302:GLY:O[1_554] | 1.16 | 1.04 |
| 4:6:281:SER:OG | 4:9:173:HIS:N[1_554] | 1.16 | 1.04 |
| 4:5:115:ASN:CG | 4:9:196:ARG:CD[1_554] | 1.16 | 1.04 |
| 4:5:276:GLU:CD | 4:8:279:TYR:N[1_554] | 1.16 | 1.04 |
| 4:4:310:ALA:C | 4:7:141:SER:N[1_554] | 1.16 | 1.04 |
| 4:5:276:GLU:CG | 4:8:278:THR:C[1_554] | 1.16 | 1.04 |
| 4:4:280:ASN:N | 4:7:174:ALA:CB[1_554] | 1.16 | 1.04 |
| 4:6:193:LEU:CB | 4:9:210:ARG:CA[1_554] | 1.16 | 1.04 |
| 4:6:162:ASN:N | 4:9:110:LEU:CD2[1_554] | 1.16 | 1.04 |
| 4:5:173:HIS:ND1 | 4:9:266:PHE:N[1_554] | 1.16 | 1.04 |
| 4:5:56:ASP:CB | 4:8:37:ARG:CZ[1_554] | 1.16 | 1.04 |
| 4:3:366:GLY:C | 4:7:235:SER:N[1_554] | 1.16 | 1.04 |
| 4:5:141:SER:C | 4:8:116:ARG:CZ[1_554] | 1.16 | 1.04 |
| 4:5:341:ILE:CD1 | 4:8:132:MET:CE[1_554] | 1.16 | 1.04 |
| 4:6:337:TYR:OH | 4:9:86:TRP:NE1[1_554] | 1.16 | 1.04 |
| 4:4:185:LEU:O | 4:7:157:ASP:O[1_554] | 1.16 | 1.04 |
| 4:5:220:ALA:CA | 4:8:335:ARG:CB[1_554] | 1.16 | 1.04 |
| 4:4:256:ARG:C | 4:7:303:THR:N[1_554] | 1.16 | 1.04 |
| 4:4:315:LYS:CD | 4:7:147:ARG:NE[1_554] | 1.16 | 1.04 |
| 4:4:173:HIS:CA | 4:8:267:ILE:CG2[1_554] | 1.16 | 1.04 |
| 4:4:185:LEU:N | 4:7:158:GLY:CA[1_554] | 1.16 | 1.04 |
| 4:6:346:LEU:CB | 4:9:368:SER:C[1_554] | 1.16 | 1.04 |
| 4:6:113:LYS:CG | 4:V:252:ASN:O[1_554] | 1.16 | 1.04 |
| 4:5:312:ARG:NE | 4:8:299:MET:CG[1_554] | 1.16 | 1.04 |
| 4:5:340:TRP:CB | 4:8:119:MET:N[1_554] | 1.16 | 1.04 |
| 4:5:328:LYS:N | 4:8:148:THR:O[1_554] | 1.16 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:26:ALA:CB | 4:7:122:ILE:CA[1_554] | 1.16 | 1.04 |
| 4:5:337:TYR:CE1 | 4:8:86:TRP:CH2[1_554] | 1.16 | 1.04 |
| 4:5:17:VAL:CA | 4:8:79:TRP:CD1[1_554] | 1.16 | 1.04 |
| 4:6:372:ARG:N | 4:V:227:MET:O[1_554] | 1.16 | 1.04 |
| 4:6:136:ILE:N | 4:9:113:LYS:CE[1_554] | 1.16 | 1.04 |
| 4:5:211:ASP:CB | 4:8:32:PRO:CG[1_554] | 1.16 | 1.04 |
| 4:6:32:PRO:CA | 4:9:78:ASN:CB[1_554] | 1.16 | 1.04 |
| 4:3:288:ASP:O | 4:8:64:ILE:CA[1_554] | 1.16 | 1.04 |
| 4:4:144:ALA:C | 4:7:370:VAL:CA[1_554] | 1.16 | 1.04 |
| 4:4:193:LEU:CG | 4:7:210:ARG:CD[1_554] | 1.17 | 1.03 |
| 4:4:143:TYR:CE2 | 4:7:368:SER:CB[1_554] | 1.17 | 1.03 |
| 4:4:208:ILE:CD1 | 4:7:59:GLN:N[1_554] | 1.17 | 1.03 |
| 4:4:333:PRO:C | 4:7:105:LEU:CB[1_554] | 1.17 | 1.03 |
| 4:6:227:MET:CB | 4:9:307:PRO:C[1_554] | 1.17 | 1.03 |
| 4:5:312:ARG:C | 4:8:298:VAL:CG1[1_554] | 1.17 | 1.03 |
| 4:6:28:ARG:CA | 4:9:126:THR:OG1[1_554] | 1.17 | 1.03 |
| 4:4:281:SER:O | 4:7:173:HIS:NE2[1_554] | 1.17 | 1.03 |
| 4:6:157:ASP:O | 4:9:73:HIS:N[1_554] | 1.17 | 1.03 |
| 4:6:294:TYR:CD2 | 4:9:166:TYR:CG[1_554] | 1.17 | 1.03 |
| 4:4:337:TYR:CZ | 4:7:86:TRP:CZ3[1_554] | 1.17 | 1.03 |
| 4:3:286:ASP:CA | 4:7:270:GLU:OE1[1_554] | 1.17 | 1.03 |
| 4:5:28:ARG:O | 4:8:83:GLU:CD[1_554] | 1.17 | 1.03 |
| 4:5:290:ARG:NE | 4:8:286:ASP:CG[1_554] | 1.17 | 1.03 |
| 4:4:311:ASP:CG | 4:7:144:ALA:CB[1_554] | 1.17 | 1.03 |
| 4:6:137:GLN:CG | 4:9:112:PRO:O[1_554] | 1.17 | 1.03 |
| 4:4:162:ASN:CA | 4:7:110:LEU:CD2[1_554] | 1.17 | 1.03 |
| 4:6:270:GLU:CA | 4:9:272:ALA:N[1_554] | 1.17 | 1.03 |
| 4:5:369:ILE:CG1 | 4:9:232:SER:OG[1_554] | 1.17 | 1.03 |
| 4:4:141:SER:N | 4:7:371:HIS:ND1[1_554] | 1.17 | 1.03 |
| 4:4:208:ILE:CD1 | 4:7:59:GLN:CA[1_554] | 1.17 | 1.03 |
| 4:4:255:PHE:CE1 | 4:7:305:MET:CG[1_554] | 1.17 | 1.03 |
| 4:6:200:PHE:N | 4:9:206:ARG:CG[1_554] | 1.17 | 1.03 |
| 4:4:259:GLU:CD | 4:7:304:THR:C[1_554] | 1.17 | 1.03 |
| 4:4:300:SER:N | 4:7:107:GLU:CG[1_554] | 1.17 | 1.03 |
| 4:4:300:SER:CA | 4:7:107:GLU:CD[1_554] | 1.17 | 1.03 |
| 4:3:109:PRO:CD | 4:7:195:GLU:CG[1_554] | 1.17 | 1.03 |
| 4:6:335:ARG:CB | 4:9:106:THR:CA[1_554] | 1.17 | 1.03 |
| 4:6:343:GLY:C | 4:9:367:PRO:CA[1_554] | 1.17 | 1.03 |
| 4:4:372:ARG:O | 4:8:255:PHE:CZ[1_554] | 1.17 | 1.03 |
| 4:6:310:ALA:O | 4:9:142:LEU:CA[1_554] | 1.17 | 1.03 |
| 4:6:30:VAL:CB | 4:9:83:GLU:N[1_554] | 1.18 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:305:MET:O | 4:7:11:ASP:OD1[1_554] | 1.18 | 1.02 |
| 4:5:290:ARG:NE | 4:8:286:ASP:CB[1_554] | 1.18 | 1.02 |
| 4:5:310:ALA:CA | 4:8:141:SER:C[1_554] | 1.18 | 1.02 |
| 4:6:191:LYS:CB | 4:9:187:ASP:N[1_554] | 1.18 | 1.02 |
| 4:4:262:PHE:CG | 4:7:153:LEU:O[1_554] | 1.18 | 1.02 |
| 4:5:192:ILE:O | 4:8:213:LYS:CB[1_554] | 1.18 | 1.02 |
| 4:6:305:MET:O | 4:9:11:ASP:OD2[1_554] | 1.18 | 1.02 |
| 4:6:349:LEU:N | 4:9:365:ALA:CA[1_554] | 1.18 | 1.02 |
| 4:4:345:ILE:CB | 4:7:366:GLY:C[1_554] | 1.18 | 1.02 |
| 4:4:198:TYR:CG | 4:7:208:ILE:N[1_554] | 1.18 | 1.02 |
| 4:4:294:TYR:O | 4:7:169:TYR:N[1_554] | 1.18 | 1.02 |
| 4:5:282:ILE:CG1 | 4:8:171:LEU:CD1[1_554] | 1.18 | 1.02 |
| 4:6:196:ARG:C | 4:9:212:ILE:CG1[1_554] | 1.18 | 1.02 |
| 4:5:193:LEU:O | 4:8:210:ARG:N[1_554] | 1.18 | 1.02 |
| 4:5:334:GLU:C | 4:8:105:LEU:C[1_554] | 1.18 | 1.02 |
| 4:6:277:THR:CA | 4:9:281:SER:OG[1_554] | 1.18 | 1.02 |
| 4:5:18:LYS:CB | 4:8:79:TRP:CZ3[1_554] | 1.18 | 1.02 |
| 4:6:178:LEU:CG | 4:9:177:ARG:C[1_554] | 1.18 | 1.02 |
| 4:4:274:ILE:CD1 | 4:7:161:HIS:CD2[1_554] | 1.18 | 1.02 |
| 4:5:327:ILE:O | 4:8:148:THR:OG1[1_554] | 1.18 | 1.02 |
| 4:4:16:LEU:N | 4:7:77:THR:CA[1_554] | 1.18 | 1.02 |
| 4:4:277:THR:CG2 | 4:7:175:ILE:O[1_554] | 1.18 | 1.02 |
| 4:5:268:GLY:CA | 4:8:264:PRO:CB[1_554] | 1.18 | 1.02 |
| 4:6:31:PHE:CD1 | 4:9:80:ASP:N[1_554] | 1.18 | 1.02 |
| 4:6:276:GLU:CG | 4:9:278:THR:C[1_554] | 1.18 | 1.02 |
| 4:6:204:ALA:C | 4:9:62:ARG:CG[1_554] | 1.18 | 1.02 |
| 4:6:290:ARG:NE | 4:9:286:ASP:CB[1_554] | 1.18 | 1.02 |
| 4:3:112:PRO:CG | 4:7:193:LEU:CD1[1_554] | 1.18 | 1.02 |
| 4:5:369:ILE:O | 4:9:228:ALA:O[1_554] | 1.18 | 1.02 |
| 4:4:113:LYS:CG | 4:8:254:ARG:N[1_554] | 1.18 | 1.02 |
| 4:5:173:HIS:O | 4:9:267:ILE:O[1_554] | 1.18 | 1.02 |
| 4:4:109:PRO:CA | 4:8:195:GLU:OE1[1_554] | 1.18 | 1.02 |
| 4:6:320:LEU:CA | 4:9:294:TYR:N[1_554] | 1.18 | 1.02 |
| 4:4:336:LYS:N | 4:7:119:MET:CE[1_554] | 1.18 | 1.02 |
| 4:4:304:THR:CB | 4:7:107:GLU:O[1_554] | 1.18 | 1.02 |
| 4:4:321:ALA:O | 4:7:292:ASP:CG[1_554] | 1.18 | 1.02 |
| 4:5:213:LYS:CE | 4:8:15:GLY:N[1_554] | 1.18 | 1.02 |
| 4:3:366:GLY:O | 4:7:234:SER:CB[1_554] | 1.18 | 1.02 |
| 4:6:322:PRO:CB | 4:9:291:LYS:NZ[1_554] | 1.18 | 1.02 |
| 4:6:338:SER:OG | 4:9:134:VAL:CG1[1_554] | 1.18 | 1.02 |
| 4:4:118:LYS:N | 4:8:237:GLU:OE1[1_554] | 1.18 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:243:PRO:CA | 4:8:60:SER:CB[1_554] | 1.18 | 1.02 |
| 4:5:262:PHE:CB | 4:8:153:LEU:CD2[1_554] | 1.19 | 1.01 |
| 4:5:153:LEU:CD1 | 4:8:163:VAL:CG2[1_554] | 1.19 | 1.01 |
| 4:6:255:PHE:C | 4:9:302:GLY:O[1_554] | 1.19 | 1.01 |
| 4:6:274:ILE:CD1 | 4:9:161:HIS:CB[1_554] | 1.19 | 1.01 |
| 4:5:369:ILE:CG2 | 4:9:232:SER:N[1_554] | 1.19 | 1.01 |
| 4:4:215:LYS:CB | 4:7:31:PHE:CA[1_554] | 1.19 | 1.01 |
| 4:5:331:ALA:CB | 4:8:140:LEU:CB[1_554] | 1.19 | 1.01 |
| 4:4:316:GLU:OE1 | 4:7:151:ILE:O[1_554] | 1.19 | 1.01 |
| 4:6:136:ILE:C | 4:9:113:LYS:CG[1_554] | 1.19 | 1.01 |
| 4:6:278:THR:N | 4:9:164:PRO:CD[1_554] | 1.19 | 1.01 |
| 4:5:196:ARG:C | 4:8:212:ILE:CB[1_554] | 1.19 | 1.01 |
| 4:4:72:GLU:O | 4:8:198:TYR:C[1_554] | 1.19 | 1.01 |
| 4:6:276:GLU:OE2 | 4:9:278:THR:C[1_554] | 1.19 | 1.01 |
| 4:4:25:ASP:CB | 4:7:124:PHE:C[1_554] | 1.19 | 1.01 |
| 4:5:305:MET:CB | 4:8:11:ASP:CG[1_554] | 1.19 | 1.01 |
| 4:4:318:THR:CB | 4:7:149:THR:O[1_554] | 1.19 | 1.01 |
| 4:4:223:PHE:CZ | 4:7:301:GLY:N[1_554] | 1.19 | 1.01 |
| 4:5:343:GLY:C | 4:8:367:PRO:CB[1_554] | 1.19 | 1.01 |
| 4:5:205:GLU:CA | 4:8:62:ARG:CZ[1_554] | 1.19 | 1.01 |
| 4:3:173:HIS:CB | 4:7:267:ILE:CG1[1_554] | 1.19 | 1.01 |
| 4:4:336:LYS:CD | 4:7:86:TRP:CZ2[1_554] | 1.19 | 1.01 |
| 4:6:114:ALA:C | 4:V:196:ARG:NH2[1_554] | 1.19 | 1.01 |
| 4:4:188:TYR:C | 4:7:183:ARG:CA[1_554] | 1.19 | 1.01 |
| 4:5:160:THR:CG2 | 4:8:161:HIS:CD2[1_554] | 1.19 | 1.01 |
| 4:6:342:GLY:CA | 4:9:370:VAL:CG1[1_554] | 1.19 | 1.01 |
| 4:4:372:ARG:CA | 4:8:226:GLU:O[1_554] | 1.19 | 1.01 |
| 4:4:157:ASP:OD2 | 4:7:72:GLU:CB[1_554] | 1.19 | 1.01 |
| 4:4:193:LEU:CG | 4:7:210:ARG:NE[1_554] | 1.19 | 1.01 |
| 4:5:340:TRP:N | 4:8:116:ARG:O[1_554] | 1.19 | 1.01 |
| 4:6:283:MET:CG | 4:9:286:ASP:C[1_554] | 1.19 | 1.01 |
| 4:4:186:THR:C | 4:7:183:ARG:NE[1_554] | 1.19 | 1.01 |
| 4:5:159:VAL:CA | 4:8:177:ARG:CZ[1_554] | 1.19 | 1.01 |
| 4:6:24:ASP:CA | 4:9:124:PHE:CA[1_554] | 1.19 | 1.01 |
| 4:4:345:ILE:CA | 4:7:367:PRO:N[1_554] | 1.19 | 1.01 |
| 4:4:113:LYS:O | 4:8:251:GLY:C[1_554] | 1.19 | 1.01 |
| 4:6:15:GLY:N | 4:9:77:THR:CB[1_554] | 1.19 | 1.01 |
| 4:4:112:PRO:CG | 4:8:193:LEU:CD1[1_554] | 1.19 | 1.01 |
| 4:6:314:GLN:CA | 4:9:142:LEU:CD1[1_554] | 1.19 | 1.01 |
| 4:4:15:GLY:C | 4:7:77:THR:CG2[1_554] | 1.19 | 1.01 |
| 4:6:56:ASP:CB | 4:9:37:ARG:CZ[1_554] | 1.19 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:113:LYS:CB | 4:9:253:GLU:N[1_554] | 1.19 | 1.01 |
| 4:6:31:PHE:CG | 4:9:80:ASP:N[1_554] | 1.19 | 1.01 |
| 4:6:193:LEU:O | 4:9:210:ARG:N[1_554] | 1.19 | 1.01 |
| 4:4:210:ARG:CB | 4:7:69:TYR:CE2[1_554] | 1.20 | 1.00 |
| 4:6:62:ARG:NH1 | 4:9:67:LEU:N[1_554] | 1.20 | 1.00 |
| 4:5:193:LEU:CB | 4:8:210:ARG:CB[1_554] | 1.20 | 1.00 |
| 4:6:274:ILE:CG1 | 4:9:161:HIS:CB[1_554] | 1.20 | 1.00 |
| 4:4:340:TRP:CB | 4:7:118:LYS:CB[1_554] | 1.20 | 1.00 |
| 4:5:319:ALA:O | 4:8:294:TYR:CA[1_554] | 1.20 | 1.00 |
| 4:3:74:GLY:C | 4:7:197:GLY:C[1_554] | 1.20 | 1.00 |
| 4:5:243:PRO:CB | 4:8:60:SER:C[1_554] | 1.20 | 1.00 |
| 4:4:199:SER:CB | 4:7:206:ARG:N[1_554] | 1.20 | 1.00 |
| 4:4:315:LYS:N | 4:7:142:LEU:CG[1_554] | 1.20 | 1.00 |
| 4:5:308:GLY:CA | 4:8:338:SER:OG[1_554] | 1.20 | 1.00 |
| 4:5:166:TYR:CG | 4:V:40:HIS:ND1[1_554] | 1.20 | 1.00 |
| 4:6:213:LYS:C | 4:9:16:LEU:CD2[1_554] | 1.20 | 1.00 |
| 4:6:294:TYR:CA | 4:9:166:TYR:O[1_554] | 1.20 | 1.00 |
| 4:6:19:ALA:N | 4:9:122:ILE:CD1[1_554] | 1.20 | 1.00 |
| 4:3:369:ILE:N | 4:7:234:SER:OG[1_554] | 1.20 | 1.00 |
| 4:5:18:LYS:O | 4:8:118:LYS:CG[1_554] | 1.20 | 1.00 |
| 4:6:196:ARG:CG | 4:9:212:ILE:N[1_554] | 1.20 | 1.00 |
| 4:4:144:ALA:CA | 4:7:370:VAL:C[1_554] | 1.20 | 1.00 |
| 4:4:111:ASN:O | 4:8:253:GLU:CG[1_554] | 1.20 | 1.00 |
| 4:6:75:ILE:O | 4:V:197:GLY:O[1_554] | 1.20 | 1.00 |
| 4:5:188:TYR:CG | 4:8:181:ALA:O[1_554] | 1.20 | 1.00 |
| 4:5:26:ALA:C | 4:8:123:MET:CA[1_554] | 1.20 | 1.00 |
| 4:5:274:ILE:CB | 4:8:161:HIS:C[1_554] | 1.20 | 1.00 |
| 4:4:27:PRO:N | 4:7:122:ILE:CG1[1_554] | 1.20 | 1.00 |
| 4:6:312:ARG:NH2 | 4:9:299:MET:SD[1_554] | 1.20 | 1.00 |
| 4:5:111:ASN:OD1 | 4:9:196:ARG:CA[1_554] | 1.20 | 1.00 |
| 4:5:308:GLY:CA | 4:8:338:SER:CA[1_554] | 1.20 | 1.00 |
| 4:5:59:GLN:CD | 4:8:68:LYS:CG[1_554] | 1.20 | 1.00 |
| 4:4:275:HIS:CA | 4:7:163:VAL:N[1_554] | 1.21 | 0.99 |
| 4:6:349:LEU:CA | 4:9:365:ALA:N[1_554] | 1.21 | 0.99 |
| 4:4:277:THR:O | 4:7:174:ALA:C[1_554] | 1.21 | 0.99 |
| 4:6:305:MET:C | 4:9:11:ASP:OD2[1_554] | 1.21 | 0.99 |
| 4:4:199:SER:N | 4:7:206:ARG:C[1_554] | 1.21 | 0.99 |
| 4:5:143:TYR:CA | 4:8:372:ARG:CB[1_554] | 1.21 | 0.99 |
| 4:4:177:ARG:CZ | 4:8:194:THR:CG2[1_554] | 1.21 | 0.99 |
| 4:6:220:ALA:CA | 4:9:335:ARG:CB[1_554] | 1.21 | 0.99 |
| 4:3:74:GLY:O | 4:7:197:GLY:N[1_554] | 1.21 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:24:ASP:CG | 4:9:125:GLU:N[1_554] | 1.21 | 0.99 |
| 4:5:136:ILE:C | 4:8:113:LYS:CG[1_554] | 1.21 | 0.99 |
| 4:6:188:TYR:C | 4:9:182:GLY:O[1_554] | 1.21 | 0.99 |
| 4:5:327:ILE:CB | 4:8:149:THR:CA[1_554] | 1.21 | 0.99 |
| 4:5:227:MET:SD | 4:8:307:PRO:N[1_554] | 1.21 | 0.99 |
| 4:5:266:PHE:CG | 4:8:261:LEU:CD1[1_554] | 1.21 | 0.99 |
| 4:4:276:GLU:C | 4:7:281:SER:OG[1_554] | 1.21 | 0.99 |
| 4:5:26:ALA:CB | 4:8:123:MET:SD[1_554] | 1.21 | 0.99 |
| 4:4:194:THR:CB | 4:7:209:VAL:CG1[1_554] | 1.21 | 0.99 |
| 4:6:280:ASN:CG | 4:9:281:SER:O[1_554] | 1.21 | 0.99 |
| 4:5:185:LEU:CA | 4:8:157:ASP:O[1_554] | 1.21 | 0.99 |
| 4:4:214:GLU:O | 4:7:16:LEU:C[1_554] | 1.21 | 0.99 |
| 4:5:24:ASP:CG | 4:8:125:GLU:N[1_554] | 1.21 | 0.99 |
| 4:4:172:PRO:CG | 4:8:266:PHE:CB[1_554] | 1.21 | 0.99 |
| 4:6:213:LYS:CE | 4:9:15:GLY:N[1_554] | 1.21 | 0.99 |
| 4:5:19:ALA:O | 4:8:122:ILE:CG1[1_554] | 1.21 | 0.99 |
| 4:5:269:MET:O | 4:8:272:ALA:O[1_554] | 1.21 | 0.99 |
| 4:6:211:ASP:CG | 4:9:32:PRO:N[1_554] | 1.21 | 0.99 |
| 4:6:341:ILE:CG2 | 4:9:132:MET:SD[1_554] | 1.21 | 0.99 |
| 4:5:19:ALA:CB | 4:8:118:LYS:NZ[1_554] | 1.21 | 0.99 |
| 4:5:198:TYR:CD2 | 4:8:208:ILE:O[1_554] | 1.21 | 0.99 |
| 4:6:166:TYR:OH | 4:W:39:ARG:CA[1_554] | 1.21 | 0.99 |
| 4:4:109:PRO:CB | 4:8:195:GLU:CD[1_554] | 1.21 | 0.99 |
| 4:5:145:SER:OG | 4:8:372:ARG:NH1[1_554] | 1.21 | 0.99 |
| 4:4:310:ALA:CA | 4:7:140:LEU:N[1_554] | 1.21 | 0.99 |
| 4:6:223:PHE:CE2 | 4:9:304:THR:CB[1_554] | 1.21 | 0.99 |
| 4:4:341:ILE:CG1 | 4:7:120:THR:N[1_554] | 1.21 | 0.99 |
| 4:3:368:SER:CA | 4:7:236:LEU:CB[1_554] | 1.21 | 0.99 |
| 4:6:294:TYR:OH | 4:9:289:ILE:CD1[1_554] | 1.21 | 0.99 |
| 4:4:333:PRO:CB | 4:7:104:LEU:C[1_554] | 1.21 | 0.99 |
| 4:6:320:LEU:N | 4:9:293:LEU:C[1_554] | 1.21 | 0.99 |
| 4:5:188:TYR:CZ | 4:8:185:LEU:CG[1_554] | 1.21 | 0.99 |
| 4:6:18:LYS:CB | 4:9:79:TRP:CZ3[1_554] | 1.21 | 0.99 |
| 4:4:207:GLU:OE1 | 4:7:67:LEU:CA[1_554] | 1.21 | 0.99 |
| 4:6:253:GLU:OE1 | 4:9:213:LYS:C[1_554] | 1.21 | 0.99 |
| 4:5:136:ILE:O | 4:8:113:LYS:CG[1_554] | 1.21 | 0.99 |
| 4:5:310:ALA:C | 4:8:142:LEU:N[1_554] | 1.21 | 0.99 |
| 4:6:193:LEU:C | 4:9:210:ARG:N[1_554] | 1.21 | 0.99 |
| 4:6:198:TYR:CB | 4:9:209:VAL:N[1_554] | 1.22 | 0.98 |
| 4:5:30:VAL:CB | 4:8:83:GLU:N[1_554] | 1.22 | 0.98 |
| 4:5:310:ALA:O | 4:8:142:LEU:CA[1_554] | 1.22 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:310:ALA:CB | 4:8:140:LEU:O[1_554] | 1.22 | 0.98 |
| 4:6:317:ILE:N | 4:9:151:ILE:N[1_554] | 1.22 | 0.98 |
| 4:6:308:GLY:CA | 4:9:338:SER:CA[1_554] | 1.22 | 0.98 |
| 4:5:110:LEU:CG | 4:9:191:LYS:CD[1_554] | 1.22 | 0.98 |
| 4:5:349:LEU:N | 4:8:365:ALA:CA[1_554] | 1.22 | 0.98 |
| 4:4:117:GLU:CA | 4:8:237:GLU:CG[1_554] | 1.22 | 0.98 |
| 4:4:340:TRP:C | 4:7:117:GLU:O[1_554] | 1.22 | 0.98 |
| 4:6:195:GLU:CG | 4:9:189:LEU:CD1[1_554] | 1.22 | 0.98 |
| 4:5:281:SER:N | 4:8:174:ALA:CB[1_554] | 1.22 | 0.98 |
| 4:4:312:ARG:NE | 4:7:299:MET:CA[1_554] | 1.22 | 0.98 |
| 4:5:343:GLY:O | 4:8:367:PRO:CB[1_554] | 1.22 | 0.98 |
| 4:5:293:LEU:CG | 4:8:169:TYR:CE2[1_554] | 1.22 | 0.98 |
| 4:4:276:GLU:OE1 | 4:7:278:THR:O[1_554] | 1.22 | 0.98 |
| 4:4:309:ILE:N | 4:7:339:VAL:CA[1_554] | 1.22 | 0.98 |
| 4:4:173:HIS:CA | 4:8:267:ILE:CB[1_554] | 1.22 | 0.98 |
| 4:6:268:GLY:CA | 4:9:264:PRO:CB[1_554] | 1.22 | 0.98 |
| 4:3:74:GLY:C | 4:7:197:GLY:CA[1_554] | 1.22 | 0.98 |
| 4:6:340:TRP:N | 4:9:116:ARG:O[1_554] | 1.22 | 0.98 |
| 4:4:204:ALA:CB | 4:7:62:ARG:O[1_554] | 1.22 | 0.98 |
| 4:4:151:ILE:CG2 | 4:7:170:ALA:O[1_554] | 1.22 | 0.98 |
| 4:4:218:TYR:CE2 | 4:7:337:TYR:CD2[1_554] | 1.22 | 0.98 |
| 4:5:23:GLY:N | 4:8:362:TYR:CD2[1_554] | 1.22 | 0.98 |
| 4:4:326:LYS:C | 4:7:167:GLU:CA[1_554] | 1.22 | 0.98 |
| 4:4:269:MET:C | 4:7:272:ALA:O[1_554] | 1.22 | 0.98 |
| 4:5:271:SER:C | 4:8:277:THR:OG1[1_554] | 1.22 | 0.98 |
| 4:5:221:LEU:C | 4:8:331:ALA:CA[1_554] | 1.22 | 0.98 |
| 4:5:192:ILE:N | 4:8:186:THR:CA[1_554] | 1.22 | 0.98 |
| 4:4:222:ASP:CA | 4:7:331:ALA:C[1_554] | 1.22 | 0.98 |
| 4:6:166:TYR:OH | 4:W:39:ARG:C[1_554] | 1.22 | 0.98 |
| 4:6:59:GLN:CD | 4:9:68:LYS:CG[1_554] | 1.22 | 0.98 |
| 4:5:294:TYR:CA | 4:8:166:TYR:O[1_554] | 1.22 | 0.98 |
| 4:5:112:PRO:CA | 4:9:253:GLU:CG[1_554] | 1.22 | 0.98 |
| 4:4:75:ILE:N | 4:8:197:GLY:C[1_554] | 1.22 | 0.98 |
| 4:6:349:LEU:N | 4:9:365:ALA:N[1_554] | 1.22 | 0.98 |
| 4:3:370:VAL:O | 4:7:230:ALA:CA[1_554] | 1.23 | 0.97 |
| 4:3:357:ILE:CB | 4:7:232:SER:CA[1_554] | 1.23 | 0.97 |
| 4:4:340:TRP:N | 4:7:118:LYS:N[1_554] | 1.23 | 0.97 |
| 4:5:262:PHE:CE1 | 4:8:153:LEU:C[1_554] | 1.23 | 0.97 |
| 4:6:141:SER:CB | 4:9:116:ARG:NE[1_554] | 1.23 | 0.97 |
| 4:5:316:GLU:C | 4:8:296:ASN:O[1_554] | 1.23 | 0.97 |
| 4:6:199:SER:C | 4:9:206:ARG:CB[1_554] | 1.23 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:307:PRO:N | 4:7:11:ASP:OD2[1_554] | 1.23 | 0.97 |
| 4:3:357:ILE:CG1 | 4:7:232:SER:CA[1_554] | 1.23 | 0.97 |
| 4:6:315:LYS:O | 4:9:296:ASN:C[1_554] | 1.23 | 0.97 |
| 4:6:250:ILE:CB | 4:9:214:GLU:OE1[1_554] | 1.23 | 0.97 |
| 4:5:279:TYR:OH | 4:8:290:ARG:CG[1_554] | 1.23 | 0.97 |
| 4:4:16:LEU:CD1 | 4:7:78:ASN:CA[1_554] | 1.23 | 0.97 |
| 4:6:340:TRP:CZ2 | 4:9:122:ILE:N[1_554] | 1.23 | 0.97 |
| 4:6:188:TYR:CE1 | 4:9:185:LEU:CD1[1_554] | 1.23 | 0.97 |
| 4:6:106:THR:CG2 | 4:9:114:ALA:C[1_554] | 1.23 | 0.97 |
| 4:4:313:MET:CB | 4:7:138:ALA:C[1_554] | 1.23 | 0.97 |
| 4:6:312:ARG:CZ | 4:9:299:MET:SD[1_554] | 1.23 | 0.97 |
| 4:6:347:ALA:CB | 4:9:367:PRO:CD[1_554] | 1.23 | 0.97 |
| 4:4:113:LYS:CD | 4:8:254:ARG:C[1_554] | 1.23 | 0.97 |
| 4:4:208:ILE:CB | 4:7:59:GLN:NE2[1_554] | 1.23 | 0.97 |
| 4:5:252:ASN:OD1 | 4:8:215:LYS:C[1_554] | 1.23 | 0.97 |
| 4:6:193:LEU:CA | 4:9:210:ARG:CA[1_554] | 1.23 | 0.97 |
| 4:6:243:PRO:CA | 4:9:60:SER:CB[1_554] | 1.23 | 0.97 |
| 4:5:305:MET:C | 4:8:11:ASP:OD2[1_554] | 1.23 | 0.97 |
| 4:3:114:ALA:C | 4:7:250:ILE:C[1_554] | 1.23 | 0.97 |
| 4:6:277:THR:OG1 | 4:9:176:MET:CG[1_554] | 1.23 | 0.97 |
| 4:6:173:HIS:ND1 | 4:V:266:PHE:N[1_554] | 1.23 | 0.97 |
| 4:4:336:LYS:NZ | 4:7:86:TRP:CG[1_554] | 1.23 | 0.97 |
| 4:4:140:LEU:O | 4:7:371:HIS:CG[1_554] | 1.23 | 0.97 |
| 4:6:250:ILE:CG2 | 4:9:214:GLU:OE1[1_554] | 1.23 | 0.97 |
| 4:4:327:ILE:N | 4:7:167:GLU:CA[1_554] | 1.23 | 0.97 |
| 4:6:22:ALA:C | 4:9:362:TYR:CE2[1_554] | 1.23 | 0.97 |
| 4:6:328:LYS:N | 4:9:148:THR:O[1_554] | 1.23 | 0.97 |
| 4:3:172:PRO:CG | 4:7:266:PHE:CD2[1_554] | 1.23 | 0.97 |
| 4:6:278:THR:OG1 | 4:9:163:VAL:CA[1_554] | 1.23 | 0.97 |
| 4:5:26:ALA:N | 4:8:123:MET:CA[1_554] | 1.23 | 0.97 |
| 4:3:369:ILE:O | 4:7:229:THR:O[1_554] | 1.23 | 0.97 |
| 4:5:24:ASP:O | 4:8:124:PHE:CG[1_554] | 1.23 | 0.97 |
| 4:6:27:PRO:CA | 4:9:122:ILE:CB[1_554] | 1.23 | 0.97 |
| 4:4:345:ILE:CG1 | 4:7:366:GLY:O[1_554] | 1.23 | 0.97 |
| 4:4:294:TYR:CE1 | 4:7:166:TYR:CB[1_554] | 1.23 | 0.97 |
| 4:4:173:HIS:CB | 4:8:267:ILE:CB[1_554] | 1.23 | 0.97 |
| 4:4:316:GLU:N | 4:7:142:LEU:CD1[1_554] | 1.23 | 0.97 |
| 4:5:150:GLY:C | 4:8:169:TYR:CE1[1_554] | 1.23 | 0.97 |
| 4:5:369:ILE:CB | 4:9:232:SER:CB[1_554] | 1.23 | 0.97 |
| 4:5:156:GLY:C | 4:8:74:GLY:C[1_554] | 1.23 | 0.97 |
| 4:5:321:ALA:O | 4:8:292:ASP:N[1_554] | 1.23 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:21:PHE:CA | 4:9:125:GLU:CD[1_554] | 1.23 | 0.97 |
| 4:6:283:MET:SD | 4:9:286:ASP:O[1_554] | 1.23 | 0.97 |
| 4:4:275:HIS:O | 4:7:164:PRO:N[1_554] | 1.23 | 0.97 |
| 4:6:31:PHE:CA | 4:9:81:ASP:N[1_554] | 1.23 | 0.97 |
| 4:5:242:LEU:CG | 4:8:207:GLU:OE1[1_554] | 1.23 | 0.97 |
| 4:6:237:GLU:OE1 | 4:9:215:LYS:CE[1_554] | 1.24 | 0.96 |
| 4:6:294:TYR:OH | 4:9:289:ILE:CG1[1_554] | 1.24 | 0.96 |
| 4:5:340:TRP:CG | 4:8:118:LYS:C[1_554] | 1.24 | 0.96 |
| 4:5:337:TYR:N | 4:8:119:MET:CE[1_554] | 1.24 | 0.96 |
| 4:6:294:TYR:CG | 4:9:166:TYR:CB[1_554] | 1.24 | 0.96 |
| 4:5:317:ILE:CG2 | 4:8:150:GLY:O[1_554] | 1.24 | 0.96 |
| 4:6:345:ILE:CB | 4:9:369:ILE:CG2[1_554] | 1.24 | 0.96 |
| 4:5:188:TYR:OH | 4:8:185:LEU:CD2[1_554] | 1.24 | 0.96 |
| 4:6:25:ASP:OD2 | 4:9:129:VAL:C[1_554] | 1.24 | 0.96 |
| 4:6:137:GLN:NE2 | 4:9:112:PRO:CB[1_554] | 1.24 | 0.96 |
| 4:5:258:PRO:O | 4:8:155:SER:CB[1_554] | 1.24 | 0.96 |
| 4:2:291:LYS:CE | 4:7:39:ARG:CA[1_554] | 1.24 | 0.96 |
| 4:6:161:HIS:C | 4:9:110:LEU:CG[1_554] | 1.24 | 0.96 |
| 4:5:280:ASN:O | 4:8:284:LYS:O[1_554] | 1.24 | 0.96 |
| 4:6:109:PRO:O | 4:V:195:GLU:OE1[1_554] | 1.24 | 0.96 |
| 4:4:261:LEU:O | 4:7:161:HIS:N[1_554] | 1.24 | 0.96 |
| 4:6:196:ARG:NH1 | 4:9:215:LYS:CB[1_554] | 1.24 | 0.96 |
| 4:4:338:SER:CB | 4:7:116:ARG:CG[1_554] | 1.24 | 0.96 |
| 4:5:335:ARG:NH2 | 4:8:339:VAL:CG1[1_554] | 1.24 | 0.96 |
| 4:4:194:THR:C | 4:7:209:VAL:CG1[1_554] | 1.24 | 0.96 |
| 4:4:316:GLU:O | 4:7:150:GLY:C[1_554] | 1.24 | 0.96 |
| 4:4:109:PRO:CD | 4:8:195:GLU:CG[1_554] | 1.24 | 0.96 |
| 4:4:299:MET:N | 4:7:136:ILE:CG1[1_554] | 1.24 | 0.96 |
| 4:6:215:LYS:NZ | 4:9:31:PHE:CB[1_554] | 1.24 | 0.96 |
| 4:5:321:ALA:O | 4:8:292:ASP:CA[1_554] | 1.24 | 0.96 |
| 4:5:28:ARG:O | 4:8:83:GLU:OE2[1_554] | 1.24 | 0.96 |
| 4:6:309:ILE:CD1 | 4:9:154:ASP:OD2[1_554] | 1.24 | 0.96 |
| 4:5:349:LEU:CB | 4:8:365:ALA:CB[1_554] | 1.24 | 0.96 |
| 4:5:183:ARG:CZ | 4:8:72:GLU:OE1[1_554] | 1.24 | 0.96 |
| 4:6:157:ASP:OD1 | 4:9:71:ILE:C[1_554] | 1.24 | 0.96 |
| 4:6:18:LYS:O | 4:9:118:LYS:CG[1_554] | 1.24 | 0.96 |
| 4:4:259:GLU:CG | 4:7:304:THR:CA[1_554] | 1.24 | 0.96 |
| 4:4:196:ARG:CD | 4:7:211:ASP:CB[1_554] | 1.24 | 0.96 |
| 4:4:205:GLU:CB | 4:7:62:ARG:NE[1_554] | 1.24 | 0.96 |
| 4:6:220:ALA:N | 4:9:335:ARG:CB[1_554] | 1.24 | 0.96 |
| 4:4:317:ILE:CD1 | 4:7:165:ILE:CA[1_554] | 1.24 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:331:ALA:C | 4:9:140:LEU:CD2[1_554] | 1.24 | 0.96 |
| 4:6:312:ARG:C | 4:9:298:VAL:CB[1_554] | 1.24 | 0.96 |
| 4:3:371:HIS:CE1 | 4:7:252:ASN:O[1_554] | 1.24 | 0.96 |
| 4:5:299:MET:O | 4:8:135:ALA:C[1_554] | 1.24 | 0.96 |
| 4:5:276:GLU:OE2 | 4:8:278:THR:C[1_554] | 1.24 | 0.96 |
| 4:5:276:GLU:OE1 | 4:8:279:TYR:C[1_554] | 1.24 | 0.96 |
| 4:5:294:TYR:CD2 | 4:8:166:TYR:CG[1_554] | 1.24 | 0.96 |
| 4:5:294:TYR:CD2 | 4:8:166:TYR:CD1[1_554] | 1.24 | 0.96 |
| 4:6:24:ASP:OD2 | 4:9:125:GLU:C[1_554] | 1.24 | 0.96 |
| 4:4:317:ILE:CD1 | 4:7:165:ILE:CB[1_554] | 1.24 | 0.96 |
| 4:5:340:TRP:CZ3 | 4:8:120:THR:C[1_554] | 1.24 | 0.96 |
| 4:4:117:GLU:C | 4:8:237:GLU:CB[1_554] | 1.24 | 0.96 |
| 4:3:116:ARG:CD | 4:7:252:ASN:OD1[1_554] | 1.24 | 0.96 |
| 4:5:157:ASP:OD1 | 4:8:71:ILE:O[1_554] | 1.24 | 0.96 |
| 4:4:281:SER:CB | 4:7:173:HIS:N[1_554] | 1.24 | 0.96 |
| 4:6:184:ASP:OD1 | 4:9:73:HIS:CE1[1_554] | 1.24 | 0.96 |
| 4:5:173:HIS:CB | 4:9:267:ILE:CA[1_554] | 1.24 | 0.96 |
| 4:3:118:LYS:CB | 4:7:249:THR:OG1[1_554] | 1.25 | 0.95 |
| 4:5:198:TYR:CB | 4:8:209:VAL:N[1_554] | 1.25 | 0.95 |
| 4:5:28:ARG:CG | 4:8:126:THR:CG2[1_554] | 1.25 | 0.95 |
| 4:6:321:ALA:O | 4:9:292:ASP:CA[1_554] | 1.25 | 0.95 |
| 4:5:227:MET:C | 4:8:307:PRO:CB[1_554] | 1.25 | 0.95 |
| 4:4:329:ILE:CG2 | 4:7:139:VAL:CG1[1_554] | 1.25 | 0.95 |
| 4:4:109:PRO:C | 4:8:195:GLU:OE1[1_554] | 1.25 | 0.95 |
| 4:4:223:PHE:CE2 | 4:7:300:SER:C[1_554] | 1.25 | 0.95 |
| 4:5:297:ASN:CG | 4:8:165:ILE:CG1[1_554] | 1.25 | 0.95 |
| 4:6:334:GLU:N | 4:9:105:LEU:N[1_554] | 1.25 | 0.95 |
| 4:4:215:LYS:CD | 4:7:31:PHE:CG[1_554] | 1.25 | 0.95 |
| 4:6:183:ARG:CZ | 4:9:72:GLU:OE1[1_554] | 1.25 | 0.95 |
| 4:5:305:MET:CE | 4:8:11:ASP:CA[1_554] | 1.25 | 0.95 |
| 4:6:259:GLU:CD | 4:9:309:ILE:CD1[1_554] | 1.25 | 0.95 |
| 4:5:278:THR:OG1 | 4:8:163:VAL:CA[1_554] | 1.25 | 0.95 |
| 1:A:637:LYS:CD | 4:5:311:ASP:CG[1_556] | 1.25 | 0.95 |
| 4:5:288:ASP:CA | 4:V:62:ARG:C[1_554] | 1.25 | 0.95 |
| 4:6:283:MET:CB | 4:9:286:ASP:N[1_554] | 1.25 | 0.95 |
| 4:4:30:VAL:CG2 | 4:7:79:TRP:O[1_554] | 1.25 | 0.95 |
| 4:6:312:ARG:CG | 4:9:299:MET:C[1_554] | 1.25 | 0.95 |
| 4:4:250:ILE:CD1 | 4:7:210:ARG:NH2[1_554] | 1.25 | 0.95 |
| 4:5:317:ILE:CG1 | 4:8:150:GLY:O[1_554] | 1.25 | 0.95 |
| 4:4:154:ASP:N | 4:7:110:LEU:N[1_554] | 1.25 | 0.95 |
| 4:6:211:ASP:CG | 4:9:32:PRO:CG[1_554] | 1.25 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:215:LYS:NZ | 4:8:31:PHE:CB[1_554] | 1.25 | 0.95 |
| 4:5:278:THR:OG1 | 4:8:163:VAL:C[1_554] | 1.25 | 0.95 |
| 4:5:283:MET:SD | 4:8:286:ASP:O[1_554] | 1.25 | 0.95 |
| 4:5:193:LEU:C | 4:8:209:VAL:C[1_554] | 1.25 | 0.95 |
| 4:5:113:LYS:CG | 4:9:252:ASN:C[1_554] | 1.25 | 0.95 |
| 4:5:21:PHE:C | 4:8:125:GLU:CD[1_554] | 1.25 | 0.95 |
| 4:6:348:SER:N | 4:9:366:GLY:N[1_554] | 1.25 | 0.95 |
| 4:5:211:ASP:CG | 4:8:32:PRO:N[1_554] | 1.25 | 0.95 |
| 4:6:143:TYR:CA | 4:9:372:ARG:CB[1_554] | 1.25 | 0.95 |
| 4:5:277:THR:CG2 | 4:8:176:MET:N[1_554] | 1.25 | 0.95 |
| 4:4:266:PHE:CG | 4:7:261:LEU:CD1[1_554] | 1.25 | 0.95 |
| 4:6:277:THR:O | 4:9:174:ALA:C[1_554] | 1.25 | 0.95 |
| 4:5:21:PHE:CA | 4:8:125:GLU:CD[1_554] | 1.25 | 0.95 |
| 4:5:326:LYS:C | 4:8:167:GLU:OE2[1_554] | 1.25 | 0.95 |
| 4:4:74:GLY:O | 4:8:197:GLY:N[1_554] | 1.25 | 0.95 |
| 4:4:286:ASP:C | 4:8:270:GLU:OE1[1_554] | 1.25 | 0.95 |
| 4:5:333:PRO:CD | 4:8:104:LEU:CG[1_554] | 1.25 | 0.95 |
| 4:4:213:LYS:C | 4:7:16:LEU:CA[1_554] | 1.25 | 0.95 |
| 4:6:335:ARG:CG | 4:9:106:THR:CG2[1_554] | 1.25 | 0.95 |
| 4:5:28:ARG:CD | 4:8:126:THR:CB[1_554] | 1.26 | 0.94 |
| 4:4:161:HIS:CA | 4:7:110:LEU:CD1[1_554] | 1.26 | 0.94 |
| 4:4:188:TYR:CG | 4:7:181:ALA:C[1_554] | 1.26 | 0.94 |
| 4:4:192:ILE:CG2 | 4:7:213:LYS:CD[1_554] | 1.26 | 0.94 |
| 4:6:32:PRO:CG | 4:9:81:ASP:OD2[1_554] | 1.26 | 0.94 |
| 4:4:169:TYR:OH | 4:8:266:PHE:CD1[1_554] | 1.26 | 0.94 |
| 4:4:338:SER:O | 4:7:117:GLU:N[1_554] | 1.26 | 0.94 |
| 4:5:114:ALA:C | 4:9:196:ARG:NH2[1_554] | 1.26 | 0.94 |
| 4:6:293:LEU:CG | 4:9:169:TYR:CE2[1_554] | 1.26 | 0.94 |
| 4:3:111:ASN:OD1 | 4:7:196:ARG:CG[1_554] | 1.26 | 0.94 |
| 4:4:153:LEU:CD2 | 4:7:109:PRO:CG[1_554] | 1.26 | 0.94 |
| 4:5:180:LEU:CB | 4:8:179:ASP:N[1_554] | 1.26 | 0.94 |
| 4:5:145:SER:CB | 4:8:372:ARG:NH1[1_554] | 1.26 | 0.94 |
| 4:6:277:THR:CG2 | 4:9:176:MET:N[1_554] | 1.26 | 0.94 |
| 4:4:116:ARG:CD | 4:8:252:ASN:CG[1_554] | 1.26 | 0.94 |
| 4:6:316:GLU:OE2 | 4:9:297:ASN:ND2[1_554] | 1.26 | 0.94 |
| 4:6:342:GLY:N | 4:9:370:VAL:CG1[1_554] | 1.26 | 0.94 |
| 4:6:313:MET:CG | 4:9:152:VAL:CG2[1_554] | 1.26 | 0.94 |
| 4:4:317:ILE:CG2 | 4:7:165:ILE:N[1_554] | 1.26 | 0.94 |
| 4:6:160:THR:OG1 | 4:9:161:HIS:CE1[1_554] | 1.26 | 0.94 |
| 4:4:157:ASP:OD1 | 4:7:72:GLU:N[1_554] | 1.26 | 0.94 |
| 4:3:75:ILE:CG1 | 4:7:193:LEU:O[1_554] | 1.26 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:255:PHE:O | 4:8:304:THR:N[1_554] | 1.26 | 0.94 |
| 4:6:113:LYS:N | 4:V:253:GLU:CD[1_554] | 1.26 | 0.94 |
| 4:6:227:MET:CG | 4:9:307:PRO:CA[1_554] | 1.26 | 0.94 |
| 4:6:345:ILE:CG2 | 4:9:369:ILE:CG1[1_554] | 1.26 | 0.94 |
| 4:4:357:ILE:CD1 | 4:8:232:SER:N[1_554] | 1.26 | 0.94 |
| 4:4:27:PRO:CD | 4:7:122:ILE:CG1[1_554] | 1.26 | 0.94 |
| 4:6:156:GLY:C | 4:9:74:GLY:CA[1_554] | 1.26 | 0.94 |
| 4:6:17:VAL:CA | 4:9:79:TRP:CG[1_554] | 1.26 | 0.94 |
| 4:4:326:LYS:CA | 4:7:167:GLU:OE1[1_554] | 1.26 | 0.94 |
| 4:4:306:TYR:N | 4:7:11:ASP:OD1[1_554] | 1.26 | 0.94 |
| 4:6:19:ALA:CB | 4:9:118:LYS:NZ[1_554] | 1.26 | 0.94 |
| 4:5:56:ASP:OD2 | 4:8:81:ASP:OD1[1_554] | 1.26 | 0.94 |
| 4:5:335:ARG:C | 4:8:106:THR:C[1_554] | 1.26 | 0.94 |
| 4:5:317:ILE:CD1 | 4:8:165:ILE:O[1_554] | 1.26 | 0.94 |
| 4:5:305:MET:CA | 4:8:11:ASP:OD1[1_554] | 1.26 | 0.94 |
| 4:3:76:ILE:O | 4:7:198:TYR:CE1[1_554] | 1.26 | 0.94 |
| 4:5:262:PHE:CG | 4:8:153:LEU:CB[1_554] | 1.26 | 0.94 |
| 4:5:263:GLN:CA | 4:8:274:ILE:CB[1_554] | 1.26 | 0.94 |
| 4:3:117:GLU:OE1 | 4:7:236:LEU:O[1_554] | 1.26 | 0.94 |
| 4:3:291:LYS:CG | 4:8:64:ILE:CG1[1_554] | 1.26 | 0.94 |
| 4:4:283:MET:CB | 4:7:285:CYS:C[1_554] | 1.26 | 0.94 |
| 4:5:183:ARG:NE | 4:8:72:GLU:OE1[1_554] | 1.26 | 0.94 |
| 4:5:272:ALA:O | 4:8:277:THR:CG2[1_554] | 1.26 | 0.94 |
| 4:6:312:ARG:CG | 4:9:299:MET:CA[1_554] | 1.26 | 0.94 |
| 4:6:26:ALA:O | 4:9:122:ILE:C[1_554] | 1.27 | 0.93 |
| 4:6:181:ALA:CA | 4:9:159:VAL:CG1[1_554] | 1.27 | 0.93 |
| 4:2:291:LYS:CE | 4:7:39:ARG:O[1_554] | 1.27 | 0.93 |
| 4:6:333:PRO:CG | 4:9:104:LEU:CB[1_554] | 1.27 | 0.93 |
| 4:6:186:THR:C | 4:9:183:ARG:CG[1_554] | 1.27 | 0.93 |
| 4:4:266:PHE:CA | 4:7:261:LEU:CG[1_554] | 1.27 | 0.93 |
| 4:4:336:LYS:NZ | 4:7:86:TRP:CE2[1_554] | 1.27 | 0.93 |
| 4:6:274:ILE:O | 4:9:162:ASN:O[1_554] | 1.27 | 0.93 |
| 4:4:277:THR:O | 4:7:175:ILE:N[1_554] | 1.27 | 0.93 |
| 4:4:255:PHE:CA | 4:7:302:GLY:CA[1_554] | 1.27 | 0.93 |
| 4:6:28:ARG:O | 4:9:83:GLU:CD[1_554] | 1.27 | 0.93 |
| 4:3:173:HIS:CD2 | 4:7:264:PRO:O[1_554] | 1.27 | 0.93 |
| 4:6:286:ASP:CA | 4:V:270:GLU:CD[1_554] | 1.27 | 0.93 |
| 4:4:213:LYS:O | 4:7:16:LEU:CA[1_554] | 1.27 | 0.93 |
| 4:4:137:GLN:O | 4:7:113:LYS:CB[1_554] | 1.27 | 0.93 |
| 4:6:341:ILE:CD1 | 4:9:132:MET:CE[1_554] | 1.27 | 0.93 |
| 4:6:196:ARG:CB | 4:9:212:ILE:CA[1_554] | 1.27 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:259:GLU:OE1 | 4:7:305:MET:N[1_554] | 1.27 | 0.93 |
| 4:5:166:TYR:CZ | 4:V:39:ARG:C[1_554] | 1.27 | 0.93 |
| 4:5:326:LYS:CB | 4:8:167:GLU:CD[1_554] | 1.27 | 0.93 |
| 4:6:338:SER:CA | 4:9:134:VAL:CG2[1_554] | 1.27 | 0.93 |
| 4:6:297:ASN:N | 4:9:168:GLY:C[1_554] | 1.27 | 0.93 |
| 4:6:367:PRO:CD | 4:V:234:SER:N[1_554] | 1.27 | 0.93 |
| 4:6:307:PRO:CA | 4:9:337:TYR:C[1_554] | 1.27 | 0.93 |
| 4:2:288:ASP:C | 4:7:39:ARG:NE[1_554] | 1.27 | 0.93 |
| 4:5:173:HIS:C | 4:9:267:ILE:CA[1_554] | 1.27 | 0.93 |
| 4:6:279:TYR:OH | 4:9:290:ARG:CG[1_554] | 1.27 | 0.93 |
| 4:5:309:ILE:C | 4:8:141:SER:OG[1_554] | 1.27 | 0.93 |
| 4:5:178:LEU:O | 4:8:177:ARG:CG[1_554] | 1.27 | 0.93 |
| 4:4:113:LYS:O | 4:8:251:GLY:CA[1_554] | 1.27 | 0.93 |
| 4:6:249:THR:CA | 4:9:211:ASP:OD2[1_554] | 1.27 | 0.93 |
| 4:5:112:PRO:O | 4:9:253:GLU:CD[1_554] | 1.27 | 0.93 |
| 4:6:326:LYS:CG | 4:9:167:GLU:OE1[1_554] | 1.27 | 0.93 |
| 4:5:141:SER:CB | 4:8:116:ARG:NE[1_554] | 1.27 | 0.93 |
| 4:5:255:PHE:CG | 4:8:305:MET:CA[1_554] | 1.27 | 0.93 |
| 4:5:349:LEU:CB | 4:8:365:ALA:CA[1_554] | 1.27 | 0.93 |
| 4:4:294:TYR:CB | 4:7:166:TYR:O[1_554] | 1.27 | 0.93 |
| 4:4:357:ILE:CB | 4:8:232:SER:CA[1_554] | 1.27 | 0.93 |
| 4:6:294:TYR:C | 4:9:167:GLU:N[1_554] | 1.27 | 0.93 |
| 4:4:211:ASP:C | 4:7:32:PRO:CB[1_554] | 1.27 | 0.93 |
| 4:4:344:SER:CA | 4:7:367:PRO:CG[1_554] | 1.27 | 0.93 |
| 4:4:25:ASP:CG | 4:7:124:PHE:CB[1_554] | 1.27 | 0.93 |
| 4:5:137:GLN:CA | 4:8:113:LYS:CA[1_554] | 1.27 | 0.93 |
| 4:6:348:SER:OG | 4:9:362:TYR:C[1_554] | 1.27 | 0.93 |
| 4:5:173:HIS:CG | 4:9:267:ILE:N[1_554] | 1.27 | 0.93 |
| 4:6:304:THR:CB | 4:9:137:GLN:CG[1_554] | 1.27 | 0.93 |
| 4:3:79:TRP:CH2 | 4:7:249:THR:CG2[1_554] | 1.27 | 0.93 |
| 1:A:542:PHE:CE2 | 4:5:328:LYS:NZ[1_556] | 1.27 | 0.93 |
| 4:5:156:GLY:C | 4:8:75:ILE:N[1_554] | 1.27 | 0.93 |
| 4:5:320:LEU:CA | 4:8:294:TYR:N[1_554] | 1.27 | 0.93 |
| 4:6:335:ARG:C | 4:9:106:THR:C[1_554] | 1.28 | 0.92 |
| 4:5:24:ASP:CA | 4:8:124:PHE:CA[1_554] | 1.28 | 0.92 |
| 4:6:219:VAL:CB | 4:9:301:GLY:N[1_554] | 1.28 | 0.92 |
| 4:4:216:LEU:CA | 4:7:30:VAL:CG1[1_554] | 1.28 | 0.92 |
| 4:5:294:TYR:CB | 4:8:166:TYR:CG[1_554] | 1.28 | 0.92 |
| 4:5:219:VAL:CG1 | 4:8:300:SER:C[1_554] | 1.28 | 0.92 |
| 4:5:112:PRO:O | 4:9:253:GLU:OE1[1_554] | 1.28 | 0.92 |
| 4:4:188:TYR:CD1 | 4:7:181:ALA:O[1_554] | 1.28 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:17:VAL:CA | 4:9:79:TRP:CD1[1_554] | 1.28 | 0.92 |
| 4:3:357:ILE:CG1 | 4:7:231:ALA:C[1_554] | 1.28 | 0.92 |
| 4:6:257:CYS:N | 4:9:303:THR:CA[1_554] | 1.28 | 0.92 |
| 4:4:315:LYS:NZ | 4:7:147:ARG:CD[1_554] | 1.28 | 0.92 |
| 4:5:270:GLU:N | 4:8:271:SER:C[1_554] | 1.28 | 0.92 |
| 4:4:213:LYS:CG | 4:7:15:GLY:N[1_554] | 1.28 | 0.92 |
| 4:6:276:GLU:OE1 | 4:9:279:TYR:C[1_554] | 1.28 | 0.92 |
| 4:5:316:GLU:OE2 | 4:8:297:ASN:ND2[1_554] | 1.28 | 0.92 |
| 4:5:184:ASP:OD1 | 4:8:73:HIS:CE1[1_554] | 1.28 | 0.92 |
| 4:6:280:ASN:O | 4:9:284:LYS:O[1_554] | 1.28 | 0.92 |
| 4:6:157:ASP:O | 4:9:73:HIS:CA[1_554] | 1.28 | 0.92 |
| 4:5:274:ILE:N | 4:8:162:ASN:N[1_554] | 1.28 | 0.92 |
| 4:5:215:LYS:CA | 4:8:30:VAL:CG1[1_554] | 1.28 | 0.92 |
| 4:6:265:SER:CA | 4:9:261:LEU:O[1_554] | 1.28 | 0.92 |
| 4:4:212:ILE:N | 4:7:32:PRO:CB[1_554] | 1.28 | 0.92 |
| 4:5:164:PRO:CD | 4:8:172:PRO:CG[1_554] | 1.28 | 0.92 |
| 4:4:261:LEU:CA | 4:7:154:ASP:O[1_554] | 1.28 | 0.92 |
| 4:4:371:HIS:CB | 4:8:236:LEU:CD1[1_554] | 1.28 | 0.92 |
| 4:6:191:LYS:CA | 4:9:187:ASP:N[1_554] | 1.28 | 0.92 |
| 4:5:31:PHE:CA | 4:8:81:ASP:N[1_554] | 1.28 | 0.92 |
| 4:6:304:THR:N | 4:9:137:GLN:CD[1_554] | 1.28 | 0.92 |
| 4:6:178:LEU:CG | 4:9:177:ARG:N[1_554] | 1.28 | 0.92 |
| 4:4:214:GLU:N | 4:7:16:LEU:N[1_554] | 1.28 | 0.92 |
| 4:4:369:ILE:O | 4:8:229:THR:O[1_554] | 1.28 | 0.92 |
| 4:5:345:ILE:CG2 | 4:8:369:ILE:CG1[1_554] | 1.28 | 0.92 |
| 4:5:348:SER:N | 4:8:366:GLY:N[1_554] | 1.28 | 0.92 |
| 4:6:173:HIS:CB | 4:V:267:ILE:N[1_554] | 1.28 | 0.92 |
| 4:5:332:PRO:N | 4:8:135:ALA:CB[1_554] | 1.28 | 0.92 |
| 4:6:11:ASP:OD1 | 4:9:115:ASN:CA[1_554] | 1.28 | 0.92 |
| 4:4:187:ASP:CA | 4:7:183:ARG:CG[1_554] | 1.28 | 0.92 |
| 4:4:248:ILE:CD1 | 4:7:207:GLU:CG[1_554] | 1.28 | 0.92 |
| 4:5:318:THR:O | 4:8:292:ASP:O[1_554] | 1.28 | 0.92 |
| 4:6:151:ILE:CD1 | 4:9:171:LEU:C[1_554] | 1.28 | 0.92 |
| 4:5:181:ALA:CA | 4:8:159:VAL:CG1[1_554] | 1.28 | 0.92 |
| 4:5:188:TYR:CA | 4:8:184:ASP:N[1_554] | 1.28 | 0.92 |
| 4:6:265:SER:C | 4:9:261:LEU:C[1_554] | 1.28 | 0.92 |
| 4:6:166:TYR:CZ | 4:W:39:ARG:C[1_554] | 1.28 | 0.92 |
| 4:4:333:PRO:CG | 4:7:103:THR:O[1_554] | 1.28 | 0.92 |
| 4:5:310:ALA:C | 4:8:141:SER:O[1_554] | 1.28 | 0.92 |
| 4:6:309:ILE:C | 4:9:141:SER:OG[1_554] | 1.28 | 0.92 |
| 4:6:151:ILE:CG1 | 4:9:170:ALA:O[1_554] | 1.28 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:349:LEU:CB | 4:9:365:ALA:CA[1_554] | 1.28 | 0.92 |
| 4:6:180:LEU:CB | 4:9:178:LEU:O[1_554] | 1.28 | 0.92 |
| 4:5:312:ARG:CZ | 4:8:299:MET:SD[1_554] | 1.28 | 0.92 |
| 4:4:282:ILE:N | 4:7:173:HIS:NE2[1_554] | 1.28 | 0.92 |
| 4:4:157:ASP:OD1 | 4:7:72:GLU:CB[1_554] | 1.28 | 0.92 |
| 4:5:274:ILE:CD1 | 4:8:161:HIS:CB[1_554] | 1.28 | 0.92 |
| 4:6:313:MET:CA | 4:9:152:VAL:CG2[1_554] | 1.29 | 0.91 |
| 4:5:113:LYS:N | 4:9:253:GLU:CD[1_554] | 1.29 | 0.91 |
| 4:6:255:PHE:CB | 4:9:305:MET:CB[1_554] | 1.29 | 0.91 |
| 4:4:187:ASP:N | 4:7:183:ARG:CG[1_554] | 1.29 | 0.91 |
| 4:4:199:SER:CA | 4:7:206:ARG:CB[1_554] | 1.29 | 0.91 |
| 4:4:178:LEU:CG | 4:7:177:ARG:N[1_554] | 1.29 | 0.91 |
| 4:5:314:GLN:OE1 | 4:8:147:ARG:CB[1_554] | 1.29 | 0.91 |
| 4:4:256:ARG:CA | 4:7:302:GLY:O[1_554] | 1.29 | 0.91 |
| 4:6:28:ARG:CD | 4:9:126:THR:CB[1_554] | 1.29 | 0.91 |
| 4:4:109:PRO:CA | 4:8:195:GLU:CG[1_554] | 1.29 | 0.91 |
| 4:5:322:PRO:C | 4:8:291:LYS:NZ[1_554] | 1.29 | 0.91 |
| 4:6:18:LYS:NZ | 4:9:76:ILE:CB[1_554] | 1.29 | 0.91 |
| 4:5:342:GLY:CA | 4:8:370:VAL:CG1[1_554] | 1.29 | 0.91 |
| 4:6:269:MET:O | 4:9:272:ALA:O[1_554] | 1.29 | 0.91 |
| 4:4:154:ASP:N | 4:7:109:PRO:C[1_554] | 1.29 | 0.91 |
| 4:4:215:LYS:CG | 4:7:31:PHE:CG[1_554] | 1.29 | 0.91 |
| 4:6:32:PRO:C | 4:9:78:ASN:CB[1_554] | 1.29 | 0.91 |
| 4:5:279:TYR:N | 4:8:164:PRO:CB[1_554] | 1.29 | 0.91 |
| 4:6:343:GLY:O | 4:9:367:PRO:CB[1_554] | 1.29 | 0.91 |
| 4:4:243:PRO:CB | 4:7:61:LYS:CA[1_554] | 1.29 | 0.91 |
| 4:6:178:LEU:O | 4:9:177:ARG:CD[1_554] | 1.29 | 0.91 |
| 4:6:196:ARG:CB | 4:9:212:ILE:N[1_554] | 1.29 | 0.91 |
| 4:4:267:ILE:O | 4:7:180:LEU:CD2[1_554] | 1.29 | 0.91 |
| 4:5:249:THR:OG1 | 4:8:215:LYS:NZ[1_554] | 1.29 | 0.91 |
| 4:6:221:LEU:CA | 4:9:332:PRO:CD[1_554] | 1.29 | 0.91 |
| 4:4:272:ALA:CA | 4:7:277:THR:CG2[1_554] | 1.29 | 0.91 |
| 4:4:267:ILE:CB | 4:7:180:LEU:CB[1_554] | 1.29 | 0.91 |
| 4:5:26:ALA:N | 4:8:123:MET:C[1_554] | 1.29 | 0.91 |
| 4:3:109:PRO:C | 4:7:195:GLU:OE1[1_554] | 1.29 | 0.91 |
| 4:6:368:SER:O | 4:V:229:THR:C[1_554] | 1.29 | 0.91 |
| 4:4:198:TYR:C | 4:7:206:ARG:C[1_554] | 1.29 | 0.91 |
| 4:5:20:GLY:N | 4:8:121:GLN:OE1[1_554] | 1.29 | 0.91 |
| 4:6:304:THR:CA | 4:9:137:GLN:OE1[1_554] | 1.29 | 0.91 |
| 4:4:153:LEU:C | 4:7:109:PRO:C[1_554] | 1.29 | 0.91 |
| 4:5:342:GLY:N | 4:8:370:VAL:CG1[1_554] | 1.29 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:208:ILE:CD1 | 4:7:59:GLN:CB[1_554] | 1.29 | 0.91 |
| 4:5:369:ILE:CB | 4:9:232:SER:OG[1_554] | 1.29 | 0.91 |
| 4:4:281:SER:O | 4:7:173:HIS:CG[1_554] | 1.29 | 0.91 |
| 4:6:227:MET:CA | 4:9:307:PRO:CA[1_554] | 1.29 | 0.91 |
| 4:5:31:PHE:CD1 | 4:8:80:ASP:N[1_554] | 1.29 | 0.91 |
| 4:4:25:ASP:OD1 | 4:7:124:PHE:CB[1_554] | 1.29 | 0.91 |
| 4:5:186:THR:OG1 | 4:8:183:ARG:NH2[1_554] | 1.29 | 0.91 |
| 4:6:267:ILE:CB | 4:9:180:LEU:CD1[1_554] | 1.29 | 0.91 |
| 4:4:332:PRO:CB | 4:7:133:TYR:C[1_554] | 1.29 | 0.91 |
| 4:5:266:PHE:CE2 | 4:8:261:LEU:CD1[1_554] | 1.29 | 0.91 |
| 4:6:28:ARG:CG | 4:9:126:THR:CG2[1_554] | 1.29 | 0.91 |
| 4:6:262:PHE:CD2 | 4:9:153:LEU:O[1_554] | 1.29 | 0.91 |
| 4:3:357:ILE:CD1 | 4:7:232:SER:N[1_554] | 1.29 | 0.91 |
| 4:5:157:ASP:OD1 | 4:8:71:ILE:C[1_554] | 1.29 | 0.91 |
| 4:5:349:LEU:CG | 4:8:365:ALA:CB[1_554] | 1.29 | 0.91 |
| 4:5:18:LYS:CB | 4:8:79:TRP:CE3[1_554] | 1.29 | 0.91 |
| 4:4:185:LEU:CA | 4:7:158:GLY:N[1_554] | 1.29 | 0.91 |
| 1:A:542:PHE:CZ | 4:5:328:LYS:NZ[1_556] | 1.29 | 0.91 |
| 4:5:222:ASP:CA | 4:8:331:ALA:CB[1_554] | 1.29 | 0.91 |
| 4:6:164:PRO:CG | 4:9:172:PRO:CG[1_554] | 1.29 | 0.91 |
| 4:5:195:GLU:CG | 4:8:189:LEU:CD1[1_554] | 1.29 | 0.91 |
| 4:5:262:PHE:CD2 | 4:8:153:LEU:O[1_554] | 1.29 | 0.91 |
| 4:6:340:TRP:CZ3 | 4:9:120:THR:C[1_554] | 1.29 | 0.91 |
| 4:5:193:LEU:CB | 4:8:210:ARG:CA[1_554] | 1.29 | 0.91 |
| 4:6:278:THR:CB | 4:9:164:PRO:CD[1_554] | 1.29 | 0.91 |
| 4:5:161:HIS:CB | 4:8:110:LEU:CG[1_554] | 1.29 | 0.91 |
| 4:4:273:GLY:C | 4:7:162:ASN:N[1_554] | 1.29 | 0.91 |
| 4:6:143:TYR:CE2 | 4:9:369:ILE:O[1_554] | 1.29 | 0.91 |
| 4:4:310:ALA:CA | 4:7:140:LEU:CA[1_554] | 1.30 | 0.90 |
| 4:5:304:THR:N | 4:8:137:GLN:CD[1_554] | 1.30 | 0.90 |
| 4:5:24:ASP:OD2 | 4:8:125:GLU:C[1_554] | 1.30 | 0.90 |
| 4:4:30:VAL:CG1 | 4:7:79:TRP:C[1_554] | 1.30 | 0.90 |
| 4:6:144:ALA:N | 4:9:370:VAL:O[1_554] | 1.30 | 0.90 |
| 4:5:215:LYS:CE | 4:8:31:PHE:CB[1_554] | 1.30 | 0.90 |
| 4:6:249:THR:CG2 | 4:9:215:LYS:NZ[1_554] | 1.30 | 0.90 |
| 4:5:340:TRP:CZ2 | 4:8:121:GLN:CA[1_554] | 1.30 | 0.90 |
| 4:6:315:LYS:O | 4:9:296:ASN:CA[1_554] | 1.30 | 0.90 |
| 4:6:249:THR:O | 4:9:211:ASP:OD2[1_554] | 1.30 | 0.90 |
| 4:6:11:ASP:CG | 4:9:115:ASN:CA[1_554] | 1.30 | 0.90 |
| 4:6:312:ARG:NE | 4:9:299:MET:CG[1_554] | 1.30 | 0.90 |
| 4:4:340:TRP:CH2 | 4:7:121:GLN:CD[1_554] | 1.30 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:341:ILE:CG2 | 4:8:132:MET:SD[1_554] | 1.30 | 0.90 |
| 4:5:300:SER:C | 4:8:107:GLU:O[1_554] | 1.30 | 0.90 |
| 4:5:141:SER:CA | 4:8:116:ARG:CD[1_554] | 1.30 | 0.90 |
| 4:4:258:PRO:O | 4:7:155:SER:CA[1_554] | 1.30 | 0.90 |
| 4:6:269:MET:C | 4:9:272:ALA:O[1_554] | 1.30 | 0.90 |
| 4:5:185:LEU:CB | 4:8:158:GLY:N[1_554] | 1.30 | 0.90 |
| 4:5:157:ASP:O | 4:8:73:HIS:N[1_554] | 1.30 | 0.90 |
| 4:4:281:SER:OG | 4:7:173:HIS:CA[1_554] | 1.30 | 0.90 |
| 4:5:346:LEU:CB | 4:8:368:SER:C[1_554] | 1.30 | 0.90 |
| 4:5:325:MET:CG | 4:8:166:TYR:CE1[1_554] | 1.30 | 0.90 |
| 4:6:276:GLU:C | 4:9:281:SER:OG[1_554] | 1.30 | 0.90 |
| 4:4:15:GLY:CA | 4:7:77:THR:CB[1_554] | 1.30 | 0.90 |
| 4:6:180:LEU:CD1 | 4:9:160:THR:N[1_554] | 1.30 | 0.90 |
| 4:3:110:LEU:N | 4:7:192:ILE:CA[1_554] | 1.30 | 0.90 |
| 4:6:294:TYR:O | 4:9:167:GLU:N[1_554] | 1.30 | 0.90 |
| 4:5:312:ARG:NH2 | 4:8:299:MET:SD[1_554] | 1.30 | 0.90 |
| 4:3:113:LYS:CG | 4:7:254:ARG:N[1_554] | 1.30 | 0.90 |
| 4:4:142:LEU:C | 4:7:371:HIS:O[1_554] | 1.30 | 0.90 |
| 4:4:253:GLU:CD | 4:7:214:GLU:CB[1_554] | 1.30 | 0.90 |
| 4:4:111:ASN:OD1 | 4:8:196:ARG:CG[1_554] | 1.30 | 0.90 |
| 4:4:189:LEU:N | 4:7:183:ARG:N[1_554] | 1.30 | 0.90 |
| 4:5:207:GLU:OE2 | 4:8:67:LEU:CA[1_554] | 1.30 | 0.90 |
| 4:6:267:ILE:CB | 4:9:180:LEU:CG[1_554] | 1.30 | 0.90 |
| 4:4:293:LEU:C | 4:7:169:TYR:CD2[1_554] | 1.30 | 0.90 |
| 4:5:267:ILE:CB | 4:8:180:LEU:CG[1_554] | 1.30 | 0.90 |
| 4:3:72:GLU:O | 4:7:199:SER:N[1_554] | 1.30 | 0.90 |
| 4:6:317:ILE:CD1 | 4:9:165:ILE:O[1_554] | 1.30 | 0.90 |
| 4:6:274:ILE:N | 4:9:162:ASN:N[1_554] | 1.30 | 0.90 |
| 4:4:274:ILE:C | 4:7:163:VAL:N[1_554] | 1.30 | 0.90 |
| 4:4:329:ILE:CA | 4:7:139:VAL:CG1[1_554] | 1.30 | 0.90 |
| 4:4:255:PHE:CG | 4:7:305:MET:CG[1_554] | 1.30 | 0.90 |
| 4:6:112:PRO:O | 4:V:253:GLU:CD[1_554] | 1.30 | 0.90 |
| 4:5:283:MET:CG | 4:8:286:ASP:C[1_554] | 1.30 | 0.90 |
| 4:5:62:ARG:NH1 | 4:8:67:LEU:N[1_554] | 1.30 | 0.90 |
| 4:6:337:TYR:CE1 | 4:9:86:TRP:CH2[1_554] | 1.30 | 0.90 |
| 4:4:222:ASP:CA | 4:7:332:PRO:CD[1_554] | 1.30 | 0.90 |
| 4:5:333:PRO:CD | 4:8:104:LEU:CD1[1_554] | 1.30 | 0.90 |
| 4:5:26:ALA:N | 4:8:123:MET:CB[1_554] | 1.30 | 0.90 |
| 4:5:340:TRP:CG | 4:8:119:MET:N[1_554] | 1.30 | 0.90 |
| 4:5:317:ILE:CA | 4:8:150:GLY:C[1_554] | 1.30 | 0.90 |
| 4:6:17:VAL:C | 4:9:79:TRP:CD2[1_554] | 1.30 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:315:LYS:O | 4:8:296:ASN:CA[1_554] | 1.31 | 0.89 |
| 4:4:214:GLU:CG | 4:7:33:SER:CB[1_554] | 1.31 | 0.89 |
| 4:4:305:MET:O | 4:7:11:ASP:CB[1_554] | 1.31 | 0.89 |
| 1:D:637:LYS:CD | 4:6:311:ASP:CG[1_556] | 1.31 | 0.89 |
| 4:6:15:GLY:CA | 4:9:77:THR:CB[1_554] | 1.31 | 0.89 |
| 4:6:262:PHE:CE1 | 4:9:153:LEU:N[1_554] | 1.31 | 0.89 |
| 4:5:340:TRP:CE3 | 4:8:120:THR:C[1_554] | 1.31 | 0.89 |
| 4:4:185:LEU:CB | 4:7:158:GLY:CA[1_554] | 1.31 | 0.89 |
| 4:5:178:LEU:CG | 4:8:177:ARG:N[1_554] | 1.31 | 0.89 |
| 4:3:370:VAL:CA | 4:7:230:ALA:C[1_554] | 1.31 | 0.89 |
| 4:4:173:HIS:CD2 | 4:8:264:PRO:O[1_554] | 1.31 | 0.89 |
| 4:6:109:PRO:C | 4:V:195:GLU:OE1[1_554] | 1.31 | 0.89 |
| 4:4:371:HIS:CE1 | 4:8:252:ASN:C[1_554] | 1.31 | 0.89 |
| 4:4:369:ILE:N | 4:8:234:SER:OG[1_554] | 1.31 | 0.89 |
| 4:5:311:ASP:OD1 | 4:8:145:SER:N[1_554] | 1.31 | 0.89 |
| 4:5:218:TYR:CB | 4:8:336:LYS:CA[1_554] | 1.31 | 0.89 |
| 4:4:180:LEU:N | 4:7:179:ASP:OD1[1_554] | 1.31 | 0.89 |
| 4:4:267:ILE:CG1 | 4:7:180:LEU:CG[1_554] | 1.31 | 0.89 |
| 4:5:349:LEU:CA | 4:8:365:ALA:N[1_554] | 1.31 | 0.89 |
| 4:6:305:MET:CE | 4:9:11:ASP:CB[1_554] | 1.31 | 0.89 |
| 4:6:115:ASN:CA | 4:V:196:ARG:NH1[1_554] | 1.31 | 0.89 |
| 4:5:263:GLN:CG | 4:8:274:ILE:CG2[1_554] | 1.31 | 0.89 |
| 4:4:114:ALA:CA | 4:8:250:ILE:C[1_554] | 1.31 | 0.89 |
| 4:5:262:PHE:CE1 | 4:8:153:LEU:N[1_554] | 1.31 | 0.89 |
| 4:5:215:LYS:C | 4:8:30:VAL:CG1[1_554] | 1.31 | 0.89 |
| 4:5:173:HIS:CB | 4:9:267:ILE:N[1_554] | 1.31 | 0.89 |
| 4:6:242:LEU:CG | 4:9:207:GLU:OE1[1_554] | 1.31 | 0.89 |
| 4:6:339:VAL:C | 4:9:116:ARG:O[1_554] | 1.31 | 0.89 |
| 4:6:157:ASP:CA | 4:9:72:GLU:O[1_554] | 1.31 | 0.89 |
| 4:5:286:ASP:CA | 4:9:270:GLU:OE1[1_554] | 1.31 | 0.89 |
| 4:5:257:CYS:N | 4:8:303:THR:CA[1_554] | 1.31 | 0.89 |
| 4:6:266:PHE:CD1 | 4:9:261:LEU:CB[1_554] | 1.31 | 0.89 |
| 4:4:367:PRO:CA | 4:8:234:SER:O[1_554] | 1.31 | 0.89 |
| 4:4:193:LEU:C | 4:7:210:ARG:N[1_554] | 1.31 | 0.89 |
| 4:4:161:HIS:C | 4:7:110:LEU:CD2[1_554] | 1.31 | 0.89 |
| 4:5:189:LEU:N | 4:8:183:ARG:N[1_554] | 1.31 | 0.89 |
| 4:5:277:THR:CA | 4:8:281:SER:OG[1_554] | 1.31 | 0.89 |
| 4:4:116:ARG:CD | 4:8:252:ASN:OD1[1_554] | 1.31 | 0.89 |
| 4:5:208:ILE:CG1 | 4:8:59:GLN:CG[1_554] | 1.31 | 0.89 |
| 4:5:106:THR:CG2 | 4:8:114:ALA:C[1_554] | 1.31 | 0.89 |
| 4:6:262:PHE:CG | 4:9:153:LEU:CB[1_554] | 1.31 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:75:ILE:CA | 4:8:198:TYR:N[1_554] | 1.31 | 0.89 |
| 4:4:184:ASP:OD1 | 4:7:73:HIS:NE2[1_554] | 1.31 | 0.89 |
| 4:6:305:MET:CG | 4:9:11:ASP:OD1[1_554] | 1.31 | 0.89 |
| 4:4:142:LEU:CA | 4:7:371:HIS:O[1_554] | 1.31 | 0.89 |
| 4:4:319:ALA:CB | 4:7:296:ASN:CG[1_554] | 1.31 | 0.89 |
| 4:6:221:LEU:CB | 4:9:332:PRO:CG[1_554] | 1.31 | 0.89 |
| 4:4:219:VAL:C | 4:7:335:ARG:O[1_554] | 1.31 | 0.89 |
| 4:4:208:ILE:CG2 | 4:7:59:GLN:NE2[1_554] | 1.31 | 0.89 |
| 4:4:213:LYS:O | 4:7:16:LEU:N[1_554] | 1.31 | 0.89 |
| 4:5:286:ASP:CB | 4:9:270:GLU:CD[1_554] | 1.31 | 0.89 |
| 4:6:340:TRP:CB | 4:9:119:MET:N[1_554] | 1.31 | 0.89 |
| 4:5:278:THR:N | 4:8:164:PRO:CD[1_554] | 1.31 | 0.89 |
| 4:6:215:LYS:C | 4:9:30:VAL:CG1[1_554] | 1.31 | 0.89 |
| 4:6:252:ASN:OD1 | 4:9:215:LYS:C[1_554] | 1.32 | 0.88 |
| 4:4:268:GLY:O | 4:7:264:PRO:CB[1_554] | 1.32 | 0.88 |
| 4:6:263:GLN:CA | 4:9:274:ILE:CB[1_554] | 1.32 | 0.88 |
| 4:5:18:LYS:N | 4:8:79:TRP:CE3[1_554] | 1.32 | 0.88 |
| 4:5:17:VAL:CA | 4:8:79:TRP:CG[1_554] | 1.32 | 0.88 |
| 4:5:334:GLU:CD | 4:8:133:TYR:O[1_554] | 1.32 | 0.88 |
| 4:4:259:GLU:OE2 | 4:7:304:THR:O[1_554] | 1.32 | 0.88 |
| 4:6:188:TYR:CG | 4:9:181:ALA:O[1_554] | 1.32 | 0.88 |
| 4:5:220:ALA:CA | 4:8:335:ARG:CD[1_554] | 1.32 | 0.88 |
| 4:5:11:ASP:CG | 4:8:115:ASN:CA[1_554] | 1.32 | 0.88 |
| 4:4:240:TYR:CD2 | 4:7:56:ASP:OD2[1_554] | 1.32 | 0.88 |
| 4:6:340:TRP:CZ2 | 4:9:121:GLN:CA[1_554] | 1.32 | 0.88 |
| 4:6:141:SER:CA | 4:9:116:ARG:CZ[1_554] | 1.32 | 0.88 |
| 4:4:188:TYR:CA | 4:7:184:ASP:N[1_554] | 1.32 | 0.88 |
| 4:4:265:SER:C | 4:7:261:LEU:CA[1_554] | 1.32 | 0.88 |
| 4:6:270:GLU:C | 4:9:272:ALA:CA[1_554] | 1.32 | 0.88 |
| 4:5:193:LEU:C | 4:8:210:ARG:N[1_554] | 1.32 | 0.88 |
| 4:6:262:PHE:CE1 | 4:9:153:LEU:C[1_554] | 1.32 | 0.88 |
| 4:4:144:ALA:C | 4:7:370:VAL:O[1_554] | 1.32 | 0.88 |
| 4:4:269:MET:CB | 4:7:178:LEU:CD1[1_554] | 1.32 | 0.88 |
| 4:6:183:ARG:CD | 4:9:72:GLU:OE2[1_554] | 1.32 | 0.88 |
| 4:6:250:ILE:CG2 | 4:9:214:GLU:CD[1_554] | 1.32 | 0.88 |
| 4:4:191:LYS:CE | 4:7:185:LEU:CA[1_554] | 1.32 | 0.88 |
| 4:4:243:PRO:N | 4:7:60:SER:N[1_554] | 1.32 | 0.88 |
| 4:5:193:LEU:CA | 4:8:210:ARG:CA[1_554] | 1.32 | 0.88 |
| 4:5:270:GLU:C | 4:8:272:ALA:CA[1_554] | 1.32 | 0.88 |
| 4:4:274:ILE:C | 4:7:162:ASN:O[1_554] | 1.32 | 0.88 |
| 4:4:24:ASP:C | 4:7:125:GLU:CG[1_554] | 1.32 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:270:GLU:CA | 4:7:272:ALA:O[1_554] | 1.32 | 0.88 |
| 4:6:276:GLU:CD | 4:9:278:THR:O[1_554] | 1.32 | 0.88 |
| 4:4:337:TYR:N | 4:7:119:MET:SD[1_554] | 1.32 | 0.88 |
| 4:6:110:LEU:CG | 4:V:191:LYS:CE[1_554] | 1.32 | 0.88 |
| 4:6:310:ALA:C | 4:9:142:LEU:N[1_554] | 1.32 | 0.88 |
| 4:4:262:PHE:C | 4:7:153:LEU:CD1[1_554] | 1.32 | 0.88 |
| 4:5:319:ALA:O | 4:8:295:ALA:N[1_554] | 1.32 | 0.88 |
| 4:5:253:GLU:OE2 | 4:8:214:GLU:CA[1_554] | 1.32 | 0.88 |
| 4:6:349:LEU:C | 4:9:364:GLU:O[1_554] | 1.32 | 0.88 |
| 4:6:218:TYR:CA | 4:9:336:LYS:CB[1_554] | 1.32 | 0.88 |
| 4:5:339:VAL:C | 4:8:116:ARG:O[1_554] | 1.32 | 0.88 |
| 4:5:154:ASP:CG | 4:8:111:ASN:N[1_554] | 1.32 | 0.88 |
| 4:5:318:THR:OG1 | 4:8:296:ASN:OD1[1_554] | 1.32 | 0.88 |
| 4:4:260:THR:O | 4:7:160:THR:OG1[1_554] | 1.32 | 0.88 |
| 4:5:191:LYS:C | 4:8:186:THR:C[1_554] | 1.32 | 0.88 |
| 4:6:221:LEU:CD1 | 4:9:332:PRO:CG[1_554] | 1.32 | 0.88 |
| 4:4:30:VAL:CA | 4:7:79:TRP:C[1_554] | 1.32 | 0.88 |
| 4:5:29:ALA:N | 4:8:83:GLU:OE1[1_554] | 1.32 | 0.88 |
| 1:D:542:PHE:CE2 | 4:6:328:LYS:NZ[1_556] | 1.32 | 0.88 |
| 4:5:164:PRO:CG | 4:8:172:PRO:CG[1_554] | 1.32 | 0.88 |
| 4:5:28:ARG:CA | 4:8:126:THR:OG1[1_554] | 1.33 | 0.87 |
| 4:6:310:ALA:CB | 4:9:141:SER:N[1_554] | 1.33 | 0.87 |
| 4:4:16:LEU:CB | 4:7:78:ASN:N[1_554] | 1.33 | 0.87 |
| 4:4:274:ILE:CG1 | 4:7:161:HIS:CB[1_554] | 1.33 | 0.87 |
| 4:5:304:THR:CB | 4:8:137:GLN:CG[1_554] | 1.33 | 0.87 |
| 4:6:26:ALA:N | 4:9:123:MET:CB[1_554] | 1.33 | 0.87 |
| 4:4:335:ARG:CD | 4:7:106:THR:CA[1_554] | 1.33 | 0.87 |
| 4:6:274:ILE:CB | 4:9:161:HIS:C[1_554] | 1.33 | 0.87 |
| 4:4:30:VAL:O | 4:7:80:ASP:N[1_554] | 1.33 | 0.87 |
| 4:5:340:TRP:CZ2 | 4:8:122:ILE:N[1_554] | 1.33 | 0.87 |
| 4:4:210:ARG:CB | 4:7:69:TYR:CD2[1_554] | 1.33 | 0.87 |
| 4:6:321:ALA:O | 4:9:292:ASP:N[1_554] | 1.33 | 0.87 |
| 4:4:31:PHE:C | 4:7:78:ASN:CG[1_554] | 1.33 | 0.87 |
| 4:6:311:ASP:OD1 | 4:9:145:SER:N[1_554] | 1.33 | 0.87 |
| 4:4:331:ALA:C | 4:7:135:ALA:N[1_554] | 1.33 | 0.87 |
| 4:6:136:ILE:O | 4:9:113:LYS:CG[1_554] | 1.33 | 0.87 |
| 4:6:312:ARG:NH2 | 4:9:299:MET:CG[1_554] | 1.33 | 0.87 |
| 4:5:258:PRO:CB | 4:8:155:SER:O[1_554] | 1.33 | 0.87 |
| 4:4:182:GLY:N | 4:7:73:HIS:C[1_554] | 1.33 | 0.87 |
| 4:6:296:ASN:C | 4:9:168:GLY:O[1_554] | 1.33 | 0.87 |
| 4:4:273:GLY:CA | 4:7:162:ASN:CG[1_554] | 1.33 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:178:LEU:O | 4:8:177:ARG:CD[1_554] | 1.33 | 0.87 |
| 4:4:291:LYS:CG | 4:9:64:ILE:CG1[1_554] | 1.33 | 0.87 |
| 4:6:312:ARG:O | 4:9:298:VAL:CA[1_554] | 1.33 | 0.87 |
| 4:3:367:PRO:CA | 4:7:234:SER:O[1_554] | 1.33 | 0.87 |
| 4:6:221:LEU:C | 4:9:331:ALA:CA[1_554] | 1.33 | 0.87 |
| 4:5:346:LEU:CG | 4:8:368:SER:OG[1_554] | 1.33 | 0.87 |
| 4:4:213:LYS:CD | 4:7:15:GLY:N[1_554] | 1.33 | 0.87 |
| 4:4:111:ASN:OD1 | 4:8:196:ARG:CB[1_554] | 1.33 | 0.87 |
| 4:3:118:LYS:N | 4:7:237:GLU:OE1[1_554] | 1.33 | 0.87 |
| 4:6:283:MET:CA | 4:9:286:ASP:N[1_554] | 1.33 | 0.87 |
| 4:5:17:VAL:C | 4:8:79:TRP:CD2[1_554] | 1.33 | 0.87 |
| 4:3:370:VAL:C | 4:7:230:ALA:C[1_554] | 1.33 | 0.87 |
| 4:6:219:VAL:N | 4:9:335:ARG:O[1_554] | 1.33 | 0.87 |
| 4:4:370:VAL:C | 4:8:230:ALA:C[1_554] | 1.33 | 0.87 |
| 4:5:347:ALA:CB | 4:8:367:PRO:CD[1_554] | 1.33 | 0.87 |
| 4:6:369:ILE:O | 4:V:228:ALA:O[1_554] | 1.33 | 0.87 |
| 4:4:341:ILE:CG1 | 4:7:120:THR:CB[1_554] | 1.33 | 0.87 |
| 4:5:336:LYS:CD | 4:8:12:ASN:CG[1_554] | 1.33 | 0.87 |
| 4:5:160:THR:CB | 4:8:161:HIS:NE2[1_554] | 1.33 | 0.87 |
| 4:6:316:GLU:OE1 | 4:9:297:ASN:CB[1_554] | 1.33 | 0.87 |
| 4:6:349:LEU:CG | 4:9:365:ALA:CB[1_554] | 1.33 | 0.87 |
| 4:6:28:ARG:O | 4:9:83:GLU:OE2[1_554] | 1.33 | 0.87 |
| 4:5:334:GLU:C | 4:8:105:LEU:CB[1_554] | 1.33 | 0.87 |
| 4:4:220:ALA:CA | 4:7:335:ARG:C[1_554] | 1.33 | 0.87 |
| 4:4:272:ALA:C | 4:7:277:THR:CG2[1_554] | 1.33 | 0.87 |
| 4:3:173:HIS:CA | 4:7:267:ILE:CB[1_554] | 1.33 | 0.87 |
| 4:5:195:GLU:CA | 4:8:189:LEU:CG[1_554] | 1.33 | 0.87 |
| 4:6:294:TYR:CG | 4:9:166:TYR:CD1[1_554] | 1.33 | 0.87 |
| 4:4:319:ALA:C | 4:7:292:ASP:O[1_554] | 1.34 | 0.86 |
| 4:6:113:LYS:NZ | 4:V:254:ARG:C[1_554] | 1.34 | 0.86 |
| 4:5:24:ASP:OD2 | 4:8:125:GLU:CB[1_554] | 1.34 | 0.86 |
| 4:4:277:THR:CG2 | 4:7:175:ILE:CA[1_554] | 1.34 | 0.86 |
| 4:3:109:PRO:CA | 4:7:195:GLU:CG[1_554] | 1.34 | 0.86 |
| 4:4:75:ILE:CG1 | 4:8:193:LEU:O[1_554] | 1.34 | 0.86 |
| 4:4:204:ALA:CB | 4:7:62:ARG:CA[1_554] | 1.34 | 0.86 |
| 4:4:196:ARG:C | 4:7:208:ILE:O[1_554] | 1.34 | 0.86 |
| 4:5:337:TYR:OH | 4:8:86:TRP:NE1[1_554] | 1.34 | 0.86 |
| 4:6:249:THR:CB | 4:9:215:LYS:NZ[1_554] | 1.34 | 0.86 |
| 4:6:195:GLU:CG | 4:9:189:LEU:CG[1_554] | 1.34 | 0.86 |
| 4:5:195:GLU:CG | 4:8:189:LEU:CG[1_554] | 1.34 | 0.86 |
| 4:5:111:ASN:OD1 | 4:9:196:ARG:CB[1_554] | 1.34 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:173:HIS:CE1 | 4:V:265:SER:O[1_554] | 1.34 | 0.86 |
| 4:4:117:GLU:OE1 | 4:8:236:LEU:O[1_554] | 1.34 | 0.86 |
| 4:5:137:GLN:CG | 4:8:112:PRO:O[1_554] | 1.34 | 0.86 |
| 4:6:113:LYS:CG | 4:V:252:ASN:C[1_554] | 1.34 | 0.86 |
| 4:5:151:ILE:CG2 | 4:8:170:ALA:C[1_554] | 1.34 | 0.86 |
| 4:6:158:GLY:C | 4:9:177:ARG:NH2[1_554] | 1.34 | 0.86 |
| 4:5:31:PHE:CG | 4:8:80:ASP:N[1_554] | 1.34 | 0.86 |
| 4:6:335:ARG:NH2 | 4:9:339:VAL:CG1[1_554] | 1.34 | 0.86 |
| 4:6:369:ILE:CB | 4:V:232:SER:OG[1_554] | 1.34 | 0.86 |
| 4:5:154:ASP:OD2 | 4:8:111:ASN:N[1_554] | 1.34 | 0.86 |
| 4:4:277:THR:CB | 4:7:175:ILE:C[1_554] | 1.34 | 0.86 |
| 4:4:79:TRP:CD1 | 4:8:247:VAL:O[1_554] | 1.34 | 0.86 |
| 4:4:243:PRO:CD | 4:7:60:SER:CA[1_554] | 1.34 | 0.86 |
| 4:6:255:PHE:CA | 4:9:302:GLY:O[1_554] | 1.34 | 0.86 |
| 4:6:250:ILE:CG1 | 4:9:214:GLU:OE1[1_554] | 1.34 | 0.86 |
| 4:6:181:ALA:O | 4:9:159:VAL:N[1_554] | 1.34 | 0.86 |
| 4:6:137:GLN:CA | 4:9:113:LYS:CA[1_554] | 1.34 | 0.86 |
| 4:6:31:PHE:CB | 4:9:81:ASP:N[1_554] | 1.34 | 0.86 |
| 4:6:195:GLU:CA | 4:9:189:LEU:CG[1_554] | 1.34 | 0.86 |
| 4:5:322:PRO:CB | 4:8:291:LYS:NZ[1_554] | 1.34 | 0.86 |
| 4:6:266:PHE:CB | 4:9:261:LEU:CD2[1_554] | 1.34 | 0.86 |
| 4:4:277:THR:CA | 4:7:174:ALA:O[1_554] | 1.34 | 0.86 |
| 4:6:20:GLY:O | 4:9:121:GLN:CD[1_554] | 1.34 | 0.86 |
| 4:4:312:ARG:NH2 | 4:7:299:MET:CG[1_554] | 1.34 | 0.86 |
| 4:4:213:LYS:CE | 4:7:14:SER:O[1_554] | 1.34 | 0.86 |
| 4:4:334:GLU:OE2 | 4:7:133:TYR:N[1_554] | 1.34 | 0.86 |
| 4:6:340:TRP:CE3 | 4:9:120:THR:C[1_554] | 1.34 | 0.86 |
| 4:5:208:ILE:CA | 4:8:59:GLN:NE2[1_554] | 1.34 | 0.86 |
| 4:4:282:ILE:CB | 4:7:171:LEU:CD2[1_554] | 1.34 | 0.86 |
| 4:6:56:ASP:CG | 4:9:81:ASP:OD1[1_554] | 1.34 | 0.86 |
| 4:4:316:GLU:C | 4:7:151:ILE:N[1_554] | 1.34 | 0.86 |
| 4:4:335:ARG:NE | 4:7:106:THR:CA[1_554] | 1.34 | 0.86 |
| 4:5:267:ILE:CD1 | 4:8:180:LEU:CB[1_554] | 1.34 | 0.86 |
| 4:5:305:MET:CE | 4:8:11:ASP:CB[1_554] | 1.34 | 0.86 |
| 4:4:325:MET:O | 4:7:167:GLU:CD[1_554] | 1.34 | 0.86 |
| 4:4:153:LEU:CG | 4:7:109:PRO:CA[1_554] | 1.34 | 0.86 |
| 4:5:262:PHE:CD1 | 4:8:153:LEU:C[1_554] | 1.34 | 0.86 |
| 4:4:333:PRO:CA | 4:7:104:LEU:C[1_554] | 1.34 | 0.86 |
| 4:5:222:ASP:N | 4:8:331:ALA:CB[1_554] | 1.34 | 0.86 |
| 4:5:266:PHE:CB | 4:8:261:LEU:CD2[1_554] | 1.34 | 0.86 |
| 4:4:26:ALA:CB | 4:7:122:ILE:O[1_554] | 1.34 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:370:VAL:CG2 | 4:7:230:ALA:O[1_554] | 1.34 | 0.86 |
| 4:4:74:GLY:C | 4:8:197:GLY:CA[1_554] | 1.34 | 0.86 |
| 4:6:340:TRP:CG | 4:9:119:MET:N[1_554] | 1.34 | 0.86 |
| 4:6:317:ILE:CA | 4:9:150:GLY:C[1_554] | 1.34 | 0.86 |
| 4:5:30:VAL:CA | 4:8:79:TRP:O[1_554] | 1.35 | 0.85 |
| 4:6:280:ASN:OD1 | 4:9:281:SER:CA[1_554] | 1.35 | 0.85 |
| 4:5:339:VAL:CB | 4:8:116:ARG:N[1_554] | 1.35 | 0.85 |
| 4:6:188:TYR:CD1 | 4:9:185:LEU:CD1[1_554] | 1.35 | 0.85 |
| 4:6:173:HIS:CG | 4:V:267:ILE:N[1_554] | 1.35 | 0.85 |
| 4:6:204:ALA:CB | 4:9:62:ARG:CG[1_554] | 1.35 | 0.85 |
| 4:6:198:TYR:C | 4:9:205:GLU:O[1_554] | 1.35 | 0.85 |
| 4:6:243:PRO:CB | 4:9:60:SER:C[1_554] | 1.35 | 0.85 |
| 4:4:185:LEU:C | 4:7:157:ASP:O[1_554] | 1.35 | 0.85 |
| 4:4:117:GLU:O | 4:8:237:GLU:CG[1_554] | 1.35 | 0.85 |
| 4:6:210:ARG:NE | 4:9:33:SER:O[1_554] | 1.35 | 0.85 |
| 4:4:197:GLY:N | 4:7:208:ILE:O[1_554] | 1.35 | 0.85 |
| 4:4:213:LYS:CE | 4:7:14:SER:CA[1_554] | 1.35 | 0.85 |
| 4:5:18:LYS:N | 4:8:79:TRP:CG[1_554] | 1.35 | 0.85 |
| 4:6:190:MET:C | 4:9:186:THR:CB[1_554] | 1.35 | 0.85 |
| 4:4:267:ILE:CD1 | 4:7:180:LEU:CA[1_554] | 1.35 | 0.85 |
| 4:4:261:LEU:C | 4:7:154:ASP:O[1_554] | 1.35 | 0.85 |
| 4:5:157:ASP:OD1 | 4:8:72:GLU:N[1_554] | 1.35 | 0.85 |
| 4:4:188:TYR:CA | 4:7:183:ARG:C[1_554] | 1.35 | 0.85 |
| 4:5:25:ASP:N | 4:8:124:PHE:CA[1_554] | 1.35 | 0.85 |
| 4:5:56:ASP:CG | 4:8:81:ASP:OD1[1_554] | 1.35 | 0.85 |
| 4:6:305:MET:CA | 4:9:11:ASP:OD1[1_554] | 1.35 | 0.85 |
| 4:5:312:ARG:C | 4:8:298:VAL:CB[1_554] | 1.35 | 0.85 |
| 4:5:283:MET:CB | 4:8:286:ASP:N[1_554] | 1.35 | 0.85 |
| 4:5:196:ARG:C | 4:8:212:ILE:CG1[1_554] | 1.35 | 0.85 |
| 4:5:188:TYR:CE2 | 4:8:185:LEU:CD2[1_554] | 1.35 | 0.85 |
| 4:6:255:PHE:CG | 4:9:305:MET:CA[1_554] | 1.35 | 0.85 |
| 4:4:166:TYR:CD1 | 4:9:40:HIS:CE1[1_554] | 1.35 | 0.85 |
| 4:4:315:LYS:CE | 4:7:147:ARG:CD[1_554] | 1.35 | 0.85 |
| 4:5:295:ALA:N | 4:8:166:TYR:O[1_554] | 1.35 | 0.85 |
| 4:6:188:TYR:CZ | 4:9:185:LEU:CG[1_554] | 1.35 | 0.85 |
| 4:4:198:TYR:CG | 4:7:207:GLU:C[1_554] | 1.35 | 0.85 |
| 4:5:320:LEU:CB | 4:8:293:LEU:CB[1_554] | 1.35 | 0.85 |
| 4:5:173:HIS:O | 4:9:267:ILE:C[1_554] | 1.35 | 0.85 |
| 4:4:188:TYR:N | 4:7:183:ARG:CB[1_554] | 1.35 | 0.85 |
| 4:5:188:TYR:CD1 | 4:8:185:LEU:CD1[1_554] | 1.35 | 0.85 |
| 4:4:16:LEU:N | 4:7:77:THR:O[1_554] | 1.35 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:210:ARG:NE | 4:8:33:SER:O[1_554] | 1.35 | 0.85 |
| 4:3:173:HIS:CB | 4:7:267:ILE:CB[1_554] | 1.35 | 0.85 |
| 4:6:319:ALA:O | 4:9:294:TYR:CA[1_554] | 1.35 | 0.85 |
| 4:4:243:PRO:CA | 4:7:61:LYS:N[1_554] | 1.35 | 0.85 |
| 4:5:257:CYS:CA | 4:8:303:THR:CB[1_554] | 1.35 | 0.85 |
| 4:4:370:VAL:CA | 4:8:230:ALA:O[1_554] | 1.35 | 0.85 |
| 4:6:261:LEU:CB | 4:9:154:ASP:C[1_554] | 1.35 | 0.85 |
| 4:4:27:PRO:CG | 4:7:122:ILE:CG1[1_554] | 1.35 | 0.85 |
| 4:5:220:ALA:CB | 4:8:335:ARG:CG[1_554] | 1.35 | 0.85 |
| 4:4:213:LYS:NZ | 4:7:14:SER:CA[1_554] | 1.35 | 0.85 |
| 4:6:345:ILE:C | 4:9:369:ILE:CG2[1_554] | 1.35 | 0.85 |
| 4:6:11:ASP:O | 4:9:79:TRP:CE2[1_554] | 1.35 | 0.85 |
| 4:6:112:PRO:CA | 4:V:253:GLU:CG[1_554] | 1.35 | 0.85 |
| 4:4:198:TYR:N | 4:7:209:VAL:N[1_554] | 1.35 | 0.85 |
| 4:4:281:SER:OG | 4:7:172:PRO:C[1_554] | 1.35 | 0.85 |
| 4:4:331:ALA:CB | 4:7:135:ALA:CB[1_554] | 1.35 | 0.85 |
| 4:5:284:LYS:O | 4:9:268:GLY:C[1_554] | 1.35 | 0.85 |
| 4:6:343:GLY:C | 4:9:367:PRO:CB[1_554] | 1.35 | 0.85 |
| 4:4:311:ASP:O | 4:7:142:LEU:CA[1_554] | 1.35 | 0.85 |
| 4:5:193:LEU:O | 4:8:209:VAL:CA[1_554] | 1.35 | 0.85 |
| 4:6:340:TRP:O | 4:9:120:THR:CB[1_554] | 1.35 | 0.85 |
| 4:4:186:THR:CB | 4:7:183:ARG:NE[1_554] | 1.35 | 0.85 |
| 4:4:220:ALA:CB | 4:7:335:ARG:C[1_554] | 1.35 | 0.85 |
| 4:6:257:CYS:CA | 4:9:303:THR:CB[1_554] | 1.35 | 0.85 |
| 4:4:110:LEU:C | 4:8:192:ILE:CA[1_554] | 1.35 | 0.85 |
| 4:6:294:TYR:CB | 4:9:166:TYR:CG[1_554] | 1.35 | 0.85 |
| 4:5:204:ALA:CB | 4:8:62:ARG:CB[1_554] | 1.35 | 0.85 |
| 4:2:291:LYS:C | 4:7:40:HIS:CB[1_554] | 1.35 | 0.85 |
| 4:5:158:GLY:C | 4:8:177:ARG:NH2[1_554] | 1.35 | 0.85 |
| 4:4:79:TRP:CH2 | 4:8:249:THR:CG2[1_554] | 1.36 | 0.84 |
| 4:4:312:ARG:NE | 4:7:300:SER:N[1_554] | 1.36 | 0.84 |
| 4:6:187:ASP:O | 4:9:183:ARG:C[1_554] | 1.36 | 0.84 |
| 4:5:267:ILE:CG1 | 4:8:180:LEU:CB[1_554] | 1.36 | 0.84 |
| 4:6:150:GLY:C | 4:9:169:TYR:CE1[1_554] | 1.36 | 0.84 |
| 4:5:280:ASN:CG | 4:8:281:SER:O[1_554] | 1.36 | 0.84 |
| 4:5:17:VAL:O | 4:8:79:TRP:CA[1_554] | 1.36 | 0.84 |
| 4:6:249:THR:OG1 | 4:9:215:LYS:NZ[1_554] | 1.36 | 0.84 |
| 4:4:18:LYS:CG | 4:7:79:TRP:CE3[1_554] | 1.36 | 0.84 |
| 4:6:305:MET:CE | 4:9:11:ASP:CA[1_554] | 1.36 | 0.84 |
| 4:6:369:ILE:CG1 | 4:V:232:SER:OG[1_554] | 1.36 | 0.84 |
| 4:5:20:GLY:CA | 4:8:121:GLN:NE2[1_554] | 1.36 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:154:ASP:N | 4:8:109:PRO:O[1_554] | 1.36 | 0.84 |
| 4:4:276:GLU:CD | 4:7:278:THR:C[1_554] | 1.36 | 0.84 |
| 4:6:21:PHE:C | 4:9:125:GLU:CD[1_554] | 1.36 | 0.84 |
| 4:5:253:GLU:OE2 | 4:8:214:GLU:CB[1_554] | 1.36 | 0.84 |
| 4:4:191:LYS:CG | 4:7:185:LEU:C[1_554] | 1.36 | 0.84 |
| 4:4:140:LEU:C | 4:7:371:HIS:CG[1_554] | 1.36 | 0.84 |
| 4:5:255:PHE:CB | 4:8:305:MET:CB[1_554] | 1.36 | 0.84 |
| 4:6:267:ILE:CD1 | 4:9:180:LEU:CB[1_554] | 1.36 | 0.84 |
| 4:6:346:LEU:CG | 4:9:368:SER:CA[1_554] | 1.36 | 0.84 |
| 4:5:371:HIS:N | 4:9:231:ALA:N[1_554] | 1.36 | 0.84 |
| 4:4:368:SER:N | 4:8:236:LEU:CB[1_554] | 1.36 | 0.84 |
| 4:4:222:ASP:OD1 | 4:7:331:ALA:O[1_554] | 1.36 | 0.84 |
| 4:5:213:LYS:C | 4:8:16:LEU:CD2[1_554] | 1.36 | 0.84 |
| 4:4:193:LEU:CA | 4:7:210:ARG:CA[1_554] | 1.36 | 0.84 |
| 4:5:137:GLN:NE2 | 4:8:112:PRO:CB[1_554] | 1.36 | 0.84 |
| 4:6:335:ARG:O | 4:9:106:THR:C[1_554] | 1.36 | 0.84 |
| 4:6:173:HIS:O | 4:V:267:ILE:C[1_554] | 1.36 | 0.84 |
| 4:6:227:MET:CG | 4:9:307:PRO:N[1_554] | 1.36 | 0.84 |
| 4:4:72:GLU:O | 4:8:199:SER:N[1_554] | 1.36 | 0.84 |
| 4:6:255:PHE:O | 4:9:304:THR:N[1_554] | 1.36 | 0.84 |
| 4:6:335:ARG:CA | 4:9:106:THR:CA[1_554] | 1.36 | 0.84 |
| 4:5:339:VAL:O | 4:8:117:GLU:N[1_554] | 1.36 | 0.84 |
| 4:6:291:LYS:NZ | 4:W:64:ILE:CD1[1_554] | 1.36 | 0.84 |
| 4:4:74:GLY:C | 4:8:197:GLY:C[1_554] | 1.36 | 0.84 |
| 4:6:160:THR:OG1 | 4:9:161:HIS:NE2[1_554] | 1.36 | 0.84 |
| 4:6:333:PRO:CD | 4:9:104:LEU:CD1[1_554] | 1.36 | 0.84 |
| 4:5:349:LEU:N | 4:8:365:ALA:N[1_554] | 1.36 | 0.84 |
| 4:6:221:LEU:C | 4:9:332:PRO:N[1_554] | 1.36 | 0.84 |
| 4:4:196:ARG:NE | 4:7:211:ASP:OD2[1_554] | 1.36 | 0.84 |
| 4:4:250:ILE:CG1 | 4:7:210:ARG:NH2[1_554] | 1.36 | 0.84 |
| 4:6:188:TYR:CE2 | 4:9:185:LEU:CD2[1_554] | 1.36 | 0.84 |
| 4:6:154:ASP:OD2 | 4:9:111:ASN:N[1_554] | 1.37 | 0.83 |
| 4:6:185:LEU:CB | 4:9:157:ASP:C[1_554] | 1.37 | 0.83 |
| 4:6:192:ILE:CB | 4:9:213:LYS:CG[1_554] | 1.37 | 0.83 |
| 4:6:26:ALA:N | 4:9:123:MET:CA[1_554] | 1.37 | 0.83 |
| 4:6:275:HIS:C | 4:9:151:ILE:CG1[1_554] | 1.37 | 0.83 |
| 4:5:262:PHE:CD1 | 4:8:153:LEU:CB[1_554] | 1.37 | 0.83 |
| 4:5:338:SER:CA | 4:8:134:VAL:CG2[1_554] | 1.37 | 0.83 |
| 4:6:274:ILE:O | 4:9:163:VAL:N[1_554] | 1.37 | 0.83 |
| 4:4:213:LYS:CA | 4:7:15:GLY:C[1_554] | 1.37 | 0.83 |
| 4:5:345:ILE:CG2 | 4:8:369:ILE:CB[1_554] | 1.37 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:307:PRO:CB | 4:7:340:TRP:CB[1_554] | 1.37 | 0.83 |
| 4:6:327:ILE:CB | 4:9:149:THR:CA[1_554] | 1.37 | 0.83 |
| 4:5:367:PRO:CD | 4:9:234:SER:N[1_554] | 1.37 | 0.83 |
| 4:4:180:LEU:CD2 | 4:7:178:LEU:C[1_554] | 1.37 | 0.83 |
| 4:5:25:ASP:OD2 | 4:8:129:VAL:C[1_554] | 1.37 | 0.83 |
| 4:4:226:GLU:OE2 | 4:7:333:PRO:O[1_554] | 1.37 | 0.83 |
| 4:5:312:ARG:NH2 | 4:8:299:MET:CG[1_554] | 1.37 | 0.83 |
| 4:4:270:GLU:CB | 4:7:272:ALA:N[1_554] | 1.37 | 0.83 |
| 4:4:333:PRO:CB | 4:7:104:LEU:CA[1_554] | 1.37 | 0.83 |
| 4:6:188:TYR:OH | 4:9:185:LEU:CD2[1_554] | 1.37 | 0.83 |
| 4:4:218:TYR:CD1 | 4:7:337:TYR:CE1[1_554] | 1.37 | 0.83 |
| 4:4:280:ASN:OD1 | 4:7:281:SER:CA[1_554] | 1.37 | 0.83 |
| 4:5:189:LEU:CA | 4:8:182:GLY:O[1_554] | 1.37 | 0.83 |
| 4:4:345:ILE:CG2 | 4:7:366:GLY:O[1_554] | 1.37 | 0.83 |
| 4:4:139:VAL:O | 4:7:371:HIS:CD2[1_554] | 1.37 | 0.83 |
| 4:6:347:ALA:CA | 4:9:366:GLY:CA[1_554] | 1.37 | 0.83 |
| 4:4:140:LEU:O | 4:7:371:HIS:CB[1_554] | 1.37 | 0.83 |
| 4:4:110:LEU:N | 4:8:192:ILE:CA[1_554] | 1.37 | 0.83 |
| 4:6:192:ILE:N | 4:9:186:THR:CA[1_554] | 1.37 | 0.83 |
| 4:6:28:ARG:CG | 4:9:126:THR:CB[1_554] | 1.37 | 0.83 |
| 4:4:207:GLU:OE2 | 4:7:67:LEU:O[1_554] | 1.37 | 0.83 |
| 4:5:22:ALA:C | 4:8:362:TYR:CE2[1_554] | 1.37 | 0.83 |
| 4:6:192:ILE:CG1 | 4:9:213:LYS:CE[1_554] | 1.37 | 0.83 |
| 4:2:291:LYS:CG | 4:7:39:ARG:C[1_554] | 1.37 | 0.83 |
| 4:4:304:THR:C | 4:7:137:GLN:NE2[1_554] | 1.37 | 0.83 |
| 4:4:178:LEU:CG | 4:7:177:ARG:C[1_554] | 1.37 | 0.83 |
| 4:3:172:PRO:CG | 4:7:266:PHE:CB[1_554] | 1.37 | 0.83 |
| 4:4:337:TYR:CA | 4:7:119:MET:CG[1_554] | 1.37 | 0.83 |
| 4:6:20:GLY:N | 4:9:121:GLN:OE1[1_554] | 1.37 | 0.83 |
| 4:5:294:TYR:O | 4:8:167:GLU:N[1_554] | 1.37 | 0.83 |
| 4:4:317:ILE:CG1 | 4:7:165:ILE:CB[1_554] | 1.37 | 0.83 |
| 4:5:183:ARG:CD | 4:8:72:GLU:OE2[1_554] | 1.37 | 0.83 |
| 4:6:141:SER:N | 4:9:116:ARG:CD[1_554] | 1.37 | 0.83 |
| 4:5:166:TYR:CD1 | 4:V:40:HIS:CE1[1_554] | 1.37 | 0.83 |
| 4:6:262:PHE:CD1 | 4:9:153:LEU:C[1_554] | 1.38 | 0.82 |
| 4:4:151:ILE:CG1 | 4:7:172:PRO:CD[1_554] | 1.38 | 0.82 |
| 4:5:294:TYR:O | 4:8:166:TYR:C[1_554] | 1.38 | 0.82 |
| 4:5:185:LEU:CB | 4:8:157:ASP:C[1_554] | 1.38 | 0.82 |
| 4:4:326:LYS:CD | 4:9:45:VAL:N[1_554] | 1.38 | 0.82 |
| 4:6:178:LEU:CB | 4:9:177:ARG:CA[1_554] | 1.38 | 0.82 |
| 1:D:542:PHE:CZ | 4:6:328:LYS:NZ[1_556] | 1.38 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:333:PRO:C | 4:9:104:LEU:O[1_554] | 1.38 | 0.82 |
| 4:5:196:ARG:O | 4:8:212:ILE:CD1[1_554] | 1.38 | 0.82 |
| 4:6:275:HIS:O | 4:9:151:ILE:CG1[1_554] | 1.38 | 0.82 |
| 4:5:141:SER:O | 4:8:116:ARG:CZ[1_554] | 1.38 | 0.82 |
| 4:4:341:ILE:CG2 | 4:7:120:THR:CB[1_554] | 1.38 | 0.82 |
| 4:5:141:SER:OG | 4:8:107:GLU:OE1[1_554] | 1.38 | 0.82 |
| 4:5:27:PRO:CA | 4:8:122:ILE:CG2[1_554] | 1.38 | 0.82 |
| 4:4:192:ILE:N | 4:7:186:THR:CB[1_554] | 1.38 | 0.82 |
| 4:6:145:SER:OG | 4:9:372:ARG:NH1[1_554] | 1.38 | 0.82 |
| 4:5:273:GLY:N | 4:8:277:THR:CG2[1_554] | 1.38 | 0.82 |
| 4:5:220:ALA:N | 4:8:335:ARG:CB[1_554] | 1.38 | 0.82 |
| 4:5:227:MET:CE | 4:8:306:TYR:CB[1_554] | 1.38 | 0.82 |
| 4:4:254:ARG:NH2 | 4:7:337:TYR:OH[1_554] | 1.38 | 0.82 |
| 4:6:262:PHE:CD1 | 4:9:153:LEU:CB[1_554] | 1.38 | 0.82 |
| 4:6:191:LYS:CA | 4:9:186:THR:O[1_554] | 1.38 | 0.82 |
| 4:5:348:SER:OG | 4:8:362:TYR:C[1_554] | 1.38 | 0.82 |
| 4:4:332:PRO:N | 4:7:134:VAL:C[1_554] | 1.38 | 0.82 |
| 4:5:338:SER:OG | 4:8:134:VAL:CB[1_554] | 1.38 | 0.82 |
| 4:6:369:ILE:CB | 4:V:232:SER:CB[1_554] | 1.38 | 0.82 |
| 4:5:297:ASN:N | 4:8:168:GLY:C[1_554] | 1.38 | 0.82 |
| 4:4:277:THR:C | 4:7:175:ILE:N[1_554] | 1.38 | 0.82 |
| 4:6:173:HIS:C | 4:V:267:ILE:C[1_554] | 1.38 | 0.82 |
| 4:4:320:LEU:O | 4:7:289:ILE:O[1_554] | 1.38 | 0.82 |
| 4:6:156:GLY:C | 4:9:75:ILE:N[1_554] | 1.38 | 0.82 |
| 4:4:304:THR:O | 4:7:137:GLN:CG[1_554] | 1.38 | 0.82 |
| 4:6:286:ASP:CA | 4:V:270:GLU:OE1[1_554] | 1.38 | 0.82 |
| 4:5:188:TYR:C | 4:8:182:GLY:O[1_554] | 1.38 | 0.82 |
| 4:6:154:ASP:OD2 | 4:9:111:ASN:CB[1_554] | 1.38 | 0.82 |
| 4:5:249:THR:O | 4:8:211:ASP:OD2[1_554] | 1.38 | 0.82 |
| 4:5:210:ARG:CD | 4:8:69:TYR:CD2[1_554] | 1.38 | 0.82 |
| 4:5:19:ALA:N | 4:8:122:ILE:CD1[1_554] | 1.38 | 0.82 |
| 4:3:114:ALA:CA | 4:7:250:ILE:C[1_554] | 1.38 | 0.82 |
| 4:4:191:LYS:CA | 4:7:186:THR:C[1_554] | 1.39 | 0.81 |
| 4:4:156:GLY:CA | 4:7:75:ILE:N[1_554] | 1.39 | 0.81 |
| 4:6:215:LYS:CD | 4:9:30:VAL:O[1_554] | 1.39 | 0.81 |
| 4:5:32:PRO:CG | 4:8:81:ASP:OD2[1_554] | 1.39 | 0.81 |
| 4:4:16:LEU:CD1 | 4:7:78:ASN:CB[1_554] | 1.39 | 0.81 |
| 4:5:221:LEU:CA | 4:8:332:PRO:CD[1_554] | 1.39 | 0.81 |
| 4:3:287:ILE:O | 4:8:63:GLY:C[1_554] | 1.39 | 0.81 |
| 4:4:337:TYR:C | 4:7:119:MET:CG[1_554] | 1.39 | 0.81 |
| 4:4:208:ILE:CA | 4:7:59:GLN:NE2[1_554] | 1.39 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:336:LYS:N | 4:8:106:THR:O[1_554] | 1.39 | 0.81 |
| 4:4:328:LYS:O | 4:7:168:GLY:O[1_554] | 1.39 | 0.81 |
| 4:4:370:VAL:O | 4:8:230:ALA:CA[1_554] | 1.39 | 0.81 |
| 4:5:333:PRO:C | 4:8:104:LEU:O[1_554] | 1.39 | 0.81 |
| 4:4:263:GLN:C | 4:7:274:ILE:CD1[1_554] | 1.39 | 0.81 |
| 4:6:189:LEU:C | 4:9:186:THR:OG1[1_554] | 1.39 | 0.81 |
| 4:4:268:GLY:C | 4:7:264:PRO:CB[1_554] | 1.39 | 0.81 |
| 4:5:281:SER:C | 4:8:173:HIS:NE2[1_554] | 1.39 | 0.81 |
| 4:5:335:ARG:CA | 4:8:106:THR:CA[1_554] | 1.39 | 0.81 |
| 4:5:310:ALA:CA | 4:8:141:SER:N[1_554] | 1.39 | 0.81 |
| 4:5:18:LYS:NZ | 4:8:76:ILE:CB[1_554] | 1.39 | 0.81 |
| 4:4:369:ILE:O | 4:8:229:THR:CA[1_554] | 1.39 | 0.81 |
| 4:4:294:TYR:CD1 | 4:7:166:TYR:CA[1_554] | 1.39 | 0.81 |
| 4:5:113:LYS:NZ | 4:9:254:ARG:C[1_554] | 1.39 | 0.81 |
| 4:4:313:MET:CE | 4:7:163:VAL:CB[1_554] | 1.39 | 0.81 |
| 4:6:294:TYR:CA | 4:9:166:TYR:CA[1_554] | 1.39 | 0.81 |
| 4:5:250:ILE:CG1 | 4:8:214:GLU:OE1[1_554] | 1.39 | 0.81 |
| 4:4:303:THR:CB | 4:7:74:GLY:CA[1_554] | 1.39 | 0.81 |
| 4:6:155:SER:C | 4:9:108:ALA:CB[1_554] | 1.39 | 0.81 |
| 4:5:20:GLY:O | 4:8:121:GLN:CD[1_554] | 1.39 | 0.81 |
| 4:4:24:ASP:CB | 4:7:125:GLU:OE1[1_554] | 1.39 | 0.81 |
| 4:5:331:ALA:C | 4:8:140:LEU:CD2[1_554] | 1.39 | 0.81 |
| 4:6:220:ALA:CA | 4:9:335:ARG:CD[1_554] | 1.39 | 0.81 |
| 4:4:339:VAL:CG2 | 4:7:112:PRO:O[1_554] | 1.39 | 0.81 |
| 4:4:193:LEU:CA | 4:7:210:ARG:CG[1_554] | 1.39 | 0.81 |
| 4:6:141:SER:CA | 4:9:116:ARG:CD[1_554] | 1.39 | 0.81 |
| 4:3:113:LYS:CD | 4:7:254:ARG:C[1_554] | 1.39 | 0.81 |
| 4:3:169:TYR:OH | 4:7:266:PHE:CD1[1_554] | 1.39 | 0.81 |
| 4:4:145:SER:N | 4:7:370:VAL:C[1_554] | 1.39 | 0.81 |
| 4:5:312:ARG:O | 4:8:298:VAL:CA[1_554] | 1.39 | 0.81 |
| 4:5:282:ILE:CD1 | 4:8:171:LEU:CG[1_554] | 1.39 | 0.81 |
| 4:5:249:THR:CG2 | 4:8:215:LYS:NZ[1_554] | 1.39 | 0.81 |
| 4:6:221:LEU:CA | 4:9:332:PRO:N[1_554] | 1.39 | 0.81 |
| 4:6:193:LEU:O | 4:9:209:VAL:CA[1_554] | 1.39 | 0.81 |
| 4:6:317:ILE:CG1 | 4:9:150:GLY:O[1_554] | 1.39 | 0.81 |
| 4:5:181:ALA:O | 4:8:158:GLY:O[1_554] | 1.39 | 0.81 |
| 4:5:194:THR:N | 4:8:209:VAL:CG1[1_554] | 1.39 | 0.81 |
| 4:6:28:ARG:CB | 4:9:126:THR:CB[1_554] | 1.39 | 0.81 |
| 4:5:269:MET:C | 4:8:272:ALA:O[1_554] | 1.39 | 0.81 |
| 4:5:112:PRO:C | 4:9:253:GLU:OE2[1_554] | 1.39 | 0.81 |
| 4:4:220:ALA:N | 4:7:335:ARG:C[1_554] | 1.39 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:349:LEU:C | 4:8:364:GLU:O[1_554] | 1.39 | 0.81 |
| 4:4:336:LYS:CE | 4:7:86:TRP:CZ2[1_554] | 1.39 | 0.81 |
| 4:4:331:ALA:C | 4:7:135:ALA:CB[1_554] | 1.39 | 0.81 |
| 4:6:185:LEU:CB | 4:9:158:GLY:N[1_554] | 1.39 | 0.81 |
| 4:6:368:SER:C | 4:V:230:ALA:N[1_554] | 1.40 | 0.80 |
| 4:6:113:LYS:NZ | 4:V:255:PHE:N[1_554] | 1.40 | 0.80 |
| 4:4:314:GLN:CB | 4:7:143:TYR:N[1_554] | 1.40 | 0.80 |
| 4:4:191:LYS:CE | 4:7:185:LEU:C[1_554] | 1.40 | 0.80 |
| 4:5:340:TRP:CE2 | 4:8:118:LYS:O[1_554] | 1.40 | 0.80 |
| 4:6:318:THR:O | 4:9:292:ASP:O[1_554] | 1.40 | 0.80 |
| 4:6:145:SER:CB | 4:9:372:ARG:NH1[1_554] | 1.40 | 0.80 |
| 4:6:141:SER:OG | 4:9:107:GLU:OE1[1_554] | 1.40 | 0.80 |
| 4:4:223:PHE:C | 4:7:335:ARG:NE[1_554] | 1.40 | 0.80 |
| 4:6:29:ALA:N | 4:9:83:GLU:OE1[1_554] | 1.40 | 0.80 |
| 4:6:300:SER:OG | 4:9:107:GLU:CG[1_554] | 1.40 | 0.80 |
| 4:6:299:MET:SD | 4:9:138:ALA:C[1_554] | 1.40 | 0.80 |
| 4:5:204:ALA:CB | 4:8:62:ARG:CG[1_554] | 1.40 | 0.80 |
| 4:6:56:ASP:OD2 | 4:9:81:ASP:OD1[1_554] | 1.40 | 0.80 |
| 4:5:227:MET:CG | 4:8:307:PRO:N[1_554] | 1.40 | 0.80 |
| 4:5:211:ASP:CA | 4:8:32:PRO:CB[1_554] | 1.40 | 0.80 |
| 4:5:157:ASP:OD1 | 4:8:72:GLU:CA[1_554] | 1.40 | 0.80 |
| 4:3:289:ILE:N | 4:8:39:ARG:NH1[1_554] | 1.40 | 0.80 |
| 4:6:219:VAL:C | 4:9:335:ARG:CB[1_554] | 1.40 | 0.80 |
| 4:4:25:ASP:CB | 4:7:124:PHE:CB[1_554] | 1.40 | 0.80 |
| 4:6:31:PHE:O | 4:9:78:ASN:O[1_554] | 1.40 | 0.80 |
| 4:4:243:PRO:N | 4:7:60:SER:CB[1_554] | 1.40 | 0.80 |
| 4:5:198:TYR:C | 4:8:205:GLU:O[1_554] | 1.40 | 0.80 |
| 4:4:115:ASN:ND2 | 4:8:198:TYR:CE2[1_554] | 1.40 | 0.80 |
| 4:6:180:LEU:CB | 4:9:179:ASP:N[1_554] | 1.40 | 0.80 |
| 4:4:317:ILE:CD1 | 4:7:165:ILE:CG2[1_554] | 1.40 | 0.80 |
| 4:6:26:ALA:N | 4:9:123:MET:C[1_554] | 1.40 | 0.80 |
| 4:5:115:ASN:CA | 4:9:196:ARG:NH1[1_554] | 1.40 | 0.80 |
| 4:6:320:LEU:CB | 4:9:293:LEU:CB[1_554] | 1.40 | 0.80 |
| 4:4:178:LEU:CD2 | 4:7:177:ARG:N[1_554] | 1.40 | 0.80 |
| 4:6:286:ASP:CB | 4:V:270:GLU:CD[1_554] | 1.40 | 0.80 |
| 4:5:366:GLY:C | 4:9:234:SER:N[1_554] | 1.40 | 0.80 |
| 4:4:196:ARG:CD | 4:7:211:ASP:CG[1_554] | 1.40 | 0.80 |
| 4:4:223:PHE:CG | 4:7:304:THR:OG1[1_554] | 1.40 | 0.80 |
| 4:6:338:SER:CA | 4:9:134:VAL:CB[1_554] | 1.40 | 0.80 |
| 4:6:262:PHE:CD1 | 4:9:153:LEU:N[1_554] | 1.40 | 0.80 |
| 4:5:180:LEU:CG | 4:8:178:LEU:C[1_554] | 1.40 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:215:LYS:CG | 4:8:31:PHE:CA[1_554] | 1.40 | 0.80 |
| 4:4:370:VAL:CG2 | 4:8:230:ALA:O[1_554] | 1.40 | 0.80 |
| 4:3:116:ARG:CG | 4:7:252:ASN:CG[1_554] | 1.40 | 0.80 |
| 4:4:187:ASP:O | 4:7:183:ARG:O[1_554] | 1.40 | 0.80 |
| 4:4:316:GLU:C | 4:7:150:GLY:C[1_554] | 1.40 | 0.80 |
| 4:4:137:GLN:O | 4:7:113:LYS:N[1_554] | 1.40 | 0.80 |
| 4:5:335:ARG:C | 4:8:106:THR:O[1_554] | 1.40 | 0.80 |
| 4:6:113:LYS:CA | 4:V:253:GLU:N[1_554] | 1.40 | 0.80 |
| 4:6:187:ASP:C | 4:9:184:ASP:N[1_554] | 1.40 | 0.80 |
| 4:5:325:MET:CG | 4:8:166:TYR:CZ[1_554] | 1.40 | 0.80 |
| 4:4:243:PRO:CB | 4:7:60:SER:C[1_554] | 1.40 | 0.80 |
| 4:3:369:ILE:O | 4:7:229:THR:CA[1_554] | 1.40 | 0.80 |
| 4:5:198:TYR:CE1 | 4:8:208:ILE:CB[1_554] | 1.40 | 0.80 |
| 4:4:326:LYS:O | 4:7:167:GLU:CA[1_554] | 1.40 | 0.80 |
| 4:4:274:ILE:N | 4:7:161:HIS:C[1_554] | 1.40 | 0.80 |
| 4:5:277:THR:CA | 4:8:174:ALA:O[1_554] | 1.40 | 0.80 |
| 4:5:218:TYR:CG | 4:8:336:LYS:CB[1_554] | 1.40 | 0.80 |
| 4:5:210:ARG:NH1 | 4:8:33:SER:O[1_554] | 1.40 | 0.80 |
| 4:5:296:ASN:N | 4:8:169:TYR:N[1_554] | 1.41 | 0.79 |
| 4:4:222:ASP:CB | 4:7:332:PRO:CA[1_554] | 1.41 | 0.79 |
| 4:6:337:TYR:N | 4:9:119:MET:CE[1_554] | 1.41 | 0.79 |
| 4:6:218:TYR:CB | 4:9:336:LYS:CA[1_554] | 1.41 | 0.79 |
| 4:4:214:GLU:CA | 4:7:16:LEU:C[1_554] | 1.41 | 0.79 |
| 4:6:307:PRO:CB | 4:9:337:TYR:C[1_554] | 1.41 | 0.79 |
| 4:4:111:ASN:CG | 4:8:196:ARG:CB[1_554] | 1.41 | 0.79 |
| 4:5:299:MET:O | 4:8:136:ILE:CA[1_554] | 1.41 | 0.79 |
| 4:5:227:MET:CG | 4:8:306:TYR:O[1_554] | 1.41 | 0.79 |
| 4:6:262:PHE:CB | 4:9:153:LEU:CB[1_554] | 1.41 | 0.79 |
| 4:6:313:MET:SD | 4:9:152:VAL:N[1_554] | 1.41 | 0.79 |
| 4:5:337:TYR:OH | 4:8:86:TRP:CD2[1_554] | 1.41 | 0.79 |
| 4:4:189:LEU:N | 4:7:183:ARG:CA[1_554] | 1.41 | 0.79 |
| 4:4:113:LYS:O | 4:8:251:GLY:N[1_554] | 1.41 | 0.79 |
| 4:6:258:PRO:O | 4:9:155:SER:CB[1_554] | 1.41 | 0.79 |
| 4:5:249:THR:CB | 4:8:215:LYS:NZ[1_554] | 1.41 | 0.79 |
| 4:6:266:PHE:CA | 4:9:261:LEU:N[1_554] | 1.41 | 0.79 |
| 4:5:112:PRO:O | 4:9:253:GLU:OE2[1_554] | 1.41 | 0.79 |
| 4:5:281:SER:C | 4:8:173:HIS:CD2[1_554] | 1.41 | 0.79 |
| 4:4:193:LEU:CB | 4:7:210:ARG:CB[1_554] | 1.41 | 0.79 |
| 4:4:242:LEU:C | 4:7:60:SER:CA[1_554] | 1.41 | 0.79 |
| 4:5:295:ALA:CB | 4:8:167:GLU:O[1_554] | 1.41 | 0.79 |
| 4:6:334:GLU:CB | 4:9:105:LEU:N[1_554] | 1.41 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:113:LYS:CA | 4:9:253:GLU:N[1_554] | 1.41 | 0.79 |
| 4:5:327:ILE:C | 4:8:148:THR:C[1_554] | 1.41 | 0.79 |
| 4:4:153:LEU:CG | 4:7:109:PRO:CB[1_554] | 1.41 | 0.79 |
| 4:4:109:PRO:O | 4:8:195:GLU:OE1[1_554] | 1.41 | 0.79 |
| 4:5:11:ASP:OD1 | 4:8:115:ASN:CA[1_554] | 1.41 | 0.79 |
| 4:6:222:ASP:N | 4:9:331:ALA:C[1_554] | 1.41 | 0.79 |
| 4:6:204:ALA:CB | 4:9:62:ARG:CB[1_554] | 1.41 | 0.79 |
| 4:4:196:ARG:CB | 4:7:211:ASP:CA[1_554] | 1.41 | 0.79 |
| 4:4:156:GLY:N | 4:7:75:ILE:CG1[1_554] | 1.41 | 0.79 |
| 4:5:350:SER:N | 4:8:364:GLU:O[1_554] | 1.41 | 0.79 |
| 4:6:32:PRO:O | 4:9:78:ASN:CG[1_554] | 1.41 | 0.79 |
| 4:4:25:ASP:OD1 | 4:7:124:PHE:CG[1_554] | 1.41 | 0.79 |
| 4:5:151:ILE:CG1 | 4:8:170:ALA:O[1_554] | 1.41 | 0.79 |
| 4:4:213:LYS:CE | 4:7:15:GLY:N[1_554] | 1.41 | 0.79 |
| 4:5:210:ARG:NH2 | 4:8:33:SER:O[1_554] | 1.41 | 0.79 |
| 4:4:321:ALA:O | 4:7:292:ASP:OD2[1_554] | 1.41 | 0.79 |
| 4:6:253:GLU:OE2 | 4:9:214:GLU:CA[1_554] | 1.41 | 0.79 |
| 4:5:208:ILE:CG2 | 4:8:59:GLN:OE1[1_554] | 1.41 | 0.79 |
| 4:6:297:ASN:ND2 | 4:9:165:ILE:CG1[1_554] | 1.41 | 0.79 |
| 4:6:75:ILE:CG1 | 4:V:194:THR:C[1_554] | 1.41 | 0.79 |
| 4:6:219:VAL:O | 4:9:335:ARG:CA[1_554] | 1.41 | 0.79 |
| 4:4:315:LYS:CG | 4:7:145:SER:OG[1_554] | 1.41 | 0.79 |
| 4:4:173:HIS:CA | 4:8:267:ILE:CA[1_554] | 1.41 | 0.79 |
| 4:5:27:PRO:CB | 4:8:122:ILE:CB[1_554] | 1.41 | 0.79 |
| 4:6:340:TRP:CG | 4:9:118:LYS:C[1_554] | 1.41 | 0.79 |
| 4:6:222:ASP:N | 4:9:331:ALA:N[1_554] | 1.41 | 0.79 |
| 4:5:222:ASP:N | 4:8:331:ALA:N[1_554] | 1.41 | 0.79 |
| 4:5:219:VAL:CB | 4:8:300:SER:C[1_554] | 1.41 | 0.79 |
| 4:4:357:ILE:CG1 | 4:8:232:SER:CA[1_554] | 1.41 | 0.79 |
| 4:5:75:ILE:CD1 | 4:9:196:ARG:N[1_554] | 1.41 | 0.79 |
| 4:5:110:LEU:O | 4:9:192:ILE:O[1_554] | 1.41 | 0.79 |
| 4:5:204:ALA:O | 4:8:62:ARG:CD[1_554] | 1.41 | 0.79 |
| 4:5:196:ARG:CB | 4:8:212:ILE:N[1_554] | 1.41 | 0.79 |
| 4:6:21:PHE:C | 4:9:125:GLU:CG[1_554] | 1.41 | 0.79 |
| 4:5:156:GLY:O | 4:8:73:HIS:C[1_554] | 1.41 | 0.79 |
| 4:4:172:PRO:C | 4:8:266:PHE:O[1_554] | 1.41 | 0.79 |
| 4:6:157:ASP:C | 4:9:72:GLU:C[1_554] | 1.41 | 0.79 |
| 4:5:276:GLU:CD | 4:8:278:THR:O[1_554] | 1.41 | 0.79 |
| 4:4:191:LYS:CB | 4:7:186:THR:C[1_554] | 1.41 | 0.79 |
| 4:4:333:PRO:N | 4:7:105:LEU:N[1_554] | 1.41 | 0.79 |
| 4:6:189:LEU:N | 4:9:183:ARG:N[1_554] | 1.41 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:73:HIS:CD2 | 4:7:199:SER:OG[1_554] | 1.41 | 0.79 |
| 4:4:262:PHE:CD2 | 4:7:153:LEU:O[1_554] | 1.41 | 0.79 |
| 4:4:196:ARG:CD | 4:7:211:ASP:CA[1_554] | 1.41 | 0.79 |
| 4:6:181:ALA:N | 4:9:159:VAL:CG1[1_554] | 1.42 | 0.78 |
| 4:6:331:ALA:CA | 4:9:140:LEU:CG[1_554] | 1.42 | 0.78 |
| 4:6:75:ILE:CG1 | 4:V:194:THR:O[1_554] | 1.42 | 0.78 |
| 4:4:314:GLN:O | 4:7:142:LEU:CG[1_554] | 1.42 | 0.78 |
| 4:5:218:TYR:OH | 4:8:337:TYR:CD2[1_554] | 1.42 | 0.78 |
| 4:5:173:HIS:C | 4:9:267:ILE:C[1_554] | 1.42 | 0.78 |
| 4:6:18:LYS:CB | 4:9:79:TRP:CE3[1_554] | 1.42 | 0.78 |
| 4:4:304:THR:C | 4:7:137:GLN:CD[1_554] | 1.42 | 0.78 |
| 4:4:172:PRO:CG | 4:8:266:PHE:CD2[1_554] | 1.42 | 0.78 |
| 4:6:334:GLU:CA | 4:9:104:LEU:C[1_554] | 1.42 | 0.78 |
| 4:4:262:PHE:C | 4:7:153:LEU:CG[1_554] | 1.42 | 0.78 |
| 4:4:260:THR:O | 4:7:160:THR:CG2[1_554] | 1.42 | 0.78 |
| 4:4:333:PRO:C | 4:7:105:LEU:CG[1_554] | 1.42 | 0.78 |
| 4:4:255:PHE:O | 4:7:302:GLY:C[1_554] | 1.42 | 0.78 |
| 4:5:26:ALA:O | 4:8:123:MET:N[1_554] | 1.42 | 0.78 |
| 4:5:30:VAL:O | 4:8:80:ASP:O[1_554] | 1.42 | 0.78 |
| 4:6:315:LYS:CD | 4:9:147:ARG:CZ[1_554] | 1.42 | 0.78 |
| 4:3:110:LEU:CB | 4:7:192:ILE:CA[1_554] | 1.42 | 0.78 |
| 4:6:335:ARG:CA | 4:9:106:THR:N[1_554] | 1.42 | 0.78 |
| 4:6:273:GLY:C | 4:9:162:ASN:CB[1_554] | 1.42 | 0.78 |
| 4:4:273:GLY:C | 4:7:162:ASN:CA[1_554] | 1.42 | 0.78 |
| 4:6:299:MET:O | 4:9:136:ILE:CA[1_554] | 1.42 | 0.78 |
| 4:5:32:PRO:N | 4:8:78:ASN:ND2[1_554] | 1.42 | 0.78 |
| 4:5:137:GLN:CB | 4:8:113:LYS:N[1_554] | 1.42 | 0.78 |
| 4:4:111:ASN:CA | 4:8:192:ILE:O[1_554] | 1.42 | 0.78 |
| 4:4:265:SER:O | 4:7:261:LEU:C[1_554] | 1.42 | 0.78 |
| 4:5:113:LYS:C | 4:9:252:ASN:N[1_554] | 1.42 | 0.78 |
| 4:2:324:THR:CG2 | 4:7:61:LYS:CE[1_554] | 1.42 | 0.78 |
| 4:5:196:ARG:CZ | 4:8:211:ASP:O[1_554] | 1.42 | 0.78 |
| 4:5:18:LYS:CG | 4:8:79:TRP:CZ3[1_554] | 1.42 | 0.78 |
| 4:6:174:ALA:C | 4:9:173:HIS:CB[1_554] | 1.42 | 0.78 |
| 4:6:173:HIS:CE1 | 4:V:265:SER:CA[1_554] | 1.42 | 0.78 |
| 4:6:137:GLN:OE1 | 4:9:112:PRO:CD[1_554] | 1.42 | 0.78 |
| 4:6:191:LYS:CG | 4:9:185:LEU:C[1_554] | 1.42 | 0.78 |
| 4:5:294:TYR:CG | 4:8:166:TYR:CD1[1_554] | 1.42 | 0.78 |
| 4:4:207:GLU:CG | 4:7:67:LEU:CB[1_554] | 1.42 | 0.78 |
| 4:6:207:GLU:OE2 | 4:9:67:LEU:CA[1_554] | 1.42 | 0.78 |
| 4:3:111:ASN:O | 4:7:253:GLU:CB[1_554] | 1.42 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:367:PRO:N | 4:8:235:SER:C[1_554] | 1.42 | 0.78 |
| 4:5:343:GLY:O | 4:8:367:PRO:N[1_554] | 1.42 | 0.78 |
| 4:6:183:ARG:NE | 4:9:72:GLU:OE1[1_554] | 1.42 | 0.78 |
| 4:4:222:ASP:CG | 4:7:331:ALA:O[1_554] | 1.42 | 0.78 |
| 4:6:173:HIS:C | 4:V:267:ILE:CA[1_554] | 1.42 | 0.78 |
| 4:6:339:VAL:CB | 4:9:116:ARG:CA[1_554] | 1.42 | 0.78 |
| 4:5:326:LYS:CB | 4:8:167:GLU:OE2[1_554] | 1.42 | 0.78 |
| 4:4:144:ALA:O | 4:7:370:VAL:CB[1_554] | 1.42 | 0.78 |
| 4:6:221:LEU:CD2 | 4:9:332:PRO:CB[1_554] | 1.42 | 0.78 |
| 4:5:173:HIS:CA | 4:9:267:ILE:N[1_554] | 1.42 | 0.78 |
| 4:6:253:GLU:OE2 | 4:9:214:GLU:CB[1_554] | 1.42 | 0.78 |
| 4:5:180:LEU:CD1 | 4:8:160:THR:N[1_554] | 1.42 | 0.78 |
| 4:5:196:ARG:CG | 4:8:212:ILE:C[1_554] | 1.42 | 0.78 |
| 4:5:196:ARG:NH1 | 4:8:215:LYS:CB[1_554] | 1.42 | 0.78 |
| 4:4:26:ALA:C | 4:7:122:ILE:CA[1_554] | 1.42 | 0.78 |
| 4:4:267:ILE:CG1 | 4:7:180:LEU:CB[1_554] | 1.42 | 0.78 |
| 4:6:151:ILE:CD1 | 4:9:171:LEU:N[1_554] | 1.42 | 0.78 |
| 4:5:335:ARG:CG | 4:8:106:THR:CG2[1_554] | 1.42 | 0.78 |
| 4:6:219:VAL:CG2 | 4:9:300:SER:C[1_554] | 1.42 | 0.78 |
| 4:5:266:PHE:CG | 4:8:261:LEU:CB[1_554] | 1.42 | 0.78 |
| 4:5:110:LEU:CG | 4:9:191:LYS:CE[1_554] | 1.42 | 0.78 |
| 4:6:326:LYS:CB | 4:9:167:GLU:CD[1_554] | 1.43 | 0.77 |
| 4:5:184:ASP:O | 4:8:184:ASP:OD1[1_554] | 1.43 | 0.77 |
| 4:6:115:ASN:C | 4:V:196:ARG:NH1[1_554] | 1.43 | 0.77 |
| 4:6:366:GLY:C | 4:V:234:SER:N[1_554] | 1.43 | 0.77 |
| 4:3:113:LYS:O | 4:7:251:GLY:N[1_554] | 1.43 | 0.77 |
| 4:6:139:VAL:O | 4:9:371:HIS:O[1_554] | 1.43 | 0.77 |
| 4:6:340:TRP:CB | 4:9:119:MET:CA[1_554] | 1.43 | 0.77 |
| 4:4:157:ASP:C | 4:7:72:GLU:O[1_554] | 1.43 | 0.77 |
| 4:5:60:SER:O | 4:8:66:THR:OG1[1_554] | 1.43 | 0.77 |
| 4:5:262:PHE:CB | 4:8:153:LEU:CB[1_554] | 1.43 | 0.77 |
| 4:5:191:LYS:CA | 4:8:186:THR:O[1_554] | 1.43 | 0.77 |
| 4:4:139:VAL:CA | 4:7:113:LYS:CD[1_554] | 1.43 | 0.77 |
| 4:6:208:ILE:CG1 | 4:9:59:GLN:CG[1_554] | 1.43 | 0.77 |
| 4:4:113:LYS:CD | 4:8:255:PHE:N[1_554] | 1.43 | 0.77 |
| 4:6:60:SER:O | 4:9:66:THR:OG1[1_554] | 1.43 | 0.77 |
| 4:5:367:PRO:CD | 4:9:234:SER:CA[1_554] | 1.43 | 0.77 |
| 4:4:188:TYR:C | 4:7:182:GLY:C[1_554] | 1.43 | 0.77 |
| 4:4:261:LEU:CB | 4:7:154:ASP:O[1_554] | 1.43 | 0.77 |
| 4:4:31:PHE:O | 4:7:78:ASN:OD1[1_554] | 1.43 | 0.77 |
| 4:5:183:ARG:CG | 4:8:72:GLU:OE2[1_554] | 1.43 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:273:GLY:C | 4:7:162:ASN:CB[1_554] | 1.43 | 0.77 |
| 4:5:339:VAL:CB | 4:8:116:ARG:CA[1_554] | 1.43 | 0.77 |
| 4:3:171:LEU:O | 4:7:266:PHE:O[1_554] | 1.43 | 0.77 |
| 4:4:297:ASN:CG | 4:7:170:ALA:CB[1_554] | 1.43 | 0.77 |
| 4:6:173:HIS:N | 4:V:267:ILE:N[1_554] | 1.43 | 0.77 |
| 4:6:114:ALA:CB | 4:V:250:ILE:CA[1_554] | 1.43 | 0.77 |
| 4:4:265:SER:OG | 4:7:274:ILE:CB[1_554] | 1.43 | 0.77 |
| 4:4:318:THR:CA | 4:7:149:THR:CA[1_554] | 1.43 | 0.77 |
| 4:6:295:ALA:C | 4:9:167:GLU:C[1_554] | 1.43 | 0.77 |
| 4:6:362:TYR:CD1 | 4:V:232:SER:O[1_554] | 1.43 | 0.77 |
| 4:6:227:MET:C | 4:9:307:PRO:CB[1_554] | 1.43 | 0.77 |
| 4:4:213:LYS:C | 4:7:15:GLY:C[1_554] | 1.43 | 0.77 |
| 4:6:316:GLU:CA | 4:9:296:ASN:O[1_554] | 1.43 | 0.77 |
| 4:5:300:SER:OG | 4:8:107:GLU:CD[1_554] | 1.43 | 0.77 |
| 4:6:215:LYS:CG | 4:9:30:VAL:C[1_554] | 1.43 | 0.77 |
| 4:4:321:ALA:O | 4:7:292:ASP:CB[1_554] | 1.43 | 0.77 |
| 4:5:116:ARG:N | 4:9:196:ARG:NH1[1_554] | 1.43 | 0.77 |
| 4:6:151:ILE:CG2 | 4:9:170:ALA:C[1_554] | 1.43 | 0.77 |
| 4:4:186:THR:C | 4:7:183:ARG:CG[1_554] | 1.43 | 0.77 |
| 4:5:173:HIS:CE1 | 4:9:265:SER:CA[1_554] | 1.43 | 0.77 |
| 4:6:317:ILE:CG1 | 4:9:150:GLY:N[1_554] | 1.43 | 0.77 |
| 4:6:143:TYR:CE2 | 4:9:369:ILE:C[1_554] | 1.43 | 0.77 |
| 4:6:258:PRO:CG | 4:9:302:GLY:N[1_554] | 1.43 | 0.77 |
| 4:5:283:MET:CG | 4:8:286:ASP:CA[1_554] | 1.43 | 0.77 |
| 4:4:277:THR:CB | 4:7:176:MET:N[1_554] | 1.43 | 0.77 |
| 4:4:243:PRO:CA | 4:7:60:SER:C[1_554] | 1.43 | 0.77 |
| 4:6:336:LYS:CD | 4:9:12:ASN:CG[1_554] | 1.43 | 0.77 |
| 4:5:269:MET:CA | 4:8:271:SER:OG[1_554] | 1.43 | 0.77 |
| 4:4:156:GLY:O | 4:7:75:ILE:N[1_554] | 1.43 | 0.77 |
| 4:5:154:ASP:CA | 4:8:109:PRO:C[1_554] | 1.43 | 0.77 |
| 4:4:193:LEU:CD2 | 4:7:210:ARG:CD[1_554] | 1.43 | 0.77 |
| 4:5:219:VAL:N | 4:8:335:ARG:O[1_554] | 1.43 | 0.77 |
| 4:6:340:TRP:CA | 4:9:116:ARG:O[1_554] | 1.43 | 0.77 |
| 4:3:287:ILE:N | 4:7:270:GLU:OE1[1_554] | 1.43 | 0.77 |
| 4:5:291:LYS:NZ | 4:V:64:ILE:CD1[1_554] | 1.43 | 0.77 |
| 4:6:186:THR:OG1 | 4:9:157:ASP:OD2[1_554] | 1.43 | 0.77 |
| 4:4:260:THR:O | 4:7:160:THR:CB[1_554] | 1.43 | 0.77 |
| 4:6:319:ALA:C | 4:9:295:ALA:N[1_554] | 1.43 | 0.77 |
| 4:4:259:GLU:CD | 4:7:304:THR:O[1_554] | 1.43 | 0.77 |
| 4:6:222:ASP:N | 4:9:331:ALA:CB[1_554] | 1.43 | 0.77 |
| 4:4:294:TYR:OH | 4:7:289:ILE:CD1[1_554] | 1.44 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:219:VAL:CG1 | 4:9:300:SER:C[1_554] | 1.44 | 0.76 |
| 4:4:207:GLU:OE1 | 4:7:67:LEU:N[1_554] | 1.44 | 0.76 |
| 4:6:189:LEU:CA | 4:9:182:GLY:O[1_554] | 1.44 | 0.76 |
| 4:6:166:TYR:CG | 4:W:40:HIS:CG[1_554] | 1.44 | 0.76 |
| 4:6:243:PRO:CG | 4:9:60:SER:CA[1_554] | 1.44 | 0.76 |
| 4:5:313:MET:CG | 4:8:152:VAL:CG2[1_554] | 1.44 | 0.76 |
| 4:4:218:TYR:CD1 | 4:7:337:TYR:CD1[1_554] | 1.44 | 0.76 |
| 4:4:258:PRO:N | 4:7:156:GLY:CA[1_554] | 1.44 | 0.76 |
| 4:5:160:THR:OG1 | 4:8:161:HIS:CE1[1_554] | 1.44 | 0.76 |
| 4:5:227:MET:CG | 4:8:307:PRO:CA[1_554] | 1.44 | 0.76 |
| 4:5:312:ARG:CG | 4:8:299:MET:N[1_554] | 1.44 | 0.76 |
| 4:5:300:SER:O | 4:8:108:ALA:N[1_554] | 1.44 | 0.76 |
| 4:2:323:SER:C | 4:7:44:MET:CE[1_554] | 1.44 | 0.76 |
| 4:4:108:ALA:N | 4:8:195:GLU:O[1_554] | 1.44 | 0.76 |
| 4:5:367:PRO:CD | 4:9:234:SER:C[1_554] | 1.44 | 0.76 |
| 4:6:322:PRO:C | 4:9:291:LYS:NZ[1_554] | 1.44 | 0.76 |
| 4:3:169:TYR:CZ | 4:7:266:PHE:CE1[1_554] | 1.44 | 0.76 |
| 4:6:173:HIS:CA | 4:V:267:ILE:N[1_554] | 1.44 | 0.76 |
| 4:4:173:HIS:CG | 4:8:267:ILE:N[1_554] | 1.44 | 0.76 |
| 4:6:314:GLN:CD | 4:9:147:ARG:C[1_554] | 1.44 | 0.76 |
| 4:6:111:ASN:OD1 | 4:V:196:ARG:CB[1_554] | 1.44 | 0.76 |
| 4:5:173:HIS:N | 4:9:267:ILE:N[1_554] | 1.44 | 0.76 |
| 4:4:311:ASP:N | 4:7:141:SER:N[1_554] | 1.44 | 0.76 |
| 4:5:305:MET:CG | 4:8:11:ASP:OD1[1_554] | 1.44 | 0.76 |
| 4:4:142:LEU:C | 4:7:371:HIS:C[1_554] | 1.44 | 0.76 |
| 4:4:26:ALA:N | 4:7:121:GLN:C[1_554] | 1.44 | 0.76 |
| 4:6:350:SER:N | 4:9:364:GLU:O[1_554] | 1.44 | 0.76 |
| 4:4:180:LEU:CD1 | 4:7:160:THR:N[1_554] | 1.44 | 0.76 |
| 4:4:259:GLU:OE1 | 4:7:304:THR:CA[1_554] | 1.44 | 0.76 |
| 4:4:173:HIS:N | 4:8:266:PHE:C[1_554] | 1.44 | 0.76 |
| 4:4:111:ASN:N | 4:8:192:ILE:C[1_554] | 1.44 | 0.76 |
| 4:6:210:ARG:NH1 | 4:9:33:SER:CB[1_554] | 1.44 | 0.76 |
| 4:4:142:LEU:O | 4:7:372:ARG:N[1_554] | 1.44 | 0.76 |
| 4:4:193:LEU:C | 4:7:210:ARG:CA[1_554] | 1.44 | 0.76 |
| 4:4:341:ILE:CD1 | 4:7:120:THR:N[1_554] | 1.44 | 0.76 |
| 4:5:196:ARG:CB | 4:8:212:ILE:CA[1_554] | 1.44 | 0.76 |
| 4:4:156:GLY:CA | 4:7:75:ILE:CB[1_554] | 1.44 | 0.76 |
| 4:6:333:PRO:CD | 4:9:104:LEU:CG[1_554] | 1.44 | 0.76 |
| 4:5:157:ASP:C | 4:8:72:GLU:C[1_554] | 1.44 | 0.76 |
| 4:6:346:LEU:CA | 4:9:369:ILE:N[1_554] | 1.44 | 0.76 |
| 4:6:340:TRP:C | 4:9:120:THR:OG1[1_554] | 1.44 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:215:LYS:CE | 4:7:31:PHE:CD2[1_554] | 1.44 | 0.76 |
| 4:6:270:GLU:CA | 4:9:272:ALA:C[1_554] | 1.44 | 0.76 |
| 4:4:220:ALA:CB | 4:7:335:ARG:CB[1_554] | 1.44 | 0.76 |
| 4:5:137:GLN:OE1 | 4:8:112:PRO:CB[1_554] | 1.44 | 0.76 |
| 4:3:173:HIS:NE2 | 4:7:265:SER:C[1_554] | 1.44 | 0.76 |
| 4:6:157:ASP:O | 4:9:73:HIS:CB[1_554] | 1.44 | 0.76 |
| 4:4:372:ARG:O | 4:8:255:PHE:CE1[1_554] | 1.44 | 0.76 |
| 4:5:294:TYR:C | 4:8:167:GLU:N[1_554] | 1.44 | 0.76 |
| 4:4:243:PRO:CD | 4:7:59:GLN:O[1_554] | 1.44 | 0.76 |
| 4:4:30:VAL:CA | 4:7:80:ASP:N[1_554] | 1.44 | 0.76 |
| 4:5:372:ARG:CA | 4:9:227:MET:C[1_554] | 1.44 | 0.76 |
| 4:5:344:SER:O | 4:8:362:TYR:CE1[1_554] | 1.44 | 0.76 |
| 4:5:156:GLY:C | 4:8:74:GLY:CA[1_554] | 1.44 | 0.76 |
| 4:5:187:ASP:C | 4:8:184:ASP:N[1_554] | 1.44 | 0.76 |
| 4:5:349:LEU:N | 4:8:365:ALA:C[1_554] | 1.44 | 0.76 |
| 4:4:255:PHE:O | 4:7:301:GLY:O[1_554] | 1.44 | 0.76 |
| 4:5:115:ASN:ND2 | 4:9:196:ARG:CD[1_554] | 1.44 | 0.76 |
| 4:5:173:HIS:CB | 4:9:267:ILE:CB[1_554] | 1.44 | 0.76 |
| 4:2:326:LYS:CB | 4:7:42:GLY:CA[1_554] | 1.44 | 0.76 |
| 4:5:221:LEU:C | 4:8:332:PRO:N[1_554] | 1.44 | 0.76 |
| 4:6:327:ILE:C | 4:9:148:THR:C[1_554] | 1.44 | 0.76 |
| 4:6:197:GLY:CA | 4:9:212:ILE:CD1[1_554] | 1.44 | 0.76 |
| 4:5:155:SER:C | 4:8:108:ALA:CB[1_554] | 1.44 | 0.76 |
| 4:6:299:MET:O | 4:9:135:ALA:O[1_554] | 1.44 | 0.76 |
| 4:5:314:GLN:CA | 4:8:142:LEU:CG[1_554] | 1.44 | 0.76 |
| 4:5:200:PHE:CB | 4:8:206:ARG:CD[1_554] | 1.44 | 0.76 |
| 4:6:156:GLY:CA | 4:9:74:GLY:O[1_554] | 1.44 | 0.76 |
| 4:5:208:ILE:CD1 | 4:8:59:GLN:CB[1_554] | 1.44 | 0.76 |
| 4:5:185:LEU:O | 4:8:157:ASP:O[1_554] | 1.44 | 0.76 |
| 4:5:283:MET:CG | 4:8:286:ASP:N[1_554] | 1.44 | 0.76 |
| 4:3:75:ILE:CB | 4:7:198:TYR:CG[1_554] | 1.44 | 0.76 |
| 4:4:273:GLY:N | 4:7:162:ASN:CG[1_554] | 1.44 | 0.76 |
| 4:4:264:PRO:CB | 4:7:178:LEU:CD2[1_554] | 1.44 | 0.76 |
| 4:4:317:ILE:CA | 4:7:150:GLY:C[1_554] | 1.45 | 0.75 |
| 4:6:327:ILE:C | 4:9:148:THR:CB[1_554] | 1.45 | 0.75 |
| 4:5:307:PRO:CB | 4:8:337:TYR:C[1_554] | 1.45 | 0.75 |
| 4:6:258:PRO:CD | 4:9:303:THR:N[1_554] | 1.45 | 0.75 |
| 4:6:262:PHE:O | 4:9:153:LEU:CD1[1_554] | 1.45 | 0.75 |
| 4:4:243:PRO:CD | 4:7:60:SER:N[1_554] | 1.45 | 0.75 |
| 4:3:370:VAL:CA | 4:7:230:ALA:O[1_554] | 1.45 | 0.75 |
| 4:5:266:PHE:CA | 4:8:261:LEU:N[1_554] | 1.45 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:294:TYR:CA | 4:8:166:TYR:CA[1_554] | 1.45 | 0.75 |
| 4:5:173:HIS:CE1 | 4:9:265:SER:O[1_554] | 1.45 | 0.75 |
| 4:5:157:ASP:O | 4:8:73:HIS:CB[1_554] | 1.45 | 0.75 |
| 4:4:173:HIS:CE1 | 4:8:265:SER:C[1_554] | 1.45 | 0.75 |
| 4:6:115:ASN:ND2 | 4:V:196:ARG:CD[1_554] | 1.45 | 0.75 |
| 4:6:339:VAL:O | 4:9:116:ARG:O[1_554] | 1.45 | 0.75 |
| 4:6:75:ILE:CD1 | 4:V:196:ARG:N[1_554] | 1.45 | 0.75 |
| 4:6:181:ALA:O | 4:9:158:GLY:O[1_554] | 1.45 | 0.75 |
| 4:5:270:GLU:N | 4:8:272:ALA:N[1_554] | 1.45 | 0.75 |
| 4:4:193:LEU:C | 4:7:210:ARG:CB[1_554] | 1.45 | 0.75 |
| 4:6:338:SER:OG | 4:9:134:VAL:CB[1_554] | 1.45 | 0.75 |
| 4:4:108:ALA:CB | 4:8:195:GLU:CA[1_554] | 1.45 | 0.75 |
| 4:6:75:ILE:C | 4:V:197:GLY:CA[1_554] | 1.45 | 0.75 |
| 4:6:26:ALA:O | 4:9:123:MET:N[1_554] | 1.45 | 0.75 |
| 4:6:191:LYS:CA | 4:9:186:THR:CA[1_554] | 1.45 | 0.75 |
| 4:4:335:ARG:C | 4:7:119:MET:CE[1_554] | 1.45 | 0.75 |
| 4:6:27:PRO:CA | 4:9:122:ILE:CG2[1_554] | 1.45 | 0.75 |
| 4:3:367:PRO:N | 4:7:235:SER:C[1_554] | 1.45 | 0.75 |
| 4:4:114:ALA:C | 4:8:250:ILE:N[1_554] | 1.45 | 0.75 |
| 4:5:137:GLN:CB | 4:8:112:PRO:CA[1_554] | 1.45 | 0.75 |
| 4:4:184:ASP:N | 4:7:73:HIS:CE1[1_554] | 1.45 | 0.75 |
| 4:6:22:ALA:CA | 4:9:362:TYR:CZ[1_554] | 1.45 | 0.75 |
| 4:5:115:ASN:C | 4:9:196:ARG:NH1[1_554] | 1.45 | 0.75 |
| 4:6:281:SER:C | 4:9:173:HIS:NE2[1_554] | 1.45 | 0.75 |
| 4:5:160:THR:OG1 | 4:8:161:HIS:NE2[1_554] | 1.45 | 0.75 |
| 4:5:221:LEU:CB | 4:8:332:PRO:CG[1_554] | 1.45 | 0.75 |
| 4:4:16:LEU:CG | 4:7:78:ASN:N[1_554] | 1.45 | 0.75 |
| 4:4:273:GLY:O | 4:7:162:ASN:CA[1_554] | 1.45 | 0.75 |
| 4:5:340:TRP:CG | 4:8:118:LYS:O[1_554] | 1.45 | 0.75 |
| 4:4:178:LEU:CD1 | 4:7:177:ARG:O[1_554] | 1.45 | 0.75 |
| 4:6:334:GLU:O | 4:9:105:LEU:CA[1_554] | 1.45 | 0.75 |
| 4:5:180:LEU:CB | 4:8:178:LEU:O[1_554] | 1.45 | 0.75 |
| 4:5:109:PRO:CA | 4:9:195:GLU:OE2[1_554] | 1.45 | 0.75 |
| 4:5:318:THR:C | 4:8:292:ASP:O[1_554] | 1.45 | 0.75 |
| 4:5:258:PRO:CA | 4:8:155:SER:C[1_554] | 1.45 | 0.75 |
| 4:6:270:GLU:N | 4:9:271:SER:C[1_554] | 1.45 | 0.75 |
| 4:5:307:PRO:CA | 4:8:337:TYR:C[1_554] | 1.45 | 0.75 |
| 4:6:154:ASP:CA | 4:9:108:ALA:O[1_554] | 1.45 | 0.75 |
| 4:6:213:LYS:O | 4:9:16:LEU:CD2[1_554] | 1.45 | 0.75 |
| 4:6:263:GLN:CB | 4:9:274:ILE:CG2[1_554] | 1.45 | 0.75 |
| 4:3:115:ASN:OD1 | 4:7:249:THR:O[1_554] | 1.45 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:334:GLU:C | 4:9:105:LEU:CB[1_554] | 1.45 | 0.75 |
| 4:5:220:ALA:C | 4:8:335:ARG:CD[1_554] | 1.45 | 0.75 |
| 4:4:320:LEU:CD2 | 4:7:293:LEU:CB[1_554] | 1.45 | 0.75 |
| 4:5:157:ASP:O | 4:8:73:HIS:CA[1_554] | 1.45 | 0.75 |
| 4:6:337:TYR:OH | 4:9:86:TRP:CD2[1_554] | 1.45 | 0.75 |
| 4:6:338:SER:CB | 4:9:134:VAL:CB[1_554] | 1.45 | 0.75 |
| 4:4:325:MET:SD | 4:7:166:TYR:CE2[1_554] | 1.45 | 0.75 |
| 4:6:343:GLY:O | 4:9:367:PRO:N[1_554] | 1.45 | 0.75 |
| 4:3:370:VAL:O | 4:7:230:ALA:C[1_554] | 1.45 | 0.75 |
| 4:4:327:ILE:CA | 4:7:168:GLY:N[1_554] | 1.45 | 0.75 |
| 4:5:346:LEU:CG | 4:8:368:SER:CA[1_554] | 1.45 | 0.75 |
| 4:6:117:GLU:CG | 4:V:252:ASN:ND2[1_554] | 1.45 | 0.75 |
| 4:2:287:ILE:C | 4:7:39:ARG:CZ[1_554] | 1.45 | 0.75 |
| 4:6:186:THR:OG1 | 4:9:183:ARG:NH2[1_554] | 1.45 | 0.75 |
| 4:3:79:TRP:CD1 | 4:7:247:VAL:O[1_554] | 1.45 | 0.75 |
| 4:6:157:ASP:OD1 | 4:9:72:GLU:N[1_554] | 1.45 | 0.75 |
| 4:6:141:SER:O | 4:9:116:ARG:CZ[1_554] | 1.45 | 0.75 |
| 4:4:255:PHE:CZ | 4:7:305:MET:CE[1_554] | 1.45 | 0.75 |
| 4:5:208:ILE:CG2 | 4:8:59:GLN:CD[1_554] | 1.45 | 0.75 |
| 4:5:32:PRO:C | 4:8:78:ASN:CB[1_554] | 1.46 | 0.74 |
| 4:6:314:GLN:CG | 4:9:142:LEU:O[1_554] | 1.46 | 0.74 |
| 4:5:294:TYR:CB | 4:8:166:TYR:CB[1_554] | 1.46 | 0.74 |
| 4:5:154:ASP:OD2 | 4:8:111:ASN:CB[1_554] | 1.46 | 0.74 |
| 4:4:143:TYR:N | 4:7:371:HIS:C[1_554] | 1.46 | 0.74 |
| 4:6:312:ARG:CG | 4:9:299:MET:N[1_554] | 1.46 | 0.74 |
| 4:4:340:TRP:NE1 | 4:7:118:LYS:CD[1_554] | 1.46 | 0.74 |
| 4:6:173:HIS:ND1 | 4:V:265:SER:C[1_554] | 1.46 | 0.74 |
| 4:5:219:VAL:CG2 | 4:8:300:SER:C[1_554] | 1.46 | 0.74 |
| 4:3:371:HIS:CE1 | 4:7:252:ASN:C[1_554] | 1.46 | 0.74 |
| 4:6:222:ASP:CA | 4:9:331:ALA:CB[1_554] | 1.46 | 0.74 |
| 4:3:357:ILE:CB | 4:7:232:SER:C[1_554] | 1.46 | 0.74 |
| 4:5:333:PRO:N | 4:8:104:LEU:CG[1_554] | 1.46 | 0.74 |
| 4:4:112:PRO:CG | 4:8:193:LEU:CG[1_554] | 1.46 | 0.74 |
| 4:5:262:PHE:CD1 | 4:8:153:LEU:N[1_554] | 1.46 | 0.74 |
| 4:5:284:LYS:C | 4:9:268:GLY:O[1_554] | 1.46 | 0.74 |
| 4:6:200:PHE:C | 4:9:206:ARG:CG[1_554] | 1.46 | 0.74 |
| 4:5:265:SER:CA | 4:8:261:LEU:O[1_554] | 1.46 | 0.74 |
| 4:5:340:TRP:CB | 4:8:119:MET:CA[1_554] | 1.46 | 0.74 |
| 4:4:166:TYR:CZ | 4:9:39:ARG:O[1_554] | 1.46 | 0.74 |
| 4:6:195:GLU:CB | 4:9:189:LEU:CD2[1_554] | 1.46 | 0.74 |
| 4:5:299:MET:N | 4:8:136:ILE:CB[1_554] | 1.46 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:166:TYR:CB | 4:W:40:HIS:CE1[1_554] | 1.46 | 0.74 |
| 4:6:188:TYR:CA | 4:9:184:ASP:N[1_554] | 1.46 | 0.74 |
| 4:4:315:LYS:C | 4:7:142:LEU:CD1[1_554] | 1.46 | 0.74 |
| 4:4:191:LYS:O | 4:7:186:THR:CG2[1_554] | 1.46 | 0.74 |
| 4:5:335:ARG:N | 4:8:106:THR:N[1_554] | 1.46 | 0.74 |
| 4:6:211:ASP:CA | 4:9:32:PRO:CB[1_554] | 1.46 | 0.74 |
| 4:5:314:GLN:CD | 4:8:147:ARG:C[1_554] | 1.46 | 0.74 |
| 4:6:154:ASP:N | 4:9:109:PRO:O[1_554] | 1.46 | 0.74 |
| 4:6:273:GLY:CA | 4:9:162:ASN:CG[1_554] | 1.46 | 0.74 |
| 4:6:320:LEU:O | 4:9:290:ARG:O[1_554] | 1.46 | 0.74 |
| 4:4:116:ARG:CG | 4:8:252:ASN:CG[1_554] | 1.46 | 0.74 |
| 4:6:186:THR:N | 4:9:157:ASP:O[1_554] | 1.46 | 0.74 |
| 4:6:137:GLN:N | 4:9:113:LYS:CA[1_554] | 1.46 | 0.74 |
| 4:3:370:VAL:N | 4:7:229:THR:O[1_554] | 1.46 | 0.74 |
| 4:5:136:ILE:CG1 | 4:8:113:LYS:NZ[1_554] | 1.46 | 0.74 |
| 4:6:215:LYS:CE | 4:9:31:PHE:CB[1_554] | 1.46 | 0.74 |
| 4:5:218:TYR:CA | 4:8:336:LYS:CB[1_554] | 1.46 | 0.74 |
| 4:4:161:HIS:C | 4:7:110:LEU:CB[1_554] | 1.46 | 0.74 |
| 4:5:267:ILE:CB | 4:8:180:LEU:CD1[1_554] | 1.46 | 0.74 |
| 4:5:187:ASP:O | 4:8:183:ARG:C[1_554] | 1.46 | 0.74 |
| 4:5:222:ASP:C | 4:8:331:ALA:CB[1_554] | 1.46 | 0.74 |
| 4:4:198:TYR:CA | 4:7:208:ILE:N[1_554] | 1.46 | 0.74 |
| 4:5:166:TYR:CE1 | 4:V:40:HIS:ND1[1_554] | 1.46 | 0.74 |
| 4:6:287:ILE:C | 4:W:63:GLY:CA[1_554] | 1.46 | 0.74 |
| 4:5:115:ASN:CB | 4:9:196:ARG:CZ[1_554] | 1.46 | 0.74 |
| 4:6:151:ILE:N | 4:9:169:TYR:CD1[1_554] | 1.46 | 0.74 |
| 4:6:320:LEU:C | 4:9:293:LEU:N[1_554] | 1.46 | 0.74 |
| 4:5:263:GLN:CB | 4:8:274:ILE:CG2[1_554] | 1.46 | 0.74 |
| 4:5:141:SER:N | 4:8:116:ARG:CD[1_554] | 1.46 | 0.74 |
| 4:4:298:VAL:CG1 | 4:7:116:ARG:NH2[1_554] | 1.46 | 0.74 |
| 4:4:287:ILE:O | 4:9:63:GLY:C[1_554] | 1.46 | 0.74 |
| 4:5:265:SER:C | 4:8:261:LEU:C[1_554] | 1.46 | 0.74 |
| 4:5:213:LYS:NZ | 4:8:14:SER:C[1_554] | 1.46 | 0.74 |
| 4:6:312:ARG:CG | 4:9:299:MET:O[1_554] | 1.46 | 0.74 |
| 4:3:114:ALA:C | 4:7:250:ILE:O[1_554] | 1.46 | 0.74 |
| 4:6:332:PRO:N | 4:9:135:ALA:CB[1_554] | 1.46 | 0.74 |
| 4:4:370:VAL:N | 4:8:229:THR:O[1_554] | 1.46 | 0.74 |
| 4:4:213:LYS:CG | 4:7:15:GLY:CA[1_554] | 1.46 | 0.74 |
| 4:5:200:PHE:CB | 4:8:206:ARG:NE[1_554] | 1.46 | 0.74 |
| 4:4:259:GLU:OE1 | 4:7:304:THR:O[1_554] | 1.47 | 0.73 |
| 4:6:340:TRP:CE2 | 4:9:118:LYS:O[1_554] | 1.47 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:313:MET:CE | 4:8:163:VAL:O[1_554] | 1.47 | 0.73 |
| 4:6:183:ARG:NE | 4:9:72:GLU:OE2[1_554] | 1.47 | 0.73 |
| 4:5:300:SER:OG | 4:8:107:GLU:OE2[1_554] | 1.47 | 0.73 |
| 4:6:223:PHE:N | 4:9:331:ALA:CB[1_554] | 1.47 | 0.73 |
| 4:6:266:PHE:CE2 | 4:9:261:LEU:CD1[1_554] | 1.47 | 0.73 |
| 4:4:193:LEU:CB | 4:7:210:ARG:CD[1_554] | 1.47 | 0.73 |
| 4:5:11:ASP:O | 4:8:79:TRP:CE2[1_554] | 1.47 | 0.73 |
| 4:6:311:ASP:OD1 | 4:9:144:ALA:O[1_554] | 1.47 | 0.73 |
| 4:6:303:THR:C | 4:9:137:GLN:OE1[1_554] | 1.47 | 0.73 |
| 4:5:273:GLY:C | 4:8:162:ASN:CB[1_554] | 1.47 | 0.73 |
| 4:5:312:ARG:N | 4:8:298:VAL:CG1[1_554] | 1.47 | 0.73 |
| 4:5:264:PRO:CA | 4:8:178:LEU:CD2[1_554] | 1.47 | 0.73 |
| 4:4:289:ILE:N | 4:9:63:GLY:O[1_554] | 1.47 | 0.73 |
| 4:5:114:ALA:CB | 4:9:250:ILE:CA[1_554] | 1.47 | 0.73 |
| 4:5:218:TYR:CZ | 4:8:337:TYR:CE2[1_554] | 1.47 | 0.73 |
| 4:6:196:ARG:CG | 4:9:212:ILE:C[1_554] | 1.47 | 0.73 |
| 4:5:214:GLU:OE1 | 4:8:33:SER:CB[1_554] | 1.47 | 0.73 |
| 4:6:267:ILE:CG1 | 4:9:180:LEU:CB[1_554] | 1.47 | 0.73 |
| 4:5:151:ILE:N | 4:8:169:TYR:CD1[1_554] | 1.47 | 0.73 |
| 4:4:259:GLU:CG | 4:7:304:THR:CG2[1_554] | 1.47 | 0.73 |
| 4:6:213:LYS:NZ | 4:9:14:SER:C[1_554] | 1.47 | 0.73 |
| 4:4:262:PHE:CD1 | 4:7:153:LEU:C[1_554] | 1.47 | 0.73 |
| 4:5:227:MET:CG | 4:8:306:TYR:C[1_554] | 1.47 | 0.73 |
| 4:4:278:THR:O | 4:7:171:LEU:CB[1_554] | 1.47 | 0.73 |
| 4:6:272:ALA:CA | 4:9:277:THR:CB[1_554] | 1.47 | 0.73 |
| 4:5:296:ASN:C | 4:8:168:GLY:O[1_554] | 1.47 | 0.73 |
| 4:5:280:ASN:OD1 | 4:8:281:SER:CA[1_554] | 1.47 | 0.73 |
| 4:5:255:PHE:CD2 | 4:8:305:MET:CB[1_554] | 1.47 | 0.73 |
| 4:5:140:LEU:CB | 4:8:371:HIS:ND1[1_554] | 1.47 | 0.73 |
| 4:4:331:ALA:C | 4:7:135:ALA:CA[1_554] | 1.47 | 0.73 |
| 4:5:370:VAL:N | 4:9:231:ALA:C[1_554] | 1.47 | 0.73 |
| 4:4:215:LYS:N | 4:7:31:PHE:O[1_554] | 1.47 | 0.73 |
| 4:5:211:ASP:CA | 4:8:32:PRO:CA[1_554] | 1.47 | 0.73 |
| 4:4:312:ARG:N | 4:7:141:SER:CA[1_554] | 1.47 | 0.73 |
| 4:5:309:ILE:CG2 | 4:8:339:VAL:CG2[1_554] | 1.47 | 0.73 |
| 4:5:340:TRP:CA | 4:8:116:ARG:O[1_554] | 1.47 | 0.73 |
| 4:6:17:VAL:O | 4:9:79:TRP:CA[1_554] | 1.47 | 0.73 |
| 4:6:296:ASN:O | 4:9:169:TYR:CA[1_554] | 1.47 | 0.73 |
| 4:6:310:ALA:CA | 4:9:141:SER:N[1_554] | 1.47 | 0.73 |
| 4:5:311:ASP:N | 4:8:141:SER:C[1_554] | 1.47 | 0.73 |
| 4:5:193:LEU:CG | 4:8:210:ARG:CG[1_554] | 1.47 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:335:ARG:O | 4:9:106:THR:O[1_554] | 1.47 | 0.73 |
| 4:5:367:PRO:CA | 4:9:233:SER:C[1_554] | 1.47 | 0.73 |
| 4:4:186:THR:O | 4:7:183:ARG:CG[1_554] | 1.47 | 0.73 |
| 4:4:344:SER:CB | 4:7:367:PRO:CG[1_554] | 1.47 | 0.73 |
| 4:6:320:LEU:CA | 4:9:293:LEU:C[1_554] | 1.47 | 0.73 |
| 4:5:362:TYR:CD1 | 4:9:232:SER:O[1_554] | 1.47 | 0.73 |
| 4:6:218:TYR:CZ | 4:9:337:TYR:CE2[1_554] | 1.47 | 0.73 |
| 4:6:266:PHE:N | 4:9:261:LEU:C[1_554] | 1.47 | 0.73 |
| 4:6:325:MET:CG | 4:9:166:TYR:CE1[1_554] | 1.47 | 0.73 |
| 4:4:289:ILE:CG2 | 4:9:39:ARG:CZ[1_554] | 1.47 | 0.73 |
| 4:4:263:GLN:NE2 | 4:7:153:LEU:CD2[1_554] | 1.47 | 0.73 |
| 4:4:114:ALA:N | 4:8:250:ILE:CG2[1_554] | 1.47 | 0.73 |
| 4:4:282:ILE:CG1 | 4:7:171:LEU:CG[1_554] | 1.47 | 0.73 |
| 4:3:326:LYS:CD | 4:8:45:VAL:N[1_554] | 1.47 | 0.73 |
| 4:6:142:LEU:C | 4:9:372:ARG:CD[1_554] | 1.47 | 0.73 |
| 4:6:300:SER:OG | 4:9:107:GLU:CD[1_554] | 1.47 | 0.73 |
| 4:5:180:LEU:CD2 | 4:8:178:LEU:O[1_554] | 1.47 | 0.73 |
| 4:5:320:LEU:CD1 | 4:8:282:ILE:CG1[1_554] | 1.47 | 0.73 |
| 4:4:369:ILE:C | 4:8:229:THR:C[1_554] | 1.47 | 0.73 |
| 4:6:263:GLN:CG | 4:9:274:ILE:CG2[1_554] | 1.48 | 0.72 |
| 4:5:221:LEU:CG | 4:8:332:PRO:CD[1_554] | 1.48 | 0.72 |
| 4:6:295:ALA:CB | 4:9:167:GLU:O[1_554] | 1.48 | 0.72 |
| 4:6:283:MET:CG | 4:9:286:ASP:CA[1_554] | 1.48 | 0.72 |
| 4:6:208:ILE:CA | 4:9:59:GLN:NE2[1_554] | 1.48 | 0.72 |
| 4:6:154:ASP:CG | 4:9:111:ASN:N[1_554] | 1.48 | 0.72 |
| 4:4:178:LEU:O | 4:7:177:ARG:CD[1_554] | 1.48 | 0.72 |
| 4:5:143:TYR:CE2 | 4:8:369:ILE:O[1_554] | 1.48 | 0.72 |
| 4:6:193:LEU:CD2 | 4:9:210:ARG:NE[1_554] | 1.48 | 0.72 |
| 1:A:637:LYS:CE | 4:5:311:ASP:OD1[1_556] | 1.48 | 0.72 |
| 4:4:294:TYR:CG | 4:7:166:TYR:CB[1_554] | 1.48 | 0.72 |
| 4:5:258:PRO:CD | 4:8:303:THR:N[1_554] | 1.48 | 0.72 |
| 4:4:256:ARG:O | 4:7:303:THR:OG1[1_554] | 1.48 | 0.72 |
| 4:4:213:LYS:O | 4:7:16:LEU:CB[1_554] | 1.48 | 0.72 |
| 4:4:16:LEU:C | 4:7:77:THR:O[1_554] | 1.48 | 0.72 |
| 4:4:341:ILE:O | 4:7:367:PRO:CA[1_554] | 1.48 | 0.72 |
| 4:6:211:ASP:CA | 4:9:32:PRO:CA[1_554] | 1.48 | 0.72 |
| 4:6:198:TYR:CD1 | 4:9:208:ILE:CG1[1_554] | 1.48 | 0.72 |
| 4:6:294:TYR:O | 4:9:166:TYR:C[1_554] | 1.48 | 0.72 |
| 4:6:253:GLU:CG | 4:9:214:GLU:N[1_554] | 1.48 | 0.72 |
| 4:5:370:VAL:N | 4:9:231:ALA:N[1_554] | 1.48 | 0.72 |
| 4:5:189:LEU:C | 4:8:186:THR:OG1[1_554] | 1.48 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:23:GLY:CA | 4:8:362:TYR:CD2[1_554] | 1.48 | 0.72 |
| 4:4:329:ILE:CG2 | 4:7:139:VAL:CA[1_554] | 1.48 | 0.72 |
| 4:4:75:ILE:C | 4:8:197:GLY:O[1_554] | 1.48 | 0.72 |
| 4:4:169:TYR:CZ | 4:8:266:PHE:CE1[1_554] | 1.48 | 0.72 |
| 4:5:316:GLU:CD | 4:8:297:ASN:ND2[1_554] | 1.48 | 0.72 |
| 4:3:111:ASN:OD1 | 4:7:196:ARG:CB[1_554] | 1.48 | 0.72 |
| 4:5:315:LYS:CD | 4:8:147:ARG:CZ[1_554] | 1.48 | 0.72 |
| 4:4:111:ASN:O | 4:8:253:GLU:CB[1_554] | 1.48 | 0.72 |
| 4:6:167:GLU:OE2 | 4:W:40:HIS:C[1_554] | 1.48 | 0.72 |
| 4:6:194:THR:N | 4:9:209:VAL:CG1[1_554] | 1.48 | 0.72 |
| 4:6:346:LEU:CG | 4:9:368:SER:OG[1_554] | 1.48 | 0.72 |
| 4:5:213:LYS:O | 4:8:16:LEU:CD2[1_554] | 1.48 | 0.72 |
| 4:6:136:ILE:CA | 4:9:113:LYS:CG[1_554] | 1.48 | 0.72 |
| 4:6:155:SER:CA | 4:9:108:ALA:CB[1_554] | 1.48 | 0.72 |
| 4:6:59:GLN:CB | 4:9:68:LYS:CE[1_554] | 1.48 | 0.72 |
| 4:6:218:TYR:CD1 | 4:9:336:LYS:CG[1_554] | 1.48 | 0.72 |
| 4:4:327:ILE:CG1 | 4:7:148:THR:O[1_554] | 1.48 | 0.72 |
| 4:4:211:ASP:CA | 4:7:32:PRO:C[1_554] | 1.48 | 0.72 |
| 4:5:300:SER:OG | 4:8:107:GLU:CG[1_554] | 1.48 | 0.72 |
| 4:6:371:HIS:N | 4:V:231:ALA:N[1_554] | 1.48 | 0.72 |
| 4:6:76:ILE:N | 4:V:197:GLY:O[1_554] | 1.48 | 0.72 |
| 4:5:218:TYR:CD2 | 4:8:336:LYS:CG[1_554] | 1.48 | 0.72 |
| 4:5:157:ASP:CA | 4:8:72:GLU:C[1_554] | 1.48 | 0.72 |
| 4:6:188:TYR:CE1 | 4:9:185:LEU:CD2[1_554] | 1.48 | 0.72 |
| 4:6:290:ARG:NE | 4:9:286:ASP:OD2[1_554] | 1.48 | 0.72 |
| 4:5:335:ARG:CA | 4:8:106:THR:N[1_554] | 1.48 | 0.72 |
| 4:6:137:GLN:CB | 4:9:112:PRO:O[1_554] | 1.48 | 0.72 |
| 4:4:223:PHE:C | 4:7:335:ARG:NH2[1_554] | 1.48 | 0.72 |
| 4:5:223:PHE:CZ | 4:8:304:THR:CB[1_554] | 1.48 | 0.72 |
| 4:4:108:ALA:CA | 4:8:195:GLU:C[1_554] | 1.48 | 0.72 |
| 4:5:137:GLN:OE1 | 4:8:112:PRO:CD[1_554] | 1.48 | 0.72 |
| 4:5:299:MET:O | 4:8:135:ALA:O[1_554] | 1.48 | 0.72 |
| 4:4:205:GLU:N | 4:7:62:ARG:CD[1_554] | 1.48 | 0.72 |
| 4:4:184:ASP:OD1 | 4:7:73:HIS:CE1[1_554] | 1.48 | 0.72 |
| 4:4:278:THR:CG2 | 4:7:164:PRO:O[1_554] | 1.48 | 0.72 |
| 4:6:180:LEU:O | 4:9:159:VAL:CG1[1_554] | 1.48 | 0.72 |
| 4:4:288:ASP:CG | 4:9:65:LEU:O[1_554] | 1.48 | 0.72 |
| 4:5:223:PHE:CE1 | 4:8:304:THR:OG1[1_554] | 1.48 | 0.72 |
| 4:3:173:HIS:CG | 4:7:267:ILE:N[1_554] | 1.48 | 0.72 |
| 4:6:258:PRO:CB | 4:9:155:SER:O[1_554] | 1.48 | 0.72 |
| 4:6:295:ALA:N | 4:9:166:TYR:O[1_554] | 1.48 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:334:GLU:CD | 4:9:133:TYR:O[1_554] | 1.48 | 0.72 |
| 4:4:218:TYR:CB | 4:7:336:LYS:C[1_554] | 1.48 | 0.72 |
| 4:6:287:ILE:O | 4:W:63:GLY:N[1_554] | 1.49 | 0.71 |
| 4:6:326:LYS:CB | 4:9:167:GLU:OE2[1_554] | 1.49 | 0.71 |
| 4:5:286:ASP:CG | 4:9:270:GLU:OE1[1_554] | 1.49 | 0.71 |
| 4:2:291:LYS:CA | 4:7:40:HIS:ND1[1_554] | 1.49 | 0.71 |
| 4:6:296:ASN:C | 4:9:168:GLY:C[1_554] | 1.49 | 0.71 |
| 4:6:59:GLN:CB | 4:9:68:LYS:CG[1_554] | 1.49 | 0.71 |
| 4:4:214:GLU:N | 4:7:16:LEU:CA[1_554] | 1.49 | 0.71 |
| 4:4:338:SER:C | 4:7:116:ARG:O[1_554] | 1.49 | 0.71 |
| 4:3:108:ALA:CA | 4:7:195:GLU:C[1_554] | 1.49 | 0.71 |
| 4:6:191:LYS:CD | 4:9:185:LEU:O[1_554] | 1.49 | 0.71 |
| 4:4:115:ASN:O | 4:8:196:ARG:NH2[1_554] | 1.49 | 0.71 |
| 4:6:272:ALA:N | 4:9:277:THR:OG1[1_554] | 1.49 | 0.71 |
| 4:6:154:ASP:CA | 4:9:109:PRO:C[1_554] | 1.49 | 0.71 |
| 4:5:333:PRO:CA | 4:8:104:LEU:CD2[1_554] | 1.49 | 0.71 |
| 4:5:316:GLU:OE1 | 4:8:297:ASN:ND2[1_554] | 1.49 | 0.71 |
| 4:4:316:GLU:CD | 4:7:151:ILE:O[1_554] | 1.49 | 0.71 |
| 4:6:115:ASN:N | 4:V:196:ARG:NH1[1_554] | 1.49 | 0.71 |
| 4:4:341:ILE:CA | 4:7:117:GLU:O[1_554] | 1.49 | 0.71 |
| 4:4:312:ARG:N | 4:7:141:SER:O[1_554] | 1.49 | 0.71 |
| 4:4:173:HIS:N | 4:8:266:PHE:O[1_554] | 1.49 | 0.71 |
| 4:5:252:ASN:CB | 4:8:214:GLU:O[1_554] | 1.49 | 0.71 |
| 4:5:313:MET:SD | 4:8:152:VAL:N[1_554] | 1.49 | 0.71 |
| 4:6:116:ARG:N | 4:V:196:ARG:NH1[1_554] | 1.49 | 0.71 |
| 4:6:344:SER:O | 4:9:362:TYR:CE1[1_554] | 1.49 | 0.71 |
| 4:6:155:SER:N | 4:9:108:ALA:CB[1_554] | 1.49 | 0.71 |
| 4:6:227:MET:CB | 4:9:307:PRO:CB[1_554] | 1.49 | 0.71 |
| 4:4:171:LEU:O | 4:8:266:PHE:O[1_554] | 1.49 | 0.71 |
| 4:4:192:ILE:CB | 4:7:213:LYS:NZ[1_554] | 1.49 | 0.71 |
| 4:6:185:LEU:C | 4:9:157:ASP:C[1_554] | 1.49 | 0.71 |
| 4:6:334:GLU:N | 4:9:104:LEU:O[1_554] | 1.49 | 0.71 |
| 4:6:194:THR:CA | 4:9:209:VAL:CG2[1_554] | 1.49 | 0.71 |
| 4:6:267:ILE:C | 4:9:180:LEU:CD2[1_554] | 1.49 | 0.71 |
| 4:6:278:THR:OG1 | 4:9:164:PRO:N[1_554] | 1.49 | 0.71 |
| 4:5:220:ALA:CB | 4:8:335:ARG:CD[1_554] | 1.49 | 0.71 |
| 4:6:220:ALA:CB | 4:9:335:ARG:CG[1_554] | 1.49 | 0.71 |
| 4:6:199:SER:N | 4:9:205:GLU:C[1_554] | 1.49 | 0.71 |
| 4:6:210:ARG:NH1 | 4:9:33:SER:O[1_554] | 1.49 | 0.71 |
| 4:4:18:LYS:CG | 4:7:79:TRP:CE2[1_554] | 1.49 | 0.71 |
| 4:3:368:SER:N | 4:7:236:LEU:N[1_554] | 1.49 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:26:ALA:C | 4:8:122:ILE:C[1_554] | 1.49 | 0.71 |
| 4:3:75:ILE:CA | 4:7:198:TYR:N[1_554] | 1.49 | 0.71 |
| 4:4:187:ASP:O | 4:7:183:ARG:C[1_554] | 1.49 | 0.71 |
| 4:4:277:THR:N | 4:7:281:SER:OG[1_554] | 1.49 | 0.71 |
| 4:5:218:TYR:O | 4:8:301:GLY:C[1_554] | 1.49 | 0.71 |
| 4:4:339:VAL:CA | 4:7:116:ARG:N[1_554] | 1.49 | 0.71 |
| 4:5:320:LEU:O | 4:8:290:ARG:O[1_554] | 1.49 | 0.71 |
| 4:6:313:MET:CE | 4:9:163:VAL:O[1_554] | 1.49 | 0.71 |
| 4:4:214:GLU:O | 4:7:17:VAL:CA[1_554] | 1.49 | 0.71 |
| 4:6:20:GLY:CA | 4:9:121:GLN:NE2[1_554] | 1.49 | 0.71 |
| 4:4:115:ASN:OD1 | 4:8:249:THR:O[1_554] | 1.49 | 0.71 |
| 4:4:173:HIS:O | 4:8:267:ILE:O[1_554] | 1.49 | 0.71 |
| 4:5:137:GLN:CB | 4:8:112:PRO:O[1_554] | 1.49 | 0.71 |
| 4:5:277:THR:O | 4:8:174:ALA:O[1_554] | 1.49 | 0.71 |
| 4:4:217:CYS:O | 4:7:18:LYS:CD[1_554] | 1.49 | 0.71 |
| 4:6:115:ASN:OD1 | 4:V:196:ARG:NE[1_554] | 1.49 | 0.71 |
| 4:5:331:ALA:CA | 4:8:140:LEU:CG[1_554] | 1.49 | 0.71 |
| 4:5:320:LEU:N | 4:8:294:TYR:N[1_554] | 1.49 | 0.71 |
| 4:5:190:MET:C | 4:8:186:THR:CB[1_554] | 1.49 | 0.71 |
| 4:5:310:ALA:N | 4:8:141:SER:OG[1_554] | 1.49 | 0.71 |
| 4:6:190:MET:C | 4:9:186:THR:CG2[1_554] | 1.49 | 0.71 |
| 4:6:196:ARG:O | 4:9:212:ILE:CD1[1_554] | 1.49 | 0.71 |
| 4:5:110:LEU:N | 4:9:195:GLU:OE1[1_554] | 1.49 | 0.71 |
| 4:4:318:THR:CG2 | 4:7:149:THR:N[1_554] | 1.49 | 0.71 |
| 4:6:309:ILE:O | 4:9:141:SER:CB[1_554] | 1.49 | 0.71 |
| 4:6:27:PRO:CB | 4:9:122:ILE:CB[1_554] | 1.49 | 0.71 |
| 4:6:32:PRO:CD | 4:9:81:ASP:CG[1_554] | 1.49 | 0.71 |
| 4:6:227:MET:CE | 4:9:306:TYR:CB[1_554] | 1.49 | 0.71 |
| 4:5:342:GLY:C | 4:8:367:PRO:O[1_554] | 1.49 | 0.71 |
| 4:5:180:LEU:N | 4:8:179:ASP:OD1[1_554] | 1.49 | 0.71 |
| 4:4:213:LYS:CB | 4:7:15:GLY:C[1_554] | 1.49 | 0.71 |
| 4:3:117:GLU:OE2 | 4:7:236:LEU:O[1_554] | 1.49 | 0.71 |
| 4:3:286:ASP:C | 4:7:270:GLU:CD[1_554] | 1.49 | 0.71 |
| 4:5:76:ILE:N | 4:9:197:GLY:O[1_554] | 1.49 | 0.71 |
| 4:5:335:ARG:O | 4:8:106:THR:C[1_554] | 1.49 | 0.71 |
| 4:5:56:ASP:CB | 4:8:37:ARG:NH2[1_554] | 1.49 | 0.71 |
| 4:4:259:GLU:CB | 4:7:304:THR:N[1_554] | 1.49 | 0.71 |
| 4:4:207:GLU:CG | 4:7:67:LEU:CA[1_554] | 1.49 | 0.71 |
| 4:5:153:LEU:C | 4:8:109:PRO:CA[1_554] | 1.49 | 0.71 |
| 4:4:335:ARG:CD | 4:7:106:THR:C[1_554] | 1.50 | 0.70 |
| 4:5:299:MET:CE | 4:8:137:GLN:O[1_554] | 1.50 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:288:ASP:OD1 | 4:7:66:THR:CG2[1_554] | 1.50 | 0.70 |
| 4:5:178:LEU:CB | 4:8:177:ARG:CA[1_554] | 1.50 | 0.70 |
| 4:6:184:ASP:O | 4:9:184:ASP:OD1[1_554] | 1.50 | 0.70 |
| 4:5:18:LYS:CE | 4:8:79:TRP:CH2[1_554] | 1.50 | 0.70 |
| 4:5:114:ALA:CA | 4:9:251:GLY:CA[1_554] | 1.50 | 0.70 |
| 4:6:344:SER:C | 4:9:362:TYR:CD1[1_554] | 1.50 | 0.70 |
| 4:5:243:PRO:CA | 4:8:60:SER:CA[1_554] | 1.50 | 0.70 |
| 4:6:258:PRO:N | 4:9:303:THR:N[1_554] | 1.50 | 0.70 |
| 4:5:193:LEU:CG | 4:8:210:ARG:CA[1_554] | 1.50 | 0.70 |
| 4:6:370:VAL:N | 4:V:231:ALA:N[1_554] | 1.50 | 0.70 |
| 4:3:117:GLU:CA | 4:7:237:GLU:CB[1_554] | 1.50 | 0.70 |
| 4:5:287:ILE:C | 4:V:63:GLY:CA[1_554] | 1.50 | 0.70 |
| 4:4:368:SER:N | 4:8:236:LEU:CA[1_554] | 1.50 | 0.70 |
| 4:6:308:GLY:C | 4:9:338:SER:OG[1_554] | 1.50 | 0.70 |
| 4:5:210:ARG:CB | 4:8:69:TYR:CE2[1_554] | 1.50 | 0.70 |
| 4:5:287:ILE:O | 4:V:63:GLY:N[1_554] | 1.50 | 0.70 |
| 4:6:270:GLU:CB | 4:9:272:ALA:N[1_554] | 1.50 | 0.70 |
| 4:6:18:LYS:N | 4:9:79:TRP:CG[1_554] | 1.50 | 0.70 |
| 4:5:199:SER:N | 4:8:205:GLU:C[1_554] | 1.50 | 0.70 |
| 4:3:117:GLU:O | 4:7:237:GLU:CG[1_554] | 1.50 | 0.70 |
| 4:6:140:LEU:CB | 4:9:371:HIS:ND1[1_554] | 1.50 | 0.70 |
| 4:6:201:VAL:CG2 | 4:9:203:THR:CA[1_554] | 1.50 | 0.70 |
| 4:4:308:GLY:C | 4:7:339:VAL:CA[1_554] | 1.50 | 0.70 |
| 4:6:24:ASP:OD2 | 4:9:125:GLU:CB[1_554] | 1.50 | 0.70 |
| 4:5:316:GLU:CA | 4:8:296:ASN:O[1_554] | 1.50 | 0.70 |
| 4:5:192:ILE:CG1 | 4:8:213:LYS:CE[1_554] | 1.50 | 0.70 |
| 4:6:173:HIS:CB | 4:V:267:ILE:CB[1_554] | 1.50 | 0.70 |
| 4:4:339:VAL:N | 4:7:116:ARG:C[1_554] | 1.50 | 0.70 |
| 4:6:307:PRO:C | 4:9:337:TYR:C[1_554] | 1.50 | 0.70 |
| 4:6:23:GLY:CA | 4:9:362:TYR:CD2[1_554] | 1.50 | 0.70 |
| 4:5:334:GLU:CB | 4:8:105:LEU:N[1_554] | 1.50 | 0.70 |
| 4:5:243:PRO:CG | 4:8:60:SER:CA[1_554] | 1.50 | 0.70 |
| 4:5:205:GLU:OE2 | 4:8:203:THR:CG2[1_554] | 1.50 | 0.70 |
| 4:6:114:ALA:O | 4:V:237:GLU:OE2[1_554] | 1.50 | 0.70 |
| 4:5:282:ILE:CG1 | 4:8:171:LEU:CD2[1_554] | 1.50 | 0.70 |
| 4:6:336:LYS:N | 4:9:106:THR:O[1_554] | 1.50 | 0.70 |
| 4:6:288:ASP:CA | 4:W:63:GLY:N[1_554] | 1.50 | 0.70 |
| 4:5:262:PHE:CE1 | 4:8:153:LEU:CA[1_554] | 1.50 | 0.70 |
| 4:6:164:PRO:CD | 4:9:172:PRO:CB[1_554] | 1.50 | 0.70 |
| 4:4:147:ARG:CG | 4:7:372:ARG:CG[1_554] | 1.50 | 0.70 |
| 4:4:281:SER:C | 4:7:173:HIS:CG[1_554] | 1.50 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:259:GLU:CG | 4:9:309:ILE:CD1[1_554] | 1.50 | 0.70 |
| 4:5:316:GLU:OE1 | 4:8:297:ASN:CB[1_554] | 1.50 | 0.70 |
| 4:5:141:SER:CA | 4:8:116:ARG:CZ[1_554] | 1.50 | 0.70 |
| 4:4:322:PRO:CA | 4:7:292:ASP:OD2[1_554] | 1.50 | 0.70 |
| 4:4:173:HIS:NE2 | 4:8:265:SER:C[1_554] | 1.50 | 0.70 |
| 4:4:317:ILE:CD1 | 4:7:165:ILE:C[1_554] | 1.50 | 0.70 |
| 4:6:335:ARG:C | 4:9:106:THR:O[1_554] | 1.50 | 0.70 |
| 4:4:267:ILE:CB | 4:7:180:LEU:CG[1_554] | 1.50 | 0.70 |
| 4:6:220:ALA:C | 4:9:335:ARG:CD[1_554] | 1.50 | 0.70 |
| 4:6:227:MET:CG | 4:9:307:PRO:C[1_554] | 1.50 | 0.70 |
| 4:6:31:PHE:CG | 4:9:80:ASP:CA[1_554] | 1.50 | 0.70 |
| 4:4:154:ASP:N | 4:7:109:PRO:O[1_554] | 1.50 | 0.70 |
| 4:6:193:LEU:CG | 4:9:210:ARG:CA[1_554] | 1.50 | 0.70 |
| 4:4:218:TYR:CE2 | 4:7:337:TYR:CD1[1_554] | 1.50 | 0.70 |
| 4:4:254:ARG:NE | 4:7:337:TYR:OH[1_554] | 1.50 | 0.70 |
| 4:6:106:THR:CG2 | 4:9:114:ALA:O[1_554] | 1.50 | 0.70 |
| 4:3:372:ARG:CA | 4:7:226:GLU:C[1_554] | 1.50 | 0.70 |
| 4:6:151:ILE:CA | 4:9:170:ALA:O[1_554] | 1.50 | 0.70 |
| 4:6:218:TYR:OH | 4:9:337:TYR:CD2[1_554] | 1.50 | 0.70 |
| 4:5:346:LEU:CB | 4:8:368:SER:CB[1_554] | 1.50 | 0.70 |
| 4:4:327:ILE:CD1 | 4:7:167:GLU:N[1_554] | 1.50 | 0.70 |
| 4:6:191:LYS:C | 4:9:186:THR:C[1_554] | 1.50 | 0.70 |
| 4:6:30:VAL:O | 4:9:80:ASP:O[1_554] | 1.50 | 0.70 |
| 4:4:339:VAL:O | 4:7:117:GLU:CB[1_554] | 1.50 | 0.70 |
| 4:5:114:ALA:O | 4:9:237:GLU:OE2[1_554] | 1.50 | 0.70 |
| 4:5:274:ILE:O | 4:8:163:VAL:N[1_554] | 1.50 | 0.70 |
| 4:4:186:THR:CA | 4:7:183:ARG:CZ[1_554] | 1.50 | 0.70 |
| 4:6:295:ALA:CA | 4:9:167:GLU:CA[1_554] | 1.50 | 0.70 |
| 4:4:326:LYS:CE | 4:9:44:MET:C[1_554] | 1.50 | 0.70 |
| 4:4:210:ARG:NH1 | 4:7:70:PRO:CD[1_554] | 1.50 | 0.70 |
| 4:5:283:MET:CA | 4:8:286:ASP:N[1_554] | 1.50 | 0.70 |
| 4:5:256:ARG:CG | 4:8:306:TYR:CD1[1_554] | 1.50 | 0.70 |
| 4:5:173:HIS:CE1 | 4:9:266:PHE:N[1_554] | 1.50 | 0.70 |
| 4:3:172:PRO:CD | 4:7:266:PHE:CG[1_554] | 1.50 | 0.70 |
| 4:6:59:GLN:CG | 4:9:68:LYS:CB[1_554] | 1.50 | 0.70 |
| 4:5:215:LYS:O | 4:8:30:VAL:CG1[1_554] | 1.50 | 0.70 |
| 4:4:110:LEU:O | 4:8:192:ILE:C[1_554] | 1.50 | 0.70 |
| 4:5:31:PHE:CB | 4:8:81:ASP:N[1_554] | 1.50 | 0.70 |
| 4:5:154:ASP:OD1 | 4:8:111:ASN:CB[1_554] | 1.50 | 0.70 |
| 4:4:335:ARG:NH1 | 4:7:106:THR:CG2[1_554] | 1.50 | 0.70 |
| 4:6:166:TYR:CE2 | 4:W:39:ARG:C[1_554] | 1.50 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:299:MET:CE | 4:9:137:GLN:O[1_554] | 1.51 | 0.69 |
| 4:6:318:THR:CB | 4:9:296:ASN:CG[1_554] | 1.51 | 0.69 |
| 4:5:256:ARG:O | 4:8:303:THR:CG2[1_554] | 1.51 | 0.69 |
| 4:6:154:ASP:C | 4:9:109:PRO:N[1_554] | 1.51 | 0.69 |
| 4:2:288:ASP:C | 4:7:39:ARG:CD[1_554] | 1.51 | 0.69 |
| 4:6:339:VAL:CB | 4:9:116:ARG:N[1_554] | 1.51 | 0.69 |
| 4:5:368:SER:C | 4:9:230:ALA:N[1_554] | 1.51 | 0.69 |
| 4:5:207:GLU:OE2 | 4:8:67:LEU:C[1_554] | 1.51 | 0.69 |
| 4:3:288:ASP:OD1 | 4:8:65:LEU:O[1_554] | 1.51 | 0.69 |
| 4:5:224:GLU:CB | 4:8:310:ALA:CB[1_554] | 1.51 | 0.69 |
| 4:4:110:LEU:CB | 4:8:192:ILE:CA[1_554] | 1.51 | 0.69 |
| 4:6:210:ARG:NH2 | 4:9:33:SER:O[1_554] | 1.51 | 0.69 |
| 4:6:32:PRO:CD | 4:9:81:ASP:CB[1_554] | 1.51 | 0.69 |
| 4:5:21:PHE:C | 4:8:125:GLU:CG[1_554] | 1.51 | 0.69 |
| 4:4:188:TYR:OH | 4:7:185:LEU:CD2[1_554] | 1.51 | 0.69 |
| 4:6:338:SER:CA | 4:9:134:VAL:CG1[1_554] | 1.51 | 0.69 |
| 4:6:196:ARG:CA | 4:9:212:ILE:CG2[1_554] | 1.51 | 0.69 |
| 4:6:110:LEU:O | 4:V:192:ILE:O[1_554] | 1.51 | 0.69 |
| 4:3:173:HIS:N | 4:7:266:PHE:C[1_554] | 1.51 | 0.69 |
| 4:4:274:ILE:CA | 4:7:162:ASN:N[1_554] | 1.51 | 0.69 |
| 4:6:221:LEU:C | 4:9:331:ALA:O[1_554] | 1.51 | 0.69 |
| 4:3:326:LYS:CE | 4:8:44:MET:C[1_554] | 1.51 | 0.69 |
| 4:6:214:GLU:N | 4:9:16:LEU:CB[1_554] | 1.51 | 0.69 |
| 4:6:136:ILE:CG1 | 4:9:113:LYS:NZ[1_554] | 1.51 | 0.69 |
| 4:5:195:GLU:CG | 4:8:189:LEU:CB[1_554] | 1.51 | 0.69 |
| 4:6:307:PRO:CB | 4:9:337:TYR:CB[1_554] | 1.51 | 0.69 |
| 4:5:155:SER:N | 4:8:108:ALA:CB[1_554] | 1.51 | 0.69 |
| 4:5:281:SER:CB | 4:8:174:ALA:N[1_554] | 1.51 | 0.69 |
| 4:4:110:LEU:O | 4:8:193:LEU:N[1_554] | 1.51 | 0.69 |
| 4:5:166:TYR:CG | 4:V:40:HIS:CD2[1_554] | 1.51 | 0.69 |
| 4:4:305:MET:C | 4:7:11:ASP:CG[1_554] | 1.51 | 0.69 |
| 4:4:194:THR:C | 4:7:209:VAL:CA[1_554] | 1.51 | 0.69 |
| 4:5:262:PHE:O | 4:8:153:LEU:CD1[1_554] | 1.51 | 0.69 |
| 4:3:288:ASP:CG | 4:8:65:LEU:O[1_554] | 1.51 | 0.69 |
| 4:4:114:ALA:C | 4:8:250:ILE:CA[1_554] | 1.51 | 0.69 |
| 4:5:289:ILE:CA | 4:V:63:GLY:O[1_554] | 1.51 | 0.69 |
| 4:4:325:MET:C | 4:7:167:GLU:CG[1_554] | 1.51 | 0.69 |
| 4:5:301:GLY:CA | 4:8:108:ALA:N[1_554] | 1.51 | 0.69 |
| 4:6:109:PRO:CA | 4:V:195:GLU:OE2[1_554] | 1.51 | 0.69 |
| 4:5:32:PRO:CD | 4:8:81:ASP:OD2[1_554] | 1.51 | 0.69 |
| 4:4:211:ASP:CA | 4:7:33:SER:N[1_554] | 1.51 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:137:GLN:CB | 4:9:113:LYS:N[1_554] | 1.51 | 0.69 |
| 4:6:33:SER:CB | 4:9:77:THR:O[1_554] | 1.51 | 0.69 |
| 4:5:59:GLN:CB | 4:8:68:LYS:CG[1_554] | 1.51 | 0.69 |
| 4:5:157:ASP:CB | 4:8:72:GLU:N[1_554] | 1.51 | 0.69 |
| 4:6:300:SER:O | 4:9:107:GLU:C[1_554] | 1.51 | 0.69 |
| 4:5:259:GLU:CG | 4:8:309:ILE:CD1[1_554] | 1.51 | 0.69 |
| 4:4:115:ASN:CA | 4:8:249:THR:C[1_554] | 1.51 | 0.69 |
| 4:4:259:GLU:CB | 4:7:304:THR:CG2[1_554] | 1.51 | 0.69 |
| 4:6:31:PHE:CD1 | 4:9:80:ASP:CA[1_554] | 1.51 | 0.69 |
| 4:4:191:LYS:CE | 4:7:185:LEU:O[1_554] | 1.51 | 0.69 |
| 4:6:266:PHE:CG | 4:9:261:LEU:CB[1_554] | 1.51 | 0.69 |
| 4:6:210:ARG:CD | 4:9:69:TYR:CD2[1_554] | 1.51 | 0.69 |
| 4:5:180:LEU:O | 4:8:159:VAL:CG1[1_554] | 1.51 | 0.69 |
| 4:3:109:PRO:O | 4:7:195:GLU:OE1[1_554] | 1.51 | 0.69 |
| 4:4:18:LYS:N | 4:7:79:TRP:CD1[1_554] | 1.51 | 0.69 |
| 1:D:637:LYS:CE | 4:6:311:ASP:CB[1_556] | 1.51 | 0.69 |
| 4:6:283:MET:CG | 4:9:286:ASP:O[1_554] | 1.51 | 0.69 |
| 4:6:166:TYR:OH | 4:W:39:ARG:N[1_554] | 1.51 | 0.69 |
| 4:3:367:PRO:CG | 4:7:235:SER:CA[1_554] | 1.51 | 0.69 |
| 4:6:329:ILE:CD1 | 4:9:142:LEU:CD2[1_554] | 1.51 | 0.69 |
| 4:4:286:ASP:N | 4:8:270:GLU:CD[1_554] | 1.51 | 0.69 |
| 4:4:289:ILE:N | 4:9:39:ARG:NH1[1_554] | 1.51 | 0.69 |
| 4:5:222:ASP:N | 4:8:331:ALA:C[1_554] | 1.51 | 0.69 |
| 4:5:346:LEU:N | 4:8:366:GLY:O[1_554] | 1.51 | 0.69 |
| 4:5:261:LEU:CB | 4:8:154:ASP:C[1_554] | 1.51 | 0.69 |
| 4:5:335:ARG:O | 4:8:106:THR:O[1_554] | 1.52 | 0.68 |
| 4:4:262:PHE:CD1 | 4:7:154:ASP:N[1_554] | 1.52 | 0.68 |
| 4:6:272:ALA:CA | 4:9:277:THR:CA[1_554] | 1.52 | 0.68 |
| 4:5:303:THR:C | 4:8:137:GLN:OE1[1_554] | 1.52 | 0.68 |
| 4:3:289:ILE:CG2 | 4:8:39:ARG:NE[1_554] | 1.52 | 0.68 |
| 4:6:284:LYS:O | 4:V:268:GLY:C[1_554] | 1.52 | 0.68 |
| 4:4:17:VAL:C | 4:7:79:TRP:CD1[1_554] | 1.52 | 0.68 |
| 4:4:188:TYR:CA | 4:7:183:ARG:N[1_554] | 1.52 | 0.68 |
| 4:6:157:ASP:CB | 4:9:72:GLU:N[1_554] | 1.52 | 0.68 |
| 4:5:215:LYS:N | 4:8:16:LEU:CG[1_554] | 1.52 | 0.68 |
| 4:5:296:ASN:O | 4:8:169:TYR:CA[1_554] | 1.52 | 0.68 |
| 4:5:113:LYS:NZ | 4:9:255:PHE:N[1_554] | 1.52 | 0.68 |
| 4:4:180:LEU:CG | 4:7:178:LEU:O[1_554] | 1.52 | 0.68 |
| 4:5:267:ILE:C | 4:8:180:LEU:CD2[1_554] | 1.52 | 0.68 |
| 4:5:154:ASP:CA | 4:8:108:ALA:O[1_554] | 1.52 | 0.68 |
| 4:6:200:PHE:CB | 4:9:206:ARG:NE[1_554] | 1.52 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:289:ILE:O | 4:7:40:HIS:NE2[1_554] | 1.52 | 0.68 |
| 4:5:195:GLU:N | 4:8:209:VAL:CG2[1_554] | 1.52 | 0.68 |
| 4:5:223:PHE:N | 4:8:331:ALA:CB[1_554] | 1.52 | 0.68 |
| 4:5:181:ALA:O | 4:8:159:VAL:N[1_554] | 1.52 | 0.68 |
| 4:5:214:GLU:CD | 4:8:33:SER:CB[1_554] | 1.52 | 0.68 |
| 4:5:270:GLU:CB | 4:8:272:ALA:N[1_554] | 1.52 | 0.68 |
| 4:5:318:THR:OG1 | 4:8:296:ASN:CB[1_554] | 1.52 | 0.68 |
| 4:6:367:PRO:CD | 4:V:234:SER:CA[1_554] | 1.52 | 0.68 |
| 4:6:32:PRO:CD | 4:9:81:ASP:OD2[1_554] | 1.52 | 0.68 |
| 4:5:262:PHE:CZ | 4:8:153:LEU:C[1_554] | 1.52 | 0.68 |
| 4:3:166:TYR:CD1 | 4:8:40:HIS:CE1[1_554] | 1.52 | 0.68 |
| 4:6:333:PRO:N | 4:9:104:LEU:CG[1_554] | 1.52 | 0.68 |
| 4:5:115:ASN:CA | 4:9:196:ARG:NH2[1_554] | 1.52 | 0.68 |
| 4:4:339:VAL:CG1 | 4:7:114:ALA:CA[1_554] | 1.52 | 0.68 |
| 4:3:173:HIS:O | 4:7:267:ILE:CA[1_554] | 1.52 | 0.68 |
| 4:3:115:ASN:CA | 4:7:249:THR:C[1_554] | 1.52 | 0.68 |
| 4:6:205:GLU:CD | 4:7:288:ASP:OD2[1_554] | 1.52 | 0.68 |
| 4:4:317:ILE:N | 4:7:150:GLY:C[1_554] | 1.52 | 0.68 |
| 4:5:345:ILE:C | 4:8:366:GLY:O[1_554] | 1.52 | 0.68 |
| 4:5:339:VAL:O | 4:8:116:ARG:O[1_554] | 1.52 | 0.68 |
| 4:5:369:ILE:CG2 | 4:9:232:SER:CB[1_554] | 1.52 | 0.68 |
| 4:6:11:ASP:OD1 | 4:9:115:ASN:CB[1_554] | 1.52 | 0.68 |
| 4:6:300:SER:O | 4:9:107:GLU:O[1_554] | 1.52 | 0.68 |
| 1:A:637:LYS:NZ | 4:5:311:ASP:CB[1_556] | 1.52 | 0.68 |
| 4:6:370:VAL:N | 4:V:231:ALA:CB[1_554] | 1.52 | 0.68 |
| 4:5:296:ASN:C | 4:8:169:TYR:CA[1_554] | 1.52 | 0.68 |
| 4:6:11:ASP:O | 4:9:79:TRP:CZ2[1_554] | 1.52 | 0.68 |
| 4:6:300:SER:OG | 4:9:107:GLU:OE2[1_554] | 1.52 | 0.68 |
| 4:4:340:TRP:CB | 4:7:118:LYS:N[1_554] | 1.52 | 0.68 |
| 4:5:286:ASP:N | 4:9:270:GLU:CD[1_554] | 1.52 | 0.68 |
| 4:4:334:GLU:CB | 4:7:132:MET:CE[1_554] | 1.52 | 0.68 |
| 4:5:155:SER:CA | 4:8:108:ALA:CB[1_554] | 1.52 | 0.68 |
| 4:3:291:LYS:N | 4:8:64:ILE:CG2[1_554] | 1.52 | 0.68 |
| 4:4:288:ASP:CB | 4:9:65:LEU:O[1_554] | 1.52 | 0.68 |
| 4:4:185:LEU:O | 4:7:157:ASP:C[1_554] | 1.52 | 0.68 |
| 4:4:174:ALA:O | 4:7:173:HIS:CB[1_554] | 1.52 | 0.68 |
| 4:4:274:ILE:CD1 | 4:7:161:HIS:CB[1_554] | 1.52 | 0.68 |
| 4:5:335:ARG:CG | 4:8:106:THR:CA[1_554] | 1.52 | 0.68 |
| 4:4:18:LYS:CD | 4:7:79:TRP:NE1[1_554] | 1.52 | 0.68 |
| 4:5:109:PRO:CA | 4:9:195:GLU:CD[1_554] | 1.52 | 0.68 |
| 4:5:312:ARG:CG | 4:8:299:MET:O[1_554] | 1.52 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:263:GLN:N | 4:8:274:ILE:CG1[1_554] | 1.52 | 0.68 |
| 4:5:345:ILE:C | 4:8:369:ILE:CG2[1_554] | 1.52 | 0.68 |
| 4:5:347:ALA:CA | 4:8:366:GLY:CA[1_554] | 1.52 | 0.68 |
| 4:4:308:GLY:O | 4:7:141:SER:OG[1_554] | 1.52 | 0.68 |
| 4:5:28:ARG:CG | 4:8:126:THR:CB[1_554] | 1.52 | 0.68 |
| 4:4:207:GLU:CB | 4:7:67:LEU:CG[1_554] | 1.52 | 0.68 |
| 4:5:181:ALA:N | 4:8:159:VAL:CG1[1_554] | 1.52 | 0.68 |
| 4:5:326:LYS:CB | 4:8:167:GLU:OE1[1_554] | 1.52 | 0.68 |
| 4:6:280:ASN:ND2 | 4:9:281:SER:O[1_554] | 1.52 | 0.68 |
| 4:6:313:MET:C | 4:9:142:LEU:CD1[1_554] | 1.52 | 0.68 |
| 4:3:74:GLY:C | 4:7:198:TYR:N[1_554] | 1.52 | 0.68 |
| 4:4:114:ALA:C | 4:8:250:ILE:O[1_554] | 1.52 | 0.68 |
| 4:6:219:VAL:O | 4:9:335:ARG:CB[1_554] | 1.52 | 0.68 |
| 4:6:180:LEU:CD2 | 4:9:178:LEU:O[1_554] | 1.52 | 0.68 |
| 4:5:340:TRP:O | 4:8:120:THR:CB[1_554] | 1.52 | 0.68 |
| 4:2:289:ILE:O | 4:7:40:HIS:CE1[1_554] | 1.52 | 0.68 |
| 4:6:257:CYS:O | 4:9:303:THR:CB[1_554] | 1.52 | 0.68 |
| 4:5:143:TYR:CE2 | 4:8:369:ILE:C[1_554] | 1.52 | 0.68 |
| 4:5:180:LEU:CD1 | 4:8:178:LEU:O[1_554] | 1.52 | 0.68 |
| 4:6:300:SER:O | 4:9:108:ALA:N[1_554] | 1.52 | 0.68 |
| 4:6:370:VAL:N | 4:V:231:ALA:C[1_554] | 1.53 | 0.67 |
| 4:6:283:MET:CG | 4:9:286:ASP:N[1_554] | 1.53 | 0.67 |
| 4:4:308:GLY:N | 4:7:339:VAL:CA[1_554] | 1.53 | 0.67 |
| 4:5:113:LYS:CB | 4:9:252:ASN:CA[1_554] | 1.53 | 0.67 |
| 4:6:309:ILE:CG2 | 4:9:339:VAL:CG2[1_554] | 1.53 | 0.67 |
| 4:5:314:GLN:CG | 4:8:142:LEU:O[1_554] | 1.53 | 0.67 |
| 4:5:166:TYR:CB | 4:V:40:HIS:CE1[1_554] | 1.53 | 0.67 |
| 4:6:319:ALA:CB | 4:9:295:ALA:CA[1_554] | 1.53 | 0.67 |
| 4:6:191:LYS:N | 4:9:186:THR:C[1_554] | 1.53 | 0.67 |
| 4:6:115:ASN:CA | 4:V:196:ARG:NE[1_554] | 1.53 | 0.67 |
| 4:4:196:ARG:N | 4:7:209:VAL:C[1_554] | 1.53 | 0.67 |
| 4:4:137:GLN:OE1 | 4:7:112:PRO:CB[1_554] | 1.53 | 0.67 |
| 4:5:267:ILE:CB | 4:8:180:LEU:CB[1_554] | 1.53 | 0.67 |
| 4:6:59:GLN:OE1 | 4:9:67:LEU:O[1_554] | 1.53 | 0.67 |
| 4:6:25:ASP:N | 4:9:124:PHE:CA[1_554] | 1.53 | 0.67 |
| 4:4:219:VAL:CG1 | 4:7:300:SER:CB[1_554] | 1.53 | 0.67 |
| 4:5:274:ILE:CB | 4:8:162:ASN:N[1_554] | 1.53 | 0.67 |
| 4:6:335:ARG:N | 4:9:106:THR:N[1_554] | 1.53 | 0.67 |
| 4:4:321:ALA:CB | 4:7:149:THR:CG2[1_554] | 1.53 | 0.67 |
| 4:3:109:PRO:CB | 4:7:195:GLU:CG[1_554] | 1.53 | 0.67 |
| 4:5:17:VAL:C | 4:8:79:TRP:CB[1_554] | 1.53 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:30:VAL:CA | 4:9:79:TRP:O[1_554] | 1.53 | 0.67 |
| 4:4:300:SER:CA | 4:7:107:GLU:CB[1_554] | 1.53 | 0.67 |
| 4:4:327:ILE:CA | 4:7:167:GLU:C[1_554] | 1.53 | 0.67 |
| 4:6:110:LEU:N | 4:V:195:GLU:OE1[1_554] | 1.53 | 0.67 |
| 4:5:180:LEU:CD2 | 4:8:178:LEU:CB[1_554] | 1.53 | 0.67 |
| 4:5:320:LEU:CA | 4:8:293:LEU:C[1_554] | 1.53 | 0.67 |
| 4:6:158:GLY:N | 4:9:72:GLU:O[1_554] | 1.53 | 0.67 |
| 4:6:166:TYR:OH | 4:W:40:HIS:N[1_554] | 1.53 | 0.67 |
| 4:5:140:LEU:CD1 | 4:8:113:LYS:O[1_554] | 1.53 | 0.67 |
| 4:6:345:ILE:CG2 | 4:9:369:ILE:CB[1_554] | 1.53 | 0.67 |
| 4:5:304:THR:CA | 4:8:137:GLN:CD[1_554] | 1.53 | 0.67 |
| 4:5:59:GLN:CB | 4:8:68:LYS:CE[1_554] | 1.53 | 0.67 |
| 4:6:280:ASN:CG | 4:9:281:SER:C[1_554] | 1.53 | 0.67 |
| 4:3:368:SER:N | 4:7:236:LEU:CB[1_554] | 1.53 | 0.67 |
| 4:5:151:ILE:CG2 | 4:8:170:ALA:O[1_554] | 1.53 | 0.67 |
| 4:4:314:GLN:C | 4:7:142:LEU:CD2[1_554] | 1.53 | 0.67 |
| 4:4:311:ASP:C | 4:7:142:LEU:N[1_554] | 1.53 | 0.67 |
| 4:6:289:ILE:N | 4:W:64:ILE:N[1_554] | 1.53 | 0.67 |
| 4:6:166:TYR:CG | 4:W:40:HIS:CD2[1_554] | 1.53 | 0.67 |
| 4:4:191:LYS:CA | 4:7:186:THR:CA[1_554] | 1.53 | 0.67 |
| 4:5:207:GLU:CD | 4:8:67:LEU:CB[1_554] | 1.53 | 0.67 |
| 4:5:340:TRP:CH2 | 4:8:121:GLN:CA[1_554] | 1.53 | 0.67 |
| 4:5:139:VAL:O | 4:8:371:HIS:O[1_554] | 1.53 | 0.67 |
| 4:5:295:ALA:C | 4:8:167:GLU:C[1_554] | 1.53 | 0.67 |
| 4:4:300:SER:N | 4:7:107:GLU:CD[1_554] | 1.53 | 0.67 |
| 4:6:193:LEU:O | 4:9:209:VAL:O[1_554] | 1.53 | 0.67 |
| 4:4:193:LEU:CD2 | 4:7:210:ARG:NE[1_554] | 1.53 | 0.67 |
| 4:6:197:GLY:N | 4:9:212:ILE:CD1[1_554] | 1.53 | 0.67 |
| 4:6:208:ILE:CG2 | 4:9:59:GLN:CG[1_554] | 1.53 | 0.67 |
| 4:5:31:PHE:CG | 4:8:80:ASP:CB[1_554] | 1.53 | 0.67 |
| 4:5:275:HIS:O | 4:8:151:ILE:CG1[1_554] | 1.53 | 0.67 |
| 4:6:335:ARG:CA | 4:9:105:LEU:C[1_554] | 1.53 | 0.67 |
| 4:5:314:GLN:CD | 4:8:147:ARG:O[1_554] | 1.53 | 0.67 |
| 4:6:187:ASP:C | 4:9:183:ARG:O[1_554] | 1.53 | 0.67 |
| 4:3:326:LYS:CD | 4:8:44:MET:CA[1_554] | 1.53 | 0.67 |
| 4:6:24:ASP:CA | 4:9:124:PHE:CB[1_554] | 1.53 | 0.67 |
| 4:6:205:GLU:OE2 | 4:7:288:ASP:CG[1_554] | 1.53 | 0.67 |
| 4:6:296:ASN:N | 4:9:169:TYR:N[1_554] | 1.53 | 0.67 |
| 4:3:172:PRO:C | 4:7:266:PHE:O[1_554] | 1.53 | 0.67 |
| 4:4:305:MET:CB | 4:7:12:ASN:N[1_554] | 1.53 | 0.67 |
| 4:4:192:ILE:CG1 | 4:7:213:LYS:CE[1_554] | 1.53 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:318:THR:OG1 | 4:7:149:THR:O[1_554] | 1.53 | 0.67 |
| 4:4:261:LEU:O | 4:7:161:HIS:O[1_554] | 1.53 | 0.67 |
| 4:4:178:LEU:CB | 4:7:177:ARG:CB[1_554] | 1.53 | 0.67 |
| 4:6:193:LEU:CG | 4:9:210:ARG:CG[1_554] | 1.53 | 0.67 |
| 4:4:345:ILE:CA | 4:7:366:GLY:CA[1_554] | 1.53 | 0.67 |
| 4:6:273:GLY:N | 4:9:277:THR:CG2[1_554] | 1.54 | 0.66 |
| 4:6:215:LYS:CG | 4:9:31:PHE:CA[1_554] | 1.54 | 0.66 |
| 4:6:270:GLU:N | 4:9:272:ALA:N[1_554] | 1.54 | 0.66 |
| 4:4:160:THR:N | 4:7:177:ARG:NH1[1_554] | 1.54 | 0.66 |
| 4:6:349:LEU:N | 4:9:365:ALA:C[1_554] | 1.54 | 0.66 |
| 4:6:288:ASP:N | 4:W:63:GLY:CA[1_554] | 1.54 | 0.66 |
| 4:4:210:ARG:CA | 4:7:69:TYR:CE2[1_554] | 1.54 | 0.66 |
| 4:6:321:ALA:C | 4:9:292:ASP:CB[1_554] | 1.54 | 0.66 |
| 4:6:277:THR:CA | 4:9:174:ALA:O[1_554] | 1.54 | 0.66 |
| 4:6:312:ARG:N | 4:9:298:VAL:CG1[1_554] | 1.54 | 0.66 |
| 4:3:284:LYS:C | 4:7:268:GLY:C[1_554] | 1.54 | 0.66 |
| 4:5:205:GLU:CD | 4:8:203:THR:OG1[1_554] | 1.54 | 0.66 |
| 4:6:336:LYS:CE | 4:9:10:CYS:SG[1_554] | 1.54 | 0.66 |
| 4:5:322:PRO:O | 4:8:292:ASP:OD2[1_554] | 1.54 | 0.66 |
| 4:4:159:VAL:O | 4:7:177:ARG:NH1[1_554] | 1.54 | 0.66 |
| 4:4:270:GLU:O | 4:7:272:ALA:CB[1_554] | 1.54 | 0.66 |
| 4:5:253:GLU:CG | 4:8:214:GLU:N[1_554] | 1.54 | 0.66 |
| 4:6:31:PHE:CB | 4:9:80:ASP:CA[1_554] | 1.54 | 0.66 |
| 4:5:318:THR:CB | 4:8:296:ASN:CG[1_554] | 1.54 | 0.66 |
| 4:3:110:LEU:C | 4:7:192:ILE:CA[1_554] | 1.54 | 0.66 |
| 4:4:325:MET:C | 4:7:167:GLU:CD[1_554] | 1.54 | 0.66 |
| 4:4:256:ARG:CA | 4:7:302:GLY:C[1_554] | 1.54 | 0.66 |
| 4:5:185:LEU:C | 4:8:157:ASP:C[1_554] | 1.54 | 0.66 |
| 4:6:278:THR:C | 4:9:164:PRO:CG[1_554] | 1.54 | 0.66 |
| 4:6:156:GLY:O | 4:9:73:HIS:C[1_554] | 1.54 | 0.66 |
| 4:4:337:TYR:N | 4:7:119:MET:CB[1_554] | 1.54 | 0.66 |
| 4:4:275:HIS:ND1 | 4:7:152:VAL:O[1_554] | 1.54 | 0.66 |
| 4:5:215:LYS:CD | 4:8:30:VAL:O[1_554] | 1.54 | 0.66 |
| 4:4:266:PHE:CE2 | 4:7:303:THR:O[1_554] | 1.54 | 0.66 |
| 4:6:299:MET:C | 4:9:136:ILE:N[1_554] | 1.54 | 0.66 |
| 4:5:167:GLU:OE2 | 4:V:40:HIS:C[1_554] | 1.54 | 0.66 |
| 4:4:315:LYS:CD | 4:7:147:ARG:CD[1_554] | 1.54 | 0.66 |
| 4:5:263:GLN:O | 4:8:274:ILE:CD1[1_554] | 1.54 | 0.66 |
| 4:6:340:TRP:CE3 | 4:9:120:THR:CA[1_554] | 1.54 | 0.66 |
| 4:4:32:PRO:CD | 4:7:78:ASN:ND2[1_554] | 1.54 | 0.66 |
| 4:5:275:HIS:C | 4:8:151:ILE:CG1[1_554] | 1.54 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:345:ILE:CG1 | 4:9:357:ILE:CG2[1_554] | 1.54 | 0.66 |
| 4:5:21:PHE:CB | 4:8:125:GLU:CD[1_554] | 1.54 | 0.66 |
| 4:5:150:GLY:CA | 4:8:169:TYR:CD1[1_554] | 1.54 | 0.66 |
| 4:6:312:ARG:CD | 4:9:299:MET:CB[1_554] | 1.54 | 0.66 |
| 4:6:195:GLU:N | 4:9:209:VAL:CG2[1_554] | 1.54 | 0.66 |
| 4:5:276:GLU:OE1 | 4:8:280:ASN:N[1_554] | 1.54 | 0.66 |
| 4:4:181:ALA:C | 4:7:73:HIS:CA[1_554] | 1.54 | 0.66 |
| 4:5:151:ILE:CA | 4:8:170:ALA:O[1_554] | 1.54 | 0.66 |
| 4:3:372:ARG:O | 4:7:255:PHE:CE1[1_554] | 1.54 | 0.66 |
| 4:5:192:ILE:CB | 4:8:213:LYS:CG[1_554] | 1.54 | 0.66 |
| 4:4:142:LEU:N | 4:7:371:HIS:O[1_554] | 1.54 | 0.66 |
| 4:4:287:ILE:O | 4:9:63:GLY:N[1_554] | 1.54 | 0.66 |
| 4:6:316:GLU:CD | 4:9:297:ASN:ND2[1_554] | 1.54 | 0.66 |
| 4:5:191:LYS:O | 4:8:186:THR:O[1_554] | 1.54 | 0.66 |
| 4:4:335:ARG:CG | 4:7:106:THR:O[1_554] | 1.54 | 0.66 |
| 4:6:75:ILE:O | 4:V:197:GLY:C[1_554] | 1.54 | 0.66 |
| 4:3:110:LEU:C | 4:7:192:ILE:O[1_554] | 1.54 | 0.66 |
| 4:4:299:MET:CG | 4:7:136:ILE:CA[1_554] | 1.54 | 0.66 |
| 4:5:211:ASP:CB | 4:8:32:PRO:CA[1_554] | 1.54 | 0.66 |
| 4:6:282:ILE:CG1 | 4:9:171:LEU:CD2[1_554] | 1.54 | 0.66 |
| 4:6:301:GLY:CA | 4:9:108:ALA:N[1_554] | 1.54 | 0.66 |
| 4:5:75:ILE:O | 4:9:197:GLY:C[1_554] | 1.54 | 0.66 |
| 4:4:161:HIS:O | 4:7:110:LEU:CB[1_554] | 1.54 | 0.66 |
| 4:4:253:GLU:OE1 | 4:7:214:GLU:CG[1_554] | 1.54 | 0.66 |
| 4:5:273:GLY:CA | 4:8:162:ASN:CG[1_554] | 1.54 | 0.66 |
| 4:6:339:VAL:O | 4:9:117:GLU:N[1_554] | 1.54 | 0.66 |
| 4:3:111:ASN:CG | 4:7:196:ARG:CB[1_554] | 1.54 | 0.66 |
| 4:6:31:PHE:CG | 4:9:80:ASP:CB[1_554] | 1.55 | 0.65 |
| 4:5:115:ASN:OD1 | 4:9:196:ARG:NE[1_554] | 1.55 | 0.65 |
| 4:4:188:TYR:CA | 4:7:183:ARG:CA[1_554] | 1.55 | 0.65 |
| 4:4:76:ILE:C | 4:8:198:TYR:CE1[1_554] | 1.55 | 0.65 |
| 4:4:153:LEU:O | 4:7:108:ALA:O[1_554] | 1.55 | 0.65 |
| 4:5:283:MET:CE | 4:8:286:ASP:O[1_554] | 1.55 | 0.65 |
| 4:5:221:LEU:O | 4:8:332:PRO:N[1_554] | 1.55 | 0.65 |
| 4:5:178:LEU:CD2 | 4:8:177:ARG:CA[1_554] | 1.55 | 0.65 |
| 4:5:21:PHE:O | 4:8:125:GLU:CG[1_554] | 1.55 | 0.65 |
| 4:5:266:PHE:N | 4:8:261:LEU:C[1_554] | 1.55 | 0.65 |
| 4:6:188:TYR:C | 4:9:182:GLY:C[1_554] | 1.55 | 0.65 |
| 4:4:188:TYR:N | 4:7:183:ARG:CA[1_554] | 1.55 | 0.65 |
| 4:3:173:HIS:N | 4:7:266:PHE:O[1_554] | 1.55 | 0.65 |
| 4:6:31:PHE:CB | 4:9:80:ASP:C[1_554] | 1.55 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:104:LEU:CD2 | 4:9:117:GLU:OE1[1_554] | 1.55 | 0.65 |
| 4:3:368:SER:N | 4:7:236:LEU:CA[1_554] | 1.55 | 0.65 |
| 4:6:270:GLU:CB | 4:9:272:ALA:CA[1_554] | 1.55 | 0.65 |
| 4:4:279:TYR:CB | 4:7:164:PRO:CB[1_554] | 1.55 | 0.65 |
| 4:5:299:MET:SD | 4:8:138:ALA:C[1_554] | 1.55 | 0.65 |
| 4:6:211:ASP:CB | 4:9:32:PRO:CA[1_554] | 1.55 | 0.65 |
| 4:4:368:SER:N | 4:8:236:LEU:N[1_554] | 1.55 | 0.65 |
| 4:5:344:SER:C | 4:8:362:TYR:CD1[1_554] | 1.55 | 0.65 |
| 4:6:200:PHE:CB | 4:9:206:ARG:CD[1_554] | 1.55 | 0.65 |
| 4:5:221:LEU:CD2 | 4:8:332:PRO:CB[1_554] | 1.55 | 0.65 |
| 4:4:243:PRO:CD | 4:7:59:GLN:C[1_554] | 1.55 | 0.65 |
| 4:6:18:LYS:CE | 4:9:79:TRP:CH2[1_554] | 1.55 | 0.65 |
| 4:5:257:CYS:C | 4:8:303:THR:OG1[1_554] | 1.55 | 0.65 |
| 4:6:299:MET:CA | 4:9:136:ILE:C[1_554] | 1.55 | 0.65 |
| 4:3:284:LYS:O | 4:7:269:MET:N[1_554] | 1.55 | 0.65 |
| 4:5:11:ASP:O | 4:8:79:TRP:NE1[1_554] | 1.55 | 0.65 |
| 4:4:253:GLU:OE2 | 4:7:214:GLU:OE1[1_554] | 1.55 | 0.65 |
| 4:5:186:THR:N | 4:8:157:ASP:O[1_554] | 1.55 | 0.65 |
| 4:5:349:LEU:CD2 | 4:8:365:ALA:CB[1_554] | 1.55 | 0.65 |
| 4:4:117:GLU:C | 4:8:237:GLU:CD[1_554] | 1.55 | 0.65 |
| 4:3:173:HIS:CE1 | 4:7:265:SER:C[1_554] | 1.55 | 0.65 |
| 4:3:367:PRO:C | 4:7:236:LEU:N[1_554] | 1.55 | 0.65 |
| 4:2:324:THR:N | 4:7:44:MET:SD[1_554] | 1.55 | 0.65 |
| 4:6:180:LEU:CG | 4:9:178:LEU:C[1_554] | 1.55 | 0.65 |
| 4:4:336:LYS:NZ | 4:7:86:TRP:NE1[1_554] | 1.55 | 0.65 |
| 4:6:325:MET:CG | 4:9:166:TYR:CZ[1_554] | 1.55 | 0.65 |
| 4:6:340:TRP:CD1 | 4:9:119:MET:N[1_554] | 1.55 | 0.65 |
| 4:5:31:PHE:CB | 4:8:80:ASP:CA[1_554] | 1.55 | 0.65 |
| 4:6:21:PHE:CB | 4:9:125:GLU:CD[1_554] | 1.55 | 0.65 |
| 4:4:180:LEU:CB | 4:7:179:ASP:N[1_554] | 1.55 | 0.65 |
| 4:6:30:VAL:CB | 4:9:82:MET:C[1_554] | 1.55 | 0.65 |
| 4:5:137:GLN:N | 4:8:113:LYS:CA[1_554] | 1.55 | 0.65 |
| 4:6:183:ARG:CG | 4:9:72:GLU:OE2[1_554] | 1.55 | 0.65 |
| 4:6:227:MET:CG | 4:9:306:TYR:O[1_554] | 1.55 | 0.65 |
| 4:5:266:PHE:CD2 | 4:8:261:LEU:CG[1_554] | 1.55 | 0.65 |
| 4:5:156:GLY:CA | 4:8:74:GLY:O[1_554] | 1.55 | 0.65 |
| 4:6:180:LEU:C | 4:9:159:VAL:CG1[1_554] | 1.55 | 0.65 |
| 4:5:196:ARG:CD | 4:8:212:ILE:N[1_554] | 1.55 | 0.65 |
| 4:5:320:LEU:C | 4:8:293:LEU:N[1_554] | 1.55 | 0.65 |
| 4:4:336:LYS:CG | 4:7:86:TRP:CZ2[1_554] | 1.55 | 0.65 |
| 4:5:280:ASN:ND2 | 4:8:281:SER:O[1_554] | 1.55 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:211:ASP:O | 4:7:32:PRO:C[1_554] | 1.55 | 0.65 |
| 4:6:333:PRO:CA | 4:9:104:LEU:CD2[1_554] | 1.55 | 0.65 |
| 4:6:140:LEU:CD1 | 4:9:113:LYS:O[1_554] | 1.55 | 0.65 |
| 4:5:194:THR:CA | 4:8:209:VAL:CG2[1_554] | 1.55 | 0.65 |
| 4:5:300:SER:O | 4:8:108:ALA:CA[1_554] | 1.55 | 0.65 |
| 1:D:637:LYS:CE | 4:6:311:ASP:OD1[1_556] | 1.55 | 0.65 |
| 4:5:312:ARG:CD | 4:8:299:MET:CB[1_554] | 1.55 | 0.65 |
| 4:6:188:TYR:O | 4:9:182:GLY:O[1_554] | 1.55 | 0.65 |
| 4:5:24:ASP:CA | 4:8:124:PHE:CB[1_554] | 1.55 | 0.65 |
| 4:5:156:GLY:CA | 4:8:75:ILE:N[1_554] | 1.55 | 0.65 |
| 4:3:289:ILE:CG2 | 4:8:39:ARG:CZ[1_554] | 1.55 | 0.65 |
| 4:5:183:ARG:NE | 4:8:72:GLU:OE2[1_554] | 1.55 | 0.65 |
| 4:6:282:ILE:CD1 | 4:9:171:LEU:CG[1_554] | 1.55 | 0.65 |
| 4:6:314:GLN:CA | 4:9:142:LEU:CG[1_554] | 1.56 | 0.64 |
| 4:3:367:PRO:CD | 4:7:235:SER:CB[1_554] | 1.56 | 0.64 |
| 4:4:287:ILE:C | 4:9:63:GLY:CA[1_554] | 1.56 | 0.64 |
| 4:5:219:VAL:O | 4:8:335:ARG:CA[1_554] | 1.56 | 0.64 |
| 4:4:145:SER:OG | 4:7:372:ARG:CZ[1_554] | 1.56 | 0.64 |
| 4:5:249:THR:O | 4:8:211:ASP:CB[1_554] | 1.56 | 0.64 |
| 4:5:28:ARG:CB | 4:8:126:THR:CB[1_554] | 1.56 | 0.64 |
| 4:4:293:LEU:C | 4:7:169:TYR:CB[1_554] | 1.56 | 0.64 |
| 4:6:278:THR:CG2 | 4:9:164:PRO:CA[1_554] | 1.56 | 0.64 |
| 4:4:311:ASP:CB | 4:7:144:ALA:CB[1_554] | 1.56 | 0.64 |
| 1:A:637:LYS:CE | 4:5:311:ASP:CB[1_556] | 1.56 | 0.64 |
| 4:6:200:PHE:CZ | 4:9:207:GLU:O[1_554] | 1.56 | 0.64 |
| 4:5:330:ILE:N | 4:8:139:VAL:CG1[1_554] | 1.56 | 0.64 |
| 4:5:32:PRO:CD | 4:8:81:ASP:CG[1_554] | 1.56 | 0.64 |
| 4:5:16:LEU:CA | 4:8:78:ASN:N[1_554] | 1.56 | 0.64 |
| 4:6:137:GLN:CB | 4:9:112:PRO:CA[1_554] | 1.56 | 0.64 |
| 4:6:157:ASP:OD1 | 4:9:72:GLU:CA[1_554] | 1.56 | 0.64 |
| 4:4:199:SER:C | 4:7:206:ARG:CB[1_554] | 1.56 | 0.64 |
| 4:5:112:PRO:CA | 4:9:253:GLU:CD[1_554] | 1.56 | 0.64 |
| 4:4:191:LYS:CA | 4:7:186:THR:CB[1_554] | 1.56 | 0.64 |
| 4:4:113:LYS:CB | 4:8:254:ARG:N[1_554] | 1.56 | 0.64 |
| 4:5:255:PHE:O | 4:8:303:THR:C[1_554] | 1.56 | 0.64 |
| 4:6:162:ASN:OD1 | 4:9:175:ILE:CG2[1_554] | 1.56 | 0.64 |
| 4:6:33:SER:OG | 4:9:77:THR:O[1_554] | 1.56 | 0.64 |
| 4:5:173:HIS:ND1 | 4:9:265:SER:C[1_554] | 1.56 | 0.64 |
| 4:4:180:LEU:O | 4:7:159:VAL:CG1[1_554] | 1.56 | 0.64 |
| 4:6:166:TYR:CD1 | 4:W:40:HIS:CE1[1_554] | 1.56 | 0.64 |
| 4:5:193:LEU:CD2 | 4:8:210:ARG:NE[1_554] | 1.56 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:210:ARG:O | 4:9:15:GLY:C[1_554] | 1.56 | 0.64 |
| 4:6:294:TYR:N | 4:9:166:TYR:O[1_554] | 1.56 | 0.64 |
| 4:5:191:LYS:N | 4:8:186:THR:C[1_554] | 1.56 | 0.64 |
| 4:2:326:LYS:CD | 4:7:42:GLY:CA[1_554] | 1.56 | 0.64 |
| 4:4:142:LEU:C | 4:7:372:ARG:N[1_554] | 1.56 | 0.64 |
| 4:4:262:PHE:CD2 | 4:7:154:ASP:CA[1_554] | 1.56 | 0.64 |
| 4:5:219:VAL:CG1 | 4:8:300:SER:N[1_554] | 1.56 | 0.64 |
| 4:6:219:VAL:CB | 4:9:300:SER:C[1_554] | 1.56 | 0.64 |
| 4:4:330:ILE:CG2 | 4:7:133:TYR:OH[1_554] | 1.56 | 0.64 |
| 4:5:140:LEU:CA | 4:8:371:HIS:CG[1_554] | 1.56 | 0.64 |
| 4:4:338:SER:O | 4:7:116:ARG:O[1_554] | 1.56 | 0.64 |
| 4:5:309:ILE:O | 4:8:141:SER:CB[1_554] | 1.56 | 0.64 |
| 4:4:220:ALA:CA | 4:7:335:ARG:O[1_554] | 1.56 | 0.64 |
| 4:5:297:ASN:ND2 | 4:8:165:ILE:CG1[1_554] | 1.56 | 0.64 |
| 4:5:208:ILE:CG2 | 4:8:59:GLN:CG[1_554] | 1.56 | 0.64 |
| 4:3:291:LYS:NZ | 4:8:64:ILE:O[1_554] | 1.56 | 0.64 |
| 4:3:75:ILE:C | 4:7:197:GLY:O[1_554] | 1.56 | 0.64 |
| 4:6:155:SER:N | 4:9:108:ALA:C[1_554] | 1.56 | 0.64 |
| 4:4:308:GLY:CA | 4:7:339:VAL:CA[1_554] | 1.56 | 0.64 |
| 4:6:140:LEU:CD2 | 4:9:371:HIS:CB[1_554] | 1.56 | 0.64 |
| 4:6:194:THR:C | 4:9:209:VAL:CB[1_554] | 1.56 | 0.64 |
| 4:6:113:LYS:O | 4:V:252:ASN:CG[1_554] | 1.56 | 0.64 |
| 4:5:338:SER:CA | 4:8:134:VAL:CB[1_554] | 1.56 | 0.64 |
| 4:4:18:LYS:CE | 4:7:79:TRP:CZ2[1_554] | 1.56 | 0.64 |
| 4:6:185:LEU:CA | 4:9:157:ASP:C[1_554] | 1.56 | 0.64 |
| 4:6:276:GLU:N | 4:9:151:ILE:CD1[1_554] | 1.56 | 0.64 |
| 4:4:243:PRO:CG | 4:7:61:LYS:N[1_554] | 1.56 | 0.64 |
| 4:5:195:GLU:OE1 | 4:8:257:CYS:SG[1_554] | 1.56 | 0.64 |
| 4:4:186:THR:OG1 | 4:7:183:ARG:CZ[1_554] | 1.56 | 0.64 |
| 4:6:221:LEU:CB | 4:9:332:PRO:N[1_554] | 1.56 | 0.64 |
| 4:6:286:ASP:CG | 4:V:270:GLU:OE1[1_554] | 1.56 | 0.64 |
| 4:5:277:THR:C | 4:8:174:ALA:O[1_554] | 1.56 | 0.64 |
| 4:5:278:THR:OG1 | 4:8:164:PRO:N[1_554] | 1.56 | 0.64 |
| 4:6:180:LEU:N | 4:9:179:ASP:OD1[1_554] | 1.56 | 0.64 |
| 4:5:75:ILE:CG1 | 4:9:194:THR:C[1_554] | 1.56 | 0.64 |
| 4:4:189:LEU:CB | 4:7:157:ASP:OD1[1_554] | 1.56 | 0.64 |
| 4:4:357:ILE:CB | 4:8:232:SER:C[1_554] | 1.56 | 0.64 |
| 4:5:300:SER:O | 4:8:107:GLU:C[1_554] | 1.56 | 0.64 |
| 4:5:341:ILE:C | 4:8:370:VAL:CG1[1_554] | 1.56 | 0.64 |
| 4:4:357:ILE:CG2 | 4:8:232:SER:CA[1_554] | 1.56 | 0.64 |
| 4:6:16:LEU:CD1 | 4:9:70:PRO:CB[1_554] | 1.56 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:114:ALA:C | 4:7:250:ILE:N[1_554] | 1.56 | 0.64 |
| 4:6:56:ASP:CA | 4:9:37:ARG:NH1[1_554] | 1.56 | 0.64 |
| 4:5:338:SER:CB | 4:8:134:VAL:CB[1_554] | 1.56 | 0.64 |
| 4:5:174:ALA:C | 4:8:173:HIS:CB[1_554] | 1.56 | 0.64 |
| 4:5:200:PHE:CB | 4:8:206:ARG:CG[1_554] | 1.56 | 0.64 |
| 4:4:282:ILE:CD1 | 4:7:171:LEU:CD2[1_554] | 1.56 | 0.64 |
| 4:5:59:GLN:CG | 4:8:68:LYS:CB[1_554] | 1.56 | 0.64 |
| 4:5:218:TYR:CD1 | 4:8:336:LYS:CG[1_554] | 1.56 | 0.64 |
| 4:4:335:ARG:CD | 4:7:107:GLU:N[1_554] | 1.57 | 0.63 |
| 4:5:166:TYR:OH | 4:V:40:HIS:N[1_554] | 1.57 | 0.63 |
| 4:6:32:PRO:N | 4:9:78:ASN:ND2[1_554] | 1.57 | 0.63 |
| 4:5:106:THR:CG2 | 4:8:114:ALA:O[1_554] | 1.57 | 0.63 |
| 4:3:326:LYS:CD | 4:8:44:MET:C[1_554] | 1.57 | 0.63 |
| 4:6:218:TYR:CG | 4:9:336:LYS:CB[1_554] | 1.57 | 0.63 |
| 4:6:198:TYR:CE1 | 4:9:208:ILE:CB[1_554] | 1.57 | 0.63 |
| 4:4:262:PHE:CB | 4:7:153:LEU:CA[1_554] | 1.57 | 0.63 |
| 4:6:318:THR:C | 4:9:292:ASP:O[1_554] | 1.57 | 0.63 |
| 4:6:112:PRO:C | 4:V:253:GLU:OE2[1_554] | 1.57 | 0.63 |
| 4:6:321:ALA:N | 4:9:292:ASP:C[1_554] | 1.57 | 0.63 |
| 4:5:75:ILE:C | 4:9:197:GLY:CA[1_554] | 1.57 | 0.63 |
| 4:6:274:ILE:CB | 4:9:161:HIS:O[1_554] | 1.57 | 0.63 |
| 4:3:115:ASN:ND2 | 4:7:198:TYR:CE2[1_554] | 1.57 | 0.63 |
| 4:5:186:THR:CB | 4:8:183:ARG:CZ[1_554] | 1.57 | 0.63 |
| 4:6:320:LEU:N | 4:9:294:TYR:N[1_554] | 1.57 | 0.63 |
| 4:5:210:ARG:O | 4:8:15:GLY:C[1_554] | 1.57 | 0.63 |
| 4:6:187:ASP:CA | 4:9:183:ARG:CG[1_554] | 1.57 | 0.63 |
| 4:3:76:ILE:C | 4:7:198:TYR:CE1[1_554] | 1.57 | 0.63 |
| 4:6:256:ARG:C | 4:9:303:THR:CA[1_554] | 1.57 | 0.63 |
| 4:5:272:ALA:CA | 4:8:277:THR:CB[1_554] | 1.57 | 0.63 |
| 4:6:259:GLU:OE2 | 4:9:309:ILE:CG2[1_554] | 1.57 | 0.63 |
| 4:5:256:ARG:C | 4:8:303:THR:CA[1_554] | 1.57 | 0.63 |
| 4:6:198:TYR:CB | 4:9:208:ILE:C[1_554] | 1.57 | 0.63 |
| 4:6:113:LYS:C | 4:V:252:ASN:N[1_554] | 1.57 | 0.63 |
| 4:5:196:ARG:O | 4:8:212:ILE:CB[1_554] | 1.57 | 0.63 |
| 4:5:194:THR:C | 4:8:209:VAL:CB[1_554] | 1.57 | 0.63 |
| 4:6:368:SER:O | 4:V:230:ALA:CA[1_554] | 1.57 | 0.63 |
| 4:5:320:LEU:O | 4:8:290:ARG:C[1_554] | 1.57 | 0.63 |
| 4:6:157:ASP:CA | 4:9:72:GLU:C[1_554] | 1.57 | 0.63 |
| 4:4:110:LEU:CD1 | 4:8:191:LYS:CB[1_554] | 1.57 | 0.63 |
| 4:4:317:ILE:O | 4:7:150:GLY:N[1_554] | 1.57 | 0.63 |
| 4:5:215:LYS:CG | 4:8:30:VAL:C[1_554] | 1.57 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:346:LEU:CA | 4:8:369:ILE:N[1_554] | 1.57 | 0.63 |
| 4:5:320:LEU:N | 4:8:293:LEU:CA[1_554] | 1.57 | 0.63 |
| 4:4:214:GLU:N | 4:7:15:GLY:C[1_554] | 1.57 | 0.63 |
| 4:3:166:TYR:CZ | 4:8:39:ARG:O[1_554] | 1.57 | 0.63 |
| 4:6:112:PRO:O | 4:V:253:GLU:OE2[1_554] | 1.57 | 0.63 |
| 4:4:277:THR:OG1 | 4:7:176:MET:N[1_554] | 1.57 | 0.63 |
| 4:4:259:GLU:O | 4:7:155:SER:CB[1_554] | 1.57 | 0.63 |
| 4:4:243:PRO:N | 4:7:60:SER:C[1_554] | 1.57 | 0.63 |
| 4:3:173:HIS:CA | 4:7:267:ILE:CA[1_554] | 1.57 | 0.63 |
| 4:6:346:LEU:CD2 | 4:9:368:SER:CB[1_554] | 1.57 | 0.63 |
| 4:5:319:ALA:C | 4:8:295:ALA:N[1_554] | 1.57 | 0.63 |
| 4:4:311:ASP:CA | 4:7:140:LEU:O[1_554] | 1.57 | 0.63 |
| 4:3:111:ASN:N | 4:7:192:ILE:C[1_554] | 1.57 | 0.63 |
| 4:6:297:ASN:OD1 | 4:9:165:ILE:CA[1_554] | 1.57 | 0.63 |
| 4:4:226:GLU:CD | 4:7:333:PRO:C[1_554] | 1.57 | 0.63 |
| 4:6:331:ALA:CA | 4:9:140:LEU:CD2[1_554] | 1.57 | 0.63 |
| 4:4:267:ILE:CB | 4:7:180:LEU:CD1[1_554] | 1.57 | 0.63 |
| 4:4:309:ILE:N | 4:7:339:VAL:CB[1_554] | 1.57 | 0.63 |
| 4:4:303:THR:OG1 | 4:7:74:GLY:N[1_554] | 1.57 | 0.63 |
| 4:4:319:ALA:CB | 4:7:296:ASN:CA[1_554] | 1.57 | 0.63 |
| 4:6:295:ALA:O | 4:9:167:GLU:O[1_554] | 1.57 | 0.63 |
| 4:4:372:ARG:CA | 4:8:226:GLU:C[1_554] | 1.57 | 0.63 |
| 4:5:166:TYR:CG | 4:V:40:HIS:CG[1_554] | 1.57 | 0.63 |
| 4:4:289:ILE:CG2 | 4:9:39:ARG:NE[1_554] | 1.57 | 0.63 |
| 4:4:74:GLY:C | 4:8:198:TYR:N[1_554] | 1.57 | 0.63 |
| 4:6:347:ALA:N | 4:9:366:GLY:O[1_554] | 1.57 | 0.63 |
| 4:6:200:PHE:CB | 4:9:206:ARG:CG[1_554] | 1.57 | 0.63 |
| 4:5:340:TRP:CH2 | 4:8:121:GLN:O[1_554] | 1.57 | 0.63 |
| 4:4:282:ILE:CG2 | 4:7:171:LEU:CD2[1_554] | 1.57 | 0.63 |
| 4:4:337:TYR:N | 4:7:119:MET:CG[1_554] | 1.57 | 0.63 |
| 4:5:166:TYR:CD1 | 4:V:40:HIS:CG[1_554] | 1.57 | 0.63 |
| 4:6:166:TYR:CE1 | 4:W:40:HIS:ND1[1_554] | 1.57 | 0.63 |
| 4:6:368:SER:CA | 4:V:229:THR:O[1_554] | 1.57 | 0.63 |
| 4:6:316:GLU:OE1 | 4:9:297:ASN:ND2[1_554] | 1.57 | 0.63 |
| 4:4:223:PHE:CB | 4:7:335:ARG:CD[1_554] | 1.57 | 0.63 |
| 4:4:257:CYS:O | 4:7:156:GLY:O[1_554] | 1.57 | 0.63 |
| 4:6:314:GLN:CD | 4:9:147:ARG:O[1_554] | 1.57 | 0.63 |
| 4:5:214:GLU:N | 4:8:16:LEU:N[1_554] | 1.57 | 0.63 |
| 4:6:222:ASP:C | 4:9:331:ALA:CB[1_554] | 1.57 | 0.63 |
| 4:4:26:ALA:CA | 4:7:121:GLN:C[1_554] | 1.57 | 0.63 |
| 4:6:172:PRO:CA | 4:V:266:PHE:O[1_554] | 1.57 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:219:VAL:C | 4:8:335:ARG:CB[1_554] | 1.57 | 0.63 |
| 4:5:221:LEU:CA | 4:8:332:PRO:N[1_554] | 1.57 | 0.63 |
| 4:6:167:GLU:OE2 | 4:W:41:GLN:CA[1_554] | 1.57 | 0.63 |
| 4:4:215:LYS:N | 4:7:17:VAL:N[1_554] | 1.58 | 0.62 |
| 4:4:315:LYS:CD | 4:7:147:ARG:CG[1_554] | 1.58 | 0.62 |
| 4:6:277:THR:O | 4:9:174:ALA:O[1_554] | 1.58 | 0.62 |
| 4:4:367:PRO:CA | 4:8:236:LEU:N[1_554] | 1.58 | 0.62 |
| 4:6:205:GLU:CA | 4:9:62:ARG:NH2[1_554] | 1.58 | 0.62 |
| 4:6:341:ILE:C | 4:9:370:VAL:CG1[1_554] | 1.58 | 0.62 |
| 4:6:110:LEU:N | 4:V:195:GLU:OE2[1_554] | 1.58 | 0.62 |
| 4:6:204:ALA:O | 4:9:62:ARG:CD[1_554] | 1.58 | 0.62 |
| 4:5:115:ASN:CA | 4:9:196:ARG:NE[1_554] | 1.58 | 0.62 |
| 4:3:367:PRO:CA | 4:7:234:SER:C[1_554] | 1.58 | 0.62 |
| 4:6:256:ARG:CG | 4:9:306:TYR:CD1[1_554] | 1.58 | 0.62 |
| 4:6:205:GLU:OE2 | 4:9:203:THR:CG2[1_554] | 1.58 | 0.62 |
| 4:5:31:PHE:O | 4:8:78:ASN:O[1_554] | 1.58 | 0.62 |
| 4:4:218:TYR:CG | 4:7:337:TYR:CE1[1_554] | 1.58 | 0.62 |
| 4:6:28:ARG:CD | 4:9:126:THR:CA[1_554] | 1.58 | 0.62 |
| 4:6:340:TRP:CG | 4:9:119:MET:CA[1_554] | 1.58 | 0.62 |
| 4:4:222:ASP:C | 4:7:331:ALA:C[1_554] | 1.58 | 0.62 |
| 4:4:265:SER:C | 4:7:261:LEU:C[1_554] | 1.58 | 0.62 |
| 4:3:113:LYS:CD | 4:7:255:PHE:N[1_554] | 1.58 | 0.62 |
| 4:4:332:PRO:CD | 4:7:135:ALA:N[1_554] | 1.58 | 0.62 |
| 4:4:333:PRO:N | 4:7:133:TYR:O[1_554] | 1.58 | 0.62 |
| 4:6:18:LYS:CG | 4:9:79:TRP:CZ3[1_554] | 1.58 | 0.62 |
| 4:6:26:ALA:O | 4:9:123:MET:CA[1_554] | 1.58 | 0.62 |
| 4:5:326:LYS:O | 4:8:167:GLU:CG[1_554] | 1.58 | 0.62 |
| 4:4:260:THR:C | 4:7:160:THR:OG1[1_554] | 1.58 | 0.62 |
| 4:6:185:LEU:O | 4:9:157:ASP:O[1_554] | 1.58 | 0.62 |
| 4:6:257:CYS:C | 4:9:303:THR:OG1[1_554] | 1.58 | 0.62 |
| 4:5:346:LEU:CB | 4:8:368:SER:N[1_554] | 1.58 | 0.62 |
| 4:4:299:MET:CG | 4:7:136:ILE:CG2[1_554] | 1.58 | 0.62 |
| 4:3:372:ARG:CG | 4:7:227:MET:C[1_554] | 1.58 | 0.62 |
| 4:5:317:ILE:N | 4:8:150:GLY:C[1_554] | 1.58 | 0.62 |
| 4:6:278:THR:CB | 4:9:164:PRO:CA[1_554] | 1.58 | 0.62 |
| 4:3:112:PRO:CG | 4:7:193:LEU:CG[1_554] | 1.58 | 0.62 |
| 4:6:367:PRO:CD | 4:V:234:SER:C[1_554] | 1.58 | 0.62 |
| 4:4:156:GLY:N | 4:7:75:ILE:CD1[1_554] | 1.58 | 0.62 |
| 4:6:320:LEU:O | 4:9:290:ARG:C[1_554] | 1.58 | 0.62 |
| 4:5:166:TYR:OH | 4:V:39:ARG:N[1_554] | 1.58 | 0.62 |
| 4:3:288:ASP:CB | 4:8:65:LEU:O[1_554] | 1.58 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:295:ALA:O | 4:8:167:GLU:O[1_554] | 1.58 | 0.62 |
| 4:5:104:LEU:CD2 | 4:8:117:GLU:OE1[1_554] | 1.58 | 0.62 |
| 4:4:75:ILE:CA | 4:8:197:GLY:C[1_554] | 1.58 | 0.62 |
| 4:5:368:SER:O | 4:9:230:ALA:CA[1_554] | 1.58 | 0.62 |
| 4:6:227:MET:CG | 4:9:306:TYR:C[1_554] | 1.58 | 0.62 |
| 4:5:345:ILE:CG2 | 4:8:369:ILE:CG2[1_554] | 1.58 | 0.62 |
| 4:5:164:PRO:CD | 4:8:172:PRO:CB[1_554] | 1.58 | 0.62 |
| 4:6:338:SER:OG | 4:9:134:VAL:CA[1_554] | 1.58 | 0.62 |
| 4:4:320:LEU:CB | 4:7:293:LEU:CA[1_554] | 1.58 | 0.62 |
| 4:4:372:ARG:C | 4:8:255:PHE:CZ[1_554] | 1.58 | 0.62 |
| 4:5:113:LYS:CB | 4:9:252:ASN:O[1_554] | 1.58 | 0.62 |
| 4:5:196:ARG:CA | 4:8:212:ILE:CG2[1_554] | 1.58 | 0.62 |
| 4:4:336:LYS:NZ | 4:7:86:TRP:CD1[1_554] | 1.58 | 0.62 |
| 4:6:310:ALA:N | 4:9:141:SER:OG[1_554] | 1.58 | 0.62 |
| 4:4:226:GLU:OE1 | 4:7:333:PRO:CA[1_554] | 1.58 | 0.62 |
| 4:5:334:GLU:N | 4:8:104:LEU:O[1_554] | 1.58 | 0.62 |
| 4:6:106:THR:C | 4:9:114:ALA:CB[1_554] | 1.58 | 0.62 |
| 4:5:267:ILE:CD1 | 4:8:180:LEU:CA[1_554] | 1.58 | 0.62 |
| 4:4:326:LYS:CD | 4:9:44:MET:C[1_554] | 1.58 | 0.62 |
| 4:6:221:LEU:O | 4:9:332:PRO:N[1_554] | 1.58 | 0.62 |
| 4:4:371:HIS:N | 4:8:230:ALA:CA[1_554] | 1.58 | 0.62 |
| 4:5:32:PRO:O | 4:8:78:ASN:CG[1_554] | 1.58 | 0.62 |
| 4:4:188:TYR:CG | 4:7:182:GLY:N[1_554] | 1.58 | 0.62 |
| 4:6:267:ILE:CD1 | 4:9:180:LEU:CA[1_554] | 1.58 | 0.62 |
| 4:6:274:ILE:N | 4:9:162:ASN:CA[1_554] | 1.58 | 0.62 |
| 4:4:188:TYR:CD2 | 4:7:181:ALA:C[1_554] | 1.58 | 0.62 |
| 4:5:276:GLU:O | 4:8:281:SER:CB[1_554] | 1.58 | 0.62 |
| 4:5:162:ASN:ND2 | 4:8:175:ILE:CB[1_554] | 1.58 | 0.62 |
| 4:4:309:ILE:CA | 4:7:339:VAL:CG2[1_554] | 1.58 | 0.62 |
| 4:3:108:ALA:CB | 4:7:195:GLU:CA[1_554] | 1.58 | 0.62 |
| 4:6:24:ASP:OD2 | 4:9:125:GLU:N[1_554] | 1.58 | 0.62 |
| 4:6:297:ASN:O | 4:9:139:VAL:CG1[1_554] | 1.58 | 0.62 |
| 4:6:194:THR:CB | 4:9:209:VAL:CG1[1_554] | 1.58 | 0.62 |
| 4:5:110:LEU:C | 4:9:192:ILE:CA[1_554] | 1.58 | 0.62 |
| 4:5:327:ILE:C | 4:8:148:THR:CB[1_554] | 1.58 | 0.62 |
| 4:4:223:PHE:CB | 4:7:335:ARG:NE[1_554] | 1.58 | 0.62 |
| 4:4:110:LEU:C | 4:8:192:ILE:O[1_554] | 1.58 | 0.62 |
| 4:5:340:TRP:CE3 | 4:8:120:THR:CA[1_554] | 1.58 | 0.62 |
| 4:4:198:TYR:CD2 | 4:7:207:GLU:O[1_554] | 1.59 | 0.61 |
| 4:4:367:PRO:O | 4:8:236:LEU:CG[1_554] | 1.59 | 0.61 |
| 4:6:281:SER:C | 4:9:173:HIS:CD2[1_554] | 1.59 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:371:HIS:CA | 4:9:230:ALA:CB[1_554] | 1.59 | 0.61 |
| 4:3:367:PRO:CA | 4:7:236:LEU:N[1_554] | 1.59 | 0.61 |
| 4:5:227:MET:CG | 4:8:307:PRO:C[1_554] | 1.59 | 0.61 |
| 4:5:191:LYS:CG | 4:8:185:LEU:C[1_554] | 1.59 | 0.61 |
| 4:4:213:LYS:NZ | 4:7:14:SER:C[1_554] | 1.59 | 0.61 |
| 4:6:261:LEU:N | 4:9:155:SER:OG[1_554] | 1.59 | 0.61 |
| 4:6:215:LYS:N | 4:9:16:LEU:CG[1_554] | 1.59 | 0.61 |
| 4:4:278:THR:OG1 | 4:7:163:VAL:CG1[1_554] | 1.59 | 0.61 |
| 4:6:180:LEU:CD2 | 4:9:178:LEU:CB[1_554] | 1.59 | 0.61 |
| 4:4:213:LYS:CD | 4:7:14:SER:C[1_554] | 1.59 | 0.61 |
| 4:5:137:GLN:CA | 4:8:112:PRO:C[1_554] | 1.59 | 0.61 |
| 4:6:191:LYS:CB | 4:9:186:THR:C[1_554] | 1.59 | 0.61 |
| 4:5:317:ILE:CG1 | 4:8:150:GLY:N[1_554] | 1.59 | 0.61 |
| 4:4:219:VAL:O | 4:7:338:SER:N[1_554] | 1.59 | 0.61 |
| 4:5:254:ARG:NH1 | 4:8:336:LYS:NZ[1_554] | 1.59 | 0.61 |
| 4:6:137:GLN:OE1 | 4:9:112:PRO:CB[1_554] | 1.59 | 0.61 |
| 4:6:223:PHE:CZ | 4:9:304:THR:CB[1_554] | 1.59 | 0.61 |
| 4:4:255:PHE:O | 4:7:302:GLY:CA[1_554] | 1.59 | 0.61 |
| 4:5:22:ALA:CA | 4:8:362:TYR:CZ[1_554] | 1.59 | 0.61 |
| 4:4:154:ASP:OD2 | 4:7:111:ASN:O[1_554] | 1.59 | 0.61 |
| 4:6:27:PRO:N | 4:9:123:MET:N[1_554] | 1.59 | 0.61 |
| 4:6:348:SER:O | 4:9:364:GLU:C[1_554] | 1.59 | 0.61 |
| 4:6:208:ILE:CG2 | 4:9:59:GLN:CD[1_554] | 1.59 | 0.61 |
| 4:6:369:ILE:N | 4:V:229:THR:C[1_554] | 1.59 | 0.61 |
| 4:6:340:TRP:CG | 4:9:118:LYS:O[1_554] | 1.59 | 0.61 |
| 4:4:240:TYR:CG | 4:7:56:ASP:OD2[1_554] | 1.59 | 0.61 |
| 4:4:198:TYR:CG | 4:7:208:ILE:CA[1_554] | 1.59 | 0.61 |
| 4:5:191:LYS:N | 4:8:187:ASP:N[1_554] | 1.59 | 0.61 |
| 4:5:262:PHE:CG | 4:8:153:LEU:CG[1_554] | 1.59 | 0.61 |
| 4:6:367:PRO:N | 4:V:233:SER:CA[1_554] | 1.59 | 0.61 |
| 4:4:339:VAL:CB | 4:7:115:ASN:CA[1_554] | 1.59 | 0.61 |
| 4:4:192:ILE:CD1 | 4:7:213:LYS:NZ[1_554] | 1.59 | 0.61 |
| 4:4:276:GLU:OE2 | 4:7:278:THR:O[1_554] | 1.59 | 0.61 |
| 4:3:110:LEU:O | 4:7:192:ILE:C[1_554] | 1.59 | 0.61 |
| 4:3:108:ALA:N | 4:7:195:GLU:O[1_554] | 1.59 | 0.61 |
| 4:6:32:PRO:C | 4:9:78:ASN:CG[1_554] | 1.59 | 0.61 |
| 4:3:114:ALA:N | 4:7:250:ILE:C[1_554] | 1.59 | 0.61 |
| 4:6:219:VAL:CG1 | 4:9:300:SER:N[1_554] | 1.59 | 0.61 |
| 4:5:295:ALA:CA | 4:8:167:GLU:CA[1_554] | 1.59 | 0.61 |
| 4:5:151:ILE:CD1 | 4:8:171:LEU:N[1_554] | 1.59 | 0.61 |
| 4:6:106:THR:CB | 4:9:114:ALA:C[1_554] | 1.59 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:278:THR:CB | 4:9:163:VAL:C[1_554] | 1.59 | 0.61 |
| 4:5:172:PRO:CA | 4:9:266:PHE:O[1_554] | 1.59 | 0.61 |
| 4:6:113:LYS:CB | 4:V:252:ASN:CA[1_554] | 1.59 | 0.61 |
| 4:5:327:ILE:CA | 4:8:149:THR:OG1[1_554] | 1.59 | 0.61 |
| 4:5:322:PRO:CD | 4:8:289:ILE:CA[1_554] | 1.59 | 0.61 |
| 4:4:73:HIS:CD2 | 4:8:199:SER:OG[1_554] | 1.59 | 0.61 |
| 4:6:296:ASN:CA | 4:9:168:GLY:C[1_554] | 1.59 | 0.61 |
| 4:5:272:ALA:N | 4:8:277:THR:OG1[1_554] | 1.59 | 0.61 |
| 4:6:223:PHE:CE1 | 4:9:304:THR:OG1[1_554] | 1.59 | 0.61 |
| 4:5:112:PRO:C | 4:9:253:GLU:CG[1_554] | 1.59 | 0.61 |
| 4:5:274:ILE:CB | 4:8:161:HIS:O[1_554] | 1.59 | 0.61 |
| 4:6:56:ASP:CB | 4:9:37:ARG:NH2[1_554] | 1.59 | 0.61 |
| 4:5:164:PRO:N | 4:8:172:PRO:CB[1_554] | 1.59 | 0.61 |
| 4:4:306:TYR:CA | 4:7:11:ASP:OD2[1_554] | 1.59 | 0.61 |
| 4:6:274:ILE:C | 4:9:163:VAL:N[1_554] | 1.59 | 0.61 |
| 4:2:291:LYS:CD | 4:7:39:ARG:CB[1_554] | 1.59 | 0.61 |
| 4:4:311:ASP:O | 4:7:142:LEU:N[1_554] | 1.59 | 0.61 |
| 4:6:309:ILE:CB | 4:9:141:SER:OG[1_554] | 1.59 | 0.61 |
| 4:6:343:GLY:O | 4:9:367:PRO:C[1_554] | 1.59 | 0.61 |
| 4:3:111:ASN:C | 4:7:253:GLU:CG[1_554] | 1.59 | 0.61 |
| 4:5:334:GLU:CA | 4:8:104:LEU:C[1_554] | 1.59 | 0.61 |
| 4:6:178:LEU:O | 4:9:177:ARG:CB[1_554] | 1.59 | 0.61 |
| 4:6:296:ASN:C | 4:9:169:TYR:N[1_554] | 1.59 | 0.61 |
| 4:6:208:ILE:CG2 | 4:9:59:GLN:OE1[1_554] | 1.59 | 0.61 |
| 4:5:346:LEU:N | 4:8:369:ILE:N[1_554] | 1.59 | 0.61 |
| 4:5:227:MET:SD | 4:8:306:TYR:CA[1_554] | 1.59 | 0.61 |
| 4:5:154:ASP:CB | 4:8:111:ASN:N[1_554] | 1.59 | 0.61 |
| 4:5:75:ILE:CA | 4:9:198:TYR:N[1_554] | 1.59 | 0.61 |
| 4:4:185:LEU:C | 4:7:157:ASP:C[1_554] | 1.59 | 0.61 |
| 4:4:318:THR:C | 4:7:149:THR:O[1_554] | 1.59 | 0.61 |
| 4:4:75:ILE:CD1 | 4:8:193:LEU:C[1_554] | 1.59 | 0.61 |
| 4:6:166:TYR:CD1 | 4:W:40:HIS:CG[1_554] | 1.59 | 0.61 |
| 4:4:299:MET:CB | 4:7:136:ILE:CB[1_554] | 1.59 | 0.61 |
| 4:6:335:ARG:C | 4:9:106:THR:CA[1_554] | 1.59 | 0.61 |
| 4:4:26:ALA:C | 4:7:122:ILE:N[1_554] | 1.59 | 0.61 |
| 4:3:110:LEU:O | 4:7:193:LEU:N[1_554] | 1.60 | 0.60 |
| 4:6:281:SER:CB | 4:9:174:ALA:N[1_554] | 1.60 | 0.60 |
| 4:6:326:LYS:CB | 4:9:167:GLU:OE1[1_554] | 1.60 | 0.60 |
| 4:5:157:ASP:O | 4:8:72:GLU:C[1_554] | 1.60 | 0.60 |
| 4:6:346:LEU:N | 4:9:369:ILE:N[1_554] | 1.60 | 0.60 |
| 4:6:150:GLY:CA | 4:9:169:TYR:CD1[1_554] | 1.60 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:372:ARG:N | 4:7:226:GLU:O[1_554] | 1.60 | 0.60 |
| 4:4:313:MET:CG | 4:7:138:ALA:CA[1_554] | 1.60 | 0.60 |
| 4:6:11:ASP:O | 4:9:79:TRP:NE1[1_554] | 1.60 | 0.60 |
| 4:3:286:ASP:N | 4:7:270:GLU:CD[1_554] | 1.60 | 0.60 |
| 4:4:326:LYS:CA | 4:7:167:GLU:CD[1_554] | 1.60 | 0.60 |
| 4:4:19:ALA:N | 4:7:118:LYS:NZ[1_554] | 1.60 | 0.60 |
| 4:4:332:PRO:O | 4:7:105:LEU:C[1_554] | 1.60 | 0.60 |
| 4:4:327:ILE:C | 4:7:168:GLY:N[1_554] | 1.60 | 0.60 |
| 4:4:173:HIS:O | 4:8:267:ILE:C[1_554] | 1.60 | 0.60 |
| 4:4:161:HIS:C | 4:7:110:LEU:CD1[1_554] | 1.60 | 0.60 |
| 4:6:154:ASP:CA | 4:9:109:PRO:CA[1_554] | 1.60 | 0.60 |
| 4:6:259:GLU:CB | 4:9:304:THR:CA[1_554] | 1.60 | 0.60 |
| 4:6:261:LEU:CG | 4:9:154:ASP:O[1_554] | 1.60 | 0.60 |
| 4:6:326:LYS:O | 4:9:167:GLU:CG[1_554] | 1.60 | 0.60 |
| 4:6:317:ILE:CA | 4:9:150:GLY:CA[1_554] | 1.60 | 0.60 |
| 4:4:369:ILE:CG2 | 4:8:234:SER:N[1_554] | 1.60 | 0.60 |
| 4:5:142:LEU:C | 4:8:372:ARG:CD[1_554] | 1.60 | 0.60 |
| 4:4:256:ARG:CA | 4:7:303:THR:CA[1_554] | 1.60 | 0.60 |
| 4:4:277:THR:C | 4:7:174:ALA:C[1_554] | 1.60 | 0.60 |
| 4:5:278:THR:C | 4:8:164:PRO:CG[1_554] | 1.60 | 0.60 |
| 4:4:311:ASP:O | 4:7:141:SER:O[1_554] | 1.60 | 0.60 |
| 4:5:75:ILE:CG1 | 4:9:194:THR:O[1_554] | 1.60 | 0.60 |
| 4:4:24:ASP:O | 4:7:362:TYR:OH[1_554] | 1.60 | 0.60 |
| 4:5:166:TYR:CD2 | 4:V:40:HIS:NE2[1_554] | 1.60 | 0.60 |
| 4:6:188:TYR:CD1 | 4:9:185:LEU:CG[1_554] | 1.60 | 0.60 |
| 4:6:21:PHE:O | 4:9:125:GLU:CG[1_554] | 1.60 | 0.60 |
| 4:4:370:VAL:O | 4:8:230:ALA:C[1_554] | 1.60 | 0.60 |
| 4:5:159:VAL:O | 4:8:177:ARG:NH1[1_554] | 1.60 | 0.60 |
| 4:5:319:ALA:CB | 4:8:295:ALA:CA[1_554] | 1.60 | 0.60 |
| 4:6:137:GLN:CD | 4:9:112:PRO:CA[1_554] | 1.60 | 0.60 |
| 4:4:196:ARG:CB | 4:7:210:ARG:C[1_554] | 1.60 | 0.60 |
| 4:5:178:LEU:CD1 | 4:8:177:ARG:O[1_554] | 1.60 | 0.60 |
| 4:3:115:ASN:N | 4:7:250:ILE:C[1_554] | 1.60 | 0.60 |
| 4:5:186:THR:OG1 | 4:8:157:ASP:OD2[1_554] | 1.60 | 0.60 |
| 4:4:172:PRO:CD | 4:8:266:PHE:CG[1_554] | 1.60 | 0.60 |
| 4:6:196:ARG:CZ | 4:9:211:ASP:O[1_554] | 1.60 | 0.60 |
| 4:5:349:LEU:N | 4:8:366:GLY:N[1_554] | 1.60 | 0.60 |
| 4:4:276:GLU:CB | 4:7:281:SER:CB[1_554] | 1.60 | 0.60 |
| 4:5:338:SER:CA | 4:8:134:VAL:CG1[1_554] | 1.60 | 0.60 |
| 4:4:257:CYS:SG | 4:7:157:ASP:CA[1_554] | 1.60 | 0.60 |
| 4:4:288:ASP:OD1 | 4:9:65:LEU:O[1_554] | 1.60 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:191:LYS:CA | 4:8:186:THR:CA[1_554] | 1.60 | 0.60 |
| 4:3:111:ASN:CA | 4:7:192:ILE:O[1_554] | 1.60 | 0.60 |
| 4:5:31:PHE:O | 4:8:78:ASN:CA[1_554] | 1.60 | 0.60 |
| 4:5:286:ASP:CA | 4:9:270:GLU:CG[1_554] | 1.60 | 0.60 |
| 4:4:325:MET:CG | 4:7:166:TYR:CD2[1_554] | 1.60 | 0.60 |
| 4:5:19:ALA:CA | 4:8:118:LYS:NZ[1_554] | 1.60 | 0.60 |
| 4:6:157:ASP:O | 4:9:72:GLU:C[1_554] | 1.60 | 0.60 |
| 4:5:113:LYS:O | 4:9:252:ASN:CG[1_554] | 1.60 | 0.60 |
| 4:5:319:ALA:O | 4:8:294:TYR:N[1_554] | 1.60 | 0.60 |
| 4:4:297:ASN:CG | 4:7:170:ALA:N[1_554] | 1.60 | 0.60 |
| 4:6:314:GLN:OE1 | 4:9:147:ARG:CA[1_554] | 1.60 | 0.60 |
| 4:5:27:PRO:N | 4:8:123:MET:N[1_554] | 1.60 | 0.60 |
| 4:6:113:LYS:CG | 4:V:253:GLU:N[1_554] | 1.60 | 0.60 |
| 4:4:140:LEU:CD2 | 4:7:117:GLU:OE2[1_554] | 1.60 | 0.60 |
| 4:4:325:MET:CB | 4:7:166:TYR:CZ[1_554] | 1.60 | 0.60 |
| 4:6:305:MET:CA | 4:9:11:ASP:CG[1_554] | 1.60 | 0.60 |
| 4:5:204:ALA:CB | 4:8:62:ARG:CA[1_554] | 1.60 | 0.60 |
| 4:4:192:ILE:N | 4:7:186:THR:CA[1_554] | 1.60 | 0.60 |
| 4:4:327:ILE:CA | 4:7:167:GLU:CA[1_554] | 1.60 | 0.60 |
| 4:5:75:ILE:CA | 4:9:197:GLY:N[1_554] | 1.60 | 0.60 |
| 4:6:153:LEU:C | 4:9:109:PRO:CA[1_554] | 1.60 | 0.60 |
| 4:6:286:ASP:N | 4:V:270:GLU:CD[1_554] | 1.60 | 0.60 |
| 4:5:340:TRP:C | 4:8:120:THR:OG1[1_554] | 1.60 | 0.60 |
| 4:5:257:CYS:CB | 4:8:303:THR:OG1[1_554] | 1.60 | 0.60 |
| 4:6:190:MET:CE | 4:9:206:ARG:NH2[1_554] | 1.61 | 0.59 |
| 1:D:637:LYS:NZ | 4:6:311:ASP:N[1_556] | 1.61 | 0.59 |
| 4:6:262:PHE:CE1 | 4:9:153:LEU:CA[1_554] | 1.61 | 0.59 |
| 4:5:219:VAL:CA | 4:8:301:GLY:N[1_554] | 1.61 | 0.59 |
| 4:4:338:SER:CA | 4:7:116:ARG:CA[1_554] | 1.61 | 0.59 |
| 4:4:16:LEU:CD2 | 4:7:70:PRO:O[1_554] | 1.61 | 0.59 |
| 4:6:167:GLU:CD | 4:W:41:GLN:N[1_554] | 1.61 | 0.59 |
| 4:6:29:ALA:CB | 4:9:83:GLU:OE1[1_554] | 1.61 | 0.59 |
| 4:4:141:SER:N | 4:7:371:HIS:CE1[1_554] | 1.61 | 0.59 |
| 4:4:255:PHE:C | 4:7:302:GLY:O[1_554] | 1.61 | 0.59 |
| 4:4:143:TYR:CA | 4:7:372:ARG:N[1_554] | 1.61 | 0.59 |
| 4:5:332:PRO:CD | 4:8:135:ALA:CA[1_554] | 1.61 | 0.59 |
| 4:6:190:MET:CG | 4:9:206:ARG:NH2[1_554] | 1.61 | 0.59 |
| 4:3:372:ARG:CD | 4:7:227:MET:CB[1_554] | 1.61 | 0.59 |
| 4:5:367:PRO:CD | 4:9:234:SER:O[1_554] | 1.61 | 0.59 |
| 4:4:313:MET:CA | 4:7:138:ALA:O[1_554] | 1.61 | 0.59 |
| 4:5:317:ILE:CA | 4:8:151:ILE:N[1_554] | 1.61 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:227:MET:CB | 4:8:307:PRO:CB[1_554] | 1.61 | 0.59 |
| 4:4:137:GLN:C | 4:7:113:LYS:CA[1_554] | 1.61 | 0.59 |
| 4:6:14:SER:O | 4:9:77:THR:CG2[1_554] | 1.61 | 0.59 |
| 4:5:193:LEU:CD2 | 4:8:210:ARG:CB[1_554] | 1.61 | 0.59 |
| 4:6:145:SER:N | 4:9:372:ARG:CZ[1_554] | 1.61 | 0.59 |
| 4:4:154:ASP:CG | 4:7:111:ASN:N[1_554] | 1.61 | 0.59 |
| 4:6:278:THR:C | 4:9:164:PRO:CB[1_554] | 1.61 | 0.59 |
| 4:6:269:MET:CA | 4:9:271:SER:OG[1_554] | 1.61 | 0.59 |
| 4:4:339:VAL:C | 4:7:117:GLU:N[1_554] | 1.61 | 0.59 |
| 4:6:113:LYS:NZ | 4:V:254:ARG:CA[1_554] | 1.61 | 0.59 |
| 4:6:164:PRO:N | 4:9:172:PRO:CB[1_554] | 1.61 | 0.59 |
| 4:5:211:ASP:OD1 | 4:8:32:PRO:N[1_554] | 1.61 | 0.59 |
| 4:6:26:ALA:CA | 4:9:123:MET:CG[1_554] | 1.61 | 0.59 |
| 4:6:255:PHE:CD1 | 4:9:305:MET:CB[1_554] | 1.61 | 0.59 |
| 4:6:340:TRP:CD2 | 4:9:120:THR:N[1_554] | 1.61 | 0.59 |
| 4:4:166:TYR:CG | 4:9:40:HIS:NE2[1_554] | 1.61 | 0.59 |
| 4:5:369:ILE:N | 4:9:229:THR:C[1_554] | 1.61 | 0.59 |
| 4:5:321:ALA:CA | 4:8:289:ILE:O[1_554] | 1.61 | 0.59 |
| 4:6:151:ILE:CB | 4:9:170:ALA:C[1_554] | 1.61 | 0.59 |
| 4:6:318:THR:C | 4:9:296:ASN:ND2[1_554] | 1.61 | 0.59 |
| 4:6:151:ILE:CG1 | 4:9:170:ALA:C[1_554] | 1.61 | 0.59 |
| 4:4:367:PRO:CG | 4:8:235:SER:CA[1_554] | 1.61 | 0.59 |
| 4:4:109:PRO:N | 4:8:195:GLU:CB[1_554] | 1.61 | 0.59 |
| 4:5:193:LEU:O | 4:8:209:VAL:O[1_554] | 1.61 | 0.59 |
| 4:6:294:TYR:CB | 4:9:166:TYR:CB[1_554] | 1.61 | 0.59 |
| 4:6:166:TYR:CZ | 4:W:40:HIS:N[1_554] | 1.61 | 0.59 |
| 4:6:114:ALA:N | 4:V:253:GLU:OE2[1_554] | 1.61 | 0.59 |
| 4:6:193:LEU:CD1 | 4:9:210:ARG:O[1_554] | 1.61 | 0.59 |
| 4:5:154:ASP:CG | 4:8:111:ASN:CB[1_554] | 1.61 | 0.59 |
| 4:5:281:SER:OG | 4:8:173:HIS:CA[1_554] | 1.61 | 0.59 |
| 4:4:215:LYS:CB | 4:7:31:PHE:C[1_554] | 1.61 | 0.59 |
| 4:4:209:VAL:CG1 | 4:7:69:TYR:OH[1_554] | 1.61 | 0.59 |
| 4:6:342:GLY:C | 4:9:367:PRO:O[1_554] | 1.61 | 0.59 |
| 4:6:17:VAL:CB | 4:9:79:TRP:CD1[1_554] | 1.61 | 0.59 |
| 4:6:258:PRO:CA | 4:9:155:SER:C[1_554] | 1.61 | 0.59 |
| 4:6:172:PRO:CG | 4:V:266:PHE:CA[1_554] | 1.61 | 0.59 |
| 4:5:340:TRP:N | 4:8:116:ARG:C[1_554] | 1.61 | 0.59 |
| 4:5:283:MET:CG | 4:8:285:CYS:C[1_554] | 1.61 | 0.59 |
| 4:4:161:HIS:CA | 4:7:110:LEU:CG[1_554] | 1.61 | 0.59 |
| 4:5:278:THR:CG2 | 4:8:164:PRO:CA[1_554] | 1.61 | 0.59 |
| 4:6:75:ILE:CA | 4:V:197:GLY:N[1_554] | 1.61 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:313:MET:SD | 4:9:152:VAL:CB[1_554] | 1.61 | 0.59 |
| 4:6:367:PRO:CD | 4:V:233:SER:C[1_554] | 1.61 | 0.59 |
| 4:3:113:LYS:CG | 4:7:254:ARG:CB[1_554] | 1.61 | 0.59 |
| 4:5:219:VAL:O | 4:8:335:ARG:CB[1_554] | 1.61 | 0.59 |
| 4:5:321:ALA:C | 4:8:292:ASP:CB[1_554] | 1.61 | 0.59 |
| 4:6:299:MET:N | 4:9:136:ILE:CB[1_554] | 1.61 | 0.59 |
| 4:6:304:THR:OG1 | 4:9:137:GLN:CB[1_554] | 1.61 | 0.59 |
| 4:4:211:ASP:C | 4:7:32:PRO:C[1_554] | 1.61 | 0.59 |
| 4:5:196:ARG:CD | 4:8:212:ILE:CA[1_554] | 1.61 | 0.59 |
| 4:6:366:GLY:C | 4:V:233:SER:C[1_554] | 1.61 | 0.59 |
| 4:5:188:TYR:O | 4:8:186:THR:N[1_554] | 1.62 | 0.58 |
| 4:4:75:ILE:CB | 4:8:198:TYR:CG[1_554] | 1.62 | 0.58 |
| 4:4:335:ARG:CG | 4:7:106:THR:CA[1_554] | 1.62 | 0.58 |
| 4:5:197:GLY:CA | 4:8:212:ILE:CD1[1_554] | 1.62 | 0.58 |
| 4:6:346:LEU:CB | 4:9:369:ILE:N[1_554] | 1.62 | 0.58 |
| 4:4:255:PHE:O | 4:7:301:GLY:C[1_554] | 1.62 | 0.58 |
| 4:5:258:PRO:CG | 4:8:302:GLY:N[1_554] | 1.62 | 0.58 |
| 4:5:210:ARG:NH1 | 4:8:33:SER:CB[1_554] | 1.62 | 0.58 |
| 4:6:367:PRO:CA | 4:V:233:SER:C[1_554] | 1.62 | 0.58 |
| 4:4:166:TYR:CD1 | 4:9:40:HIS:CD2[1_554] | 1.62 | 0.58 |
| 4:5:106:THR:OG1 | 4:8:114:ALA:CB[1_554] | 1.62 | 0.58 |
| 4:5:219:VAL:CB | 4:8:300:SER:CA[1_554] | 1.62 | 0.58 |
| 4:5:334:GLU:OE1 | 4:8:133:TYR:CA[1_554] | 1.62 | 0.58 |
| 4:4:286:ASP:C | 4:8:270:GLU:CD[1_554] | 1.62 | 0.58 |
| 4:3:369:ILE:C | 4:7:229:THR:C[1_554] | 1.62 | 0.58 |
| 4:4:311:ASP:CA | 4:7:141:SER:O[1_554] | 1.62 | 0.58 |
| 4:4:222:ASP:O | 4:7:332:PRO:C[1_554] | 1.62 | 0.58 |
| 4:5:307:PRO:C | 4:8:337:TYR:C[1_554] | 1.62 | 0.58 |
| 4:6:196:ARG:C | 4:9:212:ILE:CD1[1_554] | 1.62 | 0.58 |
| 4:3:74:GLY:O | 4:7:197:GLY:C[1_554] | 1.62 | 0.58 |
| 4:6:289:ILE:CA | 4:W:63:GLY:O[1_554] | 1.62 | 0.58 |
| 4:6:309:ILE:N | 4:9:338:SER:CB[1_554] | 1.62 | 0.58 |
| 4:6:277:THR:CG2 | 4:9:175:ILE:CA[1_554] | 1.62 | 0.58 |
| 4:6:253:GLU:OE2 | 4:9:214:GLU:C[1_554] | 1.62 | 0.58 |
| 4:6:191:LYS:N | 4:9:186:THR:CA[1_554] | 1.62 | 0.58 |
| 4:6:259:GLU:CA | 4:9:304:THR:CG2[1_554] | 1.62 | 0.58 |
| 4:4:305:MET:CE | 4:7:10:CYS:O[1_554] | 1.62 | 0.58 |
| 4:4:266:PHE:CB | 4:7:261:LEU:CG[1_554] | 1.62 | 0.58 |
| 4:5:300:SER:C | 4:8:108:ALA:N[1_554] | 1.62 | 0.58 |
| 4:3:75:ILE:N | 4:7:198:TYR:CA[1_554] | 1.62 | 0.58 |
| 4:4:140:LEU:O | 4:7:371:HIS:ND1[1_554] | 1.62 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:275:HIS:C | 4:9:151:ILE:CD1[1_554] | 1.62 | 0.58 |
| 4:5:322:PRO:CG | 4:8:288:ASP:C[1_554] | 1.62 | 0.58 |
| 4:4:188:TYR:O | 4:7:182:GLY:C[1_554] | 1.62 | 0.58 |
| 4:5:255:PHE:CD1 | 4:8:305:MET:CB[1_554] | 1.62 | 0.58 |
| 4:6:208:ILE:CD1 | 4:9:59:GLN:CB[1_554] | 1.62 | 0.58 |
| 4:5:114:ALA:N | 4:9:251:GLY:N[1_554] | 1.62 | 0.58 |
| 4:6:283:MET:CA | 4:9:285:CYS:C[1_554] | 1.62 | 0.58 |
| 4:5:186:THR:O | 4:8:183:ARG:CG[1_554] | 1.62 | 0.58 |
| 4:4:307:PRO:C | 4:7:340:TRP:N[1_554] | 1.62 | 0.58 |
| 4:4:310:ALA:CB | 4:7:140:LEU:N[1_554] | 1.62 | 0.58 |
| 4:4:274:ILE:CB | 4:7:161:HIS:CB[1_554] | 1.62 | 0.58 |
| 4:4:333:PRO:C | 4:7:105:LEU:CA[1_554] | 1.62 | 0.58 |
| 4:5:287:ILE:O | 4:V:63:GLY:CA[1_554] | 1.62 | 0.58 |
| 4:6:346:LEU:N | 4:9:366:GLY:O[1_554] | 1.62 | 0.58 |
| 4:4:287:ILE:N | 4:8:270:GLU:OE1[1_554] | 1.62 | 0.58 |
| 4:4:155:SER:CB | 4:7:108:ALA:CB[1_554] | 1.62 | 0.58 |
| 4:5:270:GLU:CA | 4:8:272:ALA:C[1_554] | 1.62 | 0.58 |
| 4:4:326:LYS:CD | 4:9:44:MET:CA[1_554] | 1.62 | 0.58 |
| 4:5:145:SER:N | 4:8:372:ARG:CZ[1_554] | 1.62 | 0.58 |
| 4:6:150:GLY:O | 4:9:169:TYR:CD1[1_554] | 1.62 | 0.58 |
| 4:6:188:TYR:O | 4:9:186:THR:N[1_554] | 1.62 | 0.58 |
| 4:4:332:PRO:CB | 4:7:134:VAL:CA[1_554] | 1.62 | 0.58 |
| 4:6:265:SER:C | 4:9:261:LEU:O[1_554] | 1.62 | 0.58 |
| 4:5:346:LEU:CD2 | 4:8:368:SER:CB[1_554] | 1.62 | 0.58 |
| 4:6:196:ARG:O | 4:9:212:ILE:CB[1_554] | 1.62 | 0.58 |
| 4:6:372:ARG:CA | 4:V:227:MET:C[1_554] | 1.62 | 0.58 |
| 4:5:341:ILE:CA | 4:8:120:THR:CB[1_554] | 1.62 | 0.58 |
| 4:4:277:THR:CB | 4:7:175:ILE:CA[1_554] | 1.62 | 0.58 |
| 4:6:296:ASN:C | 4:9:169:TYR:CA[1_554] | 1.62 | 0.58 |
| 4:4:340:TRP:CA | 4:7:117:GLU:C[1_554] | 1.62 | 0.58 |
| 4:6:173:HIS:CD2 | 4:V:268:GLY:N[1_554] | 1.62 | 0.58 |
| 4:6:115:ASN:CB | 4:V:196:ARG:CZ[1_554] | 1.62 | 0.58 |
| 4:6:205:GLU:CB | 4:9:62:ARG:NH2[1_554] | 1.62 | 0.58 |
| 4:5:158:GLY:N | 4:8:72:GLU:O[1_554] | 1.62 | 0.58 |
| 4:5:147:ARG:O | 4:8:372:ARG:CG[1_554] | 1.62 | 0.58 |
| 4:5:286:ASP:N | 4:9:270:GLU:OE2[1_554] | 1.62 | 0.58 |
| 4:5:256:ARG:CB | 4:8:306:TYR:CZ[1_554] | 1.62 | 0.58 |
| 4:5:172:PRO:CG | 4:9:266:PHE:CB[1_554] | 1.62 | 0.58 |
| 4:6:288:ASP:CG | 4:W:62:ARG:O[1_554] | 1.62 | 0.58 |
| 4:6:220:ALA:CB | 4:9:335:ARG:CD[1_554] | 1.62 | 0.58 |
| 4:5:370:VAL:CB | 4:9:231:ALA:CA[1_554] | 1.62 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:637:LYS:CE | 4:5:311:ASP:CG[1_556] | 1.62 | 0.58 |
| 4:4:274:ILE:CG1 | 4:7:161:HIS:CG[1_554] | 1.62 | 0.58 |
| 4:6:263:GLN:O | 4:9:274:ILE:CD1[1_554] | 1.62 | 0.58 |
| 4:6:297:ASN:OD1 | 4:9:165:ILE:CG1[1_554] | 1.62 | 0.58 |
| 4:5:32:PRO:N | 4:8:78:ASN:CG[1_554] | 1.62 | 0.58 |
| 4:6:11:ASP:N | 4:9:118:LYS:CB[1_554] | 1.62 | 0.58 |
| 4:6:114:ALA:CA | 4:V:251:GLY:CA[1_554] | 1.62 | 0.58 |
| 4:6:112:PRO:C | 4:V:253:GLU:CG[1_554] | 1.62 | 0.58 |
| 4:4:311:ASP:OD2 | 4:7:144:ALA:CB[1_554] | 1.62 | 0.58 |
| 4:6:114:ALA:O | 4:V:196:ARG:NH2[1_554] | 1.62 | 0.58 |
| 4:6:17:VAL:C | 4:9:79:TRP:CB[1_554] | 1.62 | 0.58 |
| 4:4:257:CYS:C | 4:7:156:GLY:CA[1_554] | 1.63 | 0.57 |
| 4:4:255:PHE:O | 4:7:302:GLY:N[1_554] | 1.63 | 0.57 |
| 4:6:16:LEU:CB | 4:9:76:ILE:CG2[1_554] | 1.63 | 0.57 |
| 4:5:114:ALA:O | 4:9:237:GLU:CD[1_554] | 1.63 | 0.57 |
| 4:4:372:ARG:CD | 4:8:227:MET:CB[1_554] | 1.63 | 0.57 |
| 4:5:33:SER:CB | 4:8:77:THR:O[1_554] | 1.63 | 0.57 |
| 4:6:215:LYS:O | 4:9:30:VAL:CG1[1_554] | 1.63 | 0.57 |
| 4:5:312:ARG:NE | 4:8:299:MET:CA[1_554] | 1.63 | 0.57 |
| 4:4:310:ALA:CB | 4:7:140:LEU:CG[1_554] | 1.63 | 0.57 |
| 4:6:24:ASP:CB | 4:9:124:PHE:O[1_554] | 1.63 | 0.57 |
| 4:6:280:ASN:OD1 | 4:9:281:SER:C[1_554] | 1.63 | 0.57 |
| 4:4:210:ARG:CD | 4:7:69:TYR:CB[1_554] | 1.63 | 0.57 |
| 4:5:159:VAL:N | 4:8:177:ARG:NH2[1_554] | 1.63 | 0.57 |
| 4:5:321:ALA:O | 4:8:292:ASP:CB[1_554] | 1.63 | 0.57 |
| 4:4:253:GLU:CD | 4:7:214:GLU:CD[1_554] | 1.63 | 0.57 |
| 4:6:224:GLU:CB | 4:9:310:ALA:CB[1_554] | 1.63 | 0.57 |
| 4:3:77:THR:CB | 4:7:246:GLN:OE1[1_554] | 1.63 | 0.57 |
| 4:6:311:ASP:N | 4:9:141:SER:C[1_554] | 1.63 | 0.57 |
| 4:5:200:PHE:C | 4:8:206:ARG:CG[1_554] | 1.63 | 0.57 |
| 4:4:197:GLY:C | 4:7:208:ILE:C[1_554] | 1.63 | 0.57 |
| 4:5:14:SER:O | 4:8:77:THR:CG2[1_554] | 1.63 | 0.57 |
| 4:6:221:LEU:CG | 4:9:332:PRO:CD[1_554] | 1.63 | 0.57 |
| 4:3:173:HIS:O | 4:7:267:ILE:O[1_554] | 1.63 | 0.57 |
| 4:6:219:VAL:CB | 4:9:300:SER:CA[1_554] | 1.63 | 0.57 |
| 4:5:223:PHE:CG | 4:8:304:THR:O[1_554] | 1.63 | 0.57 |
| 4:5:115:ASN:OD1 | 4:9:249:THR:O[1_554] | 1.63 | 0.57 |
| 4:4:340:TRP:CA | 4:7:118:LYS:CA[1_554] | 1.63 | 0.57 |
| 4:5:59:GLN:OE1 | 4:8:67:LEU:O[1_554] | 1.63 | 0.57 |
| 4:5:31:PHE:CD1 | 4:8:80:ASP:CA[1_554] | 1.63 | 0.57 |
| 4:5:259:GLU:CD | 4:8:309:ILE:CG1[1_554] | 1.63 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:30:VAL:CG1 | 4:9:82:MET:CA[1_554] | 1.63 | 0.57 |
| 4:4:242:LEU:O | 4:7:60:SER:OG[1_554] | 1.63 | 0.57 |
| 4:6:252:ASN:CB | 4:9:214:GLU:O[1_554] | 1.63 | 0.57 |
| 4:5:288:ASP:CA | 4:V:63:GLY:N[1_554] | 1.63 | 0.57 |
| 4:4:333:PRO:CA | 4:7:105:LEU:CA[1_554] | 1.63 | 0.57 |
| 4:4:188:TYR:CB | 4:7:181:ALA:O[1_554] | 1.63 | 0.57 |
| 4:4:340:TRP:CG | 4:7:118:LYS:CA[1_554] | 1.63 | 0.57 |
| 4:3:371:HIS:N | 4:7:230:ALA:CA[1_554] | 1.63 | 0.57 |
| 4:5:317:ILE:CG1 | 4:8:150:GLY:C[1_554] | 1.63 | 0.57 |
| 4:5:288:ASP:N | 4:V:63:GLY:CA[1_554] | 1.63 | 0.57 |
| 4:5:327:ILE:CG2 | 4:8:149:THR:CA[1_554] | 1.63 | 0.57 |
| 4:6:336:LYS:CA | 4:9:106:THR:O[1_554] | 1.63 | 0.57 |
| 4:5:369:ILE:C | 4:9:228:ALA:O[1_554] | 1.63 | 0.57 |
| 4:6:267:ILE:CB | 4:9:180:LEU:CB[1_554] | 1.63 | 0.57 |
| 4:5:154:ASP:OD2 | 4:8:111:ASN:C[1_554] | 1.63 | 0.57 |
| 4:6:25:ASP:CG | 4:9:129:VAL:O[1_554] | 1.63 | 0.57 |
| 4:4:218:TYR:CE1 | 4:7:337:TYR:CE1[1_554] | 1.63 | 0.57 |
| 4:6:263:GLN:N | 4:9:274:ILE:CG1[1_554] | 1.63 | 0.57 |
| 4:4:371:HIS:CE1 | 4:8:252:ASN:CA[1_554] | 1.63 | 0.57 |
| 4:4:313:MET:CE | 4:7:163:VAL:CG1[1_554] | 1.63 | 0.57 |
| 4:3:115:ASN:O | 4:7:196:ARG:NH2[1_554] | 1.63 | 0.57 |
| 4:6:276:GLU:O | 4:9:281:SER:CB[1_554] | 1.63 | 0.57 |
| 4:5:368:SER:CA | 4:9:229:THR:O[1_554] | 1.63 | 0.57 |
| 4:4:151:ILE:CD1 | 4:7:171:LEU:C[1_554] | 1.63 | 0.57 |
| 4:4:200:PHE:N | 4:7:206:ARG:CB[1_554] | 1.63 | 0.57 |
| 4:6:110:LEU:C | 4:V:192:ILE:CA[1_554] | 1.63 | 0.57 |
| 4:5:62:ARG:NH1 | 4:8:67:LEU:O[1_554] | 1.63 | 0.57 |
| 4:5:162:ASN:OD1 | 4:8:175:ILE:CG2[1_554] | 1.63 | 0.57 |
| 4:4:265:SER:C | 4:7:261:LEU:O[1_554] | 1.63 | 0.57 |
| 4:6:200:PHE:N | 4:9:206:ARG:CA[1_554] | 1.63 | 0.57 |
| 4:6:166:TYR:CD2 | 4:W:40:HIS:NE2[1_554] | 1.63 | 0.57 |
| 4:5:280:ASN:CB | 4:8:284:LYS:CB[1_554] | 1.63 | 0.57 |
| 4:4:314:GLN:C | 4:7:142:LEU:CB[1_554] | 1.63 | 0.57 |
| 4:6:24:ASP:OD1 | 4:9:124:PHE:O[1_554] | 1.63 | 0.57 |
| 4:5:187:ASP:CA | 4:8:183:ARG:CG[1_554] | 1.63 | 0.57 |
| 4:5:117:GLU:CG | 4:9:252:ASN:ND2[1_554] | 1.63 | 0.57 |
| 4:6:113:LYS:CB | 4:V:252:ASN:O[1_554] | 1.63 | 0.57 |
| 4:6:218:TYR:CD2 | 4:9:336:LYS:CG[1_554] | 1.63 | 0.57 |
| 4:4:143:TYR:N | 4:7:372:ARG:N[1_554] | 1.63 | 0.57 |
| 4:3:173:HIS:C | 4:7:267:ILE:CB[1_554] | 1.63 | 0.57 |
| 4:6:340:TRP:CH2 | 4:9:121:GLN:O[1_554] | 1.63 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:299:MET:CE | 4:8:139:VAL:N[1_554] | 1.63 | 0.57 |
| 4:4:204:ALA:C | 4:7:62:ARG:CG[1_554] | 1.63 | 0.57 |
| 4:4:297:ASN:CG | 4:7:170:ALA:CA[1_554] | 1.63 | 0.57 |
| 4:5:310:ALA:CB | 4:8:141:SER:CA[1_554] | 1.63 | 0.57 |
| 4:5:298:VAL:O | 4:8:136:ILE:CD1[1_554] | 1.63 | 0.57 |
| 4:4:117:GLU:N | 4:8:237:GLU:OE2[1_554] | 1.63 | 0.57 |
| 4:4:222:ASP:C | 4:7:332:PRO:N[1_554] | 1.63 | 0.57 |
| 4:6:337:TYR:CZ | 4:9:86:TRP:NE1[1_554] | 1.63 | 0.57 |
| 4:6:317:ILE:CG2 | 4:9:150:GLY:C[1_554] | 1.63 | 0.57 |
| 4:4:370:VAL:C | 4:8:230:ALA:CB[1_554] | 1.63 | 0.57 |
| 4:4:333:PRO:O | 4:7:105:LEU:CA[1_554] | 1.63 | 0.57 |
| 4:4:113:LYS:CG | 4:8:254:ARG:C[1_554] | 1.63 | 0.57 |
| 4:4:117:GLU:OE2 | 4:8:236:LEU:O[1_554] | 1.63 | 0.57 |
| 4:5:117:GLU:OE2 | 4:9:236:LEU:CG[1_554] | 1.63 | 0.57 |
| 4:4:193:LEU:CD1 | 4:7:210:ARG:CZ[1_554] | 1.63 | 0.57 |
| 4:4:188:TYR:CE1 | 4:7:185:LEU:CB[1_554] | 1.63 | 0.57 |
| 4:5:195:GLU:CB | 4:8:189:LEU:CD2[1_554] | 1.63 | 0.57 |
| 4:5:328:LYS:O | 4:8:168:GLY:CA[1_554] | 1.63 | 0.57 |
| 4:4:207:GLU:OE2 | 4:7:68:LYS:N[1_554] | 1.63 | 0.57 |
| 4:5:341:ILE:O | 4:8:120:THR:CG2[1_554] | 1.63 | 0.57 |
| 4:3:114:ALA:N | 4:7:250:ILE:CG2[1_554] | 1.63 | 0.57 |
| 4:5:214:GLU:N | 4:8:16:LEU:CB[1_554] | 1.64 | 0.56 |
| 4:5:191:LYS:CD | 4:8:185:LEU:O[1_554] | 1.64 | 0.56 |
| 1:D:637:LYS:NZ | 4:6:311:ASP:CB[1_556] | 1.64 | 0.56 |
| 4:3:369:ILE:CG2 | 4:7:234:SER:N[1_554] | 1.64 | 0.56 |
| 4:5:261:LEU:N | 4:8:155:SER:OG[1_554] | 1.64 | 0.56 |
| 4:3:289:ILE:N | 4:8:63:GLY:O[1_554] | 1.64 | 0.56 |
| 4:5:215:LYS:CD | 4:8:31:PHE:CA[1_554] | 1.64 | 0.56 |
| 4:6:59:GLN:NE2 | 4:9:68:LYS:CG[1_554] | 1.64 | 0.56 |
| 4:5:334:GLU:O | 4:8:105:LEU:CA[1_554] | 1.64 | 0.56 |
| 4:6:313:MET:SD | 4:9:152:VAL:CA[1_554] | 1.64 | 0.56 |
| 4:4:333:PRO:O | 4:7:105:LEU:CD2[1_554] | 1.64 | 0.56 |
| 4:5:113:LYS:CG | 4:9:253:GLU:N[1_554] | 1.64 | 0.56 |
| 4:5:258:PRO:N | 4:8:155:SER:O[1_554] | 1.64 | 0.56 |
| 4:6:62:ARG:NH1 | 4:9:67:LEU:O[1_554] | 1.64 | 0.56 |
| 4:6:24:ASP:CG | 4:9:124:PHE:C[1_554] | 1.64 | 0.56 |
| 4:6:348:SER:OG | 4:9:362:TYR:CA[1_554] | 1.64 | 0.56 |
| 4:4:280:ASN:CA | 4:7:174:ALA:CB[1_554] | 1.64 | 0.56 |
| 4:6:218:TYR:CE1 | 4:9:337:TYR:CZ[1_554] | 1.64 | 0.56 |
| 4:5:188:TYR:O | 4:8:182:GLY:O[1_554] | 1.64 | 0.56 |
| 4:5:221:LEU:CB | 4:8:332:PRO:N[1_554] | 1.64 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:208:ILE:CG1 | 4:7:59:GLN:CB[1_554] | 1.64 | 0.56 |
| 4:4:328:LYS:N | 4:7:168:GLY:N[1_554] | 1.64 | 0.56 |
| 4:6:335:ARG:CA | 4:9:105:LEU:O[1_554] | 1.64 | 0.56 |
| 4:6:137:GLN:CG | 4:9:112:PRO:CA[1_554] | 1.64 | 0.56 |
| 4:6:156:GLY:C | 4:9:74:GLY:N[1_554] | 1.64 | 0.56 |
| 4:5:313:MET:C | 4:8:142:LEU:CD1[1_554] | 1.64 | 0.56 |
| 4:5:143:TYR:CA | 4:8:372:ARG:CA[1_554] | 1.64 | 0.56 |
| 4:4:188:TYR:CE1 | 4:7:185:LEU:CD2[1_554] | 1.64 | 0.56 |
| 4:5:258:PRO:N | 4:8:303:THR:N[1_554] | 1.64 | 0.56 |
| 4:3:371:HIS:CE1 | 4:7:252:ASN:CA[1_554] | 1.64 | 0.56 |
| 4:4:32:PRO:N | 4:7:78:ASN:CG[1_554] | 1.64 | 0.56 |
| 4:4:192:ILE:CA | 4:7:213:LYS:CD[1_554] | 1.64 | 0.56 |
| 4:6:337:TYR:CD1 | 4:9:86:TRP:CZ2[1_554] | 1.64 | 0.56 |
| 4:5:113:LYS:NZ | 4:9:254:ARG:CA[1_554] | 1.64 | 0.56 |
| 4:4:117:GLU:CA | 4:8:237:GLU:CB[1_554] | 1.64 | 0.56 |
| 4:6:218:TYR:CB | 4:9:336:LYS:CG[1_554] | 1.64 | 0.56 |
| 4:6:32:PRO:O | 4:9:78:ASN:OD1[1_554] | 1.64 | 0.56 |
| 4:5:196:ARG:C | 4:8:212:ILE:CD1[1_554] | 1.64 | 0.56 |
| 4:6:284:LYS:C | 4:V:268:GLY:O[1_554] | 1.64 | 0.56 |
| 4:5:326:LYS:CA | 4:8:167:GLU:CD[1_554] | 1.64 | 0.56 |
| 4:4:143:TYR:CE2 | 4:7:368:SER:OG[1_554] | 1.64 | 0.56 |
| 4:4:116:ARG:CB | 4:8:252:ASN:OD1[1_554] | 1.64 | 0.56 |
| 4:6:367:PRO:O | 4:V:230:ALA:C[1_554] | 1.64 | 0.56 |
| 4:6:320:LEU:CD1 | 4:9:282:ILE:CG1[1_554] | 1.64 | 0.56 |
| 4:5:327:ILE:CG2 | 4:8:148:THR:C[1_554] | 1.64 | 0.56 |
| 4:6:182:GLY:CA | 4:9:14:SER:OG[1_554] | 1.64 | 0.56 |
| 4:4:372:ARG:N | 4:8:226:GLU:O[1_554] | 1.64 | 0.56 |
| 4:4:253:GLU:OE1 | 4:7:214:GLU:CA[1_554] | 1.64 | 0.56 |
| 4:6:318:THR:OG1 | 4:9:296:ASN:CB[1_554] | 1.64 | 0.56 |
| 4:6:109:PRO:O | 4:V:195:GLU:CD[1_554] | 1.64 | 0.56 |
| 4:4:154:ASP:N | 4:7:110:LEU:CA[1_554] | 1.64 | 0.56 |
| 4:6:317:ILE:CG1 | 4:9:150:GLY:C[1_554] | 1.64 | 0.56 |
| 4:3:173:HIS:O | 4:7:267:ILE:C[1_554] | 1.64 | 0.56 |
| 4:6:278:THR:CA | 4:9:164:PRO:CG[1_554] | 1.64 | 0.56 |
| 4:5:164:PRO:CA | 4:8:172:PRO:CG[1_554] | 1.64 | 0.56 |
| 4:5:25:ASP:CG | 4:8:129:VAL:O[1_554] | 1.64 | 0.56 |
| 4:3:291:LYS:CB | 4:8:64:ILE:CD1[1_554] | 1.64 | 0.56 |
| 4:6:322:PRO:O | 4:9:292:ASP:OD2[1_554] | 1.64 | 0.56 |
| 4:6:214:GLU:OE1 | 4:9:33:SER:CB[1_554] | 1.64 | 0.56 |
| 4:6:154:ASP:OD1 | 4:9:111:ASN:CB[1_554] | 1.64 | 0.56 |
| 4:5:311:ASP:OD1 | 4:8:144:ALA:O[1_554] | 1.64 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:188:TYR:CE1 | 4:8:185:LEU:CD2[1_554] | 1.64 | 0.56 |
| 4:6:346:LEU:CB | 4:9:368:SER:N[1_554] | 1.64 | 0.56 |
| 4:5:28:ARG:CD | 4:8:126:THR:CA[1_554] | 1.64 | 0.56 |
| 4:6:267:ILE:CG2 | 4:9:180:LEU:CD1[1_554] | 1.64 | 0.56 |
| 4:6:223:PHE:CG | 4:9:304:THR:O[1_554] | 1.64 | 0.56 |
| 4:4:286:ASP:CB | 4:8:270:GLU:OE1[1_554] | 1.64 | 0.56 |
| 4:3:117:GLU:CB | 4:7:237:GLU:CB[1_554] | 1.64 | 0.56 |
| 4:6:166:TYR:C | 4:W:40:HIS:CD2[1_554] | 1.64 | 0.56 |
| 4:4:173:HIS:O | 4:8:267:ILE:CA[1_554] | 1.64 | 0.56 |
| 4:3:108:ALA:CB | 4:7:196:ARG:N[1_554] | 1.64 | 0.56 |
| 4:5:166:TYR:CE2 | 4:V:39:ARG:C[1_554] | 1.64 | 0.56 |
| 4:4:161:HIS:CA | 4:7:110:LEU:CB[1_554] | 1.64 | 0.56 |
| 4:6:62:ARG:NH1 | 4:9:67:LEU:CA[1_554] | 1.64 | 0.56 |
| 4:5:201:VAL:CG2 | 4:8:203:THR:CA[1_554] | 1.64 | 0.56 |
| 4:5:187:ASP:C | 4:8:183:ARG:O[1_554] | 1.64 | 0.56 |
| 4:5:301:GLY:N | 4:8:108:ALA:N[1_554] | 1.64 | 0.56 |
| 4:4:338:SER:CA | 4:7:116:ARG:O[1_554] | 1.64 | 0.56 |
| 4:5:188:TYR:C | 4:8:182:GLY:C[1_554] | 1.64 | 0.56 |
| 4:5:189:LEU:O | 4:8:186:THR:CB[1_554] | 1.64 | 0.56 |
| 4:6:312:ARG:NE | 4:9:299:MET:CA[1_554] | 1.64 | 0.56 |
| 4:5:242:LEU:CD1 | 4:8:207:GLU:OE1[1_554] | 1.64 | 0.56 |
| 4:5:180:LEU:CD2 | 4:8:178:LEU:C[1_554] | 1.64 | 0.56 |
| 4:5:115:ASN:N | 4:9:196:ARG:NH1[1_554] | 1.64 | 0.56 |
| 4:6:195:GLU:CG | 4:9:189:LEU:CB[1_554] | 1.65 | 0.55 |
| 4:4:178:LEU:CG | 4:7:177:ARG:CB[1_554] | 1.65 | 0.55 |
| 4:6:193:LEU:CD2 | 4:9:210:ARG:CB[1_554] | 1.65 | 0.55 |
| 4:6:218:TYR:O | 4:9:301:GLY:C[1_554] | 1.65 | 0.55 |
| 4:6:157:ASP:OD2 | 4:9:72:GLU:N[1_554] | 1.65 | 0.55 |
| 4:4:322:PRO:N | 4:7:292:ASP:OD2[1_554] | 1.65 | 0.55 |
| 4:5:327:ILE:C | 4:8:148:THR:O[1_554] | 1.65 | 0.55 |
| 4:4:190:MET:CG | 4:7:206:ARG:NH2[1_554] | 1.65 | 0.55 |
| 4:3:117:GLU:CB | 4:7:237:GLU:N[1_554] | 1.65 | 0.55 |
| 4:4:16:LEU:CB | 4:7:77:THR:C[1_554] | 1.65 | 0.55 |
| 4:5:218:TYR:CE1 | 4:8:337:TYR:CZ[1_554] | 1.65 | 0.55 |
| 4:5:372:ARG:N | 4:9:227:MET:C[1_554] | 1.65 | 0.55 |
| 4:5:109:PRO:O | 4:9:195:GLU:CD[1_554] | 1.65 | 0.55 |
| 4:5:31:PHE:CG | 4:8:80:ASP:CA[1_554] | 1.65 | 0.55 |
| 4:5:114:ALA:CB | 4:9:250:ILE:O[1_554] | 1.65 | 0.55 |
| 4:6:321:ALA:CB | 4:9:292:ASP:CB[1_554] | 1.65 | 0.55 |
| 4:6:369:ILE:CG2 | 4:V:232:SER:CB[1_554] | 1.65 | 0.55 |
| 4:4:18:LYS:CD | 4:7:79:TRP:CG[1_554] | 1.65 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:255:PHE:CD2 | 4:9:305:MET:CB[1_554] | 1.65 | 0.55 |
| 4:4:340:TRP:C | 4:7:118:LYS:N[1_554] | 1.65 | 0.55 |
| 4:5:299:MET:CA | 4:8:136:ILE:C[1_554] | 1.65 | 0.55 |
| 4:5:16:LEU:N | 4:8:77:THR:CA[1_554] | 1.65 | 0.55 |
| 4:4:303:THR:N | 4:7:74:GLY:O[1_554] | 1.65 | 0.55 |
| 4:6:188:TYR:CE1 | 4:9:185:LEU:CB[1_554] | 1.65 | 0.55 |
| 4:6:264:PRO:CA | 4:9:178:LEU:CD2[1_554] | 1.65 | 0.55 |
| 4:5:249:THR:C | 4:8:211:ASP:CG[1_554] | 1.65 | 0.55 |
| 4:4:188:TYR:CE1 | 4:7:185:LEU:CG[1_554] | 1.65 | 0.55 |
| 4:5:154:ASP:CG | 4:8:111:ASN:CA[1_554] | 1.65 | 0.55 |
| 4:4:143:TYR:C | 4:7:372:ARG:N[1_554] | 1.65 | 0.55 |
| 4:5:214:GLU:CD | 4:8:33:SER:OG[1_554] | 1.65 | 0.55 |
| 4:6:316:GLU:CG | 4:9:298:VAL:N[1_554] | 1.65 | 0.55 |
| 4:6:335:ARG:CG | 4:9:106:THR:CA[1_554] | 1.65 | 0.55 |
| 4:5:339:VAL:CG1 | 4:8:115:ASN:C[1_554] | 1.65 | 0.55 |
| 1:D:637:LYS:CE | 4:6:311:ASP:CA[1_556] | 1.65 | 0.55 |
| 4:3:75:ILE:CA | 4:7:197:GLY:C[1_554] | 1.65 | 0.55 |
| 4:4:75:ILE:N | 4:8:198:TYR:CA[1_554] | 1.65 | 0.55 |
| 4:4:281:SER:O | 4:7:173:HIS:CE1[1_554] | 1.65 | 0.55 |
| 4:6:310:ALA:O | 4:9:141:SER:C[1_554] | 1.65 | 0.55 |
| 4:6:259:GLU:CD | 4:9:309:ILE:CG1[1_554] | 1.65 | 0.55 |
| 4:6:334:GLU:OE1 | 4:9:133:TYR:CA[1_554] | 1.65 | 0.55 |
| 4:4:315:LYS:N | 4:7:142:LEU:CD1[1_554] | 1.65 | 0.55 |
| 4:5:340:TRP:CD1 | 4:8:118:LYS:CA[1_554] | 1.65 | 0.55 |
| 4:5:272:ALA:CA | 4:8:277:THR:CA[1_554] | 1.65 | 0.55 |
| 4:4:162:ASN:N | 4:7:110:LEU:CG[1_554] | 1.65 | 0.55 |
| 4:4:16:LEU:CA | 4:7:78:ASN:N[1_554] | 1.65 | 0.55 |
| 4:6:207:GLU:CD | 4:9:67:LEU:CB[1_554] | 1.65 | 0.55 |
| 4:6:367:PRO:CD | 4:V:234:SER:O[1_554] | 1.65 | 0.55 |
| 4:5:227:MET:CA | 4:8:307:PRO:CG[1_554] | 1.65 | 0.55 |
| 4:5:137:GLN:OE1 | 4:8:112:PRO:CG[1_554] | 1.65 | 0.55 |
| 4:6:137:GLN:CA | 4:9:112:PRO:C[1_554] | 1.65 | 0.55 |
| 4:4:184:ASP:CG | 4:7:73:HIS:CE1[1_554] | 1.65 | 0.55 |
| 4:6:191:LYS:N | 4:9:186:THR:CB[1_554] | 1.65 | 0.55 |
| 4:5:27:PRO:CA | 4:8:122:ILE:CA[1_554] | 1.65 | 0.55 |
| 4:4:260:THR:C | 4:7:155:SER:OG[1_554] | 1.65 | 0.55 |
| 4:4:181:ALA:CB | 4:7:73:HIS:CB[1_554] | 1.65 | 0.55 |
| 4:4:299:MET:CG | 4:7:136:ILE:CB[1_554] | 1.65 | 0.55 |
| 4:4:185:LEU:CD1 | 4:7:158:GLY:C[1_554] | 1.65 | 0.55 |
| 4:6:369:ILE:C | 4:V:228:ALA:O[1_554] | 1.65 | 0.55 |
| 4:5:366:GLY:C | 4:9:233:SER:C[1_554] | 1.65 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:290:ARG:NE | 4:8:286:ASP:OD2[1_554] | 1.65 | 0.55 |
| 4:5:296:ASN:CA | 4:8:168:GLY:C[1_554] | 1.65 | 0.55 |
| 4:4:345:ILE:CB | 4:7:367:PRO:N[1_554] | 1.65 | 0.55 |
| 4:5:309:ILE:N | 4:8:141:SER:OG[1_554] | 1.65 | 0.55 |
| 4:5:198:TYR:CE2 | 4:8:208:ILE:O[1_554] | 1.65 | 0.55 |
| 4:4:114:ALA:N | 4:8:250:ILE:C[1_554] | 1.65 | 0.55 |
| 4:4:223:PHE:CD2 | 4:7:304:THR:OG1[1_554] | 1.65 | 0.55 |
| 4:4:258:PRO:CA | 4:7:155:SER:C[1_554] | 1.65 | 0.55 |
| 4:2:292:ASP:N | 4:7:40:HIS:NE2[1_554] | 1.65 | 0.55 |
| 4:4:213:LYS:CA | 4:7:16:LEU:N[1_554] | 1.65 | 0.55 |
| 4:6:304:THR:CA | 4:9:137:GLN:CD[1_554] | 1.65 | 0.55 |
| 4:4:274:ILE:O | 4:7:162:ASN:C[1_554] | 1.65 | 0.55 |
| 4:3:174:ALA:N | 4:7:267:ILE:CA[1_554] | 1.65 | 0.55 |
| 4:6:162:ASN:OD1 | 4:9:175:ILE:CA[1_554] | 1.65 | 0.55 |
| 4:5:296:ASN:C | 4:8:168:GLY:C[1_554] | 1.65 | 0.55 |
| 4:5:180:LEU:C | 4:8:159:VAL:CG1[1_554] | 1.65 | 0.55 |
| 4:5:340:TRP:CH2 | 4:8:122:ILE:N[1_554] | 1.65 | 0.55 |
| 4:6:334:GLU:C | 4:9:105:LEU:N[1_554] | 1.65 | 0.55 |
| 4:5:335:ARG:CA | 4:8:105:LEU:C[1_554] | 1.65 | 0.55 |
| 4:6:300:SER:O | 4:9:108:ALA:CA[1_554] | 1.65 | 0.55 |
| 4:5:182:GLY:CA | 4:8:14:SER:OG[1_554] | 1.65 | 0.55 |
| 4:5:307:PRO:CB | 4:8:337:TYR:CB[1_554] | 1.65 | 0.55 |
| 4:4:218:TYR:C | 4:7:336:LYS:O[1_554] | 1.65 | 0.55 |
| 4:5:274:ILE:C | 4:8:163:VAL:N[1_554] | 1.65 | 0.55 |
| 4:5:16:LEU:CB | 4:8:76:ILE:CG2[1_554] | 1.65 | 0.55 |
| 4:4:115:ASN:CA | 4:8:249:THR:O[1_554] | 1.65 | 0.55 |
| 4:4:269:MET:O | 4:7:272:ALA:O[1_554] | 1.65 | 0.55 |
| 4:4:344:SER:N | 4:7:367:PRO:CG[1_554] | 1.65 | 0.55 |
| 4:4:271:SER:O | 4:7:277:THR:CB[1_554] | 1.65 | 0.55 |
| 4:5:280:ASN:OD1 | 4:8:280:ASN:O[1_554] | 1.65 | 0.55 |
| 4:4:199:SER:CA | 4:7:206:ARG:N[1_554] | 1.65 | 0.55 |
| 4:4:198:TYR:C | 4:7:206:ARG:O[1_554] | 1.65 | 0.55 |
| 4:2:291:LYS:CG | 4:7:40:HIS:CA[1_554] | 1.65 | 0.55 |
| 4:6:253:GLU:CG | 4:9:214:GLU:CA[1_554] | 1.66 | 0.54 |
| 4:6:185:LEU:N | 4:9:158:GLY:CA[1_554] | 1.66 | 0.54 |
| 4:4:26:ALA:CB | 4:7:123:MET:N[1_554] | 1.66 | 0.54 |
| 4:5:208:ILE:CA | 4:8:59:GLN:CD[1_554] | 1.66 | 0.54 |
| 4:4:281:SER:C | 4:7:173:HIS:CE1[1_554] | 1.66 | 0.54 |
| 4:3:77:THR:CG2 | 4:7:246:GLN:CD[1_554] | 1.66 | 0.54 |
| 4:5:214:GLU:OE2 | 4:8:33:SER:CB[1_554] | 1.66 | 0.54 |
| 4:4:109:PRO:CB | 4:8:195:GLU:CG[1_554] | 1.66 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:195:GLU:OE1 | 4:9:257:CYS:SG[1_554] | 1.66 | 0.54 |
| 4:5:15:GLY:C | 4:8:77:THR:CB[1_554] | 1.66 | 0.54 |
| 4:4:338:SER:C | 4:7:117:GLU:N[1_554] | 1.66 | 0.54 |
| 4:6:147:ARG:O | 4:9:372:ARG:CG[1_554] | 1.66 | 0.54 |
| 4:6:75:ILE:CA | 4:V:198:TYR:N[1_554] | 1.66 | 0.54 |
| 4:3:109:PRO:N | 4:7:195:GLU:CB[1_554] | 1.66 | 0.54 |
| 1:D:637:LYS:NZ | 4:6:311:ASP:C[1_556] | 1.66 | 0.54 |
| 4:6:11:ASP:OD1 | 4:9:115:ASN:CG[1_554] | 1.66 | 0.54 |
| 4:4:312:ARG:NH2 | 4:7:299:MET:CB[1_554] | 1.66 | 0.54 |
| 4:5:294:TYR:CB | 4:8:166:TYR:CA[1_554] | 1.66 | 0.54 |
| 4:5:17:VAL:CB | 4:8:79:TRP:CD1[1_554] | 1.66 | 0.54 |
| 4:6:340:TRP:NE1 | 4:9:118:LYS:C[1_554] | 1.66 | 0.54 |
| 4:3:109:PRO:CG | 4:7:195:GLU:CG[1_554] | 1.66 | 0.54 |
| 4:6:300:SER:N | 4:9:136:ILE:CA[1_554] | 1.66 | 0.54 |
| 4:6:257:CYS:CB | 4:9:303:THR:OG1[1_554] | 1.66 | 0.54 |
| 4:5:136:ILE:CA | 4:8:113:LYS:CG[1_554] | 1.66 | 0.54 |
| 4:5:185:LEU:CA | 4:8:157:ASP:C[1_554] | 1.66 | 0.54 |
| 4:4:277:THR:CG2 | 4:7:176:MET:N[1_554] | 1.66 | 0.54 |
| 4:4:113:LYS:CB | 4:8:254:ARG:CA[1_554] | 1.66 | 0.54 |
| 4:3:116:ARG:CB | 4:7:252:ASN:OD1[1_554] | 1.66 | 0.54 |
| 4:5:137:GLN:CG | 4:8:112:PRO:CA[1_554] | 1.66 | 0.54 |
| 4:4:308:GLY:CA | 4:7:338:SER:O[1_554] | 1.66 | 0.54 |
| 4:4:258:PRO:O | 4:7:155:SER:C[1_554] | 1.66 | 0.54 |
| 4:6:346:LEU:CD2 | 4:9:368:SER:CA[1_554] | 1.66 | 0.54 |
| 4:5:198:TYR:CD1 | 4:8:208:ILE:CG1[1_554] | 1.66 | 0.54 |
| 4:4:215:LYS:O | 4:7:17:VAL:O[1_554] | 1.66 | 0.54 |
| 4:4:188:TYR:N | 4:7:183:ARG:C[1_554] | 1.66 | 0.54 |
| 4:6:327:ILE:CA | 4:9:149:THR:OG1[1_554] | 1.66 | 0.54 |
| 4:3:113:LYS:CG | 4:7:254:ARG:C[1_554] | 1.66 | 0.54 |
| 4:5:346:LEU:CD1 | 4:8:368:SER:CB[1_554] | 1.66 | 0.54 |
| 4:4:291:LYS:NZ | 4:9:64:ILE:O[1_554] | 1.66 | 0.54 |
| 4:4:195:GLU:CB | 4:7:189:LEU:CD2[1_554] | 1.66 | 0.54 |
| 4:6:346:LEU:O | 4:9:365:ALA:C[1_554] | 1.66 | 0.54 |
| 4:4:185:LEU:CA | 4:7:157:ASP:C[1_554] | 1.66 | 0.54 |
| 4:5:296:ASN:C | 4:8:169:TYR:N[1_554] | 1.66 | 0.54 |
| 4:4:227:MET:CE | 4:7:305:MET:C[1_554] | 1.66 | 0.54 |
| 4:6:227:MET:CA | 4:9:307:PRO:CG[1_554] | 1.66 | 0.54 |
| 4:4:221:LEU:C | 4:7:332:PRO:CD[1_554] | 1.66 | 0.54 |
| 4:6:278:THR:N | 4:9:164:PRO:CG[1_554] | 1.66 | 0.54 |
| 4:5:267:ILE:CG2 | 4:8:180:LEU:CD1[1_554] | 1.66 | 0.54 |
| 4:6:26:ALA:C | 4:9:122:ILE:C[1_554] | 1.66 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:367:PRO:C | 4:8:236:LEU:N[1_554] | 1.66 | 0.54 |
| 4:5:145:SER:CA | 4:8:372:ARG:CZ[1_554] | 1.66 | 0.54 |
| 4:6:256:ARG:O | 4:9:303:THR:CG2[1_554] | 1.66 | 0.54 |
| 4:5:190:MET:C | 4:8:186:THR:CG2[1_554] | 1.66 | 0.54 |
| 4:6:329:ILE:CG1 | 4:9:142:LEU:CD2[1_554] | 1.66 | 0.54 |
| 4:6:112:PRO:CA | 4:V:253:GLU:CD[1_554] | 1.66 | 0.54 |
| 4:4:326:LYS:N | 4:7:167:GLU:CD[1_554] | 1.66 | 0.54 |
| 4:5:277:THR:CG2 | 4:8:175:ILE:CA[1_554] | 1.66 | 0.54 |
| 4:6:334:GLU:CG | 4:9:103:THR:O[1_554] | 1.66 | 0.54 |
| 4:4:282:ILE:CG1 | 4:7:171:LEU:CB[1_554] | 1.66 | 0.54 |
| 4:4:59:GLN:CG | 4:7:68:LYS:CG[1_554] | 1.66 | 0.54 |
| 4:3:166:TYR:CD1 | 4:8:40:HIS:CD2[1_554] | 1.66 | 0.54 |
| 4:5:180:LEU:CA | 4:8:179:ASP:OD1[1_554] | 1.66 | 0.54 |
| 4:4:370:VAL:CA | 4:8:230:ALA:CA[1_554] | 1.66 | 0.54 |
| 4:4:369:ILE:O | 4:8:230:ALA:N[1_554] | 1.66 | 0.54 |
| 4:6:159:VAL:N | 4:9:177:ARG:NH2[1_554] | 1.66 | 0.54 |
| 4:6:188:TYR:CD1 | 4:9:185:LEU:CB[1_554] | 1.66 | 0.54 |
| 4:5:336:LYS:CA | 4:8:106:THR:O[1_554] | 1.66 | 0.54 |
| 4:4:277:THR:O | 4:7:174:ALA:CA[1_554] | 1.66 | 0.54 |
| 4:5:257:CYS:O | 4:8:303:THR:CB[1_554] | 1.66 | 0.54 |
| 4:6:320:LEU:CB | 4:9:293:LEU:C[1_554] | 1.66 | 0.54 |
| 4:5:337:TYR:CE2 | 4:8:86:TRP:CE2[1_554] | 1.66 | 0.54 |
| 1:D:637:LYS:CE | 4:6:311:ASP:CG[1_556] | 1.66 | 0.54 |
| 4:5:30:VAL:CG1 | 4:8:82:MET:CA[1_554] | 1.66 | 0.54 |
| 4:5:16:LEU:CD1 | 4:8:70:PRO:CB[1_554] | 1.66 | 0.54 |
| 4:6:184:ASP:OD1 | 4:9:73:HIS:ND1[1_554] | 1.66 | 0.54 |
| 4:5:305:MET:SD | 4:8:106:THR:OG1[1_554] | 1.66 | 0.54 |
| 4:5:221:LEU:C | 4:8:331:ALA:O[1_554] | 1.66 | 0.54 |
| 4:5:30:VAL:CB | 4:8:82:MET:C[1_554] | 1.66 | 0.54 |
| 4:5:155:SER:N | 4:8:108:ALA:C[1_554] | 1.66 | 0.54 |
| 4:6:154:ASP:CG | 4:9:111:ASN:CB[1_554] | 1.66 | 0.54 |
| 4:5:190:MET:CG | 4:8:206:ARG:NH2[1_554] | 1.66 | 0.54 |
| 4:4:331:ALA:N | 4:7:135:ALA:CB[1_554] | 1.66 | 0.54 |
| 4:5:274:ILE:N | 4:8:162:ASN:CA[1_554] | 1.66 | 0.54 |
| 4:6:262:PHE:CZ | 4:9:153:LEU:C[1_554] | 1.66 | 0.54 |
| 4:5:109:PRO:N | 4:9:195:GLU:CG[1_554] | 1.66 | 0.54 |
| 4:4:256:ARG:CA | 4:7:303:THR:N[1_554] | 1.66 | 0.54 |
| 4:5:32:PRO:C | 4:8:78:ASN:CG[1_554] | 1.66 | 0.54 |
| 4:6:205:GLU:CD | 4:9:203:THR:OG1[1_554] | 1.66 | 0.54 |
| 4:6:317:ILE:CA | 4:9:151:ILE:N[1_554] | 1.66 | 0.54 |
| 4:4:340:TRP:CG | 4:7:118:LYS:CD[1_554] | 1.66 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:218:TYR:O | 4:8:302:GLY:N[1_554] | 1.67 | 0.53 |
| 4:4:299:MET:C | 4:7:107:GLU:CG[1_554] | 1.67 | 0.53 |
| 4:5:157:ASP:CB | 4:8:72:GLU:O[1_554] | 1.67 | 0.53 |
| 4:5:17:VAL:O | 4:8:79:TRP:CB[1_554] | 1.67 | 0.53 |
| 4:6:207:GLU:OE2 | 4:9:67:LEU:CB[1_554] | 1.67 | 0.53 |
| 4:5:274:ILE:N | 4:8:162:ASN:OD1[1_554] | 1.67 | 0.53 |
| 4:4:293:LEU:CG | 4:7:169:TYR:OH[1_554] | 1.67 | 0.53 |
| 4:5:139:VAL:C | 4:8:371:HIS:CE1[1_554] | 1.67 | 0.53 |
| 4:5:305:MET:CA | 4:8:11:ASP:CG[1_554] | 1.67 | 0.53 |
| 4:4:223:PHE:CE1 | 4:7:301:GLY:O[1_554] | 1.67 | 0.53 |
| 4:5:185:LEU:N | 4:8:158:GLY:CA[1_554] | 1.67 | 0.53 |
| 4:4:198:TYR:C | 4:7:205:GLU:O[1_554] | 1.67 | 0.53 |
| 4:4:154:ASP:CB | 4:7:111:ASN:CA[1_554] | 1.67 | 0.53 |
| 4:4:309:ILE:N | 4:7:339:VAL:CG2[1_554] | 1.67 | 0.53 |
| 4:4:112:PRO:O | 4:8:253:GLU:OE2[1_554] | 1.67 | 0.53 |
| 4:4:197:GLY:C | 4:7:208:ILE:CG2[1_554] | 1.67 | 0.53 |
| 4:4:199:SER:N | 4:7:206:ARG:CA[1_554] | 1.67 | 0.53 |
| 4:5:340:TRP:CD1 | 4:8:119:MET:N[1_554] | 1.67 | 0.53 |
| 4:4:220:ALA:CB | 4:7:335:ARG:N[1_554] | 1.67 | 0.53 |
| 4:5:343:GLY:O | 4:8:367:PRO:C[1_554] | 1.67 | 0.53 |
| 4:4:27:PRO:CD | 4:7:122:ILE:CB[1_554] | 1.67 | 0.53 |
| 4:6:24:ASP:CB | 4:9:124:PHE:CA[1_554] | 1.67 | 0.53 |
| 4:4:327:ILE:CG2 | 4:7:148:THR:C[1_554] | 1.67 | 0.53 |
| 4:6:295:ALA:N | 4:9:167:GLU:C[1_554] | 1.67 | 0.53 |
| 4:4:333:PRO:CB | 4:7:104:LEU:N[1_554] | 1.67 | 0.53 |
| 4:4:74:GLY:O | 4:8:197:GLY:C[1_554] | 1.67 | 0.53 |
| 4:4:204:ALA:O | 4:7:62:ARG:CG[1_554] | 1.67 | 0.53 |
| 4:6:301:GLY:CA | 4:9:107:GLU:C[1_554] | 1.67 | 0.53 |
| 4:6:321:ALA:CA | 4:9:292:ASP:CB[1_554] | 1.67 | 0.53 |
| 4:6:346:LEU:CB | 4:9:368:SER:CB[1_554] | 1.67 | 0.53 |
| 4:3:114:ALA:N | 4:7:250:ILE:O[1_554] | 1.67 | 0.53 |
| 4:6:295:ALA:N | 4:9:167:GLU:CA[1_554] | 1.67 | 0.53 |
| 4:6:240:TYR:OH | 4:9:56:ASP:OD2[1_554] | 1.67 | 0.53 |
| 4:4:317:ILE:CB | 4:7:165:ILE:N[1_554] | 1.67 | 0.53 |
| 4:4:24:ASP:CB | 4:7:125:GLU:CD[1_554] | 1.67 | 0.53 |
| 4:5:205:GLU:OE2 | 4:8:203:THR:OG1[1_554] | 1.67 | 0.53 |
| 4:6:188:TYR:N | 4:9:183:ARG:CA[1_554] | 1.67 | 0.53 |
| 4:5:260:THR:CG2 | 4:8:180:LEU:O[1_554] | 1.67 | 0.53 |
| 4:5:310:ALA:O | 4:8:141:SER:C[1_554] | 1.67 | 0.53 |
| 4:5:275:HIS:C | 4:8:151:ILE:CD1[1_554] | 1.67 | 0.53 |
| 4:5:214:GLU:OE1 | 4:8:33:SER:CA[1_554] | 1.67 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:75:ILE:CD1 | 4:7:193:LEU:C[1_554] | 1.67 | 0.53 |
| 4:6:274:ILE:N | 4:9:162:ASN:CG[1_554] | 1.67 | 0.53 |
| 4:5:32:PRO:CD | 4:8:81:ASP:CB[1_554] | 1.67 | 0.53 |
| 4:4:263:GLN:CD | 4:7:153:LEU:CD2[1_554] | 1.67 | 0.53 |
| 4:3:357:ILE:CG2 | 4:7:232:SER:CA[1_554] | 1.67 | 0.53 |
| 4:6:243:PRO:CA | 4:9:60:SER:CA[1_554] | 1.67 | 0.53 |
| 4:5:294:TYR:CZ | 4:8:289:ILE:CD1[1_554] | 1.67 | 0.53 |
| 4:4:210:ARG:CD | 4:7:69:TYR:CA[1_554] | 1.67 | 0.53 |
| 4:4:263:GLN:CA | 4:7:274:ILE:CG1[1_554] | 1.67 | 0.53 |
| 4:4:270:GLU:N | 4:7:272:ALA:C[1_554] | 1.67 | 0.53 |
| 4:5:265:SER:OG | 4:8:261:LEU:O[1_554] | 1.67 | 0.53 |
| 4:6:305:MET:CA | 4:9:11:ASP:OD2[1_554] | 1.67 | 0.53 |
| 4:4:240:TYR:OH | 4:7:56:ASP:N[1_554] | 1.67 | 0.53 |
| 4:6:173:HIS:CE1 | 4:V:266:PHE:N[1_554] | 1.67 | 0.53 |
| 4:5:188:TYR:CE1 | 4:8:185:LEU:CB[1_554] | 1.67 | 0.53 |
| 4:6:204:ALA:C | 4:9:62:ARG:NE[1_554] | 1.67 | 0.53 |
| 4:5:299:MET:C | 4:8:136:ILE:N[1_554] | 1.67 | 0.53 |
| 4:4:293:LEU:CA | 4:7:169:TYR:CD2[1_554] | 1.67 | 0.53 |
| 4:6:214:GLU:CD | 4:9:33:SER:CB[1_554] | 1.67 | 0.53 |
| 4:5:300:SER:CB | 4:8:107:GLU:CD[1_554] | 1.67 | 0.53 |
| 4:6:274:ILE:CB | 4:9:162:ASN:N[1_554] | 1.67 | 0.53 |
| 4:6:320:LEU:CB | 4:9:293:LEU:CA[1_554] | 1.67 | 0.53 |
| 4:5:263:GLN:CB | 4:8:274:ILE:CB[1_554] | 1.67 | 0.53 |
| 4:6:310:ALA:CB | 4:9:141:SER:CA[1_554] | 1.67 | 0.53 |
| 4:5:348:SER:O | 4:8:364:GLU:C[1_554] | 1.67 | 0.53 |
| 4:4:321:ALA:C | 4:7:292:ASP:OD2[1_554] | 1.67 | 0.53 |
| 4:5:207:GLU:OE2 | 4:8:67:LEU:CB[1_554] | 1.67 | 0.53 |
| 4:6:267:ILE:CG1 | 4:9:180:LEU:CD1[1_554] | 1.67 | 0.53 |
| 4:6:196:ARG:CG | 4:9:211:ASP:C[1_554] | 1.67 | 0.53 |
| 4:6:190:MET:CE | 4:9:206:ARG:CZ[1_554] | 1.67 | 0.53 |
| 4:6:310:ALA:CA | 4:9:142:LEU:N[1_554] | 1.67 | 0.53 |
| 4:4:367:PRO:CA | 4:8:234:SER:C[1_554] | 1.67 | 0.53 |
| 4:5:11:ASP:OD1 | 4:8:115:ASN:CB[1_554] | 1.67 | 0.53 |
| 4:6:208:ILE:CA | 4:9:59:GLN:CD[1_554] | 1.67 | 0.53 |
| 4:6:322:PRO:CA | 4:9:291:LYS:CE[1_554] | 1.67 | 0.53 |
| 4:6:31:PHE:O | 4:9:78:ASN:CA[1_554] | 1.67 | 0.53 |
| 4:6:180:LEU:CD1 | 4:9:178:LEU:O[1_554] | 1.67 | 0.53 |
| 4:4:289:ILE:CG2 | 4:9:39:ARG:NH2[1_554] | 1.67 | 0.53 |
| 4:4:117:GLU:O | 4:8:237:GLU:CB[1_554] | 1.67 | 0.53 |
| 4:4:208:ILE:CG2 | 4:7:59:GLN:OE1[1_554] | 1.68 | 0.52 |
| 4:4:24:ASP:N | 4:7:125:GLU:OE1[1_554] | 1.68 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:337:TYR:CD1 | 4:8:86:TRP:CZ2[1_554] | 1.68 | 0.52 |
| 4:5:26:ALA:CA | 4:8:123:MET:CG[1_554] | 1.68 | 0.52 |
| 4:5:261:LEU:CG | 4:8:154:ASP:O[1_554] | 1.68 | 0.52 |
| 4:5:297:ASN:OD1 | 4:8:165:ILE:CA[1_554] | 1.68 | 0.52 |
| 4:6:254:ARG:NH1 | 4:9:336:LYS:NZ[1_554] | 1.68 | 0.52 |
| 4:6:253:GLU:OE1 | 4:9:214:GLU:CA[1_554] | 1.68 | 0.52 |
| 4:4:215:LYS:CG | 4:7:31:PHE:CB[1_554] | 1.68 | 0.52 |
| 4:6:319:ALA:CA | 4:9:296:ASN:N[1_554] | 1.68 | 0.52 |
| 4:5:161:HIS:C | 4:8:110:LEU:CD2[1_554] | 1.68 | 0.52 |
| 4:4:259:GLU:CD | 4:7:304:THR:CB[1_554] | 1.68 | 0.52 |
| 4:6:204:ALA:CA | 4:9:62:ARG:CD[1_554] | 1.68 | 0.52 |
| 4:5:329:ILE:CD1 | 4:8:142:LEU:CD2[1_554] | 1.68 | 0.52 |
| 4:6:317:ILE:N | 4:9:150:GLY:C[1_554] | 1.68 | 0.52 |
| 4:5:308:GLY:C | 4:8:338:SER:OG[1_554] | 1.68 | 0.52 |
| 4:6:204:ALA:CB | 4:9:62:ARG:CA[1_554] | 1.68 | 0.52 |
| 4:5:193:LEU:CD1 | 4:8:210:ARG:O[1_554] | 1.68 | 0.52 |
| 4:6:178:LEU:CB | 4:9:177:ARG:CB[1_554] | 1.68 | 0.52 |
| 4:4:142:LEU:C | 4:7:372:ARG:CA[1_554] | 1.68 | 0.52 |
| 4:5:318:THR:O | 4:8:292:ASP:C[1_554] | 1.68 | 0.52 |
| 4:6:280:ASN:OD1 | 4:9:281:SER:N[1_554] | 1.68 | 0.52 |
| 4:5:289:ILE:N | 4:V:64:ILE:N[1_554] | 1.68 | 0.52 |
| 4:6:321:ALA:O | 4:9:292:ASP:CB[1_554] | 1.68 | 0.52 |
| 4:4:182:GLY:CA | 4:7:14:SER:OG[1_554] | 1.68 | 0.52 |
| 4:4:142:LEU:CG | 4:7:372:ARG:O[1_554] | 1.68 | 0.52 |
| 4:5:173:HIS:CB | 4:9:267:ILE:CG1[1_554] | 1.68 | 0.52 |
| 4:4:190:MET:O | 4:7:186:THR:CG2[1_554] | 1.68 | 0.52 |
| 4:5:333:PRO:CD | 4:8:104:LEU:CB[1_554] | 1.68 | 0.52 |
| 4:5:223:PHE:CD1 | 4:8:304:THR:C[1_554] | 1.68 | 0.52 |
| 4:5:56:ASP:OD1 | 4:8:80:ASP:OD1[1_554] | 1.68 | 0.52 |
| 4:4:311:ASP:CA | 4:7:141:SER:C[1_554] | 1.68 | 0.52 |
| 4:6:201:VAL:CG2 | 4:9:203:THR:N[1_554] | 1.68 | 0.52 |
| 4:6:341:ILE:O | 4:9:120:THR:CG2[1_554] | 1.68 | 0.52 |
| 4:5:270:GLU:C | 4:8:272:ALA:N[1_554] | 1.68 | 0.52 |
| 4:5:137:GLN:CD | 4:8:112:PRO:CA[1_554] | 1.68 | 0.52 |
| 4:4:211:ASP:CG | 4:7:32:PRO:O[1_554] | 1.68 | 0.52 |
| 4:4:157:ASP:CG | 4:7:72:GLU:CA[1_554] | 1.68 | 0.52 |
| 4:4:16:LEU:CD1 | 4:7:78:ASN:C[1_554] | 1.68 | 0.52 |
| 4:6:340:TRP:CD2 | 4:9:119:MET:C[1_554] | 1.68 | 0.52 |
| 4:4:218:TYR:CD2 | 4:7:337:TYR:CD2[1_554] | 1.68 | 0.52 |
| 4:3:173:HIS:O | 4:7:267:ILE:CB[1_554] | 1.68 | 0.52 |
| 4:6:327:ILE:CG2 | 4:9:148:THR:C[1_554] | 1.68 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:115:ASN:N | 4:8:250:ILE:C[1_554] | 1.68 | 0.52 |
| 4:6:210:ARG:CB | 4:9:69:TYR:CE2[1_554] | 1.68 | 0.52 |
| 4:4:327:ILE:CB | 4:7:148:THR:C[1_554] | 1.68 | 0.52 |
| 4:6:277:THR:N | 4:9:281:SER:CB[1_554] | 1.68 | 0.52 |
| 4:5:337:TYR:CD1 | 4:8:86:TRP:CH2[1_554] | 1.68 | 0.52 |
| 4:6:299:MET:SD | 4:9:138:ALA:CA[1_554] | 1.68 | 0.52 |
| 4:5:277:THR:N | 4:8:281:SER:CB[1_554] | 1.68 | 0.52 |
| 4:6:211:ASP:O | 4:9:16:LEU:CD1[1_554] | 1.68 | 0.52 |
| 4:4:213:LYS:NZ | 4:7:14:SER:O[1_554] | 1.68 | 0.52 |
| 4:3:112:PRO:O | 4:7:253:GLU:OE2[1_554] | 1.68 | 0.52 |
| 4:5:315:LYS:CE | 4:8:147:ARG:NH1[1_554] | 1.68 | 0.52 |
| 4:5:173:HIS:CA | 4:9:267:ILE:CB[1_554] | 1.68 | 0.52 |
| 4:4:266:PHE:N | 4:7:261:LEU:CD2[1_554] | 1.68 | 0.52 |
| 4:6:265:SER:CB | 4:9:261:LEU:O[1_554] | 1.68 | 0.52 |
| 4:3:169:TYR:OH | 4:7:266:PHE:CZ[1_554] | 1.68 | 0.52 |
| 4:5:155:SER:OG | 4:8:161:HIS:CE1[1_554] | 1.68 | 0.52 |
| 4:6:283:MET:CE | 4:9:286:ASP:O[1_554] | 1.68 | 0.52 |
| 4:6:154:ASP:CA | 4:9:108:ALA:C[1_554] | 1.68 | 0.52 |
| 4:5:274:ILE:CG1 | 4:8:161:HIS:CA[1_554] | 1.68 | 0.52 |
| 4:6:339:VAL:CA | 4:9:116:ARG:CG[1_554] | 1.68 | 0.52 |
| 4:5:300:SER:O | 4:8:107:GLU:O[1_554] | 1.68 | 0.52 |
| 4:6:321:ALA:C | 4:9:292:ASP:N[1_554] | 1.68 | 0.52 |
| 4:4:183:ARG:N | 4:7:73:HIS:N[1_554] | 1.68 | 0.52 |
| 4:3:115:ASN:O | 4:7:237:GLU:OE1[1_554] | 1.68 | 0.52 |
| 4:3:117:GLU:N | 4:7:237:GLU:OE2[1_554] | 1.68 | 0.52 |
| 4:3:372:ARG:C | 4:7:255:PHE:CZ[1_554] | 1.68 | 0.52 |
| 4:3:113:LYS:CE | 4:7:254:ARG:CG[1_554] | 1.68 | 0.52 |
| 4:6:164:PRO:CA | 4:9:172:PRO:CG[1_554] | 1.68 | 0.52 |
| 4:6:258:PRO:N | 4:9:155:SER:O[1_554] | 1.68 | 0.52 |
| 4:4:27:PRO:CA | 4:7:122:ILE:CG1[1_554] | 1.68 | 0.52 |
| 4:5:178:LEU:CB | 4:8:177:ARG:CB[1_554] | 1.68 | 0.52 |
| 4:6:115:ASN:CA | 4:V:196:ARG:NH2[1_554] | 1.68 | 0.52 |
| 4:4:200:PHE:CA | 4:7:206:ARG:CG[1_554] | 1.68 | 0.52 |
| 4:4:309:ILE:C | 4:7:137:GLN:O[1_554] | 1.68 | 0.52 |
| 4:5:196:ARG:NE | 4:8:211:ASP:C[1_554] | 1.68 | 0.52 |
| 4:6:349:LEU:N | 4:9:366:GLY:N[1_554] | 1.68 | 0.52 |
| 4:6:339:VAL:CG1 | 4:9:115:ASN:C[1_554] | 1.68 | 0.52 |
| 4:6:340:TRP:CH2 | 4:9:121:GLN:CA[1_554] | 1.68 | 0.52 |
| 4:4:243:PRO:CD | 4:7:60:SER:C[1_554] | 1.68 | 0.52 |
| 4:4:222:ASP:CB | 4:7:331:ALA:C[1_554] | 1.68 | 0.52 |
| 4:6:335:ARG:C | 4:9:106:THR:N[1_554] | 1.68 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:156:GLY:CA | 4:9:75:ILE:N[1_554] | 1.69 | 0.51 |
| 4:4:299:MET:SD | 4:7:136:ILE:CG2[1_554] | 1.69 | 0.51 |
| 4:6:315:LYS:CE | 4:9:147:ARG:NH1[1_554] | 1.69 | 0.51 |
| 4:5:11:ASP:OD1 | 4:8:115:ASN:CG[1_554] | 1.69 | 0.51 |
| 4:5:276:GLU:N | 4:8:151:ILE:CD1[1_554] | 1.69 | 0.51 |
| 4:4:194:THR:O | 4:7:209:VAL:CG2[1_554] | 1.69 | 0.51 |
| 4:4:255:PHE:CD1 | 4:7:305:MET:CB[1_554] | 1.69 | 0.51 |
| 4:5:340:TRP:CG | 4:8:119:MET:CA[1_554] | 1.69 | 0.51 |
| 4:5:293:LEU:CA | 4:8:169:TYR:CD2[1_554] | 1.69 | 0.51 |
| 4:5:197:GLY:N | 4:8:212:ILE:CD1[1_554] | 1.69 | 0.51 |
| 4:4:110:LEU:C | 4:8:192:ILE:CB[1_554] | 1.69 | 0.51 |
| 4:3:116:ARG:C | 4:7:237:GLU:CD[1_554] | 1.69 | 0.51 |
| 4:5:191:LYS:C | 4:8:186:THR:O[1_554] | 1.69 | 0.51 |
| 4:4:188:TYR:CZ | 4:7:185:LEU:CD2[1_554] | 1.69 | 0.51 |
| 4:5:243:PRO:CG | 4:8:59:GLN:O[1_554] | 1.69 | 0.51 |
| 4:4:371:HIS:NE2 | 4:8:252:ASN:O[1_554] | 1.69 | 0.51 |
| 4:4:198:TYR:O | 4:7:206:ARG:O[1_554] | 1.69 | 0.51 |
| 4:4:333:PRO:C | 4:7:105:LEU:N[1_554] | 1.69 | 0.51 |
| 4:6:340:TRP:CG | 4:9:119:MET:C[1_554] | 1.69 | 0.51 |
| 4:4:300:SER:C | 4:7:107:GLU:CB[1_554] | 1.69 | 0.51 |
| 4:6:178:LEU:CD1 | 4:9:177:ARG:O[1_554] | 1.69 | 0.51 |
| 4:4:336:LYS:CD | 4:7:86:TRP:CE2[1_554] | 1.69 | 0.51 |
| 4:4:215:LYS:CG | 4:7:31:PHE:CD2[1_554] | 1.69 | 0.51 |
| 4:5:17:VAL:N | 4:8:79:TRP:N[1_554] | 1.69 | 0.51 |
| 4:6:302:GLY:CA | 4:9:12:ASN:O[1_554] | 1.69 | 0.51 |
| 4:4:288:ASP:O | 4:9:65:LEU:N[1_554] | 1.69 | 0.51 |
| 4:4:221:LEU:O | 4:7:332:PRO:CB[1_554] | 1.69 | 0.51 |
| 4:4:291:LYS:N | 4:9:64:ILE:CG2[1_554] | 1.69 | 0.51 |
| 4:5:24:ASP:OD1 | 4:8:125:GLU:CA[1_554] | 1.69 | 0.51 |
| 4:4:337:TYR:OH | 4:7:86:TRP:CZ3[1_554] | 1.69 | 0.51 |
| 4:5:180:LEU:CD2 | 4:8:178:LEU:CA[1_554] | 1.69 | 0.51 |
| 4:5:329:ILE:CG1 | 4:8:142:LEU:CD2[1_554] | 1.69 | 0.51 |
| 4:4:77:THR:CB | 4:8:246:GLN:OE1[1_554] | 1.69 | 0.51 |
| 4:6:196:ARG:CD | 4:9:211:ASP:O[1_554] | 1.69 | 0.51 |
| 4:5:153:LEU:CG | 4:8:109:PRO:CG[1_554] | 1.69 | 0.51 |
| 4:4:221:LEU:N | 4:7:338:SER:OG[1_554] | 1.69 | 0.51 |
| 4:6:207:GLU:OE2 | 4:9:67:LEU:C[1_554] | 1.69 | 0.51 |
| 4:6:297:ASN:OD1 | 4:9:165:ILE:CB[1_554] | 1.69 | 0.51 |
| 4:5:278:THR:CB | 4:8:163:VAL:C[1_554] | 1.69 | 0.51 |
| 4:6:346:LEU:C | 4:9:366:GLY:O[1_554] | 1.69 | 0.51 |
| 4:4:144:ALA:O | 4:7:370:VAL:C[1_554] | 1.69 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:196:ARG:CD | 4:7:211:ASP:C[1_554] | 1.69 | 0.51 |
| 4:5:340:TRP:CE3 | 4:8:120:THR:N[1_554] | 1.69 | 0.51 |
| 4:4:291:LYS:CD | 4:9:64:ILE:CD1[1_554] | 1.69 | 0.51 |
| 4:2:326:LYS:CG | 4:7:42:GLY:CA[1_554] | 1.69 | 0.51 |
| 4:5:113:LYS:N | 4:9:253:GLU:N[1_554] | 1.69 | 0.51 |
| 4:4:15:GLY:N | 4:7:77:THR:OG1[1_554] | 1.69 | 0.51 |
| 4:5:154:ASP:C | 4:8:109:PRO:N[1_554] | 1.69 | 0.51 |
| 4:4:345:ILE:CG1 | 4:7:366:GLY:C[1_554] | 1.69 | 0.51 |
| 4:5:154:ASP:CA | 4:8:109:PRO:CA[1_554] | 1.69 | 0.51 |
| 4:4:30:VAL:C | 4:7:80:ASP:CA[1_554] | 1.69 | 0.51 |
| 4:6:109:PRO:CA | 4:V:195:GLU:CD[1_554] | 1.69 | 0.51 |
| 4:4:25:ASP:N | 4:7:125:GLU:N[1_554] | 1.69 | 0.51 |
| 4:4:258:PRO:CA | 4:7:156:GLY:N[1_554] | 1.69 | 0.51 |
| 4:6:276:GLU:OE2 | 4:9:278:THR:CA[1_554] | 1.69 | 0.51 |
| 4:4:304:THR:OG1 | 4:7:107:GLU:CA[1_554] | 1.69 | 0.51 |
| 4:5:317:ILE:C | 4:8:150:GLY:CA[1_554] | 1.69 | 0.51 |
| 4:4:304:THR:CG2 | 4:7:108:ALA:N[1_554] | 1.69 | 0.51 |
| 4:5:192:ILE:N | 4:8:186:THR:N[1_554] | 1.69 | 0.51 |
| 4:5:198:TYR:CD2 | 4:8:208:ILE:CA[1_554] | 1.69 | 0.51 |
| 4:6:24:ASP:CA | 4:9:124:PHE:O[1_554] | 1.69 | 0.51 |
| 4:6:270:GLU:N | 4:9:272:ALA:O[1_554] | 1.69 | 0.51 |
| 4:5:308:GLY:N | 4:8:338:SER:C[1_554] | 1.69 | 0.51 |
| 4:2:288:ASP:CA | 4:7:39:ARG:NE[1_554] | 1.69 | 0.51 |
| 4:4:24:ASP:CB | 4:7:125:GLU:CB[1_554] | 1.69 | 0.51 |
| 4:6:327:ILE:CD1 | 4:9:149:THR:OG1[1_554] | 1.69 | 0.51 |
| 4:6:60:SER:OG | 4:9:37:ARG:CG[1_554] | 1.69 | 0.51 |
| 4:5:253:GLU:OE2 | 4:8:214:GLU:C[1_554] | 1.69 | 0.51 |
| 4:4:199:SER:C | 4:7:206:ARG:CG[1_554] | 1.69 | 0.51 |
| 4:5:275:HIS:N | 4:8:162:ASN:CA[1_554] | 1.69 | 0.51 |
| 4:5:172:PRO:CG | 4:9:266:PHE:CA[1_554] | 1.69 | 0.51 |
| 4:6:178:LEU:CD2 | 4:9:177:ARG:CA[1_554] | 1.69 | 0.51 |
| 4:4:184:ASP:CB | 4:7:73:HIS:CE1[1_554] | 1.69 | 0.51 |
| 4:4:257:CYS:O | 4:7:156:GLY:N[1_554] | 1.69 | 0.51 |
| 4:4:195:GLU:CG | 4:7:189:LEU:CG[1_554] | 1.69 | 0.51 |
| 4:4:258:PRO:CA | 4:7:155:SER:O[1_554] | 1.69 | 0.51 |
| 4:6:151:ILE:CG2 | 4:9:170:ALA:O[1_554] | 1.69 | 0.51 |
| 4:5:320:LEU:CA | 4:8:293:LEU:CA[1_554] | 1.69 | 0.51 |
| 4:6:327:ILE:C | 4:9:148:THR:CA[1_554] | 1.69 | 0.51 |
| 4:6:372:ARG:O | 4:V:227:MET:SD[1_554] | 1.69 | 0.51 |
| 4:3:114:ALA:C | 4:7:250:ILE:CA[1_554] | 1.70 | 0.50 |
| 4:6:294:TYR:CB | 4:9:166:TYR:CA[1_554] | 1.70 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:317:ILE:C | 4:9:150:GLY:CA[1_554] | 1.70 | 0.50 |
| 4:3:115:ASN:OD1 | 4:7:249:THR:C[1_554] | 1.70 | 0.50 |
| 4:5:274:ILE:N | 4:8:162:ASN:CG[1_554] | 1.70 | 0.50 |
| 4:5:187:ASP:N | 4:8:183:ARG:CD[1_554] | 1.70 | 0.50 |
| 4:6:93:GLU:OE2 | 4:9:80:ASP:OD2[1_554] | 1.70 | 0.50 |
| 4:5:31:PHE:CB | 4:8:80:ASP:C[1_554] | 1.70 | 0.50 |
| 4:4:274:ILE:N | 4:7:162:ASN:CA[1_554] | 1.70 | 0.50 |
| 4:3:367:PRO:O | 4:7:236:LEU:CG[1_554] | 1.70 | 0.50 |
| 4:4:279:TYR:CE2 | 4:7:285:CYS:CB[1_554] | 1.70 | 0.50 |
| 4:5:213:LYS:NZ | 4:8:14:SER:CB[1_554] | 1.70 | 0.50 |
| 4:5:309:ILE:CD1 | 4:8:154:ASP:CG[1_554] | 1.70 | 0.50 |
| 4:6:10:CYS:CA | 4:9:118:LYS:CD[1_554] | 1.70 | 0.50 |
| 4:6:137:GLN:OE1 | 4:9:112:PRO:N[1_554] | 1.70 | 0.50 |
| 4:5:11:ASP:O | 4:8:79:TRP:CZ2[1_554] | 1.70 | 0.50 |
| 4:6:249:THR:N | 4:9:211:ASP:OD2[1_554] | 1.70 | 0.50 |
| 4:5:199:SER:N | 4:8:206:ARG:N[1_554] | 1.70 | 0.50 |
| 4:4:185:LEU:CA | 4:7:157:ASP:O[1_554] | 1.70 | 0.50 |
| 4:5:280:ASN:CG | 4:8:281:SER:C[1_554] | 1.70 | 0.50 |
| 4:4:302:GLY:O | 4:7:12:ASN:O[1_554] | 1.70 | 0.50 |
| 4:5:255:PHE:CG | 4:8:305:MET:CG[1_554] | 1.70 | 0.50 |
| 4:4:223:PHE:O | 4:7:335:ARG:NE[1_554] | 1.70 | 0.50 |
| 4:5:267:ILE:N | 4:8:180:LEU:CD1[1_554] | 1.70 | 0.50 |
| 4:4:280:ASN:OD1 | 4:7:281:SER:C[1_554] | 1.70 | 0.50 |
| 4:6:348:SER:CB | 4:9:362:TYR:C[1_554] | 1.70 | 0.50 |
| 4:6:214:GLU:OE2 | 4:9:33:SER:CB[1_554] | 1.70 | 0.50 |
| 4:5:188:TYR:CA | 4:8:183:ARG:C[1_554] | 1.70 | 0.50 |
| 4:4:26:ALA:CA | 4:7:122:ILE:C[1_554] | 1.70 | 0.50 |
| 4:5:31:PHE:N | 4:8:79:TRP:C[1_554] | 1.70 | 0.50 |
| 4:6:276:GLU:OE1 | 4:9:280:ASN:N[1_554] | 1.70 | 0.50 |
| 4:6:340:TRP:C | 4:9:120:THR:CB[1_554] | 1.70 | 0.50 |
| 4:5:340:TRP:NE1 | 4:8:118:LYS:C[1_554] | 1.70 | 0.50 |
| 4:4:317:ILE:N | 4:7:150:GLY:O[1_554] | 1.70 | 0.50 |
| 4:5:191:LYS:CB | 4:8:186:THR:C[1_554] | 1.70 | 0.50 |
| 4:4:300:SER:N | 4:7:107:GLU:OE2[1_554] | 1.70 | 0.50 |
| 4:5:27:PRO:O | 4:8:122:ILE:CG2[1_554] | 1.70 | 0.50 |
| 4:6:299:MET:CE | 4:9:139:VAL:N[1_554] | 1.70 | 0.50 |
| 4:6:21:PHE:CB | 4:9:125:GLU:CG[1_554] | 1.70 | 0.50 |
| 4:5:196:ARG:CD | 4:8:211:ASP:C[1_554] | 1.70 | 0.50 |
| 4:3:287:ILE:O | 4:8:63:GLY:N[1_554] | 1.70 | 0.50 |
| 4:5:151:ILE:CB | 4:8:170:ALA:C[1_554] | 1.70 | 0.50 |
| 4:4:174:ALA:N | 4:8:267:ILE:CA[1_554] | 1.70 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:283:MET:CG | 4:8:286:ASP:O[1_554] | 1.70 | 0.50 |
| 4:4:336:LYS:CE | 4:7:86:TRP:CD2[1_554] | 1.70 | 0.50 |
| 4:4:173:HIS:ND1 | 4:8:266:PHE:N[1_554] | 1.70 | 0.50 |
| 4:6:347:ALA:N | 4:9:367:PRO:N[1_554] | 1.70 | 0.50 |
| 4:4:243:PRO:CA | 4:7:60:SER:OG[1_554] | 1.70 | 0.50 |
| 4:5:156:GLY:C | 4:8:74:GLY:N[1_554] | 1.70 | 0.50 |
| 4:5:319:ALA:CA | 4:8:295:ALA:N[1_554] | 1.70 | 0.50 |
| 4:5:299:MET:C | 4:8:136:ILE:CB[1_554] | 1.70 | 0.50 |
| 4:6:14:SER:C | 4:9:77:THR:CB[1_554] | 1.70 | 0.50 |
| 4:5:344:SER:C | 4:8:362:TYR:CE1[1_554] | 1.70 | 0.50 |
| 4:4:173:HIS:C | 4:8:267:ILE:CB[1_554] | 1.70 | 0.50 |
| 4:5:369:ILE:CG2 | 4:9:232:SER:C[1_554] | 1.70 | 0.50 |
| 4:3:177:ARG:NH2 | 4:7:194:THR:CG2[1_554] | 1.70 | 0.50 |
| 4:5:370:VAL:N | 4:9:231:ALA:CB[1_554] | 1.70 | 0.50 |
| 4:5:249:THR:N | 4:8:211:ASP:OD2[1_554] | 1.70 | 0.50 |
| 4:5:338:SER:OG | 4:8:134:VAL:CA[1_554] | 1.70 | 0.50 |
| 4:4:256:ARG:C | 4:7:303:THR:CB[1_554] | 1.70 | 0.50 |
| 4:4:279:TYR:CD2 | 4:7:285:CYS:SG[1_554] | 1.70 | 0.50 |
| 4:4:262:PHE:CB | 4:7:153:LEU:O[1_554] | 1.70 | 0.50 |
| 4:6:269:MET:CB | 4:9:178:LEU:CD1[1_554] | 1.70 | 0.50 |
| 4:5:269:MET:CB | 4:8:178:LEU:CD1[1_554] | 1.70 | 0.50 |
| 4:4:215:LYS:CB | 4:7:31:PHE:O[1_554] | 1.70 | 0.50 |
| 4:5:304:THR:OG1 | 4:8:137:GLN:CB[1_554] | 1.70 | 0.50 |
| 4:4:279:TYR:C | 4:7:285:CYS:SG[1_554] | 1.70 | 0.50 |
| 4:6:106:THR:OG1 | 4:9:114:ALA:CB[1_554] | 1.70 | 0.50 |
| 4:5:319:ALA:CA | 4:8:296:ASN:N[1_554] | 1.70 | 0.50 |
| 4:5:208:ILE:CB | 4:8:59:GLN:NE2[1_554] | 1.70 | 0.50 |
| 4:4:311:ASP:O | 4:7:141:SER:C[1_554] | 1.70 | 0.50 |
| 4:5:112:PRO:CG | 4:9:193:LEU:CD1[1_554] | 1.70 | 0.50 |
| 4:4:160:THR:CG2 | 4:7:161:HIS:NE2[1_554] | 1.70 | 0.50 |
| 4:4:337:TYR:CB | 4:7:119:MET:N[1_554] | 1.70 | 0.50 |
| 4:5:196:ARG:CG | 4:8:211:ASP:C[1_554] | 1.70 | 0.50 |
| 4:6:276:GLU:CB | 4:9:278:THR:O[1_554] | 1.70 | 0.50 |
| 4:6:191:LYS:N | 4:9:187:ASP:N[1_554] | 1.70 | 0.50 |
| 4:6:196:ARG:CZ | 4:9:215:LYS:CG[1_554] | 1.70 | 0.50 |
| 4:6:345:ILE:C | 4:9:366:GLY:O[1_554] | 1.70 | 0.50 |
| 4:2:291:LYS:O | 4:7:40:HIS:CB[1_554] | 1.70 | 0.50 |
| 4:3:110:LEU:CD1 | 4:7:191:LYS:CB[1_554] | 1.70 | 0.50 |
| 4:4:207:GLU:OE2 | 4:7:67:LEU:CA[1_554] | 1.70 | 0.50 |
| 4:4:333:PRO:CD | 4:7:133:TYR:O[1_554] | 1.70 | 0.50 |
| 4:5:243:PRO:CB | 4:8:60:SER:O[1_554] | 1.70 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:299:MET:SD | 4:8:138:ALA:CA[1_554] | 1.70 | 0.50 |
| 4:6:328:LYS:N | 4:9:148:THR:C[1_554] | 1.70 | 0.50 |
| 4:5:184:ASP:OD2 | 4:8:179:ASP:CB[1_554] | 1.70 | 0.50 |
| 4:6:140:LEU:CA | 4:9:371:HIS:CG[1_554] | 1.70 | 0.50 |
| 4:5:270:GLU:N | 4:8:271:SER:O[1_554] | 1.70 | 0.50 |
| 4:5:302:GLY:O | 4:8:12:ASN:O[1_554] | 1.70 | 0.50 |
| 4:3:111:ASN:ND2 | 4:7:196:ARG:CD[1_554] | 1.70 | 0.50 |
| 4:5:154:ASP:O | 4:8:110:LEU:N[1_554] | 1.70 | 0.50 |
| 4:4:344:SER:C | 4:7:367:PRO:CG[1_554] | 1.70 | 0.50 |
| 4:4:305:MET:CA | 4:7:106:THR:OG1[1_554] | 1.70 | 0.50 |
| 4:4:310:ALA:CA | 4:7:140:LEU:C[1_554] | 1.71 | 0.49 |
| 4:4:310:ALA:C | 4:7:140:LEU:CA[1_554] | 1.71 | 0.49 |
| 4:5:262:PHE:CG | 4:8:153:LEU:C[1_554] | 1.71 | 0.49 |
| 4:5:319:ALA:C | 4:8:294:TYR:N[1_554] | 1.71 | 0.49 |
| 4:4:158:GLY:O | 4:7:177:ARG:NH2[1_554] | 1.71 | 0.49 |
| 4:6:265:SER:N | 4:9:261:LEU:O[1_554] | 1.71 | 0.49 |
| 4:4:191:LYS:C | 4:7:186:THR:CG2[1_554] | 1.71 | 0.49 |
| 4:6:272:ALA:CA | 4:9:277:THR:CG2[1_554] | 1.71 | 0.49 |
| 4:5:205:GLU:OE2 | 4:8:203:THR:CB[1_554] | 1.71 | 0.49 |
| 4:5:178:LEU:CG | 4:8:177:ARG:O[1_554] | 1.71 | 0.49 |
| 4:5:270:GLU:CB | 4:8:272:ALA:CA[1_554] | 1.71 | 0.49 |
| 4:6:262:PHE:CE1 | 4:9:153:LEU:O[1_554] | 1.71 | 0.49 |
| 4:5:372:ARG:O | 4:9:227:MET:SD[1_554] | 1.71 | 0.49 |
| 4:6:320:LEU:CA | 4:9:293:LEU:CA[1_554] | 1.71 | 0.49 |
| 4:5:267:ILE:CD1 | 4:8:180:LEU:N[1_554] | 1.71 | 0.49 |
| 4:5:297:ASN:OD1 | 4:8:165:ILE:CG1[1_554] | 1.71 | 0.49 |
| 4:4:278:THR:N | 4:7:164:PRO:CD[1_554] | 1.71 | 0.49 |
| 4:5:294:TYR:N | 4:8:166:TYR:O[1_554] | 1.71 | 0.49 |
| 4:6:16:LEU:CA | 4:9:78:ASN:N[1_554] | 1.71 | 0.49 |
| 4:5:11:ASP:OD1 | 4:8:115:ASN:OD1[1_554] | 1.71 | 0.49 |
| 4:6:261:LEU:N | 4:9:155:SER:CB[1_554] | 1.71 | 0.49 |
| 4:6:328:LYS:O | 4:9:168:GLY:CA[1_554] | 1.71 | 0.49 |
| 4:5:288:ASP:C | 4:V:63:GLY:CA[1_554] | 1.71 | 0.49 |
| 4:6:266:PHE:CD2 | 4:9:261:LEU:CG[1_554] | 1.71 | 0.49 |
| 4:4:195:GLU:O | 4:7:212:ILE:CB[1_554] | 1.71 | 0.49 |
| 4:4:195:GLU:OE2 | 4:7:257:CYS:SG[1_554] | 1.71 | 0.49 |
| 4:4:332:PRO:CG | 4:7:134:VAL:O[1_554] | 1.71 | 0.49 |
| 4:6:142:LEU:O | 4:9:372:ARG:CZ[1_554] | 1.71 | 0.49 |
| 4:6:266:PHE:CB | 4:9:261:LEU:CB[1_554] | 1.71 | 0.49 |
| 4:5:288:ASP:CG | 4:V:62:ARG:O[1_554] | 1.71 | 0.49 |
| 4:4:213:LYS:NZ | 4:7:14:SER:CB[1_554] | 1.71 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:249:THR:O | 4:9:211:ASP:CB[1_554] | 1.71 | 0.49 |
| 4:5:310:ALA:CA | 4:8:142:LEU:N[1_554] | 1.71 | 0.49 |
| 4:5:297:ASN:O | 4:8:139:VAL:CG1[1_554] | 1.71 | 0.49 |
| 4:6:154:ASP:CA | 4:9:109:PRO:N[1_554] | 1.71 | 0.49 |
| 4:5:219:VAL:CG2 | 4:8:301:GLY:CA[1_554] | 1.71 | 0.49 |
| 4:4:263:GLN:C | 4:7:274:ILE:CG1[1_554] | 1.71 | 0.49 |
| 4:4:204:ALA:CA | 4:7:62:ARG:CB[1_554] | 1.71 | 0.49 |
| 4:5:278:THR:CA | 4:8:164:PRO:CG[1_554] | 1.71 | 0.49 |
| 4:6:340:TRP:CH2 | 4:9:122:ILE:N[1_554] | 1.71 | 0.49 |
| 4:4:331:ALA:CA | 4:7:135:ALA:C[1_554] | 1.71 | 0.49 |
| 4:6:322:PRO:CB | 4:9:291:LYS:CE[1_554] | 1.71 | 0.49 |
| 4:6:262:PHE:CG | 4:9:153:LEU:CG[1_554] | 1.71 | 0.49 |
| 4:5:308:GLY:N | 4:8:338:SER:CB[1_554] | 1.71 | 0.49 |
| 4:5:24:ASP:OD2 | 4:8:125:GLU:N[1_554] | 1.71 | 0.49 |
| 4:4:215:LYS:CD | 4:7:31:PHE:CD2[1_554] | 1.71 | 0.49 |
| 4:5:30:VAL:N | 4:8:79:TRP:O[1_554] | 1.71 | 0.49 |
| 4:5:32:PRO:O | 4:8:78:ASN:OD1[1_554] | 1.71 | 0.49 |
| 4:5:26:ALA:O | 4:8:123:MET:CA[1_554] | 1.71 | 0.49 |
| 4:6:218:TYR:C | 4:9:336:LYS:CA[1_554] | 1.71 | 0.49 |
| 4:6:172:PRO:CG | 4:V:266:PHE:CB[1_554] | 1.71 | 0.49 |
| 4:6:211:ASP:OD1 | 4:9:32:PRO:N[1_554] | 1.71 | 0.49 |
| 4:6:280:ASN:OD1 | 4:9:280:ASN:O[1_554] | 1.71 | 0.49 |
| 4:4:335:ARG:NH2 | 4:7:106:THR:CB[1_554] | 1.71 | 0.49 |
| 4:4:253:GLU:CB | 4:7:214:GLU:CG[1_554] | 1.71 | 0.49 |
| 4:4:31:PHE:N | 4:7:78:ASN:OD1[1_554] | 1.71 | 0.49 |
| 4:5:283:MET:CA | 4:8:285:CYS:C[1_554] | 1.71 | 0.49 |
| 4:4:180:LEU:CB | 4:7:178:LEU:C[1_554] | 1.71 | 0.49 |
| 4:4:274:ILE:O | 4:7:163:VAL:CA[1_554] | 1.71 | 0.49 |
| 4:5:372:ARG:CA | 4:9:227:MET:CA[1_554] | 1.71 | 0.49 |
| 4:4:267:ILE:CA | 4:7:180:LEU:CG[1_554] | 1.71 | 0.49 |
| 4:4:117:GLU:CB | 4:8:237:GLU:CB[1_554] | 1.71 | 0.49 |
| 4:5:255:PHE:CE1 | 4:8:306:TYR:N[1_554] | 1.71 | 0.49 |
| 4:5:204:ALA:C | 4:8:62:ARG:NE[1_554] | 1.71 | 0.49 |
| 4:4:212:ILE:N | 4:7:32:PRO:CA[1_554] | 1.71 | 0.49 |
| 4:6:345:ILE:CG2 | 4:9:369:ILE:CG2[1_554] | 1.71 | 0.49 |
| 4:5:24:ASP:CA | 4:8:124:PHE:O[1_554] | 1.71 | 0.49 |
| 4:6:326:LYS:C | 4:9:167:GLU:CD[1_554] | 1.71 | 0.49 |
| 4:5:30:VAL:O | 4:8:80:ASP:C[1_554] | 1.71 | 0.49 |
| 4:4:177:ARG:NH1 | 4:8:194:THR:OG1[1_554] | 1.71 | 0.49 |
| 4:5:260:THR:N | 4:8:155:SER:OG[1_554] | 1.71 | 0.49 |
| 4:4:366:GLY:O | 4:8:234:SER:OG[1_554] | 1.71 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:17:VAL:N | 4:9:79:TRP:N[1_554] | 1.71 | 0.49 |
| 4:3:287:ILE:C | 4:8:63:GLY:CA[1_554] | 1.71 | 0.49 |
| 4:5:340:TRP:CD2 | 4:8:120:THR:N[1_554] | 1.71 | 0.49 |
| 4:4:188:TYR:N | 4:7:184:ASP:N[1_554] | 1.71 | 0.49 |
| 4:3:117:GLU:O | 4:7:237:GLU:CB[1_554] | 1.72 | 0.48 |
| 4:6:113:LYS:CE | 4:V:252:ASN:O[1_554] | 1.72 | 0.48 |
| 4:4:162:ASN:CB | 4:7:172:PRO:O[1_554] | 1.72 | 0.48 |
| 4:4:332:PRO:CG | 4:7:134:VAL:N[1_554] | 1.72 | 0.48 |
| 4:5:313:MET:SD | 4:8:152:VAL:CB[1_554] | 1.72 | 0.48 |
| 4:4:280:ASN:ND2 | 4:7:281:SER:C[1_554] | 1.72 | 0.48 |
| 4:4:269:MET:CB | 4:7:178:LEU:CG[1_554] | 1.72 | 0.48 |
| 4:5:278:THR:CB | 4:8:164:PRO:CA[1_554] | 1.72 | 0.48 |
| 4:5:296:ASN:CA | 4:8:169:TYR:N[1_554] | 1.72 | 0.48 |
| 4:6:327:ILE:CG1 | 4:9:149:THR:C[1_554] | 1.72 | 0.48 |
| 4:5:186:THR:O | 4:8:183:ARG:CB[1_554] | 1.72 | 0.48 |
| 4:6:320:LEU:N | 4:9:292:ASP:O[1_554] | 1.72 | 0.48 |
| 4:5:317:ILE:CA | 4:8:150:GLY:CA[1_554] | 1.72 | 0.48 |
| 4:4:185:LEU:CG | 4:7:159:VAL:N[1_554] | 1.72 | 0.48 |
| 4:5:341:ILE:C | 4:8:120:THR:OG1[1_554] | 1.72 | 0.48 |
| 4:6:286:ASP:CA | 4:V:270:GLU:CG[1_554] | 1.72 | 0.48 |
| 4:4:226:GLU:CG | 4:7:333:PRO:O[1_554] | 1.72 | 0.48 |
| 4:6:268:GLY:O | 4:9:264:PRO:CB[1_554] | 1.72 | 0.48 |
| 4:4:258:PRO:CA | 4:7:156:GLY:CA[1_554] | 1.72 | 0.48 |
| 4:6:299:MET:C | 4:9:136:ILE:CB[1_554] | 1.72 | 0.48 |
| 4:6:369:ILE:CB | 4:V:232:SER:N[1_554] | 1.72 | 0.48 |
| 4:4:16:LEU:CD1 | 4:7:78:ASN:N[1_554] | 1.72 | 0.48 |
| 4:4:154:ASP:CA | 4:7:110:LEU:C[1_554] | 1.72 | 0.48 |
| 4:6:111:ASN:O | 4:V:256:ARG:NH2[1_554] | 1.72 | 0.48 |
| 4:5:173:HIS:CD2 | 4:9:268:GLY:N[1_554] | 1.72 | 0.48 |
| 4:6:330:ILE:N | 4:9:139:VAL:CG1[1_554] | 1.72 | 0.48 |
| 4:4:196:ARG:CB | 4:7:211:ASP:C[1_554] | 1.72 | 0.48 |
| 4:6:307:PRO:O | 4:9:338:SER:N[1_554] | 1.72 | 0.48 |
| 4:5:334:GLU:CG | 4:8:103:THR:O[1_554] | 1.72 | 0.48 |
| 4:5:258:PRO:O | 4:8:155:SER:CA[1_554] | 1.72 | 0.48 |
| 4:3:173:HIS:ND1 | 4:7:266:PHE:N[1_554] | 1.72 | 0.48 |
| 4:4:284:LYS:C | 4:8:268:GLY:C[1_554] | 1.72 | 0.48 |
| 4:5:31:PHE:C | 4:8:78:ASN:CG[1_554] | 1.72 | 0.48 |
| 4:2:324:THR:CG2 | 4:7:61:LYS:CG[1_554] | 1.72 | 0.48 |
| 4:6:218:TYR:CZ | 4:9:337:TYR:CD2[1_554] | 1.72 | 0.48 |
| 4:6:267:ILE:N | 4:9:180:LEU:CD1[1_554] | 1.72 | 0.48 |
| 4:6:249:THR:C | 4:9:211:ASP:CG[1_554] | 1.72 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:265:SER:C | 4:8:261:LEU:O[1_554] | 1.72 | 0.48 |
| 4:5:336:LYS:CE | 4:8:10:CYS:SG[1_554] | 1.72 | 0.48 |
| 4:4:367:PRO:CD | 4:8:235:SER:O[1_554] | 1.72 | 0.48 |
| 4:6:320:LEU:N | 4:9:293:LEU:CA[1_554] | 1.72 | 0.48 |
| 4:6:277:THR:C | 4:9:174:ALA:O[1_554] | 1.72 | 0.48 |
| 4:6:279:TYR:OH | 4:9:290:ARG:CB[1_554] | 1.72 | 0.48 |
| 4:6:340:TRP:CE3 | 4:9:120:THR:N[1_554] | 1.72 | 0.48 |
| 4:3:173:HIS:NE2 | 4:7:265:SER:CA[1_554] | 1.72 | 0.48 |
| 4:4:281:SER:O | 4:7:173:HIS:ND1[1_554] | 1.72 | 0.48 |
| 4:6:223:PHE:CD1 | 4:9:335:ARG:NE[1_554] | 1.72 | 0.48 |
| 4:6:275:HIS:O | 4:9:151:ILE:CD1[1_554] | 1.72 | 0.48 |
| 4:5:20:GLY:N | 4:8:121:GLN:CD[1_554] | 1.72 | 0.48 |
| 4:5:30:VAL:C | 4:8:79:TRP:O[1_554] | 1.72 | 0.48 |
| 4:6:184:ASP:OD2 | 4:9:179:ASP:CB[1_554] | 1.72 | 0.48 |
| 4:4:338:SER:CB | 4:7:116:ARG:CB[1_554] | 1.72 | 0.48 |
| 4:5:184:ASP:OD1 | 4:8:73:HIS:NE2[1_554] | 1.72 | 0.48 |
| 4:6:288:ASP:C | 4:W:63:GLY:CA[1_554] | 1.72 | 0.48 |
| 4:5:259:GLU:CA | 4:8:304:THR:CG2[1_554] | 1.72 | 0.48 |
| 4:4:268:GLY:N | 4:7:180:LEU:CD2[1_554] | 1.72 | 0.48 |
| 4:5:218:TYR:CZ | 4:8:337:TYR:CD2[1_554] | 1.72 | 0.48 |
| 4:4:284:LYS:O | 4:8:269:MET:N[1_554] | 1.72 | 0.48 |
| 4:2:287:ILE:O | 4:7:39:ARG:NH2[1_554] | 1.72 | 0.48 |
| 4:6:213:LYS:NZ | 4:9:15:GLY:N[1_554] | 1.72 | 0.48 |
| 4:4:335:ARG:CZ | 4:7:106:THR:CA[1_554] | 1.72 | 0.48 |
| 4:4:327:ILE:CD1 | 4:7:149:THR:OG1[1_554] | 1.72 | 0.48 |
| 4:5:283:MET:CG | 4:8:285:CYS:O[1_554] | 1.72 | 0.48 |
| 4:5:110:LEU:CD1 | 4:9:191:LYS:CB[1_554] | 1.72 | 0.48 |
| 4:5:316:GLU:N | 4:8:296:ASN:O[1_554] | 1.72 | 0.48 |
| 4:5:20:GLY:C | 4:8:121:GLN:CD[1_554] | 1.72 | 0.48 |
| 4:6:260:THR:CA | 4:9:155:SER:OG[1_554] | 1.72 | 0.48 |
| 4:6:308:GLY:N | 4:9:338:SER:CB[1_554] | 1.72 | 0.48 |
| 4:6:294:TYR:OH | 4:9:289:ILE:CB[1_554] | 1.72 | 0.48 |
| 4:6:287:ILE:O | 4:W:63:GLY:CA[1_554] | 1.72 | 0.48 |
| 4:3:117:GLU:C | 4:7:237:GLU:CD[1_554] | 1.72 | 0.48 |
| 4:5:262:PHE:CG | 4:8:153:LEU:CA[1_554] | 1.72 | 0.48 |
| 4:6:346:LEU:CD1 | 4:9:368:SER:CB[1_554] | 1.72 | 0.48 |
| 4:5:345:ILE:CG1 | 4:8:357:ILE:CG2[1_554] | 1.72 | 0.48 |
| 4:4:118:LYS:N | 4:8:237:GLU:CD[1_554] | 1.72 | 0.48 |
| 4:5:157:ASP:OD2 | 4:8:72:GLU:CG[1_554] | 1.72 | 0.48 |
| 4:4:153:LEU:CG | 4:7:109:PRO:CG[1_554] | 1.72 | 0.48 |
| 4:4:305:MET:SD | 4:7:12:ASN:ND2[1_554] | 1.72 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:296:ASN:N | 4:8:168:GLY:C[1_554] | 1.72 | 0.48 |
| 4:5:195:GLU:C | 4:8:189:LEU:CD2[1_554] | 1.72 | 0.48 |
| 4:6:255:PHE:O | 4:9:303:THR:C[1_554] | 1.72 | 0.48 |
| 4:6:340:TRP:N | 4:9:116:ARG:C[1_554] | 1.72 | 0.48 |
| 4:6:308:GLY:O | 4:9:338:SER:OG[1_554] | 1.72 | 0.48 |
| 4:6:141:SER:OG | 4:9:107:GLU:CD[1_554] | 1.72 | 0.48 |
| 4:4:219:VAL:CG1 | 4:7:300:SER:OG[1_554] | 1.72 | 0.48 |
| 4:4:112:PRO:CG | 4:8:193:LEU:CD2[1_554] | 1.72 | 0.48 |
| 4:4:240:TYR:OH | 4:7:55:GLY:C[1_554] | 1.72 | 0.48 |
| 4:6:329:ILE:CG1 | 4:9:142:LEU:CB[1_554] | 1.72 | 0.48 |
| 4:6:319:ALA:N | 4:9:296:ASN:ND2[1_554] | 1.72 | 0.48 |
| 4:5:166:TYR:C | 4:V:40:HIS:CD2[1_554] | 1.72 | 0.48 |
| 4:6:186:THR:CB | 4:9:183:ARG:CZ[1_554] | 1.72 | 0.48 |
| 4:6:136:ILE:C | 4:9:113:LYS:CA[1_554] | 1.72 | 0.48 |
| 4:5:214:GLU:C | 4:8:16:LEU:CG[1_554] | 1.72 | 0.48 |
| 4:4:109:PRO:CA | 4:8:195:GLU:OE2[1_554] | 1.72 | 0.48 |
| 4:5:253:GLU:OE1 | 4:8:213:LYS:O[1_554] | 1.72 | 0.48 |
| 4:5:178:LEU:CD2 | 4:8:177:ARG:N[1_554] | 1.72 | 0.48 |
| 4:4:240:TYR:OH | 4:7:56:ASP:CA[1_554] | 1.72 | 0.48 |
| 4:5:160:THR:N | 4:8:177:ARG:CD[1_554] | 1.73 | 0.47 |
| 4:4:75:ILE:CA | 4:8:198:TYR:CA[1_554] | 1.73 | 0.47 |
| 4:6:30:VAL:CG1 | 4:9:82:MET:CG[1_554] | 1.73 | 0.47 |
| 4:5:265:SER:CB | 4:8:261:LEU:O[1_554] | 1.73 | 0.47 |
| 4:5:56:ASP:CA | 4:8:37:ARG:NH1[1_554] | 1.73 | 0.47 |
| 4:3:284:LYS:CA | 4:7:268:GLY:O[1_554] | 1.73 | 0.47 |
| 4:5:208:ILE:CG1 | 4:8:59:GLN:CB[1_554] | 1.73 | 0.47 |
| 4:5:336:LYS:CD | 4:8:12:ASN:ND2[1_554] | 1.73 | 0.47 |
| 4:5:200:PHE:CZ | 4:8:207:GLU:O[1_554] | 1.73 | 0.47 |
| 4:6:221:LEU:CG | 4:9:332:PRO:CA[1_554] | 1.73 | 0.47 |
| 4:5:347:ALA:N | 4:8:367:PRO:N[1_554] | 1.73 | 0.47 |
| 4:5:24:ASP:CB | 4:8:124:PHE:O[1_554] | 1.73 | 0.47 |
| 4:4:270:GLU:C | 4:7:272:ALA:CB[1_554] | 1.73 | 0.47 |
| 4:6:191:LYS:O | 4:9:186:THR:O[1_554] | 1.73 | 0.47 |
| 4:5:166:TYR:CZ | 4:V:40:HIS:N[1_554] | 1.73 | 0.47 |
| 4:6:349:LEU:CD2 | 4:9:365:ALA:CB[1_554] | 1.73 | 0.47 |
| 4:4:187:ASP:C | 4:7:183:ARG:C[1_554] | 1.73 | 0.47 |
| 4:6:272:ALA:C | 4:9:277:THR:CB[1_554] | 1.73 | 0.47 |
| 4:5:326:LYS:C | 4:8:167:GLU:CD[1_554] | 1.73 | 0.47 |
| 4:6:319:ALA:CA | 4:9:295:ALA:N[1_554] | 1.73 | 0.47 |
| 4:5:322:PRO:CB | 4:8:288:ASP:O[1_554] | 1.73 | 0.47 |
| 4:5:194:THR:CB | 4:8:209:VAL:CG1[1_554] | 1.73 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:370:VAL:CG1 | 4:8:230:ALA:O[1_554] | 1.73 | 0.47 |
| 4:4:162:ASN:OD1 | 4:7:175:ILE:CB[1_554] | 1.73 | 0.47 |
| 4:5:314:GLN:OE1 | 4:8:147:ARG:CA[1_554] | 1.73 | 0.47 |
| 4:6:347:ALA:C | 4:9:366:GLY:N[1_554] | 1.73 | 0.47 |
| 4:6:28:ARG:N | 4:9:122:ILE:CG2[1_554] | 1.73 | 0.47 |
| 4:6:372:ARG:N | 4:V:227:MET:C[1_554] | 1.73 | 0.47 |
| 4:5:25:ASP:C | 4:8:123:MET:CB[1_554] | 1.73 | 0.47 |
| 4:6:196:ARG:CD | 4:9:212:ILE:N[1_554] | 1.73 | 0.47 |
| 4:4:299:MET:SD | 4:7:136:ILE:C[1_554] | 1.73 | 0.47 |
| 4:5:319:ALA:N | 4:8:292:ASP:O[1_554] | 1.73 | 0.47 |
| 4:6:314:GLN:CD | 4:9:147:ARG:CA[1_554] | 1.73 | 0.47 |
| 4:6:227:MET:SD | 4:9:306:TYR:CA[1_554] | 1.73 | 0.47 |
| 4:3:288:ASP:O | 4:8:65:LEU:N[1_554] | 1.73 | 0.47 |
| 4:6:17:VAL:CG1 | 4:9:79:TRP:CD1[1_554] | 1.73 | 0.47 |
| 4:5:199:SER:N | 4:8:206:ARG:CA[1_554] | 1.73 | 0.47 |
| 4:5:208:ILE:CD1 | 4:8:59:GLN:CG[1_554] | 1.73 | 0.47 |
| 4:5:214:GLU:N | 4:8:16:LEU:CA[1_554] | 1.73 | 0.47 |
| 4:6:335:ARG:N | 4:9:105:LEU:CA[1_554] | 1.73 | 0.47 |
| 4:6:157:ASP:CB | 4:9:72:GLU:O[1_554] | 1.73 | 0.47 |
| 4:4:145:SER:OG | 4:7:372:ARG:CD[1_554] | 1.73 | 0.47 |
| 4:5:211:ASP:O | 4:8:16:LEU:CD1[1_554] | 1.73 | 0.47 |
| 4:4:144:ALA:CB | 4:7:371:HIS:N[1_554] | 1.73 | 0.47 |
| 4:5:322:PRO:CA | 4:8:291:LYS:CE[1_554] | 1.73 | 0.47 |
| 4:4:298:VAL:C | 4:7:136:ILE:CG1[1_554] | 1.73 | 0.47 |
| 4:5:267:ILE:CA | 4:8:180:LEU:CD2[1_554] | 1.73 | 0.47 |
| 4:4:309:ILE:CB | 4:7:339:VAL:CG2[1_554] | 1.73 | 0.47 |
| 4:6:214:GLU:C | 4:9:16:LEU:CG[1_554] | 1.73 | 0.47 |
| 4:4:367:PRO:CD | 4:8:235:SER:CB[1_554] | 1.73 | 0.47 |
| 4:6:308:GLY:N | 4:9:338:SER:C[1_554] | 1.73 | 0.47 |
| 4:5:198:TYR:CB | 4:8:208:ILE:C[1_554] | 1.73 | 0.47 |
| 4:6:214:GLU:N | 4:9:16:LEU:N[1_554] | 1.73 | 0.47 |
| 4:6:159:VAL:O | 4:9:177:ARG:NH1[1_554] | 1.73 | 0.47 |
| 4:6:62:ARG:CZ | 4:9:67:LEU:O[1_554] | 1.73 | 0.47 |
| 4:5:327:ILE:N | 4:8:149:THR:OG1[1_554] | 1.73 | 0.47 |
| 4:4:310:ALA:O | 4:7:139:VAL:O[1_554] | 1.73 | 0.47 |
| 4:5:207:GLU:OE2 | 4:8:68:LYS:N[1_554] | 1.73 | 0.47 |
| 4:4:188:TYR:CE2 | 4:7:182:GLY:CA[1_554] | 1.73 | 0.47 |
| 4:2:288:ASP:O | 4:7:39:ARG:CD[1_554] | 1.73 | 0.47 |
| 4:6:327:ILE:CA | 4:9:149:THR:N[1_554] | 1.73 | 0.47 |
| 4:4:173:HIS:NE2 | 4:8:265:SER:CA[1_554] | 1.73 | 0.47 |
| 4:5:327:ILE:CD1 | 4:8:149:THR:OG1[1_554] | 1.73 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:329:ILE:CG2 | 4:7:139:VAL:CG2[1_554] | 1.73 | 0.47 |
| 4:5:293:LEU:CB | 4:8:169:TYR:CD2[1_554] | 1.73 | 0.47 |
| 1:A:637:LYS:NZ | 4:5:311:ASP:C[1_556] | 1.73 | 0.47 |
| 4:6:106:THR:OG1 | 4:9:114:ALA:C[1_554] | 1.73 | 0.47 |
| 4:6:336:LYS:N | 4:9:106:THR:N[1_554] | 1.73 | 0.47 |
| 4:6:276:GLU:OE1 | 4:9:279:TYR:CA[1_554] | 1.73 | 0.47 |
| 4:4:24:ASP:CA | 4:7:125:GLU:OE1[1_554] | 1.73 | 0.47 |
| 4:6:273:GLY:C | 4:9:162:ASN:ND2[1_554] | 1.73 | 0.47 |
| 4:5:205:GLU:CA | 4:8:62:ARG:NH2[1_554] | 1.73 | 0.47 |
| 4:6:370:VAL:CB | 4:V:231:ALA:CA[1_554] | 1.73 | 0.47 |
| 4:6:208:ILE:N | 4:9:59:GLN:CD[1_554] | 1.73 | 0.47 |
| 4:6:348:SER:C | 4:9:365:ALA:N[1_554] | 1.73 | 0.47 |
| 4:6:198:TYR:CD2 | 4:9:208:ILE:CA[1_554] | 1.73 | 0.47 |
| 4:5:321:ALA:N | 4:8:292:ASP:C[1_554] | 1.73 | 0.47 |
| 4:4:153:LEU:CD1 | 4:7:109:PRO:CB[1_554] | 1.73 | 0.47 |
| 4:5:114:ALA:O | 4:9:237:GLU:OE1[1_554] | 1.73 | 0.47 |
| 4:5:140:LEU:CD2 | 4:8:371:HIS:CB[1_554] | 1.73 | 0.47 |
| 4:3:366:GLY:CA | 4:7:235:SER:OG[1_554] | 1.73 | 0.47 |
| 4:5:196:ARG:CD | 4:8:211:ASP:O[1_554] | 1.73 | 0.47 |
| 4:6:255:PHE:CG | 4:9:305:MET:CG[1_554] | 1.73 | 0.47 |
| 4:5:259:GLU:CB | 4:8:304:THR:CA[1_554] | 1.73 | 0.47 |
| 4:6:136:ILE:N | 4:9:113:LYS:CD[1_554] | 1.73 | 0.47 |
| 4:4:372:ARG:CG | 4:8:227:MET:C[1_554] | 1.73 | 0.47 |
| 4:4:59:GLN:CG | 4:7:68:LYS:CD[1_554] | 1.73 | 0.47 |
| 4:4:153:LEU:CD2 | 4:7:109:PRO:CD[1_554] | 1.74 | 0.46 |
| 4:6:21:PHE:CA | 4:9:125:GLU:CG[1_554] | 1.74 | 0.46 |
| 4:5:223:PHE:CE1 | 4:8:304:THR:C[1_554] | 1.74 | 0.46 |
| 4:4:161:HIS:N | 4:7:110:LEU:CD1[1_554] | 1.74 | 0.46 |
| 4:5:266:PHE:CD1 | 4:8:261:LEU:CG[1_554] | 1.74 | 0.46 |
| 4:5:253:GLU:OE1 | 4:8:214:GLU:CA[1_554] | 1.74 | 0.46 |
| 4:4:198:TYR:CB | 4:7:207:GLU:CA[1_554] | 1.74 | 0.46 |
| 4:5:327:ILE:CB | 4:8:149:THR:CB[1_554] | 1.74 | 0.46 |
| 4:4:317:ILE:C | 4:7:150:GLY:CA[1_554] | 1.74 | 0.46 |
| 4:5:321:ALA:C | 4:8:292:ASP:N[1_554] | 1.74 | 0.46 |
| 4:5:62:ARG:CZ | 4:8:67:LEU:O[1_554] | 1.74 | 0.46 |
| 4:6:155:SER:OG | 4:9:161:HIS:CE1[1_554] | 1.74 | 0.46 |
| 4:4:187:ASP:C | 4:7:183:ARG:CB[1_554] | 1.74 | 0.46 |
| 4:4:320:LEU:C | 4:7:293:LEU:N[1_554] | 1.74 | 0.46 |
| 4:4:192:ILE:CA | 4:7:186:THR:OG1[1_554] | 1.74 | 0.46 |
| 4:5:313:MET:SD | 4:8:152:VAL:CA[1_554] | 1.74 | 0.46 |
| 4:6:276:GLU:CA | 4:9:151:ILE:CD1[1_554] | 1.74 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:155:SER:O | 4:8:108:ALA:CB[1_554] | 1.74 | 0.46 |
| 4:6:193:LEU:CD1 | 4:9:211:ASP:N[1_554] | 1.74 | 0.46 |
| 4:5:75:ILE:N | 4:9:197:GLY:CA[1_554] | 1.74 | 0.46 |
| 4:5:172:PRO:CG | 4:9:266:PHE:CG[1_554] | 1.74 | 0.46 |
| 4:5:212:ILE:O | 4:8:16:LEU:CD2[1_554] | 1.74 | 0.46 |
| 4:4:341:ILE:CG1 | 4:7:120:THR:C[1_554] | 1.74 | 0.46 |
| 4:4:265:SER:O | 4:7:261:LEU:N[1_554] | 1.74 | 0.46 |
| 4:5:33:SER:OG | 4:8:77:THR:O[1_554] | 1.74 | 0.46 |
| 4:5:255:PHE:CD1 | 4:8:305:MET:N[1_554] | 1.74 | 0.46 |
| 4:5:309:ILE:CB | 4:8:141:SER:OG[1_554] | 1.74 | 0.46 |
| 4:3:113:LYS:CB | 4:7:254:ARG:N[1_554] | 1.74 | 0.46 |
| 4:4:198:TYR:N | 4:7:208:ILE:C[1_554] | 1.74 | 0.46 |
| 4:5:327:ILE:CG1 | 4:8:149:THR:C[1_554] | 1.74 | 0.46 |
| 4:4:304:THR:C | 4:7:137:GLN:CG[1_554] | 1.74 | 0.46 |
| 4:6:283:MET:CG | 4:9:285:CYS:C[1_554] | 1.74 | 0.46 |
| 4:4:184:ASP:OD2 | 4:7:179:ASP:CB[1_554] | 1.74 | 0.46 |
| 4:3:117:GLU:CD | 4:7:236:LEU:C[1_554] | 1.74 | 0.46 |
| 4:5:331:ALA:CA | 4:8:140:LEU:CD2[1_554] | 1.74 | 0.46 |
| 4:6:199:SER:C | 4:9:206:ARG:N[1_554] | 1.74 | 0.46 |
| 4:5:198:TYR:CD1 | 4:8:208:ILE:CG2[1_554] | 1.74 | 0.46 |
| 4:6:155:SER:N | 4:9:109:PRO:N[1_554] | 1.74 | 0.46 |
| 4:6:160:THR:N | 4:9:177:ARG:CD[1_554] | 1.74 | 0.46 |
| 4:5:109:PRO:CB | 4:9:195:GLU:OE2[1_554] | 1.74 | 0.46 |
| 4:5:32:PRO:N | 4:8:78:ASN:CB[1_554] | 1.74 | 0.46 |
| 4:4:281:SER:N | 4:7:174:ALA:N[1_554] | 1.74 | 0.46 |
| 4:3:367:PRO:CD | 4:7:235:SER:O[1_554] | 1.74 | 0.46 |
| 4:5:59:GLN:NE2 | 4:8:68:LYS:CG[1_554] | 1.74 | 0.46 |
| 4:6:296:ASN:N | 4:9:168:GLY:C[1_554] | 1.74 | 0.46 |
| 4:4:257:CYS:N | 4:7:303:THR:N[1_554] | 1.74 | 0.46 |
| 4:4:311:ASP:O | 4:7:142:LEU:C[1_554] | 1.74 | 0.46 |
| 4:4:315:LYS:CA | 4:7:142:LEU:CD1[1_554] | 1.74 | 0.46 |
| 4:6:267:ILE:CA | 4:9:180:LEU:CD1[1_554] | 1.74 | 0.46 |
| 4:6:24:ASP:C | 4:9:124:PHE:CG[1_554] | 1.74 | 0.46 |
| 4:6:279:TYR:CG | 4:9:293:LEU:CD2[1_554] | 1.74 | 0.46 |
| 4:4:314:GLN:CA | 4:7:142:LEU:CG[1_554] | 1.74 | 0.46 |
| 4:4:109:PRO:C | 4:8:195:GLU:CD[1_554] | 1.74 | 0.46 |
| 4:6:162:ASN:ND2 | 4:9:175:ILE:CB[1_554] | 1.74 | 0.46 |
| 4:6:326:LYS:CA | 4:9:167:GLU:CD[1_554] | 1.74 | 0.46 |
| 4:6:300:SER:C | 4:9:108:ALA:N[1_554] | 1.74 | 0.46 |
| 4:6:327:ILE:CG2 | 4:9:149:THR:CA[1_554] | 1.74 | 0.46 |
| 4:5:278:THR:CG2 | 4:8:164:PRO:N[1_554] | 1.74 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:337:TYR:CZ | 4:8:86:TRP:CD2[1_554] | 1.74 | 0.46 |
| 4:6:193:LEU:CB | 4:9:210:ARG:CG[1_554] | 1.74 | 0.46 |
| 4:4:111:ASN:C | 4:8:253:GLU:CG[1_554] | 1.74 | 0.46 |
| 4:4:27:PRO:CB | 4:7:122:ILE:CD1[1_554] | 1.74 | 0.46 |
| 4:6:199:SER:C | 4:9:206:ARG:C[1_554] | 1.74 | 0.46 |
| 4:3:116:ARG:CD | 4:7:252:ASN:CB[1_554] | 1.74 | 0.46 |
| 4:4:25:ASP:C | 4:7:121:GLN:O[1_554] | 1.74 | 0.46 |
| 4:6:157:ASP:CG | 4:9:72:GLU:C[1_554] | 1.74 | 0.46 |
| 4:4:15:GLY:C | 4:7:77:THR:CB[1_554] | 1.74 | 0.46 |
| 4:4:113:LYS:CE | 4:8:254:ARG:CG[1_554] | 1.74 | 0.46 |
| 4:5:173:HIS:NE2 | 4:9:265:SER:C[1_554] | 1.74 | 0.46 |
| 4:6:114:ALA:O | 4:V:237:GLU:CD[1_554] | 1.74 | 0.46 |
| 4:5:190:MET:CE | 4:8:206:ARG:NH2[1_554] | 1.74 | 0.46 |
| 4:5:145:SER:CB | 4:8:372:ARG:CZ[1_554] | 1.74 | 0.46 |
| 4:6:274:ILE:CA | 4:9:162:ASN:C[1_554] | 1.74 | 0.46 |
| 4:4:178:LEU:CB | 4:7:177:ARG:N[1_554] | 1.74 | 0.46 |
| 4:5:260:THR:CA | 4:8:155:SER:OG[1_554] | 1.74 | 0.46 |
| 4:6:372:ARG:CA | 4:V:227:MET:CB[1_554] | 1.74 | 0.46 |
| 1:A:637:LYS:NZ | 4:5:311:ASP:N[1_556] | 1.74 | 0.46 |
| 4:5:167:GLU:OE2 | 4:V:41:GLN:CA[1_554] | 1.74 | 0.46 |
| 4:6:337:TYR:CE1 | 4:9:86:TRP:CE2[1_554] | 1.75 | 0.45 |
| 4:3:291:LYS:CD | 4:8:64:ILE:CD1[1_554] | 1.75 | 0.45 |
| 4:6:348:SER:CA | 4:9:362:TYR:O[1_554] | 1.75 | 0.45 |
| 4:6:267:ILE:O | 4:9:180:LEU:CD2[1_554] | 1.75 | 0.45 |
| 4:5:218:TYR:CB | 4:8:336:LYS:CG[1_554] | 1.75 | 0.45 |
| 4:6:339:VAL:CG1 | 4:9:116:ARG:CA[1_554] | 1.75 | 0.45 |
| 4:6:219:VAL:CG2 | 4:9:301:GLY:CA[1_554] | 1.75 | 0.45 |
| 4:5:157:ASP:CB | 4:8:72:GLU:C[1_554] | 1.75 | 0.45 |
| 4:6:181:ALA:CA | 4:9:159:VAL:CB[1_554] | 1.75 | 0.45 |
| 4:6:27:PRO:CA | 4:9:122:ILE:CA[1_554] | 1.75 | 0.45 |
| 4:6:274:ILE:CG1 | 4:9:161:HIS:C[1_554] | 1.75 | 0.45 |
| 4:5:162:ASN:OD1 | 4:8:175:ILE:CA[1_554] | 1.75 | 0.45 |
| 4:5:335:ARG:N | 4:8:105:LEU:CA[1_554] | 1.75 | 0.45 |
| 4:4:16:LEU:CG | 4:7:78:ASN:C[1_554] | 1.75 | 0.45 |
| 4:5:367:PRO:CD | 4:9:233:SER:C[1_554] | 1.75 | 0.45 |
| 4:3:289:ILE:CG2 | 4:8:39:ARG:NH2[1_554] | 1.75 | 0.45 |
| 4:5:157:ASP:CG | 4:8:72:GLU:CB[1_554] | 1.75 | 0.45 |
| 4:6:274:ILE:N | 4:9:162:ASN:OD1[1_554] | 1.75 | 0.45 |
| 4:6:193:LEU:C | 4:9:209:VAL:O[1_554] | 1.75 | 0.45 |
| 4:6:211:ASP:OD2 | 4:9:32:PRO:N[1_554] | 1.75 | 0.45 |
| 4:3:116:ARG:O | 4:7:237:GLU:CD[1_554] | 1.75 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:280:ASN:CB | 4:9:281:SER:O[1_554] | 1.75 | 0.45 |
| 4:5:346:LEU:O | 4:8:365:ALA:C[1_554] | 1.75 | 0.45 |
| 4:6:199:SER:CB | 4:9:205:GLU:C[1_554] | 1.75 | 0.45 |
| 4:3:113:LYS:CB | 4:7:254:ARG:CA[1_554] | 1.75 | 0.45 |
| 4:6:155:SER:N | 4:9:108:ALA:CA[1_554] | 1.75 | 0.45 |
| 4:4:275:HIS:O | 4:7:164:PRO:CA[1_554] | 1.75 | 0.45 |
| 4:4:281:SER:CA | 4:7:173:HIS:CD2[1_554] | 1.75 | 0.45 |
| 4:6:141:SER:OG | 4:9:116:ARG:NE[1_554] | 1.75 | 0.45 |
| 4:5:184:ASP:OD1 | 4:8:73:HIS:ND1[1_554] | 1.75 | 0.45 |
| 4:4:333:PRO:CG | 4:7:104:LEU:CA[1_554] | 1.75 | 0.45 |
| 4:5:335:ARG:C | 4:8:106:THR:CA[1_554] | 1.75 | 0.45 |
| 4:4:318:THR:C | 4:7:149:THR:C[1_554] | 1.75 | 0.45 |
| 4:5:11:ASP:OD2 | 4:8:115:ASN:CA[1_554] | 1.75 | 0.45 |
| 4:3:172:PRO:CB | 4:7:188:TYR:OH[1_554] | 1.75 | 0.45 |
| 4:5:178:LEU:O | 4:8:177:ARG:CB[1_554] | 1.75 | 0.45 |
| 4:6:340:TRP:CG | 4:9:120:THR:N[1_554] | 1.75 | 0.45 |
| 4:5:200:PHE:N | 4:8:206:ARG:CA[1_554] | 1.75 | 0.45 |
| 4:6:56:ASP:OD1 | 4:9:81:ASP:OD1[1_554] | 1.75 | 0.45 |
| 4:5:188:TYR:CD1 | 4:8:185:LEU:CG[1_554] | 1.75 | 0.45 |
| 4:6:30:VAL:N | 4:9:83:GLU:CB[1_554] | 1.75 | 0.45 |
| 4:6:19:ALA:C | 4:9:122:ILE:CG1[1_554] | 1.75 | 0.45 |
| 4:6:113:LYS:N | 4:V:253:GLU:N[1_554] | 1.75 | 0.45 |
| 4:5:272:ALA:C | 4:8:277:THR:CB[1_554] | 1.75 | 0.45 |
| 4:6:196:ARG:CD | 4:9:212:ILE:CA[1_554] | 1.75 | 0.45 |
| 4:6:11:ASP:N | 4:9:118:LYS:CG[1_554] | 1.75 | 0.45 |
| 4:5:259:GLU:OE2 | 4:8:309:ILE:CG2[1_554] | 1.75 | 0.45 |
| 4:5:294:TYR:CA | 4:8:166:TYR:CB[1_554] | 1.75 | 0.45 |
| 4:5:24:ASP:CG | 4:8:125:GLU:C[1_554] | 1.75 | 0.45 |
| 4:5:172:PRO:O | 4:9:266:PHE:O[1_554] | 1.75 | 0.45 |
| 4:6:200:PHE:CE1 | 4:9:207:GLU:CA[1_554] | 1.75 | 0.45 |
| 4:6:296:ASN:CA | 4:9:169:TYR:N[1_554] | 1.75 | 0.45 |
| 4:5:362:TYR:CE1 | 4:9:233:SER:O[1_554] | 1.75 | 0.45 |
| 4:4:326:LYS:CA | 4:7:167:GLU:CG[1_554] | 1.75 | 0.45 |
| 4:6:371:HIS:CA | 4:V:230:ALA:CB[1_554] | 1.75 | 0.45 |
| 4:4:208:ILE:C | 4:7:59:GLN:NE2[1_554] | 1.75 | 0.45 |
| 4:5:106:THR:C | 4:8:114:ALA:CB[1_554] | 1.75 | 0.45 |
| 4:6:154:ASP:O | 4:9:110:LEU:N[1_554] | 1.75 | 0.45 |
| 4:5:340:TRP:C | 4:8:116:ARG:O[1_554] | 1.75 | 0.45 |
| 4:4:111:ASN:ND2 | 4:8:196:ARG:CD[1_554] | 1.75 | 0.45 |
| 4:6:20:GLY:N | 4:9:121:GLN:CD[1_554] | 1.75 | 0.45 |
| 4:5:371:HIS:CG | 4:9:230:ALA:CB[1_554] | 1.75 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:323:SER:CB | 4:7:44:MET:CE[1_554] | 1.75 | 0.45 |
| 4:4:166:TYR:OH | 4:9:39:ARG:C[1_554] | 1.75 | 0.45 |
| 4:4:173:HIS:NE2 | 4:8:264:PRO:O[1_554] | 1.75 | 0.45 |
| 4:5:293:LEU:O | 4:8:169:TYR:O[1_554] | 1.75 | 0.45 |
| 4:5:106:THR:CB | 4:8:114:ALA:C[1_554] | 1.75 | 0.45 |
| 4:6:301:GLY:N | 4:9:108:ALA:N[1_554] | 1.75 | 0.45 |
| 4:4:268:GLY:CA | 4:7:264:PRO:CA[1_554] | 1.75 | 0.45 |
| 4:6:110:LEU:CD1 | 4:V:191:LYS:CB[1_554] | 1.75 | 0.45 |
| 4:6:196:ARG:CB | 4:9:212:ILE:CB[1_554] | 1.75 | 0.45 |
| 4:5:259:GLU:OE2 | 4:8:309:ILE:CD1[1_554] | 1.75 | 0.45 |
| 4:5:157:ASP:CG | 4:8:72:GLU:C[1_554] | 1.75 | 0.45 |
| 4:6:113:LYS:N | 4:V:253:GLU:CG[1_554] | 1.75 | 0.45 |
| 4:6:288:ASP:N | 4:W:63:GLY:N[1_554] | 1.75 | 0.45 |
| 4:5:275:HIS:O | 4:8:151:ILE:CD1[1_554] | 1.75 | 0.45 |
| 4:6:337:TYR:CE2 | 4:9:86:TRP:CE2[1_554] | 1.75 | 0.45 |
| 4:4:211:ASP:N | 4:7:34:ILE:CD1[1_554] | 1.75 | 0.45 |
| 4:4:188:TYR:C | 4:7:182:GLY:O[1_554] | 1.75 | 0.45 |
| 4:6:298:VAL:O | 4:9:136:ILE:CD1[1_554] | 1.75 | 0.45 |
| 4:3:110:LEU:C | 4:7:192:ILE:CB[1_554] | 1.75 | 0.45 |
| 4:5:276:GLU:OE2 | 4:8:278:THR:CA[1_554] | 1.75 | 0.45 |
| 4:5:173:HIS:ND1 | 4:9:267:ILE:N[1_554] | 1.75 | 0.45 |
| 4:6:337:TYR:OH | 4:9:86:TRP:CD1[1_554] | 1.75 | 0.45 |
| 4:4:183:ARG:NE | 4:7:72:GLU:CD[1_554] | 1.75 | 0.45 |
| 4:6:262:PHE:CG | 4:9:153:LEU:C[1_554] | 1.75 | 0.45 |
| 4:3:285:CYS:C | 4:7:270:GLU:OE2[1_554] | 1.75 | 0.45 |
| 4:5:110:LEU:N | 4:9:195:GLU:OE2[1_554] | 1.75 | 0.45 |
| 4:5:252:ASN:OD1 | 4:8:215:LYS:CA[1_554] | 1.75 | 0.45 |
| 4:5:114:ALA:O | 4:9:196:ARG:NH2[1_554] | 1.76 | 0.44 |
| 4:6:338:SER:OG | 4:9:134:VAL:C[1_554] | 1.76 | 0.44 |
| 4:3:115:ASN:CA | 4:7:250:ILE:N[1_554] | 1.76 | 0.44 |
| 4:5:210:ARG:CG | 4:8:69:TYR:CE2[1_554] | 1.76 | 0.44 |
| 4:6:316:GLU:OE1 | 4:9:297:ASN:CA[1_554] | 1.76 | 0.44 |
| 4:4:196:ARG:CD | 4:7:211:ASP:OD1[1_554] | 1.76 | 0.44 |
| 4:2:292:ASP:CB | 4:7:40:HIS:CD2[1_554] | 1.76 | 0.44 |
| 4:5:190:MET:CE | 4:8:206:ARG:CZ[1_554] | 1.76 | 0.44 |
| 4:5:372:ARG:CA | 4:9:227:MET:CB[1_554] | 1.76 | 0.44 |
| 4:6:319:ALA:CA | 4:9:295:ALA:C[1_554] | 1.76 | 0.44 |
| 4:5:262:PHE:CE1 | 4:8:153:LEU:O[1_554] | 1.76 | 0.44 |
| 4:4:222:ASP:OD1 | 4:7:331:ALA:C[1_554] | 1.76 | 0.44 |
| 4:5:164:PRO:CB | 4:8:172:PRO:CG[1_554] | 1.76 | 0.44 |
| 4:6:198:TYR:CE2 | 4:9:208:ILE:O[1_554] | 1.76 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:287:ILE:C | 4:W:63:GLY:N[1_554] | 1.76 | 0.44 |
| 4:4:183:ARG:CB | 4:7:72:GLU:OE2[1_554] | 1.76 | 0.44 |
| 4:6:28:ARG:CZ | 4:9:125:GLU:O[1_554] | 1.76 | 0.44 |
| 4:4:341:ILE:N | 4:7:117:GLU:CA[1_554] | 1.76 | 0.44 |
| 4:4:333:PRO:CB | 4:7:105:LEU:N[1_554] | 1.76 | 0.44 |
| 4:6:321:ALA:CA | 4:9:289:ILE:O[1_554] | 1.76 | 0.44 |
| 4:6:157:ASP:CB | 4:9:72:GLU:C[1_554] | 1.76 | 0.44 |
| 4:5:75:ILE:CB | 4:9:197:GLY:C[1_554] | 1.76 | 0.44 |
| 4:5:280:ASN:OD1 | 4:8:281:SER:N[1_554] | 1.76 | 0.44 |
| 4:5:301:GLY:CA | 4:8:107:GLU:C[1_554] | 1.76 | 0.44 |
| 4:6:276:GLU:OE1 | 4:9:279:TYR:N[1_554] | 1.76 | 0.44 |
| 4:5:143:TYR:CG | 4:8:372:ARG:N[1_554] | 1.76 | 0.44 |
| 4:5:28:ARG:C | 4:8:83:GLU:OE1[1_554] | 1.76 | 0.44 |
| 4:6:219:VAL:N | 4:9:335:ARG:C[1_554] | 1.76 | 0.44 |
| 4:5:274:ILE:CG1 | 4:8:161:HIS:C[1_554] | 1.76 | 0.44 |
| 4:4:357:ILE:CG2 | 4:8:233:SER:N[1_554] | 1.76 | 0.44 |
| 4:5:213:LYS:CD | 4:8:157:ASP:CG[1_554] | 1.76 | 0.44 |
| 4:6:256:ARG:O | 4:9:303:THR:O[1_554] | 1.76 | 0.44 |
| 4:5:294:TYR:CB | 4:8:166:TYR:CD2[1_554] | 1.76 | 0.44 |
| 4:4:156:GLY:CA | 4:7:75:ILE:CG1[1_554] | 1.76 | 0.44 |
| 4:5:347:ALA:N | 4:8:366:GLY:O[1_554] | 1.76 | 0.44 |
| 4:6:137:GLN:OE1 | 4:9:112:PRO:CG[1_554] | 1.76 | 0.44 |
| 4:6:173:HIS:ND1 | 4:V:267:ILE:N[1_554] | 1.76 | 0.44 |
| 4:4:277:THR:CA | 4:7:174:ALA:C[1_554] | 1.76 | 0.44 |
| 4:6:143:TYR:CZ | 4:9:369:ILE:O[1_554] | 1.76 | 0.44 |
| 4:5:329:ILE:CG2 | 4:8:139:VAL:CA[1_554] | 1.76 | 0.44 |
| 4:4:282:ILE:CA | 4:7:173:HIS:NE2[1_554] | 1.76 | 0.44 |
| 4:4:72:GLU:O | 4:8:198:TYR:O[1_554] | 1.76 | 0.44 |
| 4:6:24:ASP:N | 4:9:124:PHE:CB[1_554] | 1.76 | 0.44 |
| 4:5:299:MET:CA | 4:8:136:ILE:CG2[1_554] | 1.76 | 0.44 |
| 4:5:318:THR:N | 4:8:150:GLY:CA[1_554] | 1.76 | 0.44 |
| 4:4:243:PRO:CA | 4:7:60:SER:CA[1_554] | 1.76 | 0.44 |
| 4:6:75:ILE:CB | 4:V:197:GLY:C[1_554] | 1.76 | 0.44 |
| 4:6:214:GLU:CB | 4:9:17:VAL:N[1_554] | 1.76 | 0.44 |
| 4:6:265:SER:OG | 4:9:261:LEU:O[1_554] | 1.76 | 0.44 |
| 4:5:72:GLU:O | 4:9:198:TYR:O[1_554] | 1.76 | 0.44 |
| 4:5:320:LEU:CD1 | 4:8:282:ILE:CD1[1_554] | 1.76 | 0.44 |
| 4:4:243:PRO:CG | 4:7:59:GLN:O[1_554] | 1.76 | 0.44 |
| 4:4:116:ARG:CD | 4:8:252:ASN:CB[1_554] | 1.76 | 0.44 |
| 4:5:22:ALA:N | 4:8:125:GLU:CD[1_554] | 1.76 | 0.44 |
| 4:4:223:PHE:CZ | 4:7:301:GLY:CA[1_554] | 1.76 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:154:ASP:CB | 4:9:111:ASN:N[1_554] | 1.76 | 0.44 |
| 4:4:207:GLU:OE1 | 4:7:66:THR:C[1_554] | 1.76 | 0.44 |
| 4:6:341:ILE:C | 4:9:120:THR:OG1[1_554] | 1.76 | 0.44 |
| 4:6:195:GLU:CA | 4:9:189:LEU:CD2[1_554] | 1.76 | 0.44 |
| 4:6:166:TYR:CD2 | 4:W:40:HIS:CD2[1_554] | 1.76 | 0.44 |
| 4:5:114:ALA:N | 4:9:253:GLU:OE2[1_554] | 1.76 | 0.44 |
| 4:6:62:ARG:NH1 | 4:9:67:LEU:C[1_554] | 1.76 | 0.44 |
| 4:5:345:ILE:O | 4:8:366:GLY:O[1_554] | 1.76 | 0.44 |
| 4:4:260:THR:CA | 4:7:155:SER:CB[1_554] | 1.76 | 0.44 |
| 4:6:293:LEU:CG | 4:9:169:TYR:CD2[1_554] | 1.76 | 0.44 |
| 4:6:136:ILE:CB | 4:9:113:LYS:CG[1_554] | 1.76 | 0.44 |
| 4:4:291:LYS:CB | 4:9:64:ILE:CD1[1_554] | 1.76 | 0.44 |
| 4:6:211:ASP:CB | 4:9:32:PRO:CD[1_554] | 1.76 | 0.44 |
| 4:4:222:ASP:N | 4:7:332:PRO:N[1_554] | 1.76 | 0.44 |
| 4:6:253:GLU:OE1 | 4:9:213:LYS:O[1_554] | 1.76 | 0.44 |
| 4:5:369:ILE:CB | 4:9:232:SER:CA[1_554] | 1.76 | 0.44 |
| 4:4:180:LEU:CD2 | 4:7:178:LEU:CA[1_554] | 1.76 | 0.44 |
| 4:6:214:GLU:N | 4:9:16:LEU:CA[1_554] | 1.76 | 0.44 |
| 4:4:367:PRO:N | 4:8:234:SER:C[1_554] | 1.76 | 0.44 |
| 4:6:173:HIS:CA | 4:V:267:ILE:CB[1_554] | 1.76 | 0.44 |
| 4:6:136:ILE:CA | 4:9:113:LYS:CB[1_554] | 1.76 | 0.44 |
| 4:6:24:ASP:O | 4:9:124:PHE:CD2[1_554] | 1.76 | 0.44 |
| 4:5:28:ARG:N | 4:8:122:ILE:CG2[1_554] | 1.76 | 0.44 |
| 4:6:302:GLY:O | 4:9:12:ASN:O[1_554] | 1.76 | 0.44 |
| 4:6:305:MET:SD | 4:9:106:THR:OG1[1_554] | 1.76 | 0.44 |
| 4:3:116:ARG:CA | 4:7:237:GLU:OE2[1_554] | 1.77 | 0.43 |
| 4:5:281:SER:OG | 4:8:172:PRO:C[1_554] | 1.77 | 0.43 |
| 4:5:277:THR:O | 4:8:174:ALA:CA[1_554] | 1.77 | 0.43 |
| 4:5:371:HIS:ND1 | 4:9:252:ASN:CB[1_554] | 1.77 | 0.43 |
| 4:5:256:ARG:CB | 4:8:306:TYR:CE1[1_554] | 1.77 | 0.43 |
| 4:6:267:ILE:CD1 | 4:9:180:LEU:N[1_554] | 1.77 | 0.43 |
| 4:4:223:PHE:CE2 | 4:7:300:SER:O[1_554] | 1.77 | 0.43 |
| 4:6:331:ALA:CB | 4:9:140:LEU:CA[1_554] | 1.77 | 0.43 |
| 4:4:336:LYS:C | 4:7:119:MET:SD[1_554] | 1.77 | 0.43 |
| 4:6:317:ILE:CG1 | 4:9:150:GLY:CA[1_554] | 1.77 | 0.43 |
| 4:6:243:PRO:CG | 4:9:60:SER:N[1_554] | 1.77 | 0.43 |
| 4:4:113:LYS:CG | 4:8:254:ARG:CB[1_554] | 1.77 | 0.43 |
| 4:4:142:LEU:CB | 4:7:372:ARG:O[1_554] | 1.77 | 0.43 |
| 4:5:93:GLU:OE2 | 4:8:80:ASP:OD2[1_554] | 1.77 | 0.43 |
| 4:5:21:PHE:CB | 4:8:125:GLU:OE1[1_554] | 1.77 | 0.43 |
| 4:6:195:GLU:C | 4:9:189:LEU:CD2[1_554] | 1.77 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:111:ASN:OD1 | 4:9:196:ARG:CG[1_554] | 1.77 | 0.43 |
| 4:4:334:GLU:O | 4:7:119:MET:CE[1_554] | 1.77 | 0.43 |
| 4:6:258:PRO:CD | 4:9:302:GLY:N[1_554] | 1.77 | 0.43 |
| 4:5:24:ASP:C | 4:8:124:PHE:N[1_554] | 1.77 | 0.43 |
| 4:6:317:ILE:N | 4:9:296:ASN:O[1_554] | 1.77 | 0.43 |
| 4:4:181:ALA:CB | 4:7:73:HIS:O[1_554] | 1.77 | 0.43 |
| 4:6:17:VAL:CB | 4:9:79:TRP:CB[1_554] | 1.77 | 0.43 |
| 4:5:367:PRO:N | 4:9:233:SER:CA[1_554] | 1.77 | 0.43 |
| 4:4:184:ASP:OD1 | 4:7:73:HIS:CD2[1_554] | 1.77 | 0.43 |
| 4:6:333:PRO:CD | 4:9:104:LEU:CB[1_554] | 1.77 | 0.43 |
| 4:4:178:LEU:CD1 | 4:7:177:ARG:C[1_554] | 1.77 | 0.43 |
| 4:3:173:HIS:NE2 | 4:7:264:PRO:O[1_554] | 1.77 | 0.43 |
| 4:6:166:TYR:CB | 4:W:40:HIS:CD2[1_554] | 1.77 | 0.43 |
| 4:2:292:ASP:N | 4:7:40:HIS:ND1[1_554] | 1.77 | 0.43 |
| 4:6:293:LEU:CB | 4:9:169:TYR:CD2[1_554] | 1.77 | 0.43 |
| 4:5:274:ILE:CA | 4:8:162:ASN:C[1_554] | 1.77 | 0.43 |
| 4:5:327:ILE:CA | 4:8:149:THR:N[1_554] | 1.77 | 0.43 |
| 4:6:341:ILE:O | 4:9:370:VAL:CG1[1_554] | 1.77 | 0.43 |
| 4:3:73:HIS:O | 4:7:198:TYR:O[1_554] | 1.77 | 0.43 |
| 4:6:309:ILE:CD1 | 4:9:154:ASP:CG[1_554] | 1.77 | 0.43 |
| 4:5:367:PRO:O | 4:9:230:ALA:C[1_554] | 1.77 | 0.43 |
| 4:6:188:TYR:CA | 4:9:183:ARG:C[1_554] | 1.77 | 0.43 |
| 4:6:172:PRO:O | 4:V:266:PHE:O[1_554] | 1.77 | 0.43 |
| 4:5:340:TRP:C | 4:8:120:THR:CB[1_554] | 1.77 | 0.43 |
| 4:5:200:PHE:CA | 4:8:206:ARG:CD[1_554] | 1.77 | 0.43 |
| 4:6:337:TYR:CZ | 4:9:86:TRP:CD2[1_554] | 1.77 | 0.43 |
| 4:4:310:ALA:CA | 4:7:141:SER:N[1_554] | 1.77 | 0.43 |
| 4:4:144:ALA:C | 4:7:371:HIS:N[1_554] | 1.77 | 0.43 |
| 4:5:113:LYS:N | 4:9:253:GLU:CG[1_554] | 1.77 | 0.43 |
| 4:3:114:ALA:CB | 4:7:238:LYS:O[1_554] | 1.77 | 0.43 |
| 4:3:75:ILE:C | 4:7:198:TYR:CD1[1_554] | 1.77 | 0.43 |
| 4:4:314:GLN:CB | 4:7:142:LEU:C[1_554] | 1.77 | 0.43 |
| 4:6:173:HIS:CB | 4:V:267:ILE:CG1[1_554] | 1.77 | 0.43 |
| 4:4:24:ASP:CA | 4:7:125:GLU:OE2[1_554] | 1.77 | 0.43 |
| 4:5:299:MET:CB | 4:8:137:GLN:N[1_554] | 1.77 | 0.43 |
| 4:5:257:CYS:N | 4:8:303:THR:OG1[1_554] | 1.77 | 0.43 |
| 4:5:341:ILE:O | 4:8:370:VAL:CG1[1_554] | 1.77 | 0.43 |
| 4:6:256:ARG:CB | 4:9:306:TYR:CZ[1_554] | 1.77 | 0.43 |
| 4:6:157:ASP:CG | 4:9:71:ILE:C[1_554] | 1.77 | 0.43 |
| 4:4:262:PHE:CB | 4:7:153:LEU:CB[1_554] | 1.77 | 0.43 |
| 4:4:193:LEU:O | 4:7:210:ARG:CA[1_554] | 1.77 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:300:SER:CA | 4:8:107:GLU:CG[1_554] | 1.77 | 0.43 |
| 4:5:117:GLU:CD | 4:9:236:LEU:CG[1_554] | 1.77 | 0.43 |
| 4:4:207:GLU:CD | 4:7:67:LEU:N[1_554] | 1.77 | 0.43 |
| 4:4:136:ILE:O | 4:7:113:LYS:CE[1_554] | 1.77 | 0.43 |
| 4:6:305:MET:SD | 4:9:11:ASP:CA[1_554] | 1.77 | 0.43 |
| 4:5:315:LYS:N | 4:8:298:VAL:CG2[1_554] | 1.77 | 0.43 |
| 4:4:191:LYS:CA | 4:7:187:ASP:N[1_554] | 1.77 | 0.43 |
| 4:4:273:GLY:C | 4:7:162:ASN:CG[1_554] | 1.77 | 0.43 |
| 4:4:293:LEU:CG | 4:7:169:TYR:CZ[1_554] | 1.77 | 0.43 |
| 4:6:280:ASN:CB | 4:9:284:LYS:CB[1_554] | 1.77 | 0.43 |
| 4:5:188:TYR:N | 4:8:183:ARG:CA[1_554] | 1.77 | 0.43 |
| 4:6:337:TYR:CD1 | 4:9:86:TRP:CH2[1_554] | 1.77 | 0.43 |
| 4:5:14:SER:C | 4:8:77:THR:CB[1_554] | 1.77 | 0.43 |
| 4:5:191:LYS:N | 4:8:186:THR:CA[1_554] | 1.77 | 0.43 |
| 4:3:291:LYS:CD | 4:8:64:ILE:CB[1_554] | 1.77 | 0.43 |
| 4:4:253:GLU:CG | 4:7:214:GLU:OE2[1_554] | 1.77 | 0.43 |
| 4:6:22:ALA:N | 4:9:125:GLU:CD[1_554] | 1.77 | 0.43 |
| 4:5:201:VAL:CG2 | 4:8:203:THR:N[1_554] | 1.77 | 0.43 |
| 4:6:19:ALA:CA | 4:9:118:LYS:NZ[1_554] | 1.77 | 0.43 |
| 4:5:243:PRO:CG | 4:8:60:SER:N[1_554] | 1.77 | 0.43 |
| 4:5:277:THR:CG2 | 4:8:175:ILE:O[1_554] | 1.77 | 0.43 |
| 4:6:179:ASP:C | 4:9:179:ASP:OD1[1_554] | 1.77 | 0.43 |
| 4:5:337:TYR:CZ | 4:8:86:TRP:NE1[1_554] | 1.77 | 0.43 |
| 4:5:272:ALA:CA | 4:8:277:THR:CG2[1_554] | 1.77 | 0.43 |
| 4:6:299:MET:CG | 4:9:138:ALA:N[1_554] | 1.77 | 0.43 |
| 4:6:307:PRO:CA | 4:9:337:TYR:CA[1_554] | 1.77 | 0.43 |
| 4:6:319:ALA:O | 4:9:294:TYR:N[1_554] | 1.77 | 0.43 |
| 4:6:344:SER:C | 4:9:362:TYR:CE1[1_554] | 1.77 | 0.43 |
| 4:4:112:PRO:C | 4:8:253:GLU:CG[1_554] | 1.77 | 0.43 |
| 4:6:274:ILE:CG1 | 4:9:161:HIS:CA[1_554] | 1.77 | 0.43 |
| 4:6:221:LEU:CA | 4:9:331:ALA:C[1_554] | 1.77 | 0.43 |
| 4:4:79:TRP:NE1 | 4:8:247:VAL:O[1_554] | 1.77 | 0.43 |
| 4:6:154:ASP:OD1 | 4:9:108:ALA:O[1_554] | 1.77 | 0.43 |
| 4:4:256:ARG:C | 4:7:303:THR:OG1[1_554] | 1.78 | 0.42 |
| 4:4:199:SER:O | 4:7:203:THR:O[1_554] | 1.78 | 0.42 |
| 4:6:159:VAL:N | 4:9:177:ARG:NH1[1_554] | 1.78 | 0.42 |
| 4:5:367:PRO:CG | 4:9:234:SER:O[1_554] | 1.78 | 0.42 |
| 4:5:167:GLU:CD | 4:V:41:GLN:N[1_554] | 1.78 | 0.42 |
| 4:6:315:LYS:N | 4:9:298:VAL:CG2[1_554] | 1.78 | 0.42 |
| 4:6:317:ILE:CG2 | 4:9:151:ILE:CA[1_554] | 1.78 | 0.42 |
| 4:6:144:ALA:C | 4:9:372:ARG:NH2[1_554] | 1.78 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:257:CYS:C | 4:7:156:GLY:O[1_554] | 1.78 | 0.42 |
| 4:4:367:PRO:N | 4:8:236:LEU:N[1_554] | 1.78 | 0.42 |
| 4:6:322:PRO:CD | 4:9:289:ILE:CA[1_554] | 1.78 | 0.42 |
| 4:4:210:ARG:CD | 4:7:69:TYR:CG[1_554] | 1.78 | 0.42 |
| 4:6:335:ARG:O | 4:9:107:GLU:N[1_554] | 1.78 | 0.42 |
| 4:6:278:THR:CG2 | 4:9:164:PRO:N[1_554] | 1.78 | 0.42 |
| 4:6:15:GLY:C | 4:9:77:THR:CB[1_554] | 1.78 | 0.42 |
| 4:4:156:GLY:C | 4:7:75:ILE:CA[1_554] | 1.78 | 0.42 |
| 4:6:153:LEU:CG | 4:9:109:PRO:CG[1_554] | 1.78 | 0.42 |
| 4:4:191:LYS:O | 4:7:186:THR:CB[1_554] | 1.78 | 0.42 |
| 4:6:189:LEU:O | 4:9:186:THR:CB[1_554] | 1.78 | 0.42 |
| 4:5:21:PHE:C | 4:8:125:GLU:OE1[1_554] | 1.78 | 0.42 |
| 4:4:281:SER:CA | 4:7:173:HIS:CG[1_554] | 1.78 | 0.42 |
| 4:6:313:MET:O | 4:9:142:LEU:CD1[1_554] | 1.78 | 0.42 |
| 4:6:196:ARG:CD | 4:9:211:ASP:C[1_554] | 1.78 | 0.42 |
| 4:5:328:LYS:N | 4:8:148:THR:C[1_554] | 1.78 | 0.42 |
| 4:5:24:ASP:CG | 4:8:124:PHE:C[1_554] | 1.78 | 0.42 |
| 4:6:282:ILE:CB | 4:9:171:LEU:CD1[1_554] | 1.78 | 0.42 |
| 4:5:76:ILE:O | 4:9:198:TYR:CE1[1_554] | 1.78 | 0.42 |
| 4:5:320:LEU:N | 4:8:293:LEU:N[1_554] | 1.78 | 0.42 |
| 4:4:331:ALA:O | 4:7:135:ALA:CB[1_554] | 1.78 | 0.42 |
| 4:4:319:ALA:CA | 4:7:296:ASN:CB[1_554] | 1.78 | 0.42 |
| 4:6:309:ILE:N | 4:9:141:SER:OG[1_554] | 1.78 | 0.42 |
| 4:4:207:GLU:CG | 4:7:67:LEU:C[1_554] | 1.78 | 0.42 |
| 4:5:300:SER:O | 4:8:108:ALA:C[1_554] | 1.78 | 0.42 |
| 4:6:316:GLU:N | 4:9:296:ASN:O[1_554] | 1.78 | 0.42 |
| 4:5:205:GLU:CB | 4:8:62:ARG:NH2[1_554] | 1.78 | 0.42 |
| 4:6:14:SER:O | 4:9:77:THR:OG1[1_554] | 1.78 | 0.42 |
| 4:6:326:LYS:N | 4:9:167:GLU:OE2[1_554] | 1.78 | 0.42 |
| 4:4:141:SER:CA | 4:7:371:HIS:ND1[1_554] | 1.78 | 0.42 |
| 4:5:278:THR:N | 4:8:164:PRO:CG[1_554] | 1.78 | 0.42 |
| 4:3:73:HIS:CG | 4:7:199:SER:OG[1_554] | 1.78 | 0.42 |
| 4:6:307:PRO:O | 4:9:335:ARG:O[1_554] | 1.78 | 0.42 |
| 4:5:204:ALA:CA | 4:8:62:ARG:CD[1_554] | 1.78 | 0.42 |
| 4:5:162:ASN:ND2 | 4:8:175:ILE:CD1[1_554] | 1.78 | 0.42 |
| 4:4:304:THR:CB | 4:7:107:GLU:C[1_554] | 1.78 | 0.42 |
| 4:4:326:LYS:CE | 4:9:45:VAL:CA[1_554] | 1.78 | 0.42 |
| 4:4:338:SER:CA | 4:7:116:ARG:C[1_554] | 1.78 | 0.42 |
| 4:6:318:THR:CB | 4:9:296:ASN:OD1[1_554] | 1.78 | 0.42 |
| 4:5:371:HIS:N | 4:9:230:ALA:C[1_554] | 1.78 | 0.42 |
| 4:4:262:PHE:CE1 | 4:7:152:VAL:CG1[1_554] | 1.78 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:312:ARG:CZ | 4:9:299:MET:CB[1_554] | 1.78 | 0.42 |
| 4:6:369:ILE:CB | 4:V:232:SER:CA[1_554] | 1.78 | 0.42 |
| 4:5:260:THR:O | 4:8:160:THR:CG2[1_554] | 1.78 | 0.42 |
| 4:6:192:ILE:C | 4:9:213:LYS:CB[1_554] | 1.78 | 0.42 |
| 4:4:300:SER:CA | 4:7:107:GLU:OE1[1_554] | 1.78 | 0.42 |
| 4:5:15:GLY:C | 4:8:77:THR:CA[1_554] | 1.78 | 0.42 |
| 4:5:196:ARG:CB | 4:8:212:ILE:CB[1_554] | 1.78 | 0.42 |
| 4:6:113:LYS:N | 4:V:253:GLU:OE1[1_554] | 1.78 | 0.42 |
| 4:6:286:ASP:N | 4:V:270:GLU:OE2[1_554] | 1.78 | 0.42 |
| 4:4:18:LYS:CG | 4:7:79:TRP:CG[1_554] | 1.78 | 0.42 |
| 4:6:312:ARG:NH1 | 4:9:299:MET:SD[1_554] | 1.78 | 0.42 |
| 4:5:24:ASP:OD1 | 4:8:124:PHE:O[1_554] | 1.78 | 0.42 |
| 4:4:223:PHE:CE2 | 4:7:301:GLY:N[1_554] | 1.78 | 0.42 |
| 4:5:177:ARG:NH2 | 4:9:194:THR:CG2[1_554] | 1.78 | 0.42 |
| 4:6:301:GLY:C | 4:9:137:GLN:NE2[1_554] | 1.78 | 0.42 |
| 4:3:288:ASP:C | 4:8:39:ARG:NH1[1_554] | 1.78 | 0.42 |
| 4:6:289:ILE:CA | 4:W:63:GLY:C[1_554] | 1.78 | 0.42 |
| 4:6:166:TYR:CA | 4:W:40:HIS:CD2[1_554] | 1.78 | 0.42 |
| 4:4:262:PHE:O | 4:7:153:LEU:CG[1_554] | 1.78 | 0.42 |
| 4:6:262:PHE:CG | 4:9:153:LEU:O[1_554] | 1.78 | 0.42 |
| 4:6:114:ALA:N | 4:V:251:GLY:N[1_554] | 1.78 | 0.42 |
| 4:6:322:PRO:CG | 4:9:288:ASP:C[1_554] | 1.78 | 0.42 |
| 4:5:327:ILE:O | 4:8:148:THR:CA[1_554] | 1.78 | 0.42 |
| 4:2:291:LYS:CD | 4:7:40:HIS:N[1_554] | 1.78 | 0.42 |
| 4:4:275:HIS:CB | 4:7:152:VAL:N[1_554] | 1.78 | 0.42 |
| 4:6:187:ASP:N | 4:9:183:ARG:CD[1_554] | 1.78 | 0.42 |
| 4:6:113:LYS:O | 4:V:252:ASN:OD1[1_554] | 1.78 | 0.42 |
| 4:6:219:VAL:CA | 4:9:301:GLY:N[1_554] | 1.78 | 0.42 |
| 4:5:263:GLN:CB | 4:8:274:ILE:CG1[1_554] | 1.78 | 0.42 |
| 4:5:141:SER:OG | 4:8:107:GLU:CD[1_554] | 1.78 | 0.42 |
| 4:3:166:TYR:CG | 4:8:40:HIS:NE2[1_554] | 1.78 | 0.42 |
| 4:5:310:ALA:CA | 4:8:141:SER:CB[1_554] | 1.78 | 0.42 |
| 4:5:113:LYS:O | 4:9:252:ASN:N[1_554] | 1.78 | 0.42 |
| 4:5:335:ARG:CA | 4:8:105:LEU:O[1_554] | 1.78 | 0.42 |
| 4:5:278:THR:C | 4:8:164:PRO:CB[1_554] | 1.78 | 0.42 |
| 4:4:293:LEU:CB | 4:7:169:TYR:CD2[1_554] | 1.78 | 0.42 |
| 4:4:196:ARG:CB | 4:7:212:ILE:N[1_554] | 1.78 | 0.42 |
| 4:4:240:TYR:CE2 | 4:7:56:ASP:OD2[1_554] | 1.78 | 0.42 |
| 4:6:340:TRP:CD1 | 4:9:118:LYS:CA[1_554] | 1.78 | 0.42 |
| 4:5:173:HIS:CG | 4:9:264:PRO:O[1_554] | 1.78 | 0.42 |
| 4:5:29:ALA:CB | 4:8:83:GLU:OE1[1_554] | 1.78 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:260:THR:C | 4:9:155:SER:OG[1_554] | 1.79 | 0.41 |
| 4:6:341:ILE:CA | 4:9:120:THR:CB[1_554] | 1.79 | 0.41 |
| 4:5:214:GLU:CA | 4:8:16:LEU:N[1_554] | 1.79 | 0.41 |
| 4:5:198:TYR:CG | 4:8:208:ILE:N[1_554] | 1.79 | 0.41 |
| 4:5:269:MET:N | 4:8:264:PRO:CB[1_554] | 1.79 | 0.41 |
| 4:3:115:ASN:CA | 4:7:249:THR:O[1_554] | 1.79 | 0.41 |
| 4:6:196:ARG:NH1 | 4:9:215:LYS:CA[1_554] | 1.79 | 0.41 |
| 4:4:143:TYR:CE2 | 4:7:368:SER:CA[1_554] | 1.79 | 0.41 |
| 4:5:154:ASP:CA | 4:8:108:ALA:C[1_554] | 1.79 | 0.41 |
| 4:6:164:PRO:CB | 4:9:172:PRO:CG[1_554] | 1.79 | 0.41 |
| 4:4:162:ASN:ND2 | 4:7:175:ILE:CB[1_554] | 1.79 | 0.41 |
| 4:4:366:GLY:O | 4:8:234:SER:CA[1_554] | 1.79 | 0.41 |
| 4:6:258:PRO:CD | 4:9:302:GLY:C[1_554] | 1.79 | 0.41 |
| 4:4:257:CYS:C | 4:7:156:GLY:C[1_554] | 1.79 | 0.41 |
| 4:5:28:ARG:CZ | 4:8:125:GLU:O[1_554] | 1.79 | 0.41 |
| 4:4:332:PRO:C | 4:7:105:LEU:O[1_554] | 1.79 | 0.41 |
| 4:4:260:THR:CG2 | 4:7:180:LEU:O[1_554] | 1.79 | 0.41 |
| 4:4:257:CYS:O | 4:7:156:GLY:CA[1_554] | 1.79 | 0.41 |
| 4:5:327:ILE:C | 4:8:148:THR:CA[1_554] | 1.79 | 0.41 |
| 4:3:177:ARG:NH1 | 4:7:194:THR:OG1[1_554] | 1.79 | 0.41 |
| 4:6:32:PRO:N | 4:9:78:ASN:CG[1_554] | 1.79 | 0.41 |
| 4:5:340:TRP:CD2 | 4:8:118:LYS:O[1_554] | 1.79 | 0.41 |
| 4:6:345:ILE:CD1 | 4:9:357:ILE:CG2[1_554] | 1.79 | 0.41 |
| 1:D:542:PHE:CD2 | 4:6:328:LYS:NZ[1_556] | 1.79 | 0.41 |
| 4:6:253:GLU:CD | 4:9:214:GLU:CB[1_554] | 1.79 | 0.41 |
| 4:3:117:GLU:CG | 4:7:237:GLU:N[1_554] | 1.79 | 0.41 |
| 4:5:27:PRO:N | 4:8:122:ILE:C[1_554] | 1.79 | 0.41 |
| 4:4:154:ASP:OD1 | 4:7:111:ASN:C[1_554] | 1.79 | 0.41 |
| 4:5:221:LEU:CG | 4:8:332:PRO:CA[1_554] | 1.79 | 0.41 |
| 4:6:140:LEU:CD2 | 4:9:371:HIS:CG[1_554] | 1.79 | 0.41 |
| 4:3:112:PRO:CG | 4:7:193:LEU:CD2[1_554] | 1.79 | 0.41 |
| 4:4:16:LEU:CD1 | 4:7:78:ASN:O[1_554] | 1.79 | 0.41 |
| 4:5:24:ASP:C | 4:8:124:PHE:CG[1_554] | 1.79 | 0.41 |
| 4:5:318:THR:C | 4:8:296:ASN:ND2[1_554] | 1.79 | 0.41 |
| 4:6:320:LEU:CD1 | 4:9:282:ILE:CD1[1_554] | 1.79 | 0.41 |
| 4:5:294:TYR:CD1 | 4:8:166:TYR:CB[1_554] | 1.79 | 0.41 |
| 4:5:367:PRO:CA | 4:9:234:SER:N[1_554] | 1.79 | 0.41 |
| 4:5:184:ASP:N | 4:8:73:HIS:CE1[1_554] | 1.79 | 0.41 |
| 4:5:213:LYS:CG | 4:8:157:ASP:CB[1_554] | 1.79 | 0.41 |
| 4:5:215:LYS:N | 4:8:16:LEU:CB[1_554] | 1.79 | 0.41 |
| 4:5:339:VAL:CA | 4:8:116:ARG:CG[1_554] | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:320:LEU:CB | 4:7:293:LEU:CD1[1_554] | 1.79 | 0.41 |
| 4:6:258:PRO:CB | 4:9:301:GLY:CA[1_554] | 1.79 | 0.41 |
| 4:6:281:SER:OG | 4:9:173:HIS:CA[1_554] | 1.79 | 0.41 |
| 4:5:223:PHE:CD2 | 4:8:304:THR:CB[1_554] | 1.79 | 0.41 |
| 4:4:266:PHE:N | 4:7:261:LEU:CB[1_554] | 1.79 | 0.41 |
| 4:5:295:ALA:N | 4:8:167:GLU:C[1_554] | 1.79 | 0.41 |
| 4:6:294:TYR:CB | 4:9:166:TYR:C[1_554] | 1.79 | 0.41 |
| 4:6:332:PRO:CD | 4:9:135:ALA:CA[1_554] | 1.79 | 0.41 |
| 4:3:79:TRP:NE1 | 4:7:247:VAL:O[1_554] | 1.79 | 0.41 |
| 4:5:157:ASP:OD2 | 4:8:72:GLU:N[1_554] | 1.79 | 0.41 |
| 4:6:191:LYS:CG | 4:9:185:LEU:O[1_554] | 1.79 | 0.41 |
| 4:5:367:PRO:C | 4:9:233:SER:CA[1_554] | 1.79 | 0.41 |
| 4:4:283:MET:CG | 4:7:285:CYS:C[1_554] | 1.79 | 0.41 |
| 4:5:334:GLU:C | 4:8:105:LEU:N[1_554] | 1.79 | 0.41 |
| 4:6:186:THR:O | 4:9:183:ARG:CB[1_554] | 1.79 | 0.41 |
| 4:6:185:LEU:CD1 | 4:9:181:ALA:CB[1_554] | 1.79 | 0.41 |
| 4:4:204:ALA:CB | 4:7:63:GLY:N[1_554] | 1.79 | 0.41 |
| 4:3:175:ILE:CG2 | 4:7:191:LYS:CD[1_554] | 1.79 | 0.41 |
| 4:4:210:ARG:N | 4:7:69:TYR:OH[1_554] | 1.79 | 0.41 |
| 4:5:307:PRO:O | 4:8:335:ARG:O[1_554] | 1.79 | 0.41 |
| 4:6:161:HIS:C | 4:9:110:LEU:CD2[1_554] | 1.79 | 0.41 |
| 4:5:22:ALA:N | 4:8:125:GLU:OE2[1_554] | 1.79 | 0.41 |
| 4:6:220:ALA:O | 4:9:335:ARG:CD[1_554] | 1.79 | 0.41 |
| 4:5:193:LEU:CB | 4:8:210:ARG:CG[1_554] | 1.79 | 0.41 |
| 4:4:75:ILE:CG2 | 4:8:198:TYR:CB[1_554] | 1.79 | 0.41 |
| 4:6:270:GLU:N | 4:9:271:SER:O[1_554] | 1.79 | 0.41 |
| 4:5:113:LYS:N | 4:9:253:GLU:OE2[1_554] | 1.79 | 0.41 |
| 4:4:214:GLU:N | 4:7:15:GLY:O[1_554] | 1.79 | 0.41 |
| 4:6:223:PHE:CE1 | 4:9:304:THR:C[1_554] | 1.79 | 0.41 |
| 4:4:278:THR:O | 4:7:171:LEU:O[1_554] | 1.79 | 0.41 |
| 4:5:320:LEU:CB | 4:8:293:LEU:CA[1_554] | 1.79 | 0.41 |
| 4:5:56:ASP:OD1 | 4:8:81:ASP:OD1[1_554] | 1.79 | 0.41 |
| 4:4:140:LEU:N | 4:7:371:HIS:NE2[1_554] | 1.79 | 0.41 |
| 4:5:25:ASP:N | 4:8:124:PHE:N[1_554] | 1.79 | 0.41 |
| 4:4:303:THR:O | 4:7:137:GLN:OE1[1_554] | 1.79 | 0.41 |
| 4:6:343:GLY:C | 4:9:367:PRO:C[1_554] | 1.79 | 0.41 |
| 4:5:343:GLY:C | 4:8:367:PRO:C[1_554] | 1.79 | 0.41 |
| 4:5:151:ILE:CG1 | 4:8:170:ALA:C[1_554] | 1.79 | 0.41 |
| 4:4:293:LEU:O | 4:7:169:TYR:CD1[1_554] | 1.79 | 0.41 |
| 4:6:181:ALA:CB | 4:9:73:HIS:O[1_554] | 1.79 | 0.41 |
| 4:4:208:ILE:N | 4:7:67:LEU:CD1[1_554] | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:256:ARG:CD | 4:8:306:TYR:CE1[1_554] | 1.79 | 0.41 |
| 4:5:31:PHE:CB | 4:8:80:ASP:N[1_554] | 1.79 | 0.41 |
| 4:5:266:PHE:CB | 4:8:261:LEU:CB[1_554] | 1.79 | 0.41 |
| 4:4:198:TYR:CB | 4:7:207:GLU:O[1_554] | 1.79 | 0.41 |
| 4:6:340:TRP:C | 4:9:116:ARG:O[1_554] | 1.79 | 0.41 |
| 4:6:256:ARG:CB | 4:9:306:TYR:CE1[1_554] | 1.79 | 0.41 |
| 4:3:370:VAL:CA | 4:7:230:ALA:CA[1_554] | 1.79 | 0.41 |
| 4:5:337:TYR:C | 4:8:119:MET:CE[1_554] | 1.79 | 0.41 |
| 4:4:308:GLY:N | 4:7:339:VAL:N[1_554] | 1.79 | 0.41 |
| 4:4:199:SER:CA | 4:7:206:ARG:C[1_554] | 1.79 | 0.41 |
| 4:6:20:GLY:C | 4:9:121:GLN:CD[1_554] | 1.79 | 0.41 |
| 4:5:294:TYR:OH | 4:8:289:ILE:CB[1_554] | 1.79 | 0.41 |
| 4:5:198:TYR:CG | 4:8:209:VAL:N[1_554] | 1.79 | 0.41 |
| 4:5:200:PHE:CE1 | 4:8:207:GLU:CA[1_554] | 1.79 | 0.41 |
| 4:4:180:LEU:CG | 4:7:178:LEU:C[1_554] | 1.79 | 0.41 |
| 4:4:280:ASN:OD1 | 4:7:281:SER:O[1_554] | 1.79 | 0.41 |
| 4:5:299:MET:SD | 4:8:138:ALA:N[1_554] | 1.79 | 0.41 |
| 4:6:154:ASP:C | 4:9:108:ALA:C[1_554] | 1.80 | 0.40 |
| 4:6:223:PHE:CA | 4:9:335:ARG:NH2[1_554] | 1.80 | 0.40 |
| 4:5:276:GLU:CB | 4:8:278:THR:O[1_554] | 1.80 | 0.40 |
| 4:4:108:ALA:CB | 4:8:196:ARG:N[1_554] | 1.80 | 0.40 |
| 4:5:181:ALA:CB | 4:8:73:HIS:O[1_554] | 1.80 | 0.40 |
| 4:6:286:ASP:OD2 | 4:W:39:ARG:NH1[1_554] | 1.80 | 0.40 |
| 4:5:144:ALA:CB | 4:8:370:VAL:CG2[1_554] | 1.80 | 0.40 |
| 4:6:274:ILE:N | 4:9:161:HIS:C[1_554] | 1.80 | 0.40 |
| 4:6:327:ILE:CA | 4:9:148:THR:C[1_554] | 1.80 | 0.40 |
| 4:5:280:ASN:OD1 | 4:8:281:SER:C[1_554] | 1.80 | 0.40 |
| 4:4:277:THR:OG1 | 4:7:176:MET:CG[1_554] | 1.80 | 0.40 |
| 4:5:194:THR:CB | 4:8:190:MET:SD[1_554] | 1.80 | 0.40 |
| 4:4:15:GLY:N | 4:7:77:THR:CG2[1_554] | 1.80 | 0.40 |
| 4:6:327:ILE:C | 4:9:148:THR:O[1_554] | 1.80 | 0.40 |
| 4:5:325:MET:CG | 4:8:166:TYR:OH[1_554] | 1.80 | 0.40 |
| 4:6:214:GLU:CG | 4:9:16:LEU:CA[1_554] | 1.80 | 0.40 |
| 4:4:266:PHE:O | 4:7:185:LEU:CD1[1_554] | 1.80 | 0.40 |
| 4:4:337:TYR:CG | 4:7:119:MET:CA[1_554] | 1.80 | 0.40 |
| 4:6:155:SER:O | 4:9:108:ALA:CB[1_554] | 1.80 | 0.40 |
| 4:5:346:LEU:CB | 4:8:369:ILE:N[1_554] | 1.80 | 0.40 |
| 4:4:207:GLU:OE1 | 4:7:66:THR:O[1_554] | 1.80 | 0.40 |
| 4:6:151:ILE:CG2 | 4:9:169:TYR:C[1_554] | 1.80 | 0.40 |
| 4:6:214:GLU:CG | 4:9:16:LEU:N[1_554] | 1.80 | 0.40 |
| 4:6:31:PHE:N | 4:9:79:TRP:C[1_554] | 1.80 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:289:ILE:O | 4:W:64:ILE:CG2[1_554] | 1.80 | 0.40 |
| 4:3:370:VAL:C | 4:7:230:ALA:CB[1_554] | 1.80 | 0.40 |
| 4:6:186:THR:O | 4:9:183:ARG:CG[1_554] | 1.80 | 0.40 |
| 4:4:117:GLU:CB | 4:8:237:GLU:N[1_554] | 1.80 | 0.40 |
| 4:6:347:ALA:N | 4:9:366:GLY:CA[1_554] | 1.80 | 0.40 |
| 4:6:262:PHE:CG | 4:9:153:LEU:CA[1_554] | 1.80 | 0.40 |
| 4:4:223:PHE:CA | 4:7:335:ARG:CZ[1_554] | 1.80 | 0.40 |
| 4:5:371:HIS:CB | 4:9:230:ALA:CA[1_554] | 1.80 | 0.40 |
| 4:6:218:TYR:N | 4:9:336:LYS:CB[1_554] | 1.80 | 0.40 |
| 4:4:177:ARG:NH2 | 4:8:194:THR:CG2[1_554] | 1.80 | 0.40 |
| 4:4:198:TYR:CG | 4:7:207:GLU:O[1_554] | 1.80 | 0.40 |
| 4:4:253:GLU:OE2 | 4:7:214:GLU:CD[1_554] | 1.80 | 0.40 |
| 4:5:188:TYR:CD1 | 4:8:185:LEU:CB[1_554] | 1.80 | 0.40 |
| 4:6:145:SER:CA | 4:9:372:ARG:CZ[1_554] | 1.80 | 0.40 |
| 4:5:274:ILE:CA | 4:8:161:HIS:C[1_554] | 1.80 | 0.40 |
| 4:6:336:LYS:CD | 4:9:12:ASN:ND2[1_554] | 1.80 | 0.40 |
| 4:6:196:ARG:CB | 4:9:212:ILE:C[1_554] | 1.80 | 0.40 |
| 4:4:260:THR:CB | 4:7:155:SER:OG[1_554] | 1.80 | 0.40 |
| 4:4:214:GLU:O | 4:7:16:LEU:O[1_554] | 1.80 | 0.40 |
| 4:4:345:ILE:N | 4:7:367:PRO:CG[1_554] | 1.80 | 0.40 |
| 4:4:222:ASP:CG | 4:7:331:ALA:C[1_554] | 1.80 | 0.40 |
| 4:4:288:ASP:O | 4:9:64:ILE:N[1_554] | 1.80 | 0.40 |
| 4:4:178:LEU:CD1 | 4:7:177:ARG:N[1_554] | 1.80 | 0.40 |
| 4:4:25:ASP:CG | 4:7:124:PHE:CA[1_554] | 1.80 | 0.40 |
| 4:4:288:ASP:C | 4:9:63:GLY:O[1_554] | 1.80 | 0.40 |
| 4:3:117:GLU:N | 4:7:237:GLU:CD[1_554] | 1.80 | 0.40 |
| 4:5:11:ASP:N | 4:8:118:LYS:CB[1_554] | 1.80 | 0.40 |
| 4:5:327:ILE:CA | 4:8:148:THR:C[1_554] | 1.80 | 0.40 |
| 4:6:215:LYS:CD | 4:9:31:PHE:CA[1_554] | 1.80 | 0.40 |
| 4:6:193:LEU:CA | 4:9:210:ARG:N[1_554] | 1.80 | 0.40 |
| 4:4:31:PHE:CA | 4:7:78:ASN:CG[1_554] | 1.80 | 0.40 |
| 4:6:369:ILE:CA | 4:V:228:ALA:O[1_554] | 1.80 | 0.40 |
| 4:6:340:TRP:CB | 4:9:119:MET:C[1_554] | 1.80 | 0.40 |
| 4:3:73:HIS:C | 4:7:198:TYR:O[1_554] | 1.80 | 0.40 |
| 4:5:137:GLN:OE1 | 4:8:112:PRO:N[1_554] | 1.80 | 0.40 |
| 4:5:150:GLY:O | 4:8:169:TYR:CD1[1_554] | 1.80 | 0.40 |
| 4:5:317:ILE:CG2 | 4:8:151:ILE:CA[1_554] | 1.80 | 0.40 |
| 4:6:24:ASP:CG | 4:9:124:PHE:O[1_554] | 1.80 | 0.40 |
| 4:5:346:LEU:CD2 | 4:8:368:SER:CA[1_554] | 1.80 | 0.40 |
| 4:4:110:LEU:CA | 4:8:192:ILE:CG2[1_554] | 1.80 | 0.40 |
| 4:5:321:ALA:CB | 4:8:292:ASP:CB[1_554] | 1.80 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:116:ARG:N | 4:8:196:ARG:CZ[1_554] | 1.80 | 0.40 |
| 4:6:227:MET:SD | 4:9:307:PRO:CD[1_554] | 1.80 | 0.40 |
| 4:4:322:PRO:C | 4:7:292:ASP:OD2[1_554] | 1.80 | 0.40 |
| 4:4:275:HIS:CA | 4:7:163:VAL:C[1_554] | 1.80 | 0.40 |
| 4:4:297:ASN:OD1 | 4:7:170:ALA:CB[1_554] | 1.80 | 0.40 |
| 4:4:173:HIS:C | 4:8:267:ILE:C[1_554] | 1.80 | 0.40 |
| 4:6:161:HIS:CG | 4:9:110:LEU:CB[1_554] | 1.80 | 0.40 |
| 4:6:280:ASN:ND2 | 4:9:281:SER:C[1_554] | 1.80 | 0.40 |
| 4:6:266:PHE:CD1 | 4:9:261:LEU:CD1[1_554] | 1.80 | 0.40 |
| 4:4:320:LEU:CA | 4:7:293:LEU:CB[1_554] | 1.80 | 0.40 |
| 4:5:193:LEU:CD1 | 4:8:210:ARG:CA[1_554] | 1.80 | 0.40 |
| 4:4:25:ASP:CB | 4:7:125:GLU:N[1_554] | 1.80 | 0.40 |
| 4:6:157:ASP:OD2 | 4:9:72:GLU:CG[1_554] | 1.80 | 0.40 |
| 4:5:11:ASP:OD2 | 4:8:115:ASN:CB[1_554] | 1.80 | 0.40 |
| 4:4:191:LYS:O | 4:7:186:THR:CA[1_554] | 1.80 | 0.40 |
| 4:6:371:HIS:CG | 4:V:230:ALA:CB[1_554] | 1.80 | 0.40 |
| 4:5:24:ASP:CB | 4:8:124:PHE:CA[1_554] | 1.80 | 0.40 |
| 4:6:283:MET:CE | 4:9:289:ILE:N[1_554] | 1.80 | 0.40 |
| 4:5:309:ILE:N | 4:8:338:SER:CB[1_554] | 1.80 | 0.40 |
| 4:6:198:TYR:CD1 | 4:9:208:ILE:CG2[1_554] | 1.80 | 0.40 |
| 4:6:279:TYR:O | 4:9:285:CYS:CB[1_554] | 1.80 | 0.40 |
| 4:6:254:ARG:NE | 4:9:336:LYS:NZ[1_554] | 1.80 | 0.40 |
| 4:6:117:GLU:OE2 | 4:V:236:LEU:CG[1_554] | 1.80 | 0.40 |
| 4:4:191:LYS:CD | 4:7:186:THR:N[1_554] | 1.80 | 0.40 |
| 4:5:166:TYR:CA | 4:V:40:HIS:CD2[1_554] | 1.80 | 0.40 |
| 4:5:326:LYS:N | 4:8:167:GLU:OE2[1_554] | 1.80 | 0.40 |
| 4:4:136:ILE:N | 4:7:113:LYS:NZ[1_554] | 1.80 | 0.40 |
| 4:6:326:LYS:NZ | 4:W:45:VAL:CB[1_554] | 1.80 | 0.40 |
| 4:4:255:PHE:CD2 | 4:7:305:MET:SD[1_554] | 1.80 | 0.40 |
| 4:6:180:LEU:CD2 | 4:9:178:LEU:C[1_554] | 1.80 | 0.40 |
| 4:6:214:GLU:CD | 4:9:33:SER:OG[1_554] | 1.80 | 0.40 |
| 4:6:198:TYR:CG | 4:9:208:ILE:O[1_554] | 1.80 | 0.40 |
| 4:5:370:VAL:N | 4:9:232:SER:N[1_554] | 1.80 | 0.40 |
| 4:6:294:TYR:CA | 4:9:166:TYR:CB[1_554] | 1.80 | 0.40 |
| 4:4:318:THR:N | 4:7:149:THR:O[1_554] | 1.80 | 0.40 |
| 4:5:142:LEU:C | 4:8:372:ARG:CB[1_554] | 1.80 | 0.40 |
| 4:6:143:TYR:CA | 4:9:372:ARG:CA[1_554] | 1.80 | 0.40 |
| 4:6:72:GLU:O | 4:V:198:TYR:O[1_554] | 1.80 | 0.40 |
| 4:6:144:ALA:CB | 4:9:370:VAL:CG2[1_554] | 1.80 | 0.40 |
| 4:6:115:ASN:OD1 | 4:V:249:THR:O[1_554] | 1.80 | 0.40 |
| 4:5:110:LEU:O | 4:9:192:ILE:CB[1_554] | 1.81 | 0.39 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:196:ARG:C | 4:7:212:ILE:N[1_554] | 1.81 | 0.39 |
| 4:5:288:ASP:O | 4:V:63:GLY:C[1_554] | 1.81 | 0.39 |
| 4:6:242:LEU:CD1 | 4:9:207:GLU:OE1[1_554] | 1.81 | 0.39 |
| 4:6:294:TYR:CB | 4:9:166:TYR:CD2[1_554] | 1.81 | 0.39 |
| 4:6:274:ILE:CD1 | 4:9:161:HIS:C[1_554] | 1.81 | 0.39 |
| 4:6:31:PHE:CB | 4:9:80:ASP:N[1_554] | 1.81 | 0.39 |
| 4:6:213:LYS:CD | 4:9:157:ASP:CG[1_554] | 1.81 | 0.39 |
| 4:3:357:ILE:CD1 | 4:7:232:SER:CA[1_554] | 1.81 | 0.39 |
| 4:6:24:ASP:C | 4:9:124:PHE:N[1_554] | 1.81 | 0.39 |
| 4:6:139:VAL:C | 4:9:371:HIS:CE1[1_554] | 1.81 | 0.39 |
| 4:6:200:PHE:CA | 4:9:206:ARG:CB[1_554] | 1.81 | 0.39 |
| 4:5:294:TYR:CB | 4:8:166:TYR:C[1_554] | 1.81 | 0.39 |
| 4:6:367:PRO:CA | 4:V:233:SER:CB[1_554] | 1.81 | 0.39 |
| 4:6:218:TYR:CB | 4:9:336:LYS:N[1_554] | 1.81 | 0.39 |
| 4:4:316:GLU:CB | 4:7:152:VAL:N[1_554] | 1.81 | 0.39 |
| 4:5:329:ILE:CG1 | 4:8:142:LEU:CB[1_554] | 1.81 | 0.39 |
| 4:6:154:ASP:OD2 | 4:9:111:ASN:C[1_554] | 1.81 | 0.39 |
| 4:3:110:LEU:CB | 4:7:192:ILE:CB[1_554] | 1.81 | 0.39 |
| 4:5:166:TYR:CD2 | 4:V:40:HIS:CD2[1_554] | 1.81 | 0.39 |
| 4:5:113:LYS:NZ | 4:9:254:ARG:CB[1_554] | 1.81 | 0.39 |
| 4:6:191:LYS:C | 4:9:186:THR:O[1_554] | 1.81 | 0.39 |
| 4:6:269:MET:N | 4:9:264:PRO:CB[1_554] | 1.81 | 0.39 |
| 4:5:347:ALA:N | 4:8:366:GLY:CA[1_554] | 1.81 | 0.39 |
| 4:6:270:GLU:C | 4:9:272:ALA:N[1_554] | 1.81 | 0.39 |
| 4:5:218:TYR:O | 4:8:301:GLY:O[1_554] | 1.81 | 0.39 |
| 4:5:189:LEU:N | 4:8:183:ARG:CA[1_554] | 1.81 | 0.39 |
| 4:6:11:ASP:OD1 | 4:9:115:ASN:OD1[1_554] | 1.81 | 0.39 |
| 4:4:109:PRO:N | 4:8:195:GLU:CD[1_554] | 1.81 | 0.39 |
| 4:4:312:ARG:NE | 4:7:299:MET:O[1_554] | 1.81 | 0.39 |
| 4:5:172:PRO:C | 4:9:266:PHE:C[1_554] | 1.81 | 0.39 |
| 4:5:314:GLN:C | 4:8:142:LEU:CD1[1_554] | 1.81 | 0.39 |
| 4:6:294:TYR:O | 4:9:168:GLY:N[1_554] | 1.81 | 0.39 |
| 4:5:289:ILE:CA | 4:V:63:GLY:C[1_554] | 1.81 | 0.39 |
| 4:4:214:GLU:OE1 | 4:7:33:SER:OG[1_554] | 1.81 | 0.39 |
| 4:6:187:ASP:OD1 | 4:9:183:ARG:CD[1_554] | 1.81 | 0.39 |
| 4:4:27:PRO:CD | 4:7:122:ILE:CD1[1_554] | 1.81 | 0.39 |
| 4:6:110:LEU:CD2 | 4:V:191:LYS:NZ[1_554] | 1.81 | 0.39 |
| 4:6:214:GLU:OE1 | 4:9:33:SER:CA[1_554] | 1.81 | 0.39 |
| 4:4:115:ASN:CA | 4:8:250:ILE:N[1_554] | 1.81 | 0.39 |
| 4:4:357:ILE:CG1 | 4:8:231:ALA:O[1_554] | 1.81 | 0.39 |
| 4:5:289:ILE:O | 4:V:64:ILE:CG2[1_554] | 1.81 | 0.39 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:184:ASP:CA | 4:7:73:HIS:CE1[1_554] | 1.81 | 0.39 |
| 4:6:327:ILE:O | 4:9:148:THR:CA[1_554] | 1.81 | 0.39 |
| 4:4:147:ARG:O | 4:7:372:ARG:C[1_554] | 1.81 | 0.39 |
| 4:3:285:CYS:O | 4:7:270:GLU:CG[1_554] | 1.81 | 0.39 |
| 4:3:110:LEU:CG | 4:7:192:ILE:N[1_554] | 1.81 | 0.39 |
| 4:6:143:TYR:CG | 4:9:372:ARG:N[1_554] | 1.81 | 0.39 |
| 4:5:267:ILE:CG1 | 4:8:180:LEU:CD2[1_554] | 1.81 | 0.39 |
| 4:6:210:ARG:NH1 | 4:9:33:SER:C[1_554] | 1.81 | 0.39 |
| 4:6:213:LYS:NZ | 4:9:14:SER:CB[1_554] | 1.81 | 0.39 |
| 4:5:240:TYR:OH | 4:8:56:ASP:OD2[1_554] | 1.81 | 0.39 |
| 4:5:110:LEU:CB | 4:9:192:ILE:N[1_554] | 1.81 | 0.39 |
| 4:6:337:TYR:OH | 4:9:86:TRP:CG[1_554] | 1.81 | 0.39 |
| 4:5:305:MET:CA | 4:8:11:ASP:OD2[1_554] | 1.81 | 0.39 |
| 4:4:240:TYR:OH | 4:7:55:GLY:O[1_554] | 1.81 | 0.39 |
| 4:5:262:PHE:CB | 4:8:153:LEU:CD1[1_554] | 1.81 | 0.39 |
| 4:5:199:SER:N | 4:8:206:ARG:C[1_554] | 1.81 | 0.39 |
| 4:5:60:SER:CA | 4:8:66:THR:OG1[1_554] | 1.81 | 0.39 |
| 4:5:339:VAL:N | 4:8:116:ARG:CG[1_554] | 1.81 | 0.39 |
| 4:6:274:ILE:CA | 4:9:161:HIS:C[1_554] | 1.81 | 0.39 |
| 4:6:199:SER:O | 4:9:203:THR:O[1_554] | 1.81 | 0.39 |
| 4:5:369:ILE:CB | 4:9:232:SER:N[1_554] | 1.81 | 0.39 |
| 4:6:212:ILE:O | 4:9:16:LEU:CD2[1_554] | 1.81 | 0.39 |
| 4:5:199:SER:C | 4:8:206:ARG:N[1_554] | 1.81 | 0.39 |
| 4:5:327:ILE:CG1 | 4:8:149:THR:CG2[1_554] | 1.81 | 0.39 |
| 4:4:333:PRO:CG | 4:7:103:THR:C[1_554] | 1.81 | 0.39 |
| 4:5:267:ILE:CG1 | 4:8:180:LEU:CD1[1_554] | 1.81 | 0.39 |
| 4:4:337:TYR:CZ | 4:7:86:TRP:CH2[1_554] | 1.81 | 0.39 |
| 4:4:180:LEU:C | 4:7:159:VAL:CG1[1_554] | 1.81 | 0.39 |
| 4:6:223:PHE:CD1 | 4:9:304:THR:C[1_554] | 1.81 | 0.39 |
| 4:4:332:PRO:C | 4:7:133:TYR:O[1_554] | 1.81 | 0.39 |
| 4:5:333:PRO:C | 4:8:104:LEU:C[1_554] | 1.81 | 0.39 |
| 4:4:196:ARG:O | 4:7:208:ILE:O[1_554] | 1.81 | 0.39 |
| 4:5:162:ASN:N | 4:8:110:LEU:CG[1_554] | 1.81 | 0.39 |
| 1:A:637:LYS:CE | 4:5:311:ASP:CA[1_556] | 1.81 | 0.39 |
| 4:6:151:ILE:CG1 | 4:9:171:LEU:N[1_554] | 1.81 | 0.39 |
| 4:6:30:VAL:C | 4:9:79:TRP:O[1_554] | 1.81 | 0.39 |
| 4:5:276:GLU:CA | 4:8:281:SER:CB[1_554] | 1.81 | 0.39 |
| 4:6:140:LEU:CG | 4:9:371:HIS:CG[1_554] | 1.81 | 0.39 |
| 4:4:317:ILE:CB | 4:7:150:GLY:O[1_554] | 1.81 | 0.39 |
| 4:4:214:GLU:CD | 4:7:33:SER:CB[1_554] | 1.81 | 0.39 |
| 4:4:109:PRO:CG | 4:8:195:GLU:CG[1_554] | 1.81 | 0.39 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:196:ARG:NH2 | 4:9:215:LYS:CD[1_554] | 1.81 | 0.39 |
| 4:6:208:ILE:CG1 | 4:9:59:GLN:CB[1_554] | 1.81 | 0.39 |
| 4:6:243:PRO:CB | 4:9:60:SER:O[1_554] | 1.81 | 0.39 |
| 4:6:16:LEU:N | 4:9:77:THR:CA[1_554] | 1.81 | 0.39 |
| 4:4:281:SER:CA | 4:7:173:HIS:C[1_554] | 1.81 | 0.39 |
| 4:5:213:LYS:NZ | 4:8:14:SER:CA[1_554] | 1.81 | 0.39 |
| 4:4:154:ASP:OD1 | 4:7:111:ASN:CG[1_554] | 1.81 | 0.39 |
| 4:3:118:LYS:N | 4:7:237:GLU:CD[1_554] | 1.81 | 0.39 |
| 4:5:141:SER:OG | 4:8:116:ARG:NE[1_554] | 1.82 | 0.38 |
| 4:4:208:ILE:CG2 | 4:7:59:GLN:CG[1_554] | 1.82 | 0.38 |
| 4:6:172:PRO:C | 4:V:266:PHE:C[1_554] | 1.82 | 0.38 |
| 4:5:221:LEU:CD1 | 4:8:332:PRO:CB[1_554] | 1.82 | 0.38 |
| 4:5:340:TRP:CD2 | 4:8:119:MET:C[1_554] | 1.82 | 0.38 |
| 4:4:116:ARG:C | 4:8:237:GLU:CD[1_554] | 1.82 | 0.38 |
| 4:5:344:SER:CA | 4:8:362:TYR:CE1[1_554] | 1.82 | 0.38 |
| 4:6:151:ILE:CG2 | 4:9:169:TYR:O[1_554] | 1.82 | 0.38 |
| 4:6:110:LEU:CA | 4:V:195:GLU:OE1[1_554] | 1.82 | 0.38 |
| 4:4:113:LYS:CD | 4:8:254:ARG:CA[1_554] | 1.82 | 0.38 |
| 4:5:177:ARG:CZ | 4:9:194:THR:CB[1_554] | 1.82 | 0.38 |
| 4:5:24:ASP:O | 4:8:124:PHE:CD2[1_554] | 1.82 | 0.38 |
| 4:6:249:THR:O | 4:9:211:ASP:OD1[1_554] | 1.82 | 0.38 |
| 4:5:279:TYR:CA | 4:8:285:CYS:SG[1_554] | 1.82 | 0.38 |
| 4:6:333:PRO:O | 4:9:104:LEU:O[1_554] | 1.82 | 0.38 |
| 4:6:199:SER:N | 4:9:206:ARG:N[1_554] | 1.82 | 0.38 |
| 4:6:243:PRO:CB | 4:9:60:SER:CB[1_554] | 1.82 | 0.38 |
| 4:4:340:TRP:CZ2 | 4:7:121:GLN:CG[1_554] | 1.82 | 0.38 |
| 4:6:299:MET:C | 4:9:136:ILE:C[1_554] | 1.82 | 0.38 |
| 4:4:312:ARG:CD | 4:7:299:MET:C[1_554] | 1.82 | 0.38 |
| 4:4:185:LEU:CD1 | 4:7:159:VAL:CA[1_554] | 1.82 | 0.38 |
| 4:4:116:ARG:O | 4:8:237:GLU:CD[1_554] | 1.82 | 0.38 |
| 4:6:179:ASP:O | 4:9:179:ASP:CG[1_554] | 1.82 | 0.38 |
| 4:6:114:ALA:CB | 4:V:250:ILE:O[1_554] | 1.82 | 0.38 |
| 4:6:337:TYR:C | 4:9:119:MET:CE[1_554] | 1.82 | 0.38 |
| 4:6:369:ILE:CG2 | 4:V:232:SER:C[1_554] | 1.82 | 0.38 |
| 4:4:141:SER:C | 4:7:371:HIS:O[1_554] | 1.82 | 0.38 |
| 4:4:334:GLU:CD | 4:7:132:MET:SD[1_554] | 1.82 | 0.38 |
| 4:4:279:TYR:O | 4:7:285:CYS:SG[1_554] | 1.82 | 0.38 |
| 4:5:316:GLU:CG | 4:8:298:VAL:N[1_554] | 1.82 | 0.38 |
| 4:5:137:GLN:N | 4:8:113:LYS:CB[1_554] | 1.82 | 0.38 |
| 4:5:227:MET:O | 4:8:307:PRO:CB[1_554] | 1.82 | 0.38 |
| 4:6:295:ALA:C | 4:9:168:GLY:N[1_554] | 1.82 | 0.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:317:ILE:CG2 | 4:8:150:GLY:C[1_554] | 1.82 | 0.38 |
| 4:5:144:ALA:CA | 4:8:370:VAL:O[1_554] | 1.82 | 0.38 |
| 4:4:196:ARG:CG | 4:7:211:ASP:O[1_554] | 1.82 | 0.38 |
| 4:5:336:LYS:CG | 4:8:12:ASN:CG[1_554] | 1.82 | 0.38 |
| 4:6:281:SER:CB | 4:9:171:LEU:O[1_554] | 1.82 | 0.38 |
| 4:4:257:CYS:O | 4:7:156:GLY:C[1_554] | 1.82 | 0.38 |
| 4:4:30:VAL:CG1 | 4:7:79:TRP:O[1_554] | 1.82 | 0.38 |
| 4:4:299:MET:N | 4:7:136:ILE:CD1[1_554] | 1.82 | 0.38 |
| 4:6:221:LEU:CD2 | 4:9:332:PRO:CG[1_554] | 1.82 | 0.38 |
| 4:4:279:TYR:CD1 | 4:7:293:LEU:CD2[1_554] | 1.82 | 0.38 |
| 4:6:263:GLN:CB | 4:9:274:ILE:CB[1_554] | 1.82 | 0.38 |
| 4:4:366:GLY:CA | 4:8:235:SER:OG[1_554] | 1.82 | 0.38 |
| 4:5:211:ASP:OD2 | 4:8:32:PRO:N[1_554] | 1.82 | 0.38 |
| 4:5:136:ILE:C | 4:8:113:LYS:CA[1_554] | 1.82 | 0.38 |
| 4:4:268:GLY:CA | 4:7:264:PRO:CB[1_554] | 1.82 | 0.38 |
| 4:6:140:LEU:C | 4:9:116:ARG:CD[1_554] | 1.82 | 0.38 |
| 4:4:115:ASN:CA | 4:8:196:ARG:NH2[1_554] | 1.82 | 0.38 |
| 4:6:22:ALA:N | 4:9:362:TYR:OH[1_554] | 1.82 | 0.38 |
| 4:4:340:TRP:CB | 4:7:118:LYS:C[1_554] | 1.82 | 0.38 |
| 4:4:161:HIS:CB | 4:7:110:LEU:CB[1_554] | 1.82 | 0.38 |
| 4:4:275:HIS:CA | 4:7:163:VAL:CA[1_554] | 1.82 | 0.38 |
| 4:4:224:GLU:N | 4:7:331:ALA:CB[1_554] | 1.82 | 0.38 |
| 4:5:274:ILE:N | 4:8:161:HIS:C[1_554] | 1.82 | 0.38 |
| 4:4:294:TYR:CD1 | 4:7:166:TYR:N[1_554] | 1.82 | 0.38 |
| 4:4:198:TYR:O | 4:7:206:ARG:C[1_554] | 1.82 | 0.38 |
| 4:4:283:MET:CE | 4:7:289:ILE:CG2[1_554] | 1.82 | 0.38 |
| 4:3:367:PRO:N | 4:7:234:SER:C[1_554] | 1.82 | 0.38 |
| 4:5:346:LEU:C | 4:8:366:GLY:O[1_554] | 1.82 | 0.38 |
| 4:4:262:PHE:CD2 | 4:7:153:LEU:C[1_554] | 1.82 | 0.38 |
| 4:4:262:PHE:CE2 | 4:7:154:ASP:CA[1_554] | 1.82 | 0.38 |
| 4:5:348:SER:OG | 4:8:362:TYR:CA[1_554] | 1.82 | 0.38 |
| 4:5:186:THR:CG2 | 4:8:183:ARG:NE[1_554] | 1.82 | 0.38 |
| 4:5:255:PHE:CE1 | 4:8:305:MET:CA[1_554] | 1.82 | 0.38 |
| 4:6:24:ASP:OD1 | 4:9:125:GLU:CA[1_554] | 1.82 | 0.38 |
| 4:3:370:VAL:CG1 | 4:7:230:ALA:O[1_554] | 1.82 | 0.38 |
| 4:5:253:GLU:CG | 4:8:214:GLU:CA[1_554] | 1.82 | 0.38 |
| 4:4:187:ASP:C | 4:7:183:ARG:CG[1_554] | 1.82 | 0.38 |
| 4:6:154:ASP:CG | 4:9:111:ASN:CA[1_554] | 1.82 | 0.38 |
| 4:4:279:TYR:N | 4:7:164:PRO:CG[1_554] | 1.82 | 0.38 |
| 4:6:173:HIS:CG | 4:V:264:PRO:O[1_554] | 1.82 | 0.38 |
| 4:6:372:ARG:C | 4:V:227:MET:CG[1_554] | 1.82 | 0.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:31:PHE:C | 4:9:78:ASN:O[1_554] | 1.82 | 0.38 |
| 4:4:318:THR:CG2 | 4:7:148:THR:N[1_554] | 1.82 | 0.38 |
| 4:6:143:TYR:CD2 | 4:9:369:ILE:O[1_554] | 1.82 | 0.38 |
| 4:6:180:LEU:CA | 4:9:179:ASP:OD1[1_554] | 1.82 | 0.38 |
| 4:6:253:GLU:OE2 | 4:9:215:LYS:N[1_554] | 1.82 | 0.38 |
| 4:5:207:GLU:OE1 | 4:8:67:LEU:CG[1_554] | 1.82 | 0.38 |
| 4:4:305:MET:O | 4:7:11:ASP:CA[1_554] | 1.82 | 0.38 |
| 4:2:291:LYS:N | 4:7:40:HIS:CE1[1_554] | 1.82 | 0.38 |
| 4:6:136:ILE:CB | 4:9:113:LYS:CD[1_554] | 1.82 | 0.38 |
| 4:5:62:ARG:NH1 | 4:8:67:LEU:CA[1_554] | 1.82 | 0.38 |
| 4:5:193:LEU:CD1 | 4:8:211:ASP:N[1_554] | 1.82 | 0.38 |
| 4:3:76:ILE:N | 4:7:198:TYR:CE1[1_554] | 1.82 | 0.38 |
| 4:6:109:PRO:N | 4:V:195:GLU:CG[1_554] | 1.82 | 0.38 |
| 4:6:137:GLN:N | 4:9:113:LYS:CB[1_554] | 1.82 | 0.38 |
| 4:6:255:PHE:CD1 | 4:9:305:MET:O[1_554] | 1.82 | 0.38 |
| 4:4:275:HIS:CD2 | 4:7:151:ILE:CG1[1_554] | 1.82 | 0.38 |
| 4:5:191:LYS:N | 4:8:186:THR:CB[1_554] | 1.82 | 0.38 |
| 4:6:110:LEU:O | 4:V:192:ILE:CB[1_554] | 1.82 | 0.38 |
| 4:5:369:ILE:CD1 | 4:9:232:SER:OG[1_554] | 1.82 | 0.38 |
| 4:5:193:LEU:CA | 4:8:210:ARG:N[1_554] | 1.82 | 0.38 |
| 4:4:172:PRO:CD | 4:8:266:PHE:CB[1_554] | 1.82 | 0.38 |
| 4:6:343:GLY:CA | 4:9:367:PRO:O[1_554] | 1.82 | 0.38 |
| 4:4:30:VAL:CB | 4:7:80:ASP:N[1_554] | 1.82 | 0.38 |
| 4:6:75:ILE:CD1 | 4:V:195:GLU:C[1_554] | 1.82 | 0.38 |
| 4:6:347:ALA:CA | 4:9:366:GLY:C[1_554] | 1.82 | 0.38 |
| 4:5:335:ARG:O | 4:8:107:GLU:N[1_554] | 1.82 | 0.38 |
| 4:3:286:ASP:CB | 4:7:270:GLU:OE1[1_554] | 1.83 | 0.37 |
| 4:5:166:TYR:CB | 4:V:40:HIS:CD2[1_554] | 1.83 | 0.37 |
| 4:4:259:GLU:CA | 4:7:304:THR:CG2[1_554] | 1.83 | 0.37 |
| 4:6:157:ASP:C | 4:9:73:HIS:N[1_554] | 1.83 | 0.37 |
| 4:6:25:ASP:C | 4:9:123:MET:CB[1_554] | 1.83 | 0.37 |
| 4:4:337:TYR:O | 4:7:116:ARG:O[1_554] | 1.83 | 0.37 |
| 4:4:339:VAL:CB | 4:7:116:ARG:N[1_554] | 1.83 | 0.37 |
| 4:4:331:ALA:N | 4:7:135:ALA:CA[1_554] | 1.83 | 0.37 |
| 4:4:265:SER:N | 4:7:274:ILE:CD1[1_554] | 1.83 | 0.37 |
| 4:6:316:GLU:O | 4:9:296:ASN:O[1_554] | 1.83 | 0.37 |
| 4:5:27:PRO:CB | 4:8:122:ILE:CG2[1_554] | 1.83 | 0.37 |
| 4:3:173:HIS:NE2 | 4:7:266:PHE:N[1_554] | 1.83 | 0.37 |
| 4:5:300:SER:N | 4:8:136:ILE:CA[1_554] | 1.83 | 0.37 |
| 4:4:141:SER:O | 4:7:371:HIS:O[1_554] | 1.83 | 0.37 |
| 4:5:311:ASP:CA | 4:8:141:SER:O[1_554] | 1.83 | 0.37 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:340:TRP:CE2 | 4:9:122:ILE:N[1_554] | 1.83 | 0.37 |
| 4:2:291:LYS:CA | 4:7:40:HIS:CG[1_554] | 1.83 | 0.37 |
| 4:4:308:GLY:C | 4:7:338:SER:C[1_554] | 1.83 | 0.37 |
| 4:5:277:THR:C | 4:8:174:ALA:C[1_554] | 1.83 | 0.37 |
| 4:4:315:LYS:NZ | 4:7:147:ARG:NE[1_554] | 1.83 | 0.37 |
| 4:5:341:ILE:N | 4:8:120:THR:CB[1_554] | 1.83 | 0.37 |
| 4:5:304:THR:CA | 4:8:137:GLN:CG[1_554] | 1.83 | 0.37 |
| 4:6:145:SER:CB | 4:9:133:TYR:OH[1_554] | 1.83 | 0.37 |
| 4:5:185:LEU:CD1 | 4:8:181:ALA:CB[1_554] | 1.83 | 0.37 |
| 4:6:304:THR:CA | 4:9:137:GLN:CG[1_554] | 1.83 | 0.37 |
| 4:5:163:VAL:C | 4:8:172:PRO:CB[1_554] | 1.83 | 0.37 |
| 4:4:19:ALA:N | 4:7:118:LYS:CE[1_554] | 1.83 | 0.37 |
| 4:5:315:LYS:O | 4:8:296:ASN:O[1_554] | 1.83 | 0.37 |
| 4:2:287:ILE:C | 4:7:39:ARG:NH1[1_554] | 1.83 | 0.37 |
| 4:6:266:PHE:CA | 4:9:261:LEU:CB[1_554] | 1.83 | 0.37 |
| 4:6:22:ALA:N | 4:9:125:GLU:OE2[1_554] | 1.83 | 0.37 |
| 4:4:193:LEU:CD1 | 4:7:210:ARG:CD[1_554] | 1.83 | 0.37 |
| 4:5:60:SER:OG | 4:8:37:ARG:CG[1_554] | 1.83 | 0.37 |
| 4:4:301:GLY:N | 4:7:107:GLU:CB[1_554] | 1.83 | 0.37 |
| 4:6:56:ASP:OD1 | 4:9:80:ASP:OD1[1_554] | 1.83 | 0.37 |
| 4:5:31:PHE:O | 4:8:78:ASN:CB[1_554] | 1.83 | 0.37 |
| 4:6:314:GLN:NE2 | 4:9:147:ARG:CA[1_554] | 1.83 | 0.37 |
| 4:4:266:PHE:N | 4:7:261:LEU:CA[1_554] | 1.83 | 0.37 |
| 4:4:173:HIS:N | 4:8:267:ILE:N[1_554] | 1.83 | 0.37 |
| 4:4:114:ALA:N | 4:8:250:ILE:O[1_554] | 1.83 | 0.37 |
| 4:6:24:ASP:CG | 4:9:125:GLU:C[1_554] | 1.83 | 0.37 |
| 4:6:27:PRO:CA | 4:9:122:ILE:C[1_554] | 1.83 | 0.37 |
| 4:6:205:GLU:OE2 | 4:9:203:THR:OG1[1_554] | 1.83 | 0.37 |
| 4:4:169:TYR:OH | 4:8:266:PHE:CZ[1_554] | 1.83 | 0.37 |
| 4:4:157:ASP:CA | 4:7:72:GLU:C[1_554] | 1.83 | 0.37 |
| 4:5:17:VAL:CG1 | 4:8:79:TRP:CD1[1_554] | 1.83 | 0.37 |
| 4:5:173:HIS:NE2 | 4:9:265:SER:CA[1_554] | 1.83 | 0.37 |
| 4:6:312:ARG:O | 4:9:298:VAL:CG1[1_554] | 1.83 | 0.37 |
| 4:5:160:THR:N | 4:8:177:ARG:NH1[1_554] | 1.83 | 0.37 |
| 4:4:25:ASP:C | 4:7:120:THR:O[1_554] | 1.83 | 0.37 |
| 4:6:214:GLU:CG | 4:9:16:LEU:C[1_554] | 1.83 | 0.37 |
| 4:5:304:THR:CB | 4:8:137:GLN:CD[1_554] | 1.83 | 0.37 |
| 4:6:307:PRO:CB | 4:9:337:TYR:O[1_554] | 1.83 | 0.37 |
| 4:6:27:PRO:CB | 4:9:122:ILE:CG2[1_554] | 1.83 | 0.37 |
| 4:4:115:ASN:ND2 | 4:8:198:TYR:CZ[1_554] | 1.83 | 0.37 |
| 4:6:281:SER:OG | 4:9:172:PRO:C[1_554] | 1.83 | 0.37 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:173:HIS:CG | 4:8:264:PRO:O[1_554] | 1.83 | 0.37 |
| 4:4:154:ASP:CB | 4:7:110:LEU:O[1_554] | 1.83 | 0.37 |
| 4:4:191:LYS:N | 4:7:186:THR:CB[1_554] | 1.83 | 0.37 |
| 4:6:151:ILE:CG2 | 4:9:170:ALA:N[1_554] | 1.83 | 0.37 |
| 4:6:290:ARG:CZ | 4:9:286:ASP:CB[1_554] | 1.83 | 0.37 |
| 4:4:227:MET:CG | 4:7:305:MET:C[1_554] | 1.83 | 0.37 |
| 4:4:327:ILE:C | 4:7:167:GLU:C[1_554] | 1.83 | 0.37 |
| 4:4:310:ALA:N | 4:7:141:SER:N[1_554] | 1.83 | 0.37 |
| 4:3:115:ASN:ND2 | 4:7:198:TYR:OH[1_554] | 1.83 | 0.37 |
| 4:6:17:VAL:O | 4:9:79:TRP:CB[1_554] | 1.83 | 0.37 |
| 4:4:194:THR:C | 4:7:209:VAL:CG2[1_554] | 1.83 | 0.37 |
| 4:5:255:PHE:CZ | 4:8:305:MET:C[1_554] | 1.83 | 0.37 |
| 4:2:291:LYS:C | 4:7:40:HIS:ND1[1_554] | 1.83 | 0.37 |
| 4:4:191:LYS:CE | 4:7:185:LEU:CB[1_554] | 1.83 | 0.37 |
| 4:6:278:THR:CA | 4:9:164:PRO:N[1_554] | 1.83 | 0.37 |
| 4:6:9:VAL:CG1 | 4:9:117:GLU:O[1_554] | 1.83 | 0.37 |
| 4:4:201:VAL:CG2 | 4:7:203:THR:CA[1_554] | 1.83 | 0.37 |
| 4:5:302:GLY:CA | 4:8:12:ASN:O[1_554] | 1.83 | 0.37 |
| 4:5:154:ASP:CA | 4:8:109:PRO:N[1_554] | 1.83 | 0.37 |
| 4:4:340:TRP:CZ2 | 4:7:121:GLN:CD[1_554] | 1.83 | 0.37 |
| 4:4:334:GLU:N | 4:7:105:LEU:CG[1_554] | 1.83 | 0.37 |
| 4:5:294:TYR:O | 4:8:168:GLY:N[1_554] | 1.83 | 0.37 |
| 4:4:286:ASP:CB | 4:8:270:GLU:OE2[1_554] | 1.83 | 0.37 |
| 4:5:108:ALA:C | 4:9:195:GLU:CG[1_554] | 1.83 | 0.37 |
| 4:6:184:ASP:OD1 | 4:9:73:HIS:NE2[1_554] | 1.83 | 0.37 |
| 4:4:310:ALA:N | 4:7:137:GLN:O[1_554] | 1.83 | 0.37 |
| 4:5:218:TYR:CE1 | 4:8:337:TYR:CE1[1_554] | 1.83 | 0.37 |
| 4:5:31:PHE:O | 4:8:79:TRP:N[1_554] | 1.83 | 0.37 |
| 4:4:77:THR:O | 4:8:246:GLN:CD[1_554] | 1.83 | 0.37 |
| 4:5:111:ASN:CA | 4:9:192:ILE:O[1_554] | 1.83 | 0.37 |
| 4:6:344:SER:CA | 4:9:362:TYR:CE1[1_554] | 1.83 | 0.37 |
| 4:6:267:ILE:CA | 4:9:180:LEU:CD2[1_554] | 1.83 | 0.37 |
| 4:3:173:HIS:CD2 | 4:7:267:ILE:N[1_554] | 1.83 | 0.37 |
| 4:6:319:ALA:N | 4:9:292:ASP:O[1_554] | 1.83 | 0.37 |
| 4:6:300:SER:CB | 4:9:107:GLU:CD[1_554] | 1.83 | 0.37 |
| 4:5:307:PRO:O | 4:8:338:SER:N[1_554] | 1.83 | 0.37 |
| 4:4:24:ASP:CB | 4:7:125:GLU:CG[1_554] | 1.83 | 0.37 |
| 4:6:259:GLU:N | 4:9:304:THR:N[1_554] | 1.83 | 0.37 |
| 4:6:325:MET:CG | 4:9:166:TYR:OH[1_554] | 1.83 | 0.37 |
| 4:6:60:SER:CB | 4:9:37:ARG:CG[1_554] | 1.83 | 0.37 |
| 4:4:313:MET:N | 4:7:138:ALA:O[1_554] | 1.84 | 0.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:306:TYR:O | 4:7:339:VAL:CG1[1_554] | 1.84 | 0.36 |
| 4:6:207:GLU:OE1 | 4:9:67:LEU:CG[1_554] | 1.84 | 0.36 |
| 4:6:210:ARG:NH1 | 4:9:33:SER:CA[1_554] | 1.84 | 0.36 |
| 4:6:265:SER:C | 4:9:261:LEU:CA[1_554] | 1.84 | 0.36 |
| 4:4:281:SER:N | 4:7:174:ALA:CB[1_554] | 1.84 | 0.36 |
| 4:6:301:GLY:N | 4:9:107:GLU:O[1_554] | 1.84 | 0.36 |
| 4:3:117:GLU:CG | 4:7:237:GLU:CA[1_554] | 1.84 | 0.36 |
| 4:5:159:VAL:CA | 4:8:177:ARG:NH2[1_554] | 1.84 | 0.36 |
| 4:4:110:LEU:CA | 4:8:192:ILE:N[1_554] | 1.84 | 0.36 |
| 4:4:312:ARG:CZ | 4:7:299:MET:C[1_554] | 1.84 | 0.36 |
| 4:4:211:ASP:O | 4:7:31:PHE:C[1_554] | 1.84 | 0.36 |
| 4:6:59:GLN:CB | 4:9:68:LYS:NZ[1_554] | 1.84 | 0.36 |
| 4:5:214:GLU:CB | 4:8:17:VAL:N[1_554] | 1.84 | 0.36 |
| 4:5:218:TYR:CB | 4:8:336:LYS:N[1_554] | 1.84 | 0.36 |
| 4:5:227:MET:CB | 4:8:307:PRO:N[1_554] | 1.84 | 0.36 |
| 4:4:188:TYR:C | 4:7:183:ARG:C[1_554] | 1.84 | 0.36 |
| 4:5:156:GLY:O | 4:8:73:HIS:O[1_554] | 1.84 | 0.36 |
| 4:6:269:MET:SD | 4:9:178:LEU:CD1[1_554] | 1.84 | 0.36 |
| 4:6:32:PRO:N | 4:9:78:ASN:CB[1_554] | 1.84 | 0.36 |
| 4:4:185:LEU:CG | 4:7:158:GLY:N[1_554] | 1.84 | 0.36 |
| 4:6:293:LEU:CA | 4:9:169:TYR:CD2[1_554] | 1.84 | 0.36 |
| 4:6:252:ASN:OD1 | 4:9:215:LYS:CA[1_554] | 1.84 | 0.36 |
| 4:4:157:ASP:O | 4:7:72:GLU:O[1_554] | 1.84 | 0.36 |
| 4:6:260:THR:N | 4:9:155:SER:OG[1_554] | 1.84 | 0.36 |
| 4:4:255:PHE:CE1 | 4:7:305:MET:CA[1_554] | 1.84 | 0.36 |
| 4:4:285:CYS:O | 4:8:270:GLU:CG[1_554] | 1.84 | 0.36 |
| 4:6:305:MET:CB | 4:9:11:ASP:OD2[1_554] | 1.84 | 0.36 |
| 4:6:59:GLN:CD | 4:9:68:LYS:CB[1_554] | 1.84 | 0.36 |
| 4:4:77:THR:CG2 | 4:8:246:GLN:CD[1_554] | 1.84 | 0.36 |
| 4:5:276:GLU:OE1 | 4:8:279:TYR:CA[1_554] | 1.84 | 0.36 |
| 4:6:294:TYR:CZ | 4:9:289:ILE:CD1[1_554] | 1.84 | 0.36 |
| 4:3:111:ASN:O | 4:7:253:GLU:CD[1_554] | 1.84 | 0.36 |
| 4:6:161:HIS:CB | 4:9:110:LEU:CD1[1_554] | 1.84 | 0.36 |
| 4:5:140:LEU:CD1 | 4:8:117:GLU:CG[1_554] | 1.84 | 0.36 |
| 4:3:75:ILE:CA | 4:7:198:TYR:CA[1_554] | 1.84 | 0.36 |
| 4:5:272:ALA:CA | 4:8:277:THR:OG1[1_554] | 1.84 | 0.36 |
| 4:6:142:LEU:C | 4:9:372:ARG:NE[1_554] | 1.84 | 0.36 |
| 4:4:153:LEU:CA | 4:7:109:PRO:C[1_554] | 1.84 | 0.36 |
| 4:5:30:VAL:CG1 | 4:8:82:MET:CG[1_554] | 1.84 | 0.36 |
| 4:3:115:ASN:CA | 4:7:196:ARG:NH2[1_554] | 1.84 | 0.36 |
| 4:5:269:MET:O | 4:8:272:ALA:C[1_554] | 1.84 | 0.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:253:GLU:CG | 4:9:214:GLU:CB[1_554] | 1.84 | 0.36 |
| 4:4:218:TYR:OH | 4:7:27:PRO:CD[1_554] | 1.84 | 0.36 |
| 4:4:367:PRO:C | 4:8:236:LEU:CD2[1_554] | 1.84 | 0.36 |
| 4:4:141:SER:OG | 4:7:116:ARG:CB[1_554] | 1.84 | 0.36 |
| 4:5:300:SER:C | 4:8:107:GLU:CA[1_554] | 1.84 | 0.36 |
| 4:5:276:GLU:O | 4:8:281:SER:OG[1_554] | 1.84 | 0.36 |
| 4:6:30:VAL:N | 4:9:79:TRP:O[1_554] | 1.84 | 0.36 |
| 4:4:318:THR:N | 4:7:149:THR:CA[1_554] | 1.84 | 0.36 |
| 4:5:320:LEU:CB | 4:8:293:LEU:C[1_554] | 1.84 | 0.36 |
| 4:4:211:ASP:OD2 | 4:7:55:GLY:N[1_554] | 1.84 | 0.36 |
| 4:4:143:TYR:N | 4:7:371:HIS:O[1_554] | 1.84 | 0.36 |
| 4:4:335:ARG:CG | 4:7:107:GLU:N[1_554] | 1.84 | 0.36 |
| 4:6:299:MET:CB | 4:9:137:GLN:N[1_554] | 1.84 | 0.36 |
| 4:6:258:PRO:CD | 4:9:302:GLY:CA[1_554] | 1.84 | 0.36 |
| 4:3:366:GLY:O | 4:7:234:SER:CA[1_554] | 1.84 | 0.36 |
| 4:6:300:SER:C | 4:9:107:GLU:CA[1_554] | 1.84 | 0.36 |
| 4:6:188:TYR:CB | 4:9:181:ALA:C[1_554] | 1.84 | 0.36 |
| 4:4:172:PRO:CB | 4:8:188:TYR:OH[1_554] | 1.84 | 0.36 |
| 4:5:215:LYS:N | 4:8:16:LEU:CD1[1_554] | 1.84 | 0.36 |
| 4:3:110:LEU:CA | 4:7:192:ILE:CG2[1_554] | 1.84 | 0.36 |
| 4:4:212:ILE:C | 4:7:16:LEU:CD1[1_554] | 1.84 | 0.36 |
| 4:6:192:ILE:N | 4:9:186:THR:N[1_554] | 1.84 | 0.36 |
| 4:5:136:ILE:N | 4:8:113:LYS:CD[1_554] | 1.84 | 0.36 |
| 4:6:112:PRO:CG | 4:V:193:LEU:CD1[1_554] | 1.84 | 0.36 |
| 4:4:305:MET:CA | 4:7:11:ASP:OD1[1_554] | 1.84 | 0.36 |
| 4:4:255:PHE:CE2 | 4:7:305:MET:CE[1_554] | 1.84 | 0.36 |
| 4:4:335:ARG:NH1 | 4:7:106:THR:N[1_554] | 1.84 | 0.36 |
| 4:6:151:ILE:CG1 | 4:9:171:LEU:CA[1_554] | 1.84 | 0.36 |
| 4:3:109:PRO:CG | 4:7:195:GLU:OE2[1_554] | 1.84 | 0.36 |
| 4:6:272:ALA:CB | 4:9:277:THR:O[1_554] | 1.84 | 0.36 |
| 4:6:17:VAL:CB | 4:9:79:TRP:CG[1_554] | 1.84 | 0.36 |
| 4:4:218:TYR:CZ | 4:7:337:TYR:CD1[1_554] | 1.84 | 0.36 |
| 4:5:161:HIS:N | 4:8:110:LEU:CD1[1_554] | 1.84 | 0.36 |
| 4:6:255:PHE:CA | 4:9:305:MET:CG[1_554] | 1.84 | 0.36 |
| 4:5:214:GLU:CA | 4:8:16:LEU:C[1_554] | 1.84 | 0.36 |
| 4:3:370:VAL:C | 4:7:230:ALA:O[1_554] | 1.84 | 0.36 |
| 4:4:372:ARG:CA | 4:8:227:MET:N[1_554] | 1.84 | 0.36 |
| 4:3:112:PRO:CB | 4:7:250:ILE:CG1[1_554] | 1.84 | 0.36 |
| 4:4:191:LYS:C | 4:7:186:THR:OG1[1_554] | 1.84 | 0.36 |
| 4:5:265:SER:N | 4:8:261:LEU:O[1_554] | 1.84 | 0.36 |
| 4:6:266:PHE:CD1 | 4:9:261:LEU:CG[1_554] | 1.84 | 0.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:320:LEU:CA | 4:9:293:LEU:N[1_554] | 1.84 | 0.36 |
| 4:6:293:LEU:O | 4:9:169:TYR:O[1_554] | 1.84 | 0.36 |
| 4:4:218:TYR:CE1 | 4:7:337:TYR:CD1[1_554] | 1.84 | 0.36 |
| 4:5:21:PHE:CB | 4:8:125:GLU:CG[1_554] | 1.84 | 0.36 |
| 4:6:327:ILE:CB | 4:9:149:THR:CB[1_554] | 1.84 | 0.36 |
| 4:4:185:LEU:N | 4:7:158:GLY:C[1_554] | 1.84 | 0.36 |
| 4:4:173:HIS:O | 4:8:267:ILE:CB[1_554] | 1.84 | 0.36 |
| 4:3:369:ILE:O | 4:7:230:ALA:N[1_554] | 1.84 | 0.36 |
| 4:5:111:ASN:O | 4:9:256:ARG:NH2[1_554] | 1.84 | 0.36 |
| 4:4:325:MET:CG | 4:7:166:TYR:CZ[1_554] | 1.84 | 0.36 |
| 4:5:280:ASN:OD1 | 4:8:280:ASN:C[1_554] | 1.84 | 0.36 |
| 4:6:340:TRP:CB | 4:9:120:THR:N[1_554] | 1.84 | 0.36 |
| 4:5:266:PHE:CD1 | 4:8:261:LEU:CD1[1_554] | 1.84 | 0.36 |
| 4:6:280:ASN:OD1 | 4:9:280:ASN:C[1_554] | 1.84 | 0.36 |
| 4:5:321:ALA:CA | 4:8:292:ASP:CB[1_554] | 1.84 | 0.36 |
| 4:5:218:TYR:C | 4:8:336:LYS:CA[1_554] | 1.84 | 0.36 |
| 4:5:60:SER:CB | 4:8:37:ARG:CG[1_554] | 1.84 | 0.36 |
| 4:6:199:SER:CA | 4:9:205:GLU:C[1_554] | 1.84 | 0.36 |
| 4:5:210:ARG:NH1 | 4:8:33:SER:C[1_554] | 1.84 | 0.36 |
| 4:4:25:ASP:N | 4:7:125:GLU:CG[1_554] | 1.84 | 0.36 |
| 4:6:196:ARG:CA | 4:9:212:ILE:CA[1_554] | 1.85 | 0.35 |
| 4:5:282:ILE:CG1 | 4:8:171:LEU:CB[1_554] | 1.85 | 0.35 |
| 4:6:178:LEU:CG | 4:9:177:ARG:O[1_554] | 1.85 | 0.35 |
| 4:5:204:ALA:O | 4:8:62:ARG:CG[1_554] | 1.85 | 0.35 |
| 4:6:256:ARG:C | 4:9:303:THR:O[1_554] | 1.85 | 0.35 |
| 4:5:267:ILE:CA | 4:8:180:LEU:CD1[1_554] | 1.85 | 0.35 |
| 4:4:317:ILE:C | 4:7:149:THR:C[1_554] | 1.85 | 0.35 |
| 4:4:201:VAL:CG2 | 4:7:203:THR:CB[1_554] | 1.85 | 0.35 |
| 4:6:183:ARG:CZ | 4:9:72:GLU:CD[1_554] | 1.85 | 0.35 |
| 4:5:257:CYS:N | 4:8:303:THR:CB[1_554] | 1.85 | 0.35 |
| 4:3:113:LYS:O | 4:7:251:GLY:O[1_554] | 1.85 | 0.35 |
| 4:6:289:ILE:N | 4:W:63:GLY:CA[1_554] | 1.85 | 0.35 |
| 4:6:218:TYR:O | 4:9:302:GLY:N[1_554] | 1.85 | 0.35 |
| 4:4:180:LEU:C | 4:7:179:ASP:OD1[1_554] | 1.85 | 0.35 |
| 4:4:25:ASP:O | 4:7:120:THR:C[1_554] | 1.85 | 0.35 |
| 4:4:194:THR:OG1 | 4:7:209:VAL:CG1[1_554] | 1.85 | 0.35 |
| 4:6:260:THR:O | 4:9:160:THR:CG2[1_554] | 1.85 | 0.35 |
| 4:3:371:HIS:C | 4:7:230:ALA:CB[1_554] | 1.85 | 0.35 |
| 4:4:326:LYS:CA | 4:7:167:GLU:CB[1_554] | 1.85 | 0.35 |
| 4:6:163:VAL:C | 4:9:172:PRO:CB[1_554] | 1.85 | 0.35 |
| 4:5:179:ASP:C | 4:8:179:ASP:OD1[1_554] | 1.85 | 0.35 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:325:MET:C | 4:7:167:GLU:OE2[1_554] | 1.85 | 0.35 |
| 4:4:218:TYR:CE2 | 4:7:337:TYR:CE2[1_554] | 1.85 | 0.35 |
| 4:4:156:GLY:O | 4:7:74:GLY:N[1_554] | 1.85 | 0.35 |
| 4:6:372:ARG:CA | 4:V:227:MET:CA[1_554] | 1.85 | 0.35 |
| 4:6:269:MET:N | 4:9:264:PRO:CG[1_554] | 1.85 | 0.35 |
| 4:5:279:TYR:OH | 4:8:290:ARG:CB[1_554] | 1.85 | 0.35 |
| 4:6:260:THR:CG2 | 4:9:180:LEU:O[1_554] | 1.85 | 0.35 |
| 4:4:256:ARG:O | 4:7:303:THR:CG2[1_554] | 1.85 | 0.35 |
| 4:6:367:PRO:C | 4:V:233:SER:CA[1_554] | 1.85 | 0.35 |
| 4:4:16:LEU:CG | 4:7:78:ASN:CA[1_554] | 1.85 | 0.35 |
| 4:4:178:LEU:CD2 | 4:7:176:MET:C[1_554] | 1.85 | 0.35 |
| 4:6:27:PRO:O | 4:9:122:ILE:CG2[1_554] | 1.85 | 0.35 |
| 4:4:115:ASN:OD1 | 4:8:249:THR:C[1_554] | 1.85 | 0.35 |
| 4:4:329:ILE:CB | 4:7:139:VAL:CB[1_554] | 1.85 | 0.35 |
| 4:4:339:VAL:CB | 4:7:115:ASN:C[1_554] | 1.85 | 0.35 |
| 4:4:264:PRO:CA | 4:7:274:ILE:CD1[1_554] | 1.85 | 0.35 |
| 4:5:200:PHE:CA | 4:8:206:ARG:CB[1_554] | 1.85 | 0.35 |
| 4:5:18:LYS:CD | 4:8:79:TRP:CZ3[1_554] | 1.85 | 0.35 |
| 4:5:221:LEU:CD2 | 4:8:332:PRO:CG[1_554] | 1.85 | 0.35 |
| 4:5:295:ALA:N | 4:8:167:GLU:CA[1_554] | 1.85 | 0.35 |
| 4:5:262:PHE:CG | 4:8:153:LEU:O[1_554] | 1.85 | 0.35 |
| 4:6:200:PHE:CA | 4:9:206:ARG:CD[1_554] | 1.85 | 0.35 |
| 4:5:348:SER:C | 4:8:365:ALA:N[1_554] | 1.85 | 0.35 |
| 4:6:207:GLU:OE2 | 4:9:68:LYS:N[1_554] | 1.85 | 0.35 |
| 4:5:223:PHE:CA | 4:8:335:ARG:NH2[1_554] | 1.85 | 0.35 |
| 4:5:253:GLU:CD | 4:8:214:GLU:CB[1_554] | 1.85 | 0.35 |
| 4:6:371:HIS:ND1 | 4:V:252:ASN:CB[1_554] | 1.85 | 0.35 |
| 4:6:318:THR:O | 4:9:292:ASP:C[1_554] | 1.85 | 0.35 |
| 4:5:270:GLU:CA | 4:8:271:SER:C[1_554] | 1.85 | 0.35 |
| 4:6:162:ASN:ND2 | 4:9:175:ILE:CD1[1_554] | 1.85 | 0.35 |
| 4:4:223:PHE:CZ | 4:7:300:SER:C[1_554] | 1.85 | 0.35 |
| 4:4:316:GLU:CG | 4:7:152:VAL:CA[1_554] | 1.85 | 0.35 |
| 4:5:143:TYR:CZ | 4:8:369:ILE:O[1_554] | 1.85 | 0.35 |
| 4:5:211:ASP:CG | 4:8:32:PRO:CA[1_554] | 1.85 | 0.35 |
| 4:6:339:VAL:N | 4:9:116:ARG:CG[1_554] | 1.85 | 0.35 |
| 4:6:178:LEU:CD2 | 4:9:176:MET:O[1_554] | 1.85 | 0.35 |
| 4:4:253:GLU:OE2 | 4:7:214:GLU:CB[1_554] | 1.85 | 0.35 |
| 4:5:299:MET:CG | 4:8:138:ALA:N[1_554] | 1.85 | 0.35 |
| 4:4:266:PHE:CG | 4:7:261:LEU:CG[1_554] | 1.85 | 0.35 |
| 4:5:213:LYS:NZ | 4:8:15:GLY:N[1_554] | 1.85 | 0.35 |
| 4:5:211:ASP:CG | 4:8:32:PRO:CB[1_554] | 1.85 | 0.35 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:139:VAL:N | 4:7:113:LYS:CD[1_554] | 1.85 | 0.35 |
| 4:4:217:CYS:O | 4:7:18:LYS:CE[1_554] | 1.85 | 0.35 |
| 4:4:315:LYS:N | 4:7:142:LEU:CB[1_554] | 1.85 | 0.35 |
| 4:5:315:LYS:O | 4:8:297:ASN:N[1_554] | 1.85 | 0.35 |
| 4:3:357:ILE:CD1 | 4:7:232:SER:OG[1_554] | 1.85 | 0.35 |
| 4:4:75:ILE:CB | 4:8:198:TYR:CA[1_554] | 1.85 | 0.35 |
| 4:5:346:LEU:C | 4:8:365:ALA:O[1_554] | 1.85 | 0.35 |
| 4:6:335:ARG:CB | 4:9:106:THR:CB[1_554] | 1.85 | 0.35 |
| 4:6:265:SER:CB | 4:9:262:PHE:CA[1_554] | 1.85 | 0.35 |
| 4:6:340:TRP:CE3 | 4:9:119:MET:O[1_554] | 1.85 | 0.35 |
| 4:5:312:ARG:CB | 4:8:299:MET:C[1_554] | 1.85 | 0.35 |
| 4:6:288:ASP:CA | 4:W:63:GLY:CA[1_554] | 1.85 | 0.35 |
| 4:5:142:LEU:O | 4:8:372:ARG:CZ[1_554] | 1.85 | 0.35 |
| 4:5:305:MET:CE | 4:8:11:ASP:N[1_554] | 1.85 | 0.35 |
| 4:6:299:MET:SD | 4:9:138:ALA:N[1_554] | 1.85 | 0.35 |
| 4:4:188:TYR:CG | 4:7:182:GLY:CA[1_554] | 1.85 | 0.35 |
| 4:6:332:PRO:O | 4:9:104:LEU:CD2[1_554] | 1.85 | 0.35 |
| 4:6:207:GLU:CG | 4:9:67:LEU:CD1[1_554] | 1.85 | 0.35 |
| 4:4:117:GLU:N | 4:8:237:GLU:CD[1_554] | 1.85 | 0.35 |
| 4:5:343:GLY:N | 4:8:367:PRO:O[1_554] | 1.85 | 0.35 |
| 4:4:185:LEU:CB | 4:7:157:ASP:C[1_554] | 1.85 | 0.35 |
| 4:6:162:ASN:CG | 4:9:175:ILE:CD1[1_554] | 1.85 | 0.35 |
| 4:6:180:LEU:CD2 | 4:9:178:LEU:CA[1_554] | 1.85 | 0.35 |
| 4:5:250:ILE:CD1 | 4:8:210:ARG:NH2[1_554] | 1.85 | 0.35 |
| 4:4:340:TRP:CZ3 | 4:7:121:GLN:CA[1_554] | 1.85 | 0.35 |
| 4:4:281:SER:CB | 4:7:173:HIS:CA[1_554] | 1.85 | 0.35 |
| 4:4:298:VAL:CG1 | 4:7:116:ARG:CZ[1_554] | 1.85 | 0.35 |
| 4:6:59:GLN:O | 4:9:66:THR:CB[1_554] | 1.85 | 0.35 |
| 4:6:315:LYS:CG | 4:9:147:ARG:CZ[1_554] | 1.85 | 0.35 |
| 4:5:155:SER:N | 4:8:109:PRO:N[1_554] | 1.85 | 0.35 |
| 4:4:243:PRO:C | 4:7:60:SER:OG[1_554] | 1.85 | 0.35 |
| 4:4:332:PRO:CG | 4:7:134:VAL:C[1_554] | 1.85 | 0.35 |
| 4:5:333:PRO:CD | 4:8:104:LEU:CD2[1_554] | 1.85 | 0.35 |
| 4:5:144:ALA:C | 4:8:372:ARG:NH2[1_554] | 1.85 | 0.35 |
| 4:4:156:GLY:O | 4:7:73:HIS:C[1_554] | 1.85 | 0.35 |
| 4:4:194:THR:C | 4:7:209:VAL:C[1_554] | 1.85 | 0.35 |
| 4:4:197:GLY:O | 4:7:208:ILE:CG1[1_554] | 1.85 | 0.35 |
| 4:5:319:ALA:C | 4:8:293:LEU:C[1_554] | 1.85 | 0.35 |
| 4:5:367:PRO:N | 4:9:234:SER:CA[1_554] | 1.85 | 0.35 |
| 4:3:72:GLU:O | 4:7:198:TYR:O[1_554] | 1.85 | 0.35 |
| 4:6:302:GLY:C | 4:9:12:ASN:O[1_554] | 1.85 | 0.35 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:322:PRO:CB | 4:8:291:LYS:CE[1_554] | 1.85 | 0.35 |
| 4:5:31:PHE:CB | 4:8:80:ASP:CB[1_554] | 1.85 | 0.35 |
| 4:4:370:VAL:CB | 4:8:230:ALA:C[1_554] | 1.86 | 0.34 |
| 4:6:31:PHE:O | 4:9:79:TRP:N[1_554] | 1.86 | 0.34 |
| 4:5:258:PRO:C | 4:8:155:SER:O[1_554] | 1.86 | 0.34 |
| 4:6:243:PRO:CG | 4:9:59:GLN:O[1_554] | 1.86 | 0.34 |
| 4:4:174:ALA:O | 4:7:173:HIS:CA[1_554] | 1.86 | 0.34 |
| 4:4:183:ARG:CZ | 4:7:72:GLU:OE1[1_554] | 1.86 | 0.34 |
| 4:5:114:ALA:CA | 4:9:250:ILE:C[1_554] | 1.86 | 0.34 |
| 4:6:275:HIS:N | 4:9:162:ASN:CA[1_554] | 1.86 | 0.34 |
| 4:5:279:TYR:CE2 | 4:8:282:ILE:O[1_554] | 1.86 | 0.34 |
| 4:4:371:HIS:C | 4:8:230:ALA:CB[1_554] | 1.86 | 0.34 |
| 4:4:311:ASP:OD1 | 4:7:144:ALA:N[1_554] | 1.86 | 0.34 |
| 4:5:179:ASP:O | 4:8:179:ASP:CG[1_554] | 1.86 | 0.34 |
| 4:6:11:ASP:OD2 | 4:9:115:ASN:CA[1_554] | 1.86 | 0.34 |
| 4:6:305:MET:CE | 4:9:11:ASP:N[1_554] | 1.86 | 0.34 |
| 4:3:109:PRO:CG | 4:7:195:GLU:CD[1_554] | 1.86 | 0.34 |
| 4:6:205:GLU:OE2 | 4:9:203:THR:CB[1_554] | 1.86 | 0.34 |
| 4:5:315:LYS:C | 4:8:296:ASN:C[1_554] | 1.86 | 0.34 |
| 4:6:213:LYS:CA | 4:9:16:LEU:CD2[1_554] | 1.86 | 0.34 |
| 4:5:220:ALA:O | 4:8:335:ARG:CD[1_554] | 1.86 | 0.34 |
| 4:4:285:CYS:C | 4:8:270:GLU:OE2[1_554] | 1.86 | 0.34 |
| 4:5:279:TYR:O | 4:8:285:CYS:CB[1_554] | 1.86 | 0.34 |
| 4:6:214:GLU:N | 4:9:16:LEU:CG[1_554] | 1.86 | 0.34 |
| 4:5:288:ASP:CA | 4:V:63:GLY:CA[1_554] | 1.86 | 0.34 |
| 4:3:115:ASN:CG | 4:7:249:THR:C[1_554] | 1.86 | 0.34 |
| 4:5:186:THR:OG1 | 4:8:183:ARG:CZ[1_554] | 1.86 | 0.34 |
| 4:5:337:TYR:CE1 | 4:8:86:TRP:CE2[1_554] | 1.86 | 0.34 |
| 4:5:262:PHE:CE2 | 4:8:153:LEU:C[1_554] | 1.86 | 0.34 |
| 4:6:162:ASN:CA | 4:9:175:ILE:CD1[1_554] | 1.86 | 0.34 |
| 4:6:274:ILE:N | 4:9:162:ASN:CB[1_554] | 1.86 | 0.34 |
| 4:4:109:PRO:CG | 4:8:195:GLU:OE2[1_554] | 1.86 | 0.34 |
| 4:6:28:ARG:CA | 4:9:126:THR:CB[1_554] | 1.86 | 0.34 |
| 4:5:198:TYR:CA | 4:8:205:GLU:O[1_554] | 1.86 | 0.34 |
| 4:6:27:PRO:N | 4:9:122:ILE:C[1_554] | 1.86 | 0.34 |
| 4:4:187:ASP:CA | 4:7:183:ARG:CD[1_554] | 1.86 | 0.34 |
| 4:5:370:VAL:C | 4:9:231:ALA:CA[1_554] | 1.86 | 0.34 |
| 4:5:320:LEU:N | 4:8:292:ASP:O[1_554] | 1.86 | 0.34 |
| 4:4:334:GLU:CG | 4:7:132:MET:SD[1_554] | 1.86 | 0.34 |
| 4:5:161:HIS:CB | 4:8:110:LEU:CD1[1_554] | 1.86 | 0.34 |
| 4:5:62:ARG:NH1 | 4:8:67:LEU:C[1_554] | 1.86 | 0.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:32:PRO:CA | 4:8:78:ASN:CG[1_554] | 1.86 | 0.34 |
| 4:6:317:ILE:CG2 | 4:9:151:ILE:N[1_554] | 1.86 | 0.34 |
| 4:5:270:GLU:CB | 4:8:271:SER:C[1_554] | 1.86 | 0.34 |
| 4:4:273:GLY:C | 4:7:162:ASN:OD1[1_554] | 1.86 | 0.34 |
| 4:6:314:GLN:CB | 4:9:142:LEU:O[1_554] | 1.86 | 0.34 |
| 4:4:31:PHE:N | 4:7:80:ASP:N[1_554] | 1.86 | 0.34 |
| 4:6:340:TRP:CH2 | 4:9:120:THR:O[1_554] | 1.86 | 0.34 |
| 4:5:208:ILE:N | 4:8:59:GLN:CD[1_554] | 1.86 | 0.34 |
| 4:6:221:LEU:CD1 | 4:9:332:PRO:CB[1_554] | 1.86 | 0.34 |
| 4:4:299:MET:CB | 4:7:136:ILE:N[1_554] | 1.86 | 0.34 |
| 4:4:255:PHE:CE2 | 4:7:305:MET:SD[1_554] | 1.86 | 0.34 |
| 4:5:214:GLU:CG | 4:8:16:LEU:N[1_554] | 1.86 | 0.34 |
| 4:6:14:SER:CA | 4:9:77:THR:OG1[1_554] | 1.86 | 0.34 |
| 4:5:274:ILE:C | 4:8:162:ASN:CB[1_554] | 1.86 | 0.34 |
| 4:4:182:GLY:N | 4:7:74:GLY:N[1_554] | 1.86 | 0.34 |
| 4:5:243:PRO:CG | 4:8:59:GLN:C[1_554] | 1.86 | 0.34 |
| 4:6:174:ALA:O | 4:9:173:HIS:N[1_554] | 1.86 | 0.34 |
| 4:6:258:PRO:CB | 4:9:301:GLY:C[1_554] | 1.86 | 0.34 |
| 4:4:198:TYR:O | 4:7:205:GLU:O[1_554] | 1.86 | 0.34 |
| 4:6:320:LEU:N | 4:9:293:LEU:N[1_554] | 1.86 | 0.34 |
| 4:4:162:ASN:CG | 4:7:175:ILE:CB[1_554] | 1.86 | 0.34 |
| 4:6:253:GLU:CG | 4:9:214:GLU:CG[1_554] | 1.86 | 0.34 |
| 4:6:253:GLU:CD | 4:9:214:GLU:C[1_554] | 1.86 | 0.34 |
| 4:4:257:CYS:SG | 4:7:157:ASP:CB[1_554] | 1.86 | 0.34 |
| 4:4:25:ASP:OD1 | 4:7:124:PHE:CD1[1_554] | 1.86 | 0.34 |
| 4:6:141:SER:CB | 4:9:116:ARG:CZ[1_554] | 1.86 | 0.34 |
| 4:3:371:HIS:NE2 | 4:7:252:ASN:O[1_554] | 1.86 | 0.34 |
| 4:6:140:LEU:CD1 | 4:9:117:GLU:CG[1_554] | 1.86 | 0.34 |
| 4:6:114:ALA:O | 4:V:237:GLU:OE1[1_554] | 1.86 | 0.34 |
| 4:4:316:GLU:O | 4:7:150:GLY:CA[1_554] | 1.86 | 0.34 |
| 4:6:326:LYS:O | 4:9:167:GLU:CD[1_554] | 1.86 | 0.34 |
| 4:3:357:ILE:CG2 | 4:7:233:SER:N[1_554] | 1.86 | 0.34 |
| 4:4:215:LYS:O | 4:7:30:VAL:CA[1_554] | 1.86 | 0.34 |
| 4:3:372:ARG:C | 4:7:226:GLU:O[1_554] | 1.86 | 0.34 |
| 4:5:295:ALA:C | 4:8:168:GLY:N[1_554] | 1.86 | 0.34 |
| 4:4:213:LYS:N | 4:7:15:GLY:O[1_554] | 1.86 | 0.34 |
| 4:4:30:VAL:CB | 4:7:79:TRP:CA[1_554] | 1.86 | 0.34 |
| 4:6:163:VAL:CA | 4:9:172:PRO:CB[1_554] | 1.86 | 0.34 |
| 4:6:333:PRO:C | 4:9:104:LEU:C[1_554] | 1.86 | 0.34 |
| 4:5:333:PRO:O | 4:8:104:LEU:O[1_554] | 1.86 | 0.34 |
| 4:6:196:ARG:NE | 4:9:211:ASP:C[1_554] | 1.86 | 0.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:261:LEU:N | 4:8:155:SER:CB[1_554] | 1.86 | 0.34 |
| 4:6:331:ALA:C | 4:9:140:LEU:CG[1_554] | 1.86 | 0.34 |
| 4:4:136:ILE:CA | 4:7:113:LYS:NZ[1_554] | 1.86 | 0.34 |
| 4:4:137:GLN:OE1 | 4:7:112:PRO:CG[1_554] | 1.86 | 0.34 |
| 4:6:263:GLN:CA | 4:9:274:ILE:CG2[1_554] | 1.86 | 0.34 |
| 4:5:199:SER:C | 4:8:206:ARG:C[1_554] | 1.86 | 0.34 |
| 4:5:335:ARG:C | 4:8:106:THR:N[1_554] | 1.86 | 0.34 |
| 4:4:294:TYR:CZ | 4:7:166:TYR:CB[1_554] | 1.86 | 0.34 |
| 4:6:198:TYR:CB | 4:9:208:ILE:N[1_554] | 1.86 | 0.34 |
| 4:5:260:THR:C | 4:8:155:SER:OG[1_554] | 1.86 | 0.34 |
| 4:5:370:VAL:C | 4:9:231:ALA:N[1_554] | 1.86 | 0.34 |
| 4:6:178:LEU:CD2 | 4:9:177:ARG:N[1_554] | 1.86 | 0.34 |
| 4:6:198:TYR:CG | 4:9:208:ILE:CB[1_554] | 1.86 | 0.34 |
| 4:6:362:TYR:CE1 | 4:V:233:SER:O[1_554] | 1.86 | 0.34 |
| 4:3:372:ARG:C | 4:7:226:GLU:C[1_554] | 1.86 | 0.34 |
| 4:5:10:CYS:CA | 4:8:118:LYS:CD[1_554] | 1.86 | 0.34 |
| 4:4:27:PRO:CB | 4:7:122:ILE:CG1[1_554] | 1.86 | 0.34 |
| 4:6:173:HIS:NE2 | 4:V:265:SER:C[1_554] | 1.86 | 0.34 |
| 4:4:270:GLU:CA | 4:7:272:ALA:N[1_554] | 1.86 | 0.34 |
| 4:6:11:ASP:OD2 | 4:9:115:ASN:CB[1_554] | 1.86 | 0.34 |
| 4:6:318:THR:CB | 4:9:296:ASN:ND2[1_554] | 1.86 | 0.34 |
| 4:6:349:LEU:CA | 4:9:364:GLU:C[1_554] | 1.86 | 0.34 |
| 4:4:136:ILE:CB | 4:7:113:LYS:NZ[1_554] | 1.86 | 0.34 |
| 4:4:115:ASN:O | 4:8:237:GLU:OE1[1_554] | 1.86 | 0.34 |
| 4:5:28:ARG:C | 4:8:83:GLU:CD[1_554] | 1.86 | 0.34 |
| 4:5:308:GLY:O | 4:8:338:SER:OG[1_554] | 1.87 | 0.33 |
| 4:5:367:PRO:N | 4:9:233:SER:O[1_554] | 1.87 | 0.33 |
| 4:6:310:ALA:CA | 4:9:141:SER:CB[1_554] | 1.87 | 0.33 |
| 4:4:279:TYR:N | 4:7:164:PRO:CB[1_554] | 1.87 | 0.33 |
| 4:5:198:TYR:CZ | 4:8:208:ILE:CG1[1_554] | 1.87 | 0.33 |
| 4:5:207:GLU:CG | 4:8:67:LEU:CD1[1_554] | 1.87 | 0.33 |
| 4:5:270:GLU:N | 4:8:272:ALA:O[1_554] | 1.87 | 0.33 |
| 4:6:75:ILE:N | 4:V:197:GLY:CA[1_554] | 1.87 | 0.33 |
| 4:5:18:LYS:N | 4:8:79:TRP:CE2[1_554] | 1.87 | 0.33 |
| 4:6:343:GLY:N | 4:9:367:PRO:O[1_554] | 1.87 | 0.33 |
| 4:4:138:ALA:N | 4:7:113:LYS:N[1_554] | 1.87 | 0.33 |
| 4:4:195:GLU:O | 4:7:212:ILE:CG2[1_554] | 1.87 | 0.33 |
| 4:6:320:LEU:N | 4:9:292:ASP:C[1_554] | 1.87 | 0.33 |
| 4:4:311:ASP:N | 4:7:141:SER:CA[1_554] | 1.87 | 0.33 |
| 4:4:255:PHE:CZ | 4:7:305:MET:CB[1_554] | 1.87 | 0.33 |
| 4:4:214:GLU:CA | 4:7:16:LEU:CA[1_554] | 1.87 | 0.33 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:21:PHE:CB | 4:9:125:GLU:OE1[1_554] | 1.87 | 0.33 |
| 4:4:227:MET:SD | 4:7:306:TYR:N[1_554] | 1.87 | 0.33 |
| 4:5:186:THR:CA | 4:8:183:ARG:NE[1_554] | 1.87 | 0.33 |
| 4:4:210:ARG:O | 4:7:15:GLY:O[1_554] | 1.87 | 0.33 |
| 4:4:284:LYS:CA | 4:8:268:GLY:O[1_554] | 1.87 | 0.33 |
| 4:5:260:THR:C | 4:8:160:THR:OG1[1_554] | 1.87 | 0.33 |
| 4:5:177:ARG:CZ | 4:9:194:THR:OG1[1_554] | 1.87 | 0.33 |
| 4:4:338:SER:N | 4:7:119:MET:CG[1_554] | 1.87 | 0.33 |
| 4:5:345:ILE:CD1 | 4:8:357:ILE:CG2[1_554] | 1.87 | 0.33 |
| 4:5:210:ARG:NH2 | 4:8:34:ILE:CA[1_554] | 1.87 | 0.33 |
| 4:4:139:VAL:CA | 4:7:113:LYS:CG[1_554] | 1.87 | 0.33 |
| 4:6:294:TYR:CD1 | 4:9:166:TYR:CB[1_554] | 1.87 | 0.33 |
| 4:4:215:LYS:CA | 4:7:31:PHE:N[1_554] | 1.87 | 0.33 |
| 4:4:223:PHE:C | 4:7:335:ARG:NH1[1_554] | 1.87 | 0.33 |
| 4:4:157:ASP:OD2 | 4:7:72:GLU:CG[1_554] | 1.87 | 0.33 |
| 4:4:27:PRO:N | 4:7:122:ILE:CB[1_554] | 1.87 | 0.33 |
| 4:6:258:PRO:O | 4:9:155:SER:CA[1_554] | 1.87 | 0.33 |
| 4:5:297:ASN:OD1 | 4:8:165:ILE:CB[1_554] | 1.87 | 0.33 |
| 4:6:213:LYS:NZ | 4:9:14:SER:CA[1_554] | 1.87 | 0.33 |
| 4:4:16:LEU:CG | 4:7:78:ASN:O[1_554] | 1.87 | 0.33 |
| 4:6:30:VAL:CA | 4:9:83:GLU:N[1_554] | 1.87 | 0.33 |
| 4:6:367:PRO:C | 4:V:230:ALA:O[1_554] | 1.87 | 0.33 |
| 4:6:264:PRO:CA | 4:9:274:ILE:CD1[1_554] | 1.87 | 0.33 |
| 4:4:294:TYR:CD2 | 4:7:166:TYR:CD2[1_554] | 1.87 | 0.33 |
| 4:5:161:HIS:CA | 4:8:110:LEU:CB[1_554] | 1.87 | 0.33 |
| 4:3:288:ASP:C | 4:8:63:GLY:O[1_554] | 1.87 | 0.33 |
| 4:4:205:GLU:N | 4:7:62:ARG:CG[1_554] | 1.87 | 0.33 |
| 4:5:305:MET:SD | 4:8:11:ASP:CA[1_554] | 1.87 | 0.33 |
| 4:6:273:GLY:CA | 4:9:162:ASN:ND2[1_554] | 1.87 | 0.33 |
| 4:6:218:TYR:CE1 | 4:9:337:TYR:CE2[1_554] | 1.87 | 0.33 |
| 4:4:320:LEU:C | 4:7:293:LEU:CD1[1_554] | 1.87 | 0.33 |
| 4:4:250:ILE:CG1 | 4:7:210:ARG:CZ[1_554] | 1.87 | 0.33 |
| 4:4:261:LEU:N | 4:7:155:SER:CA[1_554] | 1.87 | 0.33 |
| 4:4:255:PHE:CG | 4:7:305:MET:SD[1_554] | 1.87 | 0.33 |
| 4:5:23:GLY:N | 4:8:362:TYR:CZ[1_554] | 1.87 | 0.33 |
| 4:4:191:LYS:CB | 4:7:186:THR:N[1_554] | 1.87 | 0.33 |
| 4:5:280:ASN:ND2 | 4:8:281:SER:C[1_554] | 1.87 | 0.33 |
| 4:6:207:GLU:O | 4:9:34:ILE:CD1[1_554] | 1.87 | 0.33 |
| 4:5:113:LYS:CE | 4:9:252:ASN:O[1_554] | 1.87 | 0.33 |
| 4:6:262:PHE:N | 4:9:153:LEU:CG[1_554] | 1.87 | 0.33 |
| 4:5:159:VAL:N | 4:8:177:ARG:NH1[1_554] | 1.87 | 0.33 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:319:ALA:N | 4:7:149:THR:O[1_554] | 1.87 | 0.33 |
| 4:4:178:LEU:CG | 4:7:177:ARG:O[1_554] | 1.87 | 0.33 |
| 4:6:199:SER:N | 4:9:206:ARG:C[1_554] | 1.87 | 0.33 |
| 4:5:258:PRO:C | 4:8:155:SER:CB[1_554] | 1.87 | 0.33 |
| 4:4:154:ASP:CG | 4:7:111:ASN:O[1_554] | 1.87 | 0.33 |
| 4:5:177:ARG:CZ | 4:9:194:THR:CG2[1_554] | 1.87 | 0.33 |
| 4:6:307:PRO:CA | 4:9:337:TYR:O[1_554] | 1.87 | 0.33 |
| 4:4:188:TYR:CB | 4:7:181:ALA:C[1_554] | 1.87 | 0.33 |
| 4:4:73:HIS:O | 4:8:198:TYR:O[1_554] | 1.87 | 0.33 |
| 4:6:257:CYS:CA | 4:9:303:THR:CA[1_554] | 1.87 | 0.33 |
| 4:6:290:ARG:CD | 4:9:286:ASP:OD2[1_554] | 1.87 | 0.33 |
| 4:3:172:PRO:CD | 4:7:266:PHE:CB[1_554] | 1.87 | 0.33 |
| 4:6:283:MET:CG | 4:9:285:CYS:O[1_554] | 1.87 | 0.33 |
| 4:5:315:LYS:C | 4:8:296:ASN:O[1_554] | 1.87 | 0.33 |
| 4:2:323:SER:O | 4:7:44:MET:CE[1_554] | 1.87 | 0.33 |
| 4:6:76:ILE:O | 4:V:198:TYR:CE1[1_554] | 1.87 | 0.33 |
| 4:4:155:SER:O | 4:7:74:GLY:O[1_554] | 1.87 | 0.33 |
| 4:6:327:ILE:N | 4:9:149:THR:OG1[1_554] | 1.87 | 0.33 |
| 4:5:340:TRP:CG | 4:8:119:MET:C[1_554] | 1.87 | 0.33 |
| 4:6:309:ILE:CG2 | 4:9:141:SER:OG[1_554] | 1.87 | 0.33 |
| 4:4:76:ILE:N | 4:8:198:TYR:CD1[1_554] | 1.87 | 0.33 |
| 4:4:286:ASP:CB | 4:8:270:GLU:CD[1_554] | 1.87 | 0.33 |
| 4:3:284:LYS:O | 4:7:268:GLY:CA[1_554] | 1.87 | 0.33 |
| 4:5:11:ASP:N | 4:8:118:LYS:CG[1_554] | 1.87 | 0.33 |
| 4:6:60:SER:CA | 4:9:66:THR:OG1[1_554] | 1.87 | 0.33 |
| 4:5:196:ARG:CZ | 4:8:215:LYS:CG[1_554] | 1.87 | 0.33 |
| 4:6:266:PHE:N | 4:9:261:LEU:O[1_554] | 1.87 | 0.33 |
| 4:3:113:LYS:N | 4:7:250:ILE:CG2[1_554] | 1.87 | 0.33 |
| 4:4:154:ASP:CG | 4:7:112:PRO:N[1_554] | 1.87 | 0.33 |
| 4:6:336:LYS:CG | 4:9:12:ASN:CG[1_554] | 1.87 | 0.33 |
| 4:5:293:LEU:CG | 4:8:169:TYR:CD2[1_554] | 1.87 | 0.33 |
| 4:5:18:LYS:CA | 4:8:79:TRP:CD2[1_554] | 1.87 | 0.33 |
| 4:6:26:ALA:O | 4:9:123:MET:C[1_554] | 1.87 | 0.33 |
| 4:3:366:GLY:O | 4:7:234:SER:OG[1_554] | 1.88 | 0.32 |
| 4:4:341:ILE:CB | 4:7:120:THR:OG1[1_554] | 1.88 | 0.32 |
| 4:5:140:LEU:CD2 | 4:8:371:HIS:CG[1_554] | 1.88 | 0.32 |
| 4:6:218:TYR:O | 4:9:301:GLY:O[1_554] | 1.88 | 0.32 |
| 4:6:183:ARG:NH2 | 4:9:72:GLU:OE1[1_554] | 1.88 | 0.32 |
| 4:5:199:SER:O | 4:8:203:THR:O[1_554] | 1.88 | 0.32 |
| 4:5:24:ASP:N | 4:8:124:PHE:CB[1_554] | 1.88 | 0.32 |
| 4:4:155:SER:C | 4:7:75:ILE:CD1[1_554] | 1.88 | 0.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:314:GLN:CG | 4:8:142:LEU:C[1_554] | 1.88 | 0.32 |
| 4:4:26:ALA:CA | 4:7:121:GLN:O[1_554] | 1.88 | 0.32 |
| 4:5:195:GLU:CA | 4:8:189:LEU:CD2[1_554] | 1.88 | 0.32 |
| 4:3:109:PRO:C | 4:7:195:GLU:CD[1_554] | 1.88 | 0.32 |
| 4:6:304:THR:CA | 4:9:137:GLN:CB[1_554] | 1.88 | 0.32 |
| 4:3:369:ILE:CG2 | 4:7:234:SER:CB[1_554] | 1.88 | 0.32 |
| 4:4:261:LEU:O | 4:7:161:HIS:CA[1_554] | 1.88 | 0.32 |
| 4:6:319:ALA:C | 4:9:294:TYR:N[1_554] | 1.88 | 0.32 |
| 4:4:344:SER:CA | 4:7:367:PRO:CD[1_554] | 1.88 | 0.32 |
| 4:6:208:ILE:CD1 | 4:9:59:GLN:CG[1_554] | 1.88 | 0.32 |
| 4:6:110:LEU:N | 4:V:195:GLU:CG[1_554] | 1.88 | 0.32 |
| 4:5:295:ALA:CA | 4:8:168:GLY:N[1_554] | 1.88 | 0.32 |
| 4:5:223:PHE:CD1 | 4:8:335:ARG:NE[1_554] | 1.88 | 0.32 |
| 4:4:276:GLU:O | 4:7:281:SER:OG[1_554] | 1.88 | 0.32 |
| 4:5:331:ALA:CB | 4:8:140:LEU:CA[1_554] | 1.88 | 0.32 |
| 4:4:261:LEU:O | 4:7:161:HIS:C[1_554] | 1.88 | 0.32 |
| 4:5:215:LYS:CE | 4:8:31:PHE:CA[1_554] | 1.88 | 0.32 |
| 4:5:155:SER:N | 4:8:108:ALA:CA[1_554] | 1.88 | 0.32 |
| 4:5:214:GLU:O | 4:8:16:LEU:CB[1_554] | 1.88 | 0.32 |
| 4:5:331:ALA:C | 4:8:140:LEU:CG[1_554] | 1.88 | 0.32 |
| 4:5:222:ASP:CA | 4:8:331:ALA:CA[1_554] | 1.88 | 0.32 |
| 4:5:157:ASP:CB | 4:8:72:GLU:CA[1_554] | 1.88 | 0.32 |
| 4:6:208:ILE:CB | 4:9:59:GLN:NE2[1_554] | 1.88 | 0.32 |
| 4:4:259:GLU:CB | 4:7:304:THR:CA[1_554] | 1.88 | 0.32 |
| 4:5:143:TYR:CE2 | 4:8:369:ILE:CA[1_554] | 1.88 | 0.32 |
| 4:6:210:ARG:CG | 4:9:69:TYR:CE2[1_554] | 1.88 | 0.32 |
| 4:6:267:ILE:CD1 | 4:9:180:LEU:CG[1_554] | 1.88 | 0.32 |
| 4:6:112:PRO:CD | 4:V:192:ILE:O[1_554] | 1.88 | 0.32 |
| 4:6:269:MET:O | 4:9:272:ALA:C[1_554] | 1.88 | 0.32 |
| 4:5:151:ILE:CG1 | 4:8:171:LEU:CA[1_554] | 1.88 | 0.32 |
| 4:5:211:ASP:OD1 | 4:8:32:PRO:CG[1_554] | 1.88 | 0.32 |
| 4:5:59:GLN:O | 4:8:66:THR:CB[1_554] | 1.88 | 0.32 |
| 4:6:199:SER:CA | 4:9:206:ARG:C[1_554] | 1.88 | 0.32 |
| 4:4:215:LYS:CA | 4:7:31:PHE:O[1_554] | 1.88 | 0.32 |
| 4:4:276:GLU:OE1 | 4:7:278:THR:C[1_554] | 1.88 | 0.32 |
| 4:6:30:VAL:O | 4:9:80:ASP:C[1_554] | 1.88 | 0.32 |
| 4:5:348:SER:CB | 4:8:362:TYR:C[1_554] | 1.88 | 0.32 |
| 4:4:258:PRO:N | 4:7:155:SER:O[1_554] | 1.88 | 0.32 |
| 4:4:316:GLU:CB | 4:7:151:ILE:C[1_554] | 1.88 | 0.32 |
| 1:D:411:GLU:OE2 | 4:6:226:GLU:OE1[1_556] | 1.88 | 0.32 |
| 4:5:277:THR:CB | 4:8:176:MET:N[1_554] | 1.88 | 0.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:198:TYR:CE2 | 4:9:211:ASP:CB[1_554] | 1.88 | 0.32 |
| 4:5:196:ARG:NH1 | 4:8:215:LYS:CA[1_554] | 1.88 | 0.32 |
| 4:6:321:ALA:C | 4:9:292:ASP:CA[1_554] | 1.88 | 0.32 |
| 4:4:75:ILE:C | 4:8:198:TYR:CD1[1_554] | 1.88 | 0.32 |
| 4:5:337:TYR:OH | 4:8:86:TRP:CG[1_554] | 1.88 | 0.32 |
| 4:4:75:ILE:O | 4:8:197:GLY:O[1_554] | 1.88 | 0.32 |
| 4:5:274:ILE:N | 4:8:162:ASN:CB[1_554] | 1.88 | 0.32 |
| 4:4:145:SER:CA | 4:7:370:VAL:O[1_554] | 1.88 | 0.32 |
| 4:5:273:GLY:C | 4:8:162:ASN:ND2[1_554] | 1.88 | 0.32 |
| 4:5:106:THR:OG1 | 4:8:114:ALA:C[1_554] | 1.88 | 0.32 |
| 4:4:275:HIS:O | 4:7:164:PRO:CD[1_554] | 1.88 | 0.32 |
| 4:6:198:TYR:CB | 4:9:208:ILE:CA[1_554] | 1.88 | 0.32 |
| 4:4:326:LYS:O | 4:7:167:GLU:C[1_554] | 1.88 | 0.32 |
| 1:D:542:PHE:CE1 | 4:6:328:LYS:NZ[1_556] | 1.88 | 0.32 |
| 4:5:267:ILE:CB | 4:8:180:LEU:CD2[1_554] | 1.88 | 0.32 |
| 4:3:115:ASN:ND2 | 4:7:198:TYR:CZ[1_554] | 1.88 | 0.32 |
| 4:6:267:ILE:CG1 | 4:9:180:LEU:CD2[1_554] | 1.88 | 0.32 |
| 4:4:154:ASP:OD2 | 4:7:111:ASN:CA[1_554] | 1.88 | 0.32 |
| 4:6:329:ILE:CG2 | 4:9:139:VAL:CA[1_554] | 1.88 | 0.32 |
| 4:6:368:SER:CA | 4:V:229:THR:C[1_554] | 1.88 | 0.32 |
| 4:5:347:ALA:C | 4:8:366:GLY:N[1_554] | 1.88 | 0.32 |
| 4:4:266:PHE:CE1 | 4:7:261:LEU:CD1[1_554] | 1.88 | 0.32 |
| 4:4:259:GLU:CB | 4:7:304:THR:CB[1_554] | 1.88 | 0.32 |
| 4:4:207:GLU:CD | 4:7:68:LYS:N[1_554] | 1.88 | 0.32 |
| 4:4:112:PRO:CD | 4:8:193:LEU:CG[1_554] | 1.88 | 0.32 |
| 4:6:159:VAL:CA | 4:9:177:ARG:NH2[1_554] | 1.88 | 0.32 |
| 4:6:288:ASP:N | 4:W:62:ARG:O[1_554] | 1.88 | 0.32 |
| 4:5:291:LYS:CE | 4:V:64:ILE:CG1[1_554] | 1.88 | 0.32 |
| 4:6:346:LEU:C | 4:9:365:ALA:O[1_554] | 1.88 | 0.32 |
| 4:5:314:GLN:CD | 4:8:147:ARG:CA[1_554] | 1.88 | 0.32 |
| 4:6:255:PHE:CE1 | 4:9:306:TYR:N[1_554] | 1.88 | 0.32 |
| 4:5:159:VAL:C | 4:8:177:ARG:CZ[1_554] | 1.88 | 0.32 |
| 4:6:340:TRP:CE3 | 4:9:119:MET:C[1_554] | 1.88 | 0.32 |
| 4:6:15:GLY:C | 4:9:77:THR:CA[1_554] | 1.88 | 0.32 |
| 4:6:367:PRO:CG | 4:V:234:SER:O[1_554] | 1.88 | 0.32 |
| 4:5:320:LEU:CA | 4:8:293:LEU:N[1_554] | 1.88 | 0.32 |
| 4:5:276:GLU:OE1 | 4:8:279:TYR:N[1_554] | 1.88 | 0.32 |
| 4:4:313:MET:CA | 4:7:152:VAL:CG2[1_554] | 1.88 | 0.32 |
| 4:4:18:LYS:C | 4:7:118:LYS:CE[1_554] | 1.88 | 0.32 |
| 4:6:366:GLY:O | 4:V:233:SER:N[1_554] | 1.88 | 0.32 |
| 4:5:173:HIS:NE2 | 4:9:265:SER:O[1_554] | 1.88 | 0.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:312:ARG:NH1 | 4:7:298:VAL:O[1_554] | 1.88 | 0.32 |
| 4:6:109:PRO:O | 4:V:195:GLU:OE2[1_554] | 1.88 | 0.32 |
| 4:4:308:GLY:O | 4:7:339:VAL:N[1_554] | 1.89 | 0.31 |
| 4:4:312:ARG:NH1 | 4:7:299:MET:CA[1_554] | 1.89 | 0.31 |
| 4:5:304:THR:OG1 | 4:8:137:GLN:CD[1_554] | 1.89 | 0.31 |
| 4:5:319:ALA:N | 4:8:296:ASN:ND2[1_554] | 1.89 | 0.31 |
| 4:5:15:GLY:CA | 4:8:77:THR:OG1[1_554] | 1.89 | 0.31 |
| 4:6:108:ALA:C | 4:V:195:GLU:CG[1_554] | 1.89 | 0.31 |
| 4:3:79:TRP:CZ2 | 4:7:249:THR:CG2[1_554] | 1.89 | 0.31 |
| 4:5:267:ILE:O | 4:8:180:LEU:CD2[1_554] | 1.89 | 0.31 |
| 4:6:312:ARG:CB | 4:9:299:MET:C[1_554] | 1.89 | 0.31 |
| 4:4:195:GLU:N | 4:7:209:VAL:C[1_554] | 1.89 | 0.31 |
| 1:A:542:PHE:CD2 | 4:5:328:LYS:NZ[1_556] | 1.89 | 0.31 |
| 4:4:212:ILE:O | 4:7:16:LEU:CG[1_554] | 1.89 | 0.31 |
| 4:6:113:LYS:N | 4:V:253:GLU:OE2[1_554] | 1.89 | 0.31 |
| 4:5:318:THR:CB | 4:8:296:ASN:ND2[1_554] | 1.89 | 0.31 |
| 4:4:137:GLN:CA | 4:7:113:LYS:N[1_554] | 1.89 | 0.31 |
| 4:2:291:LYS:CB | 4:7:40:HIS:N[1_554] | 1.89 | 0.31 |
| 4:5:30:VAL:N | 4:8:83:GLU:CB[1_554] | 1.89 | 0.31 |
| 4:4:314:GLN:OE1 | 4:7:147:ARG:C[1_554] | 1.89 | 0.31 |
| 4:6:188:TYR:CA | 4:9:185:LEU:N[1_554] | 1.89 | 0.31 |
| 4:3:286:ASP:CB | 4:7:270:GLU:OE2[1_554] | 1.89 | 0.31 |
| 4:4:344:SER:OG | 4:7:362:TYR:OH[1_554] | 1.89 | 0.31 |
| 4:6:299:MET:CA | 4:9:136:ILE:CG2[1_554] | 1.89 | 0.31 |
| 4:6:261:LEU:O | 4:9:161:HIS:O[1_554] | 1.89 | 0.31 |
| 4:6:28:ARG:C | 4:9:83:GLU:OE1[1_554] | 1.89 | 0.31 |
| 4:4:23:GLY:O | 4:7:125:GLU:OE2[1_554] | 1.89 | 0.31 |
| 4:5:31:PHE:O | 4:8:78:ASN:CG[1_554] | 1.89 | 0.31 |
| 4:5:110:LEU:CB | 4:9:192:ILE:CA[1_554] | 1.89 | 0.31 |
| 4:6:198:TYR:CG | 4:9:208:ILE:N[1_554] | 1.89 | 0.31 |
| 4:5:28:ARG:O | 4:8:83:GLU:OE1[1_554] | 1.89 | 0.31 |
| 4:5:310:ALA:N | 4:8:141:SER:N[1_554] | 1.89 | 0.31 |
| 4:6:162:ASN:N | 4:9:110:LEU:CG[1_554] | 1.89 | 0.31 |
| 4:5:27:PRO:CA | 4:8:122:ILE:C[1_554] | 1.89 | 0.31 |
| 4:4:312:ARG:N | 4:7:141:SER:CB[1_554] | 1.89 | 0.31 |
| 4:4:262:PHE:CD2 | 4:7:154:ASP:N[1_554] | 1.89 | 0.31 |
| 4:6:166:TYR:CD2 | 4:W:40:HIS:CE1[1_554] | 1.89 | 0.31 |
| 4:5:299:MET:CE | 4:8:138:ALA:C[1_554] | 1.89 | 0.31 |
| 4:5:287:ILE:C | 4:V:63:GLY:N[1_554] | 1.89 | 0.31 |
| 4:5:316:GLU:OE1 | 4:8:297:ASN:OD1[1_554] | 1.89 | 0.31 |
| 4:6:272:ALA:CA | 4:9:277:THR:OG1[1_554] | 1.89 | 0.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:141:SER:OG | 4:9:107:GLU:OE2[1_554] | 1.89 | 0.31 |
| 4:4:137:GLN:C | 4:7:113:LYS:CB[1_554] | 1.89 | 0.31 |
| 4:6:18:LYS:CE | 4:9:79:TRP:CZ3[1_554] | 1.89 | 0.31 |
| 4:6:190:MET:O | 4:9:186:THR:CB[1_554] | 1.89 | 0.31 |
| 4:4:325:MET:CB | 4:7:166:TYR:CE2[1_554] | 1.89 | 0.31 |
| 4:6:113:LYS:NZ | 4:V:254:ARG:CB[1_554] | 1.89 | 0.31 |
| 4:5:113:LYS:O | 4:9:252:ASN:OD1[1_554] | 1.89 | 0.31 |
| 4:5:283:MET:CB | 4:8:285:CYS:CA[1_554] | 1.89 | 0.31 |
| 4:5:312:ARG:NH1 | 4:8:299:MET:SD[1_554] | 1.89 | 0.31 |
| 4:4:173:HIS:CA | 4:8:267:ILE:N[1_554] | 1.89 | 0.31 |
| 4:6:113:LYS:O | 4:V:252:ASN:CB[1_554] | 1.89 | 0.31 |
| 4:5:266:PHE:N | 4:8:261:LEU:O[1_554] | 1.89 | 0.31 |
| 4:5:183:ARG:NH2 | 4:8:72:GLU:OE1[1_554] | 1.89 | 0.31 |
| 4:4:306:TYR:O | 4:7:339:VAL:CB[1_554] | 1.89 | 0.31 |
| 4:4:370:VAL:C | 4:8:230:ALA:O[1_554] | 1.89 | 0.31 |
| 4:5:307:PRO:CB | 4:8:337:TYR:O[1_554] | 1.89 | 0.31 |
| 4:6:187:ASP:CA | 4:9:183:ARG:CB[1_554] | 1.89 | 0.31 |
| 4:4:293:LEU:CA | 4:7:169:TYR:CG[1_554] | 1.89 | 0.31 |
| 4:4:113:LYS:O | 4:8:252:ASN:N[1_554] | 1.89 | 0.31 |
| 4:3:291:LYS:CB | 4:8:64:ILE:CG1[1_554] | 1.89 | 0.31 |
| 4:5:25:ASP:O | 4:8:123:MET:CB[1_554] | 1.89 | 0.31 |
| 4:4:339:VAL:CB | 4:7:114:ALA:C[1_554] | 1.89 | 0.31 |
| 4:4:268:GLY:C | 4:7:264:PRO:CG[1_554] | 1.89 | 0.31 |
| 4:4:309:ILE:N | 4:7:339:VAL:N[1_554] | 1.89 | 0.31 |
| 4:4:106:THR:CG2 | 4:7:114:ALA:CB[1_554] | 1.89 | 0.31 |
| 4:5:190:MET:CE | 4:8:206:ARG:NH1[1_554] | 1.89 | 0.31 |
| 4:5:372:ARG:O | 4:9:227:MET:CA[1_554] | 1.89 | 0.31 |
| 4:5:26:ALA:CA | 4:8:123:MET:N[1_554] | 1.89 | 0.31 |
| 4:6:61:LYS:N | 4:9:66:THR:OG1[1_554] | 1.89 | 0.31 |
| 4:6:151:ILE:CG2 | 4:9:170:ALA:CA[1_554] | 1.89 | 0.31 |
| 4:4:270:GLU:CB | 4:7:272:ALA:C[1_554] | 1.89 | 0.31 |
| 4:6:283:MET:CB | 4:9:285:CYS:CA[1_554] | 1.89 | 0.31 |
| 4:6:265:SER:O | 4:9:260:THR:C[1_554] | 1.89 | 0.31 |
| 4:4:198:TYR:CD1 | 4:7:208:ILE:N[1_554] | 1.89 | 0.31 |
| 4:5:113:LYS:CA | 4:9:252:ASN:C[1_554] | 1.89 | 0.31 |
| 4:6:255:PHE:CD1 | 4:9:305:MET:N[1_554] | 1.89 | 0.31 |
| 4:6:294:TYR:CE2 | 4:9:166:TYR:CD1[1_554] | 1.89 | 0.31 |
| 4:4:179:ASP:O | 4:7:179:ASP:CG[1_554] | 1.89 | 0.31 |
| 4:5:340:TRP:CE3 | 4:8:119:MET:C[1_554] | 1.89 | 0.31 |
| 4:4:262:PHE:CB | 4:7:153:LEU:CG[1_554] | 1.89 | 0.31 |
| 4:4:199:SER:CB | 4:7:206:ARG:CA[1_554] | 1.89 | 0.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:341:ILE:N | 4:9:120:THR:CB[1_554] | 1.89 | 0.31 |
| 4:4:117:GLU:CD | 4:8:236:LEU:C[1_554] | 1.89 | 0.31 |
| 4:6:318:THR:N | 4:9:150:GLY:CA[1_554] | 1.89 | 0.31 |
| 4:6:220:ALA:CB | 4:9:335:ARG:NH1[1_554] | 1.89 | 0.31 |
| 4:4:25:ASP:CA | 4:7:125:GLU:N[1_554] | 1.89 | 0.31 |
| 4:6:22:ALA:CA | 4:9:362:TYR:CE2[1_554] | 1.89 | 0.31 |
| 4:5:28:ARG:CA | 4:8:126:THR:CB[1_554] | 1.89 | 0.31 |
| 4:6:296:ASN:N | 4:9:168:GLY:CA[1_554] | 1.89 | 0.31 |
| 4:4:211:ASP:OD1 | 4:7:55:GLY:CA[1_554] | 1.89 | 0.31 |
| 4:5:307:PRO:CA | 4:8:337:TYR:CA[1_554] | 1.89 | 0.31 |
| 4:4:256:ARG:N | 4:7:302:GLY:CA[1_554] | 1.89 | 0.31 |
| 4:6:111:ASN:CA | 4:V:192:ILE:O[1_554] | 1.89 | 0.31 |
| 4:4:115:ASN:C | 4:8:196:ARG:CZ[1_554] | 1.89 | 0.31 |
| 4:4:180:LEU:CA | 4:7:179:ASP:CG[1_554] | 1.89 | 0.31 |
| 4:4:291:LYS:CD | 4:9:64:ILE:CB[1_554] | 1.89 | 0.31 |
| 4:5:266:PHE:CZ | 4:8:261:LEU:CD1[1_554] | 1.89 | 0.31 |
| 4:4:215:LYS:CE | 4:7:31:PHE:CG[1_554] | 1.89 | 0.31 |
| 4:3:76:ILE:N | 4:7:198:TYR:CD1[1_554] | 1.89 | 0.31 |
| 4:6:281:SER:OG | 4:9:174:ALA:N[1_554] | 1.89 | 0.31 |
| 4:5:319:ALA:CA | 4:8:295:ALA:C[1_554] | 1.89 | 0.31 |
| 4:4:15:GLY:O | 4:7:77:THR:CG2[1_554] | 1.89 | 0.31 |
| 4:5:268:GLY:O | 4:8:264:PRO:CB[1_554] | 1.89 | 0.31 |
| 4:5:207:GLU:CD | 4:8:67:LEU:CA[1_554] | 1.89 | 0.31 |
| 4:5:281:SER:N | 4:8:174:ALA:CA[1_554] | 1.89 | 0.31 |
| 4:5:335:ARG:CB | 4:8:106:THR:CB[1_554] | 1.89 | 0.31 |
| 4:6:301:GLY:CA | 4:9:107:GLU:CA[1_554] | 1.89 | 0.31 |
| 4:6:295:ALA:CB | 4:9:167:GLU:CB[1_554] | 1.89 | 0.31 |
| 4:5:340:TRP:CG | 4:8:120:THR:N[1_554] | 1.89 | 0.31 |
| 4:4:196:ARG:NE | 4:7:211:ASP:OD1[1_554] | 1.89 | 0.31 |
| 4:6:159:VAL:N | 4:9:177:ARG:CZ[1_554] | 1.89 | 0.31 |
| 4:5:31:PHE:N | 4:8:80:ASP:N[1_554] | 1.89 | 0.31 |
| 4:5:261:LEU:CA | 4:8:160:THR:CG2[1_554] | 1.89 | 0.31 |
| 4:4:114:ALA:CB | 4:8:238:LYS:O[1_554] | 1.90 | 0.30 |
| 4:6:31:PHE:C | 4:9:78:ASN:CG[1_554] | 1.90 | 0.30 |
| 4:3:109:PRO:N | 4:7:195:GLU:CD[1_554] | 1.90 | 0.30 |
| 4:5:22:ALA:N | 4:8:362:TYR:OH[1_554] | 1.90 | 0.30 |
| 4:5:310:ALA:C | 4:8:141:SER:CA[1_554] | 1.90 | 0.30 |
| 4:5:276:GLU:CB | 4:8:281:SER:CB[1_554] | 1.90 | 0.30 |
| 4:4:157:ASP:N | 4:7:72:GLU:O[1_554] | 1.90 | 0.30 |
| 4:4:319:ALA:CA | 4:7:296:ASN:ND2[1_554] | 1.90 | 0.30 |
| 4:5:317:ILE:CG1 | 4:8:150:GLY:CA[1_554] | 1.90 | 0.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:109:PRO:CA | 4:7:195:GLU:OE2[1_554] | 1.90 | 0.30 |
| 4:4:293:LEU:CB | 4:7:169:TYR:CZ[1_554] | 1.90 | 0.30 |
| 4:4:196:ARG:NE | 4:7:211:ASP:CB[1_554] | 1.90 | 0.30 |
| 4:4:223:PHE:O | 4:7:335:ARG:NH1[1_554] | 1.90 | 0.30 |
| 4:5:336:LYS:N | 4:8:106:THR:N[1_554] | 1.90 | 0.30 |
| 4:4:186:THR:CB | 4:7:183:ARG:NH1[1_554] | 1.90 | 0.30 |
| 4:4:274:ILE:O | 4:7:163:VAL:N[1_554] | 1.90 | 0.30 |
| 4:4:217:CYS:N | 4:7:16:LEU:CG[1_554] | 1.90 | 0.30 |
| 4:4:255:PHE:O | 4:7:303:THR:N[1_554] | 1.90 | 0.30 |
| 4:3:172:PRO:O | 4:7:188:TYR:CD1[1_554] | 1.90 | 0.30 |
| 4:6:270:GLU:CB | 4:9:271:SER:C[1_554] | 1.90 | 0.30 |
| 4:4:337:TYR:CE2 | 4:7:86:TRP:CH2[1_554] | 1.90 | 0.30 |
| 4:6:212:ILE:CG2 | 4:9:210:ARG:NH1[1_554] | 1.90 | 0.30 |
| 4:4:73:HIS:C | 4:8:198:TYR:O[1_554] | 1.90 | 0.30 |
| 4:4:342:GLY:CA | 4:7:117:GLU:CG[1_554] | 1.90 | 0.30 |
| 4:5:282:ILE:CB | 4:8:171:LEU:CD1[1_554] | 1.90 | 0.30 |
| 4:4:17:VAL:O | 4:7:79:TRP:CD1[1_554] | 1.90 | 0.30 |
| 4:4:276:GLU:CG | 4:7:151:ILE:CD1[1_554] | 1.90 | 0.30 |
| 4:6:295:ALA:CA | 4:9:168:GLY:N[1_554] | 1.90 | 0.30 |
| 4:5:21:PHE:CA | 4:8:125:GLU:CG[1_554] | 1.90 | 0.30 |
| 4:5:193:LEU:C | 4:8:209:VAL:O[1_554] | 1.90 | 0.30 |
| 4:6:145:SER:CB | 4:9:372:ARG:CZ[1_554] | 1.90 | 0.30 |
| 4:5:20:GLY:N | 4:8:121:GLN:NE2[1_554] | 1.90 | 0.30 |
| 4:6:109:PRO:CB | 4:V:195:GLU:OE2[1_554] | 1.90 | 0.30 |
| 4:6:304:THR:CB | 4:9:137:GLN:CD[1_554] | 1.90 | 0.30 |
| 4:6:260:THR:OG1 | 4:9:303:THR:CG2[1_554] | 1.90 | 0.30 |
| 4:2:289:ILE:N | 4:7:39:ARG:NE[1_554] | 1.90 | 0.30 |
| 4:5:141:SER:C | 4:8:116:ARG:NE[1_554] | 1.90 | 0.30 |
| 4:5:312:ARG:CZ | 4:8:299:MET:CB[1_554] | 1.90 | 0.30 |
| 4:4:157:ASP:O | 4:7:72:GLU:C[1_554] | 1.90 | 0.30 |
| 4:6:339:VAL:CG2 | 4:9:111:ASN:ND2[1_554] | 1.90 | 0.30 |
| 4:6:143:TYR:CE2 | 4:9:369:ILE:CA[1_554] | 1.90 | 0.30 |
| 4:5:295:ALA:CB | 4:8:167:GLU:CB[1_554] | 1.90 | 0.30 |
| 4:5:136:ILE:CB | 4:8:113:LYS:CD[1_554] | 1.90 | 0.30 |
| 4:6:194:THR:CB | 4:9:190:MET:SD[1_554] | 1.90 | 0.30 |
| 4:6:345:ILE:O | 4:9:366:GLY:O[1_554] | 1.90 | 0.30 |
| 4:4:266:PHE:CD2 | 4:7:303:THR:CG2[1_554] | 1.90 | 0.30 |
| 4:4:294:TYR:C | 4:7:169:TYR:N[1_554] | 1.90 | 0.30 |
| 4:6:196:ARG:CZ | 4:9:215:LYS:CB[1_554] | 1.90 | 0.30 |
| 4:4:267:ILE:CD1 | 4:7:180:LEU:CB[1_554] | 1.90 | 0.30 |
| 4:5:198:TYR:CG | 4:8:208:ILE:O[1_554] | 1.90 | 0.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:31:PHE:O | 4:9:78:ASN:CB[1_554] | 1.90 | 0.30 |
| 4:5:367:PRO:CA | 4:9:233:SER:CB[1_554] | 1.90 | 0.30 |
| 4:4:248:ILE:CD1 | 4:7:207:GLU:CD[1_554] | 1.90 | 0.30 |
| 4:3:175:ILE:CG1 | 4:7:191:LYS:NZ[1_554] | 1.90 | 0.30 |
| 4:6:317:ILE:CB | 4:9:150:GLY:CA[1_554] | 1.90 | 0.30 |
| 4:5:339:VAL:CG1 | 4:8:116:ARG:CA[1_554] | 1.90 | 0.30 |
| 4:5:140:LEU:CG | 4:8:371:HIS:CG[1_554] | 1.90 | 0.30 |
| 4:4:315:LYS:CE | 4:7:147:ARG:NH1[1_554] | 1.90 | 0.30 |
| 4:4:214:GLU:C | 4:7:16:LEU:CA[1_554] | 1.90 | 0.30 |
| 4:6:199:SER:N | 4:9:206:ARG:CA[1_554] | 1.90 | 0.30 |
| 4:6:177:ARG:CZ | 4:V:194:THR:OG1[1_554] | 1.90 | 0.30 |
| 4:4:281:SER:C | 4:7:173:HIS:ND1[1_554] | 1.90 | 0.30 |
| 4:6:255:PHE:O | 4:9:305:MET:N[1_554] | 1.90 | 0.30 |
| 4:5:340:TRP:CE2 | 4:8:122:ILE:N[1_554] | 1.90 | 0.30 |
| 4:6:13:GLY:CA | 4:9:76:ILE:O[1_554] | 1.90 | 0.30 |
| 4:5:317:ILE:N | 4:8:296:ASN:O[1_554] | 1.90 | 0.30 |
| 4:4:342:GLY:N | 4:7:117:GLU:CA[1_554] | 1.90 | 0.30 |
| 4:4:256:ARG:NH1 | 4:7:306:TYR:CD1[1_554] | 1.90 | 0.30 |
| 4:6:172:PRO:CG | 4:V:266:PHE:CG[1_554] | 1.90 | 0.30 |
| 4:4:262:PHE:CZ | 4:7:154:ASP:CB[1_554] | 1.90 | 0.30 |
| 4:6:300:SER:O | 4:9:108:ALA:C[1_554] | 1.90 | 0.30 |
| 4:6:220:ALA:N | 4:9:335:ARG:CD[1_554] | 1.90 | 0.30 |
| 4:4:344:SER:O | 4:7:367:PRO:CD[1_554] | 1.90 | 0.30 |
| 4:6:322:PRO:CB | 4:9:288:ASP:O[1_554] | 1.90 | 0.30 |
| 4:6:301:GLY:N | 4:9:107:GLU:N[1_554] | 1.90 | 0.30 |
| 4:3:372:ARG:CB | 4:7:227:MET:C[1_554] | 1.90 | 0.30 |
| 4:4:115:ASN:CB | 4:8:196:ARG:NE[1_554] | 1.90 | 0.30 |
| 4:3:367:PRO:CA | 4:7:235:SER:N[1_554] | 1.90 | 0.30 |
| 4:5:326:LYS:NZ | 4:V:45:VAL:CB[1_554] | 1.90 | 0.30 |
| 4:6:340:TRP:CE2 | 4:9:121:GLN:N[1_554] | 1.90 | 0.30 |
| 4:4:275:HIS:CG | 4:7:152:VAL:O[1_554] | 1.90 | 0.30 |
| 4:6:258:PRO:C | 4:9:155:SER:O[1_554] | 1.90 | 0.30 |
| 4:4:260:THR:N | 4:7:155:SER:CA[1_554] | 1.90 | 0.30 |
| 4:5:108:ALA:CB | 4:9:195:GLU:O[1_554] | 1.90 | 0.30 |
| 4:6:227:MET:CE | 4:9:306:TYR:C[1_554] | 1.90 | 0.30 |
| 4:5:110:LEU:CA | 4:9:195:GLU:OE1[1_554] | 1.90 | 0.30 |
| 4:4:340:TRP:CG | 4:7:118:LYS:CB[1_554] | 1.90 | 0.30 |
| 4:6:289:ILE:CA | 4:W:64:ILE:N[1_554] | 1.90 | 0.30 |
| 4:5:145:SER:CB | 4:8:372:ARG:NH2[1_554] | 1.90 | 0.30 |
| 4:5:266:PHE:CG | 4:8:261:LEU:CD2[1_554] | 1.90 | 0.30 |
| 4:5:258:PRO:CD | 4:8:302:GLY:N[1_554] | 1.90 | 0.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:16:LEU:CB | 4:7:78:ASN:CA[1_554] | 1.90 | 0.30 |
| 4:6:299:MET:CE | 4:9:138:ALA:C[1_554] | 1.90 | 0.30 |
| 4:4:313:MET:C | 4:7:142:LEU:CB[1_554] | 1.90 | 0.30 |
| 4:6:210:ARG:CZ | 4:9:33:SER:CA[1_554] | 1.90 | 0.30 |
| 4:5:18:LYS:CE | 4:8:79:TRP:CZ3[1_554] | 1.90 | 0.30 |
| 4:4:283:MET:CG | 4:7:286:ASP:CB[1_554] | 1.90 | 0.30 |
| 4:3:372:ARG:CA | 4:7:227:MET:N[1_554] | 1.91 | 0.29 |
| 4:6:28:ARG:C | 4:9:83:GLU:CD[1_554] | 1.91 | 0.29 |
| 4:6:198:TYR:CZ | 4:9:208:ILE:CG1[1_554] | 1.91 | 0.29 |
| 4:4:280:ASN:CG | 4:7:281:SER:C[1_554] | 1.91 | 0.29 |
| 4:6:20:GLY:O | 4:9:121:GLN:CG[1_554] | 1.91 | 0.29 |
| 4:6:60:SER:CB | 4:9:37:ARG:CA[1_554] | 1.91 | 0.29 |
| 4:6:11:ASP:CG | 4:9:115:ASN:CB[1_554] | 1.91 | 0.29 |
| 4:6:173:HIS:NE2 | 4:V:265:SER:O[1_554] | 1.91 | 0.29 |
| 4:5:113:LYS:N | 4:9:253:GLU:OE1[1_554] | 1.91 | 0.29 |
| 4:6:336:LYS:CB | 4:9:12:ASN:CG[1_554] | 1.91 | 0.29 |
| 4:2:325:MET:SD | 4:7:64:ILE:CG2[1_554] | 1.91 | 0.29 |
| 4:2:290:ARG:C | 4:7:40:HIS:ND1[1_554] | 1.91 | 0.29 |
| 4:4:272:ALA:N | 4:7:277:THR:OG1[1_554] | 1.91 | 0.29 |
| 4:6:367:PRO:N | 4:V:233:SER:O[1_554] | 1.91 | 0.29 |
| 4:5:192:ILE:CG1 | 4:8:213:LYS:NZ[1_554] | 1.91 | 0.29 |
| 4:3:357:ILE:CG1 | 4:7:231:ALA:O[1_554] | 1.91 | 0.29 |
| 4:4:293:LEU:O | 4:7:169:TYR:CD2[1_554] | 1.91 | 0.29 |
| 4:5:372:ARG:C | 4:9:227:MET:CG[1_554] | 1.91 | 0.29 |
| 4:5:340:TRP:CB | 4:8:119:MET:C[1_554] | 1.91 | 0.29 |
| 4:5:249:THR:O | 4:8:211:ASP:OD1[1_554] | 1.91 | 0.29 |
| 4:5:221:LEU:CA | 4:8:331:ALA:C[1_554] | 1.91 | 0.29 |
| 4:6:214:GLU:CA | 4:9:16:LEU:C[1_554] | 1.91 | 0.29 |
| 4:5:255:PHE:N | 4:8:302:GLY:O[1_554] | 1.91 | 0.29 |
| 4:4:294:TYR:CA | 4:7:166:TYR:O[1_554] | 1.91 | 0.29 |
| 4:4:337:TYR:CG | 4:7:119:MET:CB[1_554] | 1.91 | 0.29 |
| 4:5:196:ARG:NH1 | 4:8:215:LYS:N[1_554] | 1.91 | 0.29 |
| 4:5:318:THR:CB | 4:8:296:ASN:OD1[1_554] | 1.91 | 0.29 |
| 4:4:117:GLU:CA | 4:8:237:GLU:CD[1_554] | 1.91 | 0.29 |
| 4:5:280:ASN:ND2 | 4:8:284:LYS:N[1_554] | 1.91 | 0.29 |
| 4:5:259:GLU:OE1 | 4:8:309:ILE:CD1[1_554] | 1.91 | 0.29 |
| 4:4:144:ALA:N | 4:7:371:HIS:CB[1_554] | 1.91 | 0.29 |
| 4:5:316:GLU:OE1 | 4:8:297:ASN:CA[1_554] | 1.91 | 0.29 |
| 4:5:188:TYR:CA | 4:8:185:LEU:N[1_554] | 1.91 | 0.29 |
| 4:4:115:ASN:N | 4:8:249:THR:C[1_554] | 1.91 | 0.29 |
| 4:3:75:ILE:O | 4:7:197:GLY:O[1_554] | 1.91 | 0.29 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:19:ALA:C | 4:8:122:ILE:CG1[1_554] | 1.91 | 0.29 |
| 4:4:335:ARG:O | 4:7:119:MET:SD[1_554] | 1.91 | 0.29 |
| 4:4:309:ILE:CG1 | 4:7:137:GLN:CB[1_554] | 1.91 | 0.29 |
| 4:6:113:LYS:O | 4:V:252:ASN:N[1_554] | 1.91 | 0.29 |
| 4:3:113:LYS:CD | 4:7:254:ARG:CA[1_554] | 1.91 | 0.29 |
| 4:4:210:ARG:CZ | 4:7:70:PRO:CD[1_554] | 1.91 | 0.29 |
| 4:5:281:SER:CB | 4:8:171:LEU:O[1_554] | 1.91 | 0.29 |
| 4:5:181:ALA:CA | 4:8:159:VAL:CB[1_554] | 1.91 | 0.29 |
| 4:5:334:GLU:CA | 4:8:105:LEU:CB[1_554] | 1.91 | 0.29 |
| 4:5:349:LEU:CA | 4:8:364:GLU:C[1_554] | 1.91 | 0.29 |
| 4:6:29:ALA:CA | 4:9:83:GLU:CD[1_554] | 1.91 | 0.29 |
| 4:6:151:ILE:CD1 | 4:9:171:LEU:CB[1_554] | 1.91 | 0.29 |
| 4:5:340:TRP:CZ2 | 4:8:121:GLN:CB[1_554] | 1.91 | 0.29 |
| 4:5:207:GLU:O | 4:8:34:ILE:CD1[1_554] | 1.91 | 0.29 |
| 4:6:159:VAL:CB | 4:9:177:ARG:NH1[1_554] | 1.91 | 0.29 |
| 4:6:341:ILE:CB | 4:9:132:MET:SD[1_554] | 1.91 | 0.29 |
| 4:5:157:ASP:CG | 4:8:71:ILE:C[1_554] | 1.91 | 0.29 |
| 4:5:276:GLU:CA | 4:8:151:ILE:CD1[1_554] | 1.91 | 0.29 |
| 4:5:289:ILE:CG2 | 4:V:39:ARG:CZ[1_554] | 1.91 | 0.29 |
| 4:4:258:PRO:C | 4:7:155:SER:CA[1_554] | 1.91 | 0.29 |
| 4:3:173:HIS:CB | 4:7:267:ILE:CG2[1_554] | 1.91 | 0.29 |
| 4:5:261:LEU:O | 4:8:161:HIS:O[1_554] | 1.91 | 0.29 |
| 4:4:147:ARG:NE | 4:7:372:ARG:CD[1_554] | 1.91 | 0.29 |
| 4:4:110:LEU:CG | 4:8:192:ILE:N[1_554] | 1.91 | 0.29 |
| 4:5:140:LEU:C | 4:8:116:ARG:CD[1_554] | 1.91 | 0.29 |
| 4:4:211:ASP:CA | 4:7:32:PRO:CA[1_554] | 1.91 | 0.29 |
| 4:4:159:VAL:C | 4:7:177:ARG:CZ[1_554] | 1.91 | 0.29 |
| 4:6:207:GLU:CD | 4:9:67:LEU:CD2[1_554] | 1.91 | 0.29 |
| 4:5:154:ASP:OD1 | 4:8:108:ALA:O[1_554] | 1.91 | 0.29 |
| 4:4:210:ARG:NE | 4:7:69:TYR:CA[1_554] | 1.91 | 0.29 |
| 4:4:115:ASN:ND2 | 4:8:198:TYR:OH[1_554] | 1.91 | 0.29 |
| 4:4:340:TRP:CZ2 | 4:7:121:GLN:OE1[1_554] | 1.91 | 0.29 |
| 4:5:313:MET:CB | 4:8:152:VAL:CB[1_554] | 1.91 | 0.29 |
| 4:6:192:ILE:CG1 | 4:9:213:LYS:NZ[1_554] | 1.91 | 0.29 |
| 4:5:136:ILE:CB | 4:8:113:LYS:CG[1_554] | 1.91 | 0.29 |
| 4:4:113:LYS:NZ | 4:8:254:ARG:O[1_554] | 1.91 | 0.29 |
| 4:5:256:ARG:CB | 4:8:306:TYR:CE2[1_554] | 1.91 | 0.29 |
| 4:5:196:ARG:CB | 4:8:212:ILE:C[1_554] | 1.91 | 0.29 |
| 4:5:253:GLU:CG | 4:8:214:GLU:CG[1_554] | 1.91 | 0.29 |
| 4:5:198:TYR:CB | 4:8:208:ILE:N[1_554] | 1.91 | 0.29 |
| 4:4:256:ARG:NH2 | 4:7:213:LYS:C[1_554] | 1.91 | 0.29 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:237:GLU:OE2 | 4:8:215:LYS:CG[1_554] | 1.91 | 0.29 |
| 4:6:256:ARG:C | 4:9:303:THR:C[1_554] | 1.91 | 0.29 |
| 4:4:204:ALA:C | 4:7:62:ARG:CD[1_554] | 1.91 | 0.29 |
| 4:6:24:ASP:O | 4:9:124:PHE:CA[1_554] | 1.91 | 0.29 |
| 4:5:293:LEU:CD1 | 4:8:169:TYR:CE2[1_554] | 1.91 | 0.29 |
| 4:4:267:ILE:C | 4:7:180:LEU:CG[1_554] | 1.91 | 0.29 |
| 4:5:277:THR:OG1 | 4:8:176:MET:CB[1_554] | 1.91 | 0.29 |
| 4:3:110:LEU:CA | 4:7:192:ILE:C[1_554] | 1.91 | 0.29 |
| 4:6:255:PHE:CE1 | 4:9:305:MET:CA[1_554] | 1.91 | 0.29 |
| 4:4:143:TYR:O | 4:7:369:ILE:O[1_554] | 1.91 | 0.29 |
| 4:5:279:TYR:CG | 4:8:293:LEU:CD2[1_554] | 1.91 | 0.29 |
| 4:5:256:ARG:C | 4:8:303:THR:O[1_554] | 1.91 | 0.29 |
| 4:5:136:ILE:CA | 4:8:113:LYS:CB[1_554] | 1.91 | 0.29 |
| 4:5:326:LYS:CG | 4:8:167:GLU:CD[1_554] | 1.91 | 0.29 |
| 4:5:249:THR:CG2 | 4:8:211:ASP:OD1[1_554] | 1.91 | 0.29 |
| 4:4:345:ILE:CA | 4:7:367:PRO:CD[1_554] | 1.91 | 0.29 |
| 4:6:276:GLU:O | 4:9:281:SER:OG[1_554] | 1.91 | 0.29 |
| 4:5:18:LYS:CG | 4:8:79:TRP:CE3[1_554] | 1.91 | 0.29 |
| 4:4:173:HIS:CD2 | 4:8:267:ILE:N[1_554] | 1.91 | 0.29 |
| 4:5:340:TRP:CB | 4:8:120:THR:N[1_554] | 1.91 | 0.29 |
| 4:5:372:ARG:CA | 4:9:227:MET:O[1_554] | 1.91 | 0.29 |
| 4:5:23:GLY:CA | 4:8:362:TYR:CE2[1_554] | 1.91 | 0.29 |
| 4:4:334:GLU:C | 4:7:105:LEU:CD1[1_554] | 1.91 | 0.29 |
| 4:3:115:ASN:CB | 4:7:249:THR:C[1_554] | 1.91 | 0.29 |
| 4:4:262:PHE:N | 4:7:154:ASP:O[1_554] | 1.91 | 0.29 |
| 4:5:311:ASP:OD1 | 4:8:144:ALA:CA[1_554] | 1.91 | 0.29 |
| 4:5:316:GLU:C | 4:8:151:ILE:N[1_554] | 1.91 | 0.29 |
| 4:4:112:PRO:CB | 4:8:193:LEU:CD1[1_554] | 1.91 | 0.29 |
| 4:4:282:ILE:N | 4:7:173:HIS:CE1[1_554] | 1.91 | 0.29 |
| 4:6:111:ASN:C | 4:V:192:ILE:O[1_554] | 1.91 | 0.29 |
| 4:5:11:ASP:CB | 4:8:118:LYS:CB[1_554] | 1.91 | 0.29 |
| 4:5:221:LEU:CG | 4:8:332:PRO:N[1_554] | 1.91 | 0.29 |
| 4:4:158:GLY:C | 4:7:177:ARG:NH2[1_554] | 1.91 | 0.29 |
| 4:6:117:GLU:CD | 4:V:236:LEU:CG[1_554] | 1.91 | 0.29 |
| 4:5:194:THR:O | 4:8:209:VAL:CB[1_554] | 1.91 | 0.29 |
| 4:5:312:ARG:O | 4:8:298:VAL:CG1[1_554] | 1.92 | 0.28 |
| 4:4:195:GLU:CA | 4:7:209:VAL:O[1_554] | 1.92 | 0.28 |
| 4:5:274:ILE:C | 4:8:162:ASN:O[1_554] | 1.92 | 0.28 |
| 4:4:311:ASP:OD2 | 4:7:342:GLY:N[1_554] | 1.92 | 0.28 |
| 4:5:191:LYS:CB | 4:8:188:TYR:N[1_554] | 1.92 | 0.28 |
| 4:4:73:HIS:CG | 4:8:199:SER:OG[1_554] | 1.92 | 0.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:162:ASN:CG | 4:8:175:ILE:CD1[1_554] | 1.92 | 0.28 |
| 4:4:199:SER:N | 4:7:206:ARG:N[1_554] | 1.92 | 0.28 |
| 4:6:210:ARG:NH2 | 4:9:33:SER:CA[1_554] | 1.92 | 0.28 |
| 4:6:173:HIS:N | 4:V:267:ILE:CA[1_554] | 1.92 | 0.28 |
| 4:5:256:ARG:O | 4:8:303:THR:O[1_554] | 1.92 | 0.28 |
| 4:6:20:GLY:N | 4:9:121:GLN:NE2[1_554] | 1.92 | 0.28 |
| 4:5:302:GLY:C | 4:8:12:ASN:O[1_554] | 1.92 | 0.28 |
| 4:4:256:ARG:O | 4:7:303:THR:N[1_554] | 1.92 | 0.28 |
| 4:4:193:LEU:CG | 4:7:210:ARG:CG[1_554] | 1.92 | 0.28 |
| 4:4:154:ASP:O | 4:7:110:LEU:N[1_554] | 1.92 | 0.28 |
| 4:5:166:TYR:CZ | 4:V:39:ARG:O[1_554] | 1.92 | 0.28 |
| 4:4:304:THR:CA | 4:7:137:GLN:OE1[1_554] | 1.92 | 0.28 |
| 4:6:187:ASP:C | 4:9:183:ARG:CA[1_554] | 1.92 | 0.28 |
| 4:6:317:ILE:N | 4:9:150:GLY:CA[1_554] | 1.92 | 0.28 |
| 4:6:319:ALA:CA | 4:9:295:ALA:CA[1_554] | 1.92 | 0.28 |
| 4:4:337:TYR:CB | 4:7:119:MET:C[1_554] | 1.92 | 0.28 |
| 4:3:173:HIS:CG | 4:7:264:PRO:O[1_554] | 1.92 | 0.28 |
| 4:4:272:ALA:N | 4:7:277:THR:CG2[1_554] | 1.92 | 0.28 |
| 4:6:143:TYR:CB | 4:9:372:ARG:CB[1_554] | 1.92 | 0.28 |
| 4:5:301:GLY:C | 4:8:137:GLN:NE2[1_554] | 1.92 | 0.28 |
| 4:6:276:GLU:OE1 | 4:9:278:THR:C[1_554] | 1.92 | 0.28 |
| 4:6:297:ASN:ND2 | 4:9:165:ILE:CD1[1_554] | 1.92 | 0.28 |
| 4:4:294:TYR:O | 4:7:168:GLY:C[1_554] | 1.92 | 0.28 |
| 4:6:194:THR:CG2 | 4:9:209:VAL:CG1[1_554] | 1.92 | 0.28 |
| 4:4:188:TYR:CE2 | 4:7:182:GLY:N[1_554] | 1.92 | 0.28 |
| 4:5:115:ASN:CB | 4:9:196:ARG:NH1[1_554] | 1.92 | 0.28 |
| 4:6:315:LYS:CG | 4:9:147:ARG:NH1[1_554] | 1.92 | 0.28 |
| 4:5:301:GLY:N | 4:8:107:GLU:CB[1_554] | 1.92 | 0.28 |
| 4:6:277:THR:O | 4:9:174:ALA:CA[1_554] | 1.92 | 0.28 |
| 4:5:320:LEU:N | 4:8:292:ASP:C[1_554] | 1.92 | 0.28 |
| 4:5:15:GLY:O | 4:8:78:ASN:N[1_554] | 1.92 | 0.28 |
| 4:5:311:ASP:C | 4:8:298:VAL:CG1[1_554] | 1.92 | 0.28 |
| 4:4:253:GLU:OE2 | 4:7:214:GLU:CG[1_554] | 1.92 | 0.28 |
| 4:6:18:LYS:CD | 4:9:79:TRP:CZ3[1_554] | 1.92 | 0.28 |
| 4:4:204:ALA:O | 4:7:62:ARG:CD[1_554] | 1.92 | 0.28 |
| 4:5:338:SER:OG | 4:8:134:VAL:C[1_554] | 1.92 | 0.28 |
| 4:6:160:THR:N | 4:9:177:ARG:NH1[1_554] | 1.92 | 0.28 |
| 4:4:227:MET:CE | 4:7:306:TYR:C[1_554] | 1.92 | 0.28 |
| 4:3:112:PRO:C | 4:7:253:GLU:CG[1_554] | 1.92 | 0.28 |
| 4:4:211:ASP:OD2 | 4:7:55:GLY:CA[1_554] | 1.92 | 0.28 |
| 4:5:295:ALA:N | 4:8:166:TYR:C[1_554] | 1.92 | 0.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:323:SER:CA | 4:7:44:MET:CE[1_554] | 1.92 | 0.28 |
| 4:2:287:ILE:O | 4:7:39:ARG:NE[1_554] | 1.92 | 0.28 |
| 4:6:11:ASP:CB | 4:9:118:LYS:CB[1_554] | 1.92 | 0.28 |
| 4:5:289:ILE:N | 4:V:63:GLY:CA[1_554] | 1.92 | 0.28 |
| 4:6:177:ARG:NH2 | 4:V:194:THR:CG2[1_554] | 1.92 | 0.28 |
| 4:6:161:HIS:CA | 4:9:110:LEU:CB[1_554] | 1.92 | 0.28 |
| 4:5:290:ARG:CD | 4:8:286:ASP:CB[1_554] | 1.92 | 0.28 |
| 4:6:15:GLY:C | 4:9:77:THR:N[1_554] | 1.92 | 0.28 |
| 4:4:218:TYR:CD2 | 4:7:337:TYR:CE1[1_554] | 1.92 | 0.28 |
| 4:4:113:LYS:O | 4:8:251:GLY:O[1_554] | 1.92 | 0.28 |
| 4:6:319:ALA:N | 4:9:296:ASN:N[1_554] | 1.92 | 0.28 |
| 4:6:186:THR:CB | 4:9:157:ASP:OD2[1_554] | 1.92 | 0.28 |
| 4:5:140:LEU:N | 4:8:371:HIS:NE2[1_554] | 1.92 | 0.28 |
| 4:6:279:TYR:CA | 4:9:285:CYS:SG[1_554] | 1.92 | 0.28 |
| 4:4:261:LEU:C | 4:7:161:HIS:N[1_554] | 1.92 | 0.28 |
| 4:5:18:LYS:CE | 4:8:79:TRP:CZ2[1_554] | 1.92 | 0.28 |
| 4:5:31:PHE:C | 4:8:78:ASN:O[1_554] | 1.92 | 0.28 |
| 4:6:300:SER:CA | 4:9:107:GLU:CG[1_554] | 1.92 | 0.28 |
| 4:6:259:GLU:OE2 | 4:9:309:ILE:CD1[1_554] | 1.92 | 0.28 |
| 4:5:313:MET:O | 4:8:142:LEU:CD1[1_554] | 1.92 | 0.28 |
| 4:6:223:PHE:CD2 | 4:9:304:THR:CB[1_554] | 1.92 | 0.28 |
| 4:4:327:ILE:N | 4:7:167:GLU:C[1_554] | 1.92 | 0.28 |
| 4:4:357:ILE:CD1 | 4:8:232:SER:CA[1_554] | 1.92 | 0.28 |
| 4:4:275:HIS:N | 4:7:162:ASN:CA[1_554] | 1.92 | 0.28 |
| 4:5:184:ASP:CG | 4:8:73:HIS:CE1[1_554] | 1.92 | 0.28 |
| 4:6:293:LEU:CD1 | 4:9:169:TYR:CE2[1_554] | 1.92 | 0.28 |
| 4:5:337:TYR:OH | 4:8:86:TRP:CD1[1_554] | 1.92 | 0.28 |
| 4:6:157:ASP:CG | 4:9:72:GLU:CB[1_554] | 1.92 | 0.28 |
| 4:5:114:ALA:N | 4:9:252:ASN:N[1_554] | 1.92 | 0.28 |
| 4:6:173:HIS:NE2 | 4:V:265:SER:CA[1_554] | 1.92 | 0.28 |
| 4:6:186:THR:CG2 | 4:9:183:ARG:NE[1_554] | 1.92 | 0.28 |
| 4:6:371:HIS:CB | 4:V:230:ALA:CA[1_554] | 1.92 | 0.28 |
| 4:4:17:VAL:O | 4:7:79:TRP:CB[1_554] | 1.92 | 0.28 |
| 4:6:198:TYR:CG | 4:9:209:VAL:N[1_554] | 1.92 | 0.28 |
| 4:6:140:LEU:CG | 4:9:371:HIS:ND1[1_554] | 1.92 | 0.28 |
| 4:5:140:LEU:CB | 4:8:371:HIS:CG[1_554] | 1.92 | 0.28 |
| 4:4:299:MET:SD | 4:7:136:ILE:CB[1_554] | 1.92 | 0.28 |
| 4:6:210:ARG:C | 4:9:15:GLY:O[1_554] | 1.92 | 0.28 |
| 4:4:312:ARG:NH2 | 4:7:299:MET:CA[1_554] | 1.92 | 0.28 |
| 4:4:204:ALA:CA | 4:7:62:ARG:O[1_554] | 1.92 | 0.28 |
| 4:5:280:ASN:CB | 4:8:281:SER:O[1_554] | 1.92 | 0.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:196:ARG:CG | 4:7:211:ASP:N[1_554] | 1.92 | 0.28 |
| 4:6:331:ALA:CB | 4:9:140:LEU:CD2[1_554] | 1.92 | 0.28 |
| 4:4:317:ILE:CG1 | 4:7:165:ILE:CA[1_554] | 1.92 | 0.28 |
| 4:5:304:THR:CA | 4:8:137:GLN:CB[1_554] | 1.92 | 0.28 |
| 4:5:24:ASP:O | 4:8:124:PHE:CA[1_554] | 1.92 | 0.28 |
| 4:6:299:MET:CE | 4:9:140:LEU:N[1_554] | 1.92 | 0.28 |
| 4:4:114:ALA:N | 4:8:250:ILE:CB[1_554] | 1.92 | 0.28 |
| 4:5:286:ASP:OD2 | 4:V:39:ARG:NH1[1_554] | 1.92 | 0.28 |
| 4:3:173:HIS:CA | 4:7:267:ILE:N[1_554] | 1.92 | 0.28 |
| 4:5:17:VAL:CB | 4:8:79:TRP:CB[1_554] | 1.92 | 0.28 |
| 4:4:319:ALA:O | 4:7:292:ASP:C[1_554] | 1.92 | 0.28 |
| 4:6:106:THR:CB | 4:9:114:ALA:N[1_554] | 1.92 | 0.28 |
| 4:4:304:THR:CG2 | 4:7:107:GLU:O[1_554] | 1.92 | 0.28 |
| 4:5:256:ARG:NE | 4:8:306:TYR:CE1[1_554] | 1.92 | 0.28 |
| 4:5:188:TYR:CB | 4:8:181:ALA:C[1_554] | 1.92 | 0.28 |
| 4:5:157:ASP:O | 4:8:72:GLU:O[1_554] | 1.92 | 0.28 |
| 4:4:153:LEU:N | 4:7:109:PRO:O[1_554] | 1.92 | 0.28 |
| 4:4:144:ALA:CA | 4:7:370:VAL:CA[1_554] | 1.92 | 0.28 |
| 4:5:242:LEU:CD2 | 4:8:207:GLU:CD[1_554] | 1.92 | 0.28 |
| 4:4:18:LYS:CD | 4:7:79:TRP:CD1[1_554] | 1.92 | 0.28 |
| 4:4:164:PRO:CG | 4:7:172:PRO:CG[1_554] | 1.92 | 0.28 |
| 4:6:157:ASP:CB | 4:9:72:GLU:CA[1_554] | 1.92 | 0.28 |
| 4:5:336:LYS:CB | 4:8:12:ASN:CG[1_554] | 1.92 | 0.28 |
| 4:6:297:ASN:CB | 4:9:165:ILE:CG2[1_554] | 1.93 | 0.27 |
| 4:3:166:TYR:OH | 4:8:39:ARG:C[1_554] | 1.93 | 0.27 |
| 4:3:367:PRO:N | 4:7:236:LEU:N[1_554] | 1.93 | 0.27 |
| 4:4:191:LYS:CB | 4:7:186:THR:CA[1_554] | 1.93 | 0.27 |
| 4:5:223:PHE:CE2 | 4:8:304:THR:CG2[1_554] | 1.93 | 0.27 |
| 4:4:320:LEU:CG | 4:7:293:LEU:CG[1_554] | 1.93 | 0.27 |
| 4:6:215:LYS:N | 4:9:16:LEU:CB[1_554] | 1.93 | 0.27 |
| 4:6:106:THR:CA | 4:9:114:ALA:CA[1_554] | 1.93 | 0.27 |
| 4:6:254:ARG:CZ | 4:9:336:LYS:CE[1_554] | 1.93 | 0.27 |
| 4:6:33:SER:N | 4:9:78:ASN:CB[1_554] | 1.93 | 0.27 |
| 1:A:542:PHE:CE1 | 4:5:328:LYS:NZ[1_556] | 1.93 | 0.27 |
| 4:5:178:LEU:CD2 | 4:8:176:MET:C[1_554] | 1.93 | 0.27 |
| 4:4:310:ALA:C | 4:7:140:LEU:O[1_554] | 1.93 | 0.27 |
| 4:3:372:ARG:CG | 4:7:227:MET:N[1_554] | 1.93 | 0.27 |
| 4:4:279:TYR:CE1 | 4:7:293:LEU:CD2[1_554] | 1.93 | 0.27 |
| 4:4:313:MET:CG | 4:7:138:ALA:C[1_554] | 1.93 | 0.27 |
| 4:6:59:GLN:CA | 4:9:68:LYS:CD[1_554] | 1.93 | 0.27 |
| 4:3:113:LYS:C | 4:7:251:GLY:N[1_554] | 1.93 | 0.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:341:ILE:C | 4:7:367:PRO:CB[1_554] | 1.93 | 0.27 |
| 4:6:330:ILE:O | 4:9:139:VAL:CG1[1_554] | 1.93 | 0.27 |
| 4:5:14:SER:O | 4:8:77:THR:OG1[1_554] | 1.93 | 0.27 |
| 4:4:178:LEU:O | 4:7:177:ARG:NE[1_554] | 1.93 | 0.27 |
| 4:4:117:GLU:N | 4:8:251:GLY:CA[1_554] | 1.93 | 0.27 |
| 4:4:325:MET:CB | 4:7:166:TYR:OH[1_554] | 1.93 | 0.27 |
| 4:4:257:CYS:N | 4:7:303:THR:OG1[1_554] | 1.93 | 0.27 |
| 4:6:310:ALA:N | 4:9:141:SER:N[1_554] | 1.93 | 0.27 |
| 4:4:310:ALA:CA | 4:7:140:LEU:CB[1_554] | 1.93 | 0.27 |
| 4:4:140:LEU:N | 4:7:113:LYS:CB[1_554] | 1.93 | 0.27 |
| 4:4:338:SER:OG | 4:7:116:ARG:CG[1_554] | 1.93 | 0.27 |
| 4:6:184:ASP:N | 4:9:73:HIS:CE1[1_554] | 1.93 | 0.27 |
| 4:5:289:ILE:CG2 | 4:V:39:ARG:NH1[1_554] | 1.93 | 0.27 |
| 4:6:18:LYS:C | 4:9:122:ILE:CD1[1_554] | 1.93 | 0.27 |
| 4:5:281:SER:OG | 4:8:173:HIS:C[1_554] | 1.93 | 0.27 |
| 4:6:312:ARG:CB | 4:9:299:MET:O[1_554] | 1.93 | 0.27 |
| 4:4:117:GLU:CG | 4:8:237:GLU:CA[1_554] | 1.93 | 0.27 |
| 4:6:314:GLN:CG | 4:9:142:LEU:C[1_554] | 1.93 | 0.27 |
| 4:3:372:ARG:NE | 4:7:227:MET:O[1_554] | 1.93 | 0.27 |
| 4:6:21:PHE:CB | 4:9:125:GLU:CB[1_554] | 1.93 | 0.27 |
| 4:4:250:ILE:CG1 | 4:7:210:ARG:NH1[1_554] | 1.93 | 0.27 |
| 4:4:327:ILE:C | 4:7:168:GLY:CA[1_554] | 1.93 | 0.27 |
| 4:4:334:GLU:CA | 4:7:105:LEU:CG[1_554] | 1.93 | 0.27 |
| 4:5:154:ASP:CB | 4:8:110:LEU:N[1_554] | 1.93 | 0.27 |
| 4:5:163:VAL:CA | 4:8:172:PRO:CB[1_554] | 1.93 | 0.27 |
| 4:4:214:GLU:CB | 4:7:33:SER:OG[1_554] | 1.93 | 0.27 |
| 4:5:173:HIS:ND1 | 4:9:266:PHE:CA[1_554] | 1.93 | 0.27 |
| 4:4:257:CYS:CA | 4:7:156:GLY:O[1_554] | 1.93 | 0.27 |
| 4:5:258:PRO:CD | 4:8:302:GLY:C[1_554] | 1.93 | 0.27 |
| 4:4:264:PRO:CA | 4:7:178:LEU:CD2[1_554] | 1.93 | 0.27 |
| 4:6:325:MET:CE | 4:9:166:TYR:OH[1_554] | 1.93 | 0.27 |
| 4:4:191:LYS:CD | 4:7:185:LEU:CA[1_554] | 1.93 | 0.27 |
| 4:4:188:TYR:OH | 4:7:306:TYR:OH[1_554] | 1.93 | 0.27 |
| 4:4:274:ILE:CA | 4:7:162:ASN:C[1_554] | 1.93 | 0.27 |
| 4:6:263:GLN:CB | 4:9:274:ILE:CG1[1_554] | 1.93 | 0.27 |
| 4:4:270:GLU:CB | 4:7:272:ALA:CB[1_554] | 1.93 | 0.27 |
| 4:5:177:ARG:NH1 | 4:9:194:THR:CG2[1_554] | 1.93 | 0.27 |
| 4:6:157:ASP:N | 4:9:74:GLY:C[1_554] | 1.93 | 0.27 |
| 4:5:339:VAL:CG2 | 4:8:111:ASN:ND2[1_554] | 1.93 | 0.27 |
| 4:5:369:ILE:CA | 4:9:228:ALA:O[1_554] | 1.93 | 0.27 |
| 4:5:75:ILE:CD1 | 4:9:195:GLU:C[1_554] | 1.93 | 0.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:337:TYR:OH | 4:8:86:TRP:CZ2[1_554] | 1.93 | 0.27 |
| 4:6:15:GLY:O | 4:9:78:ASN:N[1_554] | 1.93 | 0.27 |
| 4:5:340:TRP:CD2 | 4:8:121:GLN:N[1_554] | 1.93 | 0.27 |
| 4:5:178:LEU:CD2 | 4:8:176:MET:O[1_554] | 1.93 | 0.27 |
| 4:5:109:PRO:CA | 4:9:195:GLU:CG[1_554] | 1.93 | 0.27 |
| 4:5:276:GLU:OE2 | 4:8:278:THR:N[1_554] | 1.93 | 0.27 |
| 4:5:166:TYR:CD2 | 4:V:40:HIS:CE1[1_554] | 1.93 | 0.27 |
| 4:5:110:LEU:N | 4:9:195:GLU:CG[1_554] | 1.93 | 0.27 |
| 4:6:307:PRO:CA | 4:9:338:SER:N[1_554] | 1.93 | 0.27 |
| 4:4:188:TYR:CB | 4:7:183:ARG:N[1_554] | 1.93 | 0.27 |
| 4:2:324:THR:CA | 4:7:44:MET:SD[1_554] | 1.93 | 0.27 |
| 4:4:272:ALA:C | 4:7:162:ASN:OD1[1_554] | 1.93 | 0.27 |
| 4:4:214:GLU:OE2 | 4:7:33:SER:OG[1_554] | 1.93 | 0.27 |
| 4:5:281:SER:OG | 4:8:174:ALA:N[1_554] | 1.93 | 0.27 |
| 4:6:181:ALA:C | 4:9:159:VAL:N[1_554] | 1.93 | 0.27 |
| 4:5:268:GLY:N | 4:8:264:PRO:CA[1_554] | 1.93 | 0.27 |
| 4:5:173:HIS:O | 4:9:267:ILE:CA[1_554] | 1.93 | 0.27 |
| 4:4:335:ARG:NH1 | 4:7:106:THR:CA[1_554] | 1.93 | 0.27 |
| 4:3:173:HIS:C | 4:7:267:ILE:C[1_554] | 1.93 | 0.27 |
| 4:4:178:LEU:CD2 | 4:7:176:MET:O[1_554] | 1.93 | 0.27 |
| 4:4:334:GLU:N | 4:7:105:LEU:CB[1_554] | 1.93 | 0.27 |
| 4:5:348:SER:CA | 4:8:362:TYR:O[1_554] | 1.93 | 0.27 |
| 4:6:349:LEU:CA | 4:9:365:ALA:CB[1_554] | 1.93 | 0.27 |
| 4:4:267:ILE:CG1 | 4:7:180:LEU:CA[1_554] | 1.93 | 0.27 |
| 4:5:332:PRO:O | 4:8:104:LEU:CD2[1_554] | 1.93 | 0.27 |
| 4:5:314:GLN:NE2 | 4:8:148:THR:N[1_554] | 1.93 | 0.27 |
| 4:6:213:LYS:CG | 4:9:157:ASP:CB[1_554] | 1.93 | 0.27 |
| 4:6:339:VAL:O | 4:9:116:ARG:CA[1_554] | 1.93 | 0.27 |
| 4:5:288:ASP:C | 4:V:63:GLY:O[1_554] | 1.93 | 0.27 |
| 4:4:190:MET:SD | 4:7:206:ARG:NH2[1_554] | 1.93 | 0.27 |
| 4:6:110:LEU:CB | 4:V:192:ILE:N[1_554] | 1.93 | 0.27 |
| 4:4:24:ASP:CG | 4:7:125:GLU:OE1[1_554] | 1.93 | 0.27 |
| 4:5:372:ARG:C | 4:9:227:MET:N[1_554] | 1.93 | 0.27 |
| 4:6:142:LEU:C | 4:9:372:ARG:CB[1_554] | 1.93 | 0.27 |
| 4:5:340:TRP:CE3 | 4:8:121:GLN:N[1_554] | 1.93 | 0.27 |
| 4:5:154:ASP:C | 4:8:108:ALA:C[1_554] | 1.93 | 0.27 |
| 4:4:141:SER:C | 4:7:371:HIS:ND1[1_554] | 1.93 | 0.27 |
| 4:6:327:ILE:CG1 | 4:9:149:THR:CG2[1_554] | 1.93 | 0.27 |
| 4:6:21:PHE:N | 4:9:125:GLU:CB[1_554] | 1.93 | 0.27 |
| 4:4:345:ILE:CA | 4:7:366:GLY:O[1_554] | 1.93 | 0.27 |
| 4:5:269:MET:N | 4:8:264:PRO:CG[1_554] | 1.93 | 0.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:343:GLY:CA | 4:8:367:PRO:O[1_554] | 1.93 | 0.27 |
| 4:6:278:THR:C | 4:9:164:PRO:CD[1_554] | 1.93 | 0.27 |
| 4:6:18:LYS:N | 4:9:79:TRP:CE2[1_554] | 1.93 | 0.27 |
| 4:6:25:ASP:OD1 | 4:9:131:ALA:N[1_554] | 1.93 | 0.27 |
| 4:6:322:PRO:N | 4:9:291:LYS:NZ[1_554] | 1.93 | 0.27 |
| 4:5:258:PRO:CB | 4:8:301:GLY:CA[1_554] | 1.93 | 0.27 |
| 4:6:112:PRO:CA | 4:V:253:GLU:OE1[1_554] | 1.93 | 0.27 |
| 4:3:116:ARG:N | 4:7:196:ARG:CZ[1_554] | 1.93 | 0.27 |
| 4:3:115:ASN:N | 4:7:249:THR:C[1_554] | 1.93 | 0.27 |
| 4:6:32:PRO:CA | 4:9:78:ASN:CG[1_554] | 1.93 | 0.27 |
| 4:6:141:SER:N | 4:9:116:ARG:NE[1_554] | 1.93 | 0.27 |
| 4:3:75:ILE:CG2 | 4:7:198:TYR:CB[1_554] | 1.93 | 0.27 |
| 4:6:288:ASP:N | 4:W:62:ARG:C[1_554] | 1.93 | 0.27 |
| 4:5:190:MET:O | 4:8:186:THR:CB[1_554] | 1.93 | 0.27 |
| 4:4:210:ARG:CZ | 4:7:33:SER:O[1_554] | 1.93 | 0.27 |
| 4:5:339:VAL:O | 4:8:116:ARG:CA[1_554] | 1.93 | 0.27 |
| 4:5:269:MET:SD | 4:8:178:LEU:CD1[1_554] | 1.94 | 0.26 |
| 4:5:199:SER:CB | 4:8:205:GLU:C[1_554] | 1.94 | 0.26 |
| 4:5:59:GLN:CB | 4:8:68:LYS:NZ[1_554] | 1.94 | 0.26 |
| 4:4:299:MET:CE | 4:7:137:GLN:N[1_554] | 1.94 | 0.26 |
| 4:4:76:ILE:N | 4:8:198:TYR:CE1[1_554] | 1.94 | 0.26 |
| 4:6:205:GLU:C | 4:9:62:ARG:NE[1_554] | 1.94 | 0.26 |
| 4:4:357:ILE:CB | 4:8:232:SER:N[1_554] | 1.94 | 0.26 |
| 4:5:276:GLU:O | 4:8:281:SER:C[1_554] | 1.94 | 0.26 |
| 4:5:211:ASP:CB | 4:8:32:PRO:CD[1_554] | 1.94 | 0.26 |
| 4:6:215:LYS:CG | 4:9:30:VAL:O[1_554] | 1.94 | 0.26 |
| 4:5:110:LEU:CD2 | 4:9:191:LYS:NZ[1_554] | 1.94 | 0.26 |
| 4:4:275:HIS:O | 4:7:164:PRO:CG[1_554] | 1.94 | 0.26 |
| 4:5:243:PRO:CB | 4:8:60:SER:CB[1_554] | 1.94 | 0.26 |
| 4:5:157:ASP:C | 4:8:73:HIS:N[1_554] | 1.94 | 0.26 |
| 4:6:112:PRO:N | 4:V:192:ILE:O[1_554] | 1.94 | 0.26 |
| 4:4:137:GLN:O | 4:7:113:LYS:C[1_554] | 1.94 | 0.26 |
| 4:4:267:ILE:CG2 | 4:7:180:LEU:C[1_554] | 1.94 | 0.26 |
| 4:5:314:GLN:CB | 4:8:142:LEU:O[1_554] | 1.94 | 0.26 |
| 4:6:273:GLY:O | 4:9:162:ASN:ND2[1_554] | 1.94 | 0.26 |
| 4:6:340:TRP:CZ2 | 4:9:121:GLN:N[1_554] | 1.94 | 0.26 |
| 4:6:263:GLN:O | 4:9:274:ILE:CG1[1_554] | 1.94 | 0.26 |
| 4:5:288:ASP:N | 4:V:63:GLY:N[1_554] | 1.94 | 0.26 |
| 4:3:112:PRO:CD | 4:7:193:LEU:CG[1_554] | 1.94 | 0.26 |
| 4:5:141:SER:OG | 4:8:107:GLU:OE2[1_554] | 1.94 | 0.26 |
| 4:6:218:TYR:CE1 | 4:9:337:TYR:CE1[1_554] | 1.94 | 0.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:142:LEU:N | 4:9:116:ARG:NH1[1_554] | 1.94 | 0.26 |
| 4:5:319:ALA:CA | 4:8:292:ASP:O[1_554] | 1.94 | 0.26 |
| 4:6:219:VAL:CA | 4:9:335:ARG:O[1_554] | 1.94 | 0.26 |
| 4:4:261:LEU:CA | 4:7:160:THR:CA[1_554] | 1.94 | 0.26 |
| 4:6:340:TRP:C | 4:9:120:THR:N[1_554] | 1.94 | 0.26 |
| 4:5:196:ARG:CB | 4:8:213:LYS:N[1_554] | 1.94 | 0.26 |
| 4:6:184:ASP:CG | 4:9:73:HIS:CE1[1_554] | 1.94 | 0.26 |
| 4:5:26:ALA:CB | 4:8:123:MET:CG[1_554] | 1.94 | 0.26 |
| 4:6:215:LYS:N | 4:9:16:LEU:CD1[1_554] | 1.94 | 0.26 |
| 4:5:189:LEU:CA | 4:8:182:GLY:C[1_554] | 1.94 | 0.26 |
| 4:4:140:LEU:C | 4:7:371:HIS:CE1[1_554] | 1.94 | 0.26 |
| 4:6:311:ASP:CA | 4:9:141:SER:O[1_554] | 1.94 | 0.26 |
| 4:5:253:GLU:OE2 | 4:8:215:LYS:N[1_554] | 1.94 | 0.26 |
| 4:5:270:GLU:O | 4:8:272:ALA:CA[1_554] | 1.94 | 0.26 |
| 4:5:136:ILE:O | 4:8:113:LYS:CA[1_554] | 1.94 | 0.26 |
| 4:5:194:THR:OG1 | 4:8:190:MET:CB[1_554] | 1.94 | 0.26 |
| 4:4:299:MET:CG | 4:7:136:ILE:C[1_554] | 1.94 | 0.26 |
| 4:4:113:LYS:CG | 4:8:255:PHE:N[1_554] | 1.94 | 0.26 |
| 4:5:340:TRP:CZ3 | 4:8:121:GLN:N[1_554] | 1.94 | 0.26 |
| 4:6:174:ALA:CA | 4:9:173:HIS:CB[1_554] | 1.94 | 0.26 |
| 4:6:154:ASP:CB | 4:9:109:PRO:C[1_554] | 1.94 | 0.26 |
| 4:6:257:CYS:C | 4:9:303:THR:CA[1_554] | 1.94 | 0.26 |
| 4:6:157:ASP:C | 4:9:73:HIS:CA[1_554] | 1.94 | 0.26 |
| 4:6:370:VAL:N | 4:V:232:SER:N[1_554] | 1.94 | 0.26 |
| 4:5:219:VAL:N | 4:8:335:ARG:C[1_554] | 1.94 | 0.26 |
| 4:4:311:ASP:OD1 | 4:7:144:ALA:CA[1_554] | 1.94 | 0.26 |
| 4:5:254:ARG:CZ | 4:8:336:LYS:CE[1_554] | 1.94 | 0.26 |
| 4:6:25:ASP:N | 4:9:124:PHE:N[1_554] | 1.94 | 0.26 |
| 4:5:288:ASP:N | 4:V:62:ARG:O[1_554] | 1.94 | 0.26 |
| 4:4:269:MET:CG | 4:7:178:LEU:CD1[1_554] | 1.94 | 0.26 |
| 4:6:242:LEU:CD2 | 4:9:207:GLU:CD[1_554] | 1.94 | 0.26 |
| 4:6:227:MET:CB | 4:9:307:PRO:N[1_554] | 1.94 | 0.26 |
| 4:6:136:ILE:O | 4:9:113:LYS:CA[1_554] | 1.94 | 0.26 |
| 4:6:346:LEU:CA | 4:9:366:GLY:O[1_554] | 1.94 | 0.26 |
| 4:6:186:THR:CA | 4:9:157:ASP:OD2[1_554] | 1.94 | 0.26 |
| 4:4:316:GLU:OE2 | 4:7:298:VAL:O[1_554] | 1.94 | 0.26 |
| 4:6:21:PHE:C | 4:9:125:GLU:OE1[1_554] | 1.94 | 0.26 |
| 4:6:215:LYS:CD | 4:9:30:VAL:C[1_554] | 1.94 | 0.26 |
| 4:4:257:CYS:CA | 4:7:303:THR:OG1[1_554] | 1.94 | 0.26 |
| 4:3:326:LYS:CE | 4:8:45:VAL:CA[1_554] | 1.94 | 0.26 |
| 4:6:313:MET:CG | 4:9:152:VAL:CG1[1_554] | 1.94 | 0.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:196:ARG:CG | 4:9:211:ASP:O[1_554] | 1.94 | 0.26 |
| 4:4:326:LYS:C | 4:7:167:GLU:CG[1_554] | 1.94 | 0.26 |
| 4:6:274:ILE:C | 4:9:162:ASN:CB[1_554] | 1.94 | 0.26 |
| 4:4:116:ARG:CA | 4:8:237:GLU:OE2[1_554] | 1.94 | 0.26 |
| 4:4:312:ARG:CZ | 4:7:299:MET:CB[1_554] | 1.94 | 0.26 |
| 4:6:295:ALA:N | 4:9:166:TYR:C[1_554] | 1.94 | 0.26 |
| 4:6:334:GLU:C | 4:9:105:LEU:O[1_554] | 1.94 | 0.26 |
| 4:3:172:PRO:O | 4:7:188:TYR:CE1[1_554] | 1.94 | 0.26 |
| 4:3:75:ILE:CB | 4:7:198:TYR:CA[1_554] | 1.94 | 0.26 |
| 4:6:194:THR:O | 4:9:209:VAL:CB[1_554] | 1.94 | 0.26 |
| 4:6:257:CYS:N | 4:9:303:THR:OG1[1_554] | 1.94 | 0.26 |
| 4:6:315:LYS:C | 4:9:296:ASN:C[1_554] | 1.94 | 0.26 |
| 4:4:30:VAL:C | 4:7:79:TRP:C[1_554] | 1.94 | 0.26 |
| 4:4:242:LEU:C | 4:7:60:SER:N[1_554] | 1.94 | 0.26 |
| 4:4:294:TYR:CD2 | 4:7:166:TYR:CG[1_554] | 1.94 | 0.26 |
| 4:5:159:VAL:N | 4:8:177:ARG:CZ[1_554] | 1.94 | 0.26 |
| 4:4:340:TRP:O | 4:7:117:GLU:O[1_554] | 1.94 | 0.26 |
| 4:5:254:ARG:NE | 4:8:336:LYS:NZ[1_554] | 1.94 | 0.26 |
| 4:6:316:GLU:CA | 4:9:297:ASN:CA[1_554] | 1.94 | 0.26 |
| 4:4:257:CYS:SG | 4:7:157:ASP:N[1_554] | 1.94 | 0.26 |
| 4:5:319:ALA:N | 4:8:296:ASN:N[1_554] | 1.94 | 0.26 |
| 4:4:288:ASP:C | 4:9:39:ARG:NH1[1_554] | 1.94 | 0.26 |
| 4:6:264:PRO:N | 4:9:274:ILE:CG1[1_554] | 1.94 | 0.26 |
| 4:4:178:LEU:CB | 4:7:177:ARG:CA[1_554] | 1.94 | 0.26 |
| 4:6:196:ARG:NH1 | 4:9:215:LYS:N[1_554] | 1.94 | 0.26 |
| 4:5:370:VAL:CA | 4:9:231:ALA:N[1_554] | 1.94 | 0.26 |
| 4:4:175:ILE:CG2 | 4:8:191:LYS:CD[1_554] | 1.94 | 0.26 |
| 4:6:207:GLU:CD | 4:9:67:LEU:CG[1_554] | 1.94 | 0.26 |
| 1:D:542:PHE:CZ | 4:6:328:LYS:CE[1_556] | 1.94 | 0.26 |
| 4:5:151:ILE:CG2 | 4:8:170:ALA:CA[1_554] | 1.94 | 0.26 |
| 4:4:207:GLU:CB | 4:7:67:LEU:CD1[1_554] | 1.94 | 0.26 |
| 4:6:281:SER:N | 4:9:174:ALA:CA[1_554] | 1.94 | 0.26 |
| 4:4:280:ASN:O | 4:7:284:LYS:O[1_554] | 1.94 | 0.26 |
| 4:4:218:TYR:CZ | 4:7:337:TYR:CE1[1_554] | 1.94 | 0.26 |
| 4:6:196:ARG:CB | 4:9:213:LYS:N[1_554] | 1.94 | 0.26 |
| 4:6:369:ILE:CD1 | 4:V:232:SER:OG[1_554] | 1.94 | 0.26 |
| 4:4:157:ASP:OD1 | 4:7:72:GLU:CG[1_554] | 1.95 | 0.25 |
| 4:4:339:VAL:N | 4:7:117:GLU:N[1_554] | 1.95 | 0.25 |
| 4:4:304:THR:CB | 4:7:137:GLN:NE2[1_554] | 1.95 | 0.25 |
| 4:4:273:GLY:O | 4:7:162:ASN:CG[1_554] | 1.95 | 0.25 |
| 4:4:110:LEU:CG | 4:8:191:LYS:CG[1_554] | 1.95 | 0.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:198:TYR:CG | 4:8:208:ILE:CB[1_554] | 1.95 | 0.25 |
| 4:6:190:MET:CE | 4:9:206:ARG:NH1[1_554] | 1.95 | 0.25 |
| 4:6:177:ARG:CZ | 4:V:194:THR:CB[1_554] | 1.95 | 0.25 |
| 4:6:316:GLU:CD | 4:9:297:ASN:CG[1_554] | 1.95 | 0.25 |
| 4:2:288:ASP:O | 4:7:39:ARG:CB[1_554] | 1.95 | 0.25 |
| 4:4:15:GLY:C | 4:7:77:THR:C[1_554] | 1.95 | 0.25 |
| 4:4:357:ILE:CB | 4:8:231:ALA:O[1_554] | 1.95 | 0.25 |
| 4:5:110:LEU:C | 4:9:192:ILE:O[1_554] | 1.95 | 0.25 |
| 4:5:137:GLN:OE1 | 4:8:112:PRO:CA[1_554] | 1.95 | 0.25 |
| 4:5:19:ALA:C | 4:8:121:GLN:OE1[1_554] | 1.95 | 0.25 |
| 4:6:282:ILE:CG1 | 4:9:171:LEU:CB[1_554] | 1.95 | 0.25 |
| 4:5:151:ILE:CG2 | 4:8:170:ALA:N[1_554] | 1.95 | 0.25 |
| 4:3:369:ILE:CG2 | 4:7:234:SER:CA[1_554] | 1.95 | 0.25 |
| 4:5:301:GLY:N | 4:8:107:GLU:O[1_554] | 1.95 | 0.25 |
| 4:6:313:MET:N | 4:9:298:VAL:CG1[1_554] | 1.95 | 0.25 |
| 4:4:173:HIS:CB | 4:8:267:ILE:CA[1_554] | 1.95 | 0.25 |
| 4:6:256:ARG:N | 4:9:302:GLY:O[1_554] | 1.95 | 0.25 |
| 4:4:184:ASP:OD1 | 4:7:73:HIS:ND1[1_554] | 1.95 | 0.25 |
| 4:6:259:GLU:CD | 4:9:309:ILE:CB[1_554] | 1.95 | 0.25 |
| 4:5:315:LYS:CG | 4:8:147:ARG:CZ[1_554] | 1.95 | 0.25 |
| 4:4:366:GLY:C | 4:8:234:SER:C[1_554] | 1.95 | 0.25 |
| 4:5:265:SER:CB | 4:8:262:PHE:CA[1_554] | 1.95 | 0.25 |
| 4:5:256:ARG:N | 4:8:302:GLY:O[1_554] | 1.95 | 0.25 |
| 4:5:340:TRP:CE3 | 4:8:119:MET:O[1_554] | 1.95 | 0.25 |
| 4:6:276:GLU:OE1 | 4:9:278:THR:O[1_554] | 1.95 | 0.25 |
| 4:6:263:GLN:C | 4:9:274:ILE:CB[1_554] | 1.95 | 0.25 |
| 4:4:217:CYS:SG | 4:7:16:LEU:CD2[1_554] | 1.95 | 0.25 |
| 4:6:243:PRO:CG | 4:9:59:GLN:C[1_554] | 1.95 | 0.25 |
| 4:6:335:ARG:CD | 4:9:106:THR:CG2[1_554] | 1.95 | 0.25 |
| 4:4:223:PHE:CZ | 4:7:301:GLY:O[1_554] | 1.95 | 0.25 |
| 4:4:267:ILE:CG1 | 4:7:180:LEU:O[1_554] | 1.95 | 0.25 |
| 4:4:309:ILE:CG2 | 4:7:339:VAL:CG1[1_554] | 1.95 | 0.25 |
| 4:6:319:ALA:N | 4:9:296:ASN:CB[1_554] | 1.95 | 0.25 |
| 4:6:193:LEU:CD1 | 4:9:210:ARG:CA[1_554] | 1.95 | 0.25 |
| 4:5:316:GLU:CD | 4:8:297:ASN:CG[1_554] | 1.95 | 0.25 |
| 4:4:282:ILE:CD1 | 4:7:171:LEU:CB[1_554] | 1.95 | 0.25 |
| 4:6:297:ASN:CA | 4:9:168:GLY:O[1_554] | 1.95 | 0.25 |
| 4:5:112:PRO:CA | 4:9:253:GLU:OE1[1_554] | 1.95 | 0.25 |
| 4:4:218:TYR:CZ | 4:7:27:PRO:CG[1_554] | 1.95 | 0.25 |
| 4:4:215:LYS:CG | 4:7:31:PHE:C[1_554] | 1.95 | 0.25 |
| 4:6:210:ARG:NH2 | 4:9:34:ILE:CA[1_554] | 1.95 | 0.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:75:ILE:CD1 | 4:V:194:THR:C[1_554] | 1.95 | 0.25 |
| 4:6:319:ALA:CB | 4:9:295:ALA:O[1_554] | 1.95 | 0.25 |
| 4:6:180:LEU:CD1 | 4:9:160:THR:CA[1_554] | 1.95 | 0.25 |
| 4:6:288:ASP:O | 4:W:63:GLY:C[1_554] | 1.95 | 0.25 |
| 4:4:340:TRP:CD1 | 4:7:118:LYS:CG[1_554] | 1.95 | 0.25 |
| 4:5:274:ILE:CD1 | 4:8:161:HIS:C[1_554] | 1.95 | 0.25 |
| 4:4:222:ASP:CB | 4:7:332:PRO:CD[1_554] | 1.95 | 0.25 |
| 4:5:188:TYR:CD2 | 4:8:181:ALA:O[1_554] | 1.95 | 0.25 |
| 4:4:178:LEU:O | 4:7:177:ARG:CG[1_554] | 1.95 | 0.25 |
| 4:4:272:ALA:CA | 4:7:277:THR:CB[1_554] | 1.95 | 0.25 |
| 4:6:178:LEU:CD1 | 4:9:177:ARG:C[1_554] | 1.95 | 0.25 |
| 4:4:79:TRP:CZ2 | 4:8:249:THR:CG2[1_554] | 1.95 | 0.25 |
| 4:4:343:GLY:N | 4:7:117:GLU:CB[1_554] | 1.95 | 0.25 |
| 4:5:59:GLN:CD | 4:8:68:LYS:CB[1_554] | 1.95 | 0.25 |
| 4:3:172:PRO:CB | 4:7:188:TYR:CZ[1_554] | 1.95 | 0.25 |
| 4:5:290:ARG:CZ | 4:8:286:ASP:CB[1_554] | 1.95 | 0.25 |
| 4:5:256:ARG:CA | 4:8:303:THR:O[1_554] | 1.95 | 0.25 |
| 4:3:113:LYS:O | 4:7:252:ASN:N[1_554] | 1.95 | 0.25 |
| 4:5:298:VAL:C | 4:8:136:ILE:CB[1_554] | 1.95 | 0.25 |
| 4:6:340:TRP:CD2 | 4:9:118:LYS:O[1_554] | 1.95 | 0.25 |
| 4:5:262:PHE:CD2 | 4:8:153:LEU:C[1_554] | 1.95 | 0.25 |
| 4:5:327:ILE:CG2 | 4:8:149:THR:C[1_554] | 1.95 | 0.25 |
| 4:4:161:HIS:O | 4:7:110:LEU:CD2[1_554] | 1.95 | 0.25 |
| 4:4:215:LYS:C | 4:7:17:VAL:O[1_554] | 1.95 | 0.25 |
| 4:4:173:HIS:CB | 4:8:267:ILE:CG2[1_554] | 1.95 | 0.25 |
| 4:6:310:ALA:CB | 4:9:141:SER:C[1_554] | 1.95 | 0.25 |
| 4:4:299:MET:O | 4:7:107:GLU:CG[1_554] | 1.95 | 0.25 |
| 4:5:304:THR:C | 4:8:137:GLN:CG[1_554] | 1.95 | 0.25 |
| 4:4:372:ARG:C | 4:8:226:GLU:C[1_554] | 1.95 | 0.25 |
| 4:5:205:GLU:C | 4:8:62:ARG:NE[1_554] | 1.95 | 0.25 |
| 4:5:227:MET:SD | 4:8:307:PRO:CD[1_554] | 1.95 | 0.25 |
| 4:6:60:SER:CA | 4:9:37:ARG:CB[1_554] | 1.95 | 0.25 |
| 4:4:266:PHE:CA | 4:7:261:LEU:CB[1_554] | 1.95 | 0.25 |
| 4:4:310:ALA:O | 4:7:139:VAL:C[1_554] | 1.95 | 0.25 |
| 4:6:28:ARG:NE | 4:9:126:THR:C[1_554] | 1.95 | 0.25 |
| 4:6:111:ASN:OD1 | 4:V:196:ARG:CG[1_554] | 1.95 | 0.25 |
| 4:4:138:ALA:C | 4:7:113:LYS:CG[1_554] | 1.95 | 0.25 |
| 4:4:255:PHE:C | 4:7:302:GLY:N[1_554] | 1.95 | 0.25 |
| 4:4:198:TYR:C | 4:7:207:GLU:N[1_554] | 1.95 | 0.25 |
| 4:5:207:GLU:CD | 4:8:67:LEU:CG[1_554] | 1.95 | 0.25 |
| 4:6:277:THR:CG2 | 4:9:175:ILE:O[1_554] | 1.95 | 0.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:175:ILE:CD1 | 4:8:191:LYS:CE[1_554] | 1.95 | 0.25 |
| 4:5:220:ALA:CB | 4:8:335:ARG:NE[1_554] | 1.95 | 0.25 |
| 4:4:196:ARG:CD | 4:7:211:ASP:O[1_554] | 1.95 | 0.25 |
| 4:6:219:VAL:O | 4:9:335:ARG:C[1_554] | 1.95 | 0.25 |
| 4:5:118:LYS:N | 4:9:237:GLU:OE2[1_554] | 1.95 | 0.25 |
| 4:3:366:GLY:O | 4:7:235:SER:N[1_554] | 1.95 | 0.25 |
| 4:6:211:ASP:CG | 4:9:32:PRO:CA[1_554] | 1.95 | 0.25 |
| 4:5:267:ILE:CD1 | 4:8:180:LEU:CG[1_554] | 1.95 | 0.25 |
| 4:5:151:ILE:CG1 | 4:8:171:LEU:N[1_554] | 1.95 | 0.25 |
| 4:6:137:GLN:OE1 | 4:9:112:PRO:CA[1_554] | 1.95 | 0.25 |
| 4:4:293:LEU:CG | 4:7:169:TYR:CE2[1_554] | 1.95 | 0.25 |
| 4:6:267:ILE:CB | 4:9:180:LEU:CD2[1_554] | 1.95 | 0.25 |
| 4:4:265:SER:O | 4:7:260:THR:O[1_554] | 1.95 | 0.25 |
| 4:4:243:PRO:CA | 4:7:60:SER:CB[1_554] | 1.95 | 0.25 |
| 4:4:144:ALA:CB | 4:7:370:VAL:CG1[1_554] | 1.95 | 0.25 |
| 4:4:293:LEU:O | 4:7:169:TYR:CA[1_554] | 1.95 | 0.25 |
| 4:4:305:MET:N | 4:7:137:GLN:NE2[1_554] | 1.95 | 0.25 |
| 4:6:161:HIS:N | 4:9:110:LEU:CD1[1_554] | 1.95 | 0.25 |
| 4:3:75:ILE:CB | 4:7:198:TYR:CD2[1_554] | 1.95 | 0.25 |
| 4:4:337:TYR:CA | 4:7:119:MET:CA[1_554] | 1.95 | 0.25 |
| 4:6:315:LYS:O | 4:9:297:ASN:N[1_554] | 1.95 | 0.25 |
| 4:5:255:PHE:CD1 | 4:8:305:MET:O[1_554] | 1.95 | 0.25 |
| 4:5:192:ILE:C | 4:8:213:LYS:CB[1_554] | 1.95 | 0.25 |
| 4:4:306:TYR:C | 4:7:11:ASP:CG[1_554] | 1.95 | 0.25 |
| 4:5:219:VAL:O | 4:8:335:ARG:C[1_554] | 1.95 | 0.25 |
| 4:4:143:TYR:CD2 | 4:7:368:SER:CA[1_554] | 1.96 | 0.24 |
| 4:6:200:PHE:CZ | 4:9:207:GLU:C[1_554] | 1.96 | 0.24 |
| 4:4:270:GLU:C | 4:7:272:ALA:C[1_554] | 1.96 | 0.24 |
| 4:5:337:TYR:O | 4:8:119:MET:CG[1_554] | 1.96 | 0.24 |
| 4:6:178:LEU:CD2 | 4:9:176:MET:C[1_554] | 1.96 | 0.24 |
| 4:4:24:ASP:CA | 4:7:125:GLU:CB[1_554] | 1.96 | 0.24 |
| 4:4:215:LYS:CB | 4:7:31:PHE:CB[1_554] | 1.96 | 0.24 |
| 4:4:110:LEU:C | 4:8:193:LEU:N[1_554] | 1.96 | 0.24 |
| 4:5:277:THR:O | 4:8:175:ILE:N[1_554] | 1.96 | 0.24 |
| 4:6:178:LEU:C | 4:9:177:ARG:CB[1_554] | 1.96 | 0.24 |
| 4:5:199:SER:CA | 4:8:206:ARG:C[1_554] | 1.96 | 0.24 |
| 4:4:284:LYS:O | 4:8:268:GLY:CA[1_554] | 1.96 | 0.24 |
| 4:5:316:GLU:O | 4:8:296:ASN:O[1_554] | 1.96 | 0.24 |
| 4:5:15:GLY:C | 4:8:77:THR:N[1_554] | 1.96 | 0.24 |
| 4:5:346:LEU:CA | 4:8:366:GLY:O[1_554] | 1.96 | 0.24 |
| 4:6:154:ASP:C | 4:9:109:PRO:CA[1_554] | 1.96 | 0.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:180:LEU:CB | 4:8:179:ASP:CA[1_554] | 1.96 | 0.24 |
| 4:4:108:ALA:C | 4:8:195:GLU:CG[1_554] | 1.96 | 0.24 |
| 4:4:110:LEU:CB | 4:8:192:ILE:CB[1_554] | 1.96 | 0.24 |
| 4:6:304:THR:OG1 | 4:9:137:GLN:CD[1_554] | 1.96 | 0.24 |
| 4:4:187:ASP:N | 4:7:183:ARG:CB[1_554] | 1.96 | 0.24 |
| 4:6:156:GLY:O | 4:9:73:HIS:O[1_554] | 1.96 | 0.24 |
| 4:5:143:TYR:CD2 | 4:8:369:ILE:O[1_554] | 1.96 | 0.24 |
| 4:6:11:ASP:OD2 | 4:9:115:ASN:O[1_554] | 1.96 | 0.24 |
| 4:4:181:ALA:O | 4:7:73:HIS:ND1[1_554] | 1.96 | 0.24 |
| 4:5:263:GLN:CA | 4:8:274:ILE:CD1[1_554] | 1.96 | 0.24 |
| 4:4:328:LYS:CA | 4:7:168:GLY:CA[1_554] | 1.96 | 0.24 |
| 4:3:175:ILE:CD1 | 4:7:191:LYS:CE[1_554] | 1.96 | 0.24 |
| 4:6:348:SER:O | 4:9:364:GLU:CA[1_554] | 1.96 | 0.24 |
| 4:5:196:ARG:NH2 | 4:8:215:LYS:CD[1_554] | 1.96 | 0.24 |
| 4:5:199:SER:O | 4:8:206:ARG:CB[1_554] | 1.96 | 0.24 |
| 4:5:113:LYS:O | 4:9:252:ASN:CB[1_554] | 1.96 | 0.24 |
| 4:4:240:TYR:CE2 | 4:7:56:ASP:CG[1_554] | 1.96 | 0.24 |
| 4:5:183:ARG:CZ | 4:8:72:GLU:CD[1_554] | 1.96 | 0.24 |
| 4:6:367:PRO:CA | 4:V:234:SER:N[1_554] | 1.96 | 0.24 |
| 4:2:288:ASP:O | 4:7:39:ARG:NE[1_554] | 1.96 | 0.24 |
| 4:5:348:SER:CA | 4:8:366:GLY:N[1_554] | 1.96 | 0.24 |
| 4:6:307:PRO:CG | 4:9:337:TYR:CA[1_554] | 1.96 | 0.24 |
| 4:6:314:GLN:C | 4:9:142:LEU:CD1[1_554] | 1.96 | 0.24 |
| 4:4:320:LEU:N | 4:7:293:LEU:CA[1_554] | 1.96 | 0.24 |
| 4:6:294:TYR:C | 4:9:167:GLU:CA[1_554] | 1.96 | 0.24 |
| 4:4:309:ILE:CD1 | 4:7:137:GLN:CB[1_554] | 1.96 | 0.24 |
| 4:4:25:ASP:OD2 | 4:7:124:PHE:O[1_554] | 1.96 | 0.24 |
| 4:5:299:MET:CB | 4:8:136:ILE:CA[1_554] | 1.96 | 0.24 |
| 4:6:200:PHE:O | 4:9:206:ARG:CD[1_554] | 1.96 | 0.24 |
| 4:3:110:LEU:CA | 4:7:192:ILE:N[1_554] | 1.96 | 0.24 |
| 4:5:299:MET:CE | 4:8:137:GLN:C[1_554] | 1.96 | 0.24 |
| 4:2:290:ARG:C | 4:7:40:HIS:CE1[1_554] | 1.96 | 0.24 |
| 4:4:118:LYS:CA | 4:8:237:GLU:OE1[1_554] | 1.96 | 0.24 |
| 4:4:25:ASP:CB | 4:7:124:PHE:N[1_554] | 1.96 | 0.24 |
| 4:4:222:ASP:CA | 4:7:331:ALA:CA[1_554] | 1.96 | 0.24 |
| 4:5:319:ALA:CB | 4:8:295:ALA:N[1_554] | 1.96 | 0.24 |
| 4:5:261:LEU:C | 4:8:160:THR:CG2[1_554] | 1.96 | 0.24 |
| 4:5:340:TRP:C | 4:8:120:THR:N[1_554] | 1.96 | 0.24 |
| 4:5:214:GLU:CB | 4:8:16:LEU:N[1_554] | 1.96 | 0.24 |
| 4:2:289:ILE:C | 4:7:40:HIS:CE1[1_554] | 1.96 | 0.24 |
| 4:3:113:LYS:C | 4:7:250:ILE:C[1_554] | 1.96 | 0.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:11:ASP:CG | 4:8:115:ASN:CB[1_554] | 1.96 | 0.24 |
| 4:5:265:SER:O | 4:8:260:THR:C[1_554] | 1.96 | 0.24 |
| 4:5:299:MET:C | 4:8:136:ILE:C[1_554] | 1.96 | 0.24 |
| 4:5:278:THR:C | 4:8:164:PRO:CD[1_554] | 1.96 | 0.24 |
| 4:4:154:ASP:CA | 4:7:110:LEU:N[1_554] | 1.96 | 0.24 |
| 4:6:141:SER:C | 4:9:116:ARG:NE[1_554] | 1.96 | 0.24 |
| 4:6:371:HIS:N | 4:V:230:ALA:C[1_554] | 1.96 | 0.24 |
| 4:4:318:THR:CA | 4:7:150:GLY:N[1_554] | 1.96 | 0.24 |
| 4:5:20:GLY:O | 4:8:121:GLN:CG[1_554] | 1.96 | 0.24 |
| 4:6:319:ALA:C | 4:9:294:TYR:C[1_554] | 1.96 | 0.24 |
| 4:4:333:PRO:CD | 4:7:104:LEU:CA[1_554] | 1.96 | 0.24 |
| 4:5:288:ASP:O | 4:V:64:ILE:CA[1_554] | 1.96 | 0.24 |
| 4:4:142:LEU:C | 4:7:372:ARG:C[1_554] | 1.96 | 0.24 |
| 4:4:279:TYR:CD2 | 4:7:285:CYS:CB[1_554] | 1.96 | 0.24 |
| 4:5:151:ILE:CG2 | 4:8:169:TYR:C[1_554] | 1.96 | 0.24 |
| 4:4:335:ARG:NH1 | 4:7:105:LEU:C[1_554] | 1.96 | 0.24 |
| 4:4:117:GLU:CG | 4:8:237:GLU:N[1_554] | 1.96 | 0.24 |
| 4:6:311:ASP:OD1 | 4:9:144:ALA:CA[1_554] | 1.96 | 0.24 |
| 4:3:173:HIS:N | 4:7:267:ILE:N[1_554] | 1.96 | 0.24 |
| 4:5:109:PRO:C | 4:9:195:GLU:CG[1_554] | 1.96 | 0.24 |
| 4:5:214:GLU:OE1 | 4:8:33:SER:OG[1_554] | 1.96 | 0.24 |
| 4:4:288:ASP:C | 4:9:64:ILE:CA[1_554] | 1.96 | 0.24 |
| 4:5:187:ASP:OD1 | 4:8:183:ARG:CD[1_554] | 1.96 | 0.24 |
| 4:6:280:ASN:O | 4:9:284:LYS:C[1_554] | 1.96 | 0.24 |
| 4:5:210:ARG:C | 4:8:15:GLY:O[1_554] | 1.96 | 0.24 |
| 4:5:151:ILE:CD1 | 4:8:172:PRO:N[1_554] | 1.96 | 0.24 |
| 4:4:272:ALA:CB | 4:7:277:THR:O[1_554] | 1.96 | 0.24 |
| 4:5:214:GLU:CG | 4:8:16:LEU:CA[1_554] | 1.96 | 0.24 |
| 4:5:370:VAL:C | 4:9:231:ALA:CB[1_554] | 1.96 | 0.24 |
| 4:6:219:VAL:C | 4:9:335:ARG:CA[1_554] | 1.96 | 0.24 |
| 4:5:311:ASP:O | 4:8:298:VAL:CG1[1_554] | 1.96 | 0.24 |
| 4:6:28:ARG:N | 4:9:126:THR:OG1[1_554] | 1.96 | 0.24 |
| 4:3:288:ASP:O | 4:8:64:ILE:N[1_554] | 1.96 | 0.24 |
| 4:6:214:GLU:CA | 4:9:16:LEU:N[1_554] | 1.96 | 0.24 |
| 4:5:26:ALA:C | 4:8:122:ILE:O[1_554] | 1.96 | 0.24 |
| 4:6:340:TRP:CE3 | 4:9:120:THR:O[1_554] | 1.96 | 0.24 |
| 4:6:114:ALA:N | 4:V:252:ASN:N[1_554] | 1.96 | 0.24 |
| 4:5:317:ILE:N | 4:8:150:GLY:CA[1_554] | 1.96 | 0.24 |
| 4:6:262:PHE:CD1 | 4:9:153:LEU:O[1_554] | 1.96 | 0.24 |
| 4:4:205:GLU:OE2 | 4:7:203:THR:CG2[1_554] | 1.96 | 0.24 |
| 4:4:197:GLY:N | 4:7:208:ILE:C[1_554] | 1.96 | 0.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:337:TYR:CZ | 4:8:86:TRP:CH2[1_554] | 1.96 | 0.24 |
| 4:4:198:TYR:O | 4:7:206:ARG:CA[1_554] | 1.96 | 0.24 |
| 4:5:183:ARG:CD | 4:8:72:GLU:CD[1_554] | 1.96 | 0.24 |
| 4:5:372:ARG:C | 4:9:227:MET:C[1_554] | 1.96 | 0.24 |
| 4:4:279:TYR:CG | 4:7:285:CYS:SG[1_554] | 1.96 | 0.24 |
| 4:4:319:ALA:CA | 4:7:296:ASN:CG[1_554] | 1.96 | 0.24 |
| 4:4:333:PRO:CG | 4:7:104:LEU:N[1_554] | 1.96 | 0.24 |
| 4:5:258:PRO:O | 4:8:155:SER:N[1_554] | 1.97 | 0.23 |
| 4:5:283:MET:CE | 4:8:289:ILE:N[1_554] | 1.97 | 0.23 |
| 4:6:290:ARG:CD | 4:9:286:ASP:CB[1_554] | 1.97 | 0.23 |
| 4:4:339:VAL:CA | 4:7:117:GLU:N[1_554] | 1.97 | 0.23 |
| 4:4:270:GLU:CA | 4:7:273:GLY:N[1_554] | 1.97 | 0.23 |
| 4:6:213:LYS:CE | 4:9:15:GLY:CA[1_554] | 1.97 | 0.23 |
| 4:5:261:LEU:CD2 | 4:8:160:THR:CA[1_554] | 1.97 | 0.23 |
| 4:6:256:ARG:CZ | 4:9:217:CYS:CB[1_554] | 1.97 | 0.23 |
| 4:6:221:LEU:CG | 4:9:332:PRO:N[1_554] | 1.97 | 0.23 |
| 4:3:177:ARG:CZ | 4:7:194:THR:CB[1_554] | 1.97 | 0.23 |
| 4:4:159:VAL:N | 4:7:177:ARG:NH2[1_554] | 1.97 | 0.23 |
| 4:4:320:LEU:CG | 4:7:293:LEU:CA[1_554] | 1.97 | 0.23 |
| 4:5:166:TYR:CZ | 4:V:39:ARG:CA[1_554] | 1.97 | 0.23 |
| 4:6:340:TRP:CD2 | 4:9:121:GLN:N[1_554] | 1.97 | 0.23 |
| 4:6:307:PRO:C | 4:9:338:SER:CA[1_554] | 1.97 | 0.23 |
| 4:5:290:ARG:CD | 4:8:286:ASP:OD2[1_554] | 1.97 | 0.23 |
| 4:6:334:GLU:O | 4:9:105:LEU:C[1_554] | 1.97 | 0.23 |
| 4:4:343:GLY:CA | 4:7:117:GLU:OE1[1_554] | 1.97 | 0.23 |
| 4:6:222:ASP:CA | 4:9:331:ALA:CA[1_554] | 1.97 | 0.23 |
| 4:4:299:MET:CB | 4:7:136:ILE:CG1[1_554] | 1.97 | 0.23 |
| 4:4:372:ARG:CB | 4:8:227:MET:C[1_554] | 1.97 | 0.23 |
| 4:6:162:ASN:OD1 | 4:9:175:ILE:CG1[1_554] | 1.97 | 0.23 |
| 4:5:110:LEU:C | 4:9:192:ILE:C[1_554] | 1.97 | 0.23 |
| 4:6:270:GLU:CG | 4:9:271:SER:O[1_554] | 1.97 | 0.23 |
| 4:6:198:TYR:CA | 4:9:205:GLU:O[1_554] | 1.97 | 0.23 |
| 4:6:316:GLU:OE1 | 4:9:297:ASN:OD1[1_554] | 1.97 | 0.23 |
| 4:3:113:LYS:CG | 4:7:255:PHE:N[1_554] | 1.97 | 0.23 |
| 4:6:321:ALA:N | 4:9:292:ASP:CA[1_554] | 1.97 | 0.23 |
| 4:5:191:LYS:CG | 4:8:185:LEU:O[1_554] | 1.97 | 0.23 |
| 4:4:275:HIS:ND1 | 4:7:152:VAL:C[1_554] | 1.97 | 0.23 |
| 4:6:270:GLU:N | 4:9:272:ALA:C[1_554] | 1.97 | 0.23 |
| 4:4:300:SER:CB | 4:7:107:GLU:OE2[1_554] | 1.97 | 0.23 |
| 4:6:316:GLU:CB | 4:9:298:VAL:N[1_554] | 1.97 | 0.23 |
| 4:3:117:GLU:CA | 4:7:237:GLU:CA[1_554] | 1.97 | 0.23 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:213:LYS:CB | 4:7:15:GLY:N[1_554] | 1.97 | 0.23 |
| 4:4:136:ILE:O | 4:7:113:LYS:NZ[1_554] | 1.97 | 0.23 |
| 4:6:113:LYS:N | 4:V:253:GLU:CB[1_554] | 1.97 | 0.23 |
| 4:6:342:GLY:C | 4:9:370:VAL:CG1[1_554] | 1.97 | 0.23 |
| 4:5:334:GLU:N | 4:8:105:LEU:CA[1_554] | 1.97 | 0.23 |
| 4:5:340:TRP:CH2 | 4:8:121:GLN:N[1_554] | 1.97 | 0.23 |
| 4:6:219:VAL:C | 4:9:335:ARG:C[1_554] | 1.97 | 0.23 |
| 4:5:173:HIS:N | 4:9:267:ILE:CA[1_554] | 1.97 | 0.23 |
| 4:5:186:THR:C | 4:8:183:ARG:CD[1_554] | 1.97 | 0.23 |
| 4:5:28:ARG:CA | 4:8:126:THR:CG2[1_554] | 1.97 | 0.23 |
| 4:4:154:ASP:OD2 | 4:7:112:PRO:CA[1_554] | 1.97 | 0.23 |
| 4:4:205:GLU:OE2 | 4:7:203:THR:OG1[1_554] | 1.97 | 0.23 |
| 4:6:211:ASP:CB | 4:9:32:PRO:N[1_554] | 1.97 | 0.23 |
| 4:5:312:ARG:CD | 4:8:298:VAL:C[1_554] | 1.97 | 0.23 |
| 4:5:151:ILE:N | 4:8:169:TYR:CE1[1_554] | 1.97 | 0.23 |
| 4:5:161:HIS:CG | 4:8:110:LEU:CB[1_554] | 1.97 | 0.23 |
| 4:5:212:ILE:CG2 | 4:8:210:ARG:NH1[1_554] | 1.97 | 0.23 |
| 4:5:190:MET:CG | 4:8:187:ASP:OD1[1_554] | 1.97 | 0.23 |
| 4:4:369:ILE:CG2 | 4:8:234:SER:CB[1_554] | 1.97 | 0.23 |
| 4:4:114:ALA:CA | 4:8:250:ILE:CA[1_554] | 1.97 | 0.23 |
| 4:5:142:LEU:C | 4:8:372:ARG:CG[1_554] | 1.97 | 0.23 |
| 4:4:319:ALA:CB | 4:7:296:ASN:ND2[1_554] | 1.97 | 0.23 |
| 4:5:220:ALA:N | 4:8:335:ARG:CD[1_554] | 1.97 | 0.23 |
| 4:6:23:GLY:N | 4:9:362:TYR:CZ[1_554] | 1.97 | 0.23 |
| 4:6:31:PHE:CB | 4:9:80:ASP:CB[1_554] | 1.97 | 0.23 |
| 4:6:280:ASN:CA | 4:9:281:SER:O[1_554] | 1.97 | 0.23 |
| 4:4:267:ILE:CG2 | 4:7:181:ALA:N[1_554] | 1.97 | 0.23 |
| 4:4:340:TRP:CH2 | 4:7:121:GLN:CB[1_554] | 1.97 | 0.23 |
| 4:4:339:VAL:N | 4:7:115:ASN:C[1_554] | 1.97 | 0.23 |
| 4:5:291:LYS:NZ | 4:V:64:ILE:CB[1_554] | 1.97 | 0.23 |
| 4:6:113:LYS:CA | 4:V:252:ASN:C[1_554] | 1.97 | 0.23 |
| 4:5:330:ILE:O | 4:8:139:VAL:CG1[1_554] | 1.97 | 0.23 |
| 4:6:140:LEU:CB | 4:9:371:HIS:CG[1_554] | 1.97 | 0.23 |
| 4:5:314:GLN:OE1 | 4:8:147:ARG:C[1_554] | 1.97 | 0.23 |
| 4:6:257:CYS:N | 4:9:303:THR:CB[1_554] | 1.97 | 0.23 |
| 4:6:276:GLU:CD | 4:9:279:TYR:CA[1_554] | 1.97 | 0.23 |
| 4:6:166:TYR:CZ | 4:W:39:ARG:CA[1_554] | 1.97 | 0.23 |
| 4:6:115:ASN:CB | 4:V:196:ARG:NH1[1_554] | 1.97 | 0.23 |
| 4:6:314:GLN:NE2 | 4:9:148:THR:N[1_554] | 1.97 | 0.23 |
| 4:6:211:ASP:OD2 | 4:9:32:PRO:CD[1_554] | 1.97 | 0.23 |
| 4:6:162:ASN:CB | 4:9:175:ILE:CD1[1_554] | 1.97 | 0.23 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:27:PRO:C | 4:8:122:ILE:CB[1_554] | 1.97 | 0.23 |
| 4:6:114:ALA:CA | 4:V:250:ILE:C[1_554] | 1.97 | 0.23 |
| 4:3:166:TYR:CE1 | 4:8:40:HIS:NE2[1_554] | 1.97 | 0.23 |
| 4:4:371:HIS:ND1 | 4:8:252:ASN:N[1_554] | 1.97 | 0.23 |
| 4:5:340:TRP:CE2 | 4:8:121:GLN:N[1_554] | 1.97 | 0.23 |
| 4:6:106:THR:N | 4:9:114:ALA:CB[1_554] | 1.97 | 0.23 |
| 4:6:189:LEU:N | 4:9:183:ARG:CA[1_554] | 1.97 | 0.23 |
| 4:6:192:ILE:CD1 | 4:9:213:LYS:CE[1_554] | 1.97 | 0.23 |
| 4:4:304:THR:OG1 | 4:7:107:GLU:N[1_554] | 1.97 | 0.23 |
| 4:5:314:GLN:NE2 | 4:8:147:ARG:CA[1_554] | 1.97 | 0.23 |
| 4:5:9:VAL:O | 4:8:118:LYS:CD[1_554] | 1.97 | 0.23 |
| 4:5:117:GLU:OE1 | 4:9:236:LEU:CG[1_554] | 1.97 | 0.23 |
| 4:6:192:ILE:CA | 4:9:213:LYS:CD[1_554] | 1.97 | 0.23 |
| 4:6:299:MET:CG | 4:9:137:GLN:C[1_554] | 1.97 | 0.23 |
| 4:6:157:ASP:O | 4:9:72:GLU:O[1_554] | 1.97 | 0.23 |
| 4:6:262:PHE:CB | 4:9:153:LEU:CD1[1_554] | 1.97 | 0.23 |
| 4:4:144:ALA:N | 4:7:371:HIS:C[1_554] | 1.97 | 0.23 |
| 4:5:301:GLY:CA | 4:8:107:GLU:CA[1_554] | 1.97 | 0.23 |
| 4:4:214:GLU:OE1 | 4:7:33:SER:CA[1_554] | 1.97 | 0.23 |
| 4:4:345:ILE:N | 4:7:366:GLY:C[1_554] | 1.97 | 0.23 |
| 4:6:184:ASP:CB | 4:9:158:GLY:O[1_554] | 1.97 | 0.23 |
| 4:6:312:ARG:O | 4:9:298:VAL:CG2[1_554] | 1.97 | 0.23 |
| 4:5:237:GLU:OE1 | 4:8:215:LYS:CD[1_554] | 1.97 | 0.23 |
| 4:3:115:ASN:CB | 4:7:196:ARG:NE[1_554] | 1.97 | 0.23 |
| 4:5:198:TYR:CE1 | 4:8:208:ILE:CA[1_554] | 1.97 | 0.23 |
| 4:5:263:GLN:CA | 4:8:274:ILE:CG2[1_554] | 1.97 | 0.23 |
| 4:4:15:GLY:N | 4:7:77:THR:CB[1_554] | 1.97 | 0.23 |
| 4:6:341:ILE:CG1 | 4:9:132:MET:SD[1_554] | 1.97 | 0.23 |
| 4:5:270:GLU:CG | 4:8:271:SER:O[1_554] | 1.97 | 0.23 |
| 4:5:173:HIS:CD2 | 4:9:264:PRO:O[1_554] | 1.97 | 0.23 |
| 4:6:136:ILE:CA | 4:9:113:LYS:CD[1_554] | 1.97 | 0.23 |
| 4:4:117:GLU:C | 4:8:237:GLU:OE1[1_554] | 1.97 | 0.23 |
| 4:5:256:ARG:CG | 4:8:306:TYR:CE1[1_554] | 1.97 | 0.23 |
| 4:6:154:ASP:CB | 4:9:110:LEU:N[1_554] | 1.97 | 0.23 |
| 4:4:318:THR:CB | 4:7:149:THR:C[1_554] | 1.97 | 0.23 |
| 4:5:154:ASP:CA | 4:8:110:LEU:N[1_554] | 1.97 | 0.23 |
| 4:3:112:PRO:N | 4:7:253:GLU:CG[1_554] | 1.97 | 0.23 |
| 4:5:16:LEU:N | 4:8:78:ASN:N[1_554] | 1.97 | 0.23 |
| 4:5:371:HIS:CE1 | 4:9:252:ASN:CB[1_554] | 1.98 | 0.22 |
| 4:4:266:PHE:CG | 4:7:261:LEU:CD2[1_554] | 1.98 | 0.22 |
| 4:4:276:GLU:CG | 4:7:278:THR:O[1_554] | 1.98 | 0.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:216:LEU:N | 4:7:30:VAL:CG1[1_554] | 1.98 | 0.22 |
| 4:4:340:TRP:N | 4:7:117:GLU:C[1_554] | 1.98 | 0.22 |
| 4:5:178:LEU:CD1 | 4:8:177:ARG:C[1_554] | 1.98 | 0.22 |
| 4:6:326:LYS:O | 4:9:167:GLU:OE2[1_554] | 1.98 | 0.22 |
| 4:3:292:ASP:N | 4:8:64:ILE:CG2[1_554] | 1.98 | 0.22 |
| 4:6:256:ARG:CD | 4:9:306:TYR:CE1[1_554] | 1.98 | 0.22 |
| 4:6:259:GLU:N | 4:9:304:THR:CG2[1_554] | 1.98 | 0.22 |
| 4:6:205:GLU:N | 4:9:62:ARG:CZ[1_554] | 1.98 | 0.22 |
| 4:5:346:LEU:CD1 | 4:8:368:SER:OG[1_554] | 1.98 | 0.22 |
| 4:4:113:LYS:C | 4:8:251:GLY:N[1_554] | 1.98 | 0.22 |
| 4:4:191:LYS:NZ | 4:7:185:LEU:O[1_554] | 1.98 | 0.22 |
| 4:5:24:ASP:CG | 4:8:124:PHE:O[1_554] | 1.98 | 0.22 |
| 4:5:278:THR:OG1 | 4:8:164:PRO:CD[1_554] | 1.98 | 0.22 |
| 4:5:313:MET:CG | 4:8:152:VAL:CG1[1_554] | 1.98 | 0.22 |
| 4:4:173:HIS:ND1 | 4:8:267:ILE:N[1_554] | 1.98 | 0.22 |
| 4:6:22:ALA:CB | 4:9:362:TYR:OH[1_554] | 1.98 | 0.22 |
| 4:5:227:MET:CG | 4:8:307:PRO:O[1_554] | 1.98 | 0.22 |
| 4:4:306:TYR:O | 4:7:11:ASP:OD2[1_554] | 1.98 | 0.22 |
| 4:4:191:LYS:C | 4:7:186:THR:C[1_554] | 1.98 | 0.22 |
| 4:6:289:ILE:CA | 4:W:64:ILE:CA[1_554] | 1.98 | 0.22 |
| 4:6:28:ARG:CB | 4:9:126:THR:OG1[1_554] | 1.98 | 0.22 |
| 4:4:314:GLN:N | 4:7:142:LEU:CA[1_554] | 1.98 | 0.22 |
| 4:6:270:GLU:O | 4:9:272:ALA:CA[1_554] | 1.98 | 0.22 |
| 4:6:268:GLY:C | 4:9:264:PRO:CG[1_554] | 1.98 | 0.22 |
| 4:5:213:LYS:CE | 4:8:14:SER:C[1_554] | 1.98 | 0.22 |
| 4:4:172:PRO:CA | 4:8:266:PHE:O[1_554] | 1.98 | 0.22 |
| 4:6:115:ASN:CB | 4:V:196:ARG:CG[1_554] | 1.98 | 0.22 |
| 4:5:151:ILE:CG1 | 4:8:172:PRO:N[1_554] | 1.98 | 0.22 |
| 4:6:156:GLY:CA | 4:9:74:GLY:CA[1_554] | 1.98 | 0.22 |
| 4:5:214:GLU:OE1 | 4:8:33:SER:N[1_554] | 1.98 | 0.22 |
| 4:4:262:PHE:CG | 4:7:154:ASP:CA[1_554] | 1.98 | 0.22 |
| 4:3:370:VAL:CB | 4:7:230:ALA:C[1_554] | 1.98 | 0.22 |
| 4:5:145:SER:C | 4:8:372:ARG:NH2[1_554] | 1.98 | 0.22 |
| 4:4:325:MET:CE | 4:7:166:TYR:CE2[1_554] | 1.98 | 0.22 |
| 4:4:223:PHE:CD1 | 4:7:335:ARG:CG[1_554] | 1.98 | 0.22 |
| 4:4:341:ILE:CD1 | 4:7:120:THR:CB[1_554] | 1.98 | 0.22 |
| 4:5:219:VAL:O | 4:8:335:ARG:O[1_554] | 1.98 | 0.22 |
| 4:5:207:GLU:CD | 4:8:67:LEU:CD2[1_554] | 1.98 | 0.22 |
| 4:5:276:GLU:O | 4:8:281:SER:CA[1_554] | 1.98 | 0.22 |
| 4:4:262:PHE:CG | 4:7:153:LEU:CA[1_554] | 1.98 | 0.22 |
| 4:5:137:GLN:CG | 4:8:112:PRO:CB[1_554] | 1.98 | 0.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:276:GLU:OE2 | 4:9:278:THR:N[1_554] | 1.98 | 0.22 |
| 4:5:316:GLU:CA | 4:8:297:ASN:CA[1_554] | 1.98 | 0.22 |
| 4:5:265:SER:C | 4:8:261:LEU:CA[1_554] | 1.98 | 0.22 |
| 4:3:370:VAL:CA | 4:7:229:THR:O[1_554] | 1.98 | 0.22 |
| 4:6:159:VAL:C | 4:9:177:ARG:CZ[1_554] | 1.98 | 0.22 |
| 4:6:367:PRO:CA | 4:V:233:SER:N[1_554] | 1.98 | 0.22 |
| 4:4:253:GLU:CD | 4:7:214:GLU:OE1[1_554] | 1.98 | 0.22 |
| 4:6:15:GLY:CA | 4:9:77:THR:OG1[1_554] | 1.98 | 0.22 |
| 4:6:16:LEU:N | 4:9:70:PRO:O[1_554] | 1.98 | 0.22 |
| 4:6:316:GLU:CG | 4:9:297:ASN:C[1_554] | 1.98 | 0.22 |
| 4:4:315:LYS:NZ | 4:7:296:ASN:OD1[1_554] | 1.98 | 0.22 |
| 4:5:14:SER:CA | 4:8:77:THR:OG1[1_554] | 1.98 | 0.22 |
| 4:5:111:ASN:C | 4:9:192:ILE:O[1_554] | 1.98 | 0.22 |
| 4:6:11:ASP:OD2 | 4:9:115:ASN:C[1_554] | 1.98 | 0.22 |
| 4:4:270:GLU:C | 4:7:272:ALA:CA[1_554] | 1.98 | 0.22 |
| 4:3:77:THR:O | 4:7:246:GLN:CD[1_554] | 1.98 | 0.22 |
| 4:6:162:ASN:CB | 4:9:175:ILE:CG1[1_554] | 1.98 | 0.22 |
| 4:2:287:ILE:C | 4:7:39:ARG:NH2[1_554] | 1.98 | 0.22 |
| 4:6:340:TRP:O | 4:9:120:THR:OG1[1_554] | 1.98 | 0.22 |
| 4:6:26:ALA:CB | 4:9:123:MET:CG[1_554] | 1.98 | 0.22 |
| 4:6:348:SER:CA | 4:9:366:GLY:N[1_554] | 1.98 | 0.22 |
| 4:4:186:THR:N | 4:7:183:ARG:NE[1_554] | 1.98 | 0.22 |
| 4:5:338:SER:C | 4:8:116:ARG:CG[1_554] | 1.98 | 0.22 |
| 4:5:315:LYS:CG | 4:8:147:ARG:NH1[1_554] | 1.98 | 0.22 |
| 4:5:191:LYS:CB | 4:8:187:ASP:CA[1_554] | 1.98 | 0.22 |
| 4:5:276:GLU:CD | 4:8:279:TYR:CA[1_554] | 1.98 | 0.22 |
| 4:6:227:MET:O | 4:9:307:PRO:CB[1_554] | 1.98 | 0.22 |
| 4:4:185:LEU:C | 4:7:158:GLY:N[1_554] | 1.98 | 0.22 |
| 4:4:317:ILE:CA | 4:7:150:GLY:N[1_554] | 1.98 | 0.22 |
| 4:5:223:PHE:CD2 | 4:8:304:THR:OG1[1_554] | 1.98 | 0.22 |
| 4:6:295:ALA:N | 4:9:167:GLU:CB[1_554] | 1.98 | 0.22 |
| 4:4:334:GLU:CD | 4:7:132:MET:CE[1_554] | 1.98 | 0.22 |
| 4:5:256:ARG:C | 4:8:303:THR:C[1_554] | 1.98 | 0.22 |
| 4:6:30:VAL:C | 4:9:82:MET:N[1_554] | 1.98 | 0.22 |
| 4:6:370:VAL:C | 4:V:231:ALA:CB[1_554] | 1.98 | 0.22 |
| 4:4:30:VAL:O | 4:7:80:ASP:C[1_554] | 1.98 | 0.22 |
| 4:6:113:LYS:CG | 4:V:253:GLU:CA[1_554] | 1.98 | 0.22 |
| 4:6:339:VAL:CB | 4:9:116:ARG:CB[1_554] | 1.98 | 0.22 |
| 4:4:173:HIS:NE2 | 4:8:266:PHE:N[1_554] | 1.98 | 0.22 |
| 4:4:367:PRO:C | 4:8:236:LEU:CB[1_554] | 1.98 | 0.22 |
| 4:4:372:ARG:CA | 4:8:227:MET:CA[1_554] | 1.98 | 0.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:250:ILE:CD1 | 4:9:210:ARG:NH2[1_554] | 1.98 | 0.22 |
| 4:5:319:ALA:N | 4:8:296:ASN:CB[1_554] | 1.98 | 0.22 |
| 4:4:109:PRO:CG | 4:8:195:GLU:CD[1_554] | 1.98 | 0.22 |
| 4:4:210:ARG:CB | 4:7:69:TYR:CZ[1_554] | 1.98 | 0.22 |
| 4:6:310:ALA:C | 4:9:141:SER:CA[1_554] | 1.98 | 0.22 |
| 4:5:286:ASP:N | 4:9:270:GLU:CG[1_554] | 1.98 | 0.22 |
| 4:6:255:PHE:CD2 | 4:9:305:MET:CE[1_554] | 1.98 | 0.22 |
| 4:5:218:TYR:N | 4:8:336:LYS:CB[1_554] | 1.98 | 0.22 |
| 4:4:143:TYR:N | 4:7:372:ARG:C[1_554] | 1.98 | 0.22 |
| 4:6:370:VAL:C | 4:V:231:ALA:CA[1_554] | 1.98 | 0.22 |
| 4:5:151:ILE:CG2 | 4:8:169:TYR:O[1_554] | 1.98 | 0.22 |
| 4:4:141:SER:O | 4:7:116:ARG:CD[1_554] | 1.98 | 0.22 |
| 4:4:143:TYR:CD2 | 4:7:368:SER:O[1_554] | 1.98 | 0.22 |
| 4:4:182:GLY:N | 4:7:73:HIS:N[1_554] | 1.98 | 0.22 |
| 4:6:270:GLU:C | 4:9:272:ALA:C[1_554] | 1.98 | 0.22 |
| 4:3:76:ILE:CA | 4:7:198:TYR:CE1[1_554] | 1.98 | 0.22 |
| 4:6:283:MET:N | 4:9:285:CYS:CA[1_554] | 1.98 | 0.22 |
| 4:6:118:LYS:N | 4:V:237:GLU:OE2[1_554] | 1.98 | 0.22 |
| 4:5:59:GLN:CG | 4:8:68:LYS:CD[1_554] | 1.98 | 0.22 |
| 4:6:329:ILE:CG1 | 4:9:142:LEU:CG[1_554] | 1.98 | 0.22 |
| 4:4:154:ASP:OD2 | 4:7:112:PRO:CD[1_554] | 1.99 | 0.21 |
| 4:4:279:TYR:CA | 4:7:164:PRO:CB[1_554] | 1.99 | 0.21 |
| 4:4:166:TYR:CE1 | 4:9:40:HIS:NE2[1_554] | 1.99 | 0.21 |
| 4:4:214:GLU:CA | 4:7:16:LEU:O[1_554] | 1.99 | 0.21 |
| 4:4:262:PHE:CB | 4:7:154:ASP:N[1_554] | 1.99 | 0.21 |
| 4:4:215:LYS:CG | 4:7:31:PHE:O[1_554] | 1.99 | 0.21 |
| 4:6:333:PRO:CD | 4:9:104:LEU:CD2[1_554] | 1.99 | 0.21 |
| 4:4:75:ILE:CA | 4:8:198:TYR:CB[1_554] | 1.99 | 0.21 |
| 4:4:337:TYR:O | 4:7:119:MET:N[1_554] | 1.99 | 0.21 |
| 4:6:316:GLU:CA | 4:9:296:ASN:C[1_554] | 1.99 | 0.21 |
| 4:5:321:ALA:C | 4:8:292:ASP:CA[1_554] | 1.99 | 0.21 |
| 4:4:180:LEU:CB | 4:7:179:ASP:CA[1_554] | 1.99 | 0.21 |
| 4:6:183:ARG:CD | 4:9:72:GLU:CD[1_554] | 1.99 | 0.21 |
| 4:5:109:PRO:O | 4:9:195:GLU:OE2[1_554] | 1.99 | 0.21 |
| 4:5:326:LYS:NZ | 4:V:45:VAL:CG2[1_554] | 1.99 | 0.21 |
| 4:5:186:THR:CB | 4:8:183:ARG:NH2[1_554] | 1.99 | 0.21 |
| 4:5:309:ILE:CG2 | 4:8:141:SER:OG[1_554] | 1.99 | 0.21 |
| 4:6:255:PHE:O | 4:9:302:GLY:O[1_554] | 1.99 | 0.21 |
| 4:6:16:LEU:O | 4:9:76:ILE:O[1_554] | 1.99 | 0.21 |
| 4:4:207:GLU:CA | 4:7:67:LEU:CD1[1_554] | 1.99 | 0.21 |
| 4:4:300:SER:O | 4:7:108:ALA:O[1_554] | 1.99 | 0.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:344:SER:N | 4:8:367:PRO:CA[1_554] | 1.99 | 0.21 |
| 4:5:259:GLU:N | 4:8:304:THR:N[1_554] | 1.99 | 0.21 |
| 4:5:17:VAL:CB | 4:8:79:TRP:CG[1_554] | 1.99 | 0.21 |
| 4:6:223:PHE:CE1 | 4:9:304:THR:O[1_554] | 1.99 | 0.21 |
| 4:4:183:ARG:O | 4:7:183:ARG:NH1[1_554] | 1.99 | 0.21 |
| 4:6:207:GLU:C | 4:9:59:GLN:NE2[1_554] | 1.99 | 0.21 |
| 4:6:204:ALA:O | 4:9:62:ARG:CG[1_554] | 1.99 | 0.21 |
| 4:2:291:LYS:NZ | 4:7:39:ARG:C[1_554] | 1.99 | 0.21 |
| 4:4:255:PHE:CZ | 4:7:305:MET:SD[1_554] | 1.99 | 0.21 |
| 4:3:371:HIS:ND1 | 4:7:252:ASN:N[1_554] | 1.99 | 0.21 |
| 4:5:211:ASP:OD2 | 4:8:32:PRO:CG[1_554] | 1.99 | 0.21 |
| 4:6:75:ILE:CG1 | 4:V:194:THR:CA[1_554] | 1.99 | 0.21 |
| 4:6:304:THR:O | 4:9:339:VAL:CG1[1_554] | 1.99 | 0.21 |
| 4:6:289:ILE:CG2 | 4:W:39:ARG:NH1[1_554] | 1.99 | 0.21 |
| 4:5:32:PRO:CD | 4:8:78:ASN:ND2[1_554] | 1.99 | 0.21 |
| 4:5:199:SER:CA | 4:8:205:GLU:C[1_554] | 1.99 | 0.21 |
| 4:5:326:LYS:O | 4:8:167:GLU:CD[1_554] | 1.99 | 0.21 |
| 4:4:270:GLU:CG | 4:7:271:SER:O[1_554] | 1.99 | 0.21 |
| 4:6:18:LYS:CA | 4:9:79:TRP:CD2[1_554] | 1.99 | 0.21 |
| 4:5:114:ALA:C | 4:9:251:GLY:N[1_554] | 1.99 | 0.21 |
| 4:5:319:ALA:C | 4:8:294:TYR:C[1_554] | 1.99 | 0.21 |
| 4:4:255:PHE:CD1 | 4:7:305:MET:SD[1_554] | 1.99 | 0.21 |
| 4:4:172:PRO:CB | 4:8:188:TYR:CZ[1_554] | 1.99 | 0.21 |
| 4:4:266:PHE:CD1 | 4:7:261:LEU:CG[1_554] | 1.99 | 0.21 |
| 4:6:215:LYS:CE | 4:9:31:PHE:CA[1_554] | 1.99 | 0.21 |
| 4:6:277:THR:CB | 4:9:176:MET:N[1_554] | 1.99 | 0.21 |
| 4:6:295:ALA:N | 4:9:167:GLU:N[1_554] | 1.99 | 0.21 |
| 4:4:275:HIS:O | 4:7:163:VAL:C[1_554] | 1.99 | 0.21 |
| 4:4:286:ASP:CA | 4:8:270:GLU:CG[1_554] | 1.99 | 0.21 |
| 4:6:140:LEU:C | 4:9:371:HIS:O[1_554] | 1.99 | 0.21 |
| 4:4:110:LEU:CA | 4:8:192:ILE:C[1_554] | 1.99 | 0.21 |
| 4:4:32:PRO:N | 4:7:78:ASN:ND2[1_554] | 1.99 | 0.21 |
| 4:4:220:ALA:C | 4:7:335:ARG:CB[1_554] | 1.99 | 0.21 |
| 4:6:109:PRO:C | 4:V:195:GLU:CG[1_554] | 1.99 | 0.21 |
| 4:4:314:GLN:CG | 4:7:143:TYR:CB[1_554] | 1.99 | 0.21 |
| 4:6:221:LEU:CA | 4:9:331:ALA:CA[1_554] | 1.99 | 0.21 |
| 4:5:143:TYR:CA | 4:8:372:ARG:N[1_554] | 1.99 | 0.21 |
| 4:5:143:TYR:CB | 4:8:371:HIS:C[1_554] | 1.99 | 0.21 |
| 4:6:312:ARG:CD | 4:9:298:VAL:C[1_554] | 1.99 | 0.21 |
| 4:5:266:PHE:CA | 4:8:261:LEU:CB[1_554] | 1.99 | 0.21 |
| 4:6:264:PRO:CD | 4:9:274:ILE:CD1[1_554] | 1.99 | 0.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:297:ASN:CG | 4:9:165:ILE:CB[1_554] | 1.99 | 0.21 |
| 4:3:117:GLU:N | 4:7:251:GLY:CA[1_554] | 1.99 | 0.21 |
| 4:6:192:ILE:O | 4:9:213:LYS:CA[1_554] | 1.99 | 0.21 |
| 4:5:368:SER:O | 4:9:229:THR:O[1_554] | 1.99 | 0.21 |
| 4:4:292:ASP:N | 4:9:64:ILE:CG2[1_554] | 1.99 | 0.21 |
| 4:5:151:ILE:CD1 | 4:8:171:LEU:CB[1_554] | 1.99 | 0.21 |
| 4:6:314:GLN:OE1 | 4:9:147:ARG:C[1_554] | 1.99 | 0.21 |
| 4:4:243:PRO:CG | 4:7:60:SER:C[1_554] | 1.99 | 0.21 |
| 4:5:210:ARG:NH1 | 4:8:33:SER:CA[1_554] | 1.99 | 0.21 |
| 4:4:113:LYS:N | 4:8:250:ILE:CG2[1_554] | 1.99 | 0.21 |
| 4:6:142:LEU:C | 4:9:372:ARG:CG[1_554] | 1.99 | 0.21 |
| 4:5:368:SER:CA | 4:9:229:THR:C[1_554] | 1.99 | 0.21 |
| 4:4:255:PHE:CZ | 4:7:305:MET:CG[1_554] | 1.99 | 0.21 |
| 4:6:345:ILE:C | 4:9:369:ILE:CB[1_554] | 1.99 | 0.21 |
| 4:6:257:CYS:C | 4:9:303:THR:N[1_554] | 1.99 | 0.21 |
| 4:4:306:TYR:N | 4:7:11:ASP:CG[1_554] | 1.99 | 0.21 |
| 4:5:208:ILE:CB | 4:8:59:GLN:OE1[1_554] | 1.99 | 0.21 |
| 4:5:227:MET:CB | 4:8:307:PRO:O[1_554] | 1.99 | 0.21 |
| 4:4:210:ARG:CG | 4:7:69:TYR:CG[1_554] | 1.99 | 0.21 |
| 4:5:277:THR:O | 4:8:174:ALA:CB[1_554] | 1.99 | 0.21 |
| 4:4:204:ALA:CB | 4:7:62:ARG:CB[1_554] | 1.99 | 0.21 |
| 4:4:187:ASP:N | 4:7:183:ARG:NE[1_554] | 1.99 | 0.21 |
| 4:4:183:ARG:CD | 4:7:72:GLU:OE1[1_554] | 1.99 | 0.21 |
| 4:5:334:GLU:C | 4:8:105:LEU:O[1_554] | 1.99 | 0.21 |
| 4:6:184:ASP:OD2 | 4:9:179:ASP:O[1_554] | 1.99 | 0.21 |
| 4:6:9:VAL:CB | 4:9:121:GLN:CB[1_554] | 1.99 | 0.21 |
| 4:5:59:GLN:CA | 4:8:68:LYS:CD[1_554] | 1.99 | 0.21 |
| 4:6:192:ILE:CD1 | 4:9:306:TYR:OH[1_554] | 1.99 | 0.21 |
| 4:6:211:ASP:CG | 4:9:32:PRO:CB[1_554] | 1.99 | 0.21 |
| 4:5:140:LEU:C | 4:8:371:HIS:O[1_554] | 1.99 | 0.21 |
| 4:4:366:GLY:O | 4:8:235:SER:N[1_554] | 1.99 | 0.21 |
| 4:5:115:ASN:C | 4:9:196:ARG:CZ[1_554] | 1.99 | 0.21 |
| 4:6:277:THR:OG1 | 4:9:176:MET:CB[1_554] | 1.99 | 0.21 |
| 4:3:110:LEU:C | 4:7:193:LEU:N[1_554] | 1.99 | 0.21 |
| 4:5:310:ALA:CB | 4:8:141:SER:C[1_554] | 1.99 | 0.21 |
| 4:6:276:GLU:CA | 4:9:281:SER:CB[1_554] | 1.99 | 0.21 |
| 4:5:336:LYS:C | 4:8:119:MET:CE[1_554] | 1.99 | 0.21 |
| 4:4:372:ARG:C | 4:8:226:GLU:O[1_554] | 1.99 | 0.21 |
| 4:6:31:PHE:CD2 | 4:9:78:ASN:OD1[1_554] | 1.99 | 0.21 |
| 4:6:204:ALA:N | 4:9:62:ARG:CB[1_554] | 1.99 | 0.21 |
| 4:5:283:MET:SD | 4:8:286:ASP:C[1_554] | 1.99 | 0.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:75:ILE:CG2 | 4:9:198:TYR:CD2[1_554] | 2.00 | 0.20 |
| 4:5:335:ARG:CD | 4:8:106:THR:CB[1_554] | 2.00 | 0.20 |
| 4:6:173:HIS:CB | 4:V:267:ILE:C[1_554] | 2.00 | 0.20 |
| 4:4:338:SER:CB | 4:7:116:ARG:CA[1_554] | 2.00 | 0.20 |
| 4:5:293:LEU:O | 4:8:169:TYR:CB[1_554] | 2.00 | 0.20 |
| 4:5:15:GLY:N | 4:8:77:THR:CA[1_554] | 2.00 | 0.20 |
| 4:5:141:SER:CB | 4:8:116:ARG:CZ[1_554] | 2.00 | 0.20 |
| 4:4:307:PRO:CD | 4:7:11:ASP:OD2[1_554] | 2.00 | 0.20 |
| 4:5:320:LEU:N | 4:8:293:LEU:O[1_554] | 2.00 | 0.20 |
| 4:4:111:ASN:O | 4:8:253:GLU:CD[1_554] | 2.00 | 0.20 |
| 4:5:223:PHE:O | 4:8:309:ILE:CG2[1_554] | 2.00 | 0.20 |
| 4:4:320:LEU:N | 4:7:293:LEU:N[1_554] | 2.00 | 0.20 |
| 4:6:326:LYS:NZ | 4:W:45:VAL:CG2[1_554] | 2.00 | 0.20 |
| 4:4:15:GLY:CA | 4:7:77:THR:OG1[1_554] | 2.00 | 0.20 |
| 4:6:153:LEU:O | 4:9:136:ILE:CG2[1_554] | 2.00 | 0.20 |
| 4:5:335:ARG:CG | 4:8:106:THR:OG1[1_554] | 2.00 | 0.20 |
| 4:5:73:HIS:CD2 | 4:9:199:SER:OG[1_554] | 2.00 | 0.20 |
| 4:4:189:LEU:N | 4:7:182:GLY:C[1_554] | 2.00 | 0.20 |
| 4:4:253:GLU:OE1 | 4:7:214:GLU:N[1_554] | 2.00 | 0.20 |
| 4:5:269:MET:CB | 4:8:271:SER:OG[1_554] | 2.00 | 0.20 |
| 4:4:222:ASP:C | 4:7:332:PRO:O[1_554] | 2.00 | 0.20 |
| 4:5:166:TYR:CZ | 4:V:39:ARG:CB[1_554] | 2.00 | 0.20 |
| 4:3:75:ILE:CA | 4:7:197:GLY:O[1_554] | 2.00 | 0.20 |
| 4:5:320:LEU:O | 4:8:290:ARG:CA[1_554] | 2.00 | 0.20 |
| 4:5:28:ARG:NE | 4:8:126:THR:CB[1_554] | 2.00 | 0.20 |
| 4:5:213:LYS:CE | 4:8:15:GLY:CA[1_554] | 2.00 | 0.20 |
| 4:4:199:SER:CB | 4:7:206:ARG:CB[1_554] | 2.00 | 0.20 |
| 4:5:192:ILE:CD1 | 4:8:213:LYS:CE[1_554] | 2.00 | 0.20 |
| 4:5:340:TRP:CZ2 | 4:8:121:GLN:N[1_554] | 2.00 | 0.20 |
| 1:D:637:LYS:CG | 4:6:311:ASP:CG[1_556] | 2.00 | 0.20 |
| 4:5:166:TYR:CA | 4:V:40:HIS:NE2[1_554] | 2.00 | 0.20 |
| 4:5:227:MET:N | 4:8:307:PRO:CA[1_554] | 2.00 | 0.20 |
| 4:6:15:GLY:C | 4:9:70:PRO:O[1_554] | 2.00 | 0.20 |
| 4:6:137:GLN:CG | 4:9:113:LYS:N[1_554] | 2.00 | 0.20 |
| 4:5:174:ALA:O | 4:8:173:HIS:N[1_554] | 2.00 | 0.20 |
| 4:6:144:ALA:CA | 4:9:370:VAL:O[1_554] | 2.00 | 0.20 |
| 4:4:278:THR:O | 4:7:171:LEU:CA[1_554] | 2.00 | 0.20 |
| 4:6:154:ASP:CB | 4:9:108:ALA:O[1_554] | 2.00 | 0.20 |
| 4:3:75:ILE:CA | 4:7:198:TYR:CG[1_554] | 2.00 | 0.20 |
| 4:5:218:TYR:CE1 | 4:8:337:TYR:CE2[1_554] | 2.00 | 0.20 |
| 4:6:186:THR:O | 4:9:183:ARG:CA[1_554] | 2.00 | 0.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:281:SER:N | 4:7:174:ALA:CA[1_554] | 2.00 | 0.20 |
| 4:6:341:ILE:CB | 4:9:132:MET:CE[1_554] | 2.00 | 0.20 |
| 4:4:192:ILE:O | 4:7:210:ARG:O[1_554] | 2.00 | 0.20 |
| 4:5:335:ARG:CD | 4:8:106:THR:CG2[1_554] | 2.00 | 0.20 |
| 4:4:309:ILE:O | 4:7:137:GLN:O[1_554] | 2.00 | 0.20 |
| 4:4:144:ALA:O | 4:7:370:VAL:CG2[1_554] | 2.00 | 0.20 |
| 4:6:301:GLY:N | 4:9:107:GLU:CB[1_554] | 2.00 | 0.20 |
| 4:6:270:GLU:CA | 4:9:271:SER:C[1_554] | 2.00 | 0.20 |
| 4:4:154:ASP:C | 4:7:111:ASN:N[1_554] | 2.00 | 0.20 |
| 4:5:142:LEU:C | 4:8:372:ARG:NE[1_554] | 2.00 | 0.20 |
| 4:4:162:ASN:CG | 4:7:175:ILE:CD1[1_554] | 2.00 | 0.20 |
| 4:5:340:TRP:CH2 | 4:8:120:THR:O[1_554] | 2.00 | 0.20 |
| 4:5:154:ASP:OD2 | 4:8:111:ASN:O[1_554] | 2.00 | 0.20 |
| 4:3:117:GLU:CA | 4:7:237:GLU:CD[1_554] | 2.00 | 0.20 |
| 4:5:347:ALA:CA | 4:8:366:GLY:C[1_554] | 2.00 | 0.20 |
| 4:4:308:GLY:CA | 4:7:339:VAL:C[1_554] | 2.00 | 0.20 |
| 4:6:208:ILE:CB | 4:9:59:GLN:CB[1_554] | 2.00 | 0.20 |
| 4:4:277:THR:C | 4:7:175:ILE:CA[1_554] | 2.00 | 0.20 |
| 4:5:317:ILE:CD1 | 4:8:165:ILE:C[1_554] | 2.00 | 0.20 |
| 4:6:328:LYS:CB | 4:9:148:THR:CG2[1_554] | 2.00 | 0.20 |
| 4:5:262:PHE:N | 4:8:153:LEU:CG[1_554] | 2.00 | 0.20 |
| 4:5:221:LEU:CA | 4:8:331:ALA:CA[1_554] | 2.00 | 0.20 |
| 4:2:323:SER:O | 4:7:44:MET:CG[1_554] | 2.00 | 0.20 |
| 4:6:274:ILE:O | 4:9:162:ASN:CA[1_554] | 2.00 | 0.20 |
| 4:6:277:THR:C | 4:9:174:ALA:C[1_554] | 2.00 | 0.20 |
| 4:5:26:ALA:O | 4:8:123:MET:C[1_554] | 2.00 | 0.20 |
| 4:4:223:PHE:CD1 | 4:7:304:THR:OG1[1_554] | 2.00 | 0.20 |
| 4:6:262:PHE:CE2 | 4:9:153:LEU:C[1_554] | 2.00 | 0.20 |
| 4:6:255:PHE:CZ | 4:9:305:MET:C[1_554] | 2.00 | 0.20 |
| 4:3:367:PRO:CB | 4:7:236:LEU:N[1_554] | 2.00 | 0.20 |
| 4:4:140:LEU:CD2 | 4:7:117:GLU:CD[1_554] | 2.00 | 0.20 |
| 4:6:253:GLU:OE1 | 4:9:214:GLU:C[1_554] | 2.00 | 0.20 |
| 4:5:11:ASP:OD2 | 4:8:115:ASN:C[1_554] | 2.00 | 0.20 |
| 4:5:273:GLY:O | 4:8:162:ASN:OD1[1_554] | 2.00 | 0.20 |
| 4:5:255:PHE:O | 4:8:302:GLY:O[1_554] | 2.00 | 0.20 |
| 4:6:28:ARG:NE | 4:9:126:THR:N[1_554] | 2.00 | 0.20 |
| 4:4:18:LYS:CD | 4:7:79:TRP:CZ2[1_554] | 2.00 | 0.20 |
| 4:5:214:GLU:CG | 4:8:16:LEU:C[1_554] | 2.00 | 0.20 |
| 4:4:223:PHE:N | 4:7:335:ARG:CD[1_554] | 2.00 | 0.20 |
| 4:5:205:GLU:CB | 4:8:62:ARG:NE[1_554] | 2.00 | 0.20 |
| 4:5:263:GLN:O | 4:8:274:ILE:CG1[1_554] | 2.00 | 0.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:227:MET:O | 4:8:307:PRO:CG[1_554] | 2.00 | 0.20 |
| 4:4:283:MET:CB | 4:7:285:CYS:CA[1_554] | 2.00 | 0.20 |
| 4:4:262:PHE:CA | 4:7:153:LEU:CG[1_554] | 2.00 | 0.20 |
| 4:5:280:ASN:O | 4:8:284:LYS:C[1_554] | 2.00 | 0.20 |
| 4:5:220:ALA:CB | 4:8:335:ARG:NH1[1_554] | 2.00 | 0.20 |
| 4:5:312:ARG:CB | 4:8:299:MET:O[1_554] | 2.00 | 0.20 |
| 4:5:17:VAL:O | 4:8:79:TRP:CG[1_554] | 2.00 | 0.20 |
| 4:3:75:ILE:CA | 4:7:198:TYR:CB[1_554] | 2.00 | 0.20 |
| 4:4:179:ASP:C | 4:7:179:ASP:OD1[1_554] | 2.00 | 0.20 |
| 4:4:371:HIS:ND1 | 4:8:252:ASN:C[1_554] | 2.00 | 0.20 |
| 4:4:157:ASP:CG | 4:7:72:GLU:N[1_554] | 2.00 | 0.20 |
| 4:5:16:LEU:O | 4:8:76:ILE:O[1_554] | 2.00 | 0.20 |
| 1:A:542:PHE:CZ | 4:5:328:LYS:CE[1_556] | 2.00 | 0.20 |
| 4:6:295:ALA:C | 4:9:168:GLY:CA[1_554] | 2.00 | 0.20 |
| 4:2:325:MET:CE | 4:7:64:ILE:CB[1_554] | 2.00 | 0.20 |
| 4:6:227:MET:CG | 4:9:307:PRO:O[1_554] | 2.00 | 0.20 |
| 4:6:279:TYR:CE2 | 4:9:282:ILE:O[1_554] | 2.00 | 0.20 |
| 4:5:329:ILE:O | 4:8:139:VAL:O[1_554] | 2.00 | 0.20 |
| 4:5:215:LYS:CD | 4:8:30:VAL:C[1_554] | 2.00 | 0.20 |
| 4:4:199:SER:OG | 4:7:206:ARG:N[1_554] | 2.00 | 0.20 |
| 4:6:315:LYS:O | 4:9:296:ASN:O[1_554] | 2.00 | 0.20 |
| 4:4:304:THR:CA | 4:7:137:GLN:CG[1_554] | 2.00 | 0.20 |
| 4:5:162:ASN:CB | 4:8:172:PRO:O[1_554] | 2.00 | 0.20 |
| 4:4:218:TYR:CD2 | 4:7:337:TYR:CB[1_554] | 2.00 | 0.20 |
| 4:5:340:TRP:N | 4:8:116:ARG:CA[1_554] | 2.00 | 0.20 |
| 4:5:281:SER:CA | 4:8:174:ALA:N[1_554] | 2.00 | 0.20 |
| 4:6:346:LEU:C | 4:9:366:GLY:C[1_554] | 2.00 | 0.20 |
| 4:4:272:ALA:O | 4:7:277:THR:CG2[1_554] | 2.00 | 0.20 |
| 4:6:276:GLU:O | 4:9:281:SER:C[1_554] | 2.00 | 0.20 |
| 4:6:204:ALA:O | 4:9:62:ARG:NH1[1_554] | 2.00 | 0.20 |
| 4:5:280:ASN:N | 4:8:281:SER:O[1_554] | 2.00 | 0.20 |
| 4:5:151:ILE:CG1 | 4:8:172:PRO:CD[1_554] | 2.00 | 0.20 |
| 4:5:289:ILE:CA | 4:V:64:ILE:N[1_554] | 2.01 | 0.19 |
| 4:5:340:TRP:CE3 | 4:8:120:THR:O[1_554] | 2.01 | 0.19 |
| 4:5:268:GLY:CA | 4:8:264:PRO:C[1_554] | 2.01 | 0.19 |
| 4:4:76:ILE:CA | 4:8:198:TYR:CE1[1_554] | 2.01 | 0.19 |
| 4:5:253:GLU:OE2 | 4:8:214:GLU:N[1_554] | 2.01 | 0.19 |
| 4:6:204:ALA:N | 4:9:62:ARG:CG[1_554] | 2.01 | 0.19 |
| 4:5:318:THR:CG2 | 4:8:149:THR:O[1_554] | 2.01 | 0.19 |
| 4:6:290:ARG:CZ | 4:9:286:ASP:CG[1_554] | 2.01 | 0.19 |
| 4:3:367:PRO:C | 4:7:236:LEU:CD2[1_554] | 2.01 | 0.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:311:ASP:CG | 4:7:144:ALA:CA[1_554] | 2.01 | 0.19 |
| 4:6:309:ILE:CA | 4:9:141:SER:CB[1_554] | 2.01 | 0.19 |
| 4:5:29:ALA:CA | 4:8:83:GLU:CD[1_554] | 2.01 | 0.19 |
| 4:4:197:GLY:O | 4:7:208:ILE:CA[1_554] | 2.01 | 0.19 |
| 4:4:198:TYR:C | 4:7:206:ARG:CA[1_554] | 2.01 | 0.19 |
| 4:4:345:ILE:CB | 4:7:368:SER:N[1_554] | 2.01 | 0.19 |
| 4:4:342:GLY:C | 4:7:117:GLU:CG[1_554] | 2.01 | 0.19 |
| 4:5:278:THR:CA | 4:8:164:PRO:N[1_554] | 2.01 | 0.19 |
| 4:6:214:GLU:OE1 | 4:9:33:SER:N[1_554] | 2.01 | 0.19 |
| 4:4:316:GLU:CG | 4:7:151:ILE:O[1_554] | 2.01 | 0.19 |
| 4:4:293:LEU:CA | 4:7:169:TYR:CE2[1_554] | 2.01 | 0.19 |
| 4:6:338:SER:N | 4:9:134:VAL:CG2[1_554] | 2.01 | 0.19 |
| 4:4:357:ILE:CA | 4:8:232:SER:CA[1_554] | 2.01 | 0.19 |
| 4:6:268:GLY:N | 4:9:264:PRO:CA[1_554] | 2.01 | 0.19 |
| 4:4:185:LEU:N | 4:7:158:GLY:O[1_554] | 2.01 | 0.19 |
| 4:4:342:GLY:CA | 4:7:367:PRO:O[1_554] | 2.01 | 0.19 |
| 4:5:344:SER:OG | 4:8:362:TYR:CZ[1_554] | 2.01 | 0.19 |
| 4:5:31:PHE:CD2 | 4:8:78:ASN:OD1[1_554] | 2.01 | 0.19 |
| 4:6:281:SER:OG | 4:9:173:HIS:C[1_554] | 2.01 | 0.19 |
| 4:4:300:SER:O | 4:7:108:ALA:N[1_554] | 2.01 | 0.19 |
| 4:5:317:ILE:CG2 | 4:8:151:ILE:N[1_554] | 2.01 | 0.19 |
| 4:4:223:PHE:CE2 | 4:7:300:SER:CA[1_554] | 2.01 | 0.19 |
| 4:5:140:LEU:N | 4:8:371:HIS:CG[1_554] | 2.01 | 0.19 |
| 4:4:328:LYS:C | 4:7:168:GLY:O[1_554] | 2.01 | 0.19 |
| 4:5:253:GLU:CG | 4:8:214:GLU:CB[1_554] | 2.01 | 0.19 |
| 4:4:339:VAL:N | 4:7:116:ARG:CB[1_554] | 2.01 | 0.19 |
| 4:5:295:ALA:C | 4:8:168:GLY:CA[1_554] | 2.01 | 0.19 |
| 4:4:259:GLU:N | 4:7:155:SER:C[1_554] | 2.01 | 0.19 |
| 4:5:213:LYS:CA | 4:8:16:LEU:CD2[1_554] | 2.01 | 0.19 |
| 4:4:343:GLY:N | 4:7:117:GLU:CG[1_554] | 2.01 | 0.19 |
| 4:5:295:ALA:CB | 4:8:167:GLU:C[1_554] | 2.01 | 0.19 |
| 4:6:337:TYR:OH | 4:9:86:TRP:CZ2[1_554] | 2.01 | 0.19 |
| 4:6:22:ALA:C | 4:9:362:TYR:CZ[1_554] | 2.01 | 0.19 |
| 4:3:357:ILE:CD1 | 4:7:232:SER:CB[1_554] | 2.01 | 0.19 |
| 4:3:357:ILE:CA | 4:7:232:SER:CA[1_554] | 2.01 | 0.19 |
| 4:4:181:ALA:N | 4:7:159:VAL:CG1[1_554] | 2.01 | 0.19 |
| 4:6:9:VAL:O | 4:9:118:LYS:CD[1_554] | 2.01 | 0.19 |
| 4:3:113:LYS:CD | 4:7:254:ARG:CB[1_554] | 2.01 | 0.19 |
| 4:4:340:TRP:NE1 | 4:7:118:LYS:CE[1_554] | 2.01 | 0.19 |
| 4:4:317:ILE:CB | 4:7:165:ILE:O[1_554] | 2.01 | 0.19 |
| 4:5:227:MET:CA | 4:8:307:PRO:N[1_554] | 2.01 | 0.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:171:LEU:O | 4:7:266:PHE:C[1_554] | 2.01 | 0.19 |
| 4:6:270:GLU:CA | 4:9:272:ALA:CB[1_554] | 2.01 | 0.19 |
| 4:5:9:VAL:CG1 | 4:8:117:GLU:O[1_554] | 2.01 | 0.19 |
| 4:5:154:ASP:CB | 4:8:109:PRO:C[1_554] | 2.01 | 0.19 |
| 4:5:196:ARG:CA | 4:8:212:ILE:CA[1_554] | 2.01 | 0.19 |
| 4:4:357:ILE:CD1 | 4:8:232:SER:OG[1_554] | 2.01 | 0.19 |
| 4:5:286:ASP:CB | 4:9:270:GLU:OE2[1_554] | 2.01 | 0.19 |
| 4:5:297:ASN:O | 4:8:139:VAL:CG2[1_554] | 2.01 | 0.19 |
| 4:6:211:ASP:OD2 | 4:9:32:PRO:CG[1_554] | 2.01 | 0.19 |
| 4:5:258:PRO:CD | 4:8:302:GLY:CA[1_554] | 2.01 | 0.19 |
| 4:3:289:ILE:CG1 | 4:8:39:ARG:NH2[1_554] | 2.01 | 0.19 |
| 4:6:336:LYS:NZ | 4:9:10:CYS:SG[1_554] | 2.01 | 0.19 |
| 4:5:255:PHE:CE2 | 4:8:305:MET:O[1_554] | 2.01 | 0.19 |
| 4:6:76:ILE:N | 4:V:197:GLY:C[1_554] | 2.01 | 0.19 |
| 4:4:343:GLY:N | 4:7:117:GLU:CD[1_554] | 2.01 | 0.19 |
| 4:5:250:ILE:CG2 | 4:8:214:GLU:OE2[1_554] | 2.01 | 0.19 |
| 4:6:346:LEU:N | 4:9:369:ILE:CG2[1_554] | 2.01 | 0.19 |
| 4:6:135:ALA:CB | 4:9:117:GLU:OE2[1_554] | 2.01 | 0.19 |
| 4:4:143:TYR:C | 4:7:371:HIS:N[1_554] | 2.01 | 0.19 |
| 4:6:327:ILE:CG2 | 4:9:149:THR:C[1_554] | 2.01 | 0.19 |
| 4:4:32:PRO:N | 4:7:78:ASN:OD1[1_554] | 2.01 | 0.19 |
| 4:5:21:PHE:N | 4:8:121:GLN:NE2[1_554] | 2.01 | 0.19 |
| 4:5:308:GLY:CA | 4:8:338:SER:N[1_554] | 2.01 | 0.19 |
| 4:6:300:SER:CA | 4:9:107:GLU:O[1_554] | 2.01 | 0.19 |
| 4:5:161:HIS:C | 4:8:110:LEU:CD1[1_554] | 2.01 | 0.19 |
| 4:4:366:GLY:O | 4:8:234:SER:C[1_554] | 2.01 | 0.19 |
| 4:4:211:ASP:C | 4:7:32:PRO:N[1_554] | 2.01 | 0.19 |
| 4:6:11:ASP:OD1 | 4:9:115:ASN:N[1_554] | 2.01 | 0.19 |
| 4:4:280:ASN:C | 4:7:174:ALA:CB[1_554] | 2.01 | 0.19 |
| 4:3:286:ASP:CB | 4:7:270:GLU:CD[1_554] | 2.01 | 0.19 |
| 4:4:316:GLU:OE2 | 4:7:153:LEU:N[1_554] | 2.01 | 0.19 |
| 4:6:298:VAL:C | 4:9:136:ILE:CB[1_554] | 2.01 | 0.19 |
| 4:6:62:ARG:NH2 | 4:9:67:LEU:CB[1_554] | 2.01 | 0.19 |
| 4:4:214:GLU:O | 4:7:17:VAL:C[1_554] | 2.01 | 0.19 |
| 4:3:115:ASN:ND2 | 4:7:249:THR:O[1_554] | 2.01 | 0.19 |
| 4:4:259:GLU:OE2 | 4:7:304:THR:C[1_554] | 2.01 | 0.19 |
| 4:5:11:ASP:OD1 | 4:8:115:ASN:N[1_554] | 2.01 | 0.19 |
| 4:6:311:ASP:CG | 4:9:144:ALA:C[1_554] | 2.01 | 0.19 |
| 4:6:196:ARG:C | 4:9:212:ILE:CG2[1_554] | 2.01 | 0.19 |
| 4:6:334:GLU:N | 4:9:104:LEU:CA[1_554] | 2.01 | 0.19 |
| 4:6:31:PHE:O | 4:9:78:ASN:CG[1_554] | 2.01 | 0.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:336:LYS:N | 4:8:106:THR:C[1_554] | 2.01 | 0.19 |
| 4:4:262:PHE:CD1 | 4:7:153:LEU:CA[1_554] | 2.01 | 0.19 |
| 4:6:190:MET:CG | 4:9:187:ASP:OD1[1_554] | 2.01 | 0.19 |
| 4:6:145:SER:CB | 4:9:372:ARG:NH2[1_554] | 2.01 | 0.19 |
| 4:4:186:THR:N | 4:7:183:ARG:CZ[1_554] | 2.01 | 0.19 |
| 4:5:20:GLY:CA | 4:8:121:GLN:CD[1_554] | 2.01 | 0.19 |
| 4:4:76:ILE:C | 4:8:198:TYR:CD1[1_554] | 2.01 | 0.19 |
| 4:5:327:ILE:CB | 4:8:148:THR:C[1_554] | 2.01 | 0.19 |
| 4:5:305:MET:CB | 4:8:11:ASP:OD2[1_554] | 2.01 | 0.19 |
| 4:5:283:MET:N | 4:8:285:CYS:CA[1_554] | 2.01 | 0.19 |
| 4:6:117:GLU:OE1 | 4:V:236:LEU:CG[1_554] | 2.01 | 0.19 |
| 4:4:215:LYS:CG | 4:7:31:PHE:CA[1_554] | 2.01 | 0.19 |
| 4:5:331:ALA:CB | 4:8:140:LEU:CD2[1_554] | 2.01 | 0.19 |
| 4:4:270:GLU:CG | 4:7:272:ALA:CA[1_554] | 2.01 | 0.19 |
| 4:5:30:VAL:CG2 | 4:8:83:GLU:N[1_554] | 2.01 | 0.19 |
| 4:6:291:LYS:CE | 4:W:64:ILE:CG1[1_554] | 2.01 | 0.19 |
| 4:5:145:SER:CB | 4:8:133:TYR:OH[1_554] | 2.01 | 0.19 |
| 4:4:307:PRO:CA | 4:7:340:TRP:N[1_554] | 2.01 | 0.19 |
| 4:6:115:ASN:CG | 4:V:196:ARG:CG[1_554] | 2.01 | 0.19 |
| 4:5:326:LYS:CD | 4:8:167:GLU:OE1[1_554] | 2.01 | 0.19 |
| 4:6:340:TRP:CB | 4:9:119:MET:CB[1_554] | 2.01 | 0.19 |
| 4:6:173:HIS:ND1 | 4:V:266:PHE:CA[1_554] | 2.01 | 0.19 |
| 4:5:162:ASN:CA | 4:8:110:LEU:CD2[1_554] | 2.01 | 0.19 |
| 4:6:198:TYR:CA | 4:9:209:VAL:N[1_554] | 2.01 | 0.19 |
| 4:3:114:ALA:N | 4:7:250:ILE:CB[1_554] | 2.01 | 0.19 |
| 4:5:327:ILE:CG1 | 4:8:149:THR:OG1[1_554] | 2.02 | 0.18 |
| 4:5:218:TYR:CD1 | 4:8:336:LYS:CB[1_554] | 2.02 | 0.18 |
| 4:5:26:ALA:N | 4:8:124:PHE:N[1_554] | 2.02 | 0.18 |
| 4:5:296:ASN:N | 4:8:168:GLY:CA[1_554] | 2.02 | 0.18 |
| 4:6:275:HIS:CA | 4:9:151:ILE:CG1[1_554] | 2.02 | 0.18 |
| 4:4:281:SER:CB | 4:7:174:ALA:N[1_554] | 2.02 | 0.18 |
| 4:6:221:LEU:N | 4:9:332:PRO:N[1_554] | 2.02 | 0.18 |
| 4:4:339:VAL:CG1 | 4:7:114:ALA:N[1_554] | 2.02 | 0.18 |
| 4:6:280:ASN:ND2 | 4:9:282:ILE:C[1_554] | 2.02 | 0.18 |
| 4:4:27:PRO:N | 4:7:122:ILE:CA[1_554] | 2.02 | 0.18 |
| 4:5:274:ILE:O | 4:8:162:ASN:CA[1_554] | 2.02 | 0.18 |
| 4:4:166:TYR:CE1 | 4:9:40:HIS:CE1[1_554] | 2.02 | 0.18 |
| 4:5:150:GLY:O | 4:8:169:TYR:CZ[1_554] | 2.02 | 0.18 |
| 4:6:223:PHE:CD2 | 4:9:304:THR:OG1[1_554] | 2.02 | 0.18 |
| 4:4:243:PRO:CG | 4:7:59:GLN:C[1_554] | 2.02 | 0.18 |
| 4:4:195:GLU:N | 4:7:209:VAL:CG2[1_554] | 2.02 | 0.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:210:ARG:N | 4:7:69:TYR:CZ[1_554] | 2.02 | 0.18 |
| 4:4:314:GLN:CD | 4:7:147:ARG:O[1_554] | 2.02 | 0.18 |
| 4:6:316:GLU:C | 4:9:296:ASN:C[1_554] | 2.02 | 0.18 |
| 4:6:14:SER:O | 4:9:77:THR:CB[1_554] | 2.02 | 0.18 |
| 4:4:277:THR:CA | 4:7:175:ILE:N[1_554] | 2.02 | 0.18 |
| 4:4:345:ILE:C | 4:7:366:GLY:CA[1_554] | 2.02 | 0.18 |
| 4:5:257:CYS:CA | 4:8:303:THR:CA[1_554] | 2.02 | 0.18 |
| 4:6:270:GLU:N | 4:9:272:ALA:CA[1_554] | 2.02 | 0.18 |
| 4:6:60:SER:OG | 4:9:37:ARG:CB[1_554] | 2.02 | 0.18 |
| 4:4:342:GLY:O | 4:7:368:SER:N[1_554] | 2.02 | 0.18 |
| 4:3:117:GLU:CB | 4:7:237:GLU:C[1_554] | 2.02 | 0.18 |
| 4:5:200:PHE:CZ | 4:8:207:GLU:CA[1_554] | 2.02 | 0.18 |
| 4:5:331:ALA:O | 4:8:140:LEU:CG[1_554] | 2.02 | 0.18 |
| 4:4:338:SER:C | 4:7:116:ARG:CB[1_554] | 2.02 | 0.18 |
| 4:4:112:PRO:CA | 4:8:253:GLU:CG[1_554] | 2.02 | 0.18 |
| 4:6:260:THR:CB | 4:9:155:SER:OG[1_554] | 2.02 | 0.18 |
| 4:5:198:TYR:CE2 | 4:8:211:ASP:CB[1_554] | 2.02 | 0.18 |
| 4:6:308:GLY:O | 4:9:338:SER:CB[1_554] | 2.02 | 0.18 |
| 4:4:159:VAL:CA | 4:7:177:ARG:CZ[1_554] | 2.02 | 0.18 |
| 4:6:205:GLU:CB | 4:9:62:ARG:CZ[1_554] | 2.02 | 0.18 |
| 4:6:277:THR:O | 4:9:174:ALA:CB[1_554] | 2.02 | 0.18 |
| 4:5:192:ILE:CD1 | 4:8:306:TYR:OH[1_554] | 2.02 | 0.18 |
| 4:5:223:PHE:CE1 | 4:8:304:THR:O[1_554] | 2.02 | 0.18 |
| 4:5:297:ASN:N | 4:8:169:TYR:N[1_554] | 2.02 | 0.18 |
| 4:4:319:ALA:C | 4:7:292:ASP:C[1_554] | 2.02 | 0.18 |
| 4:6:205:GLU:O | 4:9:59:GLN:OE1[1_554] | 2.02 | 0.18 |
| 4:5:344:SER:OG | 4:8:362:TYR:CE1[1_554] | 2.02 | 0.18 |
| 4:5:332:PRO:CG | 4:8:135:ALA:CB[1_554] | 2.02 | 0.18 |
| 4:4:62:ARG:NH2 | 4:7:67:LEU:O[1_554] | 2.02 | 0.18 |
| 4:4:143:TYR:CD2 | 4:7:368:SER:OG[1_554] | 2.02 | 0.18 |
| 4:6:261:LEU:CA | 4:9:160:THR:CG2[1_554] | 2.02 | 0.18 |
| 4:6:319:ALA:C | 4:9:292:ASP:O[1_554] | 2.02 | 0.18 |
| 4:6:348:SER:O | 4:9:365:ALA:N[1_554] | 2.02 | 0.18 |
| 4:3:357:ILE:CB | 4:7:232:SER:O[1_554] | 2.02 | 0.18 |
| 4:6:279:TYR:CE1 | 4:9:293:LEU:CD2[1_554] | 2.02 | 0.18 |
| 4:4:142:LEU:O | 4:7:371:HIS:C[1_554] | 2.02 | 0.18 |
| 4:3:289:ILE:N | 4:8:39:ARG:CZ[1_554] | 2.02 | 0.18 |
| 4:4:159:VAL:CA | 4:7:177:ARG:NH2[1_554] | 2.02 | 0.18 |
| 4:6:313:MET:CB | 4:9:152:VAL:CB[1_554] | 2.02 | 0.18 |
| 4:4:16:LEU:N | 4:7:77:THR:CB[1_554] | 2.02 | 0.18 |
| 4:4:339:VAL:O | 4:7:117:GLU:CA[1_554] | 2.02 | 0.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:150:GLY:O | 4:9:169:TYR:CZ[1_554] | 2.02 | 0.18 |
| 4:6:200:PHE:CZ | 4:9:207:GLU:CA[1_554] | 2.02 | 0.18 |
| 4:6:256:ARG:CA | 4:9:303:THR:O[1_554] | 2.02 | 0.18 |
| 4:4:271:SER:O | 4:7:277:THR:CG2[1_554] | 2.02 | 0.18 |
| 4:4:367:PRO:CB | 4:8:236:LEU:N[1_554] | 2.02 | 0.18 |
| 4:6:334:GLU:CG | 4:9:104:LEU:CA[1_554] | 2.02 | 0.18 |
| 4:6:328:LYS:N | 4:9:148:THR:CA[1_554] | 2.02 | 0.18 |
| 4:6:222:ASP:N | 4:9:331:ALA:O[1_554] | 2.02 | 0.18 |
| 4:3:367:PRO:CA | 4:7:235:SER:CA[1_554] | 2.02 | 0.18 |
| 4:5:193:LEU:CD1 | 4:8:210:ARG:CB[1_554] | 2.02 | 0.18 |
| 4:4:335:ARG:NH1 | 4:7:105:LEU:O[1_554] | 2.02 | 0.18 |
| 4:6:189:LEU:CA | 4:9:182:GLY:C[1_554] | 2.02 | 0.18 |
| 4:4:112:PRO:CB | 4:8:250:ILE:CG1[1_554] | 2.02 | 0.18 |
| 4:4:161:HIS:O | 4:7:110:LEU:CA[1_554] | 2.02 | 0.18 |
| 4:6:31:PHE:CD1 | 4:9:79:TRP:C[1_554] | 2.02 | 0.18 |
| 4:6:340:TRP:CH2 | 4:9:121:GLN:N[1_554] | 2.02 | 0.18 |
| 4:6:215:LYS:CB | 4:9:30:VAL:CG1[1_554] | 2.02 | 0.18 |
| 4:6:191:LYS:CB | 4:9:188:TYR:N[1_554] | 2.02 | 0.18 |
| 4:4:215:LYS:C | 4:7:31:PHE:N[1_554] | 2.02 | 0.18 |
| 4:3:175:ILE:CB | 4:7:191:LYS:CE[1_554] | 2.02 | 0.18 |
| 4:4:193:LEU:O | 4:7:210:ARG:CB[1_554] | 2.02 | 0.18 |
| 4:4:316:GLU:CB | 4:7:151:ILE:O[1_554] | 2.02 | 0.18 |
| 4:6:227:MET:CE | 4:9:306:TYR:CA[1_554] | 2.02 | 0.18 |
| 4:5:24:ASP:CB | 4:8:125:GLU:CA[1_554] | 2.02 | 0.18 |
| 4:4:214:GLU:CA | 4:7:17:VAL:N[1_554] | 2.02 | 0.18 |
| 4:5:255:PHE:CA | 4:8:305:MET:CG[1_554] | 2.02 | 0.18 |
| 4:4:264:PRO:C | 4:7:178:LEU:CD2[1_554] | 2.02 | 0.18 |
| 4:4:144:ALA:N | 4:7:370:VAL:C[1_554] | 2.02 | 0.18 |
| 4:4:24:ASP:C | 4:7:125:GLU:CD[1_554] | 2.02 | 0.18 |
| 4:6:367:PRO:CB | 4:V:233:SER:CA[1_554] | 2.02 | 0.18 |
| 4:4:276:GLU:CB | 4:7:281:SER:OG[1_554] | 2.02 | 0.18 |
| 4:4:194:THR:CA | 4:7:209:VAL:CB[1_554] | 2.02 | 0.18 |
| 4:6:297:ASN:N | 4:9:169:TYR:N[1_554] | 2.02 | 0.18 |
| 4:6:25:ASP:O | 4:9:123:MET:CB[1_554] | 2.02 | 0.18 |
| 4:5:142:LEU:O | 4:8:372:ARG:CG[1_554] | 2.02 | 0.18 |
| 4:5:11:ASP:OD2 | 4:8:115:ASN:O[1_554] | 2.02 | 0.18 |
| 4:5:75:ILE:N | 4:9:197:GLY:C[1_554] | 2.02 | 0.18 |
| 4:5:274:ILE:CD1 | 4:8:161:HIS:CG[1_554] | 2.02 | 0.18 |
| 4:5:337:TYR:CA | 4:8:119:MET:SD[1_554] | 2.02 | 0.18 |
| 4:6:153:LEU:CG | 4:9:163:VAL:CG2[1_554] | 2.02 | 0.18 |
| 4:5:143:TYR:CD2 | 4:8:368:SER:O[1_554] | 2.02 | 0.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:204:ALA:CB | 4:9:62:ARG:N[1_554] | 2.02 | 0.18 |
| 4:5:112:PRO:CB | 4:9:253:GLU:CG[1_554] | 2.02 | 0.18 |
| 4:6:276:GLU:CB | 4:9:281:SER:CB[1_554] | 2.02 | 0.18 |
| 4:4:343:GLY:N | 4:7:117:GLU:OE1[1_554] | 2.02 | 0.18 |
| 4:5:166:TYR:OH | 4:V:39:ARG:CB[1_554] | 2.02 | 0.18 |
| 4:6:193:LEU:CG | 4:9:210:ARG:C[1_554] | 2.02 | 0.18 |
| 4:5:309:ILE:CD1 | 4:8:154:ASP:OD1[1_554] | 2.02 | 0.18 |
| 4:5:143:TYR:CB | 4:8:372:ARG:CB[1_554] | 2.02 | 0.18 |
| 4:4:267:ILE:CD1 | 4:7:180:LEU:C[1_554] | 2.02 | 0.18 |
| 4:6:309:ILE:CD1 | 4:9:154:ASP:OD1[1_554] | 2.02 | 0.18 |
| 4:6:308:GLY:N | 4:9:337:TYR:C[1_554] | 2.02 | 0.18 |
| 4:6:279:TYR:OH | 4:9:290:ARG:CA[1_554] | 2.02 | 0.18 |
| 4:5:272:ALA:CB | 4:8:277:THR:O[1_554] | 2.02 | 0.18 |
| 4:5:116:ARG:CB | 4:9:252:ASN:OD1[1_554] | 2.02 | 0.18 |
| 4:6:25:ASP:CG | 4:9:129:VAL:C[1_554] | 2.02 | 0.18 |
| 4:6:265:SER:CA | 4:9:261:LEU:C[1_554] | 2.02 | 0.18 |
| 4:6:9:VAL:O | 4:9:121:GLN:OE1[1_554] | 2.02 | 0.18 |
| 4:4:18:LYS:CB | 4:7:79:TRP:CD2[1_554] | 2.02 | 0.18 |
| 4:3:173:HIS:NE2 | 4:7:265:SER:N[1_554] | 2.02 | 0.18 |
| 4:5:186:THR:O | 4:8:183:ARG:CA[1_554] | 2.03 | 0.17 |
| 4:4:75:ILE:CG1 | 4:8:193:LEU:C[1_554] | 2.03 | 0.17 |
| 4:3:77:THR:CA | 4:7:246:GLN:NE2[1_554] | 2.03 | 0.17 |
| 4:6:261:LEU:CD2 | 4:9:160:THR:CA[1_554] | 2.03 | 0.17 |
| 4:4:15:GLY:C | 4:7:77:THR:CA[1_554] | 2.03 | 0.17 |
| 4:3:166:TYR:CE1 | 4:8:39:ARG:O[1_554] | 2.03 | 0.17 |
| 4:6:166:TYR:CD2 | 4:W:40:HIS:CG[1_554] | 2.03 | 0.17 |
| 4:6:173:HIS:CA | 4:V:267:ILE:C[1_554] | 2.03 | 0.17 |
| 4:4:291:LYS:CB | 4:9:64:ILE:CG1[1_554] | 2.03 | 0.17 |
| 4:4:113:LYS:C | 4:8:250:ILE:C[1_554] | 2.03 | 0.17 |
| 4:6:321:ALA:C | 4:9:292:ASP:CG[1_554] | 2.03 | 0.17 |
| 4:4:118:LYS:CB | 4:8:249:THR:CB[1_554] | 2.03 | 0.17 |
| 4:6:367:PRO:N | 4:V:234:SER:CA[1_554] | 2.03 | 0.17 |
| 4:5:293:LEU:O | 4:8:169:TYR:CA[1_554] | 2.03 | 0.17 |
| 4:4:161:HIS:N | 4:7:110:LEU:CB[1_554] | 2.03 | 0.17 |
| 4:6:205:GLU:CB | 4:9:62:ARG:NE[1_554] | 2.03 | 0.17 |
| 4:5:22:ALA:C | 4:8:362:TYR:CZ[1_554] | 2.03 | 0.17 |
| 4:6:327:ILE:CG1 | 4:9:149:THR:OG1[1_554] | 2.03 | 0.17 |
| 4:6:320:LEU:N | 4:9:293:LEU:O[1_554] | 2.03 | 0.17 |
| 4:5:319:ALA:CA | 4:8:295:ALA:CA[1_554] | 2.03 | 0.17 |
| 4:6:186:THR:CA | 4:9:183:ARG:NE[1_554] | 2.03 | 0.17 |
| 4:6:280:ASN:ND2 | 4:9:284:LYS:N[1_554] | 2.03 | 0.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:260:THR:C | 4:9:160:THR:OG1[1_554] | 2.03 | 0.17 |
| 4:5:281:SER:CA | 4:8:173:HIS:CD2[1_554] | 2.03 | 0.17 |
| 4:4:331:ALA:CA | 4:7:135:ALA:N[1_554] | 2.03 | 0.17 |
| 4:4:208:ILE:CB | 4:7:59:GLN:CD[1_554] | 2.03 | 0.17 |
| 4:5:309:ILE:CA | 4:8:141:SER:CB[1_554] | 2.03 | 0.17 |
| 4:4:300:SER:OG | 4:7:107:GLU:OE1[1_554] | 2.03 | 0.17 |
| 4:5:339:VAL:CB | 4:8:116:ARG:CB[1_554] | 2.03 | 0.17 |
| 4:6:264:PRO:CD | 4:9:274:ILE:CA[1_554] | 2.03 | 0.17 |
| 4:5:31:PHE:C | 4:8:78:ASN:ND2[1_554] | 2.03 | 0.17 |
| 4:6:312:ARG:NH1 | 4:9:299:MET:CG[1_554] | 2.03 | 0.17 |
| 4:6:164:PRO:CG | 4:9:172:PRO:CD[1_554] | 2.03 | 0.17 |
| 4:5:307:PRO:CA | 4:8:337:TYR:O[1_554] | 2.03 | 0.17 |
| 4:6:218:TYR:CA | 4:9:336:LYS:C[1_554] | 2.03 | 0.17 |
| 4:4:75:ILE:CA | 4:8:197:GLY:O[1_554] | 2.03 | 0.17 |
| 4:5:253:GLU:CD | 4:8:214:GLU:C[1_554] | 2.03 | 0.17 |
| 4:5:327:ILE:CB | 4:8:149:THR:OG1[1_554] | 2.03 | 0.17 |
| 4:6:214:GLU:O | 4:9:16:LEU:CB[1_554] | 2.03 | 0.17 |
| 4:4:321:ALA:N | 4:7:293:LEU:CD1[1_554] | 2.03 | 0.17 |
| 4:5:261:LEU:N | 4:8:160:THR:OG1[1_554] | 2.03 | 0.17 |
| 4:6:319:ALA:C | 4:9:293:LEU:C[1_554] | 2.03 | 0.17 |
| 4:5:215:LYS:CD | 4:8:31:PHE:N[1_554] | 2.03 | 0.17 |
| 4:5:28:ARG:NE | 4:8:126:THR:N[1_554] | 2.03 | 0.17 |
| 4:5:137:GLN:CG | 4:8:113:LYS:N[1_554] | 2.03 | 0.17 |
| 4:6:336:LYS:N | 4:9:106:THR:C[1_554] | 2.03 | 0.17 |
| 4:4:345:ILE:N | 4:7:367:PRO:CA[1_554] | 2.03 | 0.17 |
| 4:2:288:ASP:N | 4:7:39:ARG:NE[1_554] | 2.03 | 0.17 |
| 4:6:143:TYR:N | 4:9:372:ARG:CG[1_554] | 2.03 | 0.17 |
| 4:6:214:GLU:CB | 4:9:16:LEU:CB[1_554] | 2.03 | 0.17 |
| 4:5:75:ILE:CG1 | 4:9:194:THR:CA[1_554] | 2.03 | 0.17 |
| 4:5:110:LEU:CA | 4:9:192:ILE:CA[1_554] | 2.03 | 0.17 |
| 4:2:326:LYS:CB | 4:7:42:GLY:C[1_554] | 2.03 | 0.17 |
| 4:4:207:GLU:CD | 4:7:67:LEU:CB[1_554] | 2.03 | 0.17 |
| 4:6:28:ARG:O | 4:9:83:GLU:OE1[1_554] | 2.03 | 0.17 |
| 4:4:338:SER:O | 4:7:117:GLU:CA[1_554] | 2.03 | 0.17 |
| 4:5:265:SER:C | 4:8:260:THR:O[1_554] | 2.03 | 0.17 |
| 4:5:185:LEU:N | 4:8:158:GLY:C[1_554] | 2.03 | 0.17 |
| 4:5:349:LEU:CA | 4:8:365:ALA:CB[1_554] | 2.03 | 0.17 |
| 4:4:220:ALA:CA | 4:7:335:ARG:CB[1_554] | 2.03 | 0.17 |
| 4:5:346:LEU:C | 4:8:366:GLY:C[1_554] | 2.03 | 0.17 |
| 4:5:106:THR:CB | 4:8:114:ALA:N[1_554] | 2.03 | 0.17 |
| 4:6:160:THR:CB | 4:9:161:HIS:CD2[1_554] | 2.03 | 0.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:290:ARG:N | 4:8:63:GLY:O[1_554] | 2.03 | 0.17 |
| 4:6:293:LEU:O | 4:9:169:TYR:N[1_554] | 2.03 | 0.17 |
| 4:5:188:TYR:C | 4:8:183:ARG:N[1_554] | 2.03 | 0.17 |
| 4:4:213:LYS:CA | 4:7:15:GLY:CA[1_554] | 2.03 | 0.17 |
| 4:6:280:ASN:N | 4:9:281:SER:O[1_554] | 2.03 | 0.17 |
| 4:5:227:MET:SD | 4:8:306:TYR:O[1_554] | 2.03 | 0.17 |
| 4:4:211:ASP:CA | 4:7:32:PRO:CB[1_554] | 2.03 | 0.17 |
| 4:4:369:ILE:CG2 | 4:8:234:SER:CA[1_554] | 2.03 | 0.17 |
| 4:4:144:ALA:CA | 4:7:371:HIS:CA[1_554] | 2.03 | 0.17 |
| 4:5:219:VAL:C | 4:8:335:ARG:C[1_554] | 2.03 | 0.17 |
| 4:5:188:TYR:C | 4:8:183:ARG:C[1_554] | 2.03 | 0.17 |
| 4:5:262:PHE:CE1 | 4:8:152:VAL:C[1_554] | 2.03 | 0.17 |
| 4:6:310:ALA:N | 4:9:141:SER:C[1_554] | 2.03 | 0.17 |
| 4:4:289:ILE:CG1 | 4:9:39:ARG:NH2[1_554] | 2.03 | 0.17 |
| 4:5:112:PRO:CD | 4:9:192:ILE:O[1_554] | 2.03 | 0.17 |
| 4:4:340:TRP:CG | 4:7:118:LYS:CG[1_554] | 2.03 | 0.17 |
| 4:4:30:VAL:CG1 | 4:7:79:TRP:N[1_554] | 2.03 | 0.17 |
| 4:5:16:LEU:N | 4:8:77:THR:C[1_554] | 2.03 | 0.17 |
| 4:4:286:ASP:OD1 | 4:8:270:GLU:OE1[1_554] | 2.03 | 0.17 |
| 4:4:166:TYR:CE1 | 4:9:39:ARG:O[1_554] | 2.03 | 0.17 |
| 4:6:294:TYR:O | 4:9:167:GLU:CA[1_554] | 2.03 | 0.17 |
| 4:4:263:GLN:N | 4:7:153:LEU:CD1[1_554] | 2.03 | 0.17 |
| 4:5:196:ARG:N | 4:8:209:VAL:O[1_554] | 2.03 | 0.17 |
| 4:6:141:SER:CA | 4:9:116:ARG:NH1[1_554] | 2.03 | 0.17 |
| 4:6:315:LYS:C | 4:9:296:ASN:O[1_554] | 2.03 | 0.17 |
| 4:6:193:LEU:C | 4:9:210:ARG:CA[1_554] | 2.03 | 0.17 |
| 4:5:17:VAL:CA | 4:8:79:TRP:NE1[1_554] | 2.03 | 0.17 |
| 4:5:289:ILE:CA | 4:V:64:ILE:CA[1_554] | 2.03 | 0.17 |
| 4:5:173:HIS:CA | 4:9:266:PHE:C[1_554] | 2.03 | 0.17 |
| 4:5:263:GLN:C | 4:8:274:ILE:CB[1_554] | 2.03 | 0.17 |
| 4:6:28:ARG:NE | 4:9:126:THR:CB[1_554] | 2.03 | 0.17 |
| 4:5:219:VAL:CA | 4:8:335:ARG:O[1_554] | 2.03 | 0.17 |
| 4:3:288:ASP:O | 4:8:64:ILE:O[1_554] | 2.03 | 0.17 |
| 4:6:62:ARG:NH1 | 4:9:66:THR:C[1_554] | 2.03 | 0.17 |
| 4:3:112:PRO:CA | 4:7:253:GLU:CG[1_554] | 2.03 | 0.17 |
| 4:5:366:GLY:O | 4:9:233:SER:N[1_554] | 2.03 | 0.17 |
| 4:6:112:PRO:CB | 4:V:253:GLU:CG[1_554] | 2.03 | 0.17 |
| 4:3:112:PRO:C | 4:7:250:ILE:CG2[1_554] | 2.03 | 0.17 |
| 4:4:172:PRO:O | 4:8:188:TYR:CD1[1_554] | 2.03 | 0.17 |
| 4:5:344:SER:N | 4:8:367:PRO:CB[1_554] | 2.03 | 0.17 |
| 4:4:334:GLU:OE1 | 4:7:132:MET:SD[1_554] | 2.03 | 0.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:140:LEU:CG | 4:8:371:HIS:ND1[1_554] | 2.03 | 0.17 |
| 4:5:210:ARG:CD | 4:8:69:TYR:CE2[1_554] | 2.03 | 0.17 |
| 4:4:317:ILE:CB | 4:7:165:ILE:CA[1_554] | 2.03 | 0.17 |
| 4:3:357:ILE:CB | 4:7:232:SER:N[1_554] | 2.03 | 0.17 |
| 4:6:320:LEU:CB | 4:9:294:TYR:N[1_554] | 2.03 | 0.17 |
| 4:6:328:LYS:N | 4:9:148:THR:CB[1_554] | 2.03 | 0.17 |
| 4:5:316:GLU:CA | 4:8:151:ILE:O[1_554] | 2.03 | 0.17 |
| 4:5:162:ASN:CA | 4:8:175:ILE:CD1[1_554] | 2.03 | 0.17 |
| 4:5:136:ILE:N | 4:8:113:LYS:NZ[1_554] | 2.03 | 0.17 |
| 4:6:166:TYR:CZ | 4:W:39:ARG:O[1_554] | 2.03 | 0.17 |
| 4:4:211:ASP:CG | 4:7:55:GLY:CA[1_554] | 2.03 | 0.17 |
| 4:4:26:ALA:N | 4:7:122:ILE:N[1_554] | 2.03 | 0.17 |
| 4:4:276:GLU:CA | 4:7:281:SER:OG[1_554] | 2.03 | 0.17 |
| 4:5:348:SER:C | 4:8:366:GLY:N[1_554] | 2.03 | 0.17 |
| 4:4:140:LEU:CA | 4:7:371:HIS:CD2[1_554] | 2.03 | 0.17 |
| 4:6:309:ILE:C | 4:9:141:SER:CA[1_554] | 2.03 | 0.17 |
| 4:5:30:VAL:CA | 4:8:83:GLU:N[1_554] | 2.03 | 0.17 |
| 4:4:23:GLY:C | 4:7:125:GLU:CD[1_554] | 2.03 | 0.17 |
| 4:5:187:ASP:CA | 4:8:183:ARG:CB[1_554] | 2.03 | 0.17 |
| 4:5:136:ILE:CA | 4:8:113:LYS:CE[1_554] | 2.03 | 0.17 |
| 4:6:15:GLY:N | 4:9:77:THR:CA[1_554] | 2.03 | 0.17 |
| 4:5:214:GLU:N | 4:8:16:LEU:CG[1_554] | 2.03 | 0.17 |
| 4:4:256:ARG:NH2 | 4:7:213:LYS:O[1_554] | 2.03 | 0.17 |
| 4:4:310:ALA:C | 4:7:140:LEU:N[1_554] | 2.03 | 0.17 |
| 4:6:214:GLU:O | 4:9:18:LYS:CD[1_554] | 2.03 | 0.17 |
| 4:6:319:ALA:CB | 4:9:295:ALA:N[1_554] | 2.03 | 0.17 |
| 4:5:325:MET:CE | 4:8:166:TYR:OH[1_554] | 2.03 | 0.17 |
| 4:4:137:GLN:CB | 4:7:112:PRO:CB[1_554] | 2.03 | 0.17 |
| 4:5:113:LYS:N | 4:9:253:GLU:CB[1_554] | 2.03 | 0.17 |
| 4:4:76:ILE:O | 4:8:198:TYR:CD1[1_554] | 2.03 | 0.17 |
| 4:5:322:PRO:N | 4:8:291:LYS:NZ[1_554] | 2.03 | 0.17 |
| 4:6:319:ALA:CA | 4:9:292:ASP:O[1_554] | 2.03 | 0.17 |
| 4:5:294:TYR:O | 4:8:166:TYR:O[1_554] | 2.03 | 0.17 |
| 4:3:292:ASP:OD2 | 4:8:40:HIS:N[1_554] | 2.03 | 0.17 |
| 4:5:307:PRO:CA | 4:8:338:SER:N[1_554] | 2.03 | 0.17 |
| 4:6:308:GLY:CA | 4:9:338:SER:N[1_554] | 2.03 | 0.17 |
| 4:4:191:LYS:NZ | 4:7:257:CYS:SG[1_554] | 2.03 | 0.17 |
| 4:5:289:ILE:CG2 | 4:V:39:ARG:NH2[1_554] | 2.03 | 0.17 |
| 4:4:173:HIS:CB | 4:8:267:ILE:N[1_554] | 2.04 | 0.16 |
| 4:5:253:GLU:CD | 4:8:213:LYS:C[1_554] | 2.04 | 0.16 |
| 4:5:110:LEU:CB | 4:9:192:ILE:CG2[1_554] | 2.04 | 0.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:199:SER:CB | 4:9:206:ARG:CA[1_554] | 2.04 | 0.16 |
| 4:5:300:SER:CA | 4:8:107:GLU:O[1_554] | 2.04 | 0.16 |
| 4:4:294:TYR:CE2 | 4:7:166:TYR:CG[1_554] | 2.04 | 0.16 |
| 4:6:372:ARG:O | 4:V:227:MET:CA[1_554] | 2.04 | 0.16 |
| 4:6:321:ALA:O | 4:9:292:ASP:CG[1_554] | 2.04 | 0.16 |
| 4:6:23:GLY:CA | 4:9:362:TYR:CE2[1_554] | 2.04 | 0.16 |
| 4:6:10:CYS:CA | 4:9:118:LYS:CE[1_554] | 2.04 | 0.16 |
| 4:4:218:TYR:CG | 4:7:337:TYR:CG[1_554] | 2.04 | 0.16 |
| 4:4:197:GLY:CA | 4:7:208:ILE:O[1_554] | 2.04 | 0.16 |
| 4:5:337:TYR:CE2 | 4:8:86:TRP:CZ2[1_554] | 2.04 | 0.16 |
| 4:3:75:ILE:C | 4:7:198:TYR:CG[1_554] | 2.04 | 0.16 |
| 4:5:318:THR:O | 4:8:292:ASP:CA[1_554] | 2.04 | 0.16 |
| 4:5:153:LEU:CD2 | 4:8:109:PRO:CG[1_554] | 2.04 | 0.16 |
| 4:5:24:ASP:CA | 4:8:125:GLU:N[1_554] | 2.04 | 0.16 |
| 4:6:316:GLU:C | 4:9:151:ILE:N[1_554] | 2.04 | 0.16 |
| 4:5:62:ARG:NH1 | 4:8:66:THR:C[1_554] | 2.04 | 0.16 |
| 4:6:301:GLY:O | 4:9:137:GLN:CD[1_554] | 2.04 | 0.16 |
| 4:2:291:LYS:CD | 4:7:39:ARG:N[1_554] | 2.04 | 0.16 |
| 4:6:344:SER:CB | 4:9:120:THR:CG2[1_554] | 2.04 | 0.16 |
| 4:2:291:LYS:CD | 4:7:39:ARG:O[1_554] | 2.04 | 0.16 |
| 4:6:286:ASP:N | 4:V:270:GLU:CG[1_554] | 2.04 | 0.16 |
| 4:4:317:ILE:CG2 | 4:7:164:PRO:C[1_554] | 2.04 | 0.16 |
| 4:5:309:ILE:CB | 4:8:339:VAL:CG2[1_554] | 2.04 | 0.16 |
| 4:4:345:ILE:O | 4:7:366:GLY:CA[1_554] | 2.04 | 0.16 |
| 4:6:258:PRO:C | 4:9:155:SER:CB[1_554] | 2.04 | 0.16 |
| 4:4:318:THR:CB | 4:7:149:THR:N[1_554] | 2.04 | 0.16 |
| 4:6:269:MET:CG | 4:9:178:LEU:CD1[1_554] | 2.04 | 0.16 |
| 4:5:273:GLY:CA | 4:8:162:ASN:ND2[1_554] | 2.04 | 0.16 |
| 4:6:111:ASN:CG | 4:V:196:ARG:CA[1_554] | 2.04 | 0.16 |
| 4:3:75:ILE:CG1 | 4:7:193:LEU:C[1_554] | 2.04 | 0.16 |
| 4:6:27:PRO:CG | 4:9:86:TRP:CZ3[1_554] | 2.04 | 0.16 |
| 4:4:304:THR:CG2 | 4:7:107:GLU:C[1_554] | 2.04 | 0.16 |
| 4:6:266:PHE:N | 4:9:261:LEU:CB[1_554] | 2.04 | 0.16 |
| 4:6:273:GLY:N | 4:9:162:ASN:OD1[1_554] | 2.04 | 0.16 |
| 4:6:256:ARG:CB | 4:9:306:TYR:CE2[1_554] | 2.04 | 0.16 |
| 4:4:279:TYR:N | 4:7:164:PRO:CD[1_554] | 2.04 | 0.16 |
| 4:4:283:MET:CG | 4:7:286:ASP:C[1_554] | 2.04 | 0.16 |
| 4:6:186:THR:OG1 | 4:9:183:ARG:CZ[1_554] | 2.04 | 0.16 |
| 4:4:310:ALA:O | 4:7:141:SER:N[1_554] | 2.04 | 0.16 |
| 4:6:210:ARG:NE | 4:9:33:SER:C[1_554] | 2.04 | 0.16 |
| 4:5:56:ASP:CG | 4:8:37:ARG:NH1[1_554] | 2.04 | 0.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:227:MET:CE | 4:8:306:TYR:C[1_554] | 2.04 | 0.16 |
| 4:6:214:GLU:N | 4:9:16:LEU:CD2[1_554] | 2.04 | 0.16 |
| 4:6:258:PRO:O | 4:9:155:SER:N[1_554] | 2.04 | 0.16 |
| 4:6:164:PRO:CA | 4:9:169:TYR:OH[1_554] | 2.04 | 0.16 |
| 4:5:196:ARG:CZ | 4:8:215:LYS:CB[1_554] | 2.04 | 0.16 |
| 4:5:191:LYS:CG | 4:8:184:ASP:O[1_554] | 2.04 | 0.16 |
| 4:4:115:ASN:CG | 4:8:249:THR:C[1_554] | 2.04 | 0.16 |
| 4:6:261:LEU:CA | 4:9:154:ASP:O[1_554] | 2.04 | 0.16 |
| 4:6:345:ILE:CD1 | 4:9:357:ILE:CB[1_554] | 2.04 | 0.16 |
| 4:6:316:GLU:O | 4:9:293:LEU:O[1_554] | 2.04 | 0.16 |
| 4:3:112:PRO:CB | 4:7:193:LEU:CD1[1_554] | 2.04 | 0.16 |
| 4:4:318:THR:CA | 4:7:149:THR:N[1_554] | 2.04 | 0.16 |
| 4:4:187:ASP:C | 4:7:183:ARG:CA[1_554] | 2.04 | 0.16 |
| 4:6:183:ARG:NE | 4:9:72:GLU:CG[1_554] | 2.04 | 0.16 |
| 4:4:311:ASP:OD1 | 4:7:144:ALA:CB[1_554] | 2.04 | 0.16 |
| 4:4:25:ASP:CG | 4:7:124:PHE:C[1_554] | 2.04 | 0.16 |
| 4:3:116:ARG:CB | 4:7:252:ASN:CG[1_554] | 2.04 | 0.16 |
| 4:4:191:LYS:CG | 4:7:185:LEU:CA[1_554] | 2.04 | 0.16 |
| 4:4:25:ASP:N | 4:7:125:GLU:CB[1_554] | 2.04 | 0.16 |
| 4:5:180:LEU:CA | 4:8:179:ASP:N[1_554] | 2.04 | 0.16 |
| 4:5:186:THR:CA | 4:8:157:ASP:OD2[1_554] | 2.04 | 0.16 |
| 4:4:151:ILE:CG1 | 4:7:172:PRO:N[1_554] | 2.04 | 0.16 |
| 4:3:117:GLU:CG | 4:7:236:LEU:C[1_554] | 2.04 | 0.16 |
| 4:5:31:PHE:C | 4:8:78:ASN:CB[1_554] | 2.04 | 0.16 |
| 4:5:198:TYR:CB | 4:8:208:ILE:CA[1_554] | 2.04 | 0.16 |
| 4:4:223:PHE:CZ | 4:7:301:GLY:C[1_554] | 2.04 | 0.16 |
| 4:6:259:GLU:OE1 | 4:9:309:ILE:CD1[1_554] | 2.04 | 0.16 |
| 4:4:274:ILE:C | 4:7:163:VAL:CA[1_554] | 2.04 | 0.16 |
| 4:5:301:GLY:N | 4:8:107:GLU:N[1_554] | 2.04 | 0.16 |
| 4:4:223:PHE:CG | 4:7:335:ARG:CD[1_554] | 2.04 | 0.16 |
| 4:5:180:LEU:CG | 4:8:178:LEU:N[1_554] | 2.04 | 0.16 |
| 4:4:116:ARG:CA | 4:8:196:ARG:NH1[1_554] | 2.04 | 0.16 |
| 4:6:210:ARG:CD | 4:9:69:TYR:CE2[1_554] | 2.04 | 0.16 |
| 4:5:270:GLU:CA | 4:8:272:ALA:CB[1_554] | 2.04 | 0.16 |
| 4:5:142:LEU:N | 4:8:116:ARG:NH1[1_554] | 2.04 | 0.16 |
| 4:4:318:THR:N | 4:7:150:GLY:CA[1_554] | 2.04 | 0.16 |
| 4:5:294:TYR:CE2 | 4:8:166:TYR:CD1[1_554] | 2.04 | 0.16 |
| 4:4:315:LYS:NZ | 4:7:147:ARG:NH1[1_554] | 2.04 | 0.16 |
| 4:4:276:GLU:O | 4:7:164:PRO:CG[1_554] | 2.04 | 0.16 |
| 4:4:277:THR:OG1 | 4:7:175:ILE:C[1_554] | 2.04 | 0.16 |
| 4:5:256:ARG:NE | 4:8:306:TYR:CD1[1_554] | 2.04 | 0.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:18:LYS:O | 4:8:118:LYS:CD[1_554] | 2.04 | 0.16 |
| 4:5:191:LYS:O | 4:8:186:THR:C[1_554] | 2.04 | 0.16 |
| 4:5:61:LYS:N | 4:8:66:THR:OG1[1_554] | 2.04 | 0.16 |
| 4:6:185:LEU:N | 4:9:158:GLY:C[1_554] | 2.04 | 0.16 |
| 4:6:255:PHE:N | 4:9:302:GLY:O[1_554] | 2.04 | 0.16 |
| 4:6:311:ASP:C | 4:9:298:VAL:CG1[1_554] | 2.04 | 0.16 |
| 4:4:298:VAL:O | 4:7:136:ILE:CG1[1_554] | 2.04 | 0.16 |
| 4:6:17:VAL:N | 4:9:78:ASN:C[1_554] | 2.04 | 0.16 |
| 4:4:299:MET:SD | 4:7:136:ILE:O[1_554] | 2.04 | 0.16 |
| 4:4:276:GLU:OE2 | 4:7:279:TYR:N[1_554] | 2.04 | 0.16 |
| 4:4:339:VAL:O | 4:7:117:GLU:N[1_554] | 2.04 | 0.16 |
| 4:6:162:ASN:O | 4:9:172:PRO:O[1_554] | 2.04 | 0.16 |
| 4:3:289:ILE:CB | 4:8:39:ARG:NH2[1_554] | 2.04 | 0.16 |
| 4:5:208:ILE:CB | 4:8:59:GLN:CB[1_554] | 2.04 | 0.16 |
| 4:5:156:GLY:O | 4:8:74:GLY:C[1_554] | 2.04 | 0.16 |
| 4:4:220:ALA:C | 4:7:335:ARG:CA[1_554] | 2.04 | 0.16 |
| 4:6:368:SER:C | 4:V:230:ALA:CA[1_554] | 2.04 | 0.16 |
| 4:5:199:SER:CA | 4:8:206:ARG:CB[1_554] | 2.04 | 0.16 |
| 4:4:288:ASP:C | 4:9:63:GLY:C[1_554] | 2.04 | 0.16 |
| 4:5:258:PRO:CB | 4:8:301:GLY:C[1_554] | 2.04 | 0.16 |
| 4:4:215:LYS:O | 4:7:30:VAL:CG1[1_554] | 2.04 | 0.16 |
| 4:5:262:PHE:CD1 | 4:8:153:LEU:O[1_554] | 2.04 | 0.16 |
| 4:6:117:GLU:N | 4:V:252:ASN:OD1[1_554] | 2.04 | 0.16 |
| 4:6:335:ARG:CG | 4:9:106:THR:OG1[1_554] | 2.04 | 0.16 |
| 4:5:312:ARG:O | 4:8:298:VAL:N[1_554] | 2.04 | 0.16 |
| 4:5:111:ASN:CG | 4:9:196:ARG:CA[1_554] | 2.04 | 0.16 |
| 4:4:143:TYR:C | 4:7:368:SER:O[1_554] | 2.04 | 0.16 |
| 4:4:200:PHE:N | 4:7:206:ARG:CD[1_554] | 2.04 | 0.16 |
| 4:5:161:HIS:O | 4:8:110:LEU:CG[1_554] | 2.04 | 0.16 |
| 4:4:115:ASN:CB | 4:8:249:THR:C[1_554] | 2.04 | 0.16 |
| 4:6:166:TYR:CA | 4:W:40:HIS:NE2[1_554] | 2.04 | 0.16 |
| 4:5:188:TYR:CD2 | 4:8:181:ALA:C[1_554] | 2.04 | 0.16 |
| 4:4:154:ASP:CG | 4:7:111:ASN:CB[1_554] | 2.04 | 0.16 |
| 4:4:341:ILE:CB | 4:7:120:THR:CG2[1_554] | 2.04 | 0.16 |
| 4:5:319:ALA:C | 4:8:292:ASP:O[1_554] | 2.04 | 0.16 |
| 4:6:261:LEU:CB | 4:9:155:SER:N[1_554] | 2.04 | 0.16 |
| 4:4:154:ASP:C | 4:7:110:LEU:N[1_554] | 2.04 | 0.16 |
| 4:5:242:LEU:CG | 4:8:207:GLU:CD[1_554] | 2.04 | 0.16 |
| 4:4:299:MET:C | 4:7:107:GLU:OE2[1_554] | 2.04 | 0.16 |
| 4:6:266:PHE:CG | 4:9:261:LEU:CD2[1_554] | 2.05 | 0.15 |
| 4:4:157:ASP:N | 4:7:75:ILE:CB[1_554] | 2.05 | 0.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:271:SER:O | 4:9:277:THR:CB[1_554] | 2.05 | 0.15 |
| 4:5:314:GLN:N | 4:8:142:LEU:CG[1_554] | 2.05 | 0.15 |
| 4:5:199:SER:CB | 4:8:206:ARG:CA[1_554] | 2.05 | 0.15 |
| 4:6:217:CYS:O | 4:9:336:LYS:O[1_554] | 2.05 | 0.15 |
| 4:5:307:PRO:CG | 4:8:337:TYR:CA[1_554] | 2.05 | 0.15 |
| 4:4:184:ASP:CG | 4:7:73:HIS:NE2[1_554] | 2.05 | 0.15 |
| 4:6:199:SER:O | 4:9:207:GLU:N[1_554] | 2.05 | 0.15 |
| 4:4:282:ILE:CB | 4:7:171:LEU:CG[1_554] | 2.05 | 0.15 |
| 4:6:19:ALA:C | 4:9:121:GLN:OE1[1_554] | 2.05 | 0.15 |
| 4:6:281:SER:CA | 4:9:174:ALA:N[1_554] | 2.05 | 0.15 |
| 4:4:277:THR:O | 4:7:174:ALA:N[1_554] | 2.05 | 0.15 |
| 4:5:219:VAL:CG1 | 4:8:300:SER:CB[1_554] | 2.05 | 0.15 |
| 4:6:214:GLU:CB | 4:9:16:LEU:N[1_554] | 2.05 | 0.15 |
| 4:5:198:TYR:CD1 | 4:8:208:ILE:C[1_554] | 2.05 | 0.15 |
| 4:5:299:MET:CG | 4:8:137:GLN:N[1_554] | 2.05 | 0.15 |
| 4:4:294:TYR:CD2 | 4:7:166:TYR:CB[1_554] | 2.05 | 0.15 |
| 4:6:295:ALA:CB | 4:9:167:GLU:C[1_554] | 2.05 | 0.15 |
| 4:4:194:THR:N | 4:7:210:ARG:N[1_554] | 2.05 | 0.15 |
| 4:4:183:ARG:CD | 4:7:72:GLU:OE2[1_554] | 2.05 | 0.15 |
| 4:5:28:ARG:N | 4:8:126:THR:OG1[1_554] | 2.05 | 0.15 |
| 4:5:250:ILE:CG2 | 4:8:214:GLU:CG[1_554] | 2.05 | 0.15 |
| 4:6:256:ARG:NE | 4:9:306:TYR:CE1[1_554] | 2.05 | 0.15 |
| 4:6:185:LEU:CA | 4:9:158:GLY:N[1_554] | 2.05 | 0.15 |
| 4:5:309:ILE:CA | 4:8:300:SER:OG[1_554] | 2.05 | 0.15 |
| 4:6:27:PRO:O | 4:9:127:PHE:CE2[1_554] | 2.05 | 0.15 |
| 4:5:276:GLU:OE1 | 4:8:279:TYR:O[1_554] | 2.05 | 0.15 |
| 4:5:75:ILE:CD1 | 4:9:194:THR:C[1_554] | 2.05 | 0.15 |
| 4:4:180:LEU:CD2 | 4:7:178:LEU:N[1_554] | 2.05 | 0.15 |
| 4:6:280:ASN:N | 4:9:285:CYS:SG[1_554] | 2.05 | 0.15 |
| 4:6:370:VAL:C | 4:V:231:ALA:N[1_554] | 2.05 | 0.15 |
| 4:4:329:ILE:C | 4:7:139:VAL:CG1[1_554] | 2.05 | 0.15 |
| 4:4:183:ARG:CG | 4:7:72:GLU:CD[1_554] | 2.05 | 0.15 |
| 4:4:312:ARG:CB | 4:7:141:SER:CB[1_554] | 2.05 | 0.15 |
| 4:6:56:ASP:CA | 4:9:37:ARG:CZ[1_554] | 2.05 | 0.15 |
| 4:5:256:ARG:CG | 4:8:306:TYR:CG[1_554] | 2.05 | 0.15 |
| 4:6:278:THR:OG1 | 4:9:164:PRO:CD[1_554] | 2.05 | 0.15 |
| 4:4:210:ARG:CD | 4:7:69:TYR:CD2[1_554] | 2.05 | 0.15 |
| 4:5:297:ASN:CB | 4:8:165:ILE:CG2[1_554] | 2.05 | 0.15 |
| 4:5:136:ILE:CA | 4:8:113:LYS:CD[1_554] | 2.05 | 0.15 |
| 4:4:171:LEU:O | 4:8:266:PHE:C[1_554] | 2.05 | 0.15 |
| 4:4:318:THR:OG1 | 4:7:147:ARG:CG[1_554] | 2.05 | 0.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:341:ILE:CB | 4:8:132:MET:SD[1_554] | 2.05 | 0.15 |
| 4:6:115:ASN:C | 4:V:196:ARG:CZ[1_554] | 2.05 | 0.15 |
| 4:6:221:LEU:O | 4:9:332:PRO:CA[1_554] | 2.05 | 0.15 |
| 4:4:180:LEU:CD1 | 4:7:178:LEU:O[1_554] | 2.05 | 0.15 |
| 4:4:195:GLU:CG | 4:7:189:LEU:CB[1_554] | 2.05 | 0.15 |
| 4:4:145:SER:CB | 4:7:372:ARG:NE[1_554] | 2.05 | 0.15 |
| 4:5:60:SER:CA | 4:8:37:ARG:CB[1_554] | 2.05 | 0.15 |
| 4:5:367:PRO:C | 4:9:230:ALA:O[1_554] | 2.05 | 0.15 |
| 4:5:300:SER:O | 4:8:108:ALA:O[1_554] | 2.05 | 0.15 |
| 4:4:332:PRO:CD | 4:7:134:VAL:CA[1_554] | 2.05 | 0.15 |
| 4:6:188:TYR:CD2 | 4:9:182:GLY:CA[1_554] | 2.05 | 0.15 |
| 4:6:314:GLN:N | 4:9:142:LEU:CG[1_554] | 2.05 | 0.15 |
| 4:6:335:ARG:CZ | 4:9:339:VAL:CG1[1_554] | 2.05 | 0.15 |
| 4:5:195:GLU:CD | 4:8:189:LEU:CB[1_554] | 2.05 | 0.15 |
| 4:4:211:ASP:O | 4:7:31:PHE:O[1_554] | 2.05 | 0.15 |
| 4:4:207:GLU:CG | 4:7:68:LYS:N[1_554] | 2.05 | 0.15 |
| 4:6:21:PHE:CA | 4:9:125:GLU:CB[1_554] | 2.05 | 0.15 |
| 4:4:156:GLY:C | 4:7:75:ILE:CB[1_554] | 2.05 | 0.15 |
| 4:2:292:ASP:N | 4:7:40:HIS:CB[1_554] | 2.05 | 0.15 |
| 4:5:308:GLY:O | 4:8:338:SER:CB[1_554] | 2.05 | 0.15 |
| 4:6:180:LEU:CA | 4:9:179:ASP:N[1_554] | 2.05 | 0.15 |
| 4:6:186:THR:CB | 4:9:183:ARG:NH2[1_554] | 2.05 | 0.15 |
| 4:6:110:LEU:CB | 4:V:192:ILE:CA[1_554] | 2.05 | 0.15 |
| 4:6:140:LEU:CA | 4:9:371:HIS:O[1_554] | 2.05 | 0.15 |
| 4:5:264:PRO:CA | 4:8:274:ILE:CD1[1_554] | 2.05 | 0.15 |
| 1:A:411:GLU:OE2 | 4:5:226:GLU:OE1[1_556] | 2.05 | 0.15 |
| 4:4:113:LYS:CG | 4:8:253:GLU:C[1_554] | 2.05 | 0.15 |
| 4:5:243:PRO:C | 4:8:60:SER:CB[1_554] | 2.05 | 0.15 |
| 4:4:286:ASP:CG | 4:8:270:GLU:OE1[1_554] | 2.05 | 0.15 |
| 4:6:178:LEU:C | 4:9:177:ARG:CG[1_554] | 2.05 | 0.15 |
| 4:4:372:ARG:CG | 4:8:227:MET:N[1_554] | 2.05 | 0.15 |
| 4:4:279:TYR:CE1 | 4:7:289:ILE:CG1[1_554] | 2.05 | 0.15 |
| 4:4:314:GLN:CB | 4:7:142:LEU:CB[1_554] | 2.05 | 0.15 |
| 4:6:262:PHE:CD2 | 4:9:153:LEU:C[1_554] | 2.05 | 0.15 |
| 4:4:340:TRP:CZ3 | 4:7:121:GLN:CD[1_554] | 2.05 | 0.15 |
| 4:6:288:ASP:C | 4:W:63:GLY:N[1_554] | 2.05 | 0.15 |
| 4:6:187:ASP:O | 4:9:184:ASP:N[1_554] | 2.05 | 0.15 |
| 4:3:75:ILE:CG2 | 4:7:198:TYR:CE2[1_554] | 2.05 | 0.15 |
| 4:5:13:GLY:CA | 4:8:76:ILE:O[1_554] | 2.05 | 0.15 |
| 4:6:211:ASP:OD1 | 4:9:32:PRO:CG[1_554] | 2.05 | 0.15 |
| 4:5:281:SER:O | 4:8:173:HIS:CG[1_554] | 2.05 | 0.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:227:MET:CE | 4:8:306:TYR:CA[1_554] | 2.05 | 0.15 |
| 4:6:327:ILE:CB | 4:9:148:THR:C[1_554] | 2.05 | 0.15 |
| 4:6:9:VAL:CG2 | 4:9:367:PRO:CG[1_554] | 2.05 | 0.15 |
| 4:5:185:LEU:CA | 4:8:158:GLY:N[1_554] | 2.05 | 0.15 |
| 4:5:200:PHE:CG | 4:8:206:ARG:NE[1_554] | 2.05 | 0.15 |
| 4:4:255:PHE:CE1 | 4:7:305:MET:SD[1_554] | 2.05 | 0.15 |
| 4:4:113:LYS:CD | 4:8:254:ARG:CB[1_554] | 2.05 | 0.15 |
| 4:5:297:ASN:CA | 4:8:168:GLY:O[1_554] | 2.05 | 0.15 |
| 4:6:347:ALA:O | 4:9:366:GLY:CA[1_554] | 2.05 | 0.15 |
| 4:3:173:HIS:ND1 | 4:7:266:PHE:CA[1_554] | 2.05 | 0.15 |
| 4:4:211:ASP:OD1 | 4:7:32:PRO:O[1_554] | 2.05 | 0.15 |
| 4:5:280:ASN:CA | 4:8:281:SER:O[1_554] | 2.05 | 0.15 |
| 4:5:292:ASP:OD1 | 4:V:64:ILE:CD1[1_554] | 2.05 | 0.15 |
| 4:6:188:TYR:C | 4:9:183:ARG:N[1_554] | 2.05 | 0.15 |
| 4:4:145:SER:CB | 4:7:372:ARG:NH2[1_554] | 2.05 | 0.15 |
| 4:5:180:LEU:CG | 4:8:178:LEU:CA[1_554] | 2.05 | 0.15 |
| 4:5:279:TYR:CE1 | 4:8:293:LEU:CD2[1_554] | 2.05 | 0.15 |
| 4:4:204:ALA:CA | 4:7:62:ARG:C[1_554] | 2.05 | 0.15 |
| 4:5:242:LEU:CD1 | 4:8:207:GLU:CD[1_554] | 2.05 | 0.15 |
| 4:6:106:THR:OG1 | 4:9:114:ALA:CA[1_554] | 2.05 | 0.15 |
| 4:6:372:ARG:C | 4:V:227:MET:C[1_554] | 2.05 | 0.15 |
| 4:6:334:GLU:CA | 4:9:104:LEU:O[1_554] | 2.05 | 0.15 |
| 4:4:142:LEU:C | 4:7:372:ARG:CB[1_554] | 2.05 | 0.15 |
| 4:5:273:GLY:O | 4:8:162:ASN:ND2[1_554] | 2.05 | 0.15 |
| 4:4:287:ILE:C | 4:9:63:GLY:C[1_554] | 2.05 | 0.15 |
| 4:4:288:ASP:CA | 4:9:62:ARG:O[1_554] | 2.05 | 0.15 |
| 4:5:307:PRO:C | 4:8:338:SER:CA[1_554] | 2.05 | 0.15 |
| 4:4:335:ARG:NH1 | 4:7:106:THR:CB[1_554] | 2.05 | 0.15 |
| 4:6:191:LYS:CE | 4:9:185:LEU:O[1_554] | 2.05 | 0.15 |
| 4:6:329:ILE:CG2 | 4:9:139:VAL:O[1_554] | 2.05 | 0.15 |
| 4:6:367:PRO:CB | 4:V:233:SER:CB[1_554] | 2.05 | 0.15 |
| 4:6:31:PHE:N | 4:9:80:ASP:N[1_554] | 2.05 | 0.15 |
| 4:4:175:ILE:CG1 | 4:8:191:LYS:NZ[1_554] | 2.05 | 0.15 |
| 4:6:156:GLY:O | 4:9:74:GLY:C[1_554] | 2.05 | 0.15 |
| 4:5:259:GLU:CD | 4:8:309:ILE:CB[1_554] | 2.06 | 0.14 |
| 4:6:26:ALA:C | 4:9:122:ILE:O[1_554] | 2.06 | 0.14 |
| 4:4:112:PRO:N | 4:8:253:GLU:CG[1_554] | 2.06 | 0.14 |
| 4:4:311:ASP:CB | 4:7:141:SER:O[1_554] | 2.06 | 0.14 |
| 4:4:171:LEU:C | 4:8:266:PHE:O[1_554] | 2.06 | 0.14 |
| 4:6:200:PHE:C | 4:9:206:ARG:CD[1_554] | 2.06 | 0.14 |
| 4:4:290:ARG:N | 4:9:63:GLY:O[1_554] | 2.06 | 0.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:180:LEU:CB | 4:7:178:LEU:O[1_554] | 2.06 | 0.14 |
| 4:4:226:GLU:CB | 4:7:335:ARG:NH1[1_554] | 2.06 | 0.14 |
| 4:5:218:TYR:OH | 4:8:337:TYR:CZ[1_554] | 2.06 | 0.14 |
| 1:D:411:GLU:OE1 | 4:6:226:GLU:OE2[1_556] | 2.06 | 0.14 |
| 4:4:244:ASP:N | 4:7:60:SER:O[1_554] | 2.06 | 0.14 |
| 4:4:139:VAL:C | 4:7:371:HIS:CE1[1_554] | 2.06 | 0.14 |
| 4:5:335:ARG:CZ | 4:8:339:VAL:CG1[1_554] | 2.06 | 0.14 |
| 4:6:180:LEU:CB | 4:9:179:ASP:CA[1_554] | 2.06 | 0.14 |
| 4:6:140:LEU:CA | 4:9:371:HIS:CA[1_554] | 2.06 | 0.14 |
| 4:5:316:GLU:O | 4:8:293:LEU:O[1_554] | 2.06 | 0.14 |
| 4:4:326:LYS:N | 4:7:167:GLU:CB[1_554] | 2.06 | 0.14 |
| 4:5:196:ARG:C | 4:8:212:ILE:CG2[1_554] | 2.06 | 0.14 |
| 4:4:308:GLY:O | 4:7:338:SER:CB[1_554] | 2.06 | 0.14 |
| 4:4:198:TYR:CD1 | 4:7:208:ILE:CA[1_554] | 2.06 | 0.14 |
| 4:5:210:ARG:NH2 | 4:8:33:SER:CA[1_554] | 2.06 | 0.14 |
| 4:4:279:TYR:C | 4:7:174:ALA:CB[1_554] | 2.06 | 0.14 |
| 4:5:140:LEU:O | 4:8:371:HIS:CA[1_554] | 2.06 | 0.14 |
| 4:6:177:ARG:CZ | 4:V:194:THR:CG2[1_554] | 2.06 | 0.14 |
| 4:4:332:PRO:CA | 4:7:133:TYR:O[1_554] | 2.06 | 0.14 |
| 4:6:213:LYS:C | 4:9:16:LEU:CG[1_554] | 2.06 | 0.14 |
| 4:6:349:LEU:O | 4:9:364:GLU:O[1_554] | 2.06 | 0.14 |
| 4:4:240:TYR:CZ | 4:7:56:ASP:CA[1_554] | 2.06 | 0.14 |
| 4:4:345:ILE:CG1 | 4:7:367:PRO:N[1_554] | 2.06 | 0.14 |
| 4:6:332:PRO:CG | 4:9:135:ALA:CB[1_554] | 2.06 | 0.14 |
| 4:4:211:ASP:OD2 | 4:7:32:PRO:O[1_554] | 2.06 | 0.14 |
| 4:4:325:MET:CE | 4:7:166:TYR:CZ[1_554] | 2.06 | 0.14 |
| 4:4:215:LYS:NZ | 4:7:55:GLY:CA[1_554] | 2.06 | 0.14 |
| 4:3:115:ASN:C | 4:7:196:ARG:CZ[1_554] | 2.06 | 0.14 |
| 4:5:255:PHE:CD1 | 4:8:306:TYR:N[1_554] | 2.06 | 0.14 |
| 4:4:156:GLY:O | 4:7:74:GLY:C[1_554] | 2.06 | 0.14 |
| 4:6:349:LEU:C | 4:9:364:GLU:C[1_554] | 2.06 | 0.14 |
| 4:6:220:ALA:CB | 4:9:335:ARG:NE[1_554] | 2.06 | 0.14 |
| 4:4:197:GLY:C | 4:7:209:VAL:N[1_554] | 2.06 | 0.14 |
| 4:4:315:LYS:CB | 4:7:145:SER:OG[1_554] | 2.06 | 0.14 |
| 4:4:256:ARG:C | 4:7:302:GLY:C[1_554] | 2.06 | 0.14 |
| 4:6:296:ASN:CA | 4:9:168:GLY:O[1_554] | 2.06 | 0.14 |
| 4:3:372:ARG:CB | 4:7:227:MET:N[1_554] | 2.06 | 0.14 |
| 4:5:200:PHE:N | 4:8:206:ARG:CD[1_554] | 2.06 | 0.14 |
| 4:6:293:LEU:O | 4:9:169:TYR:CA[1_554] | 2.06 | 0.14 |
| 4:6:279:TYR:CA | 4:9:164:PRO:CB[1_554] | 2.06 | 0.14 |
| 4:6:166:TYR:CZ | 4:W:39:ARG:CB[1_554] | 2.06 | 0.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:18:LYS:NZ | 4:9:76:ILE:CG2[1_554] | 2.06 | 0.14 |
| 4:5:299:MET:CE | 4:8:140:LEU:N[1_554] | 2.06 | 0.14 |
| 4:6:188:TYR:N | 4:9:183:ARG:N[1_554] | 2.06 | 0.14 |
| 4:6:256:ARG:CB | 4:9:306:TYR:CD1[1_554] | 2.06 | 0.14 |
| 4:6:299:MET:CA | 4:9:136:ILE:O[1_554] | 2.06 | 0.14 |
| 4:4:186:THR:CA | 4:7:183:ARG:NH2[1_554] | 2.06 | 0.14 |
| 4:5:113:LYS:CG | 4:9:253:GLU:CA[1_554] | 2.06 | 0.14 |
| 4:5:308:GLY:N | 4:8:337:TYR:C[1_554] | 2.06 | 0.14 |
| 4:6:196:ARG:N | 4:9:209:VAL:O[1_554] | 2.06 | 0.14 |
| 4:6:162:ASN:CG | 4:9:175:ILE:CA[1_554] | 2.06 | 0.14 |
| 4:5:276:GLU:OE1 | 4:8:278:THR:C[1_554] | 2.06 | 0.14 |
| 4:6:276:GLU:OE1 | 4:9:279:TYR:O[1_554] | 2.06 | 0.14 |
| 4:5:210:ARG:CG | 4:8:69:TYR:CD2[1_554] | 2.06 | 0.14 |
| 4:6:256:ARG:NE | 4:9:306:TYR:CD1[1_554] | 2.06 | 0.14 |
| 4:6:340:TRP:CZ2 | 4:9:121:GLN:CB[1_554] | 2.06 | 0.14 |
| 4:5:21:PHE:N | 4:8:125:GLU:OE1[1_554] | 2.06 | 0.14 |
| 4:6:292:ASP:OD1 | 4:W:64:ILE:CD1[1_554] | 2.06 | 0.14 |
| 4:3:367:PRO:C | 4:7:236:LEU:CB[1_554] | 2.06 | 0.14 |
| 4:5:342:GLY:O | 4:8:367:PRO:C[1_554] | 2.06 | 0.14 |
| 4:4:289:ILE:O | 4:9:64:ILE:CG2[1_554] | 2.06 | 0.14 |
| 4:3:113:LYS:NZ | 4:7:254:ARG:O[1_554] | 2.06 | 0.14 |
| 4:4:75:ILE:C | 4:8:198:TYR:CG[1_554] | 2.06 | 0.14 |
| 4:3:287:ILE:O | 4:8:63:GLY:O[1_554] | 2.06 | 0.14 |
| 4:4:114:ALA:CB | 4:8:250:ILE:CB[1_554] | 2.06 | 0.14 |
| 4:4:181:ALA:CA | 4:7:159:VAL:CG1[1_554] | 2.06 | 0.14 |
| 4:6:219:VAL:CG1 | 4:9:300:SER:CB[1_554] | 2.06 | 0.14 |
| 4:5:22:ALA:CB | 4:8:362:TYR:OH[1_554] | 2.06 | 0.14 |
| 4:6:343:GLY:CA | 4:9:367:PRO:C[1_554] | 2.06 | 0.14 |
| 4:5:270:GLU:N | 4:8:272:ALA:CA[1_554] | 2.06 | 0.14 |
| 4:6:371:HIS:CE1 | 4:V:252:ASN:CB[1_554] | 2.06 | 0.14 |
| 4:6:186:THR:N | 4:9:157:ASP:C[1_554] | 2.06 | 0.14 |
| 4:3:366:GLY:C | 4:7:234:SER:C[1_554] | 2.06 | 0.14 |
| 4:4:265:SER:CA | 4:7:261:LEU:C[1_554] | 2.06 | 0.14 |
| 4:5:17:VAL:C | 4:8:79:TRP:CD1[1_554] | 2.06 | 0.14 |
| 4:6:227:MET:SD | 4:9:306:TYR:O[1_554] | 2.06 | 0.14 |
| 4:6:288:ASP:O | 4:W:64:ILE:CA[1_554] | 2.06 | 0.14 |
| 4:3:118:LYS:N | 4:7:237:GLU:CG[1_554] | 2.06 | 0.14 |
| 4:6:141:SER:CB | 4:9:107:GLU:OE2[1_554] | 2.06 | 0.14 |
| 4:6:283:MET:SD | 4:9:286:ASP:C[1_554] | 2.06 | 0.14 |
| 4:4:173:HIS:CE1 | 4:8:265:SER:CA[1_554] | 2.06 | 0.14 |
| 4:5:349:LEU:CA | 4:8:364:GLU:O[1_554] | 2.06 | 0.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:288:ASP:C | 4:8:64:ILE:CA[1_554] | 2.06 | 0.14 |
| 4:5:72:GLU:O | 4:9:198:TYR:C[1_554] | 2.06 | 0.14 |
| 4:6:266:PHE:CZ | 4:9:261:LEU:CD1[1_554] | 2.06 | 0.14 |
| 4:4:30:VAL:CA | 4:7:79:TRP:O[1_554] | 2.06 | 0.14 |
| 4:5:273:GLY:N | 4:8:162:ASN:OD1[1_554] | 2.06 | 0.14 |
| 4:5:18:LYS:C | 4:8:122:ILE:CD1[1_554] | 2.06 | 0.14 |
| 4:6:75:ILE:CD1 | 4:V:195:GLU:N[1_554] | 2.06 | 0.14 |
| 4:4:184:ASP:N | 4:7:73:HIS:ND1[1_554] | 2.06 | 0.14 |
| 4:4:186:THR:C | 4:7:183:ARG:CB[1_554] | 2.06 | 0.14 |
| 4:4:275:HIS:C | 4:7:164:PRO:N[1_554] | 2.06 | 0.14 |
| 4:5:316:GLU:CB | 4:8:151:ILE:C[1_554] | 2.06 | 0.14 |
| 4:5:195:GLU:OE1 | 4:8:257:CYS:CB[1_554] | 2.06 | 0.14 |
| 4:4:200:PHE:CD2 | 4:7:206:ARG:NE[1_554] | 2.06 | 0.14 |
| 4:4:276:GLU:OE2 | 4:7:278:THR:N[1_554] | 2.06 | 0.14 |
| 4:6:312:ARG:O | 4:9:298:VAL:N[1_554] | 2.06 | 0.14 |
| 4:5:110:LEU:CA | 4:9:192:ILE:CG2[1_554] | 2.06 | 0.14 |
| 4:5:275:HIS:N | 4:8:162:ASN:C[1_554] | 2.06 | 0.14 |
| 4:4:213:LYS:N | 4:7:15:GLY:C[1_554] | 2.06 | 0.14 |
| 4:6:276:GLU:CG | 4:9:278:THR:CA[1_554] | 2.06 | 0.14 |
| 4:6:174:ALA:C | 4:9:173:HIS:CA[1_554] | 2.06 | 0.14 |
| 4:4:341:ILE:CD1 | 4:7:119:MET:C[1_554] | 2.06 | 0.14 |
| 4:5:200:PHE:CZ | 4:8:207:GLU:C[1_554] | 2.06 | 0.14 |
| 4:5:343:GLY:O | 4:8:367:PRO:CG[1_554] | 2.06 | 0.14 |
| 4:6:372:ARG:CA | 4:V:227:MET:O[1_554] | 2.06 | 0.14 |
| 4:5:255:PHE:O | 4:8:305:MET:N[1_554] | 2.06 | 0.14 |
| 4:5:185:LEU:CB | 4:8:157:ASP:O[1_554] | 2.06 | 0.14 |
| 4:5:321:ALA:O | 4:8:292:ASP:CG[1_554] | 2.06 | 0.14 |
| 4:4:312:ARG:N | 4:7:142:LEU:N[1_554] | 2.06 | 0.14 |
| 4:6:173:HIS:O | 4:V:267:ILE:CA[1_554] | 2.06 | 0.14 |
| 4:4:220:ALA:O | 4:7:299:MET:O[1_554] | 2.06 | 0.14 |
| 4:5:156:GLY:CA | 4:8:74:GLY:CA[1_554] | 2.06 | 0.14 |
| 4:5:113:LYS:CA | 4:9:252:ASN:CA[1_554] | 2.07 | 0.13 |
| 4:6:112:PRO:CG | 4:V:193:LEU:CA[1_554] | 2.07 | 0.13 |
| 4:5:253:GLU:N | 4:8:214:GLU:CA[1_554] | 2.07 | 0.13 |
| 4:5:27:PRO:CG | 4:8:86:TRP:CZ3[1_554] | 2.07 | 0.13 |
| 4:3:149:THR:CG2 | 4:8:40:HIS:CD2[1_554] | 2.07 | 0.13 |
| 4:2:291:LYS:CB | 4:7:40:HIS:CB[1_554] | 2.07 | 0.13 |
| 4:6:137:GLN:CG | 4:9:112:PRO:CB[1_554] | 2.07 | 0.13 |
| 4:4:281:SER:CB | 4:7:172:PRO:C[1_554] | 2.07 | 0.13 |
| 4:6:140:LEU:N | 4:9:371:HIS:CG[1_554] | 2.07 | 0.13 |
| 4:5:149:THR:OG1 | 4:V:40:HIS:CB[1_554] | 2.07 | 0.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:243:PRO:CG | 4:7:62:ARG:N[1_554] | 2.07 | 0.13 |
| 4:5:188:TYR:CA | 4:8:184:ASP:CA[1_554] | 2.07 | 0.13 |
| 4:4:156:GLY:O | 4:7:73:HIS:O[1_554] | 2.07 | 0.13 |
| 4:6:157:ASP:C | 4:9:73:HIS:CB[1_554] | 2.07 | 0.13 |
| 4:6:309:ILE:CB | 4:9:339:VAL:CG2[1_554] | 2.07 | 0.13 |
| 4:6:289:ILE:CG2 | 4:W:39:ARG:CZ[1_554] | 2.07 | 0.13 |
| 4:4:314:GLN:C | 4:7:142:LEU:CD1[1_554] | 2.07 | 0.13 |
| 4:5:227:MET:CB | 4:8:308:GLY:N[1_554] | 2.07 | 0.13 |
| 4:4:342:GLY:C | 4:7:117:GLU:CD[1_554] | 2.07 | 0.13 |
| 4:6:106:THR:OG1 | 4:9:115:ASN:N[1_554] | 2.07 | 0.13 |
| 4:4:311:ASP:C | 4:7:141:SER:CA[1_554] | 2.07 | 0.13 |
| 4:6:268:GLY:CA | 4:9:264:PRO:C[1_554] | 2.07 | 0.13 |
| 4:6:30:VAL:CG2 | 4:9:83:GLU:N[1_554] | 2.07 | 0.13 |
| 4:5:256:ARG:CZ | 4:8:217:CYS:CB[1_554] | 2.07 | 0.13 |
| 4:4:196:ARG:CA | 4:7:212:ILE:CA[1_554] | 2.07 | 0.13 |
| 4:4:263:GLN:CB | 4:7:274:ILE:CG1[1_554] | 2.07 | 0.13 |
| 4:3:75:ILE:N | 4:7:197:GLY:O[1_554] | 2.07 | 0.13 |
| 4:6:304:THR:C | 4:9:137:GLN:CG[1_554] | 2.07 | 0.13 |
| 4:5:198:TYR:OH | 4:8:211:ASP:CB[1_554] | 2.07 | 0.13 |
| 4:5:75:ILE:CD1 | 4:9:197:GLY:N[1_554] | 2.07 | 0.13 |
| 4:6:136:ILE:N | 4:9:113:LYS:CB[1_554] | 2.07 | 0.13 |
| 4:5:198:TYR:CA | 4:8:209:VAL:N[1_554] | 2.07 | 0.13 |
| 4:5:259:GLU:N | 4:8:304:THR:CG2[1_554] | 2.07 | 0.13 |
| 4:5:322:PRO:O | 4:8:291:LYS:NZ[1_554] | 2.07 | 0.13 |
| 4:5:254:ARG:O | 4:8:302:GLY:CA[1_554] | 2.07 | 0.13 |
| 4:5:223:PHE:C | 4:8:309:ILE:CG2[1_554] | 2.07 | 0.13 |
| 4:6:198:TYR:CE1 | 4:9:208:ILE:CD1[1_554] | 2.07 | 0.13 |
| 4:4:332:PRO:CB | 4:7:133:TYR:O[1_554] | 2.07 | 0.13 |
| 4:4:319:ALA:O | 4:7:293:LEU:C[1_554] | 2.07 | 0.13 |
| 4:6:276:GLU:CD | 4:9:278:THR:CA[1_554] | 2.07 | 0.13 |
| 4:4:177:ARG:CZ | 4:8:194:THR:CB[1_554] | 2.07 | 0.13 |
| 4:4:222:ASP:N | 4:7:332:PRO:CG[1_554] | 2.07 | 0.13 |
| 4:5:139:VAL:C | 4:8:371:HIS:NE2[1_554] | 2.07 | 0.13 |
| 4:6:274:ILE:CD1 | 4:9:161:HIS:CG[1_554] | 2.07 | 0.13 |
| 4:4:192:ILE:N | 4:7:186:THR:N[1_554] | 2.07 | 0.13 |
| 4:3:173:HIS:CB | 4:7:267:ILE:CA[1_554] | 2.07 | 0.13 |
| 4:5:276:GLU:CG | 4:8:278:THR:CA[1_554] | 2.07 | 0.13 |
| 4:6:31:PHE:CA | 4:9:80:ASP:C[1_554] | 2.07 | 0.13 |
| 4:6:274:ILE:C | 4:9:162:ASN:O[1_554] | 2.07 | 0.13 |
| 4:3:366:GLY:O | 4:7:234:SER:C[1_554] | 2.07 | 0.13 |
| 4:4:332:PRO:N | 4:7:135:ALA:CA[1_554] | 2.07 | 0.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:311:ASP:CG | 4:8:144:ALA:C[1_554] | 2.07 | 0.13 |
| 4:6:293:LEU:C | 4:9:166:TYR:O[1_554] | 2.07 | 0.13 |
| 4:5:111:ASN:N | 4:9:192:ILE:O[1_554] | 2.07 | 0.13 |
| 4:4:316:GLU:CD | 4:7:298:VAL:O[1_554] | 2.07 | 0.13 |
| 4:6:288:ASP:CB | 4:W:62:ARG:C[1_554] | 2.07 | 0.13 |
| 4:5:159:VAL:CB | 4:8:177:ARG:NH1[1_554] | 2.07 | 0.13 |
| 4:3:369:ILE:O | 4:7:229:THR:CB[1_554] | 2.07 | 0.13 |
| 4:4:282:ILE:N | 4:7:173:HIS:CD2[1_554] | 2.07 | 0.13 |
| 4:4:194:THR:O | 4:7:209:VAL:CG1[1_554] | 2.07 | 0.13 |
| 4:5:17:VAL:N | 4:8:78:ASN:C[1_554] | 2.07 | 0.13 |
| 4:5:196:ARG:CG | 4:8:211:ASP:O[1_554] | 2.07 | 0.13 |
| 4:3:173:HIS:CE1 | 4:7:266:PHE:CA[1_554] | 2.07 | 0.13 |
| 4:6:30:VAL:CG1 | 4:9:82:MET:C[1_554] | 2.07 | 0.13 |
| 4:5:192:ILE:CA | 4:8:213:LYS:CD[1_554] | 2.07 | 0.13 |
| 4:6:307:PRO:CG | 4:9:337:TYR:CB[1_554] | 2.07 | 0.13 |
| 4:4:277:THR:CA | 4:7:175:ILE:CA[1_554] | 2.07 | 0.13 |
| 4:5:187:ASP:O | 4:8:184:ASP:N[1_554] | 2.07 | 0.13 |
| 4:5:188:TYR:CD2 | 4:8:182:GLY:CA[1_554] | 2.07 | 0.13 |
| 4:6:340:TRP:N | 4:9:116:ARG:CA[1_554] | 2.07 | 0.13 |
| 4:4:326:LYS:C | 4:7:167:GLU:C[1_554] | 2.07 | 0.13 |
| 4:6:262:PHE:CE1 | 4:9:152:VAL:C[1_554] | 2.07 | 0.13 |
| 4:3:173:HIS:CB | 4:7:267:ILE:N[1_554] | 2.07 | 0.13 |
| 4:5:33:SER:N | 4:8:78:ASN:CB[1_554] | 2.07 | 0.13 |
| 4:4:289:ILE:CB | 4:9:39:ARG:NH2[1_554] | 2.07 | 0.13 |
| 4:6:19:ALA:N | 4:9:122:ILE:CG1[1_554] | 2.07 | 0.13 |
| 4:4:240:TYR:CE2 | 4:7:32:PRO:CD[1_554] | 2.07 | 0.13 |
| 4:4:368:SER:O | 4:8:236:LEU:CD1[1_554] | 2.07 | 0.13 |
| 4:3:173:HIS:NE2 | 4:7:264:PRO:C[1_554] | 2.07 | 0.13 |
| 4:6:17:VAL:CA | 4:9:79:TRP:NE1[1_554] | 2.07 | 0.13 |
| 4:6:366:GLY:O | 4:V:232:SER:C[1_554] | 2.07 | 0.13 |
| 4:4:339:VAL:CG1 | 4:7:114:ALA:O[1_554] | 2.07 | 0.13 |
| 4:6:326:LYS:CG | 4:9:167:GLU:CD[1_554] | 2.07 | 0.13 |
| 4:5:187:ASP:C | 4:8:183:ARG:CA[1_554] | 2.07 | 0.13 |
| 4:6:219:VAL:N | 4:9:336:LYS:N[1_554] | 2.07 | 0.13 |
| 4:6:195:GLU:CB | 4:9:189:LEU:CD1[1_554] | 2.07 | 0.13 |
| 4:5:338:SER:N | 4:8:134:VAL:CG2[1_554] | 2.07 | 0.13 |
| 4:4:269:MET:CA | 4:7:271:SER:OG[1_554] | 2.07 | 0.13 |
| 4:6:17:VAL:CA | 4:9:79:TRP:CB[1_554] | 2.07 | 0.13 |
| 4:5:207:GLU:CB | 4:8:67:LEU:CG[1_554] | 2.07 | 0.13 |
| 4:6:199:SER:C | 4:9:207:GLU:N[1_554] | 2.07 | 0.13 |
| 4:4:283:MET:CE | 4:7:289:ILE:CG1[1_554] | 2.07 | 0.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:220:ALA:CB | 4:7:336:LYS:N[1_554] | 2.07 | 0.13 |
| 4:6:177:ARG:NH1 | 4:V:194:THR:CG2[1_554] | 2.07 | 0.13 |
| 4:6:273:GLY:O | 4:9:162:ASN:OD1[1_554] | 2.07 | 0.13 |
| 4:5:264:PRO:CD | 4:8:274:ILE:CD1[1_554] | 2.07 | 0.13 |
| 4:6:28:ARG:CA | 4:9:126:THR:CG2[1_554] | 2.07 | 0.13 |
| 4:6:345:ILE:CD1 | 4:9:357:ILE:CG1[1_554] | 2.07 | 0.13 |
| 4:6:174:ALA:O | 4:9:173:HIS:CG[1_554] | 2.07 | 0.13 |
| 4:6:277:THR:O | 4:9:175:ILE:N[1_554] | 2.07 | 0.13 |
| 4:4:299:MET:CG | 4:7:137:GLN:N[1_554] | 2.07 | 0.13 |
| 4:5:154:ASP:C | 4:8:109:PRO:CA[1_554] | 2.07 | 0.13 |
| 4:4:266:PHE:N | 4:7:261:LEU:CG[1_554] | 2.07 | 0.13 |
| 4:5:296:ASN:CA | 4:8:168:GLY:O[1_554] | 2.07 | 0.13 |
| 4:5:219:VAL:C | 4:8:335:ARG:O[1_554] | 2.07 | 0.13 |
| 4:6:256:ARG:NH2 | 4:9:217:CYS:CB[1_554] | 2.07 | 0.13 |
| 4:6:227:MET:CB | 4:9:308:GLY:N[1_554] | 2.07 | 0.13 |
| 4:6:219:VAL:O | 4:9:335:ARG:O[1_554] | 2.07 | 0.13 |
| 4:4:111:ASN:CB | 4:8:196:ARG:CB[1_554] | 2.07 | 0.13 |
| 4:6:140:LEU:N | 4:9:371:HIS:NE2[1_554] | 2.07 | 0.13 |
| 4:5:367:PRO:CA | 4:9:233:SER:N[1_554] | 2.07 | 0.13 |
| 4:4:316:GLU:C | 4:7:150:GLY:CA[1_554] | 2.07 | 0.13 |
| 4:4:218:TYR:CE2 | 4:7:337:TYR:CE1[1_554] | 2.07 | 0.13 |
| 4:5:211:ASP:OD2 | 4:8:32:PRO:CD[1_554] | 2.07 | 0.13 |
| 4:5:22:ALA:CA | 4:8:362:TYR:CE2[1_554] | 2.07 | 0.13 |
| 4:4:214:GLU:CB | 4:7:33:SER:CB[1_554] | 2.07 | 0.13 |
| 4:5:210:ARG:CZ | 4:8:33:SER:CA[1_554] | 2.07 | 0.13 |
| 4:4:114:ALA:O | 4:8:250:ILE:N[1_554] | 2.07 | 0.13 |
| 4:6:173:HIS:CA | 4:V:266:PHE:C[1_554] | 2.07 | 0.13 |
| 4:6:198:TYR:OH | 4:9:211:ASP:CG[1_554] | 2.07 | 0.13 |
| 4:5:341:ILE:CG1 | 4:8:132:MET:SD[1_554] | 2.07 | 0.13 |
| 4:5:252:ASN:CA | 4:8:214:GLU:O[1_554] | 2.07 | 0.13 |
| 4:6:26:ALA:CA | 4:9:123:MET:N[1_554] | 2.07 | 0.13 |
| 4:6:191:LYS:CG | 4:9:185:LEU:CA[1_554] | 2.07 | 0.13 |
| 4:4:194:THR:O | 4:7:209:VAL:N[1_554] | 2.07 | 0.13 |
| 4:5:260:THR:OG1 | 4:8:303:THR:CG2[1_554] | 2.07 | 0.13 |
| 4:6:109:PRO:CA | 4:V:195:GLU:CG[1_554] | 2.07 | 0.13 |
| 4:5:299:MET:N | 4:8:136:ILE:CA[1_554] | 2.07 | 0.13 |
| 4:5:21:PHE:N | 4:8:125:GLU:CB[1_554] | 2.07 | 0.13 |
| 4:4:189:LEU:O | 4:7:186:THR:OG1[1_554] | 2.07 | 0.13 |
| 4:4:341:ILE:N | 4:7:118:LYS:N[1_554] | 2.07 | 0.13 |
| 4:4:139:VAL:CB | 4:7:113:LYS:CE[1_554] | 2.07 | 0.13 |
| 4:6:249:THR:CG2 | 4:9:211:ASP:OD1[1_554] | 2.07 | 0.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:117:GLU:CA | 4:8:237:GLU:CA[1_554] | 2.07 | 0.13 |
| 4:5:185:LEU:CD2 | 4:8:159:VAL:O[1_554] | 2.07 | 0.13 |
| 4:4:159:VAL:CA | 4:7:177:ARG:NH1[1_554] | 2.07 | 0.13 |
| 4:4:227:MET:CB | 4:7:305:MET:O[1_554] | 2.08 | 0.12 |
| 4:5:181:ALA:C | 4:8:159:VAL:N[1_554] | 2.08 | 0.12 |
| 4:4:116:ARG:CB | 4:8:252:ASN:CG[1_554] | 2.08 | 0.12 |
| 4:6:262:PHE:C | 4:9:153:LEU:CG[1_554] | 2.08 | 0.12 |
| 4:6:336:LYS:C | 4:9:119:MET:CE[1_554] | 2.08 | 0.12 |
| 4:4:317:ILE:CA | 4:7:150:GLY:CA[1_554] | 2.08 | 0.12 |
| 4:4:75:ILE:C | 4:8:197:GLY:C[1_554] | 2.08 | 0.12 |
| 4:5:184:ASP:OD2 | 4:8:179:ASP:O[1_554] | 2.08 | 0.12 |
| 4:5:162:ASN:CG | 4:8:175:ILE:CA[1_554] | 2.08 | 0.12 |
| 4:4:266:PHE:C | 4:7:180:LEU:CD1[1_554] | 2.08 | 0.12 |
| 4:5:9:VAL:O | 4:8:121:GLN:OE1[1_554] | 2.08 | 0.12 |
| 4:4:173:HIS:N | 4:8:267:ILE:CG2[1_554] | 2.08 | 0.12 |
| 4:6:294:TYR:CD2 | 4:9:166:TYR:CE1[1_554] | 2.08 | 0.12 |
| 4:6:31:PHE:CD2 | 4:9:80:ASP:CB[1_554] | 2.08 | 0.12 |
| 4:3:111:ASN:CB | 4:7:196:ARG:CB[1_554] | 2.08 | 0.12 |
| 4:4:143:TYR:CE2 | 4:7:368:SER:C[1_554] | 2.08 | 0.12 |
| 4:6:32:PRO:O | 4:9:78:ASN:ND2[1_554] | 2.08 | 0.12 |
| 4:5:106:THR:N | 4:8:114:ALA:CB[1_554] | 2.08 | 0.12 |
| 4:4:197:GLY:N | 4:7:209:VAL:CA[1_554] | 2.08 | 0.12 |
| 4:4:297:ASN:OD1 | 4:7:169:TYR:C[1_554] | 2.08 | 0.12 |
| 4:5:204:ALA:CB | 4:8:62:ARG:C[1_554] | 2.08 | 0.12 |
| 4:5:188:TYR:OH | 4:8:185:LEU:CG[1_554] | 2.08 | 0.12 |
| 4:6:207:GLU:CD | 4:9:67:LEU:CA[1_554] | 2.08 | 0.12 |
| 4:6:254:ARG:NH2 | 4:9:336:LYS:CE[1_554] | 2.08 | 0.12 |
| 4:6:114:ALA:C | 4:V:251:GLY:N[1_554] | 2.08 | 0.12 |
| 4:5:141:SER:CB | 4:8:107:GLU:OE2[1_554] | 2.08 | 0.12 |
| 4:4:310:ALA:O | 4:7:142:LEU:N[1_554] | 2.08 | 0.12 |
| 4:4:137:GLN:CB | 4:7:112:PRO:CA[1_554] | 2.08 | 0.12 |
| 4:6:317:ILE:CB | 4:9:151:ILE:N[1_554] | 2.08 | 0.12 |
| 4:6:262:PHE:CA | 4:9:153:LEU:CD2[1_554] | 2.08 | 0.12 |
| 4:4:281:SER:CA | 4:7:174:ALA:N[1_554] | 2.08 | 0.12 |
| 4:4:280:ASN:CB | 4:7:284:LYS:CB[1_554] | 2.08 | 0.12 |
| 4:6:292:ASP:CG | 4:W:64:ILE:CD1[1_554] | 2.08 | 0.12 |
| 4:5:340:TRP:O | 4:8:117:GLU:O[1_554] | 2.08 | 0.12 |
| 4:6:178:LEU:CA | 4:9:177:ARG:CB[1_554] | 2.08 | 0.12 |
| 4:4:178:LEU:CD2 | 4:7:177:ARG:C[1_554] | 2.08 | 0.12 |
| 4:6:281:SER:O | 4:9:173:HIS:CE1[1_554] | 2.08 | 0.12 |
| 4:4:276:GLU:CD | 4:7:278:THR:CA[1_554] | 2.08 | 0.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:297:ASN:ND2 | 4:8:165:ILE:CD1[1_554] | 2.08 | 0.12 |
| 4:5:325:MET:SD | 4:8:166:TYR:CE2[1_554] | 2.08 | 0.12 |
| 4:5:274:ILE:CA | 4:8:162:ASN:CB[1_554] | 2.08 | 0.12 |
| 4:6:218:TYR:CD1 | 4:9:336:LYS:CB[1_554] | 2.08 | 0.12 |
| 4:6:191:LYS:CG | 4:9:186:THR:N[1_554] | 2.08 | 0.12 |
| 4:4:267:ILE:C | 4:7:180:LEU:CD1[1_554] | 2.08 | 0.12 |
| 4:3:367:PRO:CA | 4:7:235:SER:C[1_554] | 2.08 | 0.12 |
| 4:5:367:PRO:CB | 4:9:233:SER:CA[1_554] | 2.08 | 0.12 |
| 4:4:208:ILE:CG1 | 4:7:59:GLN:CA[1_554] | 2.08 | 0.12 |
| 4:6:335:ARG:NH1 | 4:9:140:LEU:CD1[1_554] | 2.08 | 0.12 |
| 4:6:16:LEU:N | 4:9:78:ASN:N[1_554] | 2.08 | 0.12 |
| 4:6:196:ARG:NE | 4:9:211:ASP:OD1[1_554] | 2.08 | 0.12 |
| 4:6:299:MET:CE | 4:9:137:GLN:C[1_554] | 2.08 | 0.12 |
| 4:6:143:TYR:CB | 4:9:371:HIS:C[1_554] | 2.08 | 0.12 |
| 4:3:74:GLY:C | 4:7:197:GLY:N[1_554] | 2.08 | 0.12 |
| 4:6:340:TRP:CE3 | 4:9:121:GLN:N[1_554] | 2.08 | 0.12 |
| 4:4:256:ARG:NH2 | 4:7:213:LYS:CG[1_554] | 2.08 | 0.12 |
| 4:6:75:ILE:CD1 | 4:V:194:THR:O[1_554] | 2.08 | 0.12 |
| 4:5:322:PRO:O | 4:8:292:ASP:CG[1_554] | 2.08 | 0.12 |
| 4:6:335:ARG:CD | 4:9:106:THR:CB[1_554] | 2.08 | 0.12 |
| 4:4:143:TYR:O | 4:7:368:SER:O[1_554] | 2.08 | 0.12 |
| 4:5:174:ALA:CA | 4:8:173:HIS:CB[1_554] | 2.08 | 0.12 |
| 4:5:204:ALA:CB | 4:8:62:ARG:N[1_554] | 2.08 | 0.12 |
| 4:5:304:THR:N | 4:8:137:GLN:NE2[1_554] | 2.08 | 0.12 |
| 4:6:27:PRO:C | 4:9:122:ILE:CB[1_554] | 2.08 | 0.12 |
| 4:5:41:GLN:CG | 4:7:224:GLU:CD[1_554] | 2.08 | 0.12 |
| 4:5:21:PHE:CB | 4:8:125:GLU:CB[1_554] | 2.08 | 0.12 |
| 4:6:298:VAL:O | 4:9:136:ILE:CB[1_554] | 2.08 | 0.12 |
| 4:4:259:GLU:CG | 4:7:304:THR:OG1[1_554] | 2.08 | 0.12 |
| 4:4:173:HIS:ND1 | 4:8:266:PHE:CA[1_554] | 2.08 | 0.12 |
| 4:4:299:MET:CA | 4:7:136:ILE:CB[1_554] | 2.08 | 0.12 |
| 4:3:174:ALA:CB | 4:7:268:GLY:N[1_554] | 2.08 | 0.12 |
| 4:5:30:VAL:C | 4:8:82:MET:N[1_554] | 2.08 | 0.12 |
| 4:6:173:HIS:C | 4:V:267:ILE:O[1_554] | 2.08 | 0.12 |
| 4:3:172:PRO:CD | 4:7:266:PHE:CD1[1_554] | 2.08 | 0.12 |
| 4:4:367:PRO:CA | 4:8:235:SER:N[1_554] | 2.08 | 0.12 |
| 4:4:259:GLU:C | 4:7:155:SER:OG[1_554] | 2.08 | 0.12 |
| 4:6:288:ASP:C | 4:W:63:GLY:O[1_554] | 2.08 | 0.12 |
| 4:4:267:ILE:CG1 | 4:7:180:LEU:C[1_554] | 2.08 | 0.12 |
| 4:3:173:HIS:C | 4:7:267:ILE:N[1_554] | 2.08 | 0.12 |
| 4:6:9:VAL:N | 4:9:121:GLN:CG[1_554] | 2.08 | 0.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:286:ASP:OD1 | 4:7:270:GLU:OE1[1_554] | 2.08 | 0.12 |
| 4:4:214:GLU:C | 4:7:17:VAL:CA[1_554] | 2.08 | 0.12 |
| 4:4:195:GLU:OE1 | 4:7:213:LYS:CG[1_554] | 2.08 | 0.12 |
| 4:5:17:VAL:C | 4:8:79:TRP:CA[1_554] | 2.08 | 0.12 |
| 4:6:201:VAL:CG2 | 4:9:202:THR:C[1_554] | 2.08 | 0.12 |
| 4:5:157:ASP:C | 4:8:73:HIS:CA[1_554] | 2.08 | 0.12 |
| 4:6:18:LYS:CE | 4:9:79:TRP:CZ2[1_554] | 2.08 | 0.12 |
| 4:4:18:LYS:NZ | 4:7:79:TRP:NE1[1_554] | 2.08 | 0.12 |
| 4:3:367:PRO:CG | 4:7:235:SER:C[1_554] | 2.08 | 0.12 |
| 4:4:264:PRO:C | 4:7:274:ILE:CD1[1_554] | 2.08 | 0.12 |
| 4:3:118:LYS:N | 4:7:237:GLU:CB[1_554] | 2.08 | 0.12 |
| 4:5:26:ALA:CB | 4:8:123:MET:CA[1_554] | 2.08 | 0.12 |
| 4:5:31:PHE:CD1 | 4:8:80:ASP:CB[1_554] | 2.08 | 0.12 |
| 4:4:262:PHE:CD1 | 4:7:153:LEU:N[1_554] | 2.08 | 0.12 |
| 4:4:255:PHE:CD2 | 4:7:305:MET:CG[1_554] | 2.08 | 0.12 |
| 4:5:343:GLY:O | 4:8:367:PRO:CD[1_554] | 2.08 | 0.12 |
| 4:3:113:LYS:C | 4:7:251:GLY:C[1_554] | 2.08 | 0.12 |
| 4:6:299:MET:CG | 4:9:137:GLN:N[1_554] | 2.08 | 0.12 |
| 4:6:349:LEU:C | 4:9:365:ALA:CA[1_554] | 2.08 | 0.12 |
| 4:6:299:MET:CB | 4:9:136:ILE:CA[1_554] | 2.08 | 0.12 |
| 4:5:369:ILE:O | 4:9:228:ALA:C[1_554] | 2.08 | 0.12 |
| 4:4:312:ARG:O | 4:7:152:VAL:CG2[1_554] | 2.08 | 0.12 |
| 4:4:197:GLY:C | 4:7:208:ILE:CA[1_554] | 2.08 | 0.12 |
| 4:6:370:VAL:CA | 4:V:231:ALA:N[1_554] | 2.08 | 0.12 |
| 4:5:335:ARG:NH1 | 4:8:140:LEU:CD1[1_554] | 2.08 | 0.12 |
| 4:5:21:PHE:C | 4:8:125:GLU:OE2[1_554] | 2.08 | 0.12 |
| 4:3:371:HIS:CA | 4:7:236:LEU:CD1[1_554] | 2.08 | 0.12 |
| 4:4:114:ALA:O | 4:8:250:ILE:O[1_554] | 2.08 | 0.12 |
| 4:5:137:GLN:CD | 4:8:112:PRO:CG[1_554] | 2.08 | 0.12 |
| 4:5:190:MET:CB | 4:8:187:ASP:OD1[1_554] | 2.08 | 0.12 |
| 4:5:9:VAL:CG2 | 4:8:367:PRO:CG[1_554] | 2.08 | 0.12 |
| 4:5:343:GLY:CA | 4:8:367:PRO:C[1_554] | 2.08 | 0.12 |
| 4:5:281:SER:O | 4:8:173:HIS:CE1[1_554] | 2.08 | 0.12 |
| 4:6:294:TYR:CG | 4:9:166:TYR:CA[1_554] | 2.08 | 0.12 |
| 4:6:108:ALA:CB | 4:V:195:GLU:O[1_554] | 2.08 | 0.12 |
| 4:6:293:LEU:O | 4:9:169:TYR:CB[1_554] | 2.09 | 0.11 |
| 4:5:317:ILE:CB | 4:8:150:GLY:CA[1_554] | 2.09 | 0.11 |
| 4:5:198:TYR:CD2 | 4:8:209:VAL:N[1_554] | 2.09 | 0.11 |
| 4:5:182:GLY:O | 4:8:158:GLY:CA[1_554] | 2.09 | 0.11 |
| 4:4:281:SER:CA | 4:7:173:HIS:CA[1_554] | 2.09 | 0.11 |
| 4:6:237:GLU:OE2 | 4:9:215:LYS:CG[1_554] | 2.09 | 0.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:317:ILE:CG1 | 4:7:165:ILE:CG2[1_554] | 2.09 | 0.11 |
| 4:5:327:ILE:CA | 4:8:148:THR:O[1_554] | 2.09 | 0.11 |
| 4:5:292:ASP:OD2 | 4:V:64:ILE:CB[1_554] | 2.09 | 0.11 |
| 4:6:182:GLY:O | 4:9:158:GLY:CA[1_554] | 2.09 | 0.11 |
| 4:5:141:SER:N | 4:8:116:ARG:NE[1_554] | 2.09 | 0.11 |
| 4:4:299:MET:C | 4:7:107:GLU:CD[1_554] | 2.09 | 0.11 |
| 1:A:637:LYS:CG | 4:5:311:ASP:CG[1_556] | 2.09 | 0.11 |
| 4:5:334:GLU:O | 4:8:105:LEU:C[1_554] | 2.09 | 0.11 |
| 4:6:56:ASP:CG | 4:9:37:ARG:NH1[1_554] | 2.09 | 0.11 |
| 4:5:275:HIS:CA | 4:8:151:ILE:CG1[1_554] | 2.09 | 0.11 |
| 4:5:315:LYS:NZ | 4:8:295:ALA:O[1_554] | 2.09 | 0.11 |
| 4:5:145:SER:OG | 4:8:372:ARG:CZ[1_554] | 2.09 | 0.11 |
| 4:5:341:ILE:CA | 4:8:120:THR:CG2[1_554] | 2.09 | 0.11 |
| 4:5:288:ASP:N | 4:V:62:ARG:C[1_554] | 2.09 | 0.11 |
| 4:6:274:ILE:CA | 4:9:162:ASN:CB[1_554] | 2.09 | 0.11 |
| 4:5:295:ALA:N | 4:8:167:GLU:N[1_554] | 2.09 | 0.11 |
| 4:6:252:ASN:CG | 4:9:215:LYS:O[1_554] | 2.09 | 0.11 |
| 4:5:188:TYR:CD1 | 4:8:185:LEU:N[1_554] | 2.09 | 0.11 |
| 4:3:286:ASP:CA | 4:7:270:GLU:CG[1_554] | 2.09 | 0.11 |
| 4:6:215:LYS:CD | 4:9:31:PHE:N[1_554] | 2.09 | 0.11 |
| 4:6:265:SER:C | 4:9:260:THR:O[1_554] | 2.09 | 0.11 |
| 4:6:369:ILE:CA | 4:V:232:SER:N[1_554] | 2.09 | 0.11 |
| 4:5:325:MET:SD | 4:8:166:TYR:CE1[1_554] | 2.09 | 0.11 |
| 4:5:211:ASP:CB | 4:8:32:PRO:N[1_554] | 2.09 | 0.11 |
| 4:6:151:ILE:N | 4:9:169:TYR:CE1[1_554] | 2.09 | 0.11 |
| 4:6:348:SER:C | 4:9:366:GLY:N[1_554] | 2.09 | 0.11 |
| 4:5:370:VAL:CB | 4:9:231:ALA:C[1_554] | 2.09 | 0.11 |
| 4:6:340:TRP:CB | 4:9:119:MET:CG[1_554] | 2.09 | 0.11 |
| 4:4:367:PRO:CG | 4:8:235:SER:C[1_554] | 2.09 | 0.11 |
| 4:4:341:ILE:CB | 4:7:120:THR:CA[1_554] | 2.09 | 0.11 |
| 4:4:193:LEU:N | 4:7:210:ARG:CG[1_554] | 2.09 | 0.11 |
| 4:4:298:VAL:CA | 4:7:136:ILE:CD1[1_554] | 2.09 | 0.11 |
| 4:4:271:SER:C | 4:7:277:THR:CB[1_554] | 2.09 | 0.11 |
| 4:5:60:SER:CB | 4:8:37:ARG:CA[1_554] | 2.09 | 0.11 |
| 4:4:254:ARG:NH1 | 4:7:337:TYR:OH[1_554] | 2.09 | 0.11 |
| 4:6:215:LYS:CE | 4:9:30:VAL:O[1_554] | 2.09 | 0.11 |
| 4:5:18:LYS:NZ | 4:8:76:ILE:CG2[1_554] | 2.09 | 0.11 |
| 4:5:188:TYR:CD2 | 4:8:182:GLY:N[1_554] | 2.09 | 0.11 |
| 4:5:370:VAL:CB | 4:9:231:ALA:O[1_554] | 2.09 | 0.11 |
| 4:4:340:TRP:C | 4:7:117:GLU:CA[1_554] | 2.09 | 0.11 |
| 4:5:215:LYS:CG | 4:8:30:VAL:O[1_554] | 2.09 | 0.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:341:ILE:CB | 4:8:132:MET:CE[1_554] | 2.09 | 0.11 |
| 4:5:334:GLU:CD | 4:8:133:TYR:C[1_554] | 2.09 | 0.11 |
| 4:6:281:SER:OG | 4:9:171:LEU:O[1_554] | 2.09 | 0.11 |
| 4:4:224:GLU:CB | 4:7:331:ALA:CB[1_554] | 2.09 | 0.11 |
| 4:4:263:GLN:N | 4:7:153:LEU:CG[1_554] | 2.09 | 0.11 |
| 4:5:227:MET:C | 4:8:307:PRO:CG[1_554] | 2.09 | 0.11 |
| 4:6:369:ILE:C | 4:V:231:ALA:CB[1_554] | 2.09 | 0.11 |
| 4:5:218:TYR:CA | 4:8:336:LYS:C[1_554] | 2.09 | 0.11 |
| 4:5:261:LEU:CA | 4:8:154:ASP:O[1_554] | 2.09 | 0.11 |
| 4:4:281:SER:CB | 4:7:173:HIS:C[1_554] | 2.09 | 0.11 |
| 4:5:178:LEU:CD2 | 4:8:177:ARG:C[1_554] | 2.09 | 0.11 |
| 4:6:334:GLU:CA | 4:9:105:LEU:CB[1_554] | 2.09 | 0.11 |
| 4:5:180:LEU:CA | 4:8:179:ASP:CA[1_554] | 2.09 | 0.11 |
| 4:5:22:ALA:O | 4:8:125:GLU:OE2[1_554] | 2.09 | 0.11 |
| 4:6:110:LEU:CD2 | 4:V:191:LYS:CD[1_554] | 2.09 | 0.11 |
| 4:5:10:CYS:CA | 4:8:118:LYS:CE[1_554] | 2.09 | 0.11 |
| 4:5:157:ASP:N | 4:8:74:GLY:C[1_554] | 2.09 | 0.11 |
| 4:5:175:ILE:CD1 | 4:9:191:LYS:NZ[1_554] | 2.09 | 0.11 |
| 4:4:274:ILE:C | 4:7:162:ASN:CA[1_554] | 2.09 | 0.11 |
| 4:2:287:ILE:C | 4:7:39:ARG:NE[1_554] | 2.09 | 0.11 |
| 4:6:210:ARG:CZ | 4:9:34:ILE:N[1_554] | 2.09 | 0.11 |
| 4:4:182:GLY:CA | 4:7:73:HIS:N[1_554] | 2.09 | 0.11 |
| 4:6:296:ASN:N | 4:9:168:GLY:N[1_554] | 2.09 | 0.11 |
| 4:5:341:ILE:C | 4:8:120:THR:CG2[1_554] | 2.09 | 0.11 |
| 4:6:328:LYS:CD | 4:W:45:VAL:CG2[1_554] | 2.09 | 0.11 |
| 4:6:274:ILE:CG2 | 4:9:152:VAL:O[1_554] | 2.09 | 0.11 |
| 4:4:188:TYR:O | 4:7:183:ARG:N[1_554] | 2.09 | 0.11 |
| 4:5:329:ILE:CG1 | 4:8:142:LEU:CG[1_554] | 2.09 | 0.11 |
| 4:4:199:SER:CA | 4:7:207:GLU:N[1_554] | 2.09 | 0.11 |
| 4:6:329:ILE:O | 4:9:139:VAL:O[1_554] | 2.09 | 0.11 |
| 4:3:370:VAL:CG1 | 4:7:233:SER:OG[1_554] | 2.09 | 0.11 |
| 4:4:275:HIS:N | 4:7:163:VAL:CA[1_554] | 2.09 | 0.11 |
| 4:4:294:TYR:O | 4:7:168:GLY:N[1_554] | 2.09 | 0.11 |
| 4:6:340:TRP:CH2 | 4:9:120:THR:C[1_554] | 2.09 | 0.11 |
| 4:4:25:ASP:C | 4:7:121:GLN:C[1_554] | 2.09 | 0.11 |
| 4:6:280:ASN:C | 4:9:174:ALA:CB[1_554] | 2.09 | 0.11 |
| 4:6:265:SER:O | 4:9:261:LEU:C[1_554] | 2.09 | 0.11 |
| 4:6:110:LEU:C | 4:V:192:ILE:C[1_554] | 2.09 | 0.11 |
| 4:5:157:ASP:C | 4:8:73:HIS:CB[1_554] | 2.09 | 0.11 |
| 4:6:136:ILE:CA | 4:9:113:LYS:CE[1_554] | 2.09 | 0.11 |
| 4:4:371:HIS:N | 4:8:230:ALA:CB[1_554] | 2.09 | 0.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:270:GLU:CA | 4:9:272:ALA:O[1_554] | 2.09 | 0.11 |
| 4:4:173:HIS:NE2 | 4:8:265:SER:N[1_554] | 2.09 | 0.11 |
| 4:4:253:GLU:CG | 4:7:214:GLU:OE1[1_554] | 2.09 | 0.11 |
| 4:6:340:TRP:CZ3 | 4:9:121:GLN:N[1_554] | 2.09 | 0.11 |
| 4:5:312:ARG:NH1 | 4:8:299:MET:CG[1_554] | 2.09 | 0.11 |
| 4:6:340:TRP:CZ2 | 4:9:121:GLN:O[1_554] | 2.09 | 0.11 |
| 4:3:287:ILE:C | 4:8:63:GLY:C[1_554] | 2.09 | 0.11 |
| 4:5:110:LEU:CG | 4:9:191:LYS:CG[1_554] | 2.09 | 0.11 |
| 4:5:334:GLU:N | 4:8:104:LEU:CA[1_554] | 2.09 | 0.11 |
| 4:5:186:THR:CB | 4:8:157:ASP:OD2[1_554] | 2.09 | 0.11 |
| 4:4:297:ASN:CB | 4:7:170:ALA:N[1_554] | 2.09 | 0.11 |
| 4:4:18:LYS:NZ | 4:7:76:ILE:O[1_554] | 2.09 | 0.11 |
| 4:5:276:GLU:OE1 | 4:8:278:THR:O[1_554] | 2.09 | 0.11 |
| 4:5:268:GLY:O | 4:8:269:MET:CB[1_554] | 2.09 | 0.11 |
| 4:4:320:LEU:CA | 4:7:293:LEU:CD1[1_554] | 2.09 | 0.11 |
| 4:5:205:GLU:O | 4:8:59:GLN:OE1[1_554] | 2.09 | 0.11 |
| 4:5:112:PRO:N | 4:9:192:ILE:O[1_554] | 2.09 | 0.11 |
| 4:5:193:LEU:O | 4:8:209:VAL:N[1_554] | 2.09 | 0.11 |
| 4:6:110:LEU:CG | 4:V:191:LYS:NZ[1_554] | 2.09 | 0.11 |
| 4:5:275:HIS:NE2 | 4:8:278:THR:CG2[1_554] | 2.09 | 0.11 |
| 4:4:256:ARG:N | 4:7:303:THR:N[1_554] | 2.09 | 0.11 |
| 4:5:339:VAL:C | 4:8:117:GLU:N[1_554] | 2.09 | 0.11 |
| 4:6:334:GLU:O | 4:9:105:LEU:CG[1_554] | 2.09 | 0.11 |
| 4:5:154:ASP:C | 4:8:110:LEU:N[1_554] | 2.09 | 0.11 |
| 4:4:265:SER:CB | 4:7:261:LEU:C[1_554] | 2.09 | 0.11 |
| 4:6:344:SER:N | 4:9:367:PRO:CA[1_554] | 2.09 | 0.11 |
| 4:6:17:VAL:C | 4:9:79:TRP:CA[1_554] | 2.09 | 0.11 |
| 4:5:162:ASN:CB | 4:8:175:ILE:CD1[1_554] | 2.09 | 0.11 |
| 4:5:31:PHE:C | 4:8:78:ASN:C[1_554] | 2.09 | 0.11 |
| 4:5:140:LEU:O | 4:8:116:ARG:CD[1_554] | 2.09 | 0.11 |
| 4:6:18:LYS:CG | 4:9:79:TRP:CE3[1_554] | 2.09 | 0.11 |
| 4:6:110:LEU:CG | 4:V:191:LYS:CG[1_554] | 2.10 | 0.10 |
| 4:6:372:ARG:C | 4:V:227:MET:N[1_554] | 2.10 | 0.10 |
| 4:6:140:LEU:O | 4:9:116:ARG:CD[1_554] | 2.10 | 0.10 |
| 4:6:295:ALA:CA | 4:9:167:GLU:CB[1_554] | 2.10 | 0.10 |
| 4:4:337:TYR:OH | 4:7:86:TRP:CE3[1_554] | 2.10 | 0.10 |
| 4:5:76:ILE:N | 4:9:197:GLY:C[1_554] | 2.10 | 0.10 |
| 4:4:184:ASP:OD1 | 4:7:73:HIS:CG[1_554] | 2.10 | 0.10 |
| 4:6:75:ILE:CD1 | 4:V:197:GLY:N[1_554] | 2.10 | 0.10 |
| 4:4:332:PRO:CA | 4:7:134:VAL:N[1_554] | 2.10 | 0.10 |
| 4:5:257:CYS:C | 4:8:303:THR:CA[1_554] | 2.10 | 0.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:213:LYS:CA | 4:7:15:GLY:O[1_554] | 2.10 | 0.10 |
| 4:2:291:LYS:CA | 4:7:40:HIS:CB[1_554] | 2.10 | 0.10 |
| 4:4:337:TYR:CD1 | 4:7:79:TRP:CZ3[1_554] | 2.10 | 0.10 |
| 4:2:291:LYS:C | 4:7:40:HIS:CD2[1_554] | 2.10 | 0.10 |
| 4:4:262:PHE:CE2 | 4:7:154:ASP:CB[1_554] | 2.10 | 0.10 |
| 4:4:185:LEU:O | 4:7:157:ASP:CA[1_554] | 2.10 | 0.10 |
| 4:6:110:LEU:C | 4:V:192:ILE:O[1_554] | 2.10 | 0.10 |
| 4:5:299:MET:CG | 4:8:137:GLN:C[1_554] | 2.10 | 0.10 |
| 4:4:370:VAL:CA | 4:8:229:THR:O[1_554] | 2.10 | 0.10 |
| 1:D:553:MLY:CH1 | 4:6:328:LYS:CE[1_556] | 2.10 | 0.10 |
| 4:4:370:VAL:CG2 | 4:8:230:ALA:C[1_554] | 2.10 | 0.10 |
| 4:4:113:LYS:CE | 4:8:254:ARG:CB[1_554] | 2.10 | 0.10 |
| 4:5:153:LEU:CG | 4:8:163:VAL:CG2[1_554] | 2.10 | 0.10 |
| 4:4:276:GLU:CA | 4:7:151:ILE:CD1[1_554] | 2.10 | 0.10 |
| 4:4:372:ARG:NE | 4:8:227:MET:O[1_554] | 2.10 | 0.10 |
| 4:6:193:LEU:O | 4:9:209:VAL:N[1_554] | 2.10 | 0.10 |
| 4:5:184:ASP:CB | 4:8:158:GLY:O[1_554] | 2.10 | 0.10 |
| 4:5:313:MET:N | 4:8:152:VAL:CG2[1_554] | 2.10 | 0.10 |
| 4:5:339:VAL:C | 4:8:116:ARG:CB[1_554] | 2.10 | 0.10 |
| 4:6:185:LEU:CB | 4:9:157:ASP:O[1_554] | 2.10 | 0.10 |
| 4:6:255:PHE:CE2 | 4:9:305:MET:O[1_554] | 2.10 | 0.10 |
| 4:6:280:ASN:OD1 | 4:9:281:SER:O[1_554] | 2.10 | 0.10 |
| 4:6:297:ASN:O | 4:9:139:VAL:CG2[1_554] | 2.10 | 0.10 |
| 4:5:252:ASN:CG | 4:8:215:LYS:O[1_554] | 2.10 | 0.10 |
| 4:6:145:SER:C | 4:9:372:ARG:NH2[1_554] | 2.10 | 0.10 |
| 4:6:31:PHE:CA | 4:9:81:ASP:CA[1_554] | 2.10 | 0.10 |
| 4:5:255:PHE:C | 4:8:302:GLY:C[1_554] | 2.10 | 0.10 |
| 4:6:76:ILE:N | 4:V:197:GLY:CA[1_554] | 2.10 | 0.10 |
| 4:5:254:ARG:NH2 | 4:8:336:LYS:CE[1_554] | 2.10 | 0.10 |
| 4:3:113:LYS:O | 4:7:250:ILE:C[1_554] | 2.10 | 0.10 |
| 4:4:23:GLY:CA | 4:7:125:GLU:OE2[1_554] | 2.10 | 0.10 |
| 4:6:334:GLU:OE2 | 4:9:104:LEU:CA[1_554] | 2.10 | 0.10 |
| 4:4:334:GLU:N | 4:7:105:LEU:CD1[1_554] | 2.10 | 0.10 |
| 4:3:118:LYS:CA | 4:7:237:GLU:OE1[1_554] | 2.10 | 0.10 |
| 4:6:194:THR:OG1 | 4:9:190:MET:CB[1_554] | 2.10 | 0.10 |
| 4:4:113:LYS:CE | 4:8:254:ARG:C[1_554] | 2.10 | 0.10 |
| 4:4:113:LYS:CA | 4:8:254:ARG:N[1_554] | 2.10 | 0.10 |
| 4:4:288:ASP:O | 4:9:64:ILE:O[1_554] | 2.10 | 0.10 |
| 4:6:253:GLU:N | 4:9:214:GLU:CA[1_554] | 2.10 | 0.10 |
| 4:6:328:LYS:CA | 4:9:148:THR:CG2[1_554] | 2.10 | 0.10 |
| 4:5:106:THR:CG2 | 4:8:114:ALA:CB[1_554] | 2.10 | 0.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:143:TYR:CE2 | 4:8:368:SER:O[1_554] | 2.10 | 0.10 |
| 4:6:327:ILE:CG1 | 4:9:149:THR:N[1_554] | 2.10 | 0.10 |
| 4:5:31:PHE:CA | 4:8:80:ASP:C[1_554] | 2.10 | 0.10 |
| 4:4:335:ARG:CG | 4:7:106:THR:N[1_554] | 2.10 | 0.10 |
| 4:4:160:THR:N | 4:7:177:ARG:CZ[1_554] | 2.10 | 0.10 |
| 4:5:270:GLU:C | 4:8:272:ALA:C[1_554] | 2.10 | 0.10 |
| 4:6:17:VAL:C | 4:9:79:TRP:CE3[1_554] | 2.10 | 0.10 |
| 4:2:291:LYS:CE | 4:7:39:ARG:CB[1_554] | 2.10 | 0.10 |
| 4:4:186:THR:O | 4:7:183:ARG:CD[1_554] | 2.10 | 0.10 |
| 4:5:348:SER:O | 4:8:364:GLU:CA[1_554] | 2.10 | 0.10 |
| 4:5:366:GLY:C | 4:9:234:SER:CA[1_554] | 2.10 | 0.10 |
| 4:5:200:PHE:O | 4:8:206:ARG:CD[1_554] | 2.10 | 0.10 |
| 4:4:291:LYS:NZ | 4:9:64:ILE:CB[1_554] | 2.10 | 0.10 |
| 4:6:256:ARG:CG | 4:9:306:TYR:CG[1_554] | 2.10 | 0.10 |
| 4:5:173:HIS:CG | 4:9:267:ILE:CA[1_554] | 2.10 | 0.10 |
| 4:6:331:ALA:O | 4:9:140:LEU:CG[1_554] | 2.10 | 0.10 |
| 4:3:166:TYR:CE1 | 4:8:40:HIS:CE1[1_554] | 2.10 | 0.10 |
| 4:4:76:ILE:N | 4:8:197:GLY:O[1_554] | 2.10 | 0.10 |
| 4:5:257:CYS:SG | 4:8:156:GLY:O[1_554] | 2.10 | 0.10 |
| 4:5:266:PHE:CE1 | 4:8:261:LEU:CD1[1_554] | 2.10 | 0.10 |
| 4:6:237:GLU:OE1 | 4:9:215:LYS:CD[1_554] | 2.10 | 0.10 |
| 4:4:277:THR:OG1 | 4:7:176:MET:CA[1_554] | 2.10 | 0.10 |
| 4:5:345:ILE:C | 4:8:369:ILE:CB[1_554] | 2.10 | 0.10 |
| 4:3:370:VAL:CG2 | 4:7:230:ALA:C[1_554] | 2.10 | 0.10 |
| 4:6:195:GLU:OE1 | 4:9:257:CYS:CB[1_554] | 2.10 | 0.10 |
| 4:5:316:GLU:N | 4:8:298:VAL:N[1_554] | 2.10 | 0.10 |
| 4:6:17:VAL:CG1 | 4:9:79:TRP:CG[1_554] | 2.10 | 0.10 |
| 4:4:192:ILE:CG2 | 4:7:213:LYS:CE[1_554] | 2.10 | 0.10 |
| 4:4:145:SER:CB | 4:7:372:ARG:CZ[1_554] | 2.10 | 0.10 |
| 4:4:366:GLY:C | 4:8:235:SER:CA[1_554] | 2.10 | 0.10 |
| 4:5:162:ASN:O | 4:8:172:PRO:O[1_554] | 2.10 | 0.10 |
| 4:6:339:VAL:C | 4:9:116:ARG:CB[1_554] | 2.10 | 0.10 |
| 4:4:315:LYS:N | 4:7:142:LEU:CA[1_554] | 2.10 | 0.10 |
| 4:3:171:LEU:C | 4:7:266:PHE:O[1_554] | 2.10 | 0.10 |
| 4:4:113:LYS:O | 4:8:250:ILE:C[1_554] | 2.10 | 0.10 |
| 4:4:349:LEU:CD2 | 4:7:365:ALA:O[1_554] | 2.10 | 0.10 |
| 4:4:288:ASP:C | 4:9:64:ILE:N[1_554] | 2.10 | 0.10 |
| 4:4:200:PHE:CD1 | 4:7:62:ARG:NH2[1_554] | 2.10 | 0.10 |
| 4:4:155:SER:CA | 4:7:108:ALA:CB[1_554] | 2.10 | 0.10 |
| 4:6:166:TYR:CD2 | 4:W:40:HIS:ND1[1_554] | 2.10 | 0.10 |
| 4:5:154:ASP:N | 4:8:110:LEU:N[1_554] | 2.10 | 0.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:D:542:PHE:CE2 | 4:6:328:LYS:CE[1_556] | 2.10 | 0.10 |
| 4:6:211:ASP:N | 4:9:32:PRO:CB[1_554] | 2.10 | 0.10 |
| 4:5:298:VAL:C | 4:8:136:ILE:CD1[1_554] | 2.10 | 0.10 |
| 4:3:285:CYS:N | 4:7:268:GLY:O[1_554] | 2.10 | 0.10 |
| 4:4:265:SER:O | 4:7:260:THR:C[1_554] | 2.10 | 0.10 |
| 4:5:194:THR:CG2 | 4:8:209:VAL:CG1[1_554] | 2.10 | 0.10 |
| 4:4:370:VAL:CG1 | 4:8:233:SER:OG[1_554] | 2.10 | 0.10 |
| 4:4:117:GLU:CB | 4:8:237:GLU:C[1_554] | 2.10 | 0.10 |
| 4:6:276:GLU:O | 4:9:281:SER:CA[1_554] | 2.10 | 0.10 |
| 4:6:137:GLN:CD | 4:9:112:PRO:CG[1_554] | 2.10 | 0.10 |
| 4:5:294:TYR:CG | 4:8:166:TYR:CA[1_554] | 2.10 | 0.10 |
| 4:5:143:TYR:N | 4:8:372:ARG:CG[1_554] | 2.10 | 0.10 |
| 4:6:275:HIS:NE2 | 4:9:278:THR:CG2[1_554] | 2.10 | 0.10 |
| 4:6:311:ASP:O | 4:9:298:VAL:CG1[1_554] | 2.10 | 0.10 |
| 4:5:255:PHE:CD2 | 4:8:305:MET:CE[1_554] | 2.10 | 0.10 |
| 4:4:151:ILE:CD1 | 4:7:171:LEU:CA[1_554] | 2.10 | 0.10 |
| 4:6:214:GLU:OE1 | 4:9:33:SER:OG[1_554] | 2.10 | 0.10 |
| 4:4:26:ALA:C | 4:7:121:GLN:C[1_554] | 2.10 | 0.10 |
| 4:5:207:GLU:OE1 | 4:8:67:LEU:CB[1_554] | 2.10 | 0.10 |
| 4:4:335:ARG:NE | 4:7:106:THR:C[1_554] | 2.10 | 0.10 |
| 4:5:212:ILE:O | 4:8:16:LEU:CG[1_554] | 2.10 | 0.10 |
| 4:5:115:ASN:CB | 4:9:196:ARG:CG[1_554] | 2.10 | 0.10 |
| 4:6:322:PRO:O | 4:9:292:ASP:OD1[1_554] | 2.10 | 0.10 |
| 4:6:199:SER:O | 4:9:206:ARG:CB[1_554] | 2.10 | 0.10 |
| 4:6:322:PRO:O | 4:9:292:ASP:CG[1_554] | 2.10 | 0.10 |
| 4:4:372:ARG:N | 4:8:230:ALA:CB[1_554] | 2.10 | 0.10 |
| 4:5:214:GLU:O | 4:8:18:LYS:CD[1_554] | 2.10 | 0.10 |
| 4:6:334:GLU:CB | 4:9:104:LEU:C[1_554] | 2.10 | 0.10 |
| 4:4:312:ARG:CG | 4:7:300:SER:CB[1_554] | 2.10 | 0.10 |
| 1:A:553:MLY:CH1 | 4:5:328:LYS:CE[1_556] | 2.10 | 0.10 |
| 4:6:31:PHE:C | 4:9:78:ASN:C[1_554] | 2.10 | 0.10 |
| 4:6:182:GLY:C | 4:9:158:GLY:CA[1_554] | 2.10 | 0.10 |
| 4:5:205:GLU:N | 4:8:62:ARG:CG[1_554] | 2.11 | 0.09 |
| 4:6:208:ILE:CB | 4:9:59:GLN:OE1[1_554] | 2.11 | 0.09 |
| 4:4:195:GLU:N | 4:7:209:VAL:O[1_554] | 2.11 | 0.09 |
| 4:6:180:LEU:CA | 4:9:179:ASP:CA[1_554] | 2.11 | 0.09 |
| 4:5:370:VAL:CG1 | 4:9:231:ALA:CA[1_554] | 2.11 | 0.09 |
| 4:4:207:GLU:C | 4:7:67:LEU:CD1[1_554] | 2.11 | 0.09 |
| 4:6:337:TYR:O | 4:9:119:MET:CG[1_554] | 2.11 | 0.09 |
| 4:5:215:LYS:CB | 4:8:30:VAL:CG1[1_554] | 2.11 | 0.09 |
| 4:5:335:ARG:CA | 4:8:106:THR:C[1_554] | 2.11 | 0.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:19:ALA:O | 4:9:122:ILE:CB[1_554] | 2.11 | 0.09 |
| 4:6:162:ASN:C | 4:9:172:PRO:CA[1_554] | 2.11 | 0.09 |
| 4:6:141:SER:C | 4:9:116:ARG:NH2[1_554] | 2.11 | 0.09 |
| 4:4:195:GLU:N | 4:7:209:VAL:CG1[1_554] | 2.11 | 0.09 |
| 4:5:260:THR:O | 4:8:160:THR:OG1[1_554] | 2.11 | 0.09 |
| 4:5:140:LEU:CA | 4:8:371:HIS:CE1[1_554] | 2.11 | 0.09 |
| 4:6:135:ALA:C | 4:9:113:LYS:CE[1_554] | 2.11 | 0.09 |
| 4:5:198:TYR:CD1 | 4:8:208:ILE:N[1_554] | 2.11 | 0.09 |
| 4:6:157:ASP:CA | 4:9:73:HIS:N[1_554] | 2.11 | 0.09 |
| 4:6:219:VAL:C | 4:9:335:ARG:O[1_554] | 2.11 | 0.09 |
| 4:6:286:ASP:OD2 | 4:W:39:ARG:CZ[1_554] | 2.11 | 0.09 |
| 4:6:173:HIS:CG | 4:V:267:ILE:CA[1_554] | 2.11 | 0.09 |
| 4:6:113:LYS:CE | 4:V:255:PHE:N[1_554] | 2.11 | 0.09 |
| 4:4:340:TRP:O | 4:7:117:GLU:C[1_554] | 2.11 | 0.09 |
| 4:5:326:LYS:O | 4:8:167:GLU:N[1_554] | 2.11 | 0.09 |
| 4:5:333:PRO:CG | 4:8:104:LEU:CG[1_554] | 2.11 | 0.09 |
| 4:5:255:PHE:CA | 4:8:302:GLY:C[1_554] | 2.11 | 0.09 |
| 4:2:292:ASP:N | 4:7:40:HIS:CE1[1_554] | 2.11 | 0.09 |
| 4:4:151:ILE:N | 4:7:169:TYR:CE1[1_554] | 2.11 | 0.09 |
| 4:5:316:GLU:CA | 4:8:296:ASN:C[1_554] | 2.11 | 0.09 |
| 4:3:367:PRO:CD | 4:7:235:SER:N[1_554] | 2.11 | 0.09 |
| 4:6:331:ALA:N | 4:9:140:LEU:CD2[1_554] | 2.11 | 0.09 |
| 4:6:349:LEU:CA | 4:9:364:GLU:O[1_554] | 2.11 | 0.09 |
| 4:4:369:ILE:O | 4:8:229:THR:CB[1_554] | 2.11 | 0.09 |
| 4:5:283:MET:SD | 4:8:286:ASP:N[1_554] | 2.11 | 0.09 |
| 4:4:314:GLN:CG | 4:7:143:TYR:N[1_554] | 2.11 | 0.09 |
| 4:6:191:LYS:CB | 4:9:187:ASP:CA[1_554] | 2.11 | 0.09 |
| 4:5:338:SER:O | 4:8:116:ARG:CG[1_554] | 2.11 | 0.09 |
| 4:6:338:SER:C | 4:9:116:ARG:CG[1_554] | 2.11 | 0.09 |
| 4:4:139:VAL:C | 4:7:113:LYS:CD[1_554] | 2.11 | 0.09 |
| 4:4:114:ALA:N | 4:8:250:ILE:CA[1_554] | 2.11 | 0.09 |
| 4:4:312:ARG:CZ | 4:7:300:SER:N[1_554] | 2.11 | 0.09 |
| 4:5:348:SER:O | 4:8:365:ALA:N[1_554] | 2.11 | 0.09 |
| 4:4:339:VAL:CG2 | 4:7:115:ASN:N[1_554] | 2.11 | 0.09 |
| 4:5:204:ALA:N | 4:8:62:ARG:CB[1_554] | 2.11 | 0.09 |
| 4:4:118:LYS:N | 4:8:237:GLU:CG[1_554] | 2.11 | 0.09 |
| 4:5:25:ASP:OD1 | 4:8:131:ALA:N[1_554] | 2.11 | 0.09 |
| 4:3:173:HIS:ND1 | 4:7:267:ILE:N[1_554] | 2.11 | 0.09 |
| 4:6:223:PHE:CE2 | 4:9:304:THR:CG2[1_554] | 2.11 | 0.09 |
| 4:5:288:ASP:CA | 4:V:63:GLY:C[1_554] | 2.11 | 0.09 |
| 4:6:281:SER:CA | 4:9:173:HIS:CD2[1_554] | 2.11 | 0.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:315:LYS:O | 4:9:296:ASN:CB[1_554] | 2.11 | 0.09 |
| 4:5:340:TRP:CB | 4:8:119:MET:CB[1_554] | 2.11 | 0.09 |
| 4:6:213:LYS:CE | 4:9:14:SER:C[1_554] | 2.11 | 0.09 |
| 4:4:275:HIS:CB | 4:7:152:VAL:O[1_554] | 2.11 | 0.09 |
| 4:6:327:ILE:O | 4:9:148:THR:CG2[1_554] | 2.11 | 0.09 |
| 4:3:287:ILE:C | 4:8:63:GLY:O[1_554] | 2.11 | 0.09 |
| 4:5:17:VAL:CA | 4:8:79:TRP:CB[1_554] | 2.11 | 0.09 |
| 4:6:154:ASP:CG | 4:9:108:ALA:O[1_554] | 2.11 | 0.09 |
| 4:4:195:GLU:C | 4:7:209:VAL:C[1_554] | 2.11 | 0.09 |
| 4:4:196:ARG:CG | 4:7:211:ASP:CB[1_554] | 2.11 | 0.09 |
| 4:4:367:PRO:CD | 4:8:235:SER:N[1_554] | 2.11 | 0.09 |
| 4:5:269:MET:CG | 4:8:178:LEU:CD1[1_554] | 2.11 | 0.09 |
| 4:5:315:LYS:CB | 4:8:298:VAL:CG2[1_554] | 2.11 | 0.09 |
| 4:3:177:ARG:NH1 | 4:7:194:THR:CA[1_554] | 2.11 | 0.09 |
| 4:4:198:TYR:CD2 | 4:7:207:GLU:C[1_554] | 2.11 | 0.09 |
| 4:4:18:LYS:CA | 4:7:79:TRP:CG[1_554] | 2.11 | 0.09 |
| 4:5:106:THR:OG1 | 4:8:114:ALA:CA[1_554] | 2.11 | 0.09 |
| 4:4:294:TYR:N | 4:7:169:TYR:CB[1_554] | 2.11 | 0.09 |
| 4:4:173:HIS:CE1 | 4:8:265:SER:N[1_554] | 2.11 | 0.09 |
| 4:4:267:ILE:CB | 4:7:180:LEU:CA[1_554] | 2.11 | 0.09 |
| 4:3:372:ARG:CA | 4:7:227:MET:CA[1_554] | 2.11 | 0.09 |
| 4:3:111:ASN:O | 4:7:253:GLU:OE1[1_554] | 2.11 | 0.09 |
| 4:6:182:GLY:O | 4:9:158:GLY:N[1_554] | 2.11 | 0.09 |
| 4:5:334:GLU:O | 4:8:105:LEU:CG[1_554] | 2.11 | 0.09 |
| 4:4:294:TYR:N | 4:7:169:TYR:CD2[1_554] | 2.11 | 0.09 |
| 4:5:183:ARG:NE | 4:8:72:GLU:CG[1_554] | 2.11 | 0.09 |
| 4:5:369:ILE:C | 4:9:232:SER:N[1_554] | 2.11 | 0.09 |
| 4:5:9:VAL:CB | 4:8:121:GLN:CB[1_554] | 2.11 | 0.09 |
| 4:5:189:LEU:C | 4:8:186:THR:CB[1_554] | 2.11 | 0.09 |
| 4:4:181:ALA:CA | 4:7:73:HIS:CB[1_554] | 2.11 | 0.09 |
| 4:4:339:VAL:CA | 4:7:115:ASN:C[1_554] | 2.11 | 0.09 |
| 4:5:200:PHE:C | 4:8:206:ARG:CD[1_554] | 2.11 | 0.09 |
| 4:5:205:GLU:CB | 4:8:62:ARG:CZ[1_554] | 2.11 | 0.09 |
| 4:5:173:HIS:CA | 4:9:267:ILE:CG2[1_554] | 2.11 | 0.09 |
| 4:5:106:THR:CA | 4:8:114:ALA:CA[1_554] | 2.11 | 0.09 |
| 4:3:292:ASP:OD2 | 4:8:40:HIS:CB[1_554] | 2.11 | 0.09 |
| 4:6:20:GLY:CA | 4:9:121:GLN:CD[1_554] | 2.11 | 0.09 |
| 4:4:171:LEU:CB | 4:8:265:SER:O[1_554] | 2.11 | 0.09 |
| 4:5:231:ALA:CB | 4:8:218:TYR:OH[1_554] | 2.11 | 0.09 |
| 4:4:291:LYS:CE | 4:9:64:ILE:CG1[1_554] | 2.11 | 0.09 |
| 4:5:204:ALA:C | 4:8:62:ARG:CB[1_554] | 2.11 | 0.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:213:LYS:CD | 4:7:15:GLY:CA[1_554] | 2.11 | 0.09 |
| 4:6:257:CYS:O | 4:9:303:THR:CG2[1_554] | 2.11 | 0.09 |
| 4:5:207:GLU:C | 4:8:59:GLN:NE2[1_554] | 2.11 | 0.09 |
| 4:4:278:THR:O | 4:7:171:LEU:C[1_554] | 2.11 | 0.09 |
| 4:5:298:VAL:O | 4:8:136:ILE:CB[1_554] | 2.11 | 0.09 |
| 4:4:214:GLU:OE1 | 4:7:33:SER:CB[1_554] | 2.11 | 0.09 |
| 4:4:316:GLU:CG | 4:7:298:VAL:O[1_554] | 2.11 | 0.09 |
| 4:5:156:GLY:C | 4:8:73:HIS:C[1_554] | 2.11 | 0.09 |
| 4:4:300:SER:C | 4:7:107:GLU:CG[1_554] | 2.11 | 0.09 |
| 4:3:370:VAL:C | 4:7:230:ALA:N[1_554] | 2.11 | 0.09 |
| 4:6:299:MET:CA | 4:9:136:ILE:N[1_554] | 2.11 | 0.09 |
| 4:5:143:TYR:CG | 4:8:372:ARG:CA[1_554] | 2.11 | 0.09 |
| 4:5:153:LEU:C | 4:8:109:PRO:C[1_554] | 2.11 | 0.09 |
| 4:3:368:SER:C | 4:7:234:SER:OG[1_554] | 2.11 | 0.09 |
| 4:4:75:ILE:CA | 4:8:198:TYR:CG[1_554] | 2.11 | 0.09 |
| 4:6:317:ILE:CD1 | 4:9:165:ILE:C[1_554] | 2.11 | 0.09 |
| 4:5:315:LYS:O | 4:8:296:ASN:CB[1_554] | 2.11 | 0.09 |
| 4:6:314:GLN:CD | 4:9:147:ARG:CG[1_554] | 2.11 | 0.09 |
| 4:5:258:PRO:N | 4:8:303:THR:CB[1_554] | 2.11 | 0.09 |
| 4:4:274:ILE:CA | 4:7:162:ASN:O[1_554] | 2.11 | 0.09 |
| 4:5:191:LYS:CE | 4:8:185:LEU:O[1_554] | 2.11 | 0.09 |
| 4:6:258:PRO:CG | 4:9:301:GLY:C[1_554] | 2.11 | 0.09 |
| 4:6:205:GLU:N | 4:9:62:ARG:CG[1_554] | 2.11 | 0.09 |
| 4:5:135:ALA:C | 4:8:113:LYS:CE[1_554] | 2.11 | 0.09 |
| 4:6:31:PHE:CD1 | 4:9:80:ASP:CB[1_554] | 2.11 | 0.09 |
| 4:3:287:ILE:N | 4:7:270:GLU:CD[1_554] | 2.11 | 0.09 |
| 4:5:256:ARG:O | 4:8:303:THR:CB[1_554] | 2.11 | 0.09 |
| 4:4:140:LEU:CA | 4:7:371:HIS:CG[1_554] | 2.11 | 0.09 |
| 4:6:31:PHE:N | 4:9:82:MET:N[1_554] | 2.11 | 0.09 |
| 4:4:140:LEU:CD2 | 4:7:117:GLU:OE1[1_554] | 2.11 | 0.09 |
| 4:6:290:ARG:NE | 4:9:286:ASP:OD1[1_554] | 2.11 | 0.09 |
| 4:4:314:GLN:CA | 4:7:142:LEU:CD2[1_554] | 2.11 | 0.09 |
| 4:6:178:LEU:CD1 | 4:9:177:ARG:N[1_554] | 2.11 | 0.09 |
| 4:5:334:GLU:OE1 | 4:8:133:TYR:N[1_554] | 2.11 | 0.09 |
| 4:4:181:ALA:O | 4:7:158:GLY:C[1_554] | 2.11 | 0.09 |
| 4:3:366:GLY:C | 4:7:235:SER:CA[1_554] | 2.11 | 0.09 |
| 4:6:143:TYR:CG | 4:9:372:ARG:CA[1_554] | 2.12 | 0.08 |
| 4:6:346:LEU:CD1 | 4:9:368:SER:OG[1_554] | 2.12 | 0.08 |
| 4:4:210:ARG:N | 4:7:69:TYR:CE2[1_554] | 2.12 | 0.08 |
| 4:4:211:ASP:C | 4:7:33:SER:N[1_554] | 2.12 | 0.08 |
| 4:6:108:ALA:O | 4:V:195:GLU:CG[1_554] | 2.12 | 0.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:197:GLY:C | 4:7:208:ILE:CB[1_554] | 2.12 | 0.08 |
| 4:4:154:ASP:OD1 | 4:7:111:ASN:OD1[1_554] | 2.12 | 0.08 |
| 4:4:300:SER:OG | 4:7:111:ASN:CB[1_554] | 2.12 | 0.08 |
| 4:4:332:PRO:CA | 4:7:133:TYR:C[1_554] | 2.12 | 0.08 |
| 4:5:313:MET:N | 4:8:298:VAL:CG1[1_554] | 2.12 | 0.08 |
| 4:4:337:TYR:N | 4:7:119:MET:CE[1_554] | 2.12 | 0.08 |
| 4:4:372:ARG:CB | 4:8:227:MET:N[1_554] | 2.12 | 0.08 |
| 4:3:114:ALA:CB | 4:7:250:ILE:O[1_554] | 2.12 | 0.08 |
| 4:4:219:VAL:O | 4:7:338:SER:CB[1_554] | 2.12 | 0.08 |
| 4:5:317:ILE:CB | 4:8:151:ILE:N[1_554] | 2.12 | 0.08 |
| 4:5:294:TYR:CD2 | 4:8:166:TYR:CB[1_554] | 2.12 | 0.08 |
| 4:5:275:HIS:CB | 4:8:151:ILE:CG1[1_554] | 2.12 | 0.08 |
| 4:3:114:ALA:CA | 4:7:250:ILE:CA[1_554] | 2.12 | 0.08 |
| 4:5:262:PHE:CE1 | 4:8:154:ASP:N[1_554] | 2.12 | 0.08 |
| 4:6:191:LYS:CD | 4:9:185:LEU:C[1_554] | 2.12 | 0.08 |
| 4:4:207:GLU:O | 4:7:34:ILE:CG2[1_554] | 2.12 | 0.08 |
| 4:4:282:ILE:CA | 4:7:173:HIS:CE1[1_554] | 2.12 | 0.08 |
| 4:5:334:GLU:OE1 | 4:8:134:VAL:N[1_554] | 2.12 | 0.08 |
| 4:6:185:LEU:CD2 | 4:9:159:VAL:O[1_554] | 2.12 | 0.08 |
| 4:4:186:THR:CA | 4:7:157:ASP:OD2[1_554] | 2.12 | 0.08 |
| 4:4:185:LEU:CB | 4:7:158:GLY:C[1_554] | 2.12 | 0.08 |
| 4:5:188:TYR:CG | 4:8:181:ALA:C[1_554] | 2.12 | 0.08 |
| 4:6:261:LEU:C | 4:9:160:THR:CG2[1_554] | 2.12 | 0.08 |
| 4:6:181:ALA:CB | 4:9:159:VAL:CG1[1_554] | 2.12 | 0.08 |
| 4:4:30:VAL:C | 4:7:80:ASP:CB[1_554] | 2.12 | 0.08 |
| 4:4:112:PRO:CD | 4:8:193:LEU:CB[1_554] | 2.12 | 0.08 |
| 4:4:317:ILE:CG1 | 4:7:165:ILE:O[1_554] | 2.12 | 0.08 |
| 4:5:162:ASN:OD1 | 4:8:175:ILE:CG1[1_554] | 2.12 | 0.08 |
| 4:3:175:ILE:CG2 | 4:7:191:LYS:CE[1_554] | 2.12 | 0.08 |
| 4:6:318:THR:N | 4:9:296:ASN:CB[1_554] | 2.12 | 0.08 |
| 4:5:140:LEU:CD2 | 4:8:117:GLU:OE2[1_554] | 2.12 | 0.08 |
| 4:6:208:ILE:N | 4:9:59:GLN:OE1[1_554] | 2.12 | 0.08 |
| 4:5:16:LEU:N | 4:8:70:PRO:O[1_554] | 2.12 | 0.08 |
| 4:6:283:MET:N | 4:9:286:ASP:N[1_554] | 2.12 | 0.08 |
| 4:5:260:THR:CB | 4:8:155:SER:OG[1_554] | 2.12 | 0.08 |
| 4:4:278:THR:CA | 4:7:164:PRO:CD[1_554] | 2.12 | 0.08 |
| 4:5:280:ASN:CG | 4:8:280:ASN:O[1_554] | 2.12 | 0.08 |
| 4:5:180:LEU:CD1 | 4:8:160:THR:CA[1_554] | 2.12 | 0.08 |
| 4:3:110:LEU:CG | 4:7:191:LYS:CG[1_554] | 2.12 | 0.08 |
| 4:4:174:ALA:CB | 4:8:268:GLY:N[1_554] | 2.12 | 0.08 |
| 4:3:173:HIS:N | 4:7:267:ILE:CG2[1_554] | 2.12 | 0.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:270:GLU:CB | 4:7:271:SER:C[1_554] | 2.12 | 0.08 |
| 4:6:368:SER:N | 4:V:229:THR:O[1_554] | 2.12 | 0.08 |
| 4:5:25:ASP:CG | 4:8:129:VAL:C[1_554] | 2.12 | 0.08 |
| 4:6:183:ARG:NH1 | 4:9:72:GLU:OE1[1_554] | 2.12 | 0.08 |
| 4:4:172:PRO:O | 4:8:188:TYR:CE1[1_554] | 2.12 | 0.08 |
| 4:6:198:TYR:CD1 | 4:9:208:ILE:C[1_554] | 2.12 | 0.08 |
| 4:4:226:GLU:OE1 | 4:7:334:GLU:N[1_554] | 2.12 | 0.08 |
| 4:4:262:PHE:N | 4:7:154:ASP:C[1_554] | 2.12 | 0.08 |
| 4:4:243:PRO:O | 4:7:61:LYS:CG[1_554] | 2.12 | 0.08 |
| 4:5:30:VAL:C | 4:8:79:TRP:C[1_554] | 2.12 | 0.08 |
| 4:4:340:TRP:CE2 | 4:7:118:LYS:CD[1_554] | 2.12 | 0.08 |
| 4:4:193:LEU:CG | 4:7:210:ARG:CB[1_554] | 2.12 | 0.08 |
| 4:6:59:GLN:CG | 4:9:68:LYS:CD[1_554] | 2.12 | 0.08 |
| 4:6:348:SER:C | 4:9:362:TYR:O[1_554] | 2.12 | 0.08 |
| 4:4:275:HIS:C | 4:7:163:VAL:C[1_554] | 2.12 | 0.08 |
| 4:4:273:GLY:O | 4:7:162:ASN:C[1_554] | 2.12 | 0.08 |
| 4:6:113:LYS:C | 4:V:253:GLU:OE2[1_554] | 2.12 | 0.08 |
| 4:6:367:PRO:CG | 4:V:233:SER:C[1_554] | 2.12 | 0.08 |
| 4:4:331:ALA:CB | 4:7:135:ALA:CA[1_554] | 2.12 | 0.08 |
| 4:5:370:VAL:CA | 4:9:231:ALA:C[1_554] | 2.12 | 0.08 |
| 4:4:265:SER:OG | 4:7:274:ILE:CG2[1_554] | 2.12 | 0.08 |
| 4:5:305:MET:C | 4:8:11:ASP:CG[1_554] | 2.12 | 0.08 |
| 4:4:198:TYR:CA | 4:7:205:GLU:O[1_554] | 2.12 | 0.08 |
| 4:6:200:PHE:N | 4:9:206:ARG:C[1_554] | 2.12 | 0.08 |
| 4:4:224:GLU:N | 4:7:335:ARG:CZ[1_554] | 2.12 | 0.08 |
| 4:4:335:ARG:C | 4:7:119:MET:SD[1_554] | 2.12 | 0.08 |
| 4:5:157:ASP:CA | 4:8:73:HIS:N[1_554] | 2.12 | 0.08 |
| 4:5:268:GLY:C | 4:8:264:PRO:CG[1_554] | 2.12 | 0.08 |
| 4:5:28:ARG:NE | 4:8:126:THR:C[1_554] | 2.12 | 0.08 |
| 4:4:305:MET:O | 4:7:11:ASP:OD2[1_554] | 2.12 | 0.08 |
| 4:6:327:ILE:CB | 4:9:149:THR:OG1[1_554] | 2.12 | 0.08 |
| 4:5:293:LEU:O | 4:8:169:TYR:N[1_554] | 2.12 | 0.08 |
| 4:5:188:TYR:CZ | 4:8:185:LEU:CB[1_554] | 2.12 | 0.08 |
| 4:6:154:ASP:OD2 | 4:9:111:ASN:O[1_554] | 2.12 | 0.08 |
| 4:5:312:ARG:O | 4:8:298:VAL:C[1_554] | 2.12 | 0.08 |
| 4:6:343:GLY:C | 4:9:367:PRO:O[1_554] | 2.12 | 0.08 |
| 4:4:341:ILE:CD1 | 4:7:120:THR:OG1[1_554] | 2.12 | 0.08 |
| 4:5:185:LEU:CB | 4:8:158:GLY:CA[1_554] | 2.12 | 0.08 |
| 4:4:277:THR:C | 4:7:174:ALA:O[1_554] | 2.12 | 0.08 |
| 4:4:327:ILE:CG1 | 4:7:148:THR:C[1_554] | 2.12 | 0.08 |
| 4:6:370:VAL:CG1 | 4:V:231:ALA:CA[1_554] | 2.12 | 0.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:117:GLU:C | 4:7:237:GLU:OE1[1_554] | 2.12 | 0.08 |
| 4:4:313:MET:SD | 4:7:138:ALA:CB[1_554] | 2.12 | 0.08 |
| 4:4:147:ARG:CD | 4:7:372:ARG:CD[1_554] | 2.12 | 0.08 |
| 4:5:186:THR:OG1 | 4:8:183:ARG:NE[1_554] | 2.12 | 0.08 |
| 4:5:274:ILE:CG1 | 4:8:162:ASN:N[1_554] | 2.12 | 0.08 |
| 4:5:221:LEU:O | 4:8:332:PRO:CA[1_554] | 2.12 | 0.08 |
| 4:6:312:ARG:CB | 4:9:299:MET:N[1_554] | 2.12 | 0.08 |
| 4:6:337:TYR:CB | 4:9:105:LEU:CD1[1_554] | 2.12 | 0.08 |
| 4:6:180:LEU:CG | 4:9:178:LEU:N[1_554] | 2.12 | 0.08 |
| 4:6:227:MET:N | 4:9:307:PRO:CA[1_554] | 2.12 | 0.08 |
| 4:6:210:ARG:NH1 | 4:9:33:SER:OG[1_554] | 2.12 | 0.08 |
| 4:3:117:GLU:N | 4:7:237:GLU:CG[1_554] | 2.12 | 0.08 |
| 4:6:154:ASP:CA | 4:9:110:LEU:N[1_554] | 2.12 | 0.08 |
| 4:6:292:ASP:OD2 | 4:W:64:ILE:CB[1_554] | 2.12 | 0.08 |
| 4:5:286:ASP:CA | 4:9:270:GLU:OE2[1_554] | 2.12 | 0.08 |
| 4:4:139:VAL:O | 4:7:371:HIS:CE1[1_554] | 2.12 | 0.08 |
| 4:4:310:ALA:O | 4:7:140:LEU:C[1_554] | 2.12 | 0.08 |
| 4:4:157:ASP:CG | 4:7:72:GLU:CG[1_554] | 2.12 | 0.08 |
| 4:4:270:GLU:N | 4:7:272:ALA:N[1_554] | 2.12 | 0.08 |
| 4:5:309:ILE:C | 4:8:141:SER:CA[1_554] | 2.12 | 0.08 |
| 4:3:72:GLU:O | 4:7:198:TYR:CA[1_554] | 2.12 | 0.08 |
| 4:4:278:THR:CG2 | 4:7:171:LEU:N[1_554] | 2.12 | 0.08 |
| 4:4:24:ASP:N | 4:7:125:GLU:CG[1_554] | 2.12 | 0.08 |
| 4:6:240:TYR:CZ | 4:9:56:ASP:OD2[1_554] | 2.12 | 0.08 |
| 4:6:173:HIS:CD2 | 4:V:264:PRO:O[1_554] | 2.12 | 0.08 |
| 4:5:369:ILE:CA | 4:9:232:SER:N[1_554] | 2.12 | 0.08 |
| 4:4:304:THR:N | 4:7:137:GLN:CD[1_554] | 2.12 | 0.08 |
| 4:5:190:MET:SD | 4:8:206:ARG:CZ[1_554] | 2.12 | 0.08 |
| 4:4:182:GLY:C | 4:7:73:HIS:N[1_554] | 2.12 | 0.08 |
| 4:4:333:PRO:CB | 4:7:103:THR:C[1_554] | 2.12 | 0.08 |
| 4:4:196:ARG:NH1 | 4:7:215:LYS:CG[1_554] | 2.12 | 0.08 |
| 4:4:345:ILE:CD1 | 4:7:369:ILE:CG2[1_554] | 2.12 | 0.08 |
| 4:5:191:LYS:O | 4:8:186:THR:CA[1_554] | 2.12 | 0.08 |
| 4:5:41:GLN:CB | 4:7:224:GLU:OE2[1_554] | 2.12 | 0.08 |
| 4:6:145:SER:CA | 4:9:133:TYR:CE1[1_554] | 2.12 | 0.08 |
| 4:4:173:HIS:NE2 | 4:8:264:PRO:C[1_554] | 2.12 | 0.08 |
| 4:6:28:ARG:O | 4:9:83:GLU:CG[1_554] | 2.12 | 0.08 |
| 4:4:366:GLY:CA | 4:8:235:SER:N[1_554] | 2.12 | 0.08 |
| 4:4:283:MET:SD | 4:7:286:ASP:N[1_554] | 2.12 | 0.08 |
| 4:5:151:ILE:CG1 | 4:8:171:LEU:C[1_554] | 2.12 | 0.08 |
| 4:4:199:SER:OG | 4:7:206:ARG:CB[1_554] | 2.13 | 0.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:326:LYS:O | 4:7:167:GLU:O[1_554] | 2.13 | 0.07 |
| 4:6:31:PHE:N | 4:9:79:TRP:O[1_554] | 2.13 | 0.07 |
| 4:5:153:LEU:C | 4:8:109:PRO:O[1_554] | 2.13 | 0.07 |
| 4:4:139:VAL:C | 4:7:371:HIS:CD2[1_554] | 2.13 | 0.07 |
| 4:4:154:ASP:OD1 | 4:7:111:ASN:N[1_554] | 2.13 | 0.07 |
| 4:5:279:TYR:CA | 4:8:164:PRO:CB[1_554] | 2.13 | 0.07 |
| 4:5:349:LEU:CA | 4:8:365:ALA:C[1_554] | 2.13 | 0.07 |
| 4:6:255:PHE:C | 4:9:305:MET:N[1_554] | 2.13 | 0.07 |
| 4:5:219:VAL:C | 4:8:335:ARG:CA[1_554] | 2.13 | 0.07 |
| 4:4:196:ARG:O | 4:7:212:ILE:N[1_554] | 2.13 | 0.07 |
| 4:5:344:SER:CB | 4:8:120:THR:CG2[1_554] | 2.13 | 0.07 |
| 4:5:286:ASP:OD2 | 4:V:39:ARG:CZ[1_554] | 2.13 | 0.07 |
| 4:4:337:TYR:CE2 | 4:7:86:TRP:CE3[1_554] | 2.13 | 0.07 |
| 4:4:182:GLY:CA | 4:7:73:HIS:CA[1_554] | 2.13 | 0.07 |
| 4:4:153:LEU:CD2 | 4:7:109:PRO:CA[1_554] | 2.13 | 0.07 |
| 4:4:160:THR:CB | 4:7:177:ARG:CD[1_554] | 2.13 | 0.07 |
| 4:6:269:MET:C | 4:9:272:ALA:C[1_554] | 2.13 | 0.07 |
| 4:6:263:GLN:CA | 4:9:274:ILE:CD1[1_554] | 2.13 | 0.07 |
| 4:5:196:ARG:NE | 4:8:211:ASP:OD1[1_554] | 2.13 | 0.07 |
| 4:4:281:SER:N | 4:7:173:HIS:C[1_554] | 2.13 | 0.07 |
| 4:6:316:GLU:N | 4:9:298:VAL:N[1_554] | 2.13 | 0.07 |
| 4:3:357:ILE:CB | 4:7:231:ALA:O[1_554] | 2.13 | 0.07 |
| 4:5:56:ASP:CA | 4:8:37:ARG:CZ[1_554] | 2.13 | 0.07 |
| 4:4:267:ILE:CA | 4:7:180:LEU:CD2[1_554] | 2.13 | 0.07 |
| 4:6:149:THR:OG1 | 4:W:40:HIS:CB[1_554] | 2.13 | 0.07 |
| 4:5:75:ILE:CG1 | 4:9:193:LEU:O[1_554] | 2.13 | 0.07 |
| 4:5:270:GLU:N | 4:8:272:ALA:C[1_554] | 2.13 | 0.07 |
| 4:6:256:ARG:CG | 4:9:306:TYR:CE1[1_554] | 2.13 | 0.07 |
| 4:4:340:TRP:CE3 | 4:7:121:GLN:CG[1_554] | 2.13 | 0.07 |
| 4:5:319:ALA:CB | 4:8:295:ALA:O[1_554] | 2.13 | 0.07 |
| 4:6:59:GLN:CD | 4:9:68:LYS:CA[1_554] | 2.13 | 0.07 |
| 4:5:173:HIS:C | 4:9:267:ILE:O[1_554] | 2.13 | 0.07 |
| 4:3:371:HIS:NE2 | 4:7:255:PHE:CD2[1_554] | 2.13 | 0.07 |
| 4:5:294:TYR:C | 4:8:167:GLU:CA[1_554] | 2.13 | 0.07 |
| 4:5:193:LEU:C | 4:8:210:ARG:CA[1_554] | 2.13 | 0.07 |
| 4:5:166:TYR:CE1 | 4:V:40:HIS:CG[1_554] | 2.13 | 0.07 |
| 4:6:278:THR:CG2 | 4:9:165:ILE:N[1_554] | 2.13 | 0.07 |
| 4:3:372:ARG:CD | 4:7:227:MET:CA[1_554] | 2.13 | 0.07 |
| 4:5:293:LEU:CB | 4:8:169:TYR:CE2[1_554] | 2.13 | 0.07 |
| 4:4:204:ALA:CA | 4:7:62:ARG:CA[1_554] | 2.13 | 0.07 |
| 4:5:173:HIS:ND1 | 4:9:266:PHE:C[1_554] | 2.13 | 0.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:137:GLN:CB | 4:7:112:PRO:C[1_554] | 2.13 | 0.07 |
| 4:5:210:ARG:NE | 4:8:33:SER:C[1_554] | 2.13 | 0.07 |
| 4:4:75:ILE:CB | 4:8:198:TYR:CD2[1_554] | 2.13 | 0.07 |
| 4:5:295:ALA:N | 4:8:167:GLU:CB[1_554] | 2.13 | 0.07 |
| 4:4:274:ILE:CA | 4:7:162:ASN:CA[1_554] | 2.13 | 0.07 |
| 4:4:265:SER:O | 4:7:261:LEU:O[1_554] | 2.13 | 0.07 |
| 4:5:254:ARG:NE | 4:8:336:LYS:CD[1_554] | 2.13 | 0.07 |
| 4:5:266:PHE:CB | 4:8:261:LEU:CA[1_554] | 2.13 | 0.07 |
| 4:4:210:ARG:CB | 4:7:69:TYR:CG[1_554] | 2.13 | 0.07 |
| 4:6:253:GLU:CD | 4:9:213:LYS:C[1_554] | 2.13 | 0.07 |
| 4:5:56:ASP:OD2 | 4:8:81:ASP:CG[1_554] | 2.13 | 0.07 |
| 4:4:294:TYR:CG | 4:7:166:TYR:CG[1_554] | 2.13 | 0.07 |
| 4:6:334:GLU:OE1 | 4:9:133:TYR:CB[1_554] | 2.13 | 0.07 |
| 4:5:264:PRO:N | 4:8:274:ILE:CG1[1_554] | 2.13 | 0.07 |
| 4:5:178:LEU:O | 4:8:177:ARG:NE[1_554] | 2.13 | 0.07 |
| 4:4:211:ASP:O | 4:7:32:PRO:CB[1_554] | 2.13 | 0.07 |
| 4:4:372:ARG:CG | 4:8:227:MET:CG[1_554] | 2.13 | 0.07 |
| 4:4:198:TYR:CB | 4:7:208:ILE:CA[1_554] | 2.13 | 0.07 |
| 4:5:297:ASN:CG | 4:8:165:ILE:CB[1_554] | 2.13 | 0.07 |
| 4:6:215:LYS:NZ | 4:9:31:PHE:CA[1_554] | 2.13 | 0.07 |
| 4:5:31:PHE:N | 4:8:79:TRP:O[1_554] | 2.13 | 0.07 |
| 4:4:196:ARG:CA | 4:7:209:VAL:O[1_554] | 2.13 | 0.07 |
| 4:6:337:TYR:CE2 | 4:9:86:TRP:NE1[1_554] | 2.13 | 0.07 |
| 4:6:188:TYR:CD2 | 4:9:182:GLY:N[1_554] | 2.13 | 0.07 |
| 4:6:198:TYR:OH | 4:9:211:ASP:CB[1_554] | 2.13 | 0.07 |
| 4:4:257:CYS:O | 4:7:155:SER:C[1_554] | 2.13 | 0.07 |
| 4:6:325:MET:SD | 4:9:166:TYR:CE1[1_554] | 2.13 | 0.07 |
| 4:6:114:ALA:C | 4:V:196:ARG:CZ[1_554] | 2.13 | 0.07 |
| 4:4:337:TYR:CA | 4:7:119:MET:N[1_554] | 2.13 | 0.07 |
| 4:3:172:PRO:C | 4:7:188:TYR:CE1[1_554] | 2.13 | 0.07 |
| 4:5:162:ASN:CB | 4:8:175:ILE:CG1[1_554] | 2.13 | 0.07 |
| 4:6:186:THR:C | 4:9:183:ARG:CA[1_554] | 2.13 | 0.07 |
| 4:5:75:ILE:N | 4:9:198:TYR:N[1_554] | 2.13 | 0.07 |
| 4:5:343:GLY:CA | 4:8:367:PRO:CB[1_554] | 2.13 | 0.07 |
| 4:4:210:ARG:CG | 4:7:69:TYR:CE2[1_554] | 2.13 | 0.07 |
| 4:4:301:GLY:N | 4:7:111:ASN:ND2[1_554] | 2.13 | 0.07 |
| 4:3:172:PRO:CB | 4:7:266:PHE:CD2[1_554] | 2.13 | 0.07 |
| 4:5:316:GLU:CB | 4:8:298:VAL:N[1_554] | 2.13 | 0.07 |
| 4:5:366:GLY:CA | 4:9:234:SER:CA[1_554] | 2.13 | 0.07 |
| 4:4:334:GLU:OE2 | 4:7:133:TYR:CA[1_554] | 2.13 | 0.07 |
| 4:5:274:ILE:CB | 4:8:162:ASN:CA[1_554] | 2.13 | 0.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:196:ARG:CB | 4:7:210:ARG:O[1_554] | 2.13 | 0.07 |
| 4:6:164:PRO:N | 4:9:172:PRO:CD[1_554] | 2.13 | 0.07 |
| 4:5:75:ILE:CA | 4:9:197:GLY:O[1_554] | 2.13 | 0.07 |
| 4:6:291:LYS:NZ | 4:W:64:ILE:CB[1_554] | 2.13 | 0.07 |
| 4:4:371:HIS:CA | 4:8:230:ALA:CB[1_554] | 2.13 | 0.07 |
| 4:6:286:ASP:CB | 4:V:270:GLU:OE2[1_554] | 2.13 | 0.07 |
| 4:3:367:PRO:C | 4:7:236:LEU:CA[1_554] | 2.13 | 0.07 |
| 4:6:195:GLU:CD | 4:9:189:LEU:CB[1_554] | 2.13 | 0.07 |
| 4:6:188:TYR:CD2 | 4:9:181:ALA:O[1_554] | 2.13 | 0.07 |
| 4:6:310:ALA:CA | 4:9:141:SER:O[1_554] | 2.13 | 0.07 |
| 4:4:339:VAL:C | 4:7:114:ALA:O[1_554] | 2.13 | 0.07 |
| 4:5:256:ARG:CB | 4:8:306:TYR:CD1[1_554] | 2.13 | 0.07 |
| 4:4:277:THR:OG1 | 4:7:176:MET:CB[1_554] | 2.13 | 0.07 |
| 4:4:110:LEU:O | 4:8:192:ILE:CA[1_554] | 2.13 | 0.07 |
| 4:4:336:LYS:CE | 4:7:86:TRP:CD1[1_554] | 2.13 | 0.07 |
| 4:5:288:ASP:C | 4:V:63:GLY:N[1_554] | 2.13 | 0.07 |
| 4:6:214:GLU:CA | 4:9:16:LEU:CG[1_554] | 2.13 | 0.07 |
| 4:3:108:ALA:C | 4:7:195:GLU:CG[1_554] | 2.13 | 0.07 |
| 4:5:113:LYS:C | 4:9:252:ASN:CA[1_554] | 2.13 | 0.07 |
| 4:6:161:HIS:CB | 4:9:110:LEU:CA[1_554] | 2.13 | 0.07 |
| 4:4:270:GLU:CA | 4:7:272:ALA:CB[1_554] | 2.13 | 0.07 |
| 4:4:321:ALA:C | 4:7:292:ASP:CG[1_554] | 2.13 | 0.07 |
| 4:5:294:TYR:O | 4:8:167:GLU:CA[1_554] | 2.13 | 0.07 |
| 4:5:217:CYS:O | 4:8:336:LYS:O[1_554] | 2.13 | 0.07 |
| 4:5:161:HIS:N | 4:8:110:LEU:CG[1_554] | 2.13 | 0.07 |
| 4:4:153:LEU:CB | 4:7:109:PRO:CA[1_554] | 2.13 | 0.07 |
| 4:6:288:ASP:CA | 4:W:63:GLY:C[1_554] | 2.13 | 0.07 |
| 4:4:153:LEU:CD1 | 4:7:109:PRO:CG[1_554] | 2.14 | 0.06 |
| 4:3:114:ALA:O | 4:7:250:ILE:O[1_554] | 2.14 | 0.06 |
| 4:4:294:TYR:C | 4:7:166:TYR:O[1_554] | 2.14 | 0.06 |
| 4:4:186:THR:CA | 4:7:183:ARG:CD[1_554] | 2.14 | 0.06 |
| 4:6:320:LEU:O | 4:9:290:ARG:CA[1_554] | 2.14 | 0.06 |
| 4:4:321:ALA:C | 4:7:292:ASP:CB[1_554] | 2.14 | 0.06 |
| 4:6:26:ALA:N | 4:9:124:PHE:N[1_554] | 2.14 | 0.06 |
| 4:6:344:SER:OG | 4:9:362:TYR:CE1[1_554] | 2.14 | 0.06 |
| 4:4:77:THR:C | 4:8:246:GLN:CD[1_554] | 2.14 | 0.06 |
| 4:6:283:MET:CB | 4:9:286:ASP:CA[1_554] | 2.14 | 0.06 |
| 4:4:300:SER:OG | 4:7:107:GLU:CD[1_554] | 2.14 | 0.06 |
| 4:4:195:GLU:N | 4:7:209:VAL:CB[1_554] | 2.14 | 0.06 |
| 4:4:143:TYR:CD2 | 4:7:368:SER:C[1_554] | 2.14 | 0.06 |
| 4:4:27:PRO:N | 4:7:122:ILE:N[1_554] | 2.14 | 0.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:312:ARG:CB | 4:8:299:MET:N[1_554] | 2.14 | 0.06 |
| 4:4:137:GLN:CD | 4:7:112:PRO:CB[1_554] | 2.14 | 0.06 |
| 4:6:341:ILE:C | 4:9:120:THR:CG2[1_554] | 2.14 | 0.06 |
| 4:6:56:ASP:C | 4:9:37:ARG:CZ[1_554] | 2.14 | 0.06 |
| 4:6:156:GLY:C | 4:9:73:HIS:C[1_554] | 2.14 | 0.06 |
| 4:5:178:LEU:C | 4:8:177:ARG:CB[1_554] | 2.14 | 0.06 |
| 4:5:300:SER:CB | 4:8:107:GLU:CB[1_554] | 2.14 | 0.06 |
| 4:6:242:LEU:CG | 4:9:207:GLU:CD[1_554] | 2.14 | 0.06 |
| 4:4:193:LEU:CD1 | 4:7:210:ARG:CG[1_554] | 2.14 | 0.06 |
| 4:6:294:TYR:CD2 | 4:9:166:TYR:CB[1_554] | 2.14 | 0.06 |
| 4:6:151:ILE:CD1 | 4:9:172:PRO:N[1_554] | 2.14 | 0.06 |
| 4:4:367:PRO:C | 4:8:236:LEU:CA[1_554] | 2.14 | 0.06 |
| 4:6:319:ALA:N | 4:9:296:ASN:CG[1_554] | 2.14 | 0.06 |
| 4:6:227:MET:CB | 4:9:307:PRO:O[1_554] | 2.14 | 0.06 |
| 4:5:312:ARG:CA | 4:8:298:VAL:CB[1_554] | 2.14 | 0.06 |
| 4:4:221:LEU:C | 4:7:332:PRO:CG[1_554] | 2.14 | 0.06 |
| 4:5:312:ARG:O | 4:8:298:VAL:CG2[1_554] | 2.14 | 0.06 |
| 4:6:294:TYR:CD1 | 4:9:166:TYR:CA[1_554] | 2.14 | 0.06 |
| 4:5:310:ALA:N | 4:8:141:SER:C[1_554] | 2.14 | 0.06 |
| 4:6:21:PHE:N | 4:9:121:GLN:NE2[1_554] | 2.14 | 0.06 |
| 4:6:221:LEU:N | 4:9:332:PRO:CD[1_554] | 2.14 | 0.06 |
| 4:5:327:ILE:O | 4:8:148:THR:CG2[1_554] | 2.14 | 0.06 |
| 4:5:308:GLY:N | 4:8:339:VAL:N[1_554] | 2.14 | 0.06 |
| 4:6:334:GLU:N | 4:9:105:LEU:CA[1_554] | 2.14 | 0.06 |
| 4:6:143:TYR:OH | 4:9:369:ILE:CD1[1_554] | 2.14 | 0.06 |
| 4:5:32:PRO:CA | 4:8:78:ASN:ND2[1_554] | 2.14 | 0.06 |
| 4:5:167:GLU:N | 4:V:40:HIS:CD2[1_554] | 2.14 | 0.06 |
| 4:4:173:HIS:CE1 | 4:8:266:PHE:CA[1_554] | 2.14 | 0.06 |
| 4:6:368:SER:O | 4:V:229:THR:O[1_554] | 2.14 | 0.06 |
| 4:6:218:TYR:CD1 | 4:9:336:LYS:CD[1_554] | 2.14 | 0.06 |
| 4:5:192:ILE:N | 4:8:185:LEU:C[1_554] | 2.14 | 0.06 |
| 4:4:264:PRO:CD | 4:7:274:ILE:CD1[1_554] | 2.14 | 0.06 |
| 4:4:166:TYR:CE1 | 4:9:40:HIS:CD2[1_554] | 2.14 | 0.06 |
| 4:5:334:GLU:OE2 | 4:8:104:LEU:CA[1_554] | 2.14 | 0.06 |
| 4:6:186:THR:C | 4:9:183:ARG:CD[1_554] | 2.14 | 0.06 |
| 4:5:140:LEU:CA | 4:8:371:HIS:CA[1_554] | 2.14 | 0.06 |
| 4:6:200:PHE:C | 4:9:206:ARG:CB[1_554] | 2.14 | 0.06 |
| 4:4:276:GLU:OE2 | 4:7:278:THR:CB[1_554] | 2.14 | 0.06 |
| 4:6:299:MET:N | 4:9:136:ILE:CA[1_554] | 2.14 | 0.06 |
| 4:6:18:LYS:O | 4:9:118:LYS:CD[1_554] | 2.14 | 0.06 |
| 4:6:337:TYR:CZ | 4:9:86:TRP:CH2[1_554] | 2.14 | 0.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:139:VAL:C | 4:9:371:HIS:O[1_554] | 2.14 | 0.06 |
| 4:5:301:GLY:O | 4:8:137:GLN:CD[1_554] | 2.14 | 0.06 |
| 4:4:260:THR:C | 4:7:155:SER:CB[1_554] | 2.14 | 0.06 |
| 4:6:334:GLU:OE1 | 4:9:133:TYR:N[1_554] | 2.14 | 0.06 |
| 4:6:16:LEU:N | 4:9:76:ILE:C[1_554] | 2.14 | 0.06 |
| 4:4:260:THR:CG2 | 4:7:160:THR:OG1[1_554] | 2.14 | 0.06 |
| 4:4:371:HIS:NE2 | 4:8:255:PHE:CD2[1_554] | 2.14 | 0.06 |
| 4:6:188:TYR:CD1 | 4:9:185:LEU:CA[1_554] | 2.14 | 0.06 |
| 4:6:265:SER:C | 4:9:262:PHE:N[1_554] | 2.14 | 0.06 |
| 4:6:327:ILE:C | 4:9:148:THR:OG1[1_554] | 2.14 | 0.06 |
| 4:6:255:PHE:CD1 | 4:9:306:TYR:N[1_554] | 2.14 | 0.06 |
| 4:3:113:LYS:CE | 4:7:254:ARG:CB[1_554] | 2.14 | 0.06 |
| 4:4:314:GLN:CG | 4:7:143:TYR:CA[1_554] | 2.14 | 0.06 |
| 4:5:218:TYR:CZ | 4:8:337:TYR:CZ[1_554] | 2.14 | 0.06 |
| 4:5:321:ALA:N | 4:8:292:ASP:CA[1_554] | 2.14 | 0.06 |
| 4:6:309:ILE:CA | 4:9:300:SER:OG[1_554] | 2.14 | 0.06 |
| 4:6:31:PHE:C | 4:9:78:ASN:CB[1_554] | 2.14 | 0.06 |
| 4:4:162:ASN:CG | 4:7:175:ILE:CG1[1_554] | 2.14 | 0.06 |
| 4:5:186:THR:CA | 4:8:183:ARG:CB[1_554] | 2.14 | 0.06 |
| 4:6:340:TRP:CD2 | 4:9:120:THR:C[1_554] | 2.14 | 0.06 |
| 4:3:166:TYR:CE1 | 4:8:40:HIS:CD2[1_554] | 2.14 | 0.06 |
| 4:4:154:ASP:CB | 4:7:111:ASN:C[1_554] | 2.14 | 0.06 |
| 4:5:14:SER:O | 4:8:77:THR:CB[1_554] | 2.14 | 0.06 |
| 4:5:342:GLY:CA | 4:8:371:HIS:N[1_554] | 2.14 | 0.06 |
| 4:4:304:THR:O | 4:7:137:GLN:CD[1_554] | 2.14 | 0.06 |
| 4:5:368:SER:C | 4:9:230:ALA:CA[1_554] | 2.14 | 0.06 |
| 4:4:299:MET:CE | 4:7:136:ILE:CA[1_554] | 2.14 | 0.06 |
| 4:6:257:CYS:N | 4:9:303:THR:N[1_554] | 2.14 | 0.06 |
| 4:5:117:GLU:N | 4:9:252:ASN:OD1[1_554] | 2.14 | 0.06 |
| 4:4:333:PRO:CB | 4:7:104:LEU:O[1_554] | 2.14 | 0.06 |
| 4:5:24:ASP:C | 4:8:124:PHE:C[1_554] | 2.14 | 0.06 |
| 4:6:198:TYR:OH | 4:9:240:TYR:OH[1_554] | 2.14 | 0.06 |
| 4:5:135:ALA:CB | 4:8:117:GLU:OE2[1_554] | 2.14 | 0.06 |
| 4:6:178:LEU:CB | 4:9:176:MET:C[1_554] | 2.14 | 0.06 |
| 4:4:336:LYS:CA | 4:7:119:MET:CE[1_554] | 2.14 | 0.06 |
| 4:4:120:THR:CG2 | 4:8:233:SER:CB[1_554] | 2.14 | 0.06 |
| 4:4:255:PHE:CA | 4:7:302:GLY:N[1_554] | 2.14 | 0.06 |
| 4:6:224:GLU:OE2 | 4:9:311:ASP:OD1[1_554] | 2.14 | 0.06 |
| 4:6:188:TYR:CG | 4:9:181:ALA:C[1_554] | 2.14 | 0.06 |
| 4:4:345:ILE:CB | 4:7:367:PRO:CA[1_554] | 2.14 | 0.06 |
| 4:6:151:ILE:CG1 | 4:9:172:PRO:N[1_554] | 2.14 | 0.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:188:TYR:CD1 | 4:8:185:LEU:CA[1_554] | 2.14 | 0.06 |
| 4:5:276:GLU:CD | 4:8:278:THR:CA[1_554] | 2.14 | 0.06 |
| 4:4:72:GLU:O | 4:8:199:SER:CA[1_554] | 2.14 | 0.06 |
| 4:5:214:GLU:CB | 4:8:16:LEU:O[1_554] | 2.14 | 0.06 |
| 4:4:332:PRO:CA | 4:7:134:VAL:CA[1_554] | 2.14 | 0.06 |
| 4:5:288:ASP:OD1 | 4:V:62:ARG:O[1_554] | 2.14 | 0.06 |
| 4:6:142:LEU:O | 4:9:372:ARG:CG[1_554] | 2.14 | 0.06 |
| 4:6:154:ASP:N | 4:9:109:PRO:N[1_554] | 2.14 | 0.06 |
| 4:4:264:PRO:CB | 4:7:178:LEU:CG[1_554] | 2.14 | 0.06 |
| 4:5:204:ALA:O | 4:8:62:ARG:NH1[1_554] | 2.14 | 0.06 |
| 4:6:318:THR:O | 4:9:292:ASP:CA[1_554] | 2.14 | 0.06 |
| 4:6:17:VAL:O | 4:9:79:TRP:CG[1_554] | 2.14 | 0.06 |
| 4:5:342:GLY:C | 4:8:370:VAL:CG1[1_554] | 2.14 | 0.06 |
| 4:4:166:TYR:CE1 | 4:9:40:HIS:ND1[1_554] | 2.14 | 0.06 |
| 4:4:214:GLU:C | 4:7:16:LEU:O[1_554] | 2.14 | 0.06 |
| 4:6:173:HIS:C | 4:V:268:GLY:N[1_554] | 2.14 | 0.06 |
| 4:5:305:MET:O | 4:8:11:ASP:CG[1_554] | 2.14 | 0.06 |
| 4:6:244:ASP:OD2 | 4:7:291:LYS:CE[1_554] | 2.14 | 0.06 |
| 4:4:173:HIS:CG | 4:8:267:ILE:CG1[1_554] | 2.14 | 0.06 |
| 4:5:215:LYS:NZ | 4:8:31:PHE:CA[1_554] | 2.14 | 0.06 |
| 4:6:212:ILE:O | 4:9:16:LEU:CG[1_554] | 2.15 | 0.05 |
| 4:4:263:GLN:CG | 4:7:153:LEU:CD2[1_554] | 2.15 | 0.05 |
| 4:5:15:GLY:C | 4:8:77:THR:C[1_554] | 2.15 | 0.05 |
| 4:3:372:ARG:N | 4:7:230:ALA:CB[1_554] | 2.15 | 0.05 |
| 4:6:254:ARG:O | 4:9:302:GLY:CA[1_554] | 2.15 | 0.05 |
| 4:5:198:TYR:OH | 4:8:211:ASP:CG[1_554] | 2.15 | 0.05 |
| 4:4:186:THR:O | 4:7:183:ARG:NE[1_554] | 2.15 | 0.05 |
| 4:5:264:PRO:CD | 4:8:274:ILE:CA[1_554] | 2.15 | 0.05 |
| 4:5:218:TYR:CG | 4:8:336:LYS:CA[1_554] | 2.15 | 0.05 |
| 4:5:210:ARG:CZ | 4:8:34:ILE:N[1_554] | 2.15 | 0.05 |
| 4:5:18:LYS:CD | 4:8:79:TRP:CE3[1_554] | 2.15 | 0.05 |
| 4:5:195:GLU:CB | 4:8:189:LEU:CD1[1_554] | 2.15 | 0.05 |
| 4:4:326:LYS:N | 4:7:167:GLU:OE1[1_554] | 2.15 | 0.05 |
| 4:6:110:LEU:CB | 4:V:192:ILE:CG2[1_554] | 2.15 | 0.05 |
| 4:5:214:GLU:C | 4:8:16:LEU:CA[1_554] | 2.15 | 0.05 |
| 4:4:18:LYS:O | 4:7:118:LYS:CE[1_554] | 2.15 | 0.05 |
| 4:4:27:PRO:CA | 4:7:121:GLN:OE1[1_554] | 2.15 | 0.05 |
| 4:6:219:VAL:N | 4:9:336:LYS:CA[1_554] | 2.15 | 0.05 |
| 4:6:261:LEU:CG | 4:9:154:ASP:C[1_554] | 2.15 | 0.05 |
| 4:6:347:ALA:CB | 4:9:367:PRO:N[1_554] | 2.15 | 0.05 |
| 4:5:322:PRO:CG | 4:8:289:ILE:N[1_554] | 2.15 | 0.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:136:ILE:CB | 4:8:113:LYS:NZ[1_554] | 2.15 | 0.05 |
| 4:6:310:ALA:O | 4:9:141:SER:O[1_554] | 2.15 | 0.05 |
| 4:6:11:ASP:CG | 4:9:115:ASN:C[1_554] | 2.15 | 0.05 |
| 4:3:76:ILE:C | 4:7:198:TYR:CD1[1_554] | 2.15 | 0.05 |
| 4:6:243:PRO:C | 4:9:60:SER:CB[1_554] | 2.15 | 0.05 |
| 4:6:189:LEU:C | 4:9:186:THR:CB[1_554] | 2.15 | 0.05 |
| 4:6:274:ILE:CG1 | 4:9:162:ASN:N[1_554] | 2.15 | 0.05 |
| 4:4:181:ALA:C | 4:7:73:HIS:C[1_554] | 2.15 | 0.05 |
| 4:6:256:ARG:O | 4:9:303:THR:CA[1_554] | 2.15 | 0.05 |
| 4:4:262:PHE:CA | 4:7:154:ASP:N[1_554] | 2.15 | 0.05 |
| 4:5:340:TRP:CE2 | 4:8:121:GLN:CA[1_554] | 2.15 | 0.05 |
| 4:5:311:ASP:O | 4:8:298:VAL:CG2[1_554] | 2.15 | 0.05 |
| 4:5:205:GLU:CA | 4:8:62:ARG:CD[1_554] | 2.15 | 0.05 |
| 4:5:191:LYS:CG | 4:8:185:LEU:CA[1_554] | 2.15 | 0.05 |
| 4:6:194:THR:N | 4:9:209:VAL:C[1_554] | 2.15 | 0.05 |
| 4:4:263:GLN:O | 4:7:274:ILE:CD1[1_554] | 2.15 | 0.05 |
| 4:4:112:PRO:N | 4:8:193:LEU:CD1[1_554] | 2.15 | 0.05 |
| 4:6:198:TYR:CE1 | 4:9:208:ILE:CA[1_554] | 2.15 | 0.05 |
| 4:5:117:GLU:CD | 4:9:236:LEU:CD1[1_554] | 2.15 | 0.05 |
| 4:2:292:ASP:CB | 4:7:40:HIS:NE2[1_554] | 2.15 | 0.05 |
| 4:4:77:THR:CA | 4:8:246:GLN:NE2[1_554] | 2.15 | 0.05 |
| 4:6:250:ILE:CG2 | 4:9:214:GLU:CG[1_554] | 2.15 | 0.05 |
| 4:4:210:ARG:NE | 4:7:33:SER:O[1_554] | 2.15 | 0.05 |
| 4:6:162:ASN:O | 4:9:172:PRO:C[1_554] | 2.15 | 0.05 |
| 4:4:193:LEU:N | 4:7:210:ARG:CA[1_554] | 2.15 | 0.05 |
| 4:4:345:ILE:CG1 | 4:7:367:PRO:CA[1_554] | 2.15 | 0.05 |
| 4:4:281:SER:CB | 4:7:171:LEU:O[1_554] | 2.15 | 0.05 |
| 4:4:166:TYR:CD1 | 4:9:40:HIS:ND1[1_554] | 2.15 | 0.05 |
| 4:5:304:THR:O | 4:8:339:VAL:CG1[1_554] | 2.15 | 0.05 |
| 4:5:26:ALA:N | 4:8:123:MET:O[1_554] | 2.15 | 0.05 |
| 4:4:172:PRO:CD | 4:8:266:PHE:CA[1_554] | 2.15 | 0.05 |
| 4:5:317:ILE:CD1 | 4:8:150:GLY:O[1_554] | 2.15 | 0.05 |
| 4:5:281:SER:CB | 4:8:173:HIS:C[1_554] | 2.15 | 0.05 |
| 4:6:32:PRO:CD | 4:9:78:ASN:ND2[1_554] | 2.15 | 0.05 |
| 4:5:297:ASN:CA | 4:8:170:ALA:N[1_554] | 2.15 | 0.05 |
| 4:6:167:GLU:OE1 | 4:W:41:GLN:CG[1_554] | 2.15 | 0.05 |
| 4:4:243:PRO:N | 4:7:60:SER:OG[1_554] | 2.15 | 0.05 |
| 4:5:108:ALA:O | 4:9:195:GLU:CG[1_554] | 2.15 | 0.05 |
| 4:5:314:GLN:CD | 4:8:147:ARG:CG[1_554] | 2.15 | 0.05 |
| 4:6:166:TYR:OH | 4:W:39:ARG:CB[1_554] | 2.15 | 0.05 |
| 4:4:330:ILE:CG2 | 4:7:133:TYR:CZ[1_554] | 2.15 | 0.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:219:VAL:CG1 | 4:8:301:GLY:N[1_554] | 2.15 | 0.05 |
| 4:6:275:HIS:N | 4:9:152:VAL:O[1_554] | 2.15 | 0.05 |
| 4:5:330:ILE:O | 4:8:139:VAL:CB[1_554] | 2.15 | 0.05 |
| 4:5:154:ASP:CB | 4:8:108:ALA:O[1_554] | 2.15 | 0.05 |
| 4:5:280:ASN:N | 4:8:285:CYS:SG[1_554] | 2.15 | 0.05 |
| 4:4:318:THR:CA | 4:7:149:THR:CB[1_554] | 2.15 | 0.05 |
| 4:6:338:SER:N | 4:9:134:VAL:CG1[1_554] | 2.15 | 0.05 |
| 4:4:306:TYR:CA | 4:7:11:ASP:CG[1_554] | 2.15 | 0.05 |
| 4:5:317:ILE:O | 4:8:293:LEU:CA[1_554] | 2.15 | 0.05 |
| 4:5:213:LYS:CD | 4:8:157:ASP:OD2[1_554] | 2.15 | 0.05 |
| 4:4:114:ALA:CA | 4:8:250:ILE:CB[1_554] | 2.15 | 0.05 |
| 4:5:75:ILE:CB | 4:9:198:TYR:CA[1_554] | 2.15 | 0.05 |
| 4:5:293:LEU:O | 4:8:169:TYR:C[1_554] | 2.15 | 0.05 |
| 4:4:25:ASP:N | 4:7:125:GLU:CA[1_554] | 2.15 | 0.05 |
| 4:5:249:THR:O | 4:8:211:ASP:CA[1_554] | 2.15 | 0.05 |
| 4:4:342:GLY:N | 4:7:117:GLU:CB[1_554] | 2.15 | 0.05 |
| 4:6:162:ASN:CB | 4:9:172:PRO:O[1_554] | 2.15 | 0.05 |
| 4:5:295:ALA:CA | 4:8:167:GLU:CB[1_554] | 2.15 | 0.05 |
| 4:4:281:SER:OG | 4:7:172:PRO:O[1_554] | 2.15 | 0.05 |
| 4:5:316:GLU:CG | 4:8:297:ASN:C[1_554] | 2.15 | 0.05 |
| 4:4:339:VAL:CA | 4:7:113:LYS:O[1_554] | 2.15 | 0.05 |
| 4:5:205:GLU:N | 4:8:62:ARG:CZ[1_554] | 2.15 | 0.05 |
| 4:6:31:PHE:C | 4:9:78:ASN:ND2[1_554] | 2.15 | 0.05 |
| 4:4:178:LEU:CD1 | 4:7:177:ARG:CA[1_554] | 2.15 | 0.05 |
| 4:5:326:LYS:O | 4:8:167:GLU:OE2[1_554] | 2.15 | 0.05 |
| 4:5:240:TYR:CZ | 4:8:56:ASP:OD2[1_554] | 2.15 | 0.05 |
| 4:5:340:TRP:CZ2 | 4:8:121:GLN:O[1_554] | 2.15 | 0.05 |
| 4:4:215:LYS:CA | 4:7:17:VAL:O[1_554] | 2.15 | 0.05 |
| 4:6:322:PRO:O | 4:9:291:LYS:NZ[1_554] | 2.15 | 0.05 |
| 4:5:321:ALA:C | 4:8:292:ASP:CG[1_554] | 2.15 | 0.05 |
| 4:4:76:ILE:O | 4:8:198:TYR:CZ[1_554] | 2.15 | 0.05 |
| 4:6:340:TRP:CE2 | 4:9:121:GLN:CA[1_554] | 2.15 | 0.05 |
| 4:4:370:VAL:C | 4:8:230:ALA:N[1_554] | 2.15 | 0.05 |
| 4:5:280:ASN:C | 4:8:174:ALA:CB[1_554] | 2.15 | 0.05 |
| 4:6:366:GLY:CA | 4:V:234:SER:CA[1_554] | 2.15 | 0.05 |
| 4:4:153:LEU:O | 4:7:109:PRO:O[1_554] | 2.15 | 0.05 |
| 4:5:198:TYR:CE1 | 4:8:208:ILE:CD1[1_554] | 2.15 | 0.05 |
| 4:5:336:LYS:CE | 4:8:12:ASN:OD1[1_554] | 2.15 | 0.05 |
| 4:5:62:ARG:NH2 | 4:8:67:LEU:CB[1_554] | 2.15 | 0.05 |
| 4:6:167:GLU:N | 4:W:40:HIS:CD2[1_554] | 2.15 | 0.05 |
| 4:4:136:ILE:O | 4:7:113:LYS:CB[1_554] | 2.15 | 0.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:188:TYR:CG | 4:7:182:GLY:C[1_554] | 2.15 | 0.05 |
| 4:6:254:ARG:NE | 4:9:336:LYS:CD[1_554] | 2.15 | 0.05 |
| 4:3:75:ILE:O | 4:7:198:TYR:CD1[1_554] | 2.15 | 0.05 |
| 4:6:344:SER:OG | 4:9:362:TYR:CZ[1_554] | 2.15 | 0.05 |
| 4:5:371:HIS:C | 4:9:227:MET:O[1_554] | 2.15 | 0.05 |
| 4:4:317:ILE:N | 4:7:150:GLY:CA[1_554] | 2.15 | 0.05 |
| 4:4:339:VAL:C | 4:7:117:GLU:CA[1_554] | 2.15 | 0.05 |
| 4:5:196:ARG:CB | 4:8:209:VAL:O[1_554] | 2.15 | 0.05 |
| 4:4:316:GLU:CB | 4:7:152:VAL:CA[1_554] | 2.15 | 0.05 |
| 4:6:179:ASP:C | 4:9:179:ASP:CG[1_554] | 2.15 | 0.05 |
| 4:5:294:TYR:CD1 | 4:8:166:TYR:CA[1_554] | 2.15 | 0.05 |
| 4:6:214:GLU:CB | 4:9:16:LEU:O[1_554] | 2.15 | 0.05 |
| 4:4:185:LEU:CD2 | 4:7:159:VAL:N[1_554] | 2.15 | 0.05 |
| 4:6:304:THR:CB | 4:9:137:GLN:CA[1_554] | 2.15 | 0.05 |
| 4:6:151:ILE:O | 4:9:170:ALA:CB[1_554] | 2.15 | 0.05 |
| 4:2:324:THR:N | 4:7:44:MET:CE[1_554] | 2.15 | 0.05 |
| 4:4:304:THR:CG2 | 4:7:108:ALA:C[1_554] | 2.15 | 0.05 |
| 4:5:218:TYR:O | 4:8:302:GLY:CA[1_554] | 2.15 | 0.05 |
| 4:3:114:ALA:N | 4:7:250:ILE:CA[1_554] | 2.15 | 0.05 |
| 4:6:312:ARG:CA | 4:9:298:VAL:CB[1_554] | 2.15 | 0.05 |
| 4:5:281:SER:CA | 4:8:173:HIS:C[1_554] | 2.15 | 0.05 |
| 4:5:185:LEU:O | 4:8:183:ARG:N[1_554] | 2.15 | 0.05 |
| 4:3:171:LEU:CB | 4:7:265:SER:O[1_554] | 2.15 | 0.05 |
| 4:4:30:VAL:CA | 4:7:79:TRP:CA[1_554] | 2.15 | 0.05 |
| 4:6:181:ALA:C | 4:9:158:GLY:C[1_554] | 2.15 | 0.05 |
| 4:4:275:HIS:CA | 4:7:163:VAL:O[1_554] | 2.15 | 0.05 |
| 4:6:304:THR:N | 4:9:137:GLN:NE2[1_554] | 2.15 | 0.05 |
| 4:3:172:PRO:CA | 4:7:266:PHE:O[1_554] | 2.15 | 0.05 |
| 4:5:286:ASP:OD1 | 4:9:270:GLU:OE1[1_554] | 2.15 | 0.05 |
| 4:4:331:ALA:CB | 4:7:135:ALA:C[1_554] | 2.15 | 0.05 |
| 4:6:369:ILE:C | 4:V:231:ALA:N[1_554] | 2.16 | 0.04 |
| 4:4:261:LEU:N | 4:7:154:ASP:O[1_554] | 2.16 | 0.04 |
| 4:4:344:SER:N | 4:7:367:PRO:CB[1_554] | 2.16 | 0.04 |
| 4:4:172:PRO:CD | 4:8:266:PHE:CD1[1_554] | 2.16 | 0.04 |
| 4:5:310:ALA:C | 4:8:142:LEU:CA[1_554] | 2.16 | 0.04 |
| 4:4:75:ILE:O | 4:8:198:TYR:CA[1_554] | 2.16 | 0.04 |
| 4:6:16:LEU:O | 4:9:76:ILE:C[1_554] | 2.16 | 0.04 |
| 4:4:243:PRO:C | 4:7:60:SER:C[1_554] | 2.16 | 0.04 |
| 4:3:112:PRO:N | 4:7:193:LEU:CD1[1_554] | 2.16 | 0.04 |
| 4:6:338:SER:C | 4:9:134:VAL:CG2[1_554] | 2.16 | 0.04 |
| 4:5:179:ASP:C | 4:8:179:ASP:CG[1_554] | 2.16 | 0.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:260:THR:N | 4:8:155:SER:CB[1_554] | 2.16 | 0.04 |
| 4:6:137:GLN:CD | 4:9:112:PRO:C[1_554] | 2.16 | 0.04 |
| 4:5:275:HIS:N | 4:8:162:ASN:CB[1_554] | 2.16 | 0.04 |
| 4:5:31:PHE:CD1 | 4:8:79:TRP:C[1_554] | 2.16 | 0.04 |
| 4:6:367:PRO:C | 4:V:233:SER:N[1_554] | 2.16 | 0.04 |
| 4:5:257:CYS:O | 4:8:303:THR:CG2[1_554] | 2.16 | 0.04 |
| 4:4:315:LYS:CD | 4:7:147:ARG:CB[1_554] | 2.16 | 0.04 |
| 4:6:215:LYS:CB | 4:9:30:VAL:C[1_554] | 2.16 | 0.04 |
| 4:5:299:MET:CG | 4:8:136:ILE:C[1_554] | 2.16 | 0.04 |
| 4:4:196:ARG:CA | 4:7:211:ASP:C[1_554] | 2.16 | 0.04 |
| 4:5:28:ARG:CB | 4:8:126:THR:OG1[1_554] | 2.16 | 0.04 |
| 4:4:195:GLU:OE2 | 4:7:189:LEU:CB[1_554] | 2.16 | 0.04 |
| 4:4:172:PRO:N | 4:8:266:PHE:O[1_554] | 2.16 | 0.04 |
| 4:4:317:ILE:CG1 | 4:7:165:ILE:C[1_554] | 2.16 | 0.04 |
| 4:5:309:ILE:CG1 | 4:8:154:ASP:OD2[1_554] | 2.16 | 0.04 |
| 4:4:114:ALA:CB | 4:8:250:ILE:O[1_554] | 2.16 | 0.04 |
| 4:5:264:PRO:CB | 4:8:178:LEU:CG[1_554] | 2.16 | 0.04 |
| 4:5:193:LEU:CG | 4:8:210:ARG:C[1_554] | 2.16 | 0.04 |
| 4:2:292:ASP:CA | 4:7:40:HIS:CG[1_554] | 2.16 | 0.04 |
| 4:4:136:ILE:C | 4:7:113:LYS:NZ[1_554] | 2.16 | 0.04 |
| 4:4:194:THR:N | 4:7:209:VAL:CG1[1_554] | 2.16 | 0.04 |
| 4:5:315:LYS:CE | 4:8:330:ILE:CD1[1_554] | 2.16 | 0.04 |
| 4:6:254:ARG:NE | 4:9:336:LYS:CE[1_554] | 2.16 | 0.04 |
| 4:5:211:ASP:N | 4:8:32:PRO:CB[1_554] | 2.16 | 0.04 |
| 4:6:269:MET:CB | 4:9:271:SER:OG[1_554] | 2.16 | 0.04 |
| 4:5:191:LYS:C | 4:8:186:THR:N[1_554] | 2.16 | 0.04 |
| 4:4:153:LEU:C | 4:7:109:PRO:CA[1_554] | 2.16 | 0.04 |
| 4:6:335:ARG:NH2 | 4:9:339:VAL:O[1_554] | 2.16 | 0.04 |
| 4:6:21:PHE:N | 4:9:125:GLU:OE1[1_554] | 2.16 | 0.04 |
| 4:6:218:TYR:CG | 4:9:336:LYS:CD[1_554] | 2.16 | 0.04 |
| 4:6:196:ARG:NH1 | 4:9:215:LYS:CG[1_554] | 2.16 | 0.04 |
| 4:6:348:SER:C | 4:9:364:GLU:C[1_554] | 2.16 | 0.04 |
| 4:4:21:PHE:O | 4:7:125:GLU:OE1[1_554] | 2.16 | 0.04 |
| 4:5:340:TRP:CH2 | 4:8:120:THR:C[1_554] | 2.16 | 0.04 |
| 4:6:326:LYS:CD | 4:9:167:GLU:OE1[1_554] | 2.16 | 0.04 |
| 4:6:227:MET:O | 4:9:307:PRO:CG[1_554] | 2.16 | 0.04 |
| 4:5:256:ARG:CD | 4:8:306:TYR:CG[1_554] | 2.16 | 0.04 |
| 4:6:136:ILE:N | 4:9:113:LYS:CG[1_554] | 2.16 | 0.04 |
| 4:5:30:VAL:CG1 | 4:8:82:MET:C[1_554] | 2.16 | 0.04 |
| 4:5:224:GLU:N | 4:8:310:ALA:CB[1_554] | 2.16 | 0.04 |
| 4:6:299:MET:CG | 4:9:136:ILE:C[1_554] | 2.16 | 0.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:219:VAL:CG2 | 4:8:300:SER:O[1_554] | 2.16 | 0.04 |
| 4:4:274:ILE:CD1 | 4:7:161:HIS:CA[1_554] | 2.16 | 0.04 |
| 4:4:207:GLU:CB | 4:7:67:LEU:CA[1_554] | 2.16 | 0.04 |
| 4:6:176:MET:CG | 4:9:173:HIS:O[1_554] | 2.16 | 0.04 |
| 4:6:369:ILE:CG2 | 4:V:231:ALA:C[1_554] | 2.16 | 0.04 |
| 4:5:329:ILE:CG2 | 4:8:139:VAL:O[1_554] | 2.16 | 0.04 |
| 4:6:305:MET:CG | 4:9:11:ASP:CG[1_554] | 2.16 | 0.04 |
| 4:6:310:ALA:C | 4:9:142:LEU:CA[1_554] | 2.16 | 0.04 |
| 4:5:319:ALA:C | 4:8:294:TYR:CA[1_554] | 2.16 | 0.04 |
| 4:5:199:SER:O | 4:8:207:GLU:N[1_554] | 2.16 | 0.04 |
| 4:3:368:SER:CA | 4:7:236:LEU:CA[1_554] | 2.16 | 0.04 |
| 4:4:341:ILE:CG1 | 4:7:121:GLN:N[1_554] | 2.16 | 0.04 |
| 4:4:149:THR:CG2 | 4:9:40:HIS:CD2[1_554] | 2.16 | 0.04 |
| 4:4:227:MET:CE | 4:7:306:TYR:CB[1_554] | 2.16 | 0.04 |
| 4:5:340:TRP:O | 4:8:120:THR:OG1[1_554] | 2.16 | 0.04 |
| 4:3:109:PRO:O | 4:7:192:ILE:CG2[1_554] | 2.16 | 0.04 |
| 4:6:219:VAL:C | 4:9:335:ARG:CG[1_554] | 2.16 | 0.04 |
| 4:4:142:LEU:N | 4:7:371:HIS:ND1[1_554] | 2.16 | 0.04 |
| 4:5:115:ASN:CG | 4:9:196:ARG:CG[1_554] | 2.16 | 0.04 |
| 4:6:195:GLU:O | 4:9:212:ILE:CG2[1_554] | 2.16 | 0.04 |
| 4:6:316:GLU:CA | 4:9:298:VAL:N[1_554] | 2.16 | 0.04 |
| 4:6:335:ARG:NH2 | 4:9:339:VAL:C[1_554] | 2.16 | 0.04 |
| 4:6:316:GLU:O | 4:9:296:ASN:C[1_554] | 2.16 | 0.04 |
| 4:5:199:SER:O | 4:8:206:ARG:CA[1_554] | 2.16 | 0.04 |
| 4:5:299:MET:CA | 4:8:136:ILE:N[1_554] | 2.16 | 0.04 |
| 4:6:318:THR:CA | 4:9:296:ASN:ND2[1_554] | 2.16 | 0.04 |
| 4:4:370:VAL:CA | 4:8:231:ALA:N[1_554] | 2.16 | 0.04 |
| 4:4:16:LEU:CA | 4:7:78:ASN:CA[1_554] | 2.16 | 0.04 |
| 4:4:144:ALA:O | 4:7:370:VAL:N[1_554] | 2.16 | 0.04 |
| 4:5:337:TYR:CB | 4:8:119:MET:CE[1_554] | 2.16 | 0.04 |
| 4:6:181:ALA:O | 4:9:159:VAL:CA[1_554] | 2.16 | 0.04 |
| 4:5:153:LEU:O | 4:8:136:ILE:CG2[1_554] | 2.16 | 0.04 |
| 4:3:173:HIS:CE1 | 4:7:265:SER:N[1_554] | 2.16 | 0.04 |
| 4:4:157:ASP:O | 4:7:73:HIS:CB[1_554] | 2.16 | 0.04 |
| 4:6:30:VAL:O | 4:9:82:MET:N[1_554] | 2.16 | 0.04 |
| 4:4:144:ALA:CA | 4:7:370:VAL:N[1_554] | 2.16 | 0.04 |
| 4:4:114:ALA:O | 4:8:250:ILE:C[1_554] | 2.16 | 0.04 |
| 4:5:110:LEU:C | 4:9:192:ILE:CB[1_554] | 2.16 | 0.04 |
| 4:4:17:VAL:O | 4:7:79:TRP:CG[1_554] | 2.16 | 0.04 |
| 4:6:289:ILE:CB | 4:W:63:GLY:O[1_554] | 2.16 | 0.04 |
| 4:5:337:TYR:CE2 | 4:8:86:TRP:NE1[1_554] | 2.16 | 0.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:109:PRO:O | 4:8:192:ILE:CG2[1_554] | 2.16 | 0.04 |
| 4:5:331:ALA:CB | 4:8:140:LEU:N[1_554] | 2.16 | 0.04 |
| 4:5:110:LEU:O | 4:9:193:LEU:N[1_554] | 2.16 | 0.04 |
| 4:6:253:GLU:OE2 | 4:9:214:GLU:N[1_554] | 2.16 | 0.04 |
| 4:5:315:LYS:CA | 4:8:298:VAL:CG2[1_554] | 2.16 | 0.04 |
| 4:5:144:ALA:CB | 4:8:370:VAL:O[1_554] | 2.16 | 0.04 |
| 4:4:262:PHE:CZ | 4:7:152:VAL:CG1[1_554] | 2.16 | 0.04 |
| 4:4:340:TRP:CH2 | 4:7:121:GLN:OE1[1_554] | 2.16 | 0.04 |
| 4:4:110:LEU:CD1 | 4:8:191:LYS:CD[1_554] | 2.16 | 0.04 |
| 4:6:252:ASN:CA | 4:9:214:GLU:O[1_554] | 2.16 | 0.04 |
| 4:6:305:MET:N | 4:9:11:ASP:OD1[1_554] | 2.16 | 0.04 |
| 4:6:29:ALA:N | 4:9:83:GLU:CD[1_554] | 2.16 | 0.04 |
| 4:6:266:PHE:C | 4:9:261:LEU:N[1_554] | 2.16 | 0.04 |
| 4:6:17:VAL:CA | 4:9:79:TRP:CD2[1_554] | 2.16 | 0.04 |
| 4:6:262:PHE:CA | 4:9:153:LEU:CB[1_554] | 2.16 | 0.04 |
| 4:3:111:ASN:OD1 | 4:7:196:ARG:CD[1_554] | 2.16 | 0.04 |
| 4:5:192:ILE:O | 4:8:213:LYS:CA[1_554] | 2.16 | 0.04 |
| 4:5:300:SER:CA | 4:8:107:GLU:C[1_554] | 2.16 | 0.04 |
| 4:6:190:MET:CA | 4:9:186:THR:CB[1_554] | 2.16 | 0.04 |
| 4:4:329:ILE:CG1 | 4:7:139:VAL:CG1[1_554] | 2.16 | 0.04 |
| 4:5:192:ILE:N | 4:8:185:LEU:O[1_554] | 2.16 | 0.04 |
| 4:6:164:PRO:CA | 4:9:172:PRO:CD[1_554] | 2.16 | 0.04 |
| 4:5:16:LEU:N | 4:8:76:ILE:C[1_554] | 2.16 | 0.04 |
| 4:5:31:PHE:O | 4:8:78:ASN:OD1[1_554] | 2.16 | 0.04 |
| 4:5:336:LYS:NZ | 4:8:10:CYS:SG[1_554] | 2.16 | 0.04 |
| 4:6:110:LEU:CA | 4:V:192:ILE:CG2[1_554] | 2.16 | 0.04 |
| 4:6:274:ILE:O | 4:9:163:VAL:CA[1_554] | 2.16 | 0.04 |
| 4:4:196:ARG:CZ | 4:7:211:ASP:OD2[1_554] | 2.16 | 0.04 |
| 4:6:312:ARG:O | 4:9:298:VAL:C[1_554] | 2.16 | 0.04 |
| 4:3:111:ASN:CB | 4:7:196:ARG:CG[1_554] | 2.16 | 0.04 |
| 4:5:219:VAL:CB | 4:8:300:SER:CB[1_554] | 2.16 | 0.04 |
| 4:6:180:LEU:CG | 4:9:178:LEU:CA[1_554] | 2.16 | 0.04 |
| 4:6:140:LEU:O | 4:9:370:VAL:O[1_554] | 2.16 | 0.04 |
| 4:5:280:ASN:ND2 | 4:8:282:ILE:C[1_554] | 2.16 | 0.04 |
| 4:6:260:THR:N | 4:9:155:SER:CB[1_554] | 2.16 | 0.04 |
| 4:5:292:ASP:CG | 4:V:64:ILE:CD1[1_554] | 2.16 | 0.04 |
| 4:5:195:GLU:C | 4:8:189:LEU:CG[1_554] | 2.16 | 0.04 |
| 4:4:309:ILE:C | 4:7:141:SER:N[1_554] | 2.16 | 0.04 |
| 4:6:274:ILE:CB | 4:9:162:ASN:CA[1_554] | 2.16 | 0.04 |
| 4:3:79:TRP:CZ2 | 4:7:249:THR:CB[1_554] | 2.16 | 0.04 |
| 4:6:76:ILE:CA | 4:V:197:GLY:O[1_554] | 2.16 | 0.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:173:HIS:ND1 | 4:V:266:PHE:C[1_554] | 2.17 | 0.03 |
| 4:6:317:ILE:CD1 | 4:9:150:GLY:O[1_554] | 2.17 | 0.03 |
| 4:4:16:LEU:N | 4:7:78:ASN:N[1_554] | 2.17 | 0.03 |
| 4:6:325:MET:SD | 4:9:166:TYR:CE2[1_554] | 2.17 | 0.03 |
| 4:5:335:ARG:CB | 4:8:106:THR:C[1_554] | 2.17 | 0.03 |
| 4:6:115:ASN:N | 4:V:196:ARG:NE[1_554] | 2.17 | 0.03 |
| 4:5:110:LEU:CD2 | 4:9:191:LYS:CD[1_554] | 2.17 | 0.03 |
| 4:4:315:LYS:NZ | 4:7:147:ARG:CZ[1_554] | 2.17 | 0.03 |
| 4:5:182:GLY:C | 4:8:158:GLY:CA[1_554] | 2.17 | 0.03 |
| 4:5:367:PRO:CB | 4:9:233:SER:CB[1_554] | 2.17 | 0.03 |
| 4:4:222:ASP:CA | 4:7:332:PRO:CA[1_554] | 2.17 | 0.03 |
| 4:4:172:PRO:N | 4:8:266:PHE:CA[1_554] | 2.17 | 0.03 |
| 4:5:144:ALA:N | 4:8:370:VAL:C[1_554] | 2.17 | 0.03 |
| 4:5:214:GLU:CB | 4:8:16:LEU:CB[1_554] | 2.17 | 0.03 |
| 4:6:250:ILE:CG2 | 4:9:214:GLU:OE2[1_554] | 2.17 | 0.03 |
| 4:3:75:ILE:CG1 | 4:7:198:TYR:CB[1_554] | 2.17 | 0.03 |
| 4:5:186:THR:N | 4:8:157:ASP:C[1_554] | 2.17 | 0.03 |
| 4:5:367:PRO:CG | 4:9:233:SER:C[1_554] | 2.17 | 0.03 |
| 4:4:115:ASN:ND2 | 4:8:249:THR:O[1_554] | 2.17 | 0.03 |
| 4:6:62:ARG:N | 4:9:66:THR:CG2[1_554] | 2.17 | 0.03 |
| 4:4:30:VAL:CG2 | 4:7:79:TRP:C[1_554] | 2.17 | 0.03 |
| 4:6:342:GLY:CA | 4:9:370:VAL:CB[1_554] | 2.17 | 0.03 |
| 4:5:201:VAL:CG2 | 4:8:202:THR:C[1_554] | 2.17 | 0.03 |
| 4:4:287:ILE:C | 4:9:63:GLY:O[1_554] | 2.17 | 0.03 |
| 4:6:335:ARG:CZ | 4:9:140:LEU:CD1[1_554] | 2.17 | 0.03 |
| 4:4:110:LEU:CD1 | 4:8:191:LYS:CA[1_554] | 2.17 | 0.03 |
| 4:6:161:HIS:C | 4:9:110:LEU:CD1[1_554] | 2.17 | 0.03 |
| 4:6:162:ASN:CA | 4:9:110:LEU:CD2[1_554] | 2.17 | 0.03 |
| 4:4:193:LEU:N | 4:7:186:THR:OG1[1_554] | 2.17 | 0.03 |
| 4:6:321:ALA:CA | 4:9:292:ASP:CA[1_554] | 2.17 | 0.03 |
| 4:4:205:GLU:OE1 | 4:7:62:ARG:CG[1_554] | 2.17 | 0.03 |
| 4:5:185:LEU:N | 4:8:158:GLY:O[1_554] | 2.17 | 0.03 |
| 4:4:144:ALA:CB | 4:7:370:VAL:C[1_554] | 2.17 | 0.03 |
| 4:5:151:ILE:CD1 | 4:8:171:LEU:O[1_554] | 2.17 | 0.03 |
| 4:6:143:TYR:CA | 4:9:372:ARG:N[1_554] | 2.17 | 0.03 |
| 4:6:288:ASP:OD1 | 4:W:62:ARG:O[1_554] | 2.17 | 0.03 |
| 4:4:294:TYR:CG | 4:7:166:TYR:O[1_554] | 2.17 | 0.03 |
| 4:5:164:PRO:CA | 4:8:169:TYR:OH[1_554] | 2.17 | 0.03 |
| 4:4:269:MET:O | 4:7:273:GLY:CA[1_554] | 2.17 | 0.03 |
| 4:3:173:HIS:CE1 | 4:7:265:SER:CA[1_554] | 2.17 | 0.03 |
| 4:6:341:ILE:CA | 4:9:120:THR:CG2[1_554] | 2.17 | 0.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:371:HIS:ND1 | 4:7:252:ASN:C[1_554] | 2.17 | 0.03 |
| 4:4:330:ILE:O | 4:7:136:ILE:N[1_554] | 2.17 | 0.03 |
| 4:4:222:ASP:CB | 4:7:332:PRO:CG[1_554] | 2.17 | 0.03 |
| 4:5:313:MET:CE | 4:8:163:VAL:C[1_554] | 2.17 | 0.03 |
| 4:6:256:ARG:O | 4:9:303:THR:CB[1_554] | 2.17 | 0.03 |
| 4:6:185:LEU:O | 4:9:183:ARG:N[1_554] | 2.17 | 0.03 |
| 4:6:275:HIS:CB | 4:9:151:ILE:CG1[1_554] | 2.17 | 0.03 |
| 4:5:28:ARG:O | 4:8:83:GLU:CG[1_554] | 2.17 | 0.03 |
| 4:5:253:GLU:OE1 | 4:8:214:GLU:C[1_554] | 2.17 | 0.03 |
| 4:6:113:LYS:C | 4:V:252:ASN:CA[1_554] | 2.17 | 0.03 |
| 4:6:327:ILE:N | 4:9:167:GLU:OE2[1_554] | 2.17 | 0.03 |
| 4:5:113:LYS:CE | 4:9:255:PHE:N[1_554] | 2.17 | 0.03 |
| 4:6:21:PHE:C | 4:9:125:GLU:OE2[1_554] | 2.17 | 0.03 |
| 4:6:154:ASP:CB | 4:9:109:PRO:O[1_554] | 2.17 | 0.03 |
| 4:5:14:SER:C | 4:8:77:THR:CG2[1_554] | 2.17 | 0.03 |
| 4:5:153:LEU:O | 4:8:109:PRO:CA[1_554] | 2.17 | 0.03 |
| 4:5:15:GLY:C | 4:8:78:ASN:N[1_554] | 2.17 | 0.03 |
| 4:4:187:ASP:C | 4:7:184:ASP:N[1_554] | 2.17 | 0.03 |
| 4:4:274:ILE:CG2 | 4:7:163:VAL:CG2[1_554] | 2.17 | 0.03 |
| 4:3:110:LEU:CD1 | 4:7:191:LYS:CA[1_554] | 2.17 | 0.03 |
| 4:5:185:LEU:CA | 4:8:158:GLY:CA[1_554] | 2.17 | 0.03 |
| 4:4:74:GLY:C | 4:8:197:GLY:N[1_554] | 2.17 | 0.03 |
| 4:4:181:ALA:O | 4:7:158:GLY:O[1_554] | 2.17 | 0.03 |
| 4:4:243:PRO:CB | 4:7:61:LYS:C[1_554] | 2.17 | 0.03 |
| 4:4:184:ASP:O | 4:7:184:ASP:OD1[1_554] | 2.17 | 0.03 |
| 4:4:186:THR:CG2 | 4:7:183:ARG:CZ[1_554] | 2.17 | 0.03 |
| 4:3:110:LEU:N | 4:7:192:ILE:C[1_554] | 2.17 | 0.03 |
| 4:5:367:PRO:C | 4:9:233:SER:N[1_554] | 2.17 | 0.03 |
| 4:6:223:PHE:O | 4:9:309:ILE:CG2[1_554] | 2.17 | 0.03 |
| 4:4:184:ASP:CB | 4:7:158:GLY:O[1_554] | 2.17 | 0.03 |
| 4:4:192:ILE:O | 4:7:213:LYS:CB[1_554] | 2.17 | 0.03 |
| 4:5:349:LEU:C | 4:8:365:ALA:CA[1_554] | 2.17 | 0.03 |
| 4:6:305:MET:C | 4:9:11:ASP:CG[1_554] | 2.17 | 0.03 |
| 4:6:369:ILE:O | 4:V:228:ALA:C[1_554] | 2.17 | 0.03 |
| 4:5:327:ILE:CG1 | 4:8:149:THR:N[1_554] | 2.17 | 0.03 |
| 4:4:149:THR:CG2 | 4:9:40:HIS:CG[1_554] | 2.17 | 0.03 |
| 4:4:265:SER:C | 4:7:261:LEU:CB[1_554] | 2.17 | 0.03 |
| 4:5:222:ASP:N | 4:8:331:ALA:O[1_554] | 2.17 | 0.03 |
| 4:6:136:ILE:N | 4:9:113:LYS:NZ[1_554] | 2.17 | 0.03 |
| 4:4:143:TYR:CD2 | 4:7:368:SER:CB[1_554] | 2.17 | 0.03 |
| 4:6:161:HIS:N | 4:9:110:LEU:CG[1_554] | 2.17 | 0.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:221:LEU:O | 4:7:332:PRO:CA[1_554] | 2.17 | 0.03 |
| 4:5:317:ILE:CA | 4:8:150:GLY:O[1_554] | 2.17 | 0.03 |
| 4:5:173:HIS:CA | 4:9:267:ILE:C[1_554] | 2.17 | 0.03 |
| 4:3:291:LYS:NZ | 4:8:64:ILE:C[1_554] | 2.17 | 0.03 |
| 4:4:313:MET:CB | 4:7:139:VAL:N[1_554] | 2.17 | 0.03 |
| 4:6:266:PHE:N | 4:9:261:LEU:N[1_554] | 2.17 | 0.03 |
| 4:4:345:ILE:CG2 | 4:7:369:ILE:N[1_554] | 2.17 | 0.03 |
| 4:5:328:LYS:CB | 4:8:148:THR:CG2[1_554] | 2.17 | 0.03 |
| 4:3:76:ILE:O | 4:7:198:TYR:CZ[1_554] | 2.17 | 0.03 |
| 4:5:339:VAL:CA | 4:8:116:ARG:C[1_554] | 2.17 | 0.03 |
| 4:6:224:GLU:N | 4:9:310:ALA:CB[1_554] | 2.17 | 0.03 |
| 4:5:258:PRO:CG | 4:8:155:SER:O[1_554] | 2.17 | 0.03 |
| 4:5:369:ILE:C | 4:9:231:ALA:N[1_554] | 2.17 | 0.03 |
| 4:4:332:PRO:CG | 4:7:134:VAL:CA[1_554] | 2.17 | 0.03 |
| 4:4:261:LEU:CB | 4:7:154:ASP:C[1_554] | 2.17 | 0.03 |
| 4:6:32:PRO:O | 4:9:78:ASN:CB[1_554] | 2.17 | 0.03 |
| 4:5:173:HIS:CB | 4:9:267:ILE:C[1_554] | 2.17 | 0.03 |
| 4:6:25:ASP:CA | 4:9:129:VAL:CG2[1_554] | 2.17 | 0.03 |
| 4:6:75:ILE:CG2 | 4:V:198:TYR:CD2[1_554] | 2.17 | 0.03 |
| 4:5:221:LEU:N | 4:8:332:PRO:N[1_554] | 2.17 | 0.03 |
| 4:6:24:ASP:CB | 4:9:125:GLU:CA[1_554] | 2.17 | 0.03 |
| 4:6:280:ASN:CG | 4:9:280:ASN:O[1_554] | 2.17 | 0.03 |
| 4:4:179:ASP:O | 4:7:179:ASP:OD2[1_554] | 2.17 | 0.03 |
| 4:4:367:PRO:C | 4:8:236:LEU:CG[1_554] | 2.17 | 0.03 |
| 4:6:258:PRO:N | 4:9:303:THR:CB[1_554] | 2.17 | 0.03 |
| 4:6:266:PHE:CB | 4:9:261:LEU:CA[1_554] | 2.17 | 0.03 |
| 4:6:342:GLY:CA | 4:9:371:HIS:N[1_554] | 2.17 | 0.03 |
| 4:5:113:LYS:C | 4:9:253:GLU:OE2[1_554] | 2.17 | 0.03 |
| 4:4:143:TYR:CA | 4:7:371:HIS:C[1_554] | 2.17 | 0.03 |
| 4:6:110:LEU:CA | 4:V:192:ILE:CA[1_554] | 2.17 | 0.03 |
| 4:6:25:ASP:OD2 | 4:9:130:PRO:N[1_554] | 2.17 | 0.03 |
| 4:6:304:THR:CG2 | 4:9:137:GLN:CB[1_554] | 2.17 | 0.03 |
| 4:4:345:ILE:C | 4:7:366:GLY:C[1_554] | 2.17 | 0.03 |
| 4:6:190:MET:CB | 4:9:187:ASP:OD1[1_554] | 2.17 | 0.03 |
| 4:6:24:ASP:N | 4:9:124:PHE:C[1_554] | 2.17 | 0.03 |
| 4:5:319:ALA:C | 4:8:293:LEU:O[1_554] | 2.17 | 0.03 |
| 4:4:222:ASP:CB | 4:7:331:ALA:O[1_554] | 2.17 | 0.03 |
| 4:4:218:TYR:CZ | 4:7:337:TYR:CG[1_554] | 2.17 | 0.03 |
| 4:4:217:CYS:N | 4:7:16:LEU:CB[1_554] | 2.17 | 0.03 |
| 4:6:151:ILE:CG1 | 4:9:172:PRO:CD[1_554] | 2.17 | 0.03 |
| 4:5:222:ASP:CB | 4:8:331:ALA:O[1_554] | 2.17 | 0.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:116:ARG:CA | 4:8:196:ARG:NH2[1_554] | 2.17 | 0.03 |
| 4:6:318:THR:CG2 | 4:9:149:THR:O[1_554] | 2.17 | 0.03 |
| 4:5:276:GLU:OE2 | 4:8:279:TYR:CA[1_554] | 2.17 | 0.03 |
| 4:4:31:PHE:CA | 4:7:78:ASN:ND2[1_554] | 2.17 | 0.03 |
| 4:4:327:ILE:CG2 | 4:7:148:THR:CA[1_554] | 2.17 | 0.03 |
| 4:6:150:GLY:C | 4:9:169:TYR:CG[1_554] | 2.17 | 0.03 |
| 4:4:292:ASP:OD2 | 4:9:40:HIS:N[1_554] | 2.17 | 0.03 |
| 4:6:343:GLY:O | 4:9:367:PRO:CG[1_554] | 2.17 | 0.03 |
| 4:6:75:ILE:C | 4:V:198:TYR:N[1_554] | 2.17 | 0.03 |
| 4:3:108:ALA:C | 4:7:195:GLU:C[1_554] | 2.17 | 0.03 |
| 4:6:293:LEU:O | 4:9:166:TYR:O[1_554] | 2.17 | 0.03 |
| 4:6:18:LYS:CA | 4:9:79:TRP:CZ3[1_554] | 2.17 | 0.03 |
| 4:6:294:TYR:O | 4:9:166:TYR:O[1_554] | 2.17 | 0.03 |
| 4:6:329:ILE:O | 4:9:143:TYR:CB[1_554] | 2.17 | 0.03 |
| 4:6:26:ALA:N | 4:9:123:MET:O[1_554] | 2.17 | 0.03 |
| 4:4:285:CYS:N | 4:8:268:GLY:O[1_554] | 2.17 | 0.03 |
| 4:4:113:LYS:C | 4:8:251:GLY:C[1_554] | 2.17 | 0.03 |
| 4:6:179:ASP:O | 4:9:179:ASP:OD1[1_554] | 2.17 | 0.03 |
| 4:4:140:LEU:N | 4:7:371:HIS:CE1[1_554] | 2.17 | 0.03 |
| 4:4:110:LEU:CG | 4:8:191:LYS:CD[1_554] | 2.17 | 0.03 |
| 4:5:199:SER:C | 4:8:206:ARG:CG[1_554] | 2.18 | 0.02 |
| 4:6:331:ALA:CB | 4:9:140:LEU:N[1_554] | 2.18 | 0.02 |
| 4:6:368:SER:CA | 4:V:230:ALA:N[1_554] | 2.18 | 0.02 |
| 4:2:325:MET:O | 4:7:43:VAL:O[1_554] | 2.18 | 0.02 |
| 4:6:160:THR:CB | 4:9:161:HIS:CE1[1_554] | 2.18 | 0.02 |
| 4:5:257:CYS:C | 4:8:303:THR:N[1_554] | 2.18 | 0.02 |
| 4:4:173:HIS:C | 4:8:267:ILE:N[1_554] | 2.18 | 0.02 |
| 4:5:213:LYS:C | 4:8:16:LEU:CG[1_554] | 2.18 | 0.02 |
| 4:6:151:ILE:C | 4:9:170:ALA:O[1_554] | 2.18 | 0.02 |
| 4:5:178:LEU:CD1 | 4:8:177:ARG:N[1_554] | 2.18 | 0.02 |
| 4:6:370:VAL:CB | 4:V:231:ALA:CB[1_554] | 2.18 | 0.02 |
| 4:6:23:GLY:C | 4:9:124:PHE:CB[1_554] | 2.18 | 0.02 |
| 4:5:166:TYR:CD2 | 4:V:40:HIS:CG[1_554] | 2.18 | 0.02 |
| 4:4:215:LYS:NZ | 4:7:31:PHE:CD2[1_554] | 2.18 | 0.02 |
| 4:6:110:LEU:CD1 | 4:V:191:LYS:CE[1_554] | 2.18 | 0.02 |
| 4:4:269:MET:CB | 4:7:178:LEU:CD2[1_554] | 2.18 | 0.02 |
| 4:5:162:ASN:C | 4:8:172:PRO:CA[1_554] | 2.18 | 0.02 |
| 4:4:320:LEU:CA | 4:7:292:ASP:C[1_554] | 2.18 | 0.02 |
| 4:6:24:ASP:OD2 | 4:9:125:GLU:O[1_554] | 2.18 | 0.02 |
| 4:6:332:PRO:C | 4:9:104:LEU:CG[1_554] | 2.18 | 0.02 |
| 4:4:317:ILE:C | 4:7:150:GLY:O[1_554] | 2.18 | 0.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:262:PHE:CA | 4:7:153:LEU:C[1_554] | 2.18 | 0.02 |
| 4:4:25:ASP:CA | 4:7:124:PHE:CB[1_554] | 2.18 | 0.02 |
| 4:5:204:ALA:O | 4:8:62:ARG:NE[1_554] | 2.18 | 0.02 |
| 4:6:32:PRO:CA | 4:9:78:ASN:ND2[1_554] | 2.18 | 0.02 |
| 4:5:164:PRO:CG | 4:8:172:PRO:CD[1_554] | 2.18 | 0.02 |
| 4:4:313:MET:CB | 4:7:138:ALA:CA[1_554] | 2.18 | 0.02 |
| 4:4:357:ILE:CB | 4:8:232:SER:O[1_554] | 2.18 | 0.02 |
| 4:4:193:LEU:N | 4:7:210:ARG:CB[1_554] | 2.18 | 0.02 |
| 4:5:140:LEU:CA | 4:8:371:HIS:O[1_554] | 2.18 | 0.02 |
| 4:6:188:TYR:CD1 | 4:9:185:LEU:N[1_554] | 2.18 | 0.02 |
| 4:6:140:LEU:O | 4:9:371:HIS:CA[1_554] | 2.18 | 0.02 |
| 4:6:199:SER:CA | 4:9:206:ARG:CB[1_554] | 2.18 | 0.02 |
| 4:5:341:ILE:CB | 4:8:120:THR:OG1[1_554] | 2.18 | 0.02 |
| 4:6:24:ASP:CA | 4:9:125:GLU:N[1_554] | 2.18 | 0.02 |
| 4:5:31:PHE:CD2 | 4:8:80:ASP:CB[1_554] | 2.18 | 0.02 |
| 4:4:180:LEU:CD2 | 4:7:178:LEU:CB[1_554] | 2.18 | 0.02 |
| 4:5:322:PRO:CG | 4:8:289:ILE:CA[1_554] | 2.18 | 0.02 |
| 4:6:178:LEU:O | 4:9:177:ARG:NE[1_554] | 2.18 | 0.02 |
| 4:4:154:ASP:CA | 4:7:110:LEU:CA[1_554] | 2.18 | 0.02 |
| 4:4:264:PRO:O | 4:7:178:LEU:CD2[1_554] | 2.18 | 0.02 |
| 4:5:345:ILE:CG2 | 4:8:369:ILE:CA[1_554] | 2.18 | 0.02 |
| 4:6:200:PHE:N | 4:9:206:ARG:CD[1_554] | 2.18 | 0.02 |
| 4:5:294:TYR:C | 4:8:166:TYR:CA[1_554] | 2.18 | 0.02 |
| 4:4:240:TYR:CD1 | 4:7:56:ASP:OD2[1_554] | 2.18 | 0.02 |
| 4:4:161:HIS:O | 4:7:110:LEU:N[1_554] | 2.18 | 0.02 |
| 4:3:290:ARG:C | 4:8:64:ILE:CG2[1_554] | 2.18 | 0.02 |
| 4:4:243:PRO:C | 4:7:60:SER:CB[1_554] | 2.18 | 0.02 |
| 4:6:346:LEU:CG | 4:9:368:SER:C[1_554] | 2.18 | 0.02 |
| 4:6:312:ARG:C | 4:9:298:VAL:CA[1_554] | 2.18 | 0.02 |
| 4:4:294:TYR:CB | 4:7:166:TYR:C[1_554] | 2.18 | 0.02 |
| 4:4:186:THR:CG2 | 4:7:183:ARG:NE[1_554] | 2.18 | 0.02 |
| 4:4:291:LYS:NZ | 4:9:64:ILE:C[1_554] | 2.18 | 0.02 |
| 4:6:322:PRO:C | 4:9:292:ASP:OD1[1_554] | 2.18 | 0.02 |
| 4:5:334:GLU:CG | 4:8:133:TYR:O[1_554] | 2.18 | 0.02 |
| 4:4:320:LEU:N | 4:7:292:ASP:C[1_554] | 2.18 | 0.02 |
| 1:A:542:PHE:CE2 | 4:5:328:LYS:CE[1_556] | 2.18 | 0.02 |
| 4:6:280:ASN:ND2 | 4:9:282:ILE:N[1_554] | 2.18 | 0.02 |
| 4:3:172:PRO:CA | 4:7:188:TYR:CE1[1_554] | 2.18 | 0.02 |
| 4:6:73:HIS:CD2 | 4:V:199:SER:OG[1_554] | 2.18 | 0.02 |
| 4:6:143:TYR:CD2 | 4:9:369:ILE:C[1_554] | 2.18 | 0.02 |
| 4:5:151:ILE:C | 4:8:170:ALA:O[1_554] | 2.18 | 0.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:179:ASP:O | 4:9:179:ASP:CB[1_554] | 2.18 | 0.02 |
| 4:5:271:SER:O | 4:8:277:THR:CB[1_554] | 2.18 | 0.02 |
| 1:A:637:LYS:CD | 4:5:311:ASP:OD2[1_556] | 2.18 | 0.02 |
| 1:D:636:LYS:O | 4:6:311:ASP:OD2[1_556] | 2.18 | 0.02 |
| 4:4:112:PRO:C | 4:8:250:ILE:CG2[1_554] | 2.18 | 0.02 |
| 4:5:265:SER:CA | 4:8:261:LEU:C[1_554] | 2.18 | 0.02 |
| 4:4:327:ILE:N | 4:7:167:GLU:CB[1_554] | 2.18 | 0.02 |
| 4:6:188:TYR:CD2 | 4:9:181:ALA:C[1_554] | 2.18 | 0.02 |
| 4:5:218:TYR:CG | 4:8:336:LYS:CD[1_554] | 2.18 | 0.02 |
| 4:5:75:ILE:CG2 | 4:9:198:TYR:CG[1_554] | 2.18 | 0.02 |
| 4:6:257:CYS:SG | 4:9:156:GLY:O[1_554] | 2.18 | 0.02 |
| 4:5:271:SER:N | 4:8:272:ALA:N[1_554] | 2.18 | 0.02 |
| 4:5:15:GLY:C | 4:8:70:PRO:O[1_554] | 2.18 | 0.02 |
| 4:5:141:SER:CA | 4:8:116:ARG:NH1[1_554] | 2.18 | 0.02 |
| 4:6:16:LEU:CD2 | 4:9:71:ILE:CG1[1_554] | 2.18 | 0.02 |
| 4:6:219:VAL:CB | 4:9:300:SER:CB[1_554] | 2.18 | 0.02 |
| 4:4:18:LYS:CD | 4:7:79:TRP:CE3[1_554] | 2.18 | 0.02 |
| 4:4:271:SER:C | 4:7:277:THR:CG2[1_554] | 2.18 | 0.02 |
| 4:6:194:THR:N | 4:9:209:VAL:CB[1_554] | 2.18 | 0.02 |
| 4:6:327:ILE:CA | 4:9:148:THR:O[1_554] | 2.18 | 0.02 |
| 4:6:261:LEU:CD1 | 4:9:154:ASP:C[1_554] | 2.18 | 0.02 |
| 4:6:348:SER:N | 4:9:366:GLY:C[1_554] | 2.18 | 0.02 |
| 4:6:304:THR:OG1 | 4:9:137:GLN:CA[1_554] | 2.18 | 0.02 |
| 4:4:198:TYR:N | 4:7:208:ILE:CA[1_554] | 2.18 | 0.02 |
| 4:6:207:GLU:CB | 4:9:67:LEU:CG[1_554] | 2.18 | 0.02 |
| 4:5:300:SER:CB | 4:8:107:GLU:OE2[1_554] | 2.18 | 0.02 |
| 4:5:24:ASP:OD2 | 4:8:125:GLU:O[1_554] | 2.18 | 0.02 |
| 4:5:290:ARG:NE | 4:8:286:ASP:OD1[1_554] | 2.18 | 0.02 |
| 4:5:215:LYS:CB | 4:8:30:VAL:C[1_554] | 2.18 | 0.02 |
| 4:4:367:PRO:CA | 4:8:235:SER:C[1_554] | 2.18 | 0.02 |
| 4:5:335:ARG:NH1 | 4:8:106:THR:CG2[1_554] | 2.18 | 0.02 |
| 4:5:305:MET:CG | 4:8:106:THR:OG1[1_554] | 2.18 | 0.02 |
| 4:5:328:LYS:N | 4:8:148:THR:CA[1_554] | 2.18 | 0.02 |
| 4:5:212:ILE:O | 4:8:16:LEU:CD1[1_554] | 2.18 | 0.02 |
| 4:5:214:GLU:N | 4:8:16:LEU:CD2[1_554] | 2.18 | 0.02 |
| 4:4:309:ILE:O | 4:7:141:SER:CB[1_554] | 2.18 | 0.02 |
| 4:5:299:MET:N | 4:8:136:ILE:N[1_554] | 2.18 | 0.02 |
| 4:6:299:MET:N | 4:9:136:ILE:N[1_554] | 2.18 | 0.02 |
| 4:6:316:GLU:CA | 4:9:297:ASN:N[1_554] | 2.18 | 0.02 |
| 4:5:196:ARG:N | 4:8:189:LEU:CD2[1_554] | 2.18 | 0.02 |
| 4:5:331:ALA:CB | 4:8:140:LEU:CD1[1_554] | 2.18 | 0.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:344:SER:C | 4:7:367:PRO:N[1_554] | 2.18 | 0.02 |
| 4:5:75:ILE:CD1 | 4:9:195:GLU:N[1_554] | 2.18 | 0.02 |
| 4:3:286:ASP:CG | 4:7:270:GLU:OE1[1_554] | 2.18 | 0.02 |
| 4:3:368:SER:O | 4:7:236:LEU:CD1[1_554] | 2.18 | 0.02 |
| 4:3:120:THR:CG2 | 4:7:233:SER:CB[1_554] | 2.18 | 0.02 |
| 4:3:370:VAL:O | 4:7:231:ALA:N[1_554] | 2.18 | 0.02 |
| 4:4:191:LYS:C | 4:7:186:THR:N[1_554] | 2.18 | 0.02 |
| 4:4:327:ILE:CD1 | 4:7:166:TYR:C[1_554] | 2.18 | 0.02 |
| 4:5:256:ARG:C | 4:8:303:THR:CB[1_554] | 2.18 | 0.02 |
| 4:3:117:GLU:CG | 4:7:236:LEU:O[1_554] | 2.18 | 0.02 |
| 4:5:306:TYR:O | 4:8:339:VAL:CG2[1_554] | 2.18 | 0.02 |
| 4:4:336:LYS:O | 4:7:76:ILE:CD1[1_554] | 2.18 | 0.02 |
| 4:5:143:TYR:N | 4:8:372:ARG:CA[1_554] | 2.18 | 0.02 |
| 4:4:368:SER:CA | 4:8:236:LEU:CA[1_554] | 2.18 | 0.02 |
| 4:5:334:GLU:CG | 4:8:104:LEU:CA[1_554] | 2.18 | 0.02 |
| 4:3:291:LYS:CE | 4:8:64:ILE:O[1_554] | 2.18 | 0.02 |
| 4:6:180:LEU:CD1 | 4:9:160:THR:CB[1_554] | 2.18 | 0.02 |
| 4:6:257:CYS:O | 4:9:303:THR:OG1[1_554] | 2.18 | 0.02 |
| 4:6:337:TYR:CE2 | 4:9:86:TRP:CZ2[1_554] | 2.18 | 0.02 |
| 4:5:320:LEU:CA | 4:8:293:LEU:CB[1_554] | 2.18 | 0.02 |
| 4:4:219:VAL:O | 4:7:338:SER:CA[1_554] | 2.18 | 0.02 |
| 4:4:339:VAL:CG2 | 4:7:116:ARG:N[1_554] | 2.18 | 0.02 |
| 4:5:282:ILE:N | 4:8:173:HIS:NE2[1_554] | 2.18 | 0.02 |
| 4:5:275:HIS:CE1 | 4:8:278:THR:OG1[1_554] | 2.18 | 0.02 |
| 4:4:242:LEU:C | 4:7:60:SER:OG[1_554] | 2.18 | 0.02 |
| 4:4:220:ALA:O | 4:7:300:SER:CA[1_554] | 2.18 | 0.02 |
| 4:5:316:GLU:CG | 4:8:151:ILE:O[1_554] | 2.18 | 0.02 |
| 4:6:330:ILE:O | 4:9:139:VAL:CB[1_554] | 2.18 | 0.02 |
| 4:5:370:VAL:CB | 4:9:231:ALA:CB[1_554] | 2.18 | 0.02 |
| 4:4:294:TYR:CE1 | 4:7:166:TYR:CA[1_554] | 2.18 | 0.02 |
| 4:6:190:MET:SD | 4:9:206:ARG:CZ[1_554] | 2.18 | 0.02 |
| 4:5:31:PHE:CA | 4:8:80:ASP:N[1_554] | 2.18 | 0.02 |
| 4:6:283:MET:SD | 4:9:289:ILE:CG1[1_554] | 2.18 | 0.02 |
| 4:6:280:ASN:CG | 4:9:281:SER:CA[1_554] | 2.18 | 0.02 |
| 4:5:322:PRO:O | 4:8:292:ASP:OD1[1_554] | 2.18 | 0.02 |
| 4:5:157:ASP:N | 4:8:72:GLU:O[1_554] | 2.18 | 0.02 |
| 4:6:113:LYS:CA | 4:V:252:ASN:CA[1_554] | 2.18 | 0.02 |
| 4:4:211:ASP:CB | 4:7:32:PRO:C[1_554] | 2.18 | 0.02 |
| 4:5:348:SER:N | 4:8:366:GLY:C[1_554] | 2.18 | 0.02 |
| 4:6:266:PHE:CE1 | 4:9:261:LEU:CD1[1_554] | 2.18 | 0.02 |
| 4:4:269:MET:SD | 4:7:178:LEU:CD1[1_554] | 2.18 | 0.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:219:VAL:CG1 | 4:8:300:SER:O[1_554] | 2.18 | 0.02 |
| 4:4:31:PHE:O | 4:7:78:ASN:CG[1_554] | 2.18 | 0.02 |
| 4:4:264:PRO:N | 4:7:274:ILE:CG1[1_554] | 2.18 | 0.02 |
| 4:6:157:ASP:CA | 4:9:74:GLY:N[1_554] | 2.18 | 0.02 |
| 4:4:188:TYR:CE1 | 4:7:185:LEU:CD1[1_554] | 2.18 | 0.02 |
| 4:6:25:ASP:CB | 4:9:129:VAL:CB[1_554] | 2.19 | 0.01 |
| 4:4:312:ARG:CD | 4:7:300:SER:N[1_554] | 2.19 | 0.01 |
| 4:5:154:ASP:CA | 4:8:109:PRO:O[1_554] | 2.19 | 0.01 |
| 4:6:117:GLU:CD | 4:V:236:LEU:CD1[1_554] | 2.19 | 0.01 |
| 4:4:157:ASP:C | 4:7:72:GLU:C[1_554] | 2.19 | 0.01 |
| 4:4:267:ILE:CD1 | 4:7:180:LEU:O[1_554] | 2.19 | 0.01 |
| 4:5:16:LEU:CA | 4:8:77:THR:N[1_554] | 2.19 | 0.01 |
| 4:4:299:MET:CB | 4:7:136:ILE:C[1_554] | 2.19 | 0.01 |
| 1:D:410:ASN:ND2 | 4:6:218:TYR:CD2[1_556] | 2.19 | 0.01 |
| 4:6:255:PHE:CA | 4:9:305:MET:CB[1_554] | 2.19 | 0.01 |
| 4:4:313:MET:N | 4:7:142:LEU:N[1_554] | 2.19 | 0.01 |
| 4:6:113:LYS:CD | 4:V:252:ASN:C[1_554] | 2.19 | 0.01 |
| 4:4:188:TYR:CD2 | 4:7:181:ALA:O[1_554] | 2.19 | 0.01 |
| 4:4:218:TYR:CE2 | 4:7:337:TYR:CZ[1_554] | 2.19 | 0.01 |
| 4:6:316:GLU:CA | 4:9:151:ILE:O[1_554] | 2.19 | 0.01 |
| 4:4:116:ARG:N | 4:8:196:ARG:NH1[1_554] | 2.19 | 0.01 |
| 4:4:335:ARG:NE | 4:7:106:THR:CG2[1_554] | 2.19 | 0.01 |
| 4:5:347:ALA:O | 4:8:366:GLY:CA[1_554] | 2.19 | 0.01 |
| 4:6:328:LYS:CA | 4:9:148:THR:CB[1_554] | 2.19 | 0.01 |
| 4:5:191:LYS:CD | 4:8:185:LEU:C[1_554] | 2.19 | 0.01 |
| 4:5:326:LYS:C | 4:8:149:THR:OG1[1_554] | 2.19 | 0.01 |
| 4:5:290:ARG:CZ | 4:8:286:ASP:CG[1_554] | 2.19 | 0.01 |
| 4:6:155:SER:OG | 4:9:161:HIS:ND1[1_554] | 2.19 | 0.01 |
| 4:6:260:THR:O | 4:9:160:THR:OG1[1_554] | 2.19 | 0.01 |
| 4:5:316:GLU:C | 4:8:296:ASN:C[1_554] | 2.19 | 0.01 |
| 4:6:333:PRO:N | 4:9:104:LEU:CD1[1_554] | 2.19 | 0.01 |
| 4:6:141:SER:CB | 4:9:116:ARG:NH2[1_554] | 2.19 | 0.01 |
| 4:4:308:GLY:O | 4:7:338:SER:C[1_554] | 2.19 | 0.01 |
| 4:5:204:ALA:N | 4:8:62:ARG:CG[1_554] | 2.19 | 0.01 |
| 4:4:267:ILE:CG1 | 4:7:180:LEU:CD1[1_554] | 2.19 | 0.01 |
| 4:6:191:LYS:O | 4:9:186:THR:CA[1_554] | 2.19 | 0.01 |
| 1:A:411:GLU:OE1 | 4:5:226:GLU:OE2[1_556] | 2.19 | 0.01 |
| 4:5:349:LEU:C | 4:8:364:GLU:C[1_554] | 2.19 | 0.01 |
| 4:3:116:ARG:CG | 4:7:252:ASN:ND2[1_554] | 2.19 | 0.01 |
| 4:6:348:SER:O | 4:9:364:GLU:N[1_554] | 2.19 | 0.01 |
| 4:6:59:GLN:CG | 4:9:68:LYS:CA[1_554] | 2.19 | 0.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:6:276:GLU:OE2 | 4:9:279:TYR:CA[1_554] | 2.19 | 0.01 |
| 4:5:60:SER:OG | 4:8:37:ARG:CB[1_554] | 2.19 | 0.01 |
| 4:6:223:PHE:CG | 4:9:335:ARG:NE[1_554] | 2.19 | 0.01 |
| 4:4:108:ALA:C | 4:8:195:GLU:C[1_554] | 2.19 | 0.01 |
| 4:4:119:MET:N | 4:8:237:GLU:OE1[1_554] | 2.19 | 0.01 |
| 4:6:268:GLY:O | 4:9:269:MET:CB[1_554] | 2.19 | 0.01 |
| 4:5:319:ALA:O | 4:8:294:TYR:CB[1_554] | 2.19 | 0.01 |
| 4:4:157:ASP:CB | 4:7:72:GLU:O[1_554] | 2.19 | 0.01 |
| 4:4:255:PHE:CB | 4:7:336:LYS:CB[1_554] | 2.19 | 0.01 |
| 4:6:315:LYS:NZ | 4:9:295:ALA:O[1_554] | 2.19 | 0.01 |
| 4:4:275:HIS:CG | 4:7:152:VAL:C[1_554] | 2.19 | 0.01 |
| 4:5:250:ILE:CB | 4:8:214:GLU:CD[1_554] | 2.19 | 0.01 |
| 4:6:281:SER:O | 4:9:173:HIS:CG[1_554] | 2.19 | 0.01 |
| 4:2:292:ASP:CA | 4:7:40:HIS:NE2[1_554] | 2.19 | 0.01 |
| 4:6:256:ARG:O | 4:9:303:THR:C[1_554] | 2.19 | 0.01 |
| 4:5:174:ALA:O | 4:8:173:HIS:CG[1_554] | 2.19 | 0.01 |
| 4:4:264:PRO:CB | 4:7:178:LEU:CB[1_554] | 2.19 | 0.01 |
| 4:5:173:HIS:CA | 4:9:266:PHE:O[1_554] | 2.19 | 0.01 |
| 4:5:346:LEU:N | 4:8:369:ILE:CG2[1_554] | 2.19 | 0.01 |
| 4:4:328:LYS:O | 4:7:168:GLY:C[1_554] | 2.19 | 0.01 |
| 4:3:149:THR:CG2 | 4:8:40:HIS:CG[1_554] | 2.19 | 0.01 |
| 4:3:357:ILE:CG1 | 4:7:232:SER:C[1_554] | 2.19 | 0.01 |
| 4:4:327:ILE:CG1 | 4:7:149:THR:OG1[1_554] | 2.19 | 0.01 |
| 4:6:199:SER:O | 4:9:206:ARG:CA[1_554] | 2.19 | 0.01 |
| 4:6:369:ILE:O | 4:V:231:ALA:CB[1_554] | 2.19 | 0.01 |
| 4:5:191:LYS:CG | 4:8:186:THR:N[1_554] | 2.19 | 0.01 |
| 4:4:224:GLU:N | 4:7:335:ARG:NH2[1_554] | 2.19 | 0.01 |
| 4:6:30:VAL:CB | 4:9:82:MET:CA[1_554] | 2.19 | 0.01 |
| 4:6:227:MET:CA | 4:9:307:PRO:N[1_554] | 2.19 | 0.01 |
| 4:6:186:THR:CA | 4:9:183:ARG:CB[1_554] | 2.19 | 0.01 |
| 4:4:208:ILE:N | 4:7:59:GLN:NE2[1_554] | 2.19 | 0.01 |
| 4:5:29:ALA:N | 4:8:83:GLU:CD[1_554] | 2.19 | 0.01 |
| 4:4:115:ASN:OD1 | 4:8:250:ILE:CD1[1_554] | 2.19 | 0.01 |
| 4:4:114:ALA:C | 4:8:251:GLY:N[1_554] | 2.19 | 0.01 |
| 4:4:157:ASP:CB | 4:7:72:GLU:CB[1_554] | 2.19 | 0.01 |
| 4:4:367:PRO:CA | 4:8:235:SER:CA[1_554] | 2.19 | 0.01 |
| 4:6:28:ARG:CZ | 4:9:126:THR:CA[1_554] | 2.19 | 0.01 |
| 4:5:208:ILE:N | 4:8:59:GLN:OE1[1_554] | 2.19 | 0.01 |
| 4:3:173:HIS:CG | 4:7:267:ILE:CG1[1_554] | 2.19 | 0.01 |
| 4:3:284:LYS:C | 4:7:268:GLY:CA[1_554] | 2.19 | 0.01 |
| 4:5:334:GLU:C | 4:8:106:THR:N[1_554] | 2.19 | 0.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:183:ARG:NH1 | 4:8:72:GLU:OE1[1_554] | 2.19 | 0.01 |
| 4:5:331:ALA:N | 4:8:140:LEU:CD2[1_554] | 2.19 | 0.01 |
| 4:4:198:TYR:CD2 | 4:7:208:ILE:CA[1_554] | 2.19 | 0.01 |
| 4:6:25:ASP:OD1 | 4:9:131:ALA:CA[1_554] | 2.19 | 0.01 |
| 4:5:137:GLN:C | 4:8:113:LYS:N[1_554] | 2.19 | 0.01 |
| 4:4:279:TYR:CE1 | 4:7:289:ILE:CD1[1_554] | 2.19 | 0.01 |
| 4:5:198:TYR:CE2 | 4:8:208:ILE:C[1_554] | 2.19 | 0.01 |
| 4:6:143:TYR:CD2 | 4:9:368:SER:O[1_554] | 2.19 | 0.01 |
| 4:6:24:ASP:OD2 | 4:9:126:THR:N[1_554] | 2.19 | 0.01 |
| 4:6:11:ASP:CA | 4:9:118:LYS:CB[1_554] | 2.19 | 0.01 |
| 4:5:178:LEU:C | 4:8:177:ARG:CG[1_554] | 2.19 | 0.01 |
| 4:5:340:TRP:CB | 4:8:118:LYS:C[1_554] | 2.19 | 0.01 |
| 4:5:316:GLU:O | 4:8:151:ILE:CG2[1_554] | 2.19 | 0.01 |
| 4:4:282:ILE:C | 4:7:173:HIS:NE2[1_554] | 2.19 | 0.01 |
| 4:6:337:TYR:CA | 4:9:119:MET:SD[1_554] | 2.19 | 0.01 |
| 4:3:113:LYS:CA | 4:7:254:ARG:N[1_554] | 2.19 | 0.01 |
| 4:4:357:ILE:CD1 | 4:8:232:SER:CB[1_554] | 2.19 | 0.01 |
| 4:6:173:HIS:ND1 | 4:V:265:SER:O[1_554] | 2.19 | 0.01 |
| 4:3:73:HIS:CA | 4:7:198:TYR:O[1_554] | 2.19 | 0.01 |
| 4:5:339:VAL:N | 4:8:116:ARG:CB[1_554] | 2.19 | 0.01 |
| 4:6:278:THR:OG1 | 4:9:163:VAL:CB[1_554] | 2.19 | 0.01 |
| 4:5:151:ILE:CG2 | 4:8:171:LEU:N[1_554] | 2.19 | 0.01 |
| 4:5:224:GLU:O | 4:8:308:GLY:N[1_554] | 2.19 | 0.01 |
| 4:4:274:ILE:CG1 | 4:7:161:HIS:CD2[1_554] | 2.19 | 0.01 |
| 4:5:336:LYS:NZ | 4:8:86:TRP:CD1[1_554] | 2.19 | 0.01 |
| 4:6:59:GLN:OE1 | 4:9:68:LYS:CA[1_554] | 2.19 | 0.01 |
| 4:5:223:PHE:CB | 4:8:309:ILE:CG2[1_554] | 2.19 | 0.01 |
| 4:5:327:ILE:N | 4:8:167:GLU:OE2[1_554] | 2.19 | 0.01 |
| 4:4:213:LYS:O | 4:7:16:LEU:C[1_554] | 2.19 | 0.01 |
| 4:4:255:PHE:O | 4:7:302:GLY:O[1_554] | 2.19 | 0.01 |
| 4:5:257:CYS:N | 4:8:303:THR:N[1_554] | 2.19 | 0.01 |
| 4:4:111:ASN:O | 4:8:253:GLU:OE1[1_554] | 2.19 | 0.01 |
| 4:5:339:VAL:CA | 4:8:116:ARG:N[1_554] | 2.19 | 0.01 |
| 4:5:176:MET:CG | 4:8:173:HIS:O[1_554] | 2.19 | 0.01 |
| 4:5:332:PRO:CG | 4:8:133:TYR:CE2[1_554] | 2.19 | 0.01 |
| 4:5:320:LEU:CB | 4:8:294:TYR:N[1_554] | 2.19 | 0.01 |
| 4:5:332:PRO:C | 4:8:104:LEU:CG[1_554] | 2.19 | 0.01 |
| 4:6:181:ALA:CA | 4:9:159:VAL:CG2[1_554] | 2.19 | 0.01 |
| 4:6:268:GLY:C | 4:9:264:PRO:CA[1_554] | 2.19 | 0.01 |
| 4:4:59:GLN:CB | 4:7:68:LYS:CD[1_554] | 2.19 | 0.01 |
| 4:4:181:ALA:C | 4:7:73:HIS:CB[1_554] | 2.19 | 0.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:255:PHE:C | 4:7:303:THR:N[1_554] | 2.19 | 0.01 |
| 4:4:193:LEU:O | 4:7:207:GLU:O[1_554] | 2.19 | 0.01 |
| 4:6:369:ILE:C | 4:V:231:ALA:CA[1_554] | 2.19 | 0.01 |
| 4:4:197:GLY:CA | 4:7:208:ILE:C[1_554] | 2.19 | 0.01 |
| 4:5:140:LEU:CA | 4:8:371:HIS:CB[1_554] | 2.19 | 0.01 |
| 4:4:142:LEU:N | 4:7:371:HIS:CE1[1_554] | 2.19 | 0.01 |
| 4:6:183:ARG:NH2 | 4:9:72:GLU:CB[1_554] | 2.19 | 0.01 |
| 4:3:116:ARG:N | 4:7:251:GLY:N[1_554] | 2.19 | 0.01 |
| 4:4:184:ASP:N | 4:7:73:HIS:NE2[1_554] | 2.19 | 0.01 |
| 4:6:350:SER:N | 4:9:364:GLU:C[1_554] | 2.19 | 0.01 |
| 4:4:222:ASP:CG | 4:7:332:PRO:N[1_554] | 2.19 | 0.01 |
| 4:4:174:ALA:N | 4:8:267:ILE:C[1_554] | 2.19 | 0.01 |
| 4:5:222:ASP:CA | 4:8:331:ALA:N[1_554] | 2.19 | 0.01 |
| 4:6:195:GLU:CG | 4:9:189:LEU:CD2[1_554] | 2.19 | 0.01 |
| 4:3:73:HIS:CB | 4:7:198:TYR:O[1_554] | 2.19 | 0.01 |
| 4:4:327:ILE:CA | 4:7:167:GLU:N[1_554] | 2.19 | 0.01 |
| 4:5:280:ASN:N | 4:8:174:ALA:CB[1_554] | 2.19 | 0.01 |
| 4:6:196:ARG:CG | 4:9:212:ILE:O[1_554] | 2.19 | 0.01 |
| 4:5:75:ILE:CD1 | 4:9:194:THR:O[1_554] | 2.19 | 0.01 |
| 4:5:343:GLY:C | 4:8:367:PRO:O[1_554] | 2.19 | 0.01 |
| 4:5:192:ILE:CD1 | 4:8:213:LYS:CD[1_554] | 2.19 | 0.01 |
| 4:3:110:LEU:CD1 | 4:7:192:ILE:N[1_554] | 2.19 | 0.01 |
| 4:6:28:ARG:NH2 | 4:9:125:GLU:C[1_554] | 2.19 | 0.01 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 789/840 (94%) | 651 (82%) | 112 (14%) | 26 (3%) | 4 | 35 |
| 1 | D | 789/840 (94%) | 651 (82%) | 112 (14%) | 26 (3%) | 4 | 35 |
| 1 | G | 791/840 (94%) | 652 (82%) | 112 (14%) | 27 (3%) | 4 | 35 |
| 1 | J | 791/840 (94%) | 652 (82%) | 112 (14%) | 27 (3%) | 4 | 35 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 1 | M | 787/840 (94%) | 649 (82%) | 112 (14%) | 26 (3%) | 4 | 35 |
| 1 | S | 785/840 (94%) | 648 (82%) | 110 (14%) | 27 (3%) | 4 | 35 |
| 2 | B | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 25 |
| 2 | E | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 25 |
| 2 | H | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 25 |
| 2 | K | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 25 |
| 2 | N | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 25 |
| 2 | T | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 25 |
| 3 | C | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | F | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | I | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | L | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | O | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | U | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 4 | 1 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 11 | 51 |
| 4 | 2 | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 11 | 51 |
| 4 | 3 | 370/375 (99%) | 333 (90%) | 31 (8%) | 6 (2%) | 11 | 51 |
| 4 | 4 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 11 | 51 |
| 4 | 5 | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 11 | 51 |
| 4 | 6 | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 11 | 51 |
| 4 | 7 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 11 | 51 |
| 4 | 8 | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 11 | 51 |
| 4 | 9 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 11 | 51 |
| 4 | V | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 11 | 51 |
| 4 | W | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 11 | 51 |
| 4 | X | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 11 | 51 |
| 4 | Y | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 11 | 51 |
| 4 | Z | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 11 | 51 |
| All | All | 11628/12042 (97%) | 10139 (87%) | 1198 (10%) | 291 (2%) | 10 | 41 |

All (291) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 73 | LYS |
| 1 | A | 202 | SER |
| 1 | A | 572 | LYS |
| 1 | A | 712 | PRO |
| 1 | A | 729 | ALA |
| 1 | A | 757 | GLN |
| 1 | A | 762 | HIS |
| 2 | B | 131 | GLU |
| 2 | B | 141 | PRO |
| 1 | D | 73 | LYS |
| 1 | D | 202 | SER |
| 1 | D | 572 | LYS |
| 1 | D | 712 | PRO |
| 1 | D | 729 | ALA |
| 1 | D | 757 | GLN |
| 1 | D | 762 | HIS |
| 2 | E | 131 | GLU |
| 2 | E | 141 | PRO |
| 1 | G | 73 | LYS |
| 1 | G | 202 | SER |
| 1 | G | 572 | LYS |
| 1 | G | 712 | PRO |
| 1 | G | 729 | ALA |
| 1 | G | 757 | GLN |
| 1 | G | 762 | HIS |
| 2 | H | 131 | GLU |
| 2 | H | 141 | PRO |
| 1 | J | 73 | LYS |
| 1 | J | 202 | SER |
| 1 | J | 572 | LYS |
| 1 | J | 712 | PRO |
| 1 | J | 729 | ALA |
| 1 | J | 757 | GLN |
| 1 | J | 762 | HIS |
| 1 | J | 785 | GLU |
| 2 | K | 131 | GLU |
| 2 | K | 141 | PRO |
| 1 | M | 73 | LYS |
| 1 | M | 202 | SER |
| 1 | M | 572 | LYS |
| 1 | M | 712 | PRO |
| 1 | M | 729 | ALA |
| 1 | M | 757 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 762 | HIS |
| 2 | N | 131 | GLU |
| 2 | N | 141 | PRO |
| 1 | S | 73 | LYS |
| 1 | S | 202 | SER |
| 1 | S | 572 | LYS |
| 1 | S | 712 | PRO |
| 1 | S | 729 | ALA |
| 1 | S | 757 | GLN |
| 1 | S | 762 | HIS |
| 2 | T | 131 | GLU |
| 2 | T | 141 | PRO |
| 4 | 1 | 246 | GLN |
| 4 | 2 | 246 | GLN |
| 4 | 3 | 246 | GLN |
| 4 | 4 | 246 | GLN |
| 4 | 5 | 246 | GLN |
| 4 | 6 | 246 | GLN |
| 4 | 7 | 246 | GLN |
| 4 | 8 | 246 | GLN |
| 4 | 9 | 246 | GLN |
| 4 | V | 246 | GLN |
| 4 | W | 246 | GLN |
| 4 | X | 246 | GLN |
| 4 | Y | 246 | GLN |
| 4 | Z | 246 | GLN |
| 1 | A | 11 | GLY |
| 1 | A | 21 | GLU |
| 1 | A | 219 | GLU |
| 1 | A | 517 | MET |
| 1 | A | 637 | LYS |
| 2 | B | 130 | PRO |
| 2 | B | 147 | ASN |
| 2 | B | 151 | LYS |
| 2 | B | 161 | GLU |
| 1 | D | 11 | GLY |
| 1 | D | 21 | GLU |
| 1 | D | 219 | GLU |
| 1 | D | 517 | MET |
| 1 | D | 637 | LYS |
| 2 | E | 130 | PRO |
| 2 | E | 147 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 151 | LYS |
| 1 | G | 11 | GLY |
| 1 | G | 21 | GLU |
| 1 | G | 219 | GLU |
| 1 | G | 517 | MET |
| 1 | G | 532 | ILE |
| 1 | G | 637 | LYS |
| 1 | G | 785 | GLU |
| 2 | H | 130 | PRO |
| 2 | H | 147 | ASN |
| 2 | H | 151 | LYS |
| 1 | J | 11 | GLY |
| 1 | J | 21 | GLU |
| 1 | J | 219 | GLU |
| 1 | J | 517 | MET |
| 1 | J | 637 | LYS |
| 2 | K | 130 | PRO |
| 2 | K | 147 | ASN |
| 2 | K | 151 | LYS |
| 2 | K | 161 | GLU |
| 1 | M | 11 | GLY |
| 1 | M | 21 | GLU |
| 1 | M | 219 | GLU |
| 1 | M | 517 | MET |
| 1 | M | 637 | LYS |
| 2 | N | 130 | PRO |
| 2 | N | 147 | ASN |
| 2 | N | 151 | LYS |
| 1 | S | 11 | GLY |
| 1 | S | 21 | GLU |
| 1 | S | 219 | GLU |
| 1 | S | 517 | MET |
| 1 | S | 637 | LYS |
| 2 | T | 130 | PRO |
| 2 | T | 147 | ASN |
| 2 | T | 151 | LYS |
| 4 | 1 | 274 | ILE |
| 4 | 2 | 274 | ILE |
| 4 | 3 | 274 | ILE |
| 4 | 4 | 274 | ILE |
| 4 | 5 | 274 | ILE |
| 4 | 6 | 274 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 7 | 274 | ILE |
| 4 | 8 | 274 | ILE |
| 4 | 9 | 274 | ILE |
| 4 | V | 274 | ILE |
| 4 | W | 274 | ILE |
| 4 | X | 274 | ILE |
| 4 | Y | 274 | ILE |
| 4 | Z | 274 | ILE |
| 1 | A | 58 | GLY |
| 1 | A | 294 | ASN |
| 1 | A | 532 | ILE |
| 1 | A | 644 | SER |
| 1 | D | 58 | GLY |
| 1 | D | 294 | ASN |
| 1 | D | 532 | ILE |
| 1 | D | 644 | SER |
| 2 | E | 161 | GLU |
| 1 | G | 58 | GLY |
| 1 | G | 294 | ASN |
| 1 | G | 644 | SER |
| 2 | H | 161 | GLU |
| 1 | J | 58 | GLY |
| 1 | J | 294 | ASN |
| 1 | J | 532 | ILE |
| 1 | J | 644 | SER |
| 1 | M | 58 | GLY |
| 1 | M | 294 | ASN |
| 1 | M | 532 | ILE |
| 1 | M | 644 | SER |
| 2 | N | 161 | GLU |
| 1 | S | 58 | GLY |
| 1 | S | 294 | ASN |
| 1 | S | 532 | ILE |
| 1 | S | 644 | SER |
| 2 | T | 161 | GLU |
| 4 | 1 | 233 | SER |
| 4 | 2 | 233 | SER |
| 4 | 3 | 233 | SER |
| 4 | 4 | 233 | SER |
| 4 | 5 | 233 | SER |
| 4 | 6 | 233 | SER |
| 4 | 7 | 233 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 8 | 233 | SER |
| 4 | 9 | 233 | SER |
| 4 | V | 233 | SER |
| 4 | W | 233 | SER |
| 4 | X | 233 | SER |
| 4 | Y | 233 | SER |
| 4 | Z | 233 | SER |
| 1 | A | 435 | GLU |
| 1 | A | 817 | GLN |
| 1 | D | 269 | LEU |
| 1 | D | 435 | GLU |
| 1 | D | 817 | GLN |
| 1 | G | 269 | LEU |
| 1 | G | 435 | GLU |
| 1 | G | 817 | GLN |
| 1 | J | 269 | LEU |
| 1 | J | 435 | GLU |
| 1 | J | 817 | GLN |
| 1 | M | 269 | LEU |
| 1 | M | 435 | GLU |
| 1 | M | 817 | GLN |
| 1 | S | 269 | LEU |
| 1 | S | 435 | GLU |
| 1 | S | 769 | ALA |
| 1 | S | 817 | GLN |
| 4 | 1 | 2 | GLU |
| 4 | 2 | 2 | GLU |
| 4 | 3 | 2 | GLU |
| 4 | 4 | 2 | GLU |
| 4 | 4 | 253 | GLU |
| 4 | 5 | 2 | GLU |
| 4 | 5 | 253 | GLU |
| 4 | 6 | 2 | GLU |
| 4 | 6 | 253 | GLU |
| 4 | 7 | 2 | GLU |
| 4 | 7 | 253 | GLU |
| 4 | 8 | 2 | GLU |
| 4 | 9 | 2 | GLU |
| 4 | 9 | 253 | GLU |
| 4 | V | 2 | GLU |
| 4 | V | 253 | GLU |
| 4 | W | 2 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | W | 253 | GLU |
| 4 | X | 2 | GLU |
| 4 | Y | 2 | GLU |
| 4 | Z | 2 | GLU |
| 4 | Z | 253 | GLU |
| 1 | A | 8 | ALA |
| 1 | A | 269 | LEU |
| 1 | A | 578 | HIS |
| 2 | B | 140 | PHE |
| 1 | D | 8 | ALA |
| 1 | D | 556 | ASP |
| 1 | D | 578 | HIS |
| 2 | E | 140 | PHE |
| 1 | G | 8 | ALA |
| 1 | G | 79 | SER |
| 1 | G | 578 | HIS |
| 2 | H | 140 | PHE |
| 1 | J | 8 | ALA |
| 1 | J | 578 | HIS |
| 2 | K | 140 | PHE |
| 1 | M | 8 | ALA |
| 1 | M | 578 | HIS |
| 2 | N | 140 | PHE |
| 1 | S | 8 | ALA |
| 1 | S | 578 | HIS |
| 2 | T | 140 | PHE |
| 4 | 1 | 253 | GLU |
| 4 | 2 | 253 | GLU |
| 4 | 3 | 253 | GLU |
| 4 | 8 | 253 | GLU |
| 4 | X | 253 | GLU |
| 4 | Y | 253 | GLU |
| 1 | A | 79 | SER |
| 1 | A | 199 | ILE |
| 1 | A | 556 | ASP |
| 2 | B | 142 | PRO |
| 1 | D | 79 | SER |
| 1 | D | 199 | ILE |
| 2 | E | 142 | PRO |
| 1 | G | 199 | ILE |
| 1 | G | 556 | ASP |
| 2 | H | 142 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 79 | SER |
| 1 | J | 199 | ILE |
| 1 | J | 556 | ASP |
| 2 | K | 142 | PRO |
| 1 | M | 79 | SER |
| 1 | M | 199 | ILE |
| 1 | M | 556 | ASP |
| 2 | N | 142 | PRO |
| 1 | S | 79 | SER |
| 1 | S | 199 | ILE |
| 1 | S | 556 | ASP |
| 2 | T | 142 | PRO |
| 1 | A | 840 | PRO |
| 1 | D | 287 | ILE |
| 1 | D | 840 | PRO |
| 1 | G | 840 | PRO |
| 1 | J | 840 | PRO |
| 1 | M | 840 | PRO |
| 1 | S | 840 | PRO |
| 4 | 1 | 242 | LEU |
| 4 | 2 | 242 | LEU |
| 4 | 3 | 242 | LEU |
| 4 | 4 | 242 | LEU |
| 4 | 5 | 242 | LEU |
| 4 | 6 | 242 | LEU |
| 4 | 7 | 242 | LEU |
| 4 | 8 | 242 | LEU |
| 4 | 9 | 242 | LEU |
| 4 | V | 242 | LEU |
| 4 | W | 242 | LEU |
| 4 | X | 242 | LEU |
| 4 | Y | 242 | LEU |
| 4 | Z | 242 | LEU |
| 1 | A | 287 | ILE |
| 1 | G | 287 | ILE |
| 1 | J | 287 | ILE |
| 1 | M | 287 | ILE |
| 1 | S | 287 | ILE |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 672/672 (100%) | 512 (76%) | 160 (24%) | 1 | 5 |
| 1 | D | 672/672 (100%) | 513 (76%) | 159 (24%) | 1 | 5 |
| 1 | G | 672/672 (100%) | 513 (76%) | 159 (24%) | 1 | 5 |
| 1 | J | 672/672 (100%) | 515 (77%) | 157 (23%) | 1 | 5 |
| 1 | M | 672/672 (100%) | 514 (76%) | 158 (24%) | 1 | 5 |
| 1 | S | 672/672 (100%) | 515 (77%) | 157 (23%) | 1 | 5 |
| 2 | B | 120/120 (100%) | 119 (99%) | 1 (1%) | 85 | 92 |
| 2 | E | 120/120 (100%) | 119 (99%) | 1 (1%) | 85 | 92 |
| 2 | H | 120/120 (100%) | 119 (99%) | 1 (1%) | 85 | 92 |
| 2 | K | 120/120 (100%) | 119 (99%) | 1 (1%) | 85 | 92 |
| 2 | N | 120/120 (100%) | 119 (99%) | 1 (1%) | 85 | 92 |
| 2 | T | 120/120 (100%) | 119 (99%) | 1 (1%) | 85 | 92 |
| 3 | C | 117/117 (100%) | 112 (96%) | 5 (4%) | 33 | 64 |
| 3 | F | 117/117 (100%) | 112 (96%) | 5 (4%) | 33 | 64 |
| 3 | I | 117/117 (100%) | 112 (96%) | 5 (4%) | 33 | 64 |
| 3 | L | 117/117 (100%) | 112 (96%) | 5 (4%) | 33 | 64 |
| 3 | O | 117/117 (100%) | 112 (96%) | 5 (4%) | 33 | 64 |
| 3 | U | 117/117 (100%) | 112 (96%) | 5 (4%) | 33 | 64 |
| 4 | 1 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 21 |
| 4 | 2 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 20 |
| 4 | 3 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 21 |
| 4 | 4 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 20 |
| 4 | 5 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 21 |
| 4 | 6 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 21 |
| 4 | 7 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 20 |
| 4 | 8 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 4 | 9 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 20 |
| 4 | V | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 21 |
| 4 | W | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 20 |
| 4 | X | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 21 |
| 4 | Y | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 21 |
| 4 | Z | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 20 |
| All | All | 9864/9906 (100%) | 8227 (83%) | 1637 (17%) | 6 | 16 |

All (1637) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 4 | ASP |
| 1 | A | 7 | MET |
| 1 | A | 12 | GLU |
| 1 | A | 15 | PRO |
| 1 | A | 17 | LEU |
| 1 | A | 20 | SER |
| 1 | A | 22 | LYS |
| 1 | A | 36 | SER |
| 1 | A | 37 | SER |
| 1 | A | 46 | SER |
| 1 | A | 61 | THR |
| 1 | A | 69 | THR |
| 1 | A | 70 | LEU |
| 1 | A | 72 | VAL |
| 1 | A | 73 | LYS |
| 1 | A | 75 | ASP |
| 1 | A | 76 | GLN |
| 1 | A | 97 | LEU |
| 1 | A | 106 | LEU |
| 1 | A | 109 | ARG |
| 1 | A | 114 | MET |
| 1 | A | 117 | THR |
| 1 | A | 121 | LEU |
| 1 | A | 126 | VAL |
| 1 | A | 127 | ASN |
| 1 | A | 135 | TYR |
| 1 | A | 136 | ASN |
| 1 | A | 146 | LYS |
| 1 | A | 149 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 155 | ILE |
| 1 | A | 157 | SER |
| 1 | A | 158 | ILE |
| 1 | A | 159 | SER |
| 1 | A | 165 | PHE |
| 1 | A | 167 | LEU |
| 1 | A | 169 | ASP |
| 1 | A | 173 | GLN |
| 1 | A | 178 | THR |
| 1 | A | 185 | LYS |
| 1 | A | 186 | THR |
| 1 | A | 187 | VAL |
| 1 | A | 189 | THR |
| 1 | A | 191 | ARG |
| 1 | A | 193 | ILE |
| 1 | A | 194 | GLN |
| 1 | A | 198 | THR |
| 1 | A | 199 | ILE |
| 1 | A | 218 | LEU |
| 1 | A | 219 | GLU |
| 1 | A | 221 | GLN |
| 1 | A | 223 | ILE |
| 1 | A | 227 | PRO |
| 1 | A | 229 | LEU |
| 1 | A | 244 | SER |
| 1 | A | 245 | ARG |
| 1 | A | 251 | ARG |
| 1 | A | 264 | ASP |
| 1 | A | 273 | SER |
| 1 | A | 274 | ARG |
| 1 | A | 278 | GLN |
| 1 | A | 282 | GLU |
| 1 | A | 287 | ILE |
| 1 | A | 290 | GLN |
| 1 | A | 294 | ASN |
| 1 | A | 298 | GLU |
| 1 | A | 300 | ILE |
| 1 | A | 325 | ILE |
| 1 | A | 331 | LEU |
| 1 | A | 336 | SER |
| 1 | A | 351 | ILE |
| 1 | A | 354 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 364 | LEU |
| 1 | A | 365 | LYS |
| 1 | A | 372 | GLU |
| 1 | A | 376 | GLU |
| 1 | A | 381 | GLU |
| 1 | A | 389 | LEU |
| 1 | A | 392 | LEU |
| 1 | A | 394 | SER |
| 1 | A | 399 | LYS |
| 1 | A | 405 | ARG |
| 1 | A | 410 | ASN |
| 1 | A | 439 | LEU |
| 1 | A | 447 | GLN |
| 1 | A | 448 | GLN |
| 1 | A | 449 | LEU |
| 1 | A | 453 | GLN |
| 1 | A | 455 | ARG |
| 1 | A | 457 | TYR |
| 1 | A | 462 | LEU |
| 1 | A | 471 | ASP |
| 1 | A | 474 | SER |
| 1 | A | 480 | ILE |
| 1 | A | 487 | LEU |
| 1 | A | 495 | MET |
| 1 | A | 499 | GLU |
| 1 | A | 506 | GLU |
| 1 | A | 513 | ILE |
| 1 | A | 518 | ASP |
| 1 | A | 524 | GLU |
| 1 | A | 532 | ILE |
| 1 | A | 534 | SER |
| 1 | A | 537 | GLU |
| 1 | A | 543 | PRO |
| 1 | A | 549 | SER |
| 1 | A | 561 | LYS |
| 1 | A | 562 | SER |
| 1 | A | 563 | ASN |
| 1 | A | 569 | LYS |
| 1 | A | 580 | SER |
| 1 | A | 593 | SER |
| 1 | A | 597 | GLU |
| 1 | A | 604 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 608 | ILE |
| 1 | A | 610 | LEU |
| 1 | A | 615 | SER |
| 1 | A | 621 | LEU |
| 1 | A | 625 | THR |
| 1 | A | 664 | LEU |
| 1 | A | 666 | SER |
| 1 | A | 673 | ARG |
| 1 | A | 675 | ILE |
| 1 | A | 676 | ILE |
| 1 | A | 686 | MET |
| 1 | A | 689 | GLU |
| 1 | A | 690 | LEU |
| 1 | A | 693 | HIS |
| 1 | A | 698 | ASN |
| 1 | A | 701 | LEU |
| 1 | A | 702 | GLU |
| 1 | A | 704 | ILE |
| 1 | A | 708 | ARG |
| 1 | A | 713 | SER |
| 1 | A | 714 | ARG |
| 1 | A | 716 | LEU |
| 1 | A | 719 | ASP |
| 1 | A | 722 | GLN |
| 1 | A | 723 | ARG |
| 1 | A | 727 | LEU |
| 1 | A | 728 | ASN |
| 1 | A | 745 | GLU |
| 1 | A | 752 | ASP |
| 1 | A | 753 | VAL |
| 1 | A | 754 | ASP |
| 1 | A | 762 | HIS |
| 1 | A | 774 | LEU |
| 1 | A | 785 | GLU |
| 1 | A | 787 | ILE |
| 1 | A | 793 | ARG |
| 1 | A | 799 | MET |
| 1 | A | 802 | GLU |
| 1 | A | 804 | ARG |
| 1 | A | 810 | ARG |
| 1 | A | 816 | ILE |
| 1 | A | 822 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 832 | MET |
| 1 | A | 834 | LEU |
| 1 | A | 838 | ILE |
| 1 | A | 842 | LEU |
| 1 | A | 843 | LYS |
| 2 | B | 142 | PRO |
| 3 | C | 48 | LYS |
| 3 | C | 68 | PHE |
| 3 | C | 83 | THR |
| 3 | C | 95 | ASP |
| 3 | C | 96 | LYS |
| 1 | D | 4 | ASP |
| 1 | D | 7 | MET |
| 1 | D | 12 | GLU |
| 1 | D | 15 | PRO |
| 1 | D | 17 | LEU |
| 1 | D | 20 | SER |
| 1 | D | 22 | LYS |
| 1 | D | 36 | SER |
| 1 | D | 37 | SER |
| 1 | D | 40 | VAL |
| 1 | D | 46 | SER |
| 1 | D | 61 | THR |
| 1 | D | 69 | THR |
| 1 | D | 70 | LEU |
| 1 | D | 72 | VAL |
| 1 | D | 73 | LYS |
| 1 | D | 75 | ASP |
| 1 | D | 76 | GLN |
| 1 | D | 97 | LEU |
| 1 | D | 106 | LEU |
| 1 | D | 109 | ARG |
| 1 | D | 114 | MET |
| 1 | D | 117 | THR |
| 1 | D | 121 | LEU |
| 1 | D | 126 | VAL |
| 1 | D | 127 | ASN |
| 1 | D | 135 | TYR |
| 1 | D | 136 | ASN |
| 1 | D | 146 | LYS |
| 1 | D | 149 | GLN |
| 1 | D | 155 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 157 | SER |
| 1 | D | 158 | ILE |
| 1 | D | 159 | SER |
| 1 | D | 165 | PHE |
| 1 | D | 167 | LEU |
| 1 | D | 169 | ASP |
| 1 | D | 173 | GLN |
| 1 | D | 178 | THR |
| 1 | D | 185 | LYS |
| 1 | D | 186 | THR |
| 1 | D | 187 | VAL |
| 1 | D | 189 | THR |
| 1 | D | 191 | ARG |
| 1 | D | 193 | ILE |
| 1 | D | 194 | GLN |
| 1 | D | 198 | THR |
| 1 | D | 199 | ILE |
| 1 | D | 218 | LEU |
| 1 | D | 219 | GLU |
| 1 | D | 221 | GLN |
| 1 | D | 223 | ILE |
| 1 | D | 229 | LEU |
| 1 | D | 244 | SER |
| 1 | D | 245 | ARG |
| 1 | D | 251 | ARG |
| 1 | D | 264 | ASP |
| 1 | D | 273 | SER |
| 1 | D | 274 | ARG |
| 1 | D | 278 | GLN |
| 1 | D | 282 | GLU |
| 1 | D | 287 | ILE |
| 1 | D | 290 | GLN |
| 1 | D | 294 | ASN |
| 1 | D | 298 | GLU |
| 1 | D | 300 | ILE |
| 1 | D | 325 | ILE |
| 1 | D | 331 | LEU |
| 1 | D | 336 | SER |
| 1 | D | 351 | ILE |
| 1 | D | 354 | LEU |
| 1 | D | 364 | LEU |
| 1 | D | 365 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 372 | GLU |
| 1 | D | 376 | GLU |
| 1 | D | 381 | GLU |
| 1 | D | 389 | LEU |
| 1 | D | 392 | LEU |
| 1 | D | 394 | SER |
| 1 | D | 399 | LYS |
| 1 | D | 405 | ARG |
| 1 | D | 410 | ASN |
| 1 | D | 439 | LEU |
| 1 | D | 447 | GLN |
| 1 | D | 448 | GLN |
| 1 | D | 449 | LEU |
| 1 | D | 453 | GLN |
| 1 | D | 455 | ARG |
| 1 | D | 457 | TYR |
| 1 | D | 462 | LEU |
| 1 | D | 471 | ASP |
| 1 | D | 474 | SER |
| 1 | D | 480 | ILE |
| 1 | D | 487 | LEU |
| 1 | D | 495 | MET |
| 1 | D | 499 | GLU |
| 1 | D | 506 | GLU |
| 1 | D | 513 | ILE |
| 1 | D | 518 | ASP |
| 1 | D | 524 | GLU |
| 1 | D | 532 | ILE |
| 1 | D | 534 | SER |
| 1 | D | 537 | GLU |
| 1 | D | 549 | SER |
| 1 | D | 561 | LYS |
| 1 | D | 562 | SER |
| 1 | D | 563 | ASN |
| 1 | D | 569 | LYS |
| 1 | D | 580 | SER |
| 1 | D | 593 | SER |
| 1 | D | 597 | GLU |
| 1 | D | 604 | ASN |
| 1 | D | 608 | ILE |
| 1 | D | 610 | LEU |
| 1 | D | 615 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 621 | LEU |
| 1 | D | 625 | THR |
| 1 | D | 664 | LEU |
| 1 | D | 666 | SER |
| 1 | D | 673 | ARG |
| 1 | D | 675 | ILE |
| 1 | D | 676 | ILE |
| 1 | D | 686 | MET |
| 1 | D | 689 | GLU |
| 1 | D | 690 | LEU |
| 1 | D | 693 | HIS |
| 1 | D | 698 | ASN |
| 1 | D | 701 | LEU |
| 1 | D | 702 | GLU |
| 1 | D | 704 | ILE |
| 1 | D | 708 | ARG |
| 1 | D | 713 | SER |
| 1 | D | 714 | ARG |
| 1 | D | 716 | LEU |
| 1 | D | 719 | ASP |
| 1 | D | 722 | GLN |
| 1 | D | 723 | ARG |
| 1 | D | 727 | LEU |
| 1 | D | 728 | ASN |
| 1 | D | 745 | GLU |
| 1 | D | 752 | ASP |
| 1 | D | 753 | VAL |
| 1 | D | 754 | ASP |
| 1 | D | 762 | HIS |
| 1 | D | 774 | LEU |
| 1 | D | 785 | GLU |
| 1 | D | 787 | ILE |
| 1 | D | 793 | ARG |
| 1 | D | 799 | MET |
| 1 | D | 802 | GLU |
| 1 | D | 804 | ARG |
| 1 | D | 810 | ARG |
| 1 | D | 816 | ILE |
| 1 | D | 822 | SER |
| 1 | D | 832 | MET |
| 1 | D | 834 | LEU |
| 1 | D | 838 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 842 | LEU |
| 1 | D | 843 | LYS |
| 2 | E | 142 | PRO |
| 3 | F | 48 | LYS |
| 3 | F | 68 | PHE |
| 3 | F | 83 | THR |
| 3 | F | 95 | ASP |
| 3 | F | 96 | LYS |
| 1 | G | 4 | ASP |
| 1 | G | 7 | MET |
| 1 | G | 12 | GLU |
| 1 | G | 15 | PRO |
| 1 | G | 17 | LEU |
| 1 | G | 20 | SER |
| 1 | G | 22 | LYS |
| 1 | G | 36 | SER |
| 1 | G | 37 | SER |
| 1 | G | 46 | SER |
| 1 | G | 61 | THR |
| 1 | G | 69 | THR |
| 1 | G | 70 | LEU |
| 1 | G | 72 | VAL |
| 1 | G | 73 | LYS |
| 1 | G | 75 | ASP |
| 1 | G | 76 | GLN |
| 1 | G | 97 | LEU |
| 1 | G | 106 | LEU |
| 1 | G | 109 | ARG |
| 1 | G | 114 | MET |
| 1 | G | 117 | THR |
| 1 | G | 121 | LEU |
| 1 | G | 126 | VAL |
| 1 | G | 127 | ASN |
| 1 | G | 135 | TYR |
| 1 | G | 136 | ASN |
| 1 | G | 146 | LYS |
| 1 | G | 149 | GLN |
| 1 | G | 155 | ILE |
| 1 | G | 157 | SER |
| 1 | G | 158 | ILE |
| 1 | G | 159 | SER |
| 1 | G | 165 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 167 | LEU |
| 1 | G | 169 | ASP |
| 1 | G | 173 | GLN |
| 1 | G | 178 | THR |
| 1 | G | 185 | LYS |
| 1 | G | 186 | THR |
| 1 | G | 187 | VAL |
| 1 | G | 189 | THR |
| 1 | G | 191 | ARG |
| 1 | G | 193 | ILE |
| 1 | G | 194 | GLN |
| 1 | G | 198 | THR |
| 1 | G | 199 | ILE |
| 1 | G | 218 | LEU |
| 1 | G | 219 | GLU |
| 1 | G | 221 | GLN |
| 1 | G | 223 | ILE |
| 1 | G | 229 | LEU |
| 1 | G | 243 | SER |
| 1 | G | 244 | SER |
| 1 | G | 245 | ARG |
| 1 | G | 251 | ARG |
| 1 | G | 264 | ASP |
| 1 | G | 273 | SER |
| 1 | G | 274 | ARG |
| 1 | G | 278 | GLN |
| 1 | G | 282 | GLU |
| 1 | G | 287 | ILE |
| 1 | G | 290 | GLN |
| 1 | G | 294 | ASN |
| 1 | G | 298 | GLU |
| 1 | G | 300 | ILE |
| 1 | G | 325 | ILE |
| 1 | G | 331 | LEU |
| 1 | G | 336 | SER |
| 1 | G | 351 | ILE |
| 1 | G | 354 | LEU |
| 1 | G | 364 | LEU |
| 1 | G | 365 | LYS |
| 1 | G | 372 | GLU |
| 1 | G | 376 | GLU |
| 1 | G | 381 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 389 | LEU |
| 1 | G | 392 | LEU |
| 1 | G | 394 | SER |
| 1 | G | 399 | LYS |
| 1 | G | 405 | ARG |
| 1 | G | 410 | ASN |
| 1 | G | 439 | LEU |
| 1 | G | 447 | GLN |
| 1 | G | 448 | GLN |
| 1 | G | 449 | LEU |
| 1 | G | 453 | GLN |
| 1 | G | 455 | ARG |
| 1 | G | 457 | TYR |
| 1 | G | 462 | LEU |
| 1 | G | 471 | ASP |
| 1 | G | 474 | SER |
| 1 | G | 480 | ILE |
| 1 | G | 487 | LEU |
| 1 | G | 495 | MET |
| 1 | G | 506 | GLU |
| 1 | G | 513 | ILE |
| 1 | G | 518 | ASP |
| 1 | G | 524 | GLU |
| 1 | G | 532 | ILE |
| 1 | G | 534 | SER |
| 1 | G | 537 | GLU |
| 1 | G | 543 | PRO |
| 1 | G | 549 | SER |
| 1 | G | 561 | LYS |
| 1 | G | 562 | SER |
| 1 | G | 563 | ASN |
| 1 | G | 569 | LYS |
| 1 | G | 580 | SER |
| 1 | G | 593 | SER |
| 1 | G | 597 | GLU |
| 1 | G | 604 | ASN |
| 1 | G | 608 | ILE |
| 1 | G | 610 | LEU |
| 1 | G | 615 | SER |
| 1 | G | 621 | LEU |
| 1 | G | 625 | THR |
| 1 | G | 664 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 666 | SER |
| 1 | G | 673 | ARG |
| 1 | G | 675 | ILE |
| 1 | G | 676 | ILE |
| 1 | G | 686 | MET |
| 1 | G | 689 | GLU |
| 1 | G | 690 | LEU |
| 1 | G | 693 | HIS |
| 1 | G | 698 | ASN |
| 1 | G | 701 | LEU |
| 1 | G | 702 | GLU |
| 1 | G | 704 | ILE |
| 1 | G | 708 | ARG |
| 1 | G | 713 | SER |
| 1 | G | 714 | ARG |
| 1 | G | 716 | LEU |
| 1 | G | 719 | ASP |
| 1 | G | 722 | GLN |
| 1 | G | 723 | ARG |
| 1 | G | 727 | LEU |
| 1 | G | 728 | ASN |
| 1 | G | 745 | GLU |
| 1 | G | 752 | ASP |
| 1 | G | 753 | VAL |
| 1 | G | 754 | ASP |
| 1 | G | 762 | HIS |
| 1 | G | 774 | LEU |
| 1 | G | 785 | GLU |
| 1 | G | 787 | ILE |
| 1 | G | 793 | ARG |
| 1 | G | 799 | MET |
| 1 | G | 802 | GLU |
| 1 | G | 804 | ARG |
| 1 | G | 810 | ARG |
| 1 | G | 816 | ILE |
| 1 | G | 822 | SER |
| 1 | G | 832 | MET |
| 1 | G | 834 | LEU |
| 1 | G | 838 | ILE |
| 1 | G | 842 | LEU |
| 1 | G | 843 | LYS |
| 2 | H | 142 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 48 | LYS |
| 3 | I | 68 | PHE |
| 3 | I | 83 | THR |
| 3 | I | 95 | ASP |
| 3 | I | 96 | LYS |
| 1 | J | 4 | ASP |
| 1 | J | 7 | MET |
| 1 | J | 12 | GLU |
| 1 | J | 15 | PRO |
| 1 | J | 17 | LEU |
| 1 | J | 20 | SER |
| 1 | J | 22 | LYS |
| 1 | J | 36 | SER |
| 1 | J | 37 | SER |
| 1 | J | 46 | SER |
| 1 | J | 61 | THR |
| 1 | J | 69 | THR |
| 1 | J | 70 | LEU |
| 1 | J | 72 | VAL |
| 1 | J | 73 | LYS |
| 1 | J | 75 | ASP |
| 1 | J | 76 | GLN |
| 1 | J | 97 | LEU |
| 1 | J | 106 | LEU |
| 1 | J | 109 | ARG |
| 1 | J | 114 | MET |
| 1 | J | 117 | THR |
| 1 | J | 121 | LEU |
| 1 | J | 126 | VAL |
| 1 | J | 127 | ASN |
| 1 | J | 135 | TYR |
| 1 | J | 136 | ASN |
| 1 | J | 146 | LYS |
| 1 | J | 149 | GLN |
| 1 | J | 155 | ILE |
| 1 | J | 157 | SER |
| 1 | J | 158 | ILE |
| 1 | J | 159 | SER |
| 1 | J | 165 | PHE |
| 1 | J | 167 | LEU |
| 1 | J | 169 | ASP |
| 1 | J | 173 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 178 | THR |
| 1 | J | 185 | LYS |
| 1 | J | 186 | THR |
| 1 | J | 187 | VAL |
| 1 | J | 191 | ARG |
| 1 | J | 193 | ILE |
| 1 | J | 194 | GLN |
| 1 | J | 198 | THR |
| 1 | J | 199 | ILE |
| 1 | J | 218 | LEU |
| 1 | J | 219 | GLU |
| 1 | J | 221 | GLN |
| 1 | J | 223 | ILE |
| 1 | J | 229 | LEU |
| 1 | J | 244 | SER |
| 1 | J | 245 | ARG |
| 1 | J | 251 | ARG |
| 1 | J | 264 | ASP |
| 1 | J | 273 | SER |
| 1 | J | 274 | ARG |
| 1 | J | 278 | GLN |
| 1 | J | 282 | GLU |
| 1 | J | 287 | ILE |
| 1 | J | 290 | GLN |
| 1 | J | 294 | ASN |
| 1 | J | 298 | GLU |
| 1 | J | 300 | ILE |
| 1 | J | 325 | ILE |
| 1 | J | 331 | LEU |
| 1 | J | 336 | SER |
| 1 | J | 351 | ILE |
| 1 | J | 354 | LEU |
| 1 | J | 364 | LEU |
| 1 | J | 365 | LYS |
| 1 | J | 372 | GLU |
| 1 | J | 376 | GLU |
| 1 | J | 381 | GLU |
| 1 | J | 389 | LEU |
| 1 | J | 392 | LEU |
| 1 | J | 394 | SER |
| 1 | J | 399 | LYS |
| 1 | J | 405 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 410 | ASN |
| 1 | J | 439 | LEU |
| 1 | J | 447 | GLN |
| 1 | J | 448 | GLN |
| 1 | J | 449 | LEU |
| 1 | J | 453 | GLN |
| 1 | J | 455 | ARG |
| 1 | J | 457 | TYR |
| 1 | J | 462 | LEU |
| 1 | J | 471 | ASP |
| 1 | J | 474 | SER |
| 1 | J | 480 | ILE |
| 1 | J | 487 | LEU |
| 1 | J | 495 | MET |
| 1 | J | 499 | GLU |
| 1 | J | 506 | GLU |
| 1 | J | 513 | ILE |
| 1 | J | 518 | ASP |
| 1 | J | 524 | GLU |
| 1 | J | 532 | ILE |
| 1 | J | 534 | SER |
| 1 | J | 537 | GLU |
| 1 | J | 543 | PRO |
| 1 | J | 549 | SER |
| 1 | J | 561 | LYS |
| 1 | J | 562 | SER |
| 1 | J | 563 | ASN |
| 1 | J | 569 | LYS |
| 1 | J | 580 | SER |
| 1 | J | 593 | SER |
| 1 | J | 597 | GLU |
| 1 | J | 604 | ASN |
| 1 | J | 608 | ILE |
| 1 | J | 610 | LEU |
| 1 | J | 615 | SER |
| 1 | J | 621 | LEU |
| 1 | J | 625 | THR |
| 1 | J | 664 | LEU |
| 1 | J | 666 | SER |
| 1 | J | 673 | ARG |
| 1 | J | 675 | ILE |
| 1 | J | 676 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 686 | MET |
| 1 | J | 689 | GLU |
| 1 | J | 690 | LEU |
| 1 | J | 693 | HIS |
| 1 | J | 698 | ASN |
| 1 | J | 701 | LEU |
| 1 | J | 702 | GLU |
| 1 | J | 708 | ARG |
| 1 | J | 713 | SER |
| 1 | J | 714 | ARG |
| 1 | J | 716 | LEU |
| 1 | J | 719 | ASP |
| 1 | J | 722 | GLN |
| 1 | J | 723 | ARG |
| 1 | J | 727 | LEU |
| 1 | J | 728 | ASN |
| 1 | J | 745 | GLU |
| 1 | J | 752 | ASP |
| 1 | J | 753 | VAL |
| 1 | J | 754 | ASP |
| 1 | J | 762 | HIS |
| 1 | J | 774 | LEU |
| 1 | J | 785 | GLU |
| 1 | J | 787 | ILE |
| 1 | J | 793 | ARG |
| 1 | J | 799 | MET |
| 1 | J | 802 | GLU |
| 1 | J | 804 | ARG |
| 1 | J | 810 | ARG |
| 1 | J | 816 | ILE |
| 1 | J | 822 | SER |
| 1 | J | 832 | MET |
| 1 | J | 834 | LEU |
| 1 | J | 838 | ILE |
| 1 | J | 842 | LEU |
| 1 | J | 843 | LYS |
| 2 | K | 142 | PRO |
| 3 | L | 48 | LYS |
| 3 | L | 68 | PHE |
| 3 | L | 83 | THR |
| 3 | L | 95 | ASP |
| 3 | L | 96 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 4 | ASP |
| 1 | M | 7 | MET |
| 1 | M | 12 | GLU |
| 1 | M | 15 | PRO |
| 1 | M | 17 | LEU |
| 1 | M | 20 | SER |
| 1 | M | 22 | LYS |
| 1 | M | 36 | SER |
| 1 | M | 37 | SER |
| 1 | M | 46 | SER |
| 1 | M | 61 | THR |
| 1 | M | 69 | THR |
| 1 | M | 70 | LEU |
| 1 | M | 72 | VAL |
| 1 | M | 73 | LYS |
| 1 | M | 75 | ASP |
| 1 | M | 76 | GLN |
| 1 | M | 97 | LEU |
| 1 | M | 106 | LEU |
| 1 | M | 109 | ARG |
| 1 | M | 114 | MET |
| 1 | M | 117 | THR |
| 1 | M | 121 | LEU |
| 1 | M | 126 | VAL |
| 1 | M | 127 | ASN |
| 1 | M | 135 | TYR |
| 1 | M | 136 | ASN |
| 1 | M | 146 | LYS |
| 1 | M | 149 | GLN |
| 1 | M | 155 | ILE |
| 1 | M | 157 | SER |
| 1 | M | 158 | ILE |
| 1 | M | 159 | SER |
| 1 | M | 165 | PHE |
| 1 | M | 167 | LEU |
| 1 | M | 169 | ASP |
| 1 | M | 173 | GLN |
| 1 | M | 178 | THR |
| 1 | M | 185 | LYS |
| 1 | M | 186 | THR |
| 1 | M | 187 | VAL |
| 1 | M | 189 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 191 | ARG |
| 1 | M | 193 | ILE |
| 1 | M | 194 | GLN |
| 1 | M | 198 | THR |
| 1 | M | 199 | ILE |
| 1 | M | 218 | LEU |
| 1 | M | 219 | GLU |
| 1 | M | 221 | GLN |
| 1 | M | 223 | ILE |
| 1 | M | 229 | LEU |
| 1 | M | 244 | SER |
| 1 | M | 245 | ARG |
| 1 | M | 251 | ARG |
| 1 | M | 264 | ASP |
| 1 | M | 273 | SER |
| 1 | M | 274 | ARG |
| 1 | M | 278 | GLN |
| 1 | M | 282 | GLU |
| 1 | M | 287 | ILE |
| 1 | M | 290 | GLN |
| 1 | M | 294 | ASN |
| 1 | M | 298 | GLU |
| 1 | M | 300 | ILE |
| 1 | M | 325 | ILE |
| 1 | M | 331 | LEU |
| 1 | M | 336 | SER |
| 1 | M | 351 | ILE |
| 1 | M | 354 | LEU |
| 1 | M | 364 | LEU |
| 1 | M | 365 | LYS |
| 1 | M | 372 | GLU |
| 1 | M | 376 | GLU |
| 1 | M | 381 | GLU |
| 1 | M | 389 | LEU |
| 1 | M | 392 | LEU |
| 1 | M | 394 | SER |
| 1 | M | 399 | LYS |
| 1 | M | 405 | ARG |
| 1 | M | 410 | ASN |
| 1 | M | 439 | LEU |
| 1 | M | 447 | GLN |
| 1 | M | 448 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 449 | LEU |
| 1 | M | 453 | GLN |
| 1 | M | 455 | ARG |
| 1 | M | 457 | TYR |
| 1 | M | 462 | LEU |
| 1 | M | 471 | ASP |
| 1 | M | 474 | SER |
| 1 | M | 480 | ILE |
| 1 | M | 487 | LEU |
| 1 | M | 495 | MET |
| 1 | M | 499 | GLU |
| 1 | M | 506 | GLU |
| 1 | M | 513 | ILE |
| 1 | M | 518 | ASP |
| 1 | M | 524 | GLU |
| 1 | M | 532 | ILE |
| 1 | M | 534 | SER |
| 1 | M | 537 | GLU |
| 1 | M | 543 | PRO |
| 1 | M | 549 | SER |
| 1 | M | 561 | LYS |
| 1 | M | 562 | SER |
| 1 | M | 563 | ASN |
| 1 | M | 569 | LYS |
| 1 | M | 580 | SER |
| 1 | M | 593 | SER |
| 1 | M | 597 | GLU |
| 1 | M | 604 | ASN |
| 1 | M | 608 | ILE |
| 1 | M | 610 | LEU |
| 1 | M | 615 | SER |
| 1 | M | 621 | LEU |
| 1 | M | 625 | THR |
| 1 | M | 664 | LEU |
| 1 | M | 666 | SER |
| 1 | M | 673 | ARG |
| 1 | M | 675 | ILE |
| 1 | M | 676 | ILE |
| 1 | M | 686 | MET |
| 1 | M | 689 | GLU |
| 1 | M | 690 | LEU |
| 1 | M | 693 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 698 | ASN |
| 1 | M | 701 | LEU |
| 1 | M | 702 | GLU |
| 1 | M | 708 | ARG |
| 1 | M | 713 | SER |
| 1 | M | 714 | ARG |
| 1 | M | 716 | LEU |
| 1 | M | 719 | ASP |
| 1 | M | 722 | GLN |
| 1 | M | 723 | ARG |
| 1 | M | 727 | LEU |
| 1 | M | 728 | ASN |
| 1 | M | 745 | GLU |
| 1 | M | 752 | ASP |
| 1 | M | 753 | VAL |
| 1 | M | 754 | ASP |
| 1 | M | 762 | HIS |
| 1 | M | 774 | LEU |
| 1 | M | 785 | GLU |
| 1 | M | 787 | ILE |
| 1 | M | 793 | ARG |
| 1 | M | 799 | MET |
| 1 | M | 802 | GLU |
| 1 | M | 804 | ARG |
| 1 | M | 810 | ARG |
| 1 | M | 816 | ILE |
| 1 | M | 822 | SER |
| 1 | M | 832 | MET |
| 1 | M | 834 | LEU |
| 1 | M | 838 | ILE |
| 1 | M | 842 | LEU |
| 1 | M | 843 | LYS |
| 2 | N | 142 | PRO |
| 3 | O | 48 | LYS |
| 3 | O | 68 | PHE |
| 3 | O | 83 | THR |
| 3 | O | 95 | ASP |
| 3 | O | 96 | LYS |
| 1 | S | 4 | ASP |
| 1 | S | 7 | MET |
| 1 | S | 12 | GLU |
| 1 | S | 15 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | S | 17 | LEU |
| 1 | S | 20 | SER |
| 1 | S | 22 | LYS |
| 1 | S | 36 | SER |
| 1 | S | 37 | SER |
| 1 | S | 46 | SER |
| 1 | S | 61 | THR |
| 1 | S | 69 | THR |
| 1 | S | 70 | LEU |
| 1 | S | 72 | VAL |
| 1 | S | 73 | LYS |
| 1 | S | 75 | ASP |
| 1 | S | 76 | GLN |
| 1 | S | 97 | LEU |
| 1 | S | 106 | LEU |
| 1 | S | 109 | ARG |
| 1 | S | 114 | MET |
| 1 | S | 117 | THR |
| 1 | S | 121 | LEU |
| 1 | S | 126 | VAL |
| 1 | S | 127 | ASN |
| 1 | S | 135 | TYR |
| 1 | S | 136 | ASN |
| 1 | S | 146 | LYS |
| 1 | S | 149 | GLN |
| 1 | S | 155 | ILE |
| 1 | S | 157 | SER |
| 1 | S | 158 | ILE |
| 1 | S | 159 | SER |
| 1 | S | 165 | PHE |
| 1 | S | 167 | LEU |
| 1 | S | 169 | ASP |
| 1 | S | 173 | GLN |
| 1 | S | 178 | THR |
| 1 | S | 185 | LYS |
| 1 | S | 186 | THR |
| 1 | S | 187 | VAL |
| 1 | S | 191 | ARG |
| 1 | S | 193 | ILE |
| 1 | S | 194 | GLN |
| 1 | S | 198 | THR |
| 1 | S | 199 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | S | 218 | LEU |
| 1 | S | 219 | GLU |
| 1 | S | 221 | GLN |
| 1 | S | 223 | ILE |
| 1 | S | 229 | LEU |
| 1 | S | 244 | SER |
| 1 | S | 245 | ARG |
| 1 | S | 251 | ARG |
| 1 | S | 264 | ASP |
| 1 | S | 273 | SER |
| 1 | S | 274 | ARG |
| 1 | S | 278 | GLN |
| 1 | S | 282 | GLU |
| 1 | S | 287 | ILE |
| 1 | S | 290 | GLN |
| 1 | S | 294 | ASN |
| 1 | S | 298 | GLU |
| 1 | S | 300 | ILE |
| 1 | S | 325 | ILE |
| 1 | S | 331 | LEU |
| 1 | S | 336 | SER |
| 1 | S | 351 | ILE |
| 1 | S | 354 | LEU |
| 1 | S | 364 | LEU |
| 1 | S | 365 | LYS |
| 1 | S | 372 | GLU |
| 1 | S | 376 | GLU |
| 1 | S | 381 | GLU |
| 1 | S | 389 | LEU |
| 1 | S | 392 | LEU |
| 1 | S | 394 | SER |
| 1 | S | 399 | LYS |
| 1 | S | 405 | ARG |
| 1 | S | 410 | ASN |
| 1 | S | 439 | LEU |
| 1 | S | 447 | GLN |
| 1 | S | 448 | GLN |
| 1 | S | 449 | LEU |
| 1 | S | 453 | GLN |
| 1 | S | 455 | ARG |
| 1 | S | 457 | TYR |
| 1 | S | 462 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | S | 471 | ASP |
| 1 | S | 474 | SER |
| 1 | S | 480 | ILE |
| 1 | S | 487 | LEU |
| 1 | S | 495 | MET |
| 1 | S | 499 | GLU |
| 1 | S | 506 | GLU |
| 1 | S | 513 | ILE |
| 1 | S | 518 | ASP |
| 1 | S | 524 | GLU |
| 1 | S | 532 | ILE |
| 1 | S | 534 | SER |
| 1 | S | 537 | GLU |
| 1 | S | 543 | PRO |
| 1 | S | 549 | SER |
| 1 | S | 561 | LYS |
| 1 | S | 562 | SER |
| 1 | S | 563 | ASN |
| 1 | S | 569 | LYS |
| 1 | S | 580 | SER |
| 1 | S | 593 | SER |
| 1 | S | 597 | GLU |
| 1 | S | 604 | ASN |
| 1 | S | 608 | ILE |
| 1 | S | 610 | LEU |
| 1 | S | 615 | SER |
| 1 | S | 621 | LEU |
| 1 | S | 625 | THR |
| 1 | S | 664 | LEU |
| 1 | S | 666 | SER |
| 1 | S | 673 | ARG |
| 1 | S | 675 | ILE |
| 1 | S | 676 | ILE |
| 1 | S | 686 | MET |
| 1 | S | 689 | GLU |
| 1 | S | 690 | LEU |
| 1 | S | 693 | HIS |
| 1 | S | 698 | ASN |
| 1 | S | 701 | LEU |
| 1 | S | 702 | GLU |
| 1 | S | 708 | ARG |
| 1 | S | 713 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | S | 714 | ARG |
| 1 | S | 716 | LEU |
| 1 | S | 719 | ASP |
| 1 | S | 722 | GLN |
| 1 | S | 723 | ARG |
| 1 | S | 727 | LEU |
| 1 | S | 728 | ASN |
| 1 | S | 745 | GLU |
| 1 | S | 752 | ASP |
| 1 | S | 753 | VAL |
| 1 | S | 754 | ASP |
| 1 | S | 762 | HIS |
| 1 | S | 774 | LEU |
| 1 | S | 785 | GLU |
| 1 | S | 787 | ILE |
| 1 | S | 793 | ARG |
| 1 | S | 799 | MET |
| 1 | S | 802 | GLU |
| 1 | S | 804 | ARG |
| 1 | S | 810 | ARG |
| 1 | S | 816 | ILE |
| 1 | S | 822 | SER |
| 1 | S | 832 | MET |
| 1 | S | 834 | LEU |
| 1 | S | 838 | ILE |
| 1 | S | 842 | LEU |
| 1 | S | 843 | LYS |
| 2 | T | 142 | PRO |
| 3 | U | 48 | LYS |
| 3 | U | 68 | PHE |
| 3 | U | 83 | THR |
| 3 | U | 95 | ASP |
| 3 | U | 96 | LYS |
| 4 | 1 | 33 | SER |
| 4 | 1 | 34 | ILE |
| 4 | 1 | 37 | ARG |
| 4 | 1 | 66 | THR |
| 4 | 1 | 72 | GLU |
| 4 | 1 | 80 | ASP |
| 4 | 1 | 100 | GLU |
| 4 | 1 | 109 | PRO |
| 4 | 1 | 116 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 1 | 145 | SER |
| 4 | 1 | 153 | LEU |
| 4 | 1 | 159 | VAL |
| 4 | 1 | 180 | LEU |
| 4 | 1 | 191 | LYS |
| 4 | 1 | 196 | ARG |
| 4 | 1 | 199 | SER |
| 4 | 1 | 201 | VAL |
| 4 | 1 | 206 | ARG |
| 4 | 1 | 221 | LEU |
| 4 | 1 | 223 | PHE |
| 4 | 1 | 229 | THR |
| 4 | 1 | 239 | SER |
| 4 | 1 | 242 | LEU |
| 4 | 1 | 246 | GLN |
| 4 | 1 | 263 | GLN |
| 4 | 1 | 281 | SER |
| 4 | 1 | 283 | MET |
| 4 | 1 | 287 | ILE |
| 4 | 1 | 291 | LYS |
| 4 | 1 | 293 | LEU |
| 4 | 1 | 297 | ASN |
| 4 | 1 | 299 | MET |
| 4 | 1 | 312 | ARG |
| 4 | 1 | 315 | LYS |
| 4 | 1 | 318 | THR |
| 4 | 1 | 320 | LEU |
| 4 | 1 | 327 | ILE |
| 4 | 1 | 334 | GLU |
| 4 | 1 | 349 | LEU |
| 4 | 1 | 350 | SER |
| 4 | 1 | 351 | THR |
| 4 | 1 | 354 | GLN |
| 4 | 1 | 359 | LYS |
| 4 | 1 | 360 | GLN |
| 4 | 1 | 361 | GLU |
| 4 | 1 | 368 | SER |
| 4 | 2 | 16 | LEU |
| 4 | 2 | 33 | SER |
| 4 | 2 | 34 | ILE |
| 4 | 2 | 37 | ARG |
| 4 | 2 | 66 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2 | 72 | GLU |
| 4 | 2 | 80 | ASP |
| 4 | 2 | 100 | GLU |
| 4 | 2 | 109 | PRO |
| 4 | 2 | 116 | ARG |
| 4 | 2 | 145 | SER |
| 4 | 2 | 153 | LEU |
| 4 | 2 | 159 | VAL |
| 4 | 2 | 180 | LEU |
| 4 | 2 | 191 | LYS |
| 4 | 2 | 196 | ARG |
| 4 | 2 | 199 | SER |
| 4 | 2 | 201 | VAL |
| 4 | 2 | 206 | ARG |
| 4 | 2 | 221 | LEU |
| 4 | 2 | 223 | PHE |
| 4 | 2 | 229 | THR |
| 4 | 2 | 239 | SER |
| 4 | 2 | 242 | LEU |
| 4 | 2 | 246 | GLN |
| 4 | 2 | 263 | GLN |
| 4 | 2 | 281 | SER |
| 4 | 2 | 283 | MET |
| 4 | 2 | 287 | ILE |
| 4 | 2 | 291 | LYS |
| 4 | 2 | 293 | LEU |
| 4 | 2 | 297 | ASN |
| 4 | 2 | 299 | MET |
| 4 | 2 | 312 | ARG |
| 4 | 2 | 315 | LYS |
| 4 | 2 | 318 | THR |
| 4 | 2 | 320 | LEU |
| 4 | 2 | 327 | ILE |
| 4 | 2 | 334 | GLU |
| 4 | 2 | 349 | LEU |
| 4 | 2 | 350 | SER |
| 4 | 2 | 351 | THR |
| 4 | 2 | 354 | GLN |
| 4 | 2 | 359 | LYS |
| 4 | 2 | 360 | GLN |
| 4 | 2 | 361 | GLU |
| 4 | 2 | 368 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 3 | 33 | SER |
| 4 | 3 | 34 | ILE |
| 4 | 3 | 37 | ARG |
| 4 | 3 | 66 | THR |
| 4 | 3 | 72 | GLU |
| 4 | 3 | 80 | ASP |
| 4 | 3 | 100 | GLU |
| 4 | 3 | 109 | PRO |
| 4 | 3 | 116 | ARG |
| 4 | 3 | 145 | SER |
| 4 | 3 | 153 | LEU |
| 4 | 3 | 159 | VAL |
| 4 | 3 | 180 | LEU |
| 4 | 3 | 191 | LYS |
| 4 | 3 | 196 | ARG |
| 4 | 3 | 199 | SER |
| 4 | 3 | 201 | VAL |
| 4 | 3 | 206 | ARG |
| 4 | 3 | 221 | LEU |
| 4 | 3 | 223 | PHE |
| 4 | 3 | 229 | THR |
| 4 | 3 | 239 | SER |
| 4 | 3 | 242 | LEU |
| 4 | 3 | 246 | GLN |
| 4 | 3 | 263 | GLN |
| 4 | 3 | 281 | SER |
| 4 | 3 | 283 | MET |
| 4 | 3 | 287 | ILE |
| 4 | 3 | 291 | LYS |
| 4 | 3 | 293 | LEU |
| 4 | 3 | 297 | ASN |
| 4 | 3 | 299 | MET |
| 4 | 3 | 312 | ARG |
| 4 | 3 | 315 | LYS |
| 4 | 3 | 318 | THR |
| 4 | 3 | 320 | LEU |
| 4 | 3 | 327 | ILE |
| 4 | 3 | 334 | GLU |
| 4 | 3 | 349 | LEU |
| 4 | 3 | 350 | SER |
| 4 | 3 | 351 | THR |
| 4 | 3 | 354 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 3 | 359 | LYS |
| 4 | 3 | 360 | GLN |
| 4 | 3 | 361 | GLU |
| 4 | 3 | 368 | SER |
| 4 | 4 | 16 | LEU |
| 4 | 4 | 33 | SER |
| 4 | 4 | 34 | ILE |
| 4 | 4 | 37 | ARG |
| 4 | 4 | 66 | THR |
| 4 | 4 | 72 | GLU |
| 4 | 4 | 80 | ASP |
| 4 | 4 | 100 | GLU |
| 4 | 4 | 109 | PRO |
| 4 | 4 | 116 | ARG |
| 4 | 4 | 145 | SER |
| 4 | 4 | 153 | LEU |
| 4 | 4 | 159 | VAL |
| 4 | 4 | 180 | LEU |
| 4 | 4 | 191 | LYS |
| 4 | 4 | 196 | ARG |
| 4 | 4 | 199 | SER |
| 4 | 4 | 201 | VAL |
| 4 | 4 | 206 | ARG |
| 4 | 4 | 221 | LEU |
| 4 | 4 | 223 | PHE |
| 4 | 4 | 229 | THR |
| 4 | 4 | 239 | SER |
| 4 | 4 | 242 | LEU |
| 4 | 4 | 246 | GLN |
| 4 | 4 | 263 | GLN |
| 4 | 4 | 281 | SER |
| 4 | 4 | 283 | MET |
| 4 | 4 | 287 | ILE |
| 4 | 4 | 291 | LYS |
| 4 | 4 | 293 | LEU |
| 4 | 4 | 297 | ASN |
| 4 | 4 | 299 | MET |
| 4 | 4 | 312 | ARG |
| 4 | 4 | 315 | LYS |
| 4 | 4 | 318 | THR |
| 4 | 4 | 320 | LEU |
| 4 | 4 | 327 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 4 | 334 | GLU |
| 4 | 4 | 349 | LEU |
| 4 | 4 | 350 | SER |
| 4 | 4 | 351 | THR |
| 4 | 4 | 354 | GLN |
| 4 | 4 | 359 | LYS |
| 4 | 4 | 360 | GLN |
| 4 | 4 | 361 | GLU |
| 4 | 4 | 368 | SER |
| 4 | 5 | 33 | SER |
| 4 | 5 | 34 | ILE |
| 4 | 5 | 37 | ARG |
| 4 | 5 | 66 | THR |
| 4 | 5 | 72 | GLU |
| 4 | 5 | 80 | ASP |
| 4 | 5 | 100 | GLU |
| 4 | 5 | 109 | PRO |
| 4 | 5 | 116 | ARG |
| 4 | 5 | 145 | SER |
| 4 | 5 | 153 | LEU |
| 4 | 5 | 159 | VAL |
| 4 | 5 | 180 | LEU |
| 4 | 5 | 191 | LYS |
| 4 | 5 | 196 | ARG |
| 4 | 5 | 199 | SER |
| 4 | 5 | 201 | VAL |
| 4 | 5 | 206 | ARG |
| 4 | 5 | 221 | LEU |
| 4 | 5 | 223 | PHE |
| 4 | 5 | 229 | THR |
| 4 | 5 | 239 | SER |
| 4 | 5 | 242 | LEU |
| 4 | 5 | 246 | GLN |
| 4 | 5 | 263 | GLN |
| 4 | 5 | 281 | SER |
| 4 | 5 | 283 | MET |
| 4 | 5 | 287 | ILE |
| 4 | 5 | 291 | LYS |
| 4 | 5 | 293 | LEU |
| 4 | 5 | 297 | ASN |
| 4 | 5 | 299 | MET |
| 4 | 5 | 312 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 5 | 315 | LYS |
| 4 | 5 | 318 | THR |
| 4 | 5 | 320 | LEU |
| 4 | 5 | 327 | ILE |
| 4 | 5 | 334 | GLU |
| 4 | 5 | 349 | LEU |
| 4 | 5 | 350 | SER |
| 4 | 5 | 351 | THR |
| 4 | 5 | 354 | GLN |
| 4 | 5 | 359 | LYS |
| 4 | 5 | 360 | GLN |
| 4 | 5 | 361 | GLU |
| 4 | 5 | 368 | SER |
| 4 | 6 | 33 | SER |
| 4 | 6 | 34 | ILE |
| 4 | 6 | 37 | ARG |
| 4 | 6 | 66 | THR |
| 4 | 6 | 72 | GLU |
| 4 | 6 | 80 | ASP |
| 4 | 6 | 100 | GLU |
| 4 | 6 | 109 | PRO |
| 4 | 6 | 116 | ARG |
| 4 | 6 | 145 | SER |
| 4 | 6 | 153 | LEU |
| 4 | 6 | 159 | VAL |
| 4 | 6 | 180 | LEU |
| 4 | 6 | 191 | LYS |
| 4 | 6 | 196 | ARG |
| 4 | 6 | 199 | SER |
| 4 | 6 | 201 | VAL |
| 4 | 6 | 206 | ARG |
| 4 | 6 | 221 | LEU |
| 4 | 6 | 223 | PHE |
| 4 | 6 | 229 | THR |
| 4 | 6 | 239 | SER |
| 4 | 6 | 242 | LEU |
| 4 | 6 | 246 | GLN |
| 4 | 6 | 263 | GLN |
| 4 | 6 | 281 | SER |
| 4 | 6 | 283 | MET |
| 4 | 6 | 287 | ILE |
| 4 | 6 | 291 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 6 | 293 | LEU |
| 4 | 6 | 297 | ASN |
| 4 | 6 | 299 | MET |
| 4 | 6 | 312 | ARG |
| 4 | 6 | 315 | LYS |
| 4 | 6 | 318 | THR |
| 4 | 6 | 320 | LEU |
| 4 | 6 | 327 | ILE |
| 4 | 6 | 334 | GLU |
| 4 | 6 | 349 | LEU |
| 4 | 6 | 350 | SER |
| 4 | 6 | 351 | THR |
| 4 | 6 | 354 | GLN |
| 4 | 6 | 359 | LYS |
| 4 | 6 | 360 | GLN |
| 4 | 6 | 361 | GLU |
| 4 | 6 | 368 | SER |
| 4 | 7 | 16 | LEU |
| 4 | 7 | 33 | SER |
| 4 | 7 | 34 | ILE |
| 4 | 7 | 37 | ARG |
| 4 | 7 | 66 | THR |
| 4 | 7 | 72 | GLU |
| 4 | 7 | 80 | ASP |
| 4 | 7 | 100 | GLU |
| 4 | 7 | 109 | PRO |
| 4 | 7 | 116 | ARG |
| 4 | 7 | 145 | SER |
| 4 | 7 | 153 | LEU |
| 4 | 7 | 159 | VAL |
| 4 | 7 | 180 | LEU |
| 4 | 7 | 191 | LYS |
| 4 | 7 | 196 | ARG |
| 4 | 7 | 199 | SER |
| 4 | 7 | 201 | VAL |
| 4 | 7 | 206 | ARG |
| 4 | 7 | 221 | LEU |
| 4 | 7 | 223 | PHE |
| 4 | 7 | 229 | THR |
| 4 | 7 | 239 | SER |
| 4 | 7 | 242 | LEU |
| 4 | 7 | 246 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 7 | 263 | GLN |
| 4 | 7 | 281 | SER |
| 4 | 7 | 283 | MET |
| 4 | 7 | 287 | ILE |
| 4 | 7 | 291 | LYS |
| 4 | 7 | 293 | LEU |
| 4 | 7 | 297 | ASN |
| 4 | 7 | 299 | MET |
| 4 | 7 | 312 | ARG |
| 4 | 7 | 315 | LYS |
| 4 | 7 | 318 | THR |
| 4 | 7 | 320 | LEU |
| 4 | 7 | 327 | ILE |
| 4 | 7 | 334 | GLU |
| 4 | 7 | 349 | LEU |
| 4 | 7 | 350 | SER |
| 4 | 7 | 351 | THR |
| 4 | 7 | 354 | GLN |
| 4 | 7 | 359 | LYS |
| 4 | 7 | 360 | GLN |
| 4 | 7 | 361 | GLU |
| 4 | 7 | 368 | SER |
| 4 | 8 | 16 | LEU |
| 4 | 8 | 33 | SER |
| 4 | 8 | 34 | ILE |
| 4 | 8 | 37 | ARG |
| 4 | 8 | 66 | THR |
| 4 | 8 | 72 | GLU |
| 4 | 8 | 80 | ASP |
| 4 | 8 | 100 | GLU |
| 4 | 8 | 109 | PRO |
| 4 | 8 | 116 | ARG |
| 4 | 8 | 145 | SER |
| 4 | 8 | 153 | LEU |
| 4 | 8 | 159 | VAL |
| 4 | 8 | 180 | LEU |
| 4 | 8 | 191 | LYS |
| 4 | 8 | 196 | ARG |
| 4 | 8 | 199 | SER |
| 4 | 8 | 201 | VAL |
| 4 | 8 | 206 | ARG |
| 4 | 8 | 221 | LEU |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 8 | 223 | PHE |
| 4 | 8 | 229 | THR |
| 4 | 8 | 239 | SER |
| 4 | 8 | 242 | LEU |
| 4 | 8 | 246 | GLN |
| 4 | 8 | 263 | GLN |
| 4 | 8 | 281 | SER |
| 4 | 8 | 283 | MET |
| 4 | 8 | 287 | ILE |
| 4 | 8 | 291 | LYS |
| 4 | 8 | 293 | LEU |
| 4 | 8 | 297 | ASN |
| 4 | 8 | 299 | MET |
| 4 | 8 | 312 | ARG |
| 4 | 8 | 315 | LYS |
| 4 | 8 | 318 | THR |
| 4 | 8 | 320 | LEU |
| 4 | 8 | 327 | ILE |
| 4 | 8 | 334 | GLU |
| 4 | 8 | 349 | LEU |
| 4 | 8 | 350 | SER |
| 4 | 8 | 351 | THR |
| 4 | 8 | 354 | GLN |
| 4 | 8 | 359 | LYS |
| 4 | 8 | 360 | GLN |
| 4 | 8 | 361 | GLU |
| 4 | 8 | 368 | SER |
| 4 | 9 | 16 | LEU |
| 4 | 9 | 33 | SER |
| 4 | 9 | 34 | ILE |
| 4 | 9 | 37 | ARG |
| 4 | 9 | 66 | THR |
| 4 | 9 | 72 | GLU |
| 4 | 9 | 80 | ASP |
| 4 | 9 | 100 | GLU |
| 4 | 9 | 109 | PRO |
| 4 | 9 | 116 | ARG |
| 4 | 9 | 145 | SER |
| 4 | 9 | 153 | LEU |
| 4 | 9 | 159 | VAL |
| 4 | 9 | 180 | LEU |
| 4 | 9 | 191 | LYS |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 9 | 196 | ARG |
| 4 | 9 | 199 | SER |
| 4 | 9 | 201 | VAL |
| 4 | 9 | 206 | ARG |
| 4 | 9 | 221 | LEU |
| 4 | 9 | 223 | PHE |
| 4 | 9 | 229 | THR |
| 4 | 9 | 239 | SER |
| 4 | 9 | 242 | LEU |
| 4 | 9 | 246 | GLN |
| 4 | 9 | 263 | GLN |
| 4 | 9 | 281 | SER |
| 4 | 9 | 283 | MET |
| 4 | 9 | 287 | ILE |
| 4 | 9 | 291 | LYS |
| 4 | 9 | 293 | LEU |
| 4 | 9 | 297 | ASN |
| 4 | 9 | 299 | MET |
| 4 | 9 | 312 | ARG |
| 4 | 9 | 315 | LYS |
| 4 | 9 | 318 | THR |
| 4 | 9 | 320 | LEU |
| 4 | 9 | 327 | ILE |
| 4 | 9 | 334 | GLU |
| 4 | 9 | 349 | LEU |
| 4 | 9 | 350 | SER |
| 4 | 9 | 351 | THR |
| 4 | 9 | 354 | GLN |
| 4 | 9 | 359 | LYS |
| 4 | 9 | 360 | GLN |
| 4 | 9 | 361 | GLU |
| 4 | 9 | 368 | SER |
| 4 | V | 33 | SER |
| 4 | V | 34 | ILE |
| 4 | V | 37 | ARG |
| 4 | V | 66 | THR |
| 4 | V | 72 | GLU |
| 4 | V | 80 | ASP |
| 4 | V | 100 | GLU |
| 4 | V | 109 | PRO |
| 4 | V | 116 | ARG |
| 4 | V | 145 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | V | 153 | LEU |
| 4 | V | 159 | VAL |
| 4 | V | 180 | LEU |
| 4 | V | 191 | LYS |
| 4 | V | 196 | ARG |
| 4 | V | 199 | SER |
| 4 | V | 201 | VAL |
| 4 | V | 206 | ARG |
| 4 | V | 221 | LEU |
| 4 | V | 223 | PHE |
| 4 | V | 229 | THR |
| 4 | V | 239 | SER |
| 4 | V | 242 | LEU |
| 4 | V | 246 | GLN |
| 4 | V | 263 | GLN |
| 4 | V | 281 | SER |
| 4 | V | 283 | MET |
| 4 | V | 287 | ILE |
| 4 | V | 291 | LYS |
| 4 | V | 293 | LEU |
| 4 | V | 297 | ASN |
| 4 | V | 299 | MET |
| 4 | V | 312 | ARG |
| 4 | V | 315 | LYS |
| 4 | V | 318 | THR |
| 4 | V | 320 | LEU |
| 4 | V | 327 | ILE |
| 4 | V | 334 | GLU |
| 4 | V | 349 | LEU |
| 4 | V | 350 | SER |
| 4 | V | 351 | THR |
| 4 | V | 354 | GLN |
| 4 | V | 359 | LYS |
| 4 | V | 360 | GLN |
| 4 | V | 361 | GLU |
| 4 | V | 368 | SER |
| 4 | W | 16 | LEU |
| 4 | W | 33 | SER |
| 4 | W | 34 | ILE |
| 4 | W | 37 | ARG |
| 4 | W | 66 | THR |
| 4 | W | 72 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | W | 80 | ASP |
| 4 | W | 100 | GLU |
| 4 | W | 109 | PRO |
| 4 | W | 116 | ARG |
| 4 | W | 145 | SER |
| 4 | W | 153 | LEU |
| 4 | W | 159 | VAL |
| 4 | W | 180 | LEU |
| 4 | W | 191 | LYS |
| 4 | W | 196 | ARG |
| 4 | W | 199 | SER |
| 4 | W | 201 | VAL |
| 4 | W | 206 | ARG |
| 4 | W | 221 | LEU |
| 4 | W | 223 | PHE |
| 4 | W | 229 | THR |
| 4 | W | 239 | SER |
| 4 | W | 242 | LEU |
| 4 | W | 246 | GLN |
| 4 | W | 263 | GLN |
| 4 | W | 281 | SER |
| 4 | W | 283 | MET |
| 4 | W | 287 | ILE |
| 4 | W | 291 | LYS |
| 4 | W | 293 | LEU |
| 4 | W | 297 | ASN |
| 4 | W | 299 | MET |
| 4 | W | 312 | ARG |
| 4 | W | 315 | LYS |
| 4 | W | 318 | THR |
| 4 | W | 320 | LEU |
| 4 | W | 327 | ILE |
| 4 | W | 334 | GLU |
| 4 | W | 349 | LEU |
| 4 | W | 350 | SER |
| 4 | W | 351 | THR |
| 4 | W | 354 | GLN |
| 4 | W | 359 | LYS |
| 4 | W | 360 | GLN |
| 4 | W | 361 | GLU |
| 4 | W | 368 | SER |
| 4 | X | 33 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | X | 34 | ILE |
| 4 | X | 37 | ARG |
| 4 | X | 66 | THR |
| 4 | X | 72 | GLU |
| 4 | X | 80 | ASP |
| 4 | X | 100 | GLU |
| 4 | X | 109 | PRO |
| 4 | X | 116 | ARG |
| 4 | X | 145 | SER |
| 4 | X | 153 | LEU |
| 4 | X | 159 | VAL |
| 4 | X | 180 | LEU |
| 4 | X | 191 | LYS |
| 4 | X | 196 | ARG |
| 4 | X | 199 | SER |
| 4 | X | 201 | VAL |
| 4 | X | 206 | ARG |
| 4 | X | 221 | LEU |
| 4 | X | 223 | PHE |
| 4 | X | 229 | THR |
| 4 | X | 239 | SER |
| 4 | X | 242 | LEU |
| 4 | X | 246 | GLN |
| 4 | X | 263 | GLN |
| 4 | X | 281 | SER |
| 4 | X | 283 | MET |
| 4 | X | 287 | ILE |
| 4 | X | 291 | LYS |
| 4 | X | 293 | LEU |
| 4 | X | 297 | ASN |
| 4 | X | 299 | MET |
| 4 | X | 312 | ARG |
| 4 | X | 315 | LYS |
| 4 | X | 318 | THR |
| 4 | X | 320 | LEU |
| 4 | X | 327 | ILE |
| 4 | X | 334 | GLU |
| 4 | X | 349 | LEU |
| 4 | X | 350 | SER |
| 4 | X | 351 | THR |
| 4 | X | 354 | GLN |
| 4 | X | 359 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | X | 360 | GLN |
| 4 | X | 361 | GLU |
| 4 | X | 368 | SER |
| 4 | Y | 33 | SER |
| 4 | Y | 34 | ILE |
| 4 | Y | 37 | ARG |
| 4 | Y | 66 | THR |
| 4 | Y | 72 | GLU |
| 4 | Y | 80 | ASP |
| 4 | Y | 100 | GLU |
| 4 | Y | 109 | PRO |
| 4 | Y | 116 | ARG |
| 4 | Y | 145 | SER |
| 4 | Y | 153 | LEU |
| 4 | Y | 159 | VAL |
| 4 | Y | 180 | LEU |
| 4 | Y | 191 | LYS |
| 4 | Y | 196 | ARG |
| 4 | Y | 199 | SER |
| 4 | Y | 201 | VAL |
| 4 | Y | 206 | ARG |
| 4 | Y | 221 | LEU |
| 4 | Y | 223 | PHE |
| 4 | Y | 229 | THR |
| 4 | Y | 239 | SER |
| 4 | Y | 242 | LEU |
| 4 | Y | 246 | GLN |
| 4 | Y | 263 | GLN |
| 4 | Y | 281 | SER |
| 4 | Y | 283 | MET |
| 4 | Y | 287 | ILE |
| 4 | Y | 291 | LYS |
| 4 | Y | 293 | LEU |
| 4 | Y | 297 | ASN |
| 4 | Y | 299 | MET |
| 4 | Y | 312 | ARG |
| 4 | Y | 315 | LYS |
| 4 | Y | 318 | THR |
| 4 | Y | 320 | LEU |
| 4 | Y | 327 | ILE |
| 4 | Y | 334 | GLU |
| 4 | Y | 349 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | Y | 350 | SER |
| 4 | Y | 351 | THR |
| 4 | Y | 354 | GLN |
| 4 | Y | 359 | LYS |
| 4 | Y | 360 | GLN |
| 4 | Y | 361 | GLU |
| 4 | Y | 368 | SER |
| 4 | Z | 16 | LEU |
| 4 | Z | 33 | SER |
| 4 | Z | 34 | ILE |
| 4 | Z | 37 | ARG |
| 4 | Z | 66 | THR |
| 4 | Z | 72 | GLU |
| 4 | Z | 80 | ASP |
| 4 | Z | 100 | GLU |
| 4 | Z | 109 | PRO |
| 4 | Z | 116 | ARG |
| 4 | Z | 145 | SER |
| 4 | Z | 153 | LEU |
| 4 | Z | 159 | VAL |
| 4 | Z | 180 | LEU |
| 4 | Z | 191 | LYS |
| 4 | Z | 196 | ARG |
| 4 | Z | 199 | SER |
| 4 | Z | 201 | VAL |
| 4 | Z | 206 | ARG |
| 4 | Z | 221 | LEU |
| 4 | Z | 223 | PHE |
| 4 | Z | 229 | THR |
| 4 | Z | 239 | SER |
| 4 | Z | 242 | LEU |
| 4 | Z | 246 | GLN |
| 4 | Z | 263 | GLN |
| 4 | Z | 281 | SER |
| 4 | Z | 283 | MET |
| 4 | Z | 287 | ILE |
| 4 | Z | 291 | LYS |
| 4 | Z | 293 | LEU |
| 4 | Z | 297 | ASN |
| 4 | Z | 299 | MET |
| 4 | Z | 312 | ARG |
| 4 | Z | 315 | LYS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | Z | 318 | THR |
| 4 | Z | 320 | LEU |
| 4 | Z | 327 | ILE |
| 4 | Z | 334 | GLU |
| 4 | Z | 349 | LEU |
| 4 | Z | 350 | SER |
| 4 | Z | 351 | THR |
| 4 | Z | 354 | GLN |
| 4 | Z | 359 | LYS |
| 4 | Z | 360 | GLN |
| 4 | Z | 361 | GLU |
| 4 | Z | 368 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (236) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 28 | GLN |
| 1 | A | 29 | ASN |
| 1 | A | 127 | ASN |
| 1 | A | 164 | GLN |
| 1 | A | 188 | ASN |
| 1 | A | 194 | GLN |
| 1 | A | 221 | GLN |
| 1 | A | 253 | HIS |
| 1 | A | 290 | GLN |
| 1 | A | 368 | GLN |
| 1 | A | 424 | ASN |
| 1 | A | 447 | GLN |
| 1 | A | 453 | GLN |
| 1 | A | 481 | ASN |
| 1 | A | 484 | ASN |
| 1 | A | 563 | ASN |
| 1 | A | 564 | ASN |
| 1 | A | 578 | HIS |
| 1 | A | 612 | GLN |
| 1 | A | 656 | ASN |
| 1 | A | 670 | HIS |
| 1 | A | 698 | ASN |
| 1 | A | 757 | GLN |
| 1 | A | 762 | HIS |
| 1 | A | 791 | GLN |
| 2 | B | 159 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 39 | GLN |
| 3 | C | 52 | ASN |
| 1 | D | 29 | ASN |
| 1 | D | 127 | ASN |
| 1 | D | 149 | GLN |
| 1 | D | 164 | GLN |
| 1 | D | 188 | ASN |
| 1 | D | 194 | GLN |
| 1 | D | 221 | GLN |
| 1 | D | 253 | HIS |
| 1 | D | 290 | GLN |
| 1 | D | 368 | GLN |
| 1 | D | 424 | ASN |
| 1 | D | 447 | GLN |
| 1 | D | 453 | GLN |
| 1 | D | 481 | ASN |
| 1 | D | 484 | ASN |
| 1 | D | 563 | ASN |
| 1 | D | 564 | ASN |
| 1 | D | 578 | HIS |
| 1 | D | 612 | GLN |
| 1 | D | 656 | ASN |
| 1 | D | 670 | HIS |
| 1 | D | 698 | ASN |
| 1 | D | 757 | GLN |
| 1 | D | 762 | HIS |
| 1 | D | 791 | GLN |
| 2 | E | 159 | HIS |
| 3 | F | 39 | GLN |
| 3 | F | 40 | ASN |
| 3 | F | 52 | ASN |
| 1 | G | 29 | ASN |
| 1 | G | 127 | ASN |
| 1 | G | 149 | GLN |
| 1 | G | 164 | GLN |
| 1 | G | 188 | ASN |
| 1 | G | 194 | GLN |
| 1 | G | 221 | GLN |
| 1 | G | 253 | HIS |
| 1 | G | 290 | GLN |
| 1 | G | 368 | GLN |
| 1 | G | 424 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 447 | GLN |
| 1 | G | 453 | GLN |
| 1 | G | 481 | ASN |
| 1 | G | 484 | ASN |
| 1 | G | 563 | ASN |
| 1 | G | 564 | ASN |
| 1 | G | 578 | HIS |
| 1 | G | 612 | GLN |
| 1 | G | 656 | ASN |
| 1 | G | 670 | HIS |
| 1 | G | 762 | HIS |
| 1 | G | 791 | GLN |
| 3 | I | 39 | GLN |
| 3 | I | 52 | ASN |
| 3 | I | 81 | GLN |
| 3 | I | 109 | HIS |
| 1 | J | 29 | ASN |
| 1 | J | 127 | ASN |
| 1 | J | 164 | GLN |
| 1 | J | 188 | ASN |
| 1 | J | 194 | GLN |
| 1 | J | 221 | GLN |
| 1 | J | 253 | HIS |
| 1 | J | 290 | GLN |
| 1 | J | 368 | GLN |
| 1 | J | 424 | ASN |
| 1 | J | 453 | GLN |
| 1 | J | 481 | ASN |
| 1 | J | 484 | ASN |
| 1 | J | 563 | ASN |
| 1 | J | 564 | ASN |
| 1 | J | 578 | HIS |
| 1 | J | 612 | GLN |
| 1 | J | 656 | ASN |
| 1 | J | 670 | HIS |
| 1 | J | 698 | ASN |
| 1 | J | 762 | HIS |
| 1 | J | 791 | GLN |
| 2 | K | 159 | HIS |
| 3 | L | 40 | ASN |
| 3 | L | 52 | ASN |
| 1 | M | 29 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 127 | ASN |
| 1 | M | 149 | GLN |
| 1 | M | 164 | GLN |
| 1 | M | 188 | ASN |
| 1 | M | 194 | GLN |
| 1 | M | 221 | GLN |
| 1 | M | 253 | HIS |
| 1 | M | 290 | GLN |
| 1 | M | 368 | GLN |
| 1 | M | 424 | ASN |
| 1 | M | 447 | GLN |
| 1 | M | 453 | GLN |
| 1 | M | 481 | ASN |
| 1 | M | 484 | ASN |
| 1 | M | 563 | ASN |
| 1 | M | 564 | ASN |
| 1 | M | 578 | HIS |
| 1 | M | 612 | GLN |
| 1 | M | 656 | ASN |
| 1 | M | 670 | HIS |
| 1 | M | 757 | GLN |
| 1 | M | 762 | HIS |
| 3 | O | 39 | GLN |
| 3 | O | 52 | ASN |
| 1 | S | 29 | ASN |
| 1 | S | 127 | ASN |
| 1 | S | 164 | GLN |
| 1 | S | 188 | ASN |
| 1 | S | 194 | GLN |
| 1 | S | 221 | GLN |
| 1 | S | 253 | HIS |
| 1 | S | 290 | GLN |
| 1 | S | 368 | GLN |
| 1 | S | 424 | ASN |
| 1 | S | 453 | GLN |
| 1 | S | 481 | ASN |
| 1 | S | 484 | ASN |
| 1 | S | 563 | ASN |
| 1 | S | 564 | ASN |
| 1 | S | 578 | HIS |
| 1 | S | 612 | GLN |
| 1 | S | 656 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | S | 670 | HIS |
| 1 | S | 698 | ASN |
| 2 | T | 159 | HIS |
| 3 | U | 40 | ASN |
| 3 | U | 52 | ASN |
| 4 | 1 | 41 | GLN |
| 4 | 1 | 87 | HIS |
| 4 | 1 | 92 | ASN |
| 4 | 1 | 137 | GLN |
| 4 | 1 | 252 | ASN |
| 4 | 1 | 263 | GLN |
| 4 | 1 | 354 | GLN |
| 4 | 2 | 41 | GLN |
| 4 | 2 | 92 | ASN |
| 4 | 2 | 137 | GLN |
| 4 | 2 | 252 | ASN |
| 4 | 2 | 263 | GLN |
| 4 | 3 | 41 | GLN |
| 4 | 3 | 92 | ASN |
| 4 | 3 | 137 | GLN |
| 4 | 3 | 252 | ASN |
| 4 | 3 | 263 | GLN |
| 4 | 3 | 354 | GLN |
| 4 | 4 | 49 | GLN |
| 4 | 4 | 92 | ASN |
| 4 | 4 | 137 | GLN |
| 4 | 4 | 252 | ASN |
| 4 | 4 | 263 | GLN |
| 4 | 4 | 354 | GLN |
| 4 | 5 | 41 | GLN |
| 4 | 5 | 92 | ASN |
| 4 | 5 | 137 | GLN |
| 4 | 5 | 252 | ASN |
| 4 | 5 | 263 | GLN |
| 4 | 5 | 354 | GLN |
| 4 | 6 | 41 | GLN |
| 4 | 6 | 92 | ASN |
| 4 | 6 | 137 | GLN |
| 4 | 6 | 252 | ASN |
| 4 | 6 | 263 | GLN |
| 4 | 6 | 354 | GLN |
| 4 | 7 | 41 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 7 | 92 | ASN |
| 4 | 7 | 137 | GLN |
| 4 | 7 | 252 | ASN |
| 4 | 7 | 263 | GLN |
| 4 | 7 | 354 | GLN |
| 4 | 8 | 41 | GLN |
| 4 | 8 | 92 | ASN |
| 4 | 8 | 137 | GLN |
| 4 | 8 | 252 | ASN |
| 4 | 8 | 263 | GLN |
| 4 | 9 | 41 | GLN |
| 4 | 9 | 92 | ASN |
| 4 | 9 | 137 | GLN |
| 4 | 9 | 252 | ASN |
| 4 | 9 | 263 | GLN |
| 4 | V | 41 | GLN |
| 4 | V | 92 | ASN |
| 4 | V | 137 | GLN |
| 4 | V | 252 | ASN |
| 4 | V | 263 | GLN |
| 4 | W | 41 | GLN |
| 4 | W | 92 | ASN |
| 4 | W | 137 | GLN |
| 4 | W | 252 | ASN |
| 4 | W | 263 | GLN |
| 4 | X | 41 | GLN |
| 4 | X | 92 | ASN |
| 4 | X | 137 | GLN |
| 4 | X | 252 | ASN |
| 4 | X | 263 | GLN |
| 4 | X | 354 | GLN |
| 4 | Y | 41 | GLN |
| 4 | Y | 92 | ASN |
| 4 | Y | 137 | GLN |
| 4 | Y | 252 | ASN |
| 4 | Y | 263 | GLN |
| 4 | Y | 354 | GLN |
| 4 | Z | 41 | GLN |
| 4 | Z | 92 | ASN |
| 4 | Z | 137 | GLN |
| 4 | Z | 252 | ASN |
| 4 | Z | 263 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

270 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 1 | MLY | A | 107 | 1 | 10,10,11 | 0.48 | 0 | 8,11,13 | 1.02 | 1 (12%) |
| 1 | MLY | A | 130 | 1 | 10,10,11 | 0.99 | 1 (10%) | 8,11,13 | 1.32 | 2 (25%) |
| 1 | MLY | A | 138 | 1 | 10,10,11 | 1.35 | 1 (10%) | 8,11,13 | 2.71 | 1 (12%) |
| 1 | MLY | A | 19 | 1 | 10,10,11 | 1.19 | 1 (10%) | 8,11,13 | 0.63 | 0 |
| 1 | MLY | A | 190 | 1 | 10,10,11 | 1.18 | 1 (10%) | 8,11,13 | 1.33 | 1 (12%) |
| 1 | MLY | A | 236 | 1 | 10,10,11 | 1.10 | 1 (10%) | 8,11,13 | 1.56 | 2 (25%) |
| 1 | MLY | A | 248 | 1 | 10,10,11 | 0.76 | 0 | 8,11,13 | 0.85 | 0 |
| 1 | MLY | A | 272 | 1 | 10,10,11 | 1.08 | 1 (10%) | 8,11,13 | 1.32 | 1 (12%) |
| 1 | MLY | A | 295 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 0.30 | 0 |
| 1 | MLY | A | 296 | 1 | 10,10,11 | 0.85 | 0 | 8,11,13 | 1.20 | 1 (12%) |
| 1 | MLY | A | 30 | 1 | 10,10,11 | 0.87 | 0 | 8,11,13 | 0.91 | 0 |
| 1 | MLY | A | 348 | 1 | 10,10,11 | 0.76 | 0 | 8,11,13 | 1.09 | 1 (12%) |
| 1 | MLY | A | 35 | 1 | 10,10,11 | 0.73 | 0 | 8,11,13 | 0.65 | 0 |
| 1 | MLY | A | 353 | 1 | 10,10,11 | 1.00 | 0 | 8,11,13 | 1.03 | 1 (12%) |
| 1 | MLY | A | 367 | 1 | 10,10,11 | 0.90 | 1 (10%) | 8,11,13 | 0.43 | 0 |
| 1 | MLY | A | 369 | 1 | 10,10,11 | 0.85 | 0 | 8,11,13 | 0.77 | 0 |
| 1 | MLY | A | 385 | 1 | 10,10,11 | 0.93 | 1 (10%) | 8,11,13 | 0.53 | 0 |
| 1 | MLY | A | 415 | 1 | 10,10,11 | 0.72 | 0 | 8,11,13 | 0.74 | 0 |
| 1 | MLY | A | 431 | 1 | 10,10,11 | 0.47 | 0 | 8,11,13 | 1.19 | 1 (12%) |
| 1 | MLY | A | 436 | 1 | 10,10,11 | 1.02 | 1 (10%) | 8,11,13 | 1.78 | 1 (12%) |
| 1 | MLY | A | 486 | 1 | 10,10,11 | 0.57 | 0 | 8,11,13 | 0.55 | 0 |
| 1 | MLY | A | 49 | 1 | 10,10,11 | 1.09 | 1 (10%) | 8,11,13 | 1.25 | 1 (12%) |
| 1 | MLY | A | 504 | 1 | 10,10,11 | 0.83 | 0 | 8,11,13 | 0.46 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | A | 505 | 1 | 10,10,11 | 1.43 | 2 (20%) | 8,11,13 | 0.51 | 0 |
| 1 | MLY | A | 528 | 1 | 10,10,11 | 0.85 | 0 | 8,11,13 | 1.13 | 1 (12%) |
| 1 | MLY | A | 55 | 1 | 10,10,11 | 0.95 | 1 (10%) | 8,11,13 | 1.09 | 0 |
| 1 | MLY | A | 551 | 1 | 10,10,11 | 0.62 | 0 | 8,11,13 | 0.73 | 0 |
| 1 | MLY | A | 553 | 1,4 | 10,10,11 | 0.65 | 0 | 8,11,13 | 0.65 | 0 |
| 1 | MLY | A | 59 | 1 | 10,10,11 | 0.80 | 0 | 8,11,13 | 1.16 | 1 (12%) |
| 1 | MLY | A | 598 | 1 | 10,10,11 | 1.16 | 2 (20%) | 8,11,13 | 1.30 | 1 (12%) |
| 1 | MLY | A | 600 | 1 | 10,10,11 | 0.60 | 0 | 8,11,13 | 0.98 | 1 (12%) |
| 1 | MLY | A | 613 | 1 | 10,10,11 | 0.64 | 0 | 8,11,13 | 1.10 | 1 (12%) |
| 1 | MLY | A | 617 | 1 | 10,10,11 | 0.89 | 1 (10%) | 8,11,13 | 0.59 | 0 |
| 1 | MLY | A | 63 | 1 | 10,10,11 | 0.91 | 1 (10%) | 8,11,13 | 0.79 | 0 |
| 1 | MLY | A | 659 | 1 | 10,10,11 | 0.74 | 0 | 8,11,13 | 0.84 | 0 |
| 1 | MLY | A | 681 | 1 | 10,10,11 | 0.99 | 1 (10%) | 8,11,13 | 1.44 | 1 (12%) |
| 1 | MLY | A | 764 | 1 | 10,10,11 | 0.80 | 0 | 8,11,13 | 0.50 | 0 |
| 1 | MLY | A | 768 | 1 | 10,10,11 | 0.87 | 0 | 8,11,13 | 1.96 | 1 (12%) |
| 1 | MLY | A | 782 | 1 | 10,10,11 | 0.74 | 0 | 8,11,13 | 1.55 | 1 (12%) |
| 1 | MLY | A | 827 | 1 | 10,10,11 | 1.00 | 1 (10%) | 8,11,13 | 0.93 | 1 (12%) |
| 1 | MLY | A | 833 | 1 | 10,10,11 | 1.07 | 1 (10%) | 8,11,13 | 1.11 | 1 (12%) |
| 1 | MLY | A | 837 | 1 | 10,10,11 | 0.68 | 0 | 8,11,13 | 0.55 | 0 |
| 1 | MLY | A | 839 | 1 | 10,10,11 | 0.64 | 0 | 8,11,13 | 1.51 | 1 (12%) |
| 1 | MLY | A | 84 | 1 | 10,10,11 | 0.56 | 0 | 8,11,13 | 0.79 | 0 |
| 1 | MLY | A | 87 | 1 | 10,10,11 | 1.11 | 1 (10%) | 8,11,13 | 0.59 | 0 |
| 1 | MLY | D | 107 | 1 | 10,10,11 | 0.50 | 0 | 8,11,13 | 1.03 | 1 (12%) |
| 1 | MLY | D | 130 | 1 | 10,10,11 | 0.98 | 1 (10%) | 8,11,13 | 1.34 | 2 (25%) |
| 1 | MLY | D | 138 | 1 | 10,10,11 | 1.38 | 1 (10%) | 8,11,13 | 2.70 | 1 (12%) |
| 1 | MLY | D | 19 | 1 | 10,10,11 | 1.28 | 2 (20%) | 8,11,13 | 0.63 | 0 |
| 1 | MLY | D | 190 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 1.33 | 1 (12%) |
| 1 | MLY | D | 236 | 1 | 10,10,11 | 1.11 | 1 (10%) | 8,11,13 | 1.54 | 2 (25%) |
| 1 | MLY | D | 248 | 1 | 10,10,11 | 0.79 | 0 | 8,11,13 | 0.85 | 0 |
| 1 | MLY | D | 272 | 1 | 10,10,11 | 1.03 | 1 (10%) | 8,11,13 | 1.34 | 1 (12%) |
| 1 | MLY | D | 295 | 1 | 10,10,11 | 1.12 | 1 (10%) | 8,11,13 | 0.33 | 0 |
| 1 | MLY | D | 296 | 1 | 10,10,11 | 0.85 | 0 | 8,11,13 | 1.20 | 1 (12%) |
| 1 | MLY | D | 30 | 1 | 10,10,11 | 0.90 | 0 | 8,11,13 | 0.94 | 0 |
| 1 | MLY | D | 348 | 1 | 10,10,11 | 0.76 | 0 | 8,11,13 | 1.07 | 1 (12%) |
| 1 | MLY | D | 35 | 1 | 10,10,11 | 0.74 | 0 | 8,11,13 | 0.63 | 0 |
| 1 | MLY | D | 353 | 1 | 10,10,11 | 0.97 | 0 | 8,11,13 | 1.02 | 1 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | D | 367 | 1 | 10,10,11 | 0.87 | 1 (10%) | 8,11,13 | 0.41 | 0 |
| 1 | MLY | D | 369 | 1 | 10,10,11 | 0.85 | 0 | 8,11,13 | 0.76 | 0 |
| 1 | MLY | D | 385 | 1 | 10,10,11 | 0.91 | 1 (10%) | 8,11,13 | 0.55 | 0 |
| 1 | MLY | D | 415 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.76 | 0 |
| 1 | MLY | D | 431 | 1 | 10,10,11 | 0.49 | 0 | 8,11,13 | 1.21 | 1 (12%) |
| 1 | MLY | D | 436 | 1 | 10,10,11 | 1.04 | 1 (10%) | 8,11,13 | 1.75 | 1 (12%) |
| 1 | MLY | D | 486 | 1 | 10,10,11 | 0.58 | 0 | 8,11,13 | 0.55 | 0 |
| 1 | MLY | D | 49 | 1 | 10,10,11 | 1.10 | 1 (10%) | 8,11,13 | 1.25 | 1 (12%) |
| 1 | MLY | D | 504 | 1 | 10,10,11 | 0.82 | 0 | 8,11,13 | 0.45 | 0 |
| 1 | MLY | D | 505 | 1 | 10,10,11 | 1.44 | 2 (20%) | 8,11,13 | 0.51 | 0 |
| 1 | MLY | D | 528 | 1 | 10,10,11 | 0.88 | 0 | 8,11,13 | 1.12 | 1 (12%) |
| 1 | MLY | D | 55 | 1 | 10,10,11 | 0.96 | 1 (10%) | 8,11,13 | 1.06 | 0 |
| 1 | MLY | D | 551 | 1 | 10,10,11 | 0.61 | 0 | 8,11,13 | 0.74 | 0 |
| 1 | MLY | D | 553 | 1,4 | 10,10,11 | 0.65 | 0 | 8,11,13 | 0.67 | 0 |
| 1 | MLY | D | 59 | 1 | 10,10,11 | 0.79 | 0 | 8,11,13 | 1.14 | 1 (12%) |
| 1 | MLY | D | 598 | 1 | 10,10,11 | 1.15 | 2 (20%) | 8,11,13 | 1.29 | 1 (12%) |
| 1 | MLY | D | 600 | 1 | 10,10,11 | 0.60 | 0 | 8,11,13 | 0.97 | 1 (12%) |
| 1 | MLY | D | 613 | 1 | 10,10,11 | 0.65 | 0 | 8,11,13 | 1.09 | 1 (12%) |
| 1 | MLY | D | 617 | 1 | 10,10,11 | 0.90 | 1 (10%) | 8,11,13 | 0.62 | 0 |
| 1 | MLY | D | 63 | 1 | 10,10,11 | 0.92 | 0 | 8,11,13 | 0.79 | 0 |
| 1 | MLY | D | 659 | 1 | 10,10,11 | 0.74 | 0 | 8,11,13 | 0.85 | 0 |
| 1 | MLY | D | 681 | 1 | 10,10,11 | 0.95 | 1 (10%) | 8,11,13 | 1.43 | 1 (12%) |
| 1 | MLY | D | 764 | 1 | 10,10,11 | 0.79 | 0 | 8,11,13 | 0.49 | 0 |
| 1 | MLY | D | 768 | 1 | 10,10,11 | 0.87 | 0 | 8,11,13 | 1.95 | 1 (12%) |
| 1 | MLY | D | 782 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 1.52 | 1 (12%) |
| 1 | MLY | D | 827 | 1 | 10,10,11 | 0.98 | 1 (10%) | 8,11,13 | 0.94 | 1 (12%) |
| 1 | MLY | D | 833 | 1 | 10,10,11 | 1.06 | 1 (10%) | 8,11,13 | 1.13 | 1 (12%) |
| 1 | MLY | D | 837 | 1 | 10,10,11 | 0.69 | 0 | 8,11,13 | 0.56 | 0 |
| 1 | MLY | D | 839 | 1 | 10,10,11 | 0.64 | 0 | 8,11,13 | 1.50 | 1 (12%) |
| 1 | MLY | D | 84 | 1 | 10,10,11 | 0.61 | 0 | 8,11,13 | 0.81 | 0 |
| 1 | MLY | D | 87 | 1 | 10,10,11 | 1.06 | 1 (10%) | 8,11,13 | 0.61 | 0 |
| 1 | MLY | G | 107 | 1 | 10,10,11 | 0.48 | 0 | 8,11,13 | 1.01 | 1 (12%) |
| 1 | MLY | G | 130 | 1 | 10,10,11 | 0.97 | 1 (10%) | 8,11,13 | 1.34 | 2 (25%) |
| 1 | MLY | G | 138 | 1 | 10,10,11 | 1.34 | 1 (10%) | 8,11,13 | 2.74 | 1 (12%) |
| 1 | MLY | G | 19 | 1 | 10,10,11 | 1.23 | 1 (10%) | 8,11,13 | 0.64 | 0 |
| 1 | MLY | G | 190 | 1 | 10,10,11 | 1.18 | 1 (10%) | 8,11,13 | 1.31 | 1 (12%) |
| 1 | MLY | G | 236 | 1 | 10,10,11 | 1.08 | 1 (10%) | 8,11,13 | 1.55 | 2 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | G | 248 | 1 | 10,10,11 | 0.74 | 0 | 8,11,13 | 0.86 | 0 |
| 1 | MLY | G | 272 | 1 | 10,10,11 | 1.06 | 1 (10%) | 8,11,13 | 1.32 | 1 (12%) |
| 1 | MLY | G | 295 | 1 | 10,10,11 | 1.14 | 1 (10%) | 8,11,13 | 0.30 | 0 |
| 1 | MLY | G | 296 | 1 | 10,10,11 | 0.87 | 1 (10%) | 8,11,13 | 1.19 | 1 (12%) |
| 1 | MLY | G | 30 | 1 | 10,10,11 | 0.88 | 0 | 8,11,13 | 0.91 | 0 |
| 1 | MLY | G | 348 | 1 | 10,10,11 | 0.81 | 1 (10%) | 8,11,13 | 1.08 | 1 (12%) |
| 1 | MLY | G | 35 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.64 | 0 |
| 1 | MLY | G | 353 | 1 | 10,10,11 | 0.99 | 0 | 8,11,13 | 1.01 | 1 (12%) |
| 1 | MLY | G | 367 | 1 | 10,10,11 | 0.94 | 1 (10%) | 8,11,13 | 0.44 | 0 |
| 1 | MLY | G | 369 | 1 | 10,10,11 | 0.83 | 0 | 8,11,13 | 0.78 | 0 |
| 1 | MLY | G | 385 | 1 | 10,10,11 | 0.92 | 1 (10%) | 8,11,13 | 0.54 | 0 |
| 1 | MLY | G | 415 | 1 | 10,10,11 | 0.72 | 0 | 8,11,13 | 0.73 | 0 |
| 1 | MLY | G | 431 | 1 | 10,10,11 | 0.47 | 0 | 8,11,13 | 1.18 | 1 (12%) |
| 1 | MLY | G | 436 | 1 | 10,10,11 | 1.01 | 1 (10%) | 8,11,13 | 1.78 | 1 (12%) |
| 1 | MLY | G | 486 | 1 | 10,10,11 | 0.57 | 0 | 8,11,13 | 0.55 | 0 |
| 1 | MLY | G | 49 | 1 | 10,10,11 | 1.09 | 1 (10%) | 8,11,13 | 1.23 | 1 (12%) |
| 1 | MLY | G | 504 | 1 | 10,10,11 | 0.82 | 0 | 8,11,13 | 0.45 | 0 |
| 1 | MLY | G | 505 | 1 | 10,10,11 | 1.44 | 2 (20%) | 8,11,13 | 0.50 | 0 |
| 1 | MLY | G | 528 | 1 | 10,10,11 | 0.85 | 0 | 8,11,13 | 1.13 | 1 (12%) |
| 1 | MLY | G | 55 | 1 | 10,10,11 | 1.00 | 1 (10%) | 8,11,13 | 1.10 | 0 |
| 1 | MLY | G | 551 | 1 | 10,10,11 | 0.61 | 0 | 8,11,13 | 0.74 | 0 |
| 1 | MLY | G | 553 | 1,4 | 10,10,11 | 0.65 | 0 | 8,11,13 | 0.65 | 0 |
| 1 | MLY | G | 59 | 1 | 10,10,11 | 0.77 | 0 | 8,11,13 | 1.16 | 1 (12%) |
| 1 | MLY | G | 598 | 1 | 10,10,11 | 1.14 | 2 (20%) | 8,11,13 | 1.30 | 1 (12%) |
| 1 | MLY | G | 600 | 1 | 10,10,11 | 0.62 | 0 | 8,11,13 | 0.96 | 1 (12%) |
| 1 | MLY | G | 613 | 1 | 10,10,11 | 0.65 | 0 | 8,11,13 | 1.10 | 1 (12%) |
| 1 | MLY | G | 617 | 1 | 10,10,11 | 0.88 | 1 (10%) | 8,11,13 | 0.61 | 0 |
| 1 | MLY | G | 63 | 1 | 10,10,11 | 0.89 | 0 | 8,11,13 | 0.79 | 0 |
| 1 | MLY | G | 659 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.82 | 0 |
| 1 | MLY | G | 681 | 1 | 10,10,11 | 0.96 | 1 (10%) | 8,11,13 | 1.43 | 1 (12%) |
| 1 | MLY | G | 764 | 1 | 10,10,11 | 0.77 | 0 | 8,11,13 | 0.50 | 0 |
| 1 | MLY | G | 768 | 1 | 10,10,11 | 0.89 | 0 | 8,11,13 | 1.95 | 1 (12%) |
| 1 | MLY | G | 782 | 1 | 10,10,11 | 0.72 | 0 | 8,11,13 | 1.53 | 1 (12%) |
| 1 | MLY | G | 827 | 1 | 10,10,11 | 1.04 | 1 (10%) | 8,11,13 | 0.93 | 1 (12%) |
| 1 | MLY | G | 833 | 1 | 10,10,11 | 1.08 | 1 (10%) | 8,11,13 | 1.16 | 1 (12%) |
| 1 | MLY | G | 837 | 1 | 10,10,11 | 0.67 | 0 | 8,11,13 | 0.52 | 0 |
| 1 | MLY | G | 839 | 1 | 10,10,11 | 0.68 | 0 | 8,11,13 | 1.51 | 1 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | G | 84 | 1 | 10,10,11 | 0.61 | 0 | 8,11,13 | 0.80 | 0 |
| 1 | MLY | G | 87 | 1 | 10,10,11 | 1.12 | 1 (10%) | 8,11,13 | 0.60 | 0 |
| 1 | MLY | J | 107 | 1 | 10,10,11 | 0.49 | 0 | 8,11,13 | 1.04 | 1 (12%) |
| 1 | MLY | J | 130 | 1 | 10,10,11 | 0.93 | 1 (10%) | 8,11,13 | 1.33 | 2 (25%) |
| 1 | MLY | J | 138 | 1 | 10,10,11 | 1.35 | 1 (10%) | 8,11,13 | 2.73 | 1 (12%) |
| 1 | MLY | J | 19 | 1 | 10,10,11 | 1.24 | 1 (10%) | 8,11,13 | 0.63 | 0 |
| 1 | MLY | J | 190 | 1 | 10,10,11 | 1.19 | 1 (10%) | 8,11,13 | 1.29 | 1 (12%) |
| 1 | MLY | J | 236 | 1 | 10,10,11 | 1.12 | 1 (10%) | 8,11,13 | 1.56 | 2 (25%) |
| 1 | MLY | J | 248 | 1 | 10,10,11 | 0.76 | 0 | 8,11,13 | 0.86 | 0 |
| 1 | MLY | J | 272 | 1 | 10,10,11 | 1.07 | 1 (10%) | 8,11,13 | 1.32 | 1 (12%) |
| 1 | MLY | J | 295 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 0.32 | 0 |
| 1 | MLY | J | 296 | 1 | 10,10,11 | 0.90 | 1 (10%) | 8,11,13 | 1.18 | 1 (12%) |
| 1 | MLY | J | 30 | 1 | 10,10,11 | 0.86 | 0 | 8,11,13 | 0.91 | 0 |
| 1 | MLY | J | 348 | 1 | 10,10,11 | 0.76 | 0 | 8,11,13 | 1.08 | 1 (12%) |
| 1 | MLY | J | 35 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.63 | 0 |
| 1 | MLY | J | 353 | 1 | 10,10,11 | 0.99 | 0 | 8,11,13 | 1.02 | 1 (12%) |
| 1 | MLY | J | 367 | 1 | 10,10,11 | 0.89 | 1 (10%) | 8,11,13 | 0.42 | 0 |
| 1 | MLY | J | 369 | 1 | 10,10,11 | 0.83 | 0 | 8,11,13 | 0.77 | 0 |
| 1 | MLY | J | 385 | 1 | 10,10,11 | 0.94 | 1 (10%) | 8,11,13 | 0.52 | 0 |
| 1 | MLY | J | 415 | 1 | 10,10,11 | 0.71 | 0 | 8,11,13 | 0.73 | 0 |
| 1 | MLY | J | 431 | 1 | 10,10,11 | 0.49 | 0 | 8,11,13 | 1.19 | 1 (12%) |
| 1 | MLY | J | 436 | 1 | 10,10,11 | 1.02 | 1 (10%) | 8,11,13 | 1.75 | 1 (12%) |
| 1 | MLY | J | 486 | 1 | 10,10,11 | 0.56 | 0 | 8,11,13 | 0.54 | 0 |
| 1 | MLY | J | 49 | 1 | 10,10,11 | 1.12 | 1 (10%) | 8,11,13 | 1.26 | 1 (12%) |
| 1 | MLY | J | 504 | 1 | 10,10,11 | 0.78 | 0 | 8,11,13 | 0.45 | 0 |
| 1 | MLY | J | 505 | 1 | 10,10,11 | 1.48 | 2 (20%) | 8,11,13 | 0.50 | 0 |
| 1 | MLY | J | 528 | 1 | 10,10,11 | 0.83 | 0 | 8,11,13 | 1.12 | 1 (12%) |
| 1 | MLY | J | 55 | 1 | 10,10,11 | 0.94 | 1 (10%) | 8,11,13 | 1.12 | 0 |
| 1 | MLY | J | 551 | 1 | 10,10,11 | 0.65 | 0 | 8,11,13 | 0.73 | 0 |
| 1 | MLY | J | 553 | 1,4 | 10,10,11 | 0.65 | 0 | 8,11,13 | 0.65 | 0 |
| 1 | MLY | J | 59 | 1 | 10,10,11 | 0.80 | 0 | 8,11,13 | 1.15 | 1 (12%) |
| 1 | MLY | J | 598 | 1 | 10,10,11 | 1.14 | 2 (20%) | 8,11,13 | 1.30 | 1 (12%) |
| 1 | MLY | J | 600 | 1 | 10,10,11 | 0.63 | 0 | 8,11,13 | 0.98 | 1 (12%) |
| 1 | MLY | J | 613 | 1 | 10,10,11 | 0.68 | 0 | 8,11,13 | 1.09 | 1 (12%) |
| 1 | MLY | J | 617 | 1 | 10,10,11 | 0.89 | 1 (10%) | 8,11,13 | 0.59 | 0 |
| 1 | MLY | J | 63 | 1 | 10,10,11 | 0.89 | 0 | 8,11,13 | 0.80 | 0 |
| 1 | MLY | J | 659 | 1 | 10,10,11 | 0.73 | 0 | 8,11,13 | 0.83 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | J | 681 | 1 | 10,10,11 | 0.95 | 1 (10%) | 8,11,13 | 1.43 | 1 (12%) |
| 1 | MLY | J | 764 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.52 | 0 |
| 1 | MLY | J | 768 | 1 | 10,10,11 | 0.88 | 0 | 8,11,13 | 1.94 | 1 (12%) |
| 1 | MLY | J | 782 | 1 | 10,10,11 | 0.73 | 0 | 8,11,13 | 1.55 | 1 (12%) |
| 1 | MLY | J | 827 | 1 | 10,10,11 | 1.07 | 1 (10%) | 8,11,13 | 0.92 | 1 (12%) |
| 1 | MLY | J | 833 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 1.08 | 1 (12%) |
| 1 | MLY | J | 837 | 1 | 10,10,11 | 0.67 | 0 | 8,11,13 | 0.55 | 0 |
| 1 | MLY | J | 839 | 1 | 10,10,11 | 0.65 | 0 | 8,11,13 | 1.51 | 1 (12%) |
| 1 | MLY | J | 84 | 1 | 10,10,11 | 0.58 | 0 | 8,11,13 | 0.80 | 0 |
| 1 | MLY | J | 87 | 1 | 10,10,11 | 1.11 | 1 (10%) | 8,11,13 | 0.61 | 0 |
| 1 | MLY | M | 107 | 1 | 10,10,11 | 0.50 | 0 | 8,11,13 | 1.04 | 1 (12%) |
| 1 | MLY | M | 130 | 1 | 10,10,11 | 0.93 | 0 | 8,11,13 | 1.34 | 2 (25%) |
| 1 | MLY | M | 138 | 1 | 10,10,11 | 1.35 | 1 (10%) | 8,11,13 | 2.72 | 1 (12%) |
| 1 | MLY | M | 19 | 1 | 10,10,11 | 1.22 | 1 (10%) | 8,11,13 | 0.64 | 0 |
| 1 | MLY | M | 190 | 1 | 10,10,11 | 1.18 | 1 (10%) | 8,11,13 | 1.30 | 1 (12%) |
| 1 | MLY | M | 236 | 1 | 10,10,11 | 1.10 | 1 (10%) | 8,11,13 | 1.56 | 2 (25%) |
| 1 | MLY | M | 248 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.86 | 0 |
| 1 | MLY | M | 272 | 1 | 10,10,11 | 1.08 | 1 (10%) | 8,11,13 | 1.33 | 1 (12%) |
| 1 | MLY | M | 295 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 0.32 | 0 |
| 1 | MLY | M | 296 | 1 | 10,10,11 | 0.95 | 1 (10%) | 8,11,13 | 1.19 | 1 (12%) |
| 1 | MLY | M | 30 | 1 | 10,10,11 | 0.86 | 0 | 8,11,13 | 0.93 | 0 |
| 1 | MLY | M | 348 | 1 | 10,10,11 | 0.74 | 0 | 8,11,13 | 1.06 | 1 (12%) |
| 1 | MLY | M | 35 | 1 | 10,10,11 | 0.74 | 0 | 8,11,13 | 0.64 | 0 |
| 1 | MLY | M | 353 | 1 | 10,10,11 | 0.99 | 0 | 8,11,13 | 1.03 | 1 (12%) |
| 1 | MLY | M | 367 | 1 | 10,10,11 | 0.90 | 1 (10%) | 8,11,13 | 0.41 | 0 |
| 1 | MLY | M | 369 | 1 | 10,10,11 | 0.85 | 0 | 8,11,13 | 0.77 | 0 |
| 1 | MLY | M | 385 | 1 | 10,10,11 | 0.95 | 1 (10%) | 8,11,13 | 0.53 | 0 |
| 1 | MLY | M | 415 | 1 | 10,10,11 | 0.73 | 0 | 8,11,13 | 0.74 | 0 |
| 1 | MLY | M | 431 | 1 | 10,10,11 | 0.50 | 0 | 8,11,13 | 1.18 | 1 (12%) |
| 1 | MLY | M | 436 | 1 | 10,10,11 | 1.05 | 1 (10%) | 8,11,13 | 1.75 | 1 (12%) |
| 1 | MLY | M | 486 | 1 | 10,10,11 | 0.56 | 0 | 8,11,13 | 0.55 | 0 |
| 1 | MLY | M | 49 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 1.26 | 1 (12%) |
| 1 | MLY | M | 504 | 1 | 10,10,11 | 0.78 | 0 | 8,11,13 | 0.45 | 0 |
| 1 | MLY | M | 505 | 1 | 10,10,11 | 1.46 | 2 (20%) | 8,11,13 | 0.49 | 0 |
| 1 | MLY | M | 528 | 1 | 10,10,11 | 0.84 | 0 | 8,11,13 | 1.11 | 1 (12%) |
| 1 | MLY | M | 55 | 1 | 10,10,11 | 0.94 | 1 (10%) | 8,11,13 | 1.09 | 0 |
| 1 | MLY | M | 551 | 1 | 10,10,11 | 0.63 | 0 | 8,11,13 | 0.74 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | M | 553 | 1,4 | 10,10,11 | 0.64 | 0 | 8,11,13 | 0.64 | 0 |
| 1 | MLY | M | 59 | 1 | 10,10,11 | 0.80 | 0 | 8,11,13 | 1.14 | 1 (12%) |
| 1 | MLY | M | 598 | 1 | 10,10,11 | 1.16 | 2 (20%) | 8,11,13 | 1.28 | 1 (12%) |
| 1 | MLY | M | 600 | 1 | 10,10,11 | 0.61 | 0 | 8,11,13 | 0.97 | 1 (12%) |
| 1 | MLY | M | 613 | 1 | 10,10,11 | 0.68 | 0 | 8,11,13 | 1.09 | 1 (12%) |
| 1 | MLY | M | 617 | 1 | 10,10,11 | 0.91 | 1 (10%) | 8,11,13 | 0.61 | 0 |
| 1 | MLY | M | 63 | 1 | 10,10,11 | 0.91 | 0 | 8,11,13 | 0.79 | 0 |
| 1 | MLY | M | 659 | 1 | 10,10,11 | 0.72 | 0 | 8,11,13 | 0.83 | 0 |
| 1 | MLY | M | 681 | 1 | 10,10,11 | 0.96 | 1 (10%) | 8,11,13 | 1.43 | 1 (12%) |
| 1 | MLY | M | 764 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.51 | 0 |
| 1 | MLY | M | 768 | 1 | 10,10,11 | 0.88 | 0 | 8,11,13 | 1.93 | 1 (12%) |
| 1 | MLY | M | 782 | 1 | 10,10,11 | 0.74 | 0 | 8,11,13 | 1.57 | 1 (12%) |
| 1 | MLY | M | 827 | 1 | 10,10,11 | 1.05 | 1 (10%) | 8,11,13 | 0.93 | 1 (12%) |
| 1 | MLY | M | 833 | 1 | 10,10,11 | 1.10 | 1 (10%) | 8,11,13 | 1.09 | 1 (12%) |
| 1 | MLY | M | 837 | 1 | 10,10,11 | 0.65 | 0 | 8,11,13 | 0.55 | 0 |
| 1 | MLY | M | 839 | 1 | 10,10,11 | 0.68 | 0 | 8,11,13 | 1.49 | 1 (12%) |
| 1 | MLY | M | 84 | 1 | 10,10,11 | 0.58 | 0 | 8,11,13 | 0.80 | 0 |
| 1 | MLY | M | 87 | 1 | 10,10,11 | 1.11 | 1 (10%) | 8,11,13 | 0.62 | 0 |
| 1 | MLY | S | 107 | 1 | 10,10,11 | 0.50 | 0 | 8,11,13 | 1.04 | 1 (12%) |
| 1 | MLY | S | 130 | 1 | 10,10,11 | 0.94 | 1 (10%) | 8,11,13 | 1.33 | 2 (25%) |
| 1 | MLY | S | 138 | 1 | 10,10,11 | 1.34 | 1 (10%) | 8,11,13 | 2.73 | 1 (12%) |
| 1 | MLY | S | 19 | 1 | 10,10,11 | 1.24 | 1 (10%) | 8,11,13 | 0.64 | 0 |
| 1 | MLY | S | 190 | 1 | 10,10,11 | 1.19 | 1 (10%) | 8,11,13 | 1.29 | 1 (12%) |
| 1 | MLY | S | 236 | 1 | 10,10,11 | 1.10 | 1 (10%) | 8,11,13 | 1.55 | 2 (25%) |
| 1 | MLY | S | 248 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.86 | 0 |
| 1 | MLY | S | 272 | 1 | 10,10,11 | 1.06 | 1 (10%) | 8,11,13 | 1.32 | 1 (12%) |
| 1 | MLY | S | 295 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 0.32 | 0 |
| 1 | MLY | S | 296 | 1 | 10,10,11 | 0.93 | 1 (10%) | 8,11,13 | 1.20 | 1 (12%) |
| 1 | MLY | S | 30 | 1 | 10,10,11 | 0.86 | 0 | 8,11,13 | 0.92 | 0 |
| 1 | MLY | S | 348 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 1.07 | 1 (12%) |
| 1 | MLY | S | 35 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.64 | 0 |
| 1 | MLY | S | 353 | 1 | 10,10,11 | 0.98 | 0 | 8,11,13 | 1.01 | 1 (12%) |
| 1 | MLY | S | 367 | 1 | 10,10,11 | 0.93 | 1 (10%) | 8,11,13 | 0.44 | 0 |
| 1 | MLY | S | 369 | 1 | 10,10,11 | 0.84 | 0 | 8,11,13 | 0.78 | 0 |
| 1 | MLY | S | 385 | 1 | 10,10,11 | 0.95 | 1 (10%) | 8,11,13 | 0.53 | 0 |
| 1 | MLY | S | 415 | 1 | 10,10,11 | 0.73 | 0 | 8,11,13 | 0.74 | 0 |
| 1 | MLY | S | 431 | 1 | 10,10,11 | 0.48 | 0 | 8,11,13 | 1.20 | 1 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | S | 436 | 1 | 10,10,11 | 1.02 | 1 (10%) | 8,11,13 | 1.76 | 1 (12%) |
| 1 | MLY | S | 486 | 1 | 10,10,11 | 0.56 | 0 | 8,11,13 | 0.55 | 0 |
| 1 | MLY | S | 49 | 1 | 10,10,11 | 1.15 | 1 (10%) | 8,11,13 | 1.25 | 1 (12%) |
| 1 | MLY | S | 504 | 1 | 10,10,11 | 0.79 | 0 | 8,11,13 | 0.45 | 0 |
| 1 | MLY | S | 505 | 1 | 10,10,11 | 1.46 | 2 (20%) | 8,11,13 | 0.49 | 0 |
| 1 | MLY | S | 528 | 1 | 10,10,11 | 0.83 | 0 | 8,11,13 | 1.12 | 1 (12%) |
| 1 | MLY | S | 55 | 1 | 10,10,11 | 0.95 | 1 (10%) | 8,11,13 | 1.11 | 0 |
| 1 | MLY | S | 551 | 1 | 10,10,11 | 0.65 | 0 | 8,11,13 | 0.75 | 0 |
| 1 | MLY | S | 553 | 1 | 10,10,11 | 0.64 | 0 | 8,11,13 | 0.63 | 0 |
| 1 | MLY | S | 59 | 1 | 10,10,11 | 0.79 | 0 | 8,11,13 | 1.15 | 1 (12%) |
| 1 | MLY | S | 598 | 1 | 10,10,11 | 1.17 | 2 (20%) | 8,11,13 | 1.29 | 1 (12%) |
| 1 | MLY | S | 600 | 1 | 10,10,11 | 0.63 | 0 | 8,11,13 | 0.98 | 1 (12%) |
| 1 | MLY | S | 613 | 1 | 10,10,11 | 0.66 | 0 | 8,11,13 | 1.09 | 1 (12%) |
| 1 | MLY | S | 617 | 1 | 10,10,11 | 0.92 | 1 (10%) | 8,11,13 | 0.61 | 0 |
| 1 | MLY | S | 63 | 1 | 10,10,11 | 0.88 | 0 | 8,11,13 | 0.79 | 0 |
| 1 | MLY | S | 659 | 1 | 10,10,11 | 0.72 | 0 | 8,11,13 | 0.84 | 0 |
| 1 | MLY | S | 681 | 1 | 10,10,11 | 0.94 | 1 (10%) | 8,11,13 | 1.41 | 1 (12%) |
| 1 | MLY | S | 764 | 1 | 10,10,11 | 0.75 | 0 | 8,11,13 | 0.52 | 0 |
| 1 | MLY | S | 768 | 1 | 10,10,11 | 0.88 | 0 | 8,11,13 | 1.94 | 1 (12%) |
| 1 | MLY | S | 782 | 1 | 10,10,11 | 0.73 | 0 | 8,11,13 | 1.56 | 1 (12%) |
| 1 | MLY | S | 827 | 1 | 10,10,11 | 1.04 | 1 (10%) | 8,11,13 | 0.92 | 1 (12%) |
| 1 | MLY | S | 833 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 1.09 | 1 (12%) |
| 1 | MLY | S | 837 | 1 | 10,10,11 | 0.64 | 0 | 8,11,13 | 0.54 | 0 |
| 1 | MLY | S | 839 | 1 | 10,10,11 | 0.65 | 0 | 8,11,13 | 1.50 | 1 (12%) |
| 1 | MLY | S | 84 | 1 | 10,10,11 | 0.57 | 0 | 8,11,13 | 0.79 | 0 |
| 1 | MLY | S | 87 | 1 | 10,10,11 | 1.13 | 1 (10%) | 8,11,13 | 0.63 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | MLY | A | 107 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 130 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 138 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 19 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 190 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 236 | 1 | - | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | MLY | A | 248 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 272 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 295 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 296 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 30 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 348 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 35 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 353 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 367 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 369 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 385 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 415 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 431 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 436 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 486 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 49 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 504 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 505 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 528 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 55 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 551 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 553 | 1,4 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 59 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 598 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 600 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 613 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 617 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 63 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 659 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 681 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 764 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 768 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 782 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 827 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 833 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 837 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 839 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 84 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | A | 87 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 107 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 130 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 138 | 1 | - | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | MLY | D | 19 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 190 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 236 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 248 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 272 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 295 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 296 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 30 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 348 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 35 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 353 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 367 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 369 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 385 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 415 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 431 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 436 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 486 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 49 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 504 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 505 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 528 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 55 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 551 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 553 | 1,4 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 59 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 598 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 600 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 613 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 617 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 63 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 659 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 681 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 764 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 768 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 782 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 827 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 833 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 837 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 839 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 84 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | D | 87 | 1 | - | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | MLY | G | 107 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 130 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 138 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 19 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 190 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 236 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 248 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 272 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 295 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 296 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 30 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 348 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 35 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 353 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 367 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 369 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 385 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 415 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 431 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 436 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 486 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 49 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 504 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 505 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 528 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 55 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 551 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 553 | 1,4 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 59 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 598 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 600 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 613 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 617 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 63 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 659 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 681 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 764 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 768 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 782 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 827 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 833 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 837 | 1 | - | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | MLY | G | 839 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 84 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | G | 87 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 107 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 130 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 138 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 19 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 190 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 236 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 248 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 272 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 295 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 296 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 30 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 348 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 35 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 353 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 367 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 369 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 385 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 415 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 431 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 436 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 486 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 49 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 504 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 505 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 528 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 55 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 551 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 553 | 1,4 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 59 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 598 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 600 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 613 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 617 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 63 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 659 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 681 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 764 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 768 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 782 | 1 | - | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | MLY | J | 827 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 833 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 837 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 839 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 84 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | J | 87 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 107 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 130 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 138 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 19 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 190 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 236 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 248 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 272 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 295 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 296 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 30 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 348 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 35 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 353 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 367 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 369 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 385 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 415 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 431 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 436 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 486 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 49 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 504 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 505 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 528 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 55 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 551 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 553 | 1,4 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 59 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 598 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 600 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 613 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 617 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 63 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 659 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 681 | 1 | - | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | MLY | M | 764 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 768 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 782 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 827 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 833 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 837 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 839 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 84 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | M | 87 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 107 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 130 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 138 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 19 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 190 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 236 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 248 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 272 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 295 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 296 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 30 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 348 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 35 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 353 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 367 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 369 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 385 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 415 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 431 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 436 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 486 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 49 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 504 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 505 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 528 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 55 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 551 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 553 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 59 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 598 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 600 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 613 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 617 | 1 | - | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | MLY | S | 63 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 659 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 681 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 764 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 768 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 782 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 827 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 833 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 837 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 839 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 84 | 1 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | MLY | S | 87 | 1 | - | 0/7/9/11 | 0/0/0/0 |

All (132) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | D | 138 | MLY | CB-CA | -3.78 | 1.48 | 1.53 |
| 1 | G | 138 | MLY | CB-CA | -3.67 | 1.48 | 1.53 |
| 1 | J | 138 | MLY | CB-CA | -3.63 | 1.48 | 1.53 |
| 1 | M | 138 | MLY | CB-CA | -3.62 | 1.48 | 1.53 |
| 1 | S | 138 | MLY | CB-CA | -3.59 | 1.48 | 1.53 |
| 1 | A | 138 | MLY | CB-CA | -3.59 | 1.48 | 1.53 |
| 1 | D | 19 | MLY | CB-CA | -3.17 | 1.49 | 1.53 |
| 1 | G | 87 | MLY | CB-CA | -3.13 | 1.49 | 1.53 |
| 1 | J | 19 | MLY | CB-CA | -3.13 | 1.49 | 1.53 |
| 1 | S | 19 | MLY | CB-CA | -3.11 | 1.49 | 1.53 |
| 1 | S | 87 | MLY | CB-CA | -3.10 | 1.49 | 1.53 |
| 1 | M | 19 | MLY | CB-CA | -3.07 | 1.49 | 1.53 |
| 1 | J | 87 | MLY | CB-CA | -3.04 | 1.49 | 1.53 |
| 1 | A | 87 | MLY | CB-CA | -3.04 | 1.49 | 1.53 |
| 1 | G | 19 | MLY | CB-CA | -3.04 | 1.49 | 1.53 |
| 1 | M | 87 | MLY | CB-CA | -3.01 | 1.49 | 1.53 |
| 1 | D | 436 | MLY | CB-CA | -2.97 | 1.49 | 1.53 |
| 1 | A | 19 | MLY | CB-CA | -2.95 | 1.49 | 1.53 |
| 1 | M | 436 | MLY | CB-CA | -2.93 | 1.49 | 1.53 |
| 1 | S | 49 | MLY | CB-CA | -2.91 | 1.49 | 1.53 |
| 1 | D | 87 | MLY | CB-CA | -2.88 | 1.49 | 1.53 |
| 1 | J | 436 | MLY | CB-CA | -2.86 | 1.49 | 1.53 |
| 1 | G | 436 | MLY | CB-CA | -2.84 | 1.49 | 1.53 |
| 1 | S | 436 | MLY | CB-CA | -2.83 | 1.49 | 1.53 |
| 1 | A | 436 | MLY | CB-CA | -2.80 | 1.49 | 1.53 |
| 1 | D | 49 | MLY | CB-CA | -2.79 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | M | 49 | MLY | CB-CA | -2.79 | 1.49 | 1.53 |
| 1 | J | 236 | MLY | CA-C | -2.78 | 1.46 | 1.50 |
| 1 | J | 49 | MLY | CB-CA | -2.77 | 1.49 | 1.53 |
| 1 | D | 236 | MLY | CA-C | -2.77 | 1.46 | 1.50 |
| 1 | G | 49 | MLY | CB-CA | -2.76 | 1.49 | 1.53 |
| 1 | M | 272 | MLY | CB-CA | -2.76 | 1.49 | 1.53 |
| 1 | A | 49 | MLY | CB-CA | -2.73 | 1.49 | 1.53 |
| 1 | S | 236 | MLY | CA-C | -2.72 | 1.46 | 1.50 |
| 1 | A | 272 | MLY | CB-CA | -2.70 | 1.49 | 1.53 |
| 1 | S | 272 | MLY | CB-CA | -2.70 | 1.49 | 1.53 |
| 1 | A | 236 | MLY | CA-C | -2.70 | 1.46 | 1.50 |
| 1 | M | 236 | MLY | CA-C | -2.69 | 1.46 | 1.50 |
| 1 | J | 272 | MLY | CB-CA | -2.68 | 1.50 | 1.53 |
| 1 | G | 236 | MLY | CA-C | -2.65 | 1.46 | 1.50 |
| 1 | G | 272 | MLY | CB-CA | -2.63 | 1.50 | 1.53 |
| 1 | S | 598 | MLY | CA-C | -2.61 | 1.46 | 1.50 |
| 1 | G | 190 | MLY | CB-CA | -2.55 | 1.50 | 1.53 |
| 1 | J | 190 | MLY | CB-CA | -2.55 | 1.50 | 1.53 |
| 1 | S | 190 | MLY | CB-CA | -2.54 | 1.50 | 1.53 |
| 1 | M | 598 | MLY | CA-C | -2.53 | 1.46 | 1.50 |
| 1 | A | 190 | MLY | CB-CA | -2.52 | 1.50 | 1.53 |
| 1 | D | 272 | MLY | CB-CA | -2.52 | 1.50 | 1.53 |
| 1 | J | 598 | MLY | CA-C | -2.51 | 1.47 | 1.50 |
| 1 | D | 598 | MLY | CA-C | -2.51 | 1.47 | 1.50 |
| 1 | A | 598 | MLY | CA-C | -2.51 | 1.47 | 1.50 |
| 1 | J | 833 | MLY | CB-CA | -2.50 | 1.50 | 1.53 |
| 1 | S | 385 | MLY | CB-CA | -2.48 | 1.50 | 1.53 |
| 1 | S | 833 | MLY | CB-CA | -2.48 | 1.50 | 1.53 |
| 1 | M | 385 | MLY | CB-CA | -2.47 | 1.50 | 1.53 |
| 1 | J | 385 | MLY | CB-CA | -2.47 | 1.50 | 1.53 |
| 1 | G | 598 | MLY | CA-C | -2.47 | 1.47 | 1.50 |
| 1 | M | 190 | MLY | CB-CA | -2.47 | 1.50 | 1.53 |
| 1 | D | 190 | MLY | CB-CA | -2.38 | 1.50 | 1.53 |
| 1 | M | 833 | MLY | CB-CA | -2.38 | 1.50 | 1.53 |
| 1 | A | 385 | MLY | CB-CA | -2.37 | 1.50 | 1.53 |
| 1 | G | 385 | MLY | CB-CA | -2.36 | 1.50 | 1.53 |
| 1 | J | 505 | MLY | CB-CA | -2.33 | 1.50 | 1.53 |
| 1 | M | 505 | MLY | CB-CA | -2.30 | 1.50 | 1.53 |
| 1 | A | 598 | MLY | CB-CA | -2.30 | 1.50 | 1.53 |
| 1 | D | 385 | MLY | CB-CA | -2.29 | 1.50 | 1.53 |
| 1 | S | 505 | MLY | CB-CA | -2.29 | 1.50 | 1.53 |
| 1 | M | 598 | MLY | CB-CA | -2.28 | 1.50 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | S | 617 | MLY | CB-CA | -2.26 | 1.50 | 1.53 |
| 1 | G | 598 | MLY | CB-CA | -2.26 | 1.50 | 1.53 |
| 1 | D | 598 | MLY | CB-CA | -2.26 | 1.50 | 1.53 |
| 1 | M | 617 | MLY | CB-CA | -2.25 | 1.50 | 1.53 |
| 1 | S | 598 | MLY | CB-CA | -2.23 | 1.50 | 1.53 |
| 1 | D | 617 | MLY | CB-CA | -2.23 | 1.50 | 1.53 |
| 1 | G | 833 | MLY | CB-CA | -2.22 | 1.50 | 1.53 |
| 1 | A | 833 | MLY | CB-CA | -2.21 | 1.50 | 1.53 |
| 1 | G | 505 | MLY | CB-CA | -2.20 | 1.50 | 1.53 |
| 1 | J | 617 | MLY | CB-CA | -2.20 | 1.50 | 1.53 |
| 1 | J | 598 | MLY | CB-CA | -2.19 | 1.50 | 1.53 |
| 1 | D | 833 | MLY | CB-CA | -2.18 | 1.50 | 1.53 |
| 1 | A | 617 | MLY | CB-CA | -2.17 | 1.50 | 1.53 |
| 1 | A | 505 | MLY | CB-CA | -2.15 | 1.50 | 1.53 |
| 1 | G | 617 | MLY | CB-CA | -2.14 | 1.50 | 1.53 |
| 1 | D | 505 | MLY | CB-CA | -2.09 | 1.50 | 1.53 |
| 1 | G | 348 | MLY | CB-CA | -2.07 | 1.50 | 1.53 |
| 1 | A | 63 | MLY | CB-CA | -2.00 | 1.50 | 1.53 |
| 1 | J | 130 | MLY | CA-C | 2.00 | 1.52 | 1.50 |
| 1 | D | 19 | MLY | CA-C | 2.00 | 1.52 | 1.50 |
| 1 | G | 296 | MLY | CA-C | 2.01 | 1.52 | 1.50 |
| 1 | S | 130 | MLY | CA-C | 2.02 | 1.52 | 1.50 |
| 1 | J | 296 | MLY | CA-C | 2.05 | 1.52 | 1.50 |
| 1 | D | 367 | MLY | CA-C | 2.09 | 1.53 | 1.50 |
| 1 | J | 55 | MLY | CA-C | 2.12 | 1.53 | 1.50 |
| 1 | A | 367 | MLY | CA-C | 2.13 | 1.53 | 1.50 |
| 1 | D | 130 | MLY | CA-C | 2.14 | 1.53 | 1.50 |
| 1 | M | 55 | MLY | CA-C | 2.14 | 1.53 | 1.50 |
| 1 | S | 55 | MLY | CA-C | 2.14 | 1.53 | 1.50 |
| 1 | G | 130 | MLY | CA-C | 2.15 | 1.53 | 1.50 |
| 1 | J | 367 | MLY | CA-C | 2.16 | 1.53 | 1.50 |
| 1 | M | 296 | MLY | CA-C | 2.16 | 1.53 | 1.50 |
| 1 | A | 130 | MLY | CA-C | 2.17 | 1.53 | 1.50 |
| 1 | M | 367 | MLY | CA-C | 2.17 | 1.53 | 1.50 |
| 1 | S | 296 | MLY | CA-C | 2.19 | 1.53 | 1.50 |
| 1 | A | 55 | MLY | CA-C | 2.20 | 1.53 | 1.50 |
| 1 | D | 55 | MLY | CA-C | 2.24 | 1.53 | 1.50 |
| 1 | G | 367 | MLY | CA-C | 2.26 | 1.53 | 1.50 |
| 1 | S | 367 | MLY | CA-C | 2.28 | 1.53 | 1.50 |
| 1 | S | 681 | MLY | CA-C | 2.34 | 1.53 | 1.50 |
| 1 | G | 55 | MLY | CA-C | 2.37 | 1.53 | 1.50 |
| 1 | A | 827 | MLY | CA-C | 2.38 | 1.53 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | D | 827 | MLY | CA-C | 2.43 | 1.53 | 1.50 |
| 1 | J | 681 | MLY | CA-C | 2.43 | 1.53 | 1.50 |
| 1 | G | 681 | MLY | CA-C | 2.43 | 1.53 | 1.50 |
| 1 | D | 681 | MLY | CA-C | 2.46 | 1.53 | 1.50 |
| 1 | M | 681 | MLY | CA-C | 2.47 | 1.53 | 1.50 |
| 1 | S | 827 | MLY | CA-C | 2.55 | 1.53 | 1.50 |
| 1 | G | 827 | MLY | CA-C | 2.56 | 1.53 | 1.50 |
| 1 | M | 827 | MLY | CA-C | 2.56 | 1.53 | 1.50 |
| 1 | A | 681 | MLY | CA-C | 2.61 | 1.53 | 1.50 |
| 1 | J | 827 | MLY | CA-C | 2.62 | 1.53 | 1.50 |
| 1 | A | 295 | MLY | CA-C | 2.74 | 1.53 | 1.50 |
| 1 | D | 295 | MLY | CA-C | 2.74 | 1.53 | 1.50 |
| 1 | J | 295 | MLY | CA-C | 2.81 | 1.53 | 1.50 |
| 1 | G | 295 | MLY | CA-C | 2.81 | 1.53 | 1.50 |
| 1 | M | 295 | MLY | CA-C | 2.81 | 1.53 | 1.50 |
| 1 | S | 295 | MLY | CA-C | 2.81 | 1.53 | 1.50 |
| 1 | M | 505 | MLY | CA-C | 3.70 | 1.55 | 1.50 |
| 1 | A | 505 | MLY | CA-C | 3.72 | 1.55 | 1.50 |
| 1 | S | 505 | MLY | CA-C | 3.73 | 1.55 | 1.50 |
| 1 | G | 505 | MLY | CA-C | 3.76 | 1.55 | 1.50 |
| 1 | D | 505 | MLY | CA-C | 3.79 | 1.55 | 1.50 |
| 1 | J | 505 | MLY | CA-C | 3.81 | 1.55 | 1.50 |

All (150) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | G | 138 | MLY | CB-CA-C | -7.48 | 99.33 | 111.65 |
| 1 | S | 138 | MLY | CB-CA-C | -7.44 | 99.38 | 111.65 |
| 1 | J | 138 | MLY | CB-CA-C | -7.44 | 99.39 | 111.65 |
| 1 | M | 138 | MLY | CB-CA-C | -7.43 | 99.41 | 111.65 |
| 1 | A | 138 | MLY | CB-CA-C | -7.38 | 99.49 | 111.65 |
| 1 | D | 138 | MLY | CB-CA-C | -7.35 | 99.53 | 111.65 |
| 1 | A | 768 | MLY | CB-CA-C | -5.21 | 103.06 | 111.65 |
| 1 | D | 768 | MLY | CB-CA-C | -5.16 | 103.15 | 111.65 |
| 1 | G | 768 | MLY | CB-CA-C | -5.16 | 103.15 | 111.65 |
| 1 | S | 768 | MLY | CB-CA-C | -5.14 | 103.19 | 111.65 |
| 1 | J | 768 | MLY | CB-CA-C | -5.13 | 103.19 | 111.65 |
| 1 | M | 768 | MLY | CB-CA-C | -5.12 | 103.22 | 111.65 |
| 1 | A | 436 | MLY | CB-CA-C | -4.81 | 103.72 | 111.65 |
| 1 | G | 436 | MLY | CB-CA-C | -4.81 | 103.73 | 111.65 |
| 1 | S | 436 | MLY | CB-CA-C | -4.77 | 103.79 | 111.65 |
| 1 | J | 436 | MLY | CB-CA-C | -4.74 | 103.84 | 111.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | M | 436 | MLY | CB-CA-C | -4.74 | 103.84 | 111.65 |
| 1 | D | 436 | MLY | CB-CA-C | -4.73 | 103.85 | 111.65 |
| 1 | A | 681 | MLY | CB-CA-C | -3.75 | 105.48 | 111.65 |
| 1 | G | 681 | MLY | CB-CA-C | -3.73 | 105.50 | 111.65 |
| 1 | J | 839 | MLY | CB-CA-C | -3.72 | 105.51 | 111.65 |
| 1 | J | 681 | MLY | CB-CA-C | -3.72 | 105.52 | 111.65 |
| 1 | M | 681 | MLY | CB-CA-C | -3.72 | 105.52 | 111.65 |
| 1 | D | 681 | MLY | CB-CA-C | -3.71 | 105.55 | 111.65 |
| 1 | A | 839 | MLY | CB-CA-C | -3.70 | 105.55 | 111.65 |
| 1 | G | 839 | MLY | CB-CA-C | -3.68 | 105.58 | 111.65 |
| 1 | S | 839 | MLY | CB-CA-C | -3.67 | 105.60 | 111.65 |
| 1 | M | 839 | MLY | CB-CA-C | -3.67 | 105.60 | 111.65 |
| 1 | D | 839 | MLY | CB-CA-C | -3.66 | 105.62 | 111.65 |
| 1 | S | 681 | MLY | CB-CA-C | -3.66 | 105.62 | 111.65 |
| 1 | D | 272 | MLY | CB-CA-C | -3.47 | 105.94 | 111.65 |
| 1 | M | 272 | MLY | CB-CA-C | -3.45 | 105.97 | 111.65 |
| 1 | S | 272 | MLY | CB-CA-C | -3.44 | 105.98 | 111.65 |
| 1 | J | 272 | MLY | CB-CA-C | -3.44 | 105.98 | 111.65 |
| 1 | G | 272 | MLY | CB-CA-C | -3.43 | 105.99 | 111.65 |
| 1 | A | 272 | MLY | CB-CA-C | -3.43 | 105.99 | 111.65 |
| 1 | A | 190 | MLY | CB-CA-C | -3.25 | 106.29 | 111.65 |
| 1 | D | 190 | MLY | CB-CA-C | -3.25 | 106.30 | 111.65 |
| 1 | G | 190 | MLY | CB-CA-C | -3.21 | 106.36 | 111.65 |
| 1 | J | 598 | MLY | CB-CA-C | -3.19 | 106.40 | 111.65 |
| 1 | G | 598 | MLY | CB-CA-C | -3.19 | 106.40 | 111.65 |
| 1 | D | 598 | MLY | CB-CA-C | -3.18 | 106.42 | 111.65 |
| 1 | A | 598 | MLY | CB-CA-C | -3.18 | 106.42 | 111.65 |
| 1 | J | 236 | MLY | CB-CA-C | -3.17 | 106.42 | 111.65 |
| 1 | S | 236 | MLY | CB-CA-C | -3.16 | 106.44 | 111.65 |
| 1 | S | 598 | MLY | CB-CA-C | -3.16 | 106.45 | 111.65 |
| 1 | M | 190 | MLY | CB-CA-C | -3.16 | 106.45 | 111.65 |
| 1 | M | 236 | MLY | CB-CA-C | -3.15 | 106.45 | 111.65 |
| 1 | S | 190 | MLY | CB-CA-C | -3.14 | 106.47 | 111.65 |
| 1 | J | 190 | MLY | CB-CA-C | -3.13 | 106.50 | 111.65 |
| 1 | M | 598 | MLY | CB-CA-C | -3.13 | 106.50 | 111.65 |
| 1 | A | 236 | MLY | CB-CA-C | -3.12 | 106.52 | 111.65 |
| 1 | G | 236 | MLY | CB-CA-C | -3.11 | 106.52 | 111.65 |
| 1 | D | 236 | MLY | CB-CA-C | -3.07 | 106.59 | 111.65 |
| 1 | D | 431 | MLY | CB-CA-C | -3.05 | 106.62 | 111.65 |
| 1 | S | 431 | MLY | CB-CA-C | -3.04 | 106.63 | 111.65 |
| 1 | A | 431 | MLY | CB-CA-C | -3.03 | 106.66 | 111.65 |
| 1 | G | 833 | MLY | CB-CA-C | -3.02 | 106.67 | 111.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | J | 431 | MLY | CB-CA-C | -3.01 | 106.69 | 111.65 |
| 1 | G | 431 | MLY | CB-CA-C | -2.98 | 106.74 | 111.65 |
| 1 | M | 431 | MLY | CB-CA-C | -2.96 | 106.78 | 111.65 |
| 1 | J | 49 | MLY | CB-CA-C | -2.95 | 106.79 | 111.65 |
| 1 | M | 49 | MLY | CB-CA-C | -2.95 | 106.79 | 111.65 |
| 1 | D | 833 | MLY | CB-CA-C | -2.95 | 106.79 | 111.65 |
| 1 | A | 49 | MLY | CB-CA-C | -2.93 | 106.83 | 111.65 |
| 1 | S | 49 | MLY | CB-CA-C | -2.91 | 106.86 | 111.65 |
| 1 | A | 833 | MLY | CB-CA-C | -2.90 | 106.87 | 111.65 |
| 1 | D | 49 | MLY | CB-CA-C | -2.89 | 106.89 | 111.65 |
| 1 | A | 236 | MLY | O-C-CA | -2.89 | 117.05 | 125.02 |
| 1 | D | 236 | MLY | O-C-CA | -2.88 | 117.06 | 125.02 |
| 1 | G | 49 | MLY | CB-CA-C | -2.88 | 106.91 | 111.65 |
| 1 | M | 236 | MLY | O-C-CA | -2.87 | 117.09 | 125.02 |
| 1 | G | 236 | MLY | O-C-CA | -2.87 | 117.10 | 125.02 |
| 1 | A | 296 | MLY | CB-CA-C | -2.86 | 106.94 | 111.65 |
| 1 | M | 833 | MLY | CB-CA-C | -2.86 | 106.94 | 111.65 |
| 1 | J | 236 | MLY | O-C-CA | -2.85 | 117.16 | 125.02 |
| 1 | S | 833 | MLY | CB-CA-C | -2.85 | 106.96 | 111.65 |
| 1 | S | 236 | MLY | O-C-CA | -2.83 | 117.19 | 125.02 |
| 1 | J | 833 | MLY | CB-CA-C | -2.80 | 107.03 | 111.65 |
| 1 | D | 296 | MLY | CB-CA-C | -2.80 | 107.03 | 111.65 |
| 1 | S | 296 | MLY | CB-CA-C | -2.80 | 107.04 | 111.65 |
| 1 | G | 296 | MLY | CB-CA-C | -2.77 | 107.08 | 111.65 |
| 1 | G | 528 | MLY | O-C-CA | -2.76 | 117.39 | 125.02 |
| 1 | M | 296 | MLY | CB-CA-C | -2.76 | 107.11 | 111.65 |
| 1 | D | 528 | MLY | O-C-CA | -2.75 | 117.41 | 125.02 |
| 1 | J | 296 | MLY | CB-CA-C | -2.74 | 107.14 | 111.65 |
| 1 | A | 528 | MLY | O-C-CA | -2.73 | 117.48 | 125.02 |
| 1 | J | 59 | MLY | CB-CA-C | -2.72 | 107.16 | 111.65 |
| 1 | A | 59 | MLY | CB-CA-C | -2.72 | 107.16 | 111.65 |
| 1 | J | 528 | MLY | O-C-CA | -2.72 | 117.50 | 125.02 |
| 1 | S | 528 | MLY | O-C-CA | -2.72 | 117.50 | 125.02 |
| 1 | G | 59 | MLY | CB-CA-C | -2.72 | 107.17 | 111.65 |
| 1 | S | 59 | MLY | CB-CA-C | -2.70 | 107.20 | 111.65 |
| 1 | M | 528 | MLY | O-C-CA | -2.69 | 117.58 | 125.02 |
| 1 | M | 59 | MLY | CB-CA-C | -2.68 | 107.24 | 111.65 |
| 1 | D | 59 | MLY | CB-CA-C | -2.66 | 107.26 | 111.65 |
| 1 | S | 600 | MLY | CB-CA-C | -2.50 | 107.53 | 111.65 |
| 1 | J | 600 | MLY | CB-CA-C | -2.50 | 107.53 | 111.65 |
| 1 | G | 613 | MLY | CB-CA-C | -2.49 | 107.54 | 111.65 |
| 1 | D | 600 | MLY | CB-CA-C | -2.49 | 107.54 | 111.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 613 | MLY | CB-CA-C | -2.49 | 107.55 | 111.65 |
| 1 | A | 600 | MLY | CB-CA-C | -2.48 | 107.56 | 111.65 |
| 1 | M | 107 | MLY | CB-CA-C | -2.47 | 107.58 | 111.65 |
| 1 | M | 600 | MLY | CB-CA-C | -2.47 | 107.58 | 111.65 |
| 1 | J | 107 | MLY | CB-CA-C | -2.47 | 107.59 | 111.65 |
| 1 | D | 613 | MLY | CB-CA-C | -2.47 | 107.59 | 111.65 |
| 1 | G | 600 | MLY | CB-CA-C | -2.46 | 107.59 | 111.65 |
| 1 | M | 613 | MLY | CB-CA-C | -2.46 | 107.60 | 111.65 |
| 1 | S | 107 | MLY | CB-CA-C | -2.45 | 107.61 | 111.65 |
| 1 | D | 107 | MLY | CB-CA-C | -2.44 | 107.63 | 111.65 |
| 1 | S | 613 | MLY | CB-CA-C | -2.44 | 107.64 | 111.65 |
| 1 | J | 613 | MLY | CB-CA-C | -2.44 | 107.64 | 111.65 |
| 1 | A | 107 | MLY | CB-CA-C | -2.41 | 107.69 | 111.65 |
| 1 | G | 107 | MLY | CB-CA-C | -2.40 | 107.70 | 111.65 |
| 1 | D | 827 | MLY | O-C-CA | -2.26 | 118.78 | 125.02 |
| 1 | A | 827 | MLY | O-C-CA | -2.24 | 118.83 | 125.02 |
| 1 | M | 827 | MLY | O-C-CA | -2.22 | 118.90 | 125.02 |
| 1 | G | 827 | MLY | O-C-CA | -2.21 | 118.93 | 125.02 |
| 1 | J | 827 | MLY | O-C-CA | -2.20 | 118.94 | 125.02 |
| 1 | G | 130 | MLY | O-C-CA | -2.17 | 119.02 | 125.02 |
| 1 | S | 130 | MLY | O-C-CA | -2.17 | 119.02 | 125.02 |
| 1 | S | 827 | MLY | O-C-CA | -2.17 | 119.03 | 125.02 |
| 1 | A | 130 | MLY | O-C-CA | -2.15 | 119.07 | 125.02 |
| 1 | D | 130 | MLY | O-C-CA | -2.15 | 119.07 | 125.02 |
| 1 | M | 353 | MLY | CB-CA-C | -2.14 | 108.13 | 111.65 |
| 1 | M | 130 | MLY | O-C-CA | -2.14 | 119.11 | 125.02 |
| 1 | J | 130 | MLY | O-C-CA | -2.13 | 119.13 | 125.02 |
| 1 | A | 353 | MLY | CB-CA-C | -2.13 | 108.14 | 111.65 |
| 1 | J | 353 | MLY | CB-CA-C | -2.12 | 108.15 | 111.65 |
| 1 | D | 353 | MLY | CB-CA-C | -2.11 | 108.18 | 111.65 |
| 1 | S | 353 | MLY | CB-CA-C | -2.09 | 108.21 | 111.65 |
| 1 | G | 353 | MLY | CB-CA-C | -2.04 | 108.29 | 111.65 |
| 1 | A | 130 | MLY | CB-CA-C | 2.47 | 115.72 | 111.65 |
| 1 | S | 130 | MLY | CB-CA-C | 2.50 | 115.77 | 111.65 |
| 1 | G | 130 | MLY | CB-CA-C | 2.50 | 115.78 | 111.65 |
| 1 | J | 130 | MLY | CB-CA-C | 2.51 | 115.78 | 111.65 |
| 1 | M | 130 | MLY | CB-CA-C | 2.54 | 115.84 | 111.65 |
| 1 | D | 130 | MLY | CB-CA-C | 2.54 | 115.84 | 111.65 |
| 1 | D | 348 | MLY | CB-CA-C | 2.56 | 115.87 | 111.65 |
| 1 | M | 348 | MLY | CB-CA-C | 2.57 | 115.88 | 111.65 |
| 1 | G | 348 | MLY | CB-CA-C | 2.59 | 115.93 | 111.65 |
| 1 | S | 348 | MLY | CB-CA-C | 2.60 | 115.93 | 111.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1 | J | 348 | MLY | CB-CA-C | 2.61 | 115.96 | 111.65 |
| 1 | A | 348 | MLY | CB-CA-C | 2.64 | 115.99 | 111.65 |
| 1 | D | 782 | MLY | CB-CA-C | 4.10 | 118.41 | 111.65 |
| 1 | G | 782 | MLY | CB-CA-C | 4.13 | 118.46 | 111.65 |
| 1 | J | 782 | MLY | CB-CA-C | 4.16 | 118.51 | 111.65 |
| 1 | A | 782 | MLY | CB-CA-C | 4.17 | 118.52 | 111.65 |
| 1 | S | 782 | MLY | CB-CA-C | 4.20 | 118.57 | 111.65 |
| 1 | M | 782 | MLY | CB-CA-C | 4.22 | 118.61 | 111.65 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

186 monomers are involved in 822 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 107 | MLY | 2 | 0 |
| 1 | A | 138 | MLY | 1 | 0 |
| 1 | A | 190 | MLY | 2 | 0 |
| 1 | A | 248 | MLY | 2 | 0 |
| 1 | A | 272 | MLY | 1 | 0 |
| 1 | A | 295 | MLY | 6 | 0 |
| 1 | A | 296 | MLY | 3 | 0 |
| 1 | A | 30 | MLY | 1 | 0 |
| 1 | A | 348 | MLY | 5 | 0 |
| 1 | A | 369 | MLY | 1 | 0 |
| 1 | A | 415 | MLY | 1 | 0 |
| 1 | A | 436 | MLY | 3 | 0 |
| 1 | A | 486 | MLY | 3 | 0 |
| 1 | A | 49 | MLY | 3 | 0 |
| 1 | A | 504 | MLY | 4 | 0 |
| 1 | A | 505 | MLY | 24 | 0 |
| 1 | A | 528 | MLY | 3 | 0 |
| 1 | A | 55 | MLY | 1 | 0 |
| 1 | A | 551 | MLY | 2 | 0 |
| 1 | A | 553 | MLY | 17 | 1 |
| 1 | A | 59 | MLY | 2 | 0 |
| 1 | A | 598 | MLY | 1 | 0 |
| 1 | A | 600 | MLY | 1 | 0 |
| 1 | A | 617 | MLY | 1 | 0 |
| 1 | A | 63 | MLY | 3 | 0 |
| 1 | A | 659 | MLY | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 764 | MLY | 10 | 0 |
| 1 | A | 768 | MLY | 12 | 0 |
| 1 | A | 782 | MLY | 8 | 0 |
| 1 | A | 837 | MLY | 1 | 0 |
| 1 | A | 839 | MLY | 9 | 0 |
| 1 | A | 87 | MLY | 3 | 0 |
| 1 | D | 107 | MLY | 3 | 0 |
| 1 | D | 138 | MLY | 1 | 0 |
| 1 | D | 190 | MLY | 2 | 0 |
| 1 | D | 248 | MLY | 2 | 0 |
| 1 | D | 272 | MLY | 1 | 0 |
| 1 | D | 295 | MLY | 6 | 0 |
| 1 | D | 296 | MLY | 3 | 0 |
| 1 | D | 30 | MLY | 1 | 0 |
| 1 | D | 348 | MLY | 6 | 0 |
| 1 | D | 415 | MLY | 1 | 0 |
| 1 | D | 436 | MLY | 3 | 0 |
| 1 | D | 486 | MLY | 3 | 0 |
| 1 | D | 49 | MLY | 3 | 0 |
| 1 | D | 528 | MLY | 3 | 0 |
| 1 | D | 55 | MLY | 1 | 0 |
| 1 | D | 551 | MLY | 2 | 0 |
| 1 | D | 553 | MLY | 16 | 1 |
| 1 | D | 59 | MLY | 2 | 0 |
| 1 | D | 598 | MLY | 1 | 0 |
| 1 | D | 600 | MLY | 1 | 0 |
| 1 | D | 617 | MLY | 1 | 0 |
| 1 | D | 63 | MLY | 4 | 0 |
| 1 | D | 659 | MLY | 2 | 0 |
| 1 | D | 764 | MLY | 6 | 0 |
| 1 | D | 768 | MLY | 1 | 0 |
| 1 | D | 782 | MLY | 71 | 0 |
| 1 | D | 827 | MLY | 3 | 0 |
| 1 | D | 837 | MLY | 1 | 0 |
| 1 | D | 839 | MLY | 7 | 0 |
| 1 | D | 87 | MLY | 3 | 0 |
| 1 | G | 107 | MLY | 2 | 0 |
| 1 | G | 138 | MLY | 1 | 0 |
| 1 | G | 190 | MLY | 2 | 0 |
| 1 | G | 248 | MLY | 2 | 0 |
| 1 | G | 272 | MLY | 1 | 0 |
| 1 | G | 295 | MLY | 7 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | G | 296 | MLY | 2 | 0 |
| 1 | G | 30 | MLY | 1 | 0 |
| 1 | G | 348 | MLY | 4 | 0 |
| 1 | G | 369 | MLY | 1 | 0 |
| 1 | G | 415 | MLY | 1 | 0 |
| 1 | G | 436 | MLY | 2 | 0 |
| 1 | G | 486 | MLY | 3 | 0 |
| 1 | G | 49 | MLY | 3 | 0 |
| 1 | G | 528 | MLY | 3 | 0 |
| 1 | G | 55 | MLY | 1 | 0 |
| 1 | G | 553 | MLY | 26 | 0 |
| 1 | G | 59 | MLY | 2 | 0 |
| 1 | G | 598 | MLY | 1 | 0 |
| 1 | G | 600 | MLY | 1 | 0 |
| 1 | G | 617 | MLY | 1 | 0 |
| 1 | G | 63 | MLY | 4 | 0 |
| 1 | G | 659 | MLY | 2 | 0 |
| 1 | G | 764 | MLY | 8 | 0 |
| 1 | G | 768 | MLY | 9 | 0 |
| 1 | G | 782 | MLY | 1 | 0 |
| 1 | G | 827 | MLY | 1 | 0 |
| 1 | G | 837 | MLY | 1 | 0 |
| 1 | G | 839 | MLY | 4 | 0 |
| 1 | G | 84 | MLY | 16 | 0 |
| 1 | G | 87 | MLY | 3 | 0 |
| 1 | J | 107 | MLY | 3 | 0 |
| 1 | J | 138 | MLY | 1 | 0 |
| 1 | J | 190 | MLY | 2 | 0 |
| 1 | J | 248 | MLY | 2 | 0 |
| 1 | J | 272 | MLY | 1 | 0 |
| 1 | J | 295 | MLY | 7 | 0 |
| 1 | J | 296 | MLY | 3 | 0 |
| 1 | J | 30 | MLY | 1 | 0 |
| 1 | J | 348 | MLY | 5 | 0 |
| 1 | J | 415 | MLY | 1 | 0 |
| 1 | J | 436 | MLY | 2 | 0 |
| 1 | J | 486 | MLY | 3 | 0 |
| 1 | J | 49 | MLY | 4 | 0 |
| 1 | J | 505 | MLY | 9 | 0 |
| 1 | J | 528 | MLY | 3 | 0 |
| 1 | J | 55 | MLY | 1 | 0 |
| 1 | J | 553 | MLY | 27 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | J | 59 | MLY | 2 | 0 |
| 1 | J | 598 | MLY | 1 | 0 |
| 1 | J | 600 | MLY | 1 | 0 |
| 1 | J | 617 | MLY | 1 | 0 |
| 1 | J | 63 | MLY | 4 | 0 |
| 1 | J | 659 | MLY | 2 | 0 |
| 1 | J | 764 | MLY | 7 | 0 |
| 1 | J | 768 | MLY | 9 | 0 |
| 1 | J | 782 | MLY | 1 | 0 |
| 1 | J | 837 | MLY | 1 | 0 |
| 1 | J | 839 | MLY | 15 | 0 |
| 1 | J | 84 | MLY | 43 | 0 |
| 1 | J | 87 | MLY | 3 | 0 |
| 1 | M | 107 | MLY | 4 | 0 |
| 1 | M | 138 | MLY | 1 | 0 |
| 1 | M | 190 | MLY | 2 | 0 |
| 1 | M | 248 | MLY | 2 | 0 |
| 1 | M | 272 | MLY | 1 | 0 |
| 1 | M | 295 | MLY | 6 | 0 |
| 1 | M | 296 | MLY | 3 | 0 |
| 1 | M | 30 | MLY | 1 | 0 |
| 1 | M | 348 | MLY | 6 | 0 |
| 1 | M | 35 | MLY | 13 | 0 |
| 1 | M | 369 | MLY | 1 | 0 |
| 1 | M | 415 | MLY | 1 | 0 |
| 1 | M | 436 | MLY | 2 | 0 |
| 1 | M | 486 | MLY | 3 | 0 |
| 1 | M | 49 | MLY | 3 | 0 |
| 1 | M | 505 | MLY | 2 | 0 |
| 1 | M | 528 | MLY | 3 | 0 |
| 1 | M | 55 | MLY | 1 | 0 |
| 1 | M | 551 | MLY | 1 | 0 |
| 1 | M | 553 | MLY | 17 | 0 |
| 1 | M | 59 | MLY | 2 | 0 |
| 1 | M | 598 | MLY | 1 | 0 |
| 1 | M | 600 | MLY | 1 | 0 |
| 1 | M | 617 | MLY | 1 | 0 |
| 1 | M | 63 | MLY | 4 | 0 |
| 1 | M | 659 | MLY | 2 | 0 |
| 1 | M | 764 | MLY | 5 | 0 |
| 1 | M | 768 | MLY | 1 | 0 |
| 1 | M | 782 | MLY | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | M | 837 | MLY | 1 | 0 |
| 1 | M | 839 | MLY | 7 | 0 |
| 1 | M | 84 | MLY | 23 | 0 |
| 1 | M | 87 | MLY | 3 | 0 |
| 1 | S | 107 | MLY | 3 | 0 |
| 1 | S | 138 | MLY | 1 | 0 |
| 1 | S | 190 | MLY | 2 | 0 |
| 1 | S | 248 | MLY | 2 | 0 |
| 1 | S | 272 | MLY | 1 | 0 |
| 1 | S | 295 | MLY | 6 | 0 |
| 1 | S | 296 | MLY | 3 | 0 |
| 1 | S | 30 | MLY | 1 | 0 |
| 1 | S | 348 | MLY | 6 | 0 |
| 1 | S | 369 | MLY | 1 | 0 |
| 1 | S | 415 | MLY | 1 | 0 |
| 1 | S | 436 | MLY | 2 | 0 |
| 1 | S | 486 | MLY | 3 | 0 |
| 1 | S | 49 | MLY | 3 | 0 |
| 1 | S | 505 | MLY | 8 | 0 |
| 1 | S | 528 | MLY | 3 | 0 |
| 1 | S | 55 | MLY | 1 | 0 |
| 1 | S | 553 | MLY | 3 | 0 |
| 1 | S | 59 | MLY | 2 | 0 |
| 1 | S | 598 | MLY | 1 | 0 |
| 1 | S | 600 | MLY | 1 | 0 |
| 1 | S | 617 | MLY | 1 | 0 |
| 1 | S | 63 | MLY | 3 | 0 |
| 1 | S | 659 | MLY | 2 | 0 |
| 1 | S | 764 | MLY | 31 | 0 |
| 1 | S | 782 | MLY | 1 | 0 |
| 1 | S | 837 | MLY | 1 | 0 |
| 1 | S | 839 | MLY | 15 | 0 |
| 1 | S | 84 | MLY | 14 | 0 |
| 1 | S | 87 | MLY | 3 | 0 |

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.