



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:55 PM GMT

PDB ID : 1R4M
Title : APPBP1-UBA3-NEDD8, an E1-ubiquitin-like protein complex
Authors : Walden, H.; Podgorski, M.S.; Holton, J.M.; Schulman, B.A.
Deposited on : 2003-10-07
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

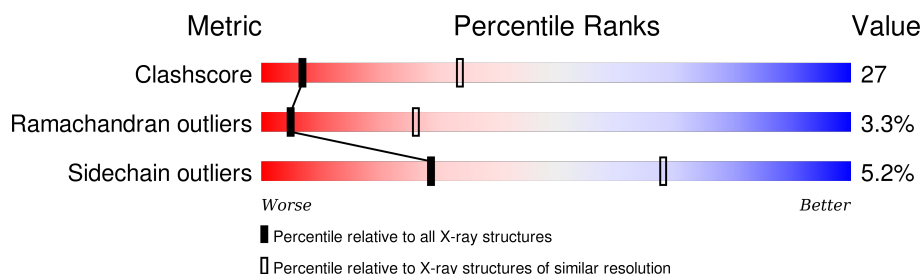
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 1912 (3.00-3.00) |
| Ramachandran outliers | 100387 | 1853 (3.00-3.00) |
| Sidechain outliers | 100360 | 1856 (3.00-3.00) |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 529 | |
| 1 | C | 529 | |
| 1 | E | 529 | |
| 1 | G | 529 | |
| 2 | B | 431 | |
| 2 | D | 431 | |
| 2 | F | 431 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | H | 431 | <div><div></div><div>52%</div><div>39%</div><div>5% • •</div></div> |
| 3 | I | 76 | <div><div></div><div>53%</div><div>42%</div><div>5%</div></div> |
| 3 | J | 76 | <div><div></div><div>57%</div><div>38%</div><div>5%</div></div> |
| 3 | K | 76 | <div><div></div><div>57%</div><div>37%</div><div>7%</div></div> |
| 3 | L | 76 | <div><div></div><div>51%</div><div>42%</div><div>7%</div></div> |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called amyloid beta precursor protein-binding protein 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 516 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4105 | 2602 | 699 | 789 | 15 | | | |
| 1 | C | 516 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4105 | 2602 | 699 | 789 | 15 | | | |
| 1 | E | 516 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4105 | 2602 | 699 | 789 | 15 | | | |
| 1 | G | 516 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4105 | 2602 | 699 | 789 | 15 | | | |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | ? | - | ASN | DELETION | UNP Q13564 |
| A | ? | - | GLU | DELETION | UNP Q13564 |
| A | ? | - | ASN | DELETION | UNP Q13564 |
| A | ? | - | GLY | DELETION | UNP Q13564 |
| A | ? | - | ALA | DELETION | UNP Q13564 |
| C | ? | - | ASN | DELETION | UNP Q13564 |
| C | ? | - | GLU | DELETION | UNP Q13564 |
| C | ? | - | ASN | DELETION | UNP Q13564 |
| C | ? | - | GLY | DELETION | UNP Q13564 |
| C | ? | - | ALA | DELETION | UNP Q13564 |
| E | ? | - | ASN | DELETION | UNP Q13564 |
| E | ? | - | GLU | DELETION | UNP Q13564 |
| E | ? | - | ASN | DELETION | UNP Q13564 |
| E | ? | - | GLY | DELETION | UNP Q13564 |
| E | ? | - | ALA | DELETION | UNP Q13564 |
| G | ? | - | ASN | DELETION | UNP Q13564 |
| G | ? | - | GLU | DELETION | UNP Q13564 |
| G | ? | - | ASN | DELETION | UNP Q13564 |
| G | ? | - | GLY | DELETION | UNP Q13564 |
| G | ? | - | ALA | DELETION | UNP Q13564 |

- Molecule 2 is a protein called ubiquitin-activating enzyme E1C.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 418 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3199 | 2038 | 549 | 595 | 17 | | | |
| 2 | D | 418 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3199 | 2038 | 549 | 595 | 17 | | | |
| 2 | F | 418 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3199 | 2038 | 549 | 595 | 17 | | | |
| 2 | H | 418 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3199 | 2038 | 549 | 595 | 17 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|------------|
| B | 216 | ALA | CYS | ENGINEERED | UNP Q8TBC4 |
| D | 216 | ALA | CYS | ENGINEERED | UNP Q8TBC4 |
| F | 216 | ALA | CYS | ENGINEERED | UNP Q8TBC4 |
| H | 216 | ALA | CYS | ENGINEERED | UNP Q8TBC4 |

- Molecule 3 is a protein called Ubiquitin-like protein NEDD8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | I | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 600 | 378 | 104 | 116 | 2 | | | |
| 3 | J | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 600 | 378 | 104 | 116 | 2 | | | |
| 3 | K | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 600 | 378 | 104 | 116 | 2 | | | |
| 3 | L | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 600 | 378 | 104 | 116 | 2 | | | |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

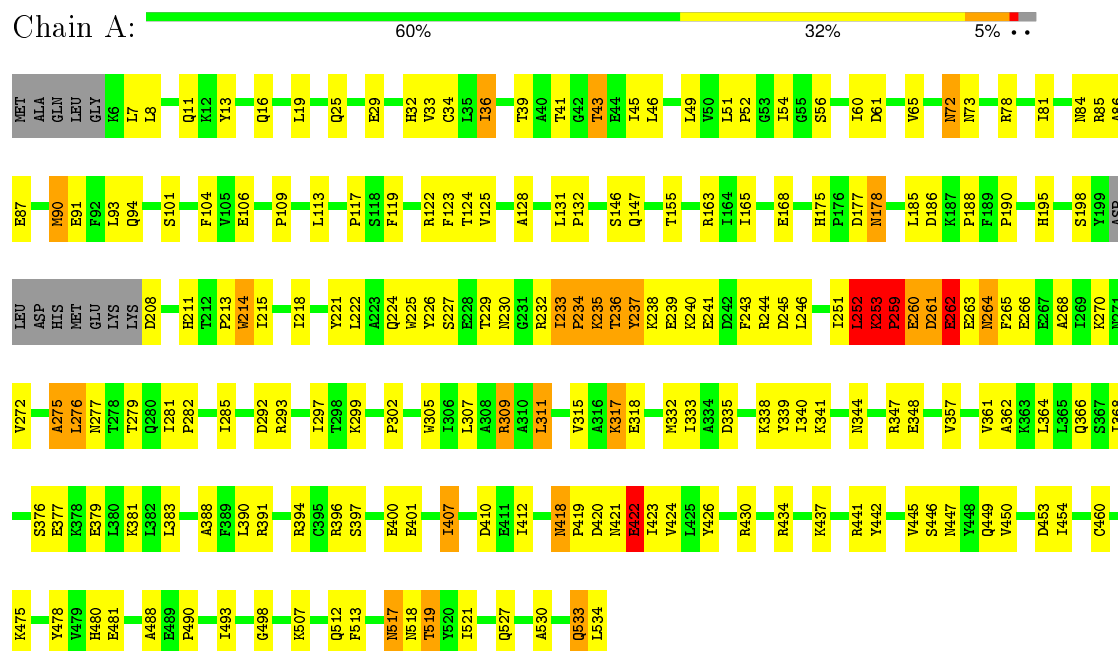
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | H | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | J | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | F | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots [i](#)

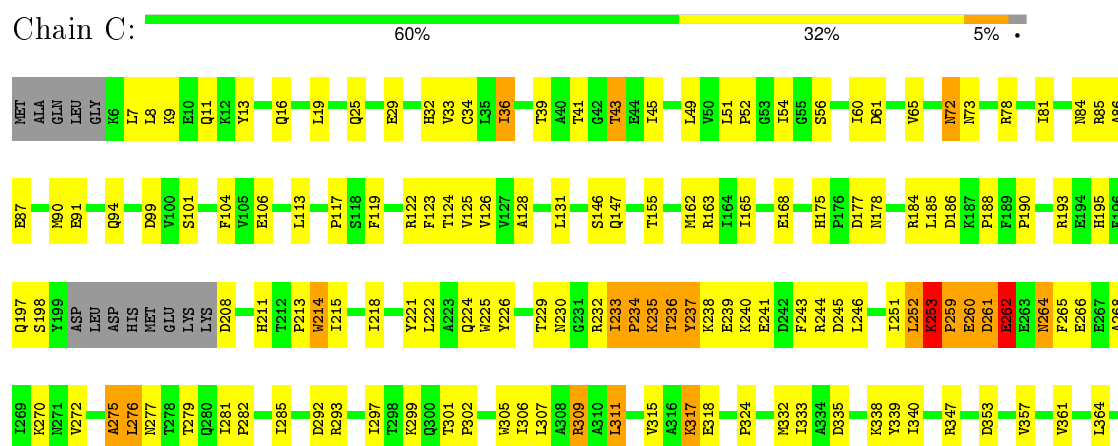
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

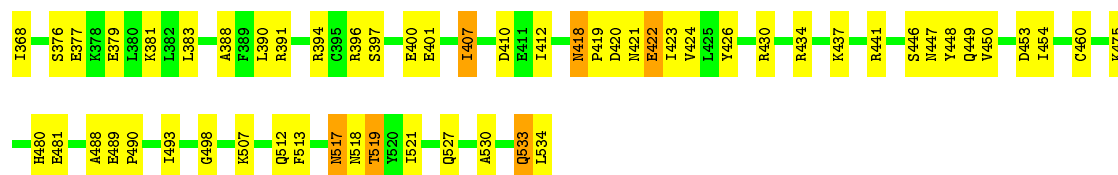
Note EDS was not executed.

- Molecule 1: amyloid beta precursor protein-binding protein 1

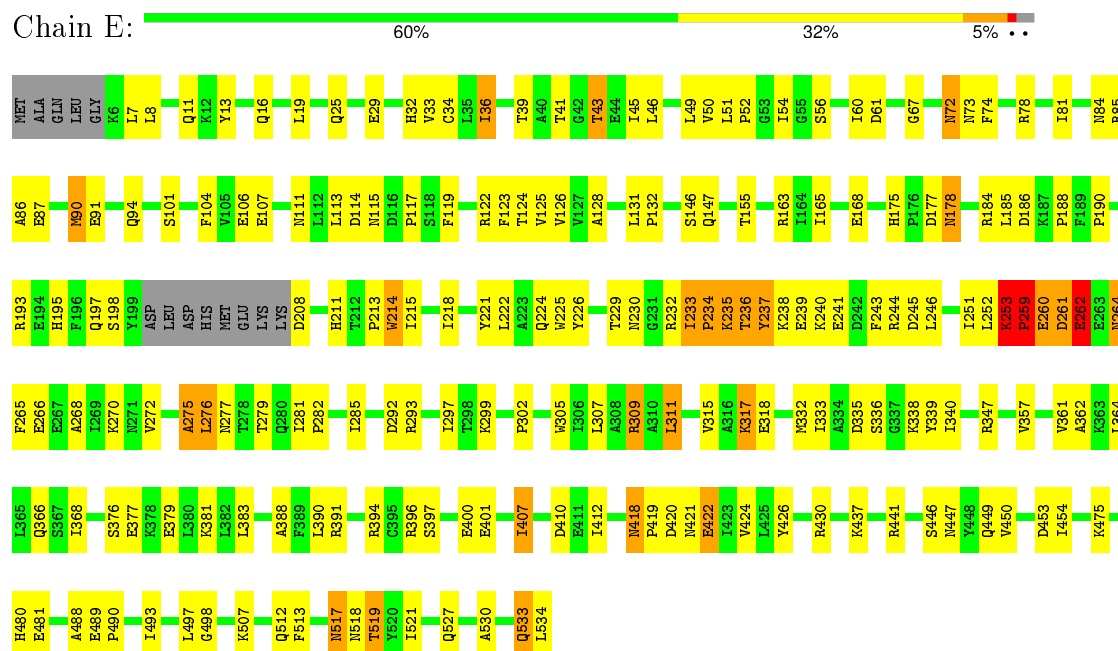


- Molecule 1: amyloid beta precursor protein-binding protein 1

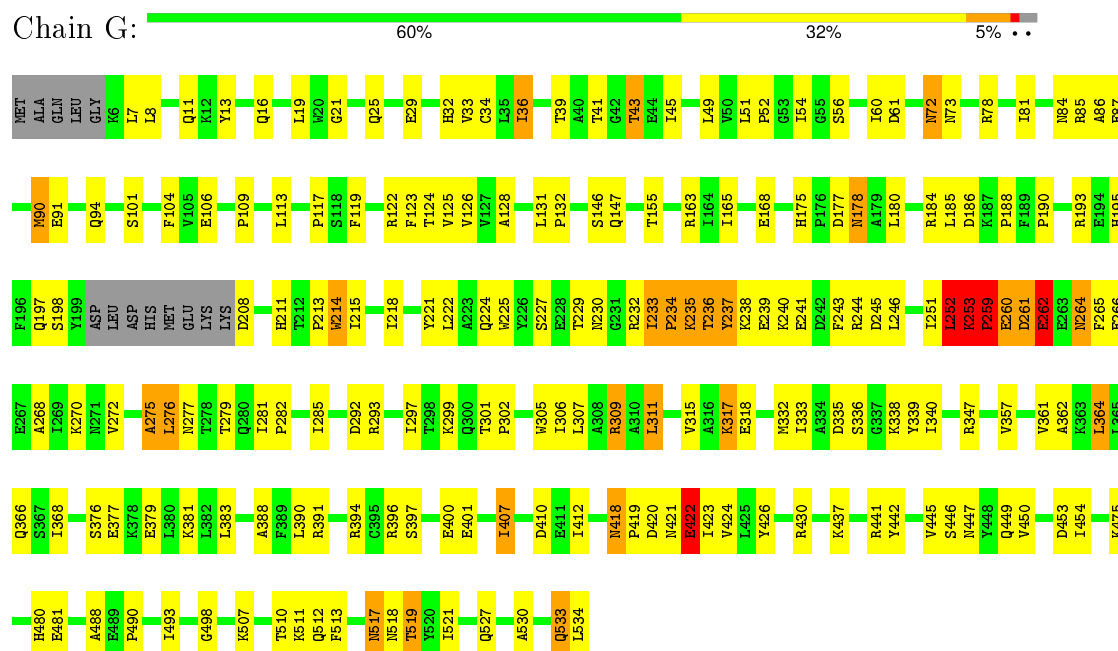




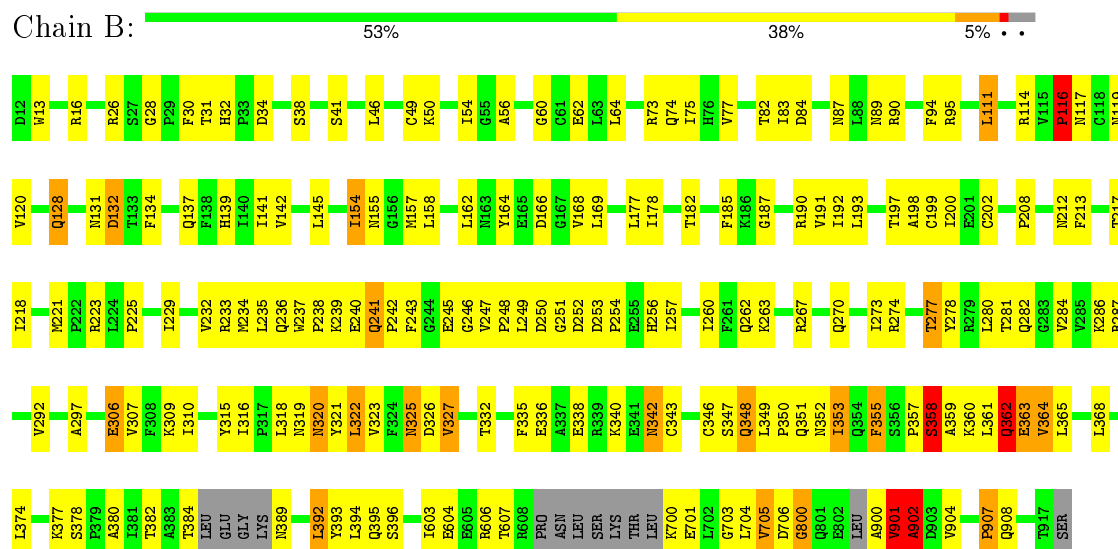
- Molecule 1: amyloid beta precursor protein-binding protein 1



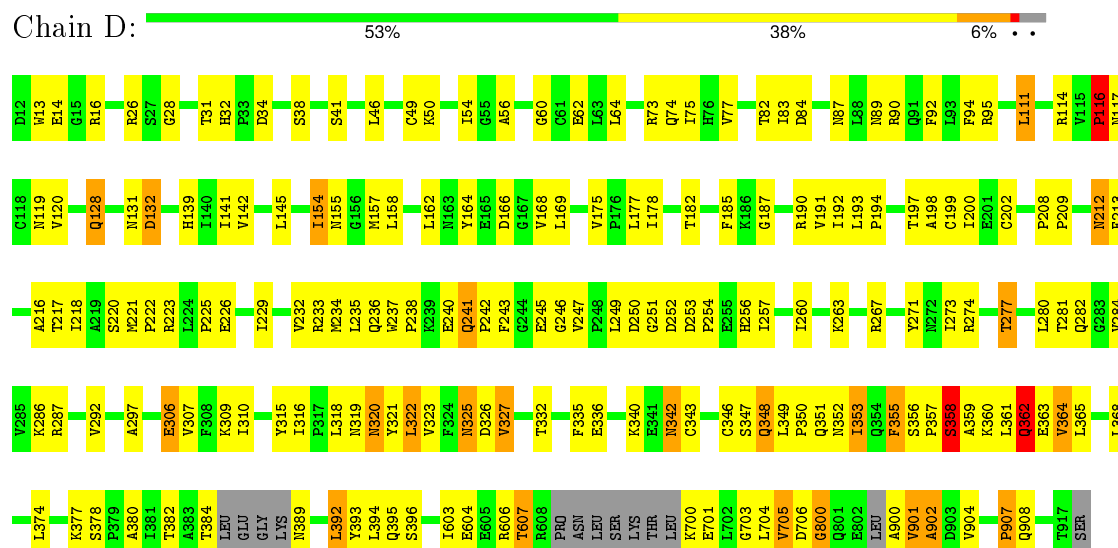
- Molecule 1: amyloid beta precursor protein-binding protein 1



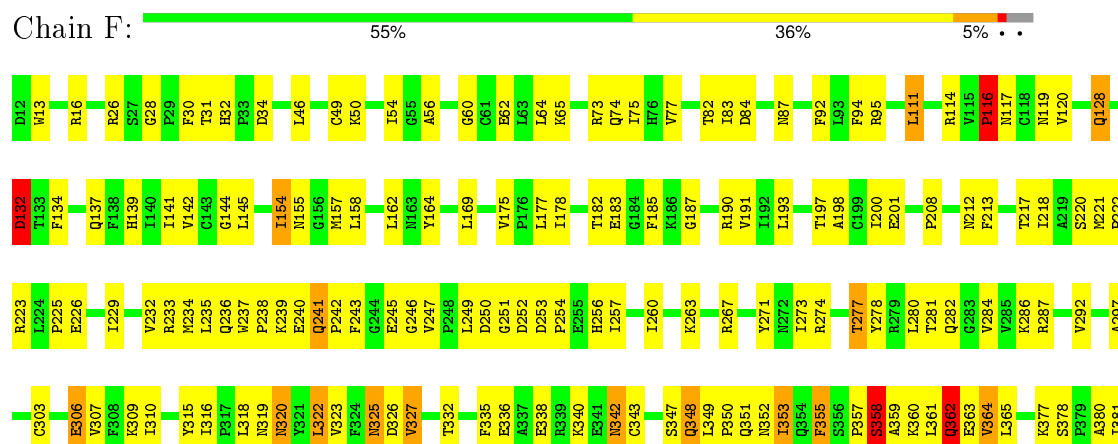
- Molecule 2: ubiquitin-activating enzyme E1C

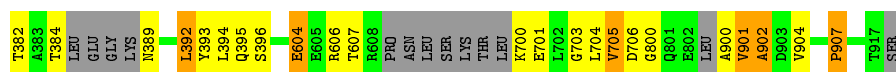


• Molecule 2: ubiquitin-activating enzyme E1C

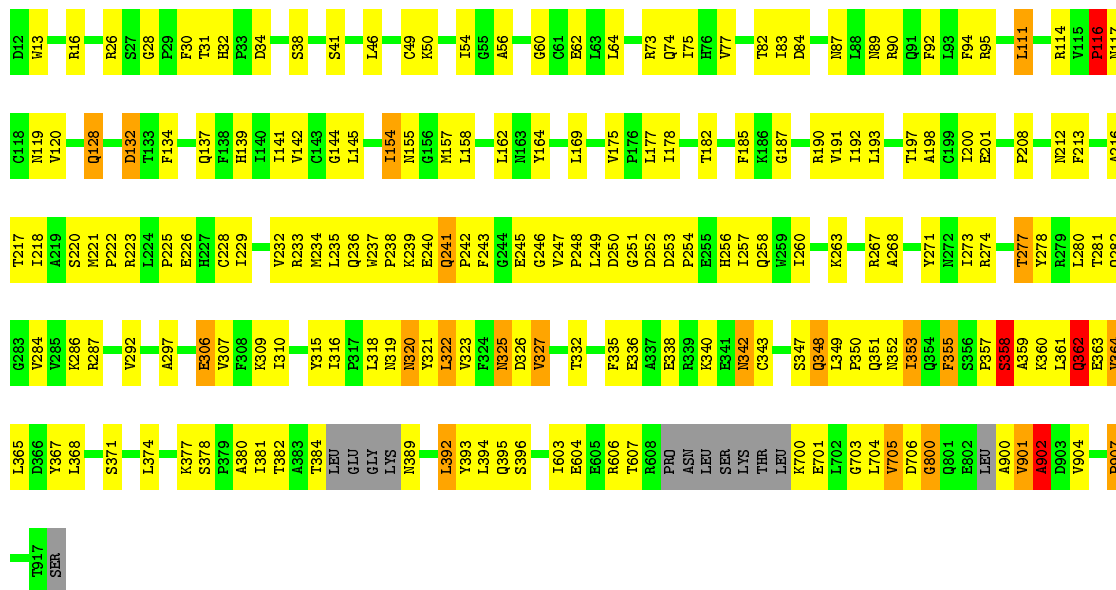


• Molecule 2: ubiquitin-activating enzyme E1C

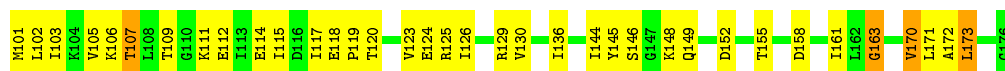




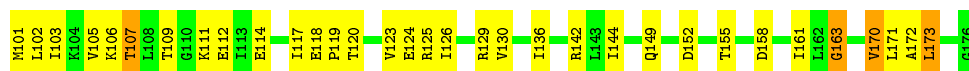
- Molecule 2: ubiquitin-activating enzyme E1C



- Molecule 3: Ubiquitin-like protein NEDD8



- Molecule 3: Ubiquitin-like protein NEDD8



- Molecule 3: Ubiquitin-like protein NEDD8



- Molecule 3: Ubiquitin-like protein NEDD8



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--|------|------|------|------|--|------|------|--|------|------|--|------|--|------|--|------|------|--|------|--|------|------|------|------|--|------|------|------|--|------|------|------|------|--|------|
| M101 | L102 | I103 | K104 | V105 | K106 | T107 | L108 | T109 | K110 | K111 | E112 | I113 | E114 | I115 | D116 | I117 | E118 | P119 | T120 | | V123 | E124 | R125 | I126 | | R129 | V130 | | G135 | I136 | | Q141 | | I144 | | K148 | Q149 | | D152 | | T155 | A156 | A157 | D158 | | I161 | L162 | G163 | | V170 | L171 | A172 | L173 | | G176 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--|------|------|------|------|--|------|------|--|------|------|--|------|--|------|--|------|------|--|------|--|------|------|------|------|--|------|------|------|--|------|------|------|------|--|------|

4 Data and refinement statistics

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

| Property | Value | Source |
|--|--|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 135.40 Å 198.90 Å 209.80 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.00 | Depositor |
| % Data completeness (in resolution range) | 99.9 (50.00-3.00) | Depositor |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.240 , 0.280 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 31620 | wwPDB-VP |
| Average B, all atoms (Å ²) | 77.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.44 | 2/4185 (0.0%) | 0.68 | 5/5661 (0.1%) |
| 1 | C | 0.44 | 3/4185 (0.1%) | 0.65 | 2/5661 (0.0%) |
| 1 | E | 0.42 | 0/4185 | 0.66 | 1/5661 (0.0%) |
| 1 | G | 0.45 | 2/4185 (0.0%) | 0.69 | 5/5661 (0.1%) |
| 2 | B | 0.44 | 0/3268 | 0.72 | 5/4447 (0.1%) |
| 2 | D | 0.43 | 0/3268 | 0.71 | 4/4447 (0.1%) |
| 2 | F | 0.45 | 0/3268 | 0.72 | 5/4447 (0.1%) |
| 2 | H | 0.44 | 0/3268 | 0.73 | 6/4447 (0.1%) |
| 3 | I | 0.38 | 0/605 | 0.72 | 1/808 (0.1%) |
| 3 | J | 0.38 | 0/605 | 0.72 | 1/808 (0.1%) |
| 3 | K | 0.38 | 0/605 | 0.73 | 1/808 (0.1%) |
| 3 | L | 0.36 | 0/605 | 0.71 | 1/808 (0.1%) |
| All | All | 0.43 | 7/32232 (0.0%) | 0.70 | 37/43664 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 1 |
| 2 | D | 0 | 1 |
| 2 | F | 0 | 1 |
| All | All | 0 | 3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | C | 253 | LYS | C-N | 6.87 | 1.47 | 1.34 |
| 1 | A | 259 | PRO | N-CA | 6.64 | 1.58 | 1.47 |
| 1 | C | 259 | PRO | N-CA | 6.41 | 1.58 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | A | 253 | LYS | C-N | 6.04 | 1.45 | 1.34 |
| 1 | G | 259 | PRO | N-CA | 5.93 | 1.57 | 1.47 |
| 1 | C | 253 | LYS | CA-C | 5.63 | 1.67 | 1.52 |
| 1 | G | 253 | LYS | C-N | 5.63 | 1.45 | 1.34 |

All (37) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1 | G | 259 | PRO | CA-N-CD | -15.83 | 89.34 | 111.50 |
| 1 | E | 259 | PRO | CA-N-CD | -14.39 | 91.35 | 111.50 |
| 1 | A | 259 | PRO | CA-N-CD | -12.29 | 94.29 | 111.50 |
| 1 | C | 252 | LEU | O-C-N | -8.30 | 109.42 | 122.70 |
| 2 | B | 800 | GLY | N-CA-C | -8.16 | 92.69 | 113.10 |
| 2 | H | 800 | GLY | N-CA-C | -8.14 | 92.74 | 113.10 |
| 2 | D | 800 | GLY | N-CA-C | -8.13 | 92.78 | 113.10 |
| 1 | A | 252 | LEU | O-C-N | -7.77 | 110.27 | 122.70 |
| 2 | F | 800 | GLY | N-CA-C | -7.37 | 94.68 | 113.10 |
| 2 | H | 355 | PHE | CA-CB-CG | -7.06 | 96.95 | 113.90 |
| 2 | F | 902 | ALA | N-CA-C | -6.65 | 93.04 | 111.00 |
| 2 | B | 392 | LEU | CA-CB-CG | -6.24 | 100.95 | 115.30 |
| 1 | A | 259 | PRO | CA-CB-CG | -6.17 | 92.28 | 104.00 |
| 2 | H | 902 | ALA | N-CA-C | -6.08 | 94.59 | 111.00 |
| 3 | K | 173 | LEU | CA-CB-CG | -6.06 | 101.36 | 115.30 |
| 1 | C | 252 | LEU | CA-C-N | 6.03 | 130.46 | 117.20 |
| 1 | G | 259 | PRO | N-CA-C | 5.95 | 127.56 | 112.10 |
| 3 | I | 173 | LEU | CA-CB-CG | -5.89 | 101.75 | 115.30 |
| 2 | B | 907 | PRO | N-CA-CB | 5.88 | 110.36 | 103.30 |
| 3 | J | 173 | LEU | CA-CB-CG | -5.88 | 101.78 | 115.30 |
| 2 | F | 907 | PRO | N-CA-CB | 5.88 | 110.36 | 103.30 |
| 2 | H | 907 | PRO | N-CA-CB | 5.84 | 110.31 | 103.30 |
| 1 | A | 252 | LEU | CA-C-N | 5.71 | 129.75 | 117.20 |
| 3 | L | 173 | LEU | CA-CB-CG | -5.69 | 102.21 | 115.30 |
| 2 | D | 907 | PRO | N-CA-CB | 5.69 | 110.13 | 103.30 |
| 2 | F | 392 | LEU | CA-CB-CG | -5.69 | 102.22 | 115.30 |
| 2 | B | 901 | VAL | CA-C-N | -5.62 | 104.84 | 117.20 |
| 2 | H | 392 | LEU | CA-CB-CG | -5.62 | 102.39 | 115.30 |
| 2 | D | 392 | LEU | CA-CB-CG | -5.61 | 102.39 | 115.30 |
| 1 | G | 252 | LEU | CA-C-N | 5.52 | 129.34 | 117.20 |
| 1 | G | 253 | LYS | CA-C-N | 5.50 | 132.49 | 117.10 |
| 1 | G | 259 | PRO | CA-CB-CG | -5.32 | 93.89 | 104.00 |
| 2 | B | 902 | ALA | N-CA-C | -5.27 | 96.76 | 111.00 |
| 2 | H | 144 | GLY | N-CA-C | -5.16 | 100.21 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 259 | PRO | N-CA-C | 5.15 | 125.49 | 112.10 |
| 2 | F | 144 | GLY | N-CA-C | -5.11 | 100.32 | 113.10 |
| 2 | D | 607 | THR | C-N-CA | 5.07 | 134.38 | 121.70 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | B | 355 | PHE | Sidechain |
| 2 | D | 355 | PHE | Sidechain |
| 2 | F | 355 | PHE | 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 | 4105 | 0 | 4063 | 201 | 0 |
| 1 | C | 4105 | 0 | 4063 | 203 | 0 |
| 1 | E | 4105 | 0 | 4063 | 218 | 0 |
| 1 | G | 4105 | 0 | 4063 | 204 | 0 |
| 2 | B | 3199 | 0 | 3066 | 196 | 0 |
| 2 | D | 3199 | 0 | 3066 | 195 | 0 |
| 2 | F | 3199 | 0 | 3062 | 189 | 0 |
| 2 | H | 3199 | 0 | 3062 | 194 | 0 |
| 3 | I | 600 | 0 | 635 | 44 | 0 |
| 3 | J | 600 | 0 | 635 | 42 | 0 |
| 3 | K | 600 | 0 | 635 | 46 | 0 |
| 3 | L | 600 | 0 | 635 | 46 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| 4 | H | 2 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| All | All | 31620 | 0 | 31048 | 1658 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (1658) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:123:VAL:HB | 3:K:152:ASP:HA | 1.31 | 1.11 |
| 1:A:252:LEU:O | 1:A:253:LYS:C | 1.90 | 1.09 |
| 3:J:123:VAL:HB | 3:J:152:ASP:HA | 1.33 | 1.08 |
| 3:I:123:VAL:HB | 3:I:152:ASP:HA | 1.30 | 1.08 |
| 2:B:274:ARG:HH22 | 1:E:107:GLU:HA | 1.18 | 1.07 |
| 1:G:252:LEU:O | 1:G:253:LYS:C | 1.93 | 1.07 |
| 3:L:107:THR:HG22 | 3:L:111:LYS:H | 1.21 | 1.06 |
| 3:L:123:VAL:HB | 3:L:152:ASP:HA | 1.35 | 1.05 |
| 1:E:211:HIS:HB3 | 1:E:335:ASP:HB2 | 1.39 | 1.05 |
| 1:A:211:HIS:HB3 | 1:A:335:ASP:HB2 | 1.39 | 1.03 |
| 1:G:211:HIS:HB3 | 1:G:335:ASP:HB2 | 1.38 | 1.03 |
| 1:C:211:HIS:HB3 | 1:C:335:ASP:HB2 | 1.40 | 1.02 |
| 3:K:107:THR:HG22 | 3:K:111:LYS:H | 1.23 | 1.02 |
| 2:B:262:GLN:NE2 | 1:E:67:GLY:H | 1.59 | 1.01 |
| 3:J:107:THR:HG22 | 3:J:111:LYS:H | 1.22 | 1.01 |
| 2:D:323:VAL:HG21 | 3:J:170:VAL:HG22 | 1.44 | 0.99 |
| 3:I:107:THR:HG22 | 3:I:111:LYS:H | 1.26 | 0.98 |
| 2:H:323:VAL:HG21 | 3:L:170:VAL:HG22 | 1.46 | 0.97 |
| 1:A:344:ASN:ND2 | 1:E:111:ASN:HD22 | 1.63 | 0.97 |
| 2:H:342:ASN:H | 2:H:342:ASN:HD22 | 0.95 | 0.95 |
| 2:F:323:VAL:HG21 | 3:K:170:VAL:HG22 | 1.49 | 0.92 |
| 2:F:342:ASN:HD22 | 2:F:342:ASN:H | 0.93 | 0.92 |
| 1:A:421:ASN:O | 1:A:424:VAL:HG23 | 1.71 | 0.91 |
| 1:E:421:ASN:O | 1:E:424:VAL:HG23 | 1.71 | 0.91 |
| 1:A:344:ASN:HD22 | 1:E:111:ASN:ND2 | 1.68 | 0.90 |
| 1:A:252:LEU:O | 1:A:253:LYS:O | 1.88 | 0.90 |
| 2:B:274:ARG:NH2 | 1:E:107:GLU:HA | 1.86 | 0.90 |
| 1:G:421:ASN:O | 1:G:424:VAL:HG23 | 1.72 | 0.90 |
| 2:B:342:ASN:HD22 | 2:B:342:ASN:N | 1.68 | 0.90 |
| 2:D:342:ASN:H | 2:D:342:ASN:HD22 | 0.92 | 0.89 |
| 2:H:64:LEU:HB3 | 2:H:111:LEU:CD1 | 2.02 | 0.89 |
| 2:F:342:ASN:HD22 | 2:F:342:ASN:N | 1.70 | 0.88 |
| 1:E:253:LYS:O | 1:E:260:GLU:N | 2.06 | 0.88 |
| 2:B:342:ASN:HD22 | 2:B:342:ASN:H | 0.92 | 0.88 |
| 1:C:421:ASN:O | 1:C:424:VAL:HG23 | 1.75 | 0.87 |
| 2:D:342:ASN:HD22 | 2:D:342:ASN:N | 1.70 | 0.87 |
| 2:B:323:VAL:HG21 | 3:I:170:VAL:HG22 | 1.55 | 0.87 |
| 2:H:342:ASN:N | 2:H:342:ASN:HD22 | 1.72 | 0.86 |
| 2:F:342:ASN:ND2 | 2:F:342:ASN:H | 1.74 | 0.86 |
| 1:E:297:ILE:HG22 | 1:E:368:ILE:HD11 | 1.58 | 0.86 |
| 2:D:64:LEU:HB3 | 2:D:111:LEU:CD1 | 2.05 | 0.86 |
| 2:F:64:LEU:HB3 | 2:F:111:LEU:CD1 | 2.05 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:901:VAL:C | 2:H:902:ALA:O | 2.04 | 0.85 |
| 2:B:342:ASN:H | 2:B:342:ASN:ND2 | 1.73 | 0.85 |
| 1:G:297:ILE:HG22 | 1:G:368:ILE:HD11 | 1.58 | 0.85 |
| 2:B:64:LEU:HB3 | 2:B:111:LEU:CD1 | 2.07 | 0.84 |
| 2:H:141:ILE:HD12 | 2:H:158:LEU:HD21 | 1.59 | 0.84 |
| 1:A:297:ILE:HG22 | 1:A:368:ILE:HD11 | 1.58 | 0.84 |
| 2:B:262:GLN:HE22 | 1:E:67:GLY:N | 1.74 | 0.84 |
| 2:B:262:GLN:HE22 | 1:E:67:GLY:H | 0.88 | 0.84 |
| 2:D:393:TYR:CE1 | 2:D:607:THR:HA | 2.13 | 0.84 |
| 2:H:342:ASN:ND2 | 2:H:342:ASN:H | 1.76 | 0.84 |
| 2:B:128:GLN:H | 2:B:128:GLN:HE21 | 1.26 | 0.84 |
| 2:F:141:ILE:HD12 | 2:F:158:LEU:HD21 | 1.60 | 0.84 |
| 2:H:128:GLN:HE21 | 2:H:128:GLN:H | 1.26 | 0.83 |
| 2:D:901:VAL:C | 2:D:902:ALA:O | 2.13 | 0.83 |
| 2:B:208:PRO:HG3 | 3:I:171:LEU:HD11 | 1.61 | 0.82 |
| 2:D:141:ILE:HD12 | 2:D:158:LEU:HD21 | 1.60 | 0.82 |
| 2:F:128:GLN:HE21 | 2:F:128:GLN:H | 1.27 | 0.82 |
| 1:C:236:THR:HG23 | 1:C:237:TYR:H | 1.45 | 0.82 |
| 2:D:128:GLN:HE21 | 2:D:128:GLN:H | 1.28 | 0.82 |
| 1:C:297:ILE:HG22 | 1:C:368:ILE:HD11 | 1.62 | 0.82 |
| 2:B:361:LEU:O | 2:B:363:GLU:N | 2.13 | 0.82 |
| 2:D:342:ASN:ND2 | 2:D:342:ASN:H | 1.73 | 0.82 |
| 2:B:352:ASN:C | 2:B:353:ILE:HD13 | 2.00 | 0.81 |
| 2:D:213:PHE:HB2 | 2:D:218:ILE:HD11 | 1.63 | 0.81 |
| 1:A:236:THR:HG23 | 1:A:237:TYR:H | 1.45 | 0.81 |
| 2:D:352:ASN:C | 2:D:353:ILE:HD13 | 2.01 | 0.81 |
| 2:D:14:GLU:HG3 | 2:H:258:GLN:HG3 | 1.62 | 0.81 |
| 3:L:107:THR:HG23 | 3:L:109:THR:H | 1.46 | 0.81 |
| 2:B:141:ILE:HD12 | 2:B:158:LEU:HD21 | 1.61 | 0.81 |
| 1:E:236:THR:HG23 | 1:E:237:TYR:H | 1.45 | 0.81 |
| 1:G:236:THR:HG23 | 1:G:237:TYR:H | 1.44 | 0.80 |
| 2:H:393:TYR:CE1 | 2:H:607:THR:HA | 2.17 | 0.79 |
| 2:F:352:ASN:C | 2:F:353:ILE:HD13 | 2.02 | 0.79 |
| 2:H:352:ASN:C | 2:H:353:ILE:HD13 | 2.02 | 0.79 |
| 3:K:107:THR:HG23 | 3:K:109:THR:H | 1.49 | 0.78 |
| 3:L:155:THR:HG23 | 3:L:158:ASP:H | 1.48 | 0.78 |
| 2:B:213:PHE:HB2 | 2:B:218:ILE:HD11 | 1.64 | 0.78 |
| 2:H:213:PHE:HB2 | 2:H:218:ILE:HD11 | 1.66 | 0.77 |
| 2:D:241:GLN:HE21 | 2:D:246:GLY:H | 1.31 | 0.77 |
| 2:D:208:PRO:HG3 | 3:J:171:LEU:HD11 | 1.66 | 0.77 |
| 3:K:155:THR:HG22 | 3:K:158:ASP:OD2 | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:128:GLN:H | 2:B:128:GLN:NE2 | 1.82 | 0.77 |
| 2:D:128:GLN:NE2 | 2:D:128:GLN:H | 1.82 | 0.77 |
| 3:J:107:THR:HG23 | 3:J:109:THR:H | 1.49 | 0.77 |
| 3:K:155:THR:HG23 | 3:K:158:ASP:H | 1.50 | 0.77 |
| 2:B:241:GLN:HE21 | 2:B:246:GLY:H | 1.32 | 0.77 |
| 3:I:107:THR:HG23 | 3:I:109:THR:H | 1.50 | 0.76 |
| 2:F:241:GLN:HE21 | 2:F:246:GLY:H | 1.31 | 0.76 |
| 2:H:241:GLN:HE21 | 2:H:246:GLY:H | 1.30 | 0.76 |
| 3:J:155:THR:HG23 | 3:J:158:ASP:H | 1.49 | 0.76 |
| 2:F:213:PHE:HB2 | 2:F:218:ILE:HD11 | 1.67 | 0.76 |
| 1:E:376:SER:OG | 1:E:379:GLU:HG3 | 1.86 | 0.76 |
| 2:D:351:GLN:HG3 | 2:D:353:ILE:HD11 | 1.68 | 0.76 |
| 1:G:297:ILE:CG2 | 1:G:368:ILE:HD11 | 2.15 | 0.75 |
| 1:A:376:SER:OG | 1:A:379:GLU:HG3 | 1.86 | 0.75 |
| 2:H:208:PRO:HG3 | 3:L:171:LEU:HD11 | 1.67 | 0.75 |
| 1:A:224:GLN:NE2 | 1:A:246:LEU:HD11 | 2.02 | 0.75 |
| 2:H:128:GLN:NE2 | 2:H:128:GLN:H | 1.83 | 0.74 |
| 3:I:155:THR:HG23 | 3:I:158:ASP:H | 1.49 | 0.74 |
| 1:E:297:ILE:CG2 | 1:E:368:ILE:HD11 | 2.17 | 0.74 |
| 1:A:297:ILE:CG2 | 1:A:368:ILE:HD11 | 2.16 | 0.74 |
| 1:A:262:GLU:HB3 | 1:A:265:PHE:HB2 | 1.69 | 0.74 |
| 2:H:353:ILE:HB | 2:H:355:PHE:CE1 | 2.23 | 0.74 |
| 3:I:155:THR:HG22 | 3:I:158:ASP:OD2 | 1.86 | 0.74 |
| 1:C:376:SER:OG | 1:C:379:GLU:HG3 | 1.87 | 0.74 |
| 2:F:208:PRO:HG3 | 3:K:171:LEU:HD11 | 1.70 | 0.74 |
| 1:C:297:ILE:CG2 | 1:C:368:ILE:HD11 | 2.18 | 0.74 |
| 2:H:185:PHE:HB3 | 2:H:326:ASP:HB2 | 1.68 | 0.74 |
| 2:D:185:PHE:HB3 | 2:D:326:ASP:HB2 | 1.69 | 0.74 |
| 2:F:128:GLN:NE2 | 2:F:128:GLN:H | 1.84 | 0.73 |
| 3:J:155:THR:HG22 | 3:J:158:ASP:OD2 | 1.88 | 0.73 |
| 2:F:353:ILE:HB | 2:F:355:PHE:CE1 | 2.24 | 0.73 |
| 1:G:252:LEU:O | 1:G:253:LYS:O | 2.06 | 0.73 |
| 1:G:262:GLU:HB3 | 1:G:265:PHE:HB2 | 1.70 | 0.73 |
| 2:B:393:TYR:CE1 | 2:B:607:THR:HA | 2.23 | 0.73 |
| 1:G:376:SER:OG | 1:G:379:GLU:HG3 | 1.87 | 0.73 |
| 1:E:224:GLN:NE2 | 1:E:246:LEU:HD11 | 2.04 | 0.73 |
| 1:E:264:ASN:N | 1:E:264:ASN:HD22 | 1.85 | 0.73 |
| 2:D:361:LEU:O | 2:D:363:GLU:N | 2.21 | 0.73 |
| 1:E:262:GLU:HB3 | 1:E:265:PHE:HB2 | 1.71 | 0.73 |
| 1:A:264:ASN:N | 1:A:264:ASN:HD22 | 1.84 | 0.73 |
| 1:G:264:ASN:N | 1:G:264:ASN:HD22 | 1.86 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:322:LEU:HD12 | 2:D:323:VAL:N | 2.04 | 0.73 |
| 2:B:267:ARG:HH11 | 2:B:267:ARG:HG2 | 1.53 | 0.73 |
| 1:C:224:GLN:NE2 | 1:C:246:LEU:HD11 | 2.04 | 0.72 |
| 1:E:317:LYS:HB3 | 1:E:318:GLU:OE1 | 1.89 | 0.72 |
| 1:C:264:ASN:HD22 | 1:C:264:ASN:N | 1.85 | 0.72 |
| 2:H:322:LEU:HD12 | 2:H:323:VAL:N | 2.05 | 0.72 |
| 2:F:361:LEU:O | 2:F:364:VAL:HG22 | 1.89 | 0.72 |
| 2:B:185:PHE:HB3 | 2:B:326:ASP:HB2 | 1.70 | 0.72 |
| 1:C:262:GLU:HB3 | 1:C:265:PHE:HB2 | 1.70 | 0.72 |
| 2:D:267:ARG:HG2 | 2:D:267:ARG:HH11 | 1.55 | 0.72 |
| 2:F:351:GLN:HG3 | 2:F:353:ILE:HD11 | 1.71 | 0.72 |
| 2:H:351:GLN:HG3 | 2:H:353:ILE:HD11 | 1.70 | 0.72 |
| 3:L:155:THR:HG22 | 3:L:158:ASP:OD2 | 1.89 | 0.72 |
| 2:F:361:LEU:O | 2:F:363:GLU:N | 2.22 | 0.72 |
| 2:H:267:ARG:HH11 | 2:H:267:ARG:HG2 | 1.55 | 0.72 |
| 2:D:361:LEU:O | 2:D:364:VAL:HG22 | 1.90 | 0.72 |
| 2:F:393:TYR:CE1 | 2:F:607:THR:HA | 2.24 | 0.72 |
| 2:H:901:VAL:O | 2:H:902:ALA:O | 2.07 | 0.71 |
| 2:B:351:GLN:HG3 | 2:B:353:ILE:HD11 | 1.71 | 0.71 |
| 2:H:703:GLY:C | 2:H:705:VAL:H | 1.93 | 0.71 |
| 2:H:361:LEU:O | 2:H:363:GLU:N | 2.23 | 0.71 |
| 1:G:224:GLN:NE2 | 1:G:246:LEU:HD11 | 2.06 | 0.71 |
| 2:D:703:GLY:C | 2:D:705:VAL:H | 1.93 | 0.71 |
| 1:A:317:LYS:HB3 | 1:A:318:GLU:OE1 | 1.90 | 0.71 |
| 3:J:124:GLU:HB2 | 3:J:152:ASP:O | 1.90 | 0.71 |
| 2:F:703:GLY:C | 2:F:705:VAL:H | 1.94 | 0.71 |
| 1:E:340:ILE:HD11 | 2:F:273:ILE:HG12 | 1.73 | 0.71 |
| 1:G:61:ASP:HB3 | 1:G:86:ALA:HB2 | 1.73 | 0.71 |
| 2:H:62:GLU:HG2 | 2:H:297:ALA:HA | 1.73 | 0.71 |
| 2:B:50:LYS:H | 2:B:139:HIS:CD2 | 2.09 | 0.71 |
| 1:A:61:ASP:HB3 | 1:A:86:ALA:HB2 | 1.72 | 0.70 |
| 2:B:353:ILE:HB | 2:B:355:PHE:CE1 | 2.26 | 0.70 |
| 2:H:901:VAL:O | 2:H:902:ALA:C | 2.30 | 0.70 |
| 1:A:224:GLN:HE22 | 1:A:246:LEU:HD11 | 1.55 | 0.70 |
| 1:E:251:ILE:HG23 | 1:E:262:GLU:HB2 | 1.73 | 0.70 |
| 2:H:348:GLN:C | 2:H:348:GLN:HE21 | 1.94 | 0.70 |
| 1:G:251:ILE:HG23 | 1:G:262:GLU:HB2 | 1.74 | 0.70 |
| 2:D:50:LYS:H | 2:D:139:HIS:CD2 | 2.10 | 0.70 |
| 2:F:185:PHE:HB3 | 2:F:326:ASP:HB2 | 1.72 | 0.70 |
| 3:I:101:MET:HB3 | 3:I:117:ILE:O | 1.92 | 0.70 |
| 1:C:251:ILE:HG23 | 1:C:262:GLU:HB2 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:61:ASP:HB3 | 1:C:86:ALA:HB2 | 1.74 | 0.70 |
| 2:H:361:LEU:O | 2:H:364:VAL:HG22 | 1.92 | 0.70 |
| 3:L:101:MET:HB3 | 3:L:117:ILE:O | 1.90 | 0.70 |
| 2:D:187:GLY:HA2 | 3:J:173:LEU:HD13 | 1.72 | 0.70 |
| 3:I:124:GLU:HB2 | 3:I:152:ASP:O | 1.92 | 0.70 |
| 3:L:124:GLU:HB2 | 3:L:152:ASP:O | 1.92 | 0.70 |
| 2:D:393:TYR:HE1 | 2:D:607:THR:HA | 1.55 | 0.70 |
| 2:B:54:ILE:HG22 | 2:B:145:LEU:HD21 | 1.73 | 0.70 |
| 3:K:123:VAL:CB | 3:K:152:ASP:HA | 2.17 | 0.70 |
| 2:H:50:LYS:H | 2:H:139:HIS:CD2 | 2.10 | 0.70 |
| 2:F:901:VAL:C | 2:F:902:ALA:O | 2.23 | 0.70 |
| 1:A:163:ARG:HG2 | 1:A:163:ARG:HH11 | 1.56 | 0.70 |
| 2:D:348:GLN:HE21 | 2:D:348:GLN:C | 1.95 | 0.70 |
| 1:A:61:ASP:OD2 | 1:A:85:ARG:HD2 | 1.92 | 0.69 |
| 2:F:62:GLU:HG2 | 2:F:297:ALA:HA | 1.74 | 0.69 |
| 1:G:317:LYS:HB3 | 1:G:318:GLU:OE1 | 1.92 | 0.69 |
| 1:E:224:GLN:HE22 | 1:E:246:LEU:HD11 | 1.58 | 0.69 |
| 1:C:224:GLN:HE22 | 1:C:246:LEU:HD11 | 1.58 | 0.69 |
| 1:E:61:ASP:HB3 | 1:E:86:ALA:HB2 | 1.75 | 0.69 |
| 1:C:517:ASN:ND2 | 1:C:517:ASN:O | 2.26 | 0.69 |
| 2:F:54:ILE:HG22 | 2:F:145:LEU:HD21 | 1.74 | 0.69 |
| 2:B:348:GLN:HE21 | 2:B:348:GLN:C | 1.95 | 0.69 |
| 2:F:267:ARG:HG2 | 2:F:267:ARG:HH11 | 1.57 | 0.69 |
| 1:E:517:ASN:O | 1:E:517:ASN:ND2 | 2.26 | 0.69 |
| 3:K:124:GLU:HB2 | 3:K:152:ASP:O | 1.93 | 0.69 |
| 2:F:348:GLN:C | 2:F:348:GLN:HE21 | 1.95 | 0.69 |
| 2:B:703:GLY:C | 2:B:705:VAL:H | 1.95 | 0.69 |
| 3:J:123:VAL:CB | 3:J:152:ASP:HA | 2.18 | 0.69 |
| 1:A:251:ILE:HG23 | 1:A:262:GLU:HB2 | 1.75 | 0.68 |
| 2:F:241:GLN:NE2 | 2:F:246:GLY:H | 1.91 | 0.68 |
| 1:C:163:ARG:HG2 | 1:C:163:ARG:HH11 | 1.59 | 0.68 |
| 2:F:322:LEU:HD12 | 2:F:323:VAL:N | 2.09 | 0.68 |
| 1:G:61:ASP:OD2 | 1:G:85:ARG:HD2 | 1.93 | 0.68 |
| 2:D:187:GLY:CA | 3:J:173:LEU:HD13 | 2.23 | 0.68 |
| 1:A:178:ASN:HD22 | 3:I:136:ILE:HG12 | 1.57 | 0.68 |
| 2:D:901:VAL:O | 2:D:902:ALA:O | 2.10 | 0.68 |
| 2:H:187:GLY:HA2 | 3:L:173:LEU:HD13 | 1.75 | 0.68 |
| 1:A:235:LYS:HB3 | 1:A:239:GLU:HB2 | 1.76 | 0.68 |
| 2:F:50:LYS:H | 2:F:139:HIS:CD2 | 2.11 | 0.68 |
| 3:I:123:VAL:CB | 3:I:152:ASP:HA | 2.17 | 0.68 |
| 1:G:340:ILE:HD11 | 2:H:273:ILE:HG12 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:322:LEU:HD12 | 2:B:323:VAL:N | 2.08 | 0.68 |
| 2:H:241:GLN:NE2 | 2:H:246:GLY:H | 1.92 | 0.68 |
| 3:K:101:MET:HB3 | 3:K:117:ILE:O | 1.93 | 0.68 |
| 1:A:264:ASN:H | 1:A:264:ASN:HD22 | 1.42 | 0.68 |
| 1:C:61:ASP:OD2 | 1:C:85:ARG:HD2 | 1.93 | 0.68 |
| 1:A:517:ASN:ND2 | 1:A:517:ASN:O | 2.26 | 0.68 |
| 1:G:224:GLN:HE22 | 1:G:246:LEU:HD11 | 1.59 | 0.68 |
| 2:D:62:GLU:HG2 | 2:D:297:ALA:HA | 1.76 | 0.68 |
| 1:C:235:LYS:HB3 | 1:C:239:GLU:HB2 | 1.74 | 0.68 |
| 1:A:240:LYS:HE2 | 1:A:276:LEU:HD12 | 1.76 | 0.67 |
| 1:C:317:LYS:HB3 | 1:C:318:GLU:OE1 | 1.94 | 0.67 |
| 1:E:163:ARG:HH11 | 1:E:163:ARG:HG2 | 1.58 | 0.67 |
| 2:B:62:GLU:HG2 | 2:B:297:ALA:HA | 1.75 | 0.67 |
| 1:C:264:ASN:HD22 | 1:C:264:ASN:H | 1.42 | 0.67 |
| 3:J:101:MET:HB3 | 3:J:117:ILE:O | 1.94 | 0.67 |
| 1:G:517:ASN:ND2 | 1:G:517:ASN:O | 2.26 | 0.67 |
| 2:D:241:GLN:NE2 | 2:D:246:GLY:H | 1.92 | 0.67 |
| 1:A:195:HIS:O | 1:A:198:SER:HB3 | 1.94 | 0.67 |
| 2:F:900:ALA:O | 2:F:901:VAL:CB | 2.43 | 0.67 |
| 1:C:177:ASP:OD2 | 2:D:327:VAL:HG21 | 1.95 | 0.67 |
| 1:A:344:ASN:ND2 | 1:E:111:ASN:ND2 | 2.31 | 0.66 |
| 1:C:260:GLU:O | 1:C:261:ASP:HB2 | 1.94 | 0.66 |
| 1:G:8:LEU:HD12 | 1:G:11:GLN:OE1 | 1.96 | 0.66 |
| 2:D:202:CYS:HG | 2:D:343:CYS:HG | 1.41 | 0.66 |
| 2:B:241:GLN:NE2 | 2:B:246:GLY:H | 1.93 | 0.66 |
| 2:F:393:TYR:HE1 | 2:F:607:THR:HA | 1.59 | 0.66 |
| 2:H:54:ILE:HG22 | 2:H:145:LEU:HD21 | 1.78 | 0.66 |
| 1:A:307:LEU:HB3 | 1:A:383:LEU:HD22 | 1.78 | 0.66 |
| 1:E:307:LEU:HB3 | 1:E:383:LEU:HD22 | 1.75 | 0.66 |
| 1:E:235:LYS:HB3 | 1:E:239:GLU:HB2 | 1.77 | 0.66 |
| 1:G:347:ARG:HH22 | 2:H:274:ARG:HD2 | 1.59 | 0.66 |
| 1:G:41:THR:O | 1:G:45:ILE:HG13 | 1.96 | 0.66 |
| 2:B:705:VAL:O | 2:B:800:GLY:O | 2.14 | 0.66 |
| 2:H:322:LEU:HD12 | 2:H:322:LEU:C | 2.16 | 0.66 |
| 1:G:163:ARG:HH11 | 1:G:163:ARG:HG2 | 1.59 | 0.66 |
| 2:D:54:ILE:HG22 | 2:D:145:LEU:HD21 | 1.78 | 0.66 |
| 1:G:235:LYS:HB3 | 1:G:239:GLU:HB2 | 1.77 | 0.66 |
| 2:F:384:THR:HA | 2:F:389:ASN:HA | 1.77 | 0.66 |
| 2:B:384:THR:HA | 2:B:389:ASN:HA | 1.78 | 0.65 |
| 1:A:401:GLU:HG3 | 1:A:533:GLN:HE22 | 1.61 | 0.65 |
| 2:D:322:LEU:HD12 | 2:D:322:LEU:C | 2.17 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:45:ILE:HG12 | 1:C:498:GLY:HA2 | 1.78 | 0.65 |
| 2:D:705:VAL:O | 2:D:800:GLY:O | 2.14 | 0.65 |
| 2:H:237:TRP:HB3 | 2:H:238:PRO:HD3 | 1.78 | 0.65 |
| 2:B:900:ALA:O | 2:B:901:VAL:CB | 2.44 | 0.65 |
| 1:A:285:ILE:HD11 | 1:A:388:ALA:HA | 1.79 | 0.65 |
| 2:H:187:GLY:CA | 3:L:173:LEU:HD13 | 2.26 | 0.65 |
| 3:K:117:ILE:HD13 | 3:K:126:ILE:HG12 | 1.78 | 0.65 |
| 2:D:384:THR:HA | 2:D:389:ASN:HA | 1.78 | 0.65 |
| 2:B:361:LEU:O | 2:B:364:VAL:HG22 | 1.97 | 0.65 |
| 2:H:384:THR:HA | 2:H:389:ASN:HA | 1.78 | 0.65 |
| 1:G:297:ILE:HD11 | 1:G:309:ARG:HG2 | 1.78 | 0.65 |
| 2:D:353:ILE:HB | 2:D:355:PHE:CE1 | 2.31 | 0.65 |
| 2:H:393:TYR:HE1 | 2:H:607:THR:HA | 1.57 | 0.65 |
| 1:E:61:ASP:OD2 | 1:E:85:ARG:HD2 | 1.97 | 0.65 |
| 1:C:195:HIS:O | 1:C:198:SER:HB3 | 1.96 | 0.65 |
| 1:E:240:LYS:HE2 | 1:E:276:LEU:HD12 | 1.78 | 0.65 |
| 1:G:401:GLU:HG3 | 1:G:533:GLN:HE22 | 1.62 | 0.64 |
| 2:B:16:ARG:NH2 | 2:B:116:PRO:HB2 | 2.13 | 0.64 |
| 2:F:322:LEU:C | 2:F:322:LEU:HD12 | 2.18 | 0.64 |
| 2:D:900:ALA:O | 2:D:901:VAL:CB | 2.45 | 0.64 |
| 1:C:297:ILE:HD11 | 1:C:309:ARG:HG2 | 1.80 | 0.64 |
| 1:E:264:ASN:HD22 | 1:E:264:ASN:H | 1.45 | 0.64 |
| 1:E:397:SER:OG | 1:E:400:GLU:HG3 | 1.97 | 0.64 |
| 1:C:422:GLU:HG3 | 1:C:530:ALA:HB3 | 1.79 | 0.64 |
| 2:B:322:LEU:HD12 | 2:B:322:LEU:C | 2.18 | 0.64 |
| 1:G:264:ASN:H | 1:G:264:ASN:HD22 | 1.45 | 0.64 |
| 1:G:240:LYS:HE2 | 1:G:276:LEU:HD12 | 1.78 | 0.64 |
| 2:F:235:LEU:O | 2:F:238:PRO:HD2 | 1.97 | 0.64 |
| 1:E:49:LEU:C | 1:E:52:PRO:HD2 | 2.18 | 0.64 |
| 1:G:397:SER:OG | 1:G:400:GLU:HG3 | 1.98 | 0.64 |
| 1:E:45:ILE:HG12 | 1:E:498:GLY:HA2 | 1.80 | 0.64 |
| 2:B:235:LEU:O | 2:B:238:PRO:HD2 | 1.98 | 0.64 |
| 1:C:51:LEU:HB2 | 1:C:52:PRO:HD3 | 1.80 | 0.64 |
| 1:E:195:HIS:O | 1:E:198:SER:HB3 | 1.98 | 0.64 |
| 2:B:277:THR:HG23 | 2:B:280:LEU:H | 1.63 | 0.64 |
| 1:C:8:LEU:HD12 | 1:C:11:GLN:OE1 | 1.98 | 0.64 |
| 1:E:8:LEU:HD12 | 1:E:11:GLN:OE1 | 1.98 | 0.63 |
| 1:C:307:LEU:HB3 | 1:C:383:LEU:HD22 | 1.80 | 0.63 |
| 1:G:422:GLU:HG3 | 1:G:530:ALA:HB3 | 1.80 | 0.63 |
| 1:C:390:LEU:O | 1:C:391:ARG:HG2 | 1.97 | 0.63 |
| 1:A:33:VAL:CG2 | 1:A:54:ILE:HD11 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:358:SER:O | 2:B:358:SER:OG | 2.14 | 0.63 |
| 1:G:260:GLU:O | 1:G:261:ASP:HB2 | 1.97 | 0.63 |
| 1:C:235:LYS:HB3 | 1:C:239:GLU:CG | 2.28 | 0.63 |
| 1:C:41:THR:O | 1:C:45:ILE:HG13 | 1.97 | 0.63 |
| 2:H:229:ILE:HD13 | 2:H:281:THR:HA | 1.80 | 0.63 |
| 2:F:187:GLY:HA2 | 3:K:173:LEU:HD13 | 1.81 | 0.63 |
| 2:D:235:LEU:O | 2:D:238:PRO:HD2 | 1.99 | 0.63 |
| 2:B:393:TYR:HE1 | 2:B:607:THR:HA | 1.62 | 0.63 |
| 2:H:335:PHE:CZ | 3:L:144:ILE:HD13 | 2.34 | 0.63 |
| 2:F:229:ILE:HD13 | 2:F:281:THR:HA | 1.80 | 0.63 |
| 2:B:95:ARG:HH11 | 2:B:95:ARG:HG3 | 1.64 | 0.63 |
| 1:C:235:LYS:HD3 | 1:C:239:GLU:HG3 | 1.80 | 0.63 |
| 1:A:8:LEU:HD12 | 1:A:11:GLN:OE1 | 1.98 | 0.63 |
| 2:F:95:ARG:HG3 | 2:F:95:ARG:HH11 | 1.63 | 0.63 |
| 2:D:393:TYR:CD1 | 2:D:607:THR:HA | 2.34 | 0.63 |
| 1:C:448:TYR:CE2 | 2:H:240:GLU:OE2 | 2.52 | 0.63 |
| 3:J:117:ILE:HD13 | 3:J:126:ILE:HG12 | 1.81 | 0.63 |
| 2:B:237:TRP:HB3 | 2:B:238:PRO:HD3 | 1.79 | 0.63 |
| 1:A:45:ILE:HG12 | 1:A:498:GLY:HA2 | 1.81 | 0.63 |
| 1:G:285:ILE:HD11 | 1:G:388:ALA:HA | 1.81 | 0.63 |
| 2:H:95:ARG:HG3 | 2:H:95:ARG:HH11 | 1.63 | 0.63 |
| 1:G:195:HIS:O | 1:G:198:SER:HB3 | 1.99 | 0.62 |
| 2:H:277:THR:HG23 | 2:H:280:LEU:H | 1.64 | 0.62 |
| 1:A:213:PRO:HB3 | 1:A:332:MET:HE2 | 1.81 | 0.62 |
| 1:E:401:GLU:HG3 | 1:E:533:GLN:HE22 | 1.64 | 0.62 |
| 1:C:241:GLU:HA | 1:C:244:ARG:HH11 | 1.65 | 0.62 |
| 2:F:277:THR:HG23 | 2:F:280:LEU:H | 1.65 | 0.62 |
| 2:B:252:ASP:O | 2:B:254:PRO:HD3 | 1.99 | 0.62 |
| 1:G:45:ILE:HG12 | 1:G:498:GLY:HA2 | 1.80 | 0.62 |
| 1:C:446:SER:HB2 | 1:C:449:GLN:HG3 | 1.79 | 0.62 |
| 1:A:297:ILE:HD11 | 1:A:309:ARG:HG2 | 1.81 | 0.62 |
| 2:F:237:TRP:HB3 | 2:F:238:PRO:HD3 | 1.82 | 0.62 |
| 1:G:307:LEU:HB3 | 1:G:383:LEU:HD22 | 1.79 | 0.62 |
| 1:A:260:GLU:O | 1:A:261:ASP:HB2 | 2.00 | 0.62 |
| 1:E:41:THR:O | 1:E:45:ILE:HG13 | 2.00 | 0.62 |
| 2:D:229:ILE:HD13 | 2:D:281:THR:HA | 1.81 | 0.62 |
| 2:B:306:GLU:OE2 | 2:B:309:LYS:HD2 | 1.98 | 0.62 |
| 2:D:95:ARG:HH11 | 2:D:95:ARG:HG3 | 1.64 | 0.62 |
| 3:K:106:LYS:HG3 | 3:K:112:GLU:HB2 | 1.81 | 0.62 |
| 1:A:396:ARG:HG3 | 1:A:534:LEU:HD11 | 1.81 | 0.62 |
| 1:E:309:ARG:HG3 | 1:E:364:LEU:HD21 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:125:ARG:HD3 | 3:K:129:ARG:NH2 | 2.15 | 0.62 |
| 1:A:51:LEU:HB2 | 1:A:52:PRO:HD3 | 1.81 | 0.62 |
| 3:K:170:VAL:HG13 | 3:K:171:LEU:N | 2.14 | 0.62 |
| 1:A:241:GLU:HA | 1:A:244:ARG:HH11 | 1.65 | 0.62 |
| 3:J:125:ARG:HD3 | 3:J:129:ARG:NH2 | 2.15 | 0.62 |
| 2:D:252:ASP:O | 2:D:254:PRO:HD3 | 2.00 | 0.62 |
| 1:C:285:ILE:HD11 | 1:C:388:ALA:HA | 1.82 | 0.62 |
| 1:E:297:ILE:HD11 | 1:E:309:ARG:HG2 | 1.81 | 0.61 |
| 1:G:241:GLU:HA | 1:G:244:ARG:HH11 | 1.65 | 0.61 |
| 1:E:347:ARG:HH22 | 2:F:274:ARG:HD2 | 1.65 | 0.61 |
| 1:C:397:SER:OG | 1:C:400:GLU:HG3 | 1.99 | 0.61 |
| 1:G:51:LEU:HB2 | 1:G:52:PRO:HD3 | 1.82 | 0.61 |
| 1:E:56:SER:HB3 | 1:E:101:SER:OG | 2.01 | 0.61 |
| 1:E:422:GLU:HG3 | 1:E:530:ALA:HB3 | 1.82 | 0.61 |
| 1:G:235:LYS:HD3 | 1:G:239:GLU:HG3 | 1.82 | 0.61 |
| 1:G:124:THR:HG22 | 1:G:125:VAL:HG23 | 1.81 | 0.61 |
| 2:H:338:GLU:HG3 | 3:L:148:LYS:HD3 | 1.82 | 0.61 |
| 3:L:106:LYS:HG3 | 3:L:112:GLU:HB2 | 1.82 | 0.61 |
| 1:C:448:TYR:HE2 | 2:H:240:GLU:OE2 | 1.84 | 0.61 |
| 1:E:235:LYS:HB3 | 1:E:239:GLU:CG | 2.30 | 0.61 |
| 1:E:235:LYS:HD3 | 1:E:239:GLU:HG3 | 1.82 | 0.61 |
| 1:A:285:ILE:CD1 | 1:A:388:ALA:HA | 2.31 | 0.61 |
| 1:C:340:ILE:HD11 | 2:D:273:ILE:HG12 | 1.82 | 0.61 |
| 2:H:252:ASP:O | 2:H:254:PRO:HD3 | 2.00 | 0.61 |
| 3:L:125:ARG:HD3 | 3:L:129:ARG:NH2 | 2.15 | 0.61 |
| 1:E:241:GLU:HA | 1:E:244:ARG:HH11 | 1.66 | 0.61 |
| 2:B:237:TRP:O | 2:B:242:PRO:HD3 | 2.01 | 0.61 |
| 1:A:49:LEU:C | 1:A:52:PRO:HD2 | 2.21 | 0.61 |
| 1:A:446:SER:HB2 | 1:A:449:GLN:HG3 | 1.81 | 0.61 |
| 1:E:390:LEU:O | 1:E:391:ARG:HG2 | 2.01 | 0.61 |
| 2:D:901:VAL:O | 2:D:902:ALA:C | 2.39 | 0.61 |
| 1:E:396:ARG:HG3 | 1:E:534:LEU:HD11 | 1.83 | 0.61 |
| 1:E:285:ILE:HD11 | 1:E:388:ALA:HA | 1.83 | 0.61 |
| 2:B:187:GLY:HA2 | 3:I:173:LEU:HD13 | 1.81 | 0.61 |
| 2:B:362:GLN:OE1 | 2:B:362:GLN:HA | 2.01 | 0.61 |
| 2:B:901:VAL:C | 2:B:902:ALA:O | 2.32 | 0.61 |
| 2:H:193:LEU:H | 2:H:197:THR:HB | 1.65 | 0.61 |
| 1:C:396:ARG:HG3 | 1:C:534:LEU:HD11 | 1.83 | 0.61 |
| 1:C:214:TRP:CZ3 | 1:C:332:MET:HB3 | 2.36 | 0.61 |
| 3:L:123:VAL:CB | 3:L:152:ASP:HA | 2.22 | 0.61 |
| 2:B:64:LEU:HD21 | 2:B:77:VAL:CG2 | 2.30 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:351:GLN:CG | 2:D:353:ILE:HD11 | 2.30 | 0.61 |
| 1:A:517:ASN:HD22 | 1:A:517:ASN:C | 2.04 | 0.61 |
| 1:A:235:LYS:HD3 | 1:A:239:GLU:HG3 | 1.83 | 0.60 |
| 2:H:237:TRP:O | 2:H:242:PRO:HD3 | 2.01 | 0.60 |
| 3:I:106:LYS:HG3 | 3:I:112:GLU:HB2 | 1.84 | 0.60 |
| 2:H:705:VAL:O | 2:H:800:GLY:O | 2.19 | 0.60 |
| 1:C:235:LYS:HE2 | 1:C:238:LYS:HB3 | 1.83 | 0.60 |
| 2:D:237:TRP:HB3 | 2:D:238:PRO:HD3 | 1.83 | 0.60 |
| 1:G:396:ARG:HG3 | 1:G:534:LEU:HD11 | 1.82 | 0.60 |
| 1:C:178:ASN:HD22 | 3:J:136:ILE:HG12 | 1.66 | 0.60 |
| 1:G:235:LYS:HE2 | 1:G:238:LYS:HB3 | 1.82 | 0.60 |
| 1:A:311:LEU:O | 1:A:315:VAL:HG23 | 2.00 | 0.60 |
| 3:J:106:LYS:HG3 | 3:J:112:GLU:HB2 | 1.82 | 0.60 |
| 2:B:202:CYS:HG | 2:B:343:CYS:HG | 1.49 | 0.60 |
| 2:F:237:TRP:O | 2:F:242:PRO:HD3 | 2.01 | 0.60 |
| 3:L:125:ARG:HD3 | 3:L:129:ARG:HH21 | 1.66 | 0.60 |
| 1:G:390:LEU:O | 1:G:391:ARG:HG2 | 2.02 | 0.60 |
| 2:D:343:CYS:O | 2:D:347:SER:HB3 | 2.01 | 0.60 |
| 3:I:117:ILE:HD13 | 3:I:126:ILE:HG12 | 1.83 | 0.60 |
| 1:A:397:SER:OG | 1:A:400:GLU:HG3 | 2.00 | 0.60 |
| 1:E:333:ILE:HA | 2:F:223:ARG:NH2 | 2.15 | 0.60 |
| 1:E:446:SER:HB2 | 1:E:449:GLN:HG3 | 1.83 | 0.60 |
| 2:H:362:GLN:OE1 | 2:H:362:GLN:HA | 2.01 | 0.60 |
| 1:G:517:ASN:ND2 | 1:G:534:LEU:HD12 | 2.16 | 0.60 |
| 1:E:450:VAL:O | 1:E:454:ILE:HG13 | 2.00 | 0.60 |
| 2:H:318:LEU:HD12 | 2:H:319:ASN:H | 1.66 | 0.60 |
| 1:A:104:PHE:HE1 | 1:A:106:GLU:HG3 | 1.66 | 0.60 |
| 2:B:54:ILE:CG2 | 2:B:145:LEU:HD21 | 2.31 | 0.60 |
| 3:I:125:ARG:HD3 | 3:I:129:ARG:NH2 | 2.16 | 0.60 |
| 2:F:343:CYS:O | 2:F:347:SER:HB3 | 2.01 | 0.60 |
| 1:A:390:LEU:O | 1:A:391:ARG:HG2 | 2.02 | 0.60 |
| 2:D:64:LEU:HD21 | 2:D:77:VAL:CG2 | 2.32 | 0.60 |
| 2:D:16:ARG:NH2 | 2:D:116:PRO:HB2 | 2.17 | 0.60 |
| 1:E:33:VAL:CG2 | 1:E:54:ILE:HD11 | 2.32 | 0.60 |
| 1:G:446:SER:HB2 | 1:G:449:GLN:HG3 | 1.83 | 0.60 |
| 1:E:178:ASN:HD22 | 3:K:136:ILE:HG12 | 1.66 | 0.60 |
| 1:C:33:VAL:CG2 | 1:C:54:ILE:HD11 | 2.31 | 0.60 |
| 2:D:362:GLN:HA | 2:D:362:GLN:OE1 | 2.01 | 0.60 |
| 2:D:50:LYS:H | 2:D:139:HIS:HD2 | 1.49 | 0.60 |
| 1:G:235:LYS:HB3 | 1:G:239:GLU:CG | 2.31 | 0.60 |
| 2:F:252:ASP:O | 2:F:254:PRO:HD3 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:358:SER:O | 2:F:358:SER:OG | 2.17 | 0.60 |
| 1:G:422:GLU:HG3 | 1:G:530:ALA:CB | 2.32 | 0.59 |
| 1:E:177:ASP:OD2 | 2:F:327:VAL:HG21 | 2.02 | 0.59 |
| 2:B:229:ILE:HD13 | 2:B:281:THR:HA | 1.83 | 0.59 |
| 1:C:517:ASN:ND2 | 1:C:534:LEU:HD12 | 2.16 | 0.59 |
| 2:H:306:GLU:OE2 | 2:H:309:LYS:HD2 | 2.01 | 0.59 |
| 2:B:325:ASN:HD21 | 2:B:327:VAL:HG22 | 1.68 | 0.59 |
| 1:E:214:TRP:CZ3 | 1:E:332:MET:HB3 | 2.38 | 0.59 |
| 3:J:125:ARG:HD3 | 3:J:129:ARG:HH21 | 1.67 | 0.59 |
| 2:F:193:LEU:H | 2:F:197:THR:HB | 1.68 | 0.59 |
| 2:H:358:SER:OG | 2:H:358:SER:O | 2.17 | 0.59 |
| 1:C:235:LYS:HB3 | 1:C:239:GLU:CB | 2.32 | 0.59 |
| 3:K:125:ARG:HD3 | 3:K:129:ARG:HH21 | 1.68 | 0.59 |
| 1:A:422:GLU:HG3 | 1:A:530:ALA:HB3 | 1.83 | 0.59 |
| 2:D:306:GLU:OE2 | 2:D:309:LYS:HD2 | 2.02 | 0.59 |
| 2:F:54:ILE:CG2 | 2:F:145:LEU:HD21 | 2.32 | 0.59 |
| 1:A:235:LYS:HB3 | 1:A:239:GLU:CG | 2.31 | 0.59 |
| 2:D:358:SER:OG | 2:D:358:SER:O | 2.19 | 0.59 |
| 1:C:401:GLU:HG3 | 1:C:533:GLN:HE22 | 1.68 | 0.59 |
| 3:K:155:THR:HG22 | 3:K:158:ASP:CG | 2.22 | 0.59 |
| 1:G:507:LYS:HG2 | 1:G:513:PHE:HB2 | 1.84 | 0.59 |
| 2:D:193:LEU:H | 2:D:197:THR:HB | 1.68 | 0.59 |
| 1:E:104:PHE:HE1 | 1:E:106:GLU:HG3 | 1.66 | 0.59 |
| 2:H:64:LEU:HD21 | 2:H:77:VAL:CG2 | 2.33 | 0.59 |
| 3:I:170:VAL:HG13 | 3:I:171:LEU:N | 2.18 | 0.59 |
| 1:A:178:ASN:ND2 | 3:I:136:ILE:HG12 | 2.17 | 0.59 |
| 2:B:16:ARG:HH22 | 2:B:116:PRO:HB2 | 1.67 | 0.59 |
| 1:G:49:LEU:C | 1:G:52:PRO:HD2 | 2.22 | 0.59 |
| 2:F:335:PHE:CZ | 3:K:144:ILE:HD13 | 2.38 | 0.59 |
| 1:A:517:ASN:ND2 | 1:A:534:LEU:HD12 | 2.17 | 0.59 |
| 1:G:285:ILE:CD1 | 1:G:388:ALA:HA | 2.33 | 0.59 |
| 1:E:309:ARG:CG | 1:E:364:LEU:HD21 | 2.32 | 0.58 |
| 2:F:187:GLY:CA | 3:K:173:LEU:HD13 | 2.33 | 0.58 |
| 2:B:187:GLY:CA | 3:I:173:LEU:HD13 | 2.32 | 0.58 |
| 1:E:488:ALA:O | 1:E:490:PRO:HD3 | 2.03 | 0.58 |
| 1:G:377:GLU:OE2 | 1:G:381:LYS:HE3 | 2.03 | 0.58 |
| 3:K:149:GLN:HG3 | 3:K:149:GLN:O | 2.02 | 0.58 |
| 1:E:285:ILE:CD1 | 1:E:388:ALA:HA | 2.33 | 0.58 |
| 3:I:125:ARG:HD3 | 3:I:129:ARG:HH21 | 1.68 | 0.58 |
| 3:J:170:VAL:HG13 | 3:J:171:LEU:N | 2.18 | 0.58 |
| 2:B:351:GLN:CG | 2:B:353:ILE:HD11 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:235:LYS:HE2 | 1:E:238:LYS:HB3 | 1.84 | 0.58 |
| 2:D:277:THR:HG23 | 2:D:280:LEU:H | 1.67 | 0.58 |
| 2:D:335:PHE:CZ | 3:J:144:ILE:HD13 | 2.39 | 0.58 |
| 2:F:306:GLU:OE2 | 2:F:309:LYS:HD2 | 2.02 | 0.58 |
| 1:A:60:ILE:HD11 | 1:A:119:PHE:HE2 | 1.68 | 0.58 |
| 1:G:309:ARG:HG3 | 1:G:364:LEU:HD21 | 1.85 | 0.58 |
| 1:C:309:ARG:HG3 | 1:C:364:LEU:HD21 | 1.85 | 0.58 |
| 1:E:377:GLU:OE2 | 1:E:381:LYS:HE3 | 2.03 | 0.58 |
| 1:E:218:ILE:O | 1:E:222:LEU:HB2 | 2.03 | 0.58 |
| 3:I:149:GLN:HG3 | 3:I:149:GLN:O | 2.02 | 0.58 |
| 2:D:237:TRP:O | 2:D:242:PRO:HD3 | 2.02 | 0.58 |
| 2:H:701:GLU:HA | 2:H:704:LEU:CB | 2.34 | 0.58 |
| 1:A:309:ARG:HG3 | 1:A:364:LEU:HD21 | 1.85 | 0.58 |
| 2:F:362:GLN:HA | 2:F:362:GLN:OE1 | 2.03 | 0.58 |
| 1:C:104:PHE:HE1 | 1:C:106:GLU:HG3 | 1.68 | 0.58 |
| 1:E:311:LEU:O | 1:E:315:VAL:HG23 | 2.04 | 0.58 |
| 1:E:260:GLU:O | 1:E:261:ASP:HB2 | 2.03 | 0.58 |
| 1:C:285:ILE:CD1 | 1:C:388:ALA:HA | 2.34 | 0.58 |
| 2:H:318:LEU:HD12 | 2:H:319:ASN:N | 2.19 | 0.58 |
| 1:G:450:VAL:O | 1:G:454:ILE:HG13 | 2.02 | 0.58 |
| 1:C:25:GLN:O | 1:C:29:GLU:HG3 | 2.04 | 0.58 |
| 2:D:325:ASN:HD21 | 2:D:327:VAL:HG22 | 1.67 | 0.58 |
| 2:F:325:ASN:HD21 | 2:F:327:VAL:HG22 | 1.69 | 0.58 |
| 1:C:454:ILE:HD13 | 1:C:480:HIS:ND1 | 2.19 | 0.58 |
| 1:A:124:THR:HG22 | 1:A:125:VAL:HG23 | 1.84 | 0.58 |
| 1:G:78:ARG:O | 1:G:81:ILE:HG13 | 2.03 | 0.58 |
| 1:C:178:ASN:ND2 | 3:J:136:ILE:HG12 | 2.18 | 0.58 |
| 2:H:235:LEU:O | 2:H:238:PRO:HD2 | 2.03 | 0.58 |
| 1:A:177:ASP:OD2 | 2:B:327:VAL:HG21 | 2.04 | 0.58 |
| 1:C:218:ILE:O | 1:C:222:LEU:HB2 | 2.04 | 0.58 |
| 2:H:343:CYS:O | 2:H:347:SER:HB3 | 2.04 | 0.58 |
| 1:C:240:LYS:HE2 | 1:C:276:LEU:HD12 | 1.85 | 0.58 |
| 2:F:132:ASP:HA | 2:F:157:MET:HE2 | 1.86 | 0.58 |
| 1:C:377:GLU:OE2 | 1:C:381:LYS:HE3 | 2.03 | 0.58 |
| 1:E:517:ASN:ND2 | 1:E:534:LEU:HD12 | 2.18 | 0.58 |
| 1:C:214:TRP:CE3 | 1:C:332:MET:HB3 | 2.39 | 0.58 |
| 1:G:214:TRP:CZ3 | 1:G:332:MET:HB3 | 2.39 | 0.58 |
| 2:F:64:LEU:HD21 | 2:F:77:VAL:CG2 | 2.33 | 0.57 |
| 2:H:351:GLN:CG | 2:H:353:ILE:HD11 | 2.33 | 0.57 |
| 2:D:164:TYR:CE2 | 2:D:169:LEU:HB2 | 2.39 | 0.57 |
| 1:G:454:ILE:HD13 | 1:G:480:HIS:ND1 | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:217:THR:HA | 2:H:221:MET:HG2 | 1.86 | 0.57 |
| 2:B:335:PHE:CZ | 3:I:144:ILE:HD13 | 2.38 | 0.57 |
| 1:G:33:VAL:CG2 | 1:G:54:ILE:HD11 | 2.34 | 0.57 |
| 1:A:235:LYS:HE2 | 1:A:238:LYS:HB3 | 1.84 | 0.57 |
| 2:D:325:ASN:ND2 | 2:D:327:VAL:HG22 | 2.18 | 0.57 |
| 1:A:454:ILE:HD13 | 1:A:480:HIS:ND1 | 2.19 | 0.57 |
| 1:E:507:LYS:HG2 | 1:E:513:PHE:HB2 | 1.85 | 0.57 |
| 3:J:155:THR:HG22 | 3:J:158:ASP:CG | 2.25 | 0.57 |
| 1:G:517:ASN:C | 1:G:517:ASN:HD22 | 2.08 | 0.57 |
| 1:E:481:GLU:HB2 | 2:F:30:PHE:HE1 | 1.69 | 0.57 |
| 2:H:393:TYR:CD1 | 2:H:607:THR:HA | 2.39 | 0.57 |
| 2:F:351:GLN:CG | 2:F:353:ILE:HD11 | 2.33 | 0.57 |
| 1:A:450:VAL:O | 1:A:454:ILE:HG13 | 2.04 | 0.57 |
| 2:H:325:ASN:HD21 | 2:H:327:VAL:HG22 | 1.70 | 0.57 |
| 2:D:243:PHE:O | 2:D:247:VAL:HG21 | 2.04 | 0.57 |
| 1:G:418:ASN:ND2 | 1:G:420:ASP:H | 2.03 | 0.57 |
| 3:L:170:VAL:HG13 | 3:L:171:LEU:N | 2.19 | 0.57 |
| 2:B:208:PRO:HG3 | 3:I:171:LEU:CD1 | 2.32 | 0.57 |
| 2:H:164:TYR:CE2 | 2:H:169:LEU:HB2 | 2.39 | 0.57 |
| 1:C:213:PRO:HB3 | 1:C:332:MET:HE2 | 1.87 | 0.57 |
| 1:E:33:VAL:HG23 | 1:E:54:ILE:HD11 | 1.85 | 0.57 |
| 1:A:56:SER:HB3 | 1:A:101:SER:OG | 2.05 | 0.57 |
| 2:H:64:LEU:HB3 | 2:H:111:LEU:HD13 | 1.86 | 0.57 |
| 1:E:124:THR:HG22 | 1:E:125:VAL:HG23 | 1.86 | 0.57 |
| 1:A:218:ILE:O | 1:A:222:LEU:HB2 | 2.03 | 0.57 |
| 1:A:33:VAL:HG23 | 1:A:54:ILE:HD11 | 1.86 | 0.57 |
| 1:G:104:PHE:HE1 | 1:G:106:GLU:HG3 | 1.69 | 0.57 |
| 1:C:309:ARG:CG | 1:C:364:LEU:HD21 | 2.35 | 0.57 |
| 3:L:155:THR:HG22 | 3:L:158:ASP:CG | 2.24 | 0.57 |
| 1:C:124:THR:HG22 | 1:C:125:VAL:HG23 | 1.86 | 0.57 |
| 1:G:218:ILE:O | 1:G:222:LEU:HB2 | 2.04 | 0.57 |
| 1:C:517:ASN:C | 1:C:517:ASN:HD22 | 2.08 | 0.57 |
| 1:E:39:THR:O | 1:E:43:THR:HB | 2.05 | 0.57 |
| 3:K:118:GLU:O | 3:K:120:THR:N | 2.38 | 0.57 |
| 3:I:155:THR:HG22 | 3:I:158:ASP:CG | 2.25 | 0.56 |
| 2:H:50:LYS:H | 2:H:139:HIS:HD2 | 1.51 | 0.56 |
| 1:C:49:LEU:C | 1:C:52:PRO:HD2 | 2.25 | 0.56 |
| 2:D:84:ASP:H | 2:D:87:ASN:ND2 | 2.03 | 0.56 |
| 2:H:178:ILE:HD11 | 2:H:310:ILE:HD12 | 1.86 | 0.56 |
| 1:A:377:GLU:OE2 | 1:A:381:LYS:HE3 | 2.05 | 0.56 |
| 2:D:701:GLU:HA | 2:D:704:LEU:CB | 2.35 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:347:ARG:HH22 | 2:D:274:ARG:HD2 | 1.70 | 0.56 |
| 2:B:199:CYS:HG | 2:B:343:CYS:HG | 1.52 | 0.56 |
| 2:B:164:TYR:CE2 | 2:B:169:LEU:HB2 | 2.40 | 0.56 |
| 1:E:235:LYS:HB3 | 1:E:239:GLU:CB | 2.36 | 0.56 |
| 3:L:118:GLU:O | 3:L:120:THR:N | 2.39 | 0.56 |
| 2:B:193:LEU:H | 2:B:197:THR:HB | 1.68 | 0.56 |
| 1:E:517:ASN:C | 1:E:517:ASN:HD22 | 2.08 | 0.56 |
| 2:H:132:ASP:HA | 2:H:157:MET:HE2 | 1.87 | 0.56 |
| 1:E:113:LEU:O | 1:E:117:PRO:HG3 | 2.06 | 0.56 |
| 3:L:149:GLN:O | 3:L:149:GLN:HG3 | 2.05 | 0.56 |
| 2:F:392:LEU:O | 2:F:606:ARG:CB | 2.54 | 0.56 |
| 1:A:36:ILE:HB | 1:A:128:ALA:HA | 1.87 | 0.56 |
| 2:B:325:ASN:ND2 | 2:B:327:VAL:HG22 | 2.20 | 0.56 |
| 1:C:450:VAL:O | 1:C:454:ILE:HG13 | 2.06 | 0.56 |
| 1:A:418:ASN:ND2 | 1:A:420:ASP:H | 2.01 | 0.56 |
| 1:C:418:ASN:ND2 | 1:C:420:ASP:H | 2.03 | 0.56 |
| 1:C:56:SER:HB3 | 1:C:101:SER:OG | 2.04 | 0.56 |
| 1:E:527:GLN:OE1 | 1:E:527:GLN:HA | 2.05 | 0.56 |
| 1:E:51:LEU:HB2 | 1:E:52:PRO:HD3 | 1.87 | 0.56 |
| 1:A:235:LYS:HB3 | 1:A:239:GLU:CB | 2.35 | 0.56 |
| 1:G:235:LYS:HB3 | 1:G:239:GLU:CB | 2.36 | 0.56 |
| 1:C:422:GLU:HG3 | 1:C:530:ALA:CB | 2.35 | 0.56 |
| 1:A:104:PHE:CE1 | 1:A:106:GLU:HG3 | 2.41 | 0.56 |
| 2:H:243:PHE:O | 2:H:247:VAL:HG21 | 2.05 | 0.56 |
| 3:J:118:GLU:O | 3:J:120:THR:N | 2.39 | 0.56 |
| 1:A:25:GLN:O | 1:A:29:GLU:HG3 | 2.06 | 0.56 |
| 1:E:104:PHE:CE1 | 1:E:106:GLU:HG3 | 2.41 | 0.56 |
| 3:J:155:THR:O | 3:J:158:ASP:HB2 | 2.06 | 0.56 |
| 1:E:422:GLU:HG3 | 1:E:530:ALA:CB | 2.36 | 0.56 |
| 2:B:217:THR:HA | 2:B:221:MET:HG2 | 1.88 | 0.56 |
| 2:B:217:THR:HG21 | 2:B:223:ARG:HH22 | 1.70 | 0.56 |
| 2:B:251:GLY:O | 2:B:286:LYS:HE3 | 2.05 | 0.56 |
| 3:L:107:THR:HG22 | 3:L:111:LYS:N | 2.06 | 0.56 |
| 2:D:208:PRO:HG3 | 3:J:171:LEU:CD1 | 2.36 | 0.56 |
| 2:F:164:TYR:CE2 | 2:F:169:LEU:HB2 | 2.41 | 0.56 |
| 1:C:60:ILE:HD11 | 1:C:119:PHE:HE2 | 1.71 | 0.56 |
| 1:G:56:SER:HB3 | 1:G:101:SER:OG | 2.06 | 0.56 |
| 2:H:16:ARG:NH2 | 2:H:116:PRO:HB2 | 2.21 | 0.56 |
| 1:C:39:THR:O | 1:C:43:THR:HB | 2.06 | 0.56 |
| 1:C:260:GLU:HG3 | 1:C:261:ASP:N | 2.21 | 0.56 |
| 1:G:25:GLN:O | 1:G:29:GLU:HG3 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:507:LYS:HG2 | 1:C:513:PHE:HB2 | 1.87 | 0.56 |
| 2:H:54:ILE:CG2 | 2:H:145:LEU:HD21 | 2.35 | 0.56 |
| 1:E:441:ARG:NH2 | 1:E:453:ASP:OD2 | 2.39 | 0.56 |
| 2:D:251:GLY:O | 2:D:257:ILE:HD11 | 2.06 | 0.56 |
| 2:F:178:ILE:HD11 | 2:F:310:ILE:HD12 | 1.87 | 0.56 |
| 3:J:149:GLN:O | 3:J:149:GLN:HG3 | 2.06 | 0.56 |
| 2:H:900:ALA:O | 2:H:901:VAL:CB | 2.53 | 0.55 |
| 1:A:309:ARG:CG | 1:A:364:LEU:HD21 | 2.36 | 0.55 |
| 3:K:155:THR:O | 3:K:158:ASP:HB2 | 2.04 | 0.55 |
| 2:F:325:ASN:ND2 | 2:F:327:VAL:HG22 | 2.21 | 0.55 |
| 1:C:113:LEU:O | 1:C:117:PRO:HG3 | 2.06 | 0.55 |
| 1:E:418:ASN:ND2 | 1:E:420:ASP:H | 2.04 | 0.55 |
| 1:A:527:GLN:OE1 | 1:A:527:GLN:HA | 2.05 | 0.55 |
| 3:L:155:THR:O | 3:L:158:ASP:HB2 | 2.04 | 0.55 |
| 2:D:54:ILE:CG2 | 2:D:145:LEU:HD21 | 2.36 | 0.55 |
| 3:I:118:GLU:O | 3:I:120:THR:N | 2.39 | 0.55 |
| 1:A:447:ASN:ND2 | 2:B:26:ARG:HH21 | 2.03 | 0.55 |
| 1:A:430:ARG:NH1 | 1:A:430:ARG:HB3 | 2.21 | 0.55 |
| 1:C:418:ASN:HD22 | 1:C:419:PRO:CD | 2.19 | 0.55 |
| 1:G:60:ILE:HD11 | 1:G:119:PHE:HE2 | 1.71 | 0.55 |
| 1:G:233:ILE:N | 1:G:234:PRO:HD3 | 2.21 | 0.55 |
| 1:E:25:GLN:O | 1:E:29:GLU:HG3 | 2.06 | 0.55 |
| 1:A:78:ARG:O | 1:A:81:ILE:HG13 | 2.05 | 0.55 |
| 2:F:50:LYS:H | 2:F:139:HIS:HD2 | 1.52 | 0.55 |
| 1:A:41:THR:O | 1:A:45:ILE:HG13 | 2.05 | 0.55 |
| 1:C:419:PRO:HB2 | 1:C:475:LYS:HE3 | 1.88 | 0.55 |
| 1:A:233:ILE:N | 1:A:234:PRO:HD3 | 2.21 | 0.55 |
| 1:E:347:ARG:HH12 | 2:F:274:ARG:HD2 | 1.71 | 0.55 |
| 2:F:217:THR:HA | 2:F:221:MET:HG2 | 1.89 | 0.55 |
| 1:C:33:VAL:HG23 | 1:C:54:ILE:HD11 | 1.87 | 0.55 |
| 1:G:177:ASP:OD2 | 2:H:327:VAL:HG21 | 2.07 | 0.55 |
| 1:C:36:ILE:HB | 1:C:128:ALA:HA | 1.89 | 0.55 |
| 1:A:441:ARG:NH2 | 1:A:453:ASP:OD2 | 2.40 | 0.55 |
| 1:A:332:MET:HG2 | 1:A:339:TYR:HE1 | 1.72 | 0.55 |
| 1:A:422:GLU:HG3 | 1:A:530:ALA:CB | 2.36 | 0.55 |
| 3:I:155:THR:O | 3:I:158:ASP:HB2 | 2.07 | 0.55 |
| 1:C:233:ILE:N | 1:C:234:PRO:HD3 | 2.22 | 0.55 |
| 1:G:332:MET:HG2 | 1:G:339:TYR:HE1 | 1.71 | 0.55 |
| 3:J:102:LEU:HD11 | 3:J:114:GLU:HG2 | 1.88 | 0.55 |
| 1:C:311:LEU:O | 1:C:315:VAL:HG23 | 2.07 | 0.55 |
| 1:A:488:ALA:O | 1:A:490:PRO:HD3 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:311:LEU:O | 1:G:315:VAL:HG23 | 2.07 | 0.55 |
| 2:F:64:LEU:HB3 | 2:F:111:LEU:HD13 | 1.86 | 0.55 |
| 3:L:117:ILE:HD13 | 3:L:126:ILE:HG12 | 1.87 | 0.55 |
| 1:E:215:ILE:HG13 | 1:E:332:MET:CE | 2.37 | 0.55 |
| 2:B:225:PRO:HG3 | 2:B:274:ARG:O | 2.07 | 0.54 |
| 1:G:309:ARG:CG | 1:G:364:LEU:HD21 | 2.37 | 0.54 |
| 1:E:233:ILE:N | 1:E:234:PRO:HD3 | 2.21 | 0.54 |
| 1:A:507:LYS:HG2 | 1:A:513:PHE:HB2 | 1.88 | 0.54 |
| 2:H:84:ASP:H | 2:H:87:ASN:ND2 | 2.05 | 0.54 |
| 1:C:527:GLN:OE1 | 1:C:527:GLN:HA | 2.06 | 0.54 |
| 2:F:243:PHE:O | 2:F:247:VAL:HG21 | 2.06 | 0.54 |
| 1:A:214:TRP:CZ3 | 1:A:332:MET:HB3 | 2.42 | 0.54 |
| 1:E:332:MET:HG2 | 1:E:339:TYR:HE1 | 1.72 | 0.54 |
| 2:F:701:GLU:HA | 2:F:704:LEU:CB | 2.37 | 0.54 |
| 2:B:178:ILE:HD11 | 2:B:310:ILE:HD12 | 1.89 | 0.54 |
| 2:H:232:VAL:HG11 | 2:H:263:LYS:HB2 | 1.89 | 0.54 |
| 2:D:217:THR:HA | 2:D:221:MET:HG2 | 1.89 | 0.54 |
| 2:D:16:ARG:HH22 | 2:D:116:PRO:HB2 | 1.72 | 0.54 |
| 1:E:214:TRP:CE3 | 1:E:332:MET:HB3 | 2.43 | 0.54 |
| 1:A:419:PRO:HB2 | 1:A:475:LYS:HE3 | 1.89 | 0.54 |
| 2:B:701:GLU:HA | 2:B:704:LEU:CB | 2.37 | 0.54 |
| 2:D:257:ILE:HD13 | 2:D:282:GLN:HG2 | 1.89 | 0.54 |
| 2:F:73:ARG:HD3 | 2:F:117:ASN:O | 2.06 | 0.54 |
| 2:B:49:CYS:HA | 2:B:139:HIS:HD2 | 1.73 | 0.54 |
| 2:B:50:LYS:H | 2:B:139:HIS:HD2 | 1.51 | 0.54 |
| 2:H:392:LEU:O | 2:H:606:ARG:CB | 2.55 | 0.54 |
| 2:B:233:ARG:HH12 | 2:B:234:MET:HB2 | 1.73 | 0.54 |
| 2:H:256:HIS:O | 2:H:260:ILE:HG13 | 2.08 | 0.54 |
| 1:E:36:ILE:HB | 1:E:128:ALA:HA | 1.90 | 0.54 |
| 1:A:340:ILE:HD11 | 2:B:273:ILE:HG12 | 1.89 | 0.54 |
| 2:F:232:VAL:HG11 | 2:F:263:LYS:HB2 | 1.90 | 0.54 |
| 1:A:39:THR:O | 1:A:43:THR:HB | 2.06 | 0.54 |
| 1:G:262:GLU:HA | 1:G:262:GLU:OE1 | 2.08 | 0.54 |
| 1:G:214:TRP:CE3 | 1:G:332:MET:HB3 | 2.43 | 0.54 |
| 2:F:251:GLY:O | 2:F:286:LYS:HE3 | 2.07 | 0.54 |
| 1:C:441:ARG:NH2 | 1:C:453:ASP:OD1 | 2.40 | 0.54 |
| 2:F:251:GLY:O | 2:F:257:ILE:HD11 | 2.07 | 0.54 |
| 1:C:208:ASP:OD1 | 1:C:211:HIS:HB2 | 2.08 | 0.54 |
| 2:B:49:CYS:HA | 2:B:139:HIS:CD2 | 2.43 | 0.54 |
| 2:B:257:ILE:HD13 | 2:B:282:GLN:HG2 | 1.90 | 0.54 |
| 1:C:441:ARG:NH2 | 1:C:453:ASP:OD2 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:392:LEU:O | 2:B:606:ARG:CB | 2.55 | 0.54 |
| 2:F:116:ARG:NH2 | 2:F:116:PRO:HB2 | 2.23 | 0.54 |
| 1:E:49:LEU:O | 1:E:52:PRO:HD2 | 2.08 | 0.54 |
| 1:A:214:TRP:CD1 | 1:A:214:TRP:C | 2.81 | 0.54 |
| 1:G:33:VAL:HG23 | 1:G:54:ILE:HD11 | 1.90 | 0.54 |
| 3:I:102:LEU:HD11 | 3:I:114:GLU:HG2 | 1.89 | 0.54 |
| 2:D:233:ARG:HH12 | 2:D:234:MET:HB2 | 1.73 | 0.54 |
| 1:C:262:GLU:OE1 | 1:C:262:GLU:HA | 2.09 | 0.53 |
| 1:E:178:ASN:ND2 | 3:K:136:ILE:HG12 | 2.23 | 0.53 |
| 2:H:32:HIS:CD2 | 2:H:34:ASP:H | 2.26 | 0.53 |
| 2:F:241:GLN:HG3 | 2:F:245:GLU:HA | 1.90 | 0.53 |
| 2:D:361:LEU:O | 2:D:364:VAL:CG2 | 2.56 | 0.53 |
| 1:E:454:ILE:HD13 | 1:E:480:HIS:ND1 | 2.23 | 0.53 |
| 1:A:447:ASN:HD22 | 2:B:26:ARG:HH21 | 1.56 | 0.53 |
| 1:G:447:ASN:ND2 | 2:H:26:ARG:HH21 | 2.07 | 0.53 |
| 1:E:78:ARG:O | 1:E:81:ILE:HG13 | 2.08 | 0.53 |
| 1:E:175:HIS:HD2 | 1:E:512:GLN:O | 1.92 | 0.53 |
| 3:K:102:LEU:HD11 | 3:K:114:GLU:HG2 | 1.90 | 0.53 |
| 2:B:243:PHE:O | 2:B:247:VAL:HG21 | 2.08 | 0.53 |
| 1:A:229:THR:O | 1:A:230:ASN:CB | 2.57 | 0.53 |
| 1:A:264:ASN:N | 1:A:264:ASN:ND2 | 2.55 | 0.53 |
| 2:B:128:GLN:NE2 | 2:B:128:GLN:N | 2.56 | 0.53 |
| 2:D:353:ILE:HB | 2:D:355:PHE:CZ | 2.43 | 0.53 |
| 1:E:163:ARG:HG3 | 1:E:519:THR:H | 1.73 | 0.53 |
| 1:G:419:PRO:HB2 | 1:G:475:LYS:HE3 | 1.90 | 0.53 |
| 1:C:488:ALA:O | 1:C:490:PRO:HD3 | 2.08 | 0.53 |
| 2:B:131:ASN:HB3 | 2:D:131:ASN:HD22 | 1.74 | 0.53 |
| 2:H:353:ILE:HB | 2:H:355:PHE:CZ | 2.42 | 0.53 |
| 1:A:163:ARG:NH2 | 1:A:518:ASN:HD21 | 2.06 | 0.53 |
| 2:D:318:LEU:HD12 | 2:D:319:ASN:H | 1.74 | 0.53 |
| 2:D:241:GLN:HG3 | 2:D:245:GLU:HA | 1.90 | 0.53 |
| 1:C:104:PHE:CE1 | 1:C:106:GLU:HG3 | 2.43 | 0.53 |
| 2:D:225:PRO:HG3 | 2:D:274:ARG:O | 2.09 | 0.53 |
| 2:B:251:GLY:O | 2:B:257:ILE:HD11 | 2.08 | 0.53 |
| 1:G:488:ALA:O | 1:G:490:PRO:HD3 | 2.08 | 0.53 |
| 2:F:208:PRO:HG3 | 3:K:171:LEU:CD1 | 2.39 | 0.53 |
| 2:D:49:CYS:HA | 2:D:139:HIS:HD2 | 1.74 | 0.53 |
| 2:H:325:ASN:ND2 | 2:H:327:VAL:HG22 | 2.23 | 0.53 |
| 1:E:418:ASN:HD22 | 1:E:419:PRO:CD | 2.22 | 0.53 |
| 2:F:256:HIS:O | 2:F:260:ILE:HG13 | 2.09 | 0.53 |
| 1:C:407:ILE:O | 1:C:407:ILE:HG23 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:185:LEU:O | 1:G:188:PRO:HD3 | 2.09 | 0.53 |
| 2:B:73:ARG:HD3 | 2:B:117:ASN:O | 2.09 | 0.53 |
| 1:C:430:ARG:NH1 | 1:C:430:ARG:HB3 | 2.23 | 0.53 |
| 1:A:208:ASP:OD1 | 1:A:211:HIS:HB2 | 2.08 | 0.53 |
| 1:E:264:ASN:N | 1:E:264:ASN:ND2 | 2.57 | 0.53 |
| 1:C:264:ASN:ND2 | 1:C:264:ASN:N | 2.57 | 0.53 |
| 2:D:49:CYS:HA | 2:D:139:HIS:CD2 | 2.44 | 0.53 |
| 2:F:49:CYS:HA | 2:F:139:HIS:CD2 | 2.43 | 0.53 |
| 3:K:117:ILE:HD11 | 3:K:126:ILE:HG23 | 1.90 | 0.53 |
| 1:C:78:ARG:O | 1:C:81:ILE:HG13 | 2.09 | 0.53 |
| 2:F:318:LEU:HD12 | 2:F:319:ASN:H | 1.73 | 0.53 |
| 1:A:262:GLU:HA | 1:A:262:GLU:OE1 | 2.08 | 0.53 |
| 2:H:340:LYS:HB3 | 2:H:342:ASN:ND2 | 2.24 | 0.53 |
| 2:F:64:LEU:HD11 | 2:F:77:VAL:HG21 | 1.90 | 0.53 |
| 2:H:251:GLY:O | 2:H:257:ILE:HD11 | 2.08 | 0.53 |
| 2:F:32:HIS:CD2 | 2:F:34:ASP:H | 2.26 | 0.53 |
| 2:H:349:LEU:HB3 | 2:H:350:PRO:CD | 2.38 | 0.53 |
| 1:G:264:ASN:N | 1:G:264:ASN:ND2 | 2.57 | 0.52 |
| 1:G:208:ASP:OD1 | 1:G:211:HIS:HB2 | 2.09 | 0.52 |
| 1:C:264:ASN:ND2 | 1:C:264:ASN:H | 2.08 | 0.52 |
| 2:H:225:PRO:HG3 | 2:H:274:ARG:O | 2.09 | 0.52 |
| 2:F:280:LEU:O | 2:F:284:VAL:HG23 | 2.09 | 0.52 |
| 1:E:488:ALA:C | 1:E:490:PRO:HD3 | 2.29 | 0.52 |
| 1:A:119:PHE:O | 1:A:122:ARG:HG3 | 2.08 | 0.52 |
| 1:G:214:TRP:CD1 | 1:G:214:TRP:C | 2.81 | 0.52 |
| 1:G:36:ILE:HB | 1:G:128:ALA:HA | 1.91 | 0.52 |
| 2:F:318:LEU:HD12 | 2:F:319:ASN:N | 2.25 | 0.52 |
| 1:G:34:CYS:HB2 | 1:G:123:PHE:CG | 2.43 | 0.52 |
| 1:C:175:HIS:HD2 | 1:C:512:GLN:O | 1.92 | 0.52 |
| 2:B:64:LEU:HB3 | 2:B:111:LEU:HD13 | 1.88 | 0.52 |
| 1:E:307:LEU:HB3 | 1:E:383:LEU:CD2 | 2.39 | 0.52 |
| 2:F:225:PRO:HG3 | 2:F:274:ARG:O | 2.09 | 0.52 |
| 1:C:418:ASN:HD22 | 1:C:419:PRO:N | 2.08 | 0.52 |
| 1:C:119:PHE:O | 1:C:122:ARG:HG3 | 2.10 | 0.52 |
| 1:E:262:GLU:HA | 1:E:262:GLU:OE1 | 2.10 | 0.52 |
| 1:E:213:PRO:HB3 | 1:E:332:MET:HE2 | 1.90 | 0.52 |
| 1:E:419:PRO:HB2 | 1:E:475:LYS:HE3 | 1.90 | 0.52 |
| 1:A:481:GLU:OE2 | 2:B:315:TYR:HE2 | 1.92 | 0.52 |
| 2:D:132:ASP:HA | 2:D:157:MET:HE2 | 1.91 | 0.52 |
| 2:F:361:LEU:O | 2:F:364:VAL:CG2 | 2.56 | 0.52 |
| 1:G:213:PRO:HB3 | 1:G:332:MET:HE2 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:104:PHE:CE1 | 1:G:106:GLU:HG3 | 2.44 | 0.52 |
| 2:H:249:LEU:CD1 | 2:H:260:ILE:HD11 | 2.40 | 0.52 |
| 2:B:131:ASN:HD22 | 2:D:131:ASN:HB3 | 1.75 | 0.52 |
| 2:D:73:ARG:HD3 | 2:D:117:ASN:O | 2.09 | 0.52 |
| 2:D:343:CYS:SG | 2:D:346:CYS:SG | 3.08 | 0.52 |
| 1:C:214:TRP:CD1 | 1:C:214:TRP:C | 2.82 | 0.52 |
| 1:E:214:TRP:CD1 | 1:E:214:TRP:C | 2.82 | 0.52 |
| 2:H:217:THR:HG21 | 2:H:223:ARG:HH22 | 1.75 | 0.52 |
| 2:F:249:LEU:CD1 | 2:F:260:ILE:HD11 | 2.40 | 0.52 |
| 2:H:257:ILE:HD13 | 2:H:282:GLN:HG2 | 1.91 | 0.52 |
| 1:G:113:LEU:O | 1:G:117:PRO:HG3 | 2.10 | 0.52 |
| 3:J:111:LYS:O | 3:J:112:GLU:HB3 | 2.10 | 0.52 |
| 1:C:253:LYS:O | 1:C:260:GLU:N | 2.42 | 0.52 |
| 1:G:235:LYS:NZ | 1:G:238:LYS:HD3 | 2.25 | 0.52 |
| 2:F:232:VAL:HA | 2:F:236:GLN:HB3 | 1.91 | 0.52 |
| 2:B:232:VAL:HG11 | 2:B:263:LYS:HB2 | 1.92 | 0.52 |
| 2:H:73:ARG:HD3 | 2:H:117:ASN:O | 2.09 | 0.52 |
| 3:J:107:THR:HG22 | 3:J:111:LYS:N | 2.07 | 0.52 |
| 2:H:351:GLN:HA | 2:H:351:GLN:HE21 | 1.75 | 0.52 |
| 2:D:46:LEU:O | 2:D:73:ARG:HB2 | 2.10 | 0.52 |
| 1:A:61:ASP:CB | 1:A:86:ALA:HB2 | 2.37 | 0.52 |
| 1:G:336:SER:HB2 | 2:H:221:MET:HA | 1.92 | 0.52 |
| 2:D:318:LEU:HD12 | 2:D:319:ASN:N | 2.25 | 0.52 |
| 2:D:351:GLN:HE21 | 2:D:351:GLN:HA | 1.75 | 0.52 |
| 2:H:49:CYS:HA | 2:H:139:HIS:CD2 | 2.44 | 0.52 |
| 1:G:215:ILE:H | 1:G:332:MET:HE3 | 1.75 | 0.52 |
| 2:H:142:VAL:HG21 | 2:H:307:VAL:HG21 | 1.91 | 0.52 |
| 1:A:264:ASN:H | 1:A:264:ASN:ND2 | 2.06 | 0.52 |
| 2:F:49:CYS:HA | 2:F:139:HIS:HD2 | 1.73 | 0.52 |
| 1:E:215:ILE:H | 1:E:332:MET:HE3 | 1.74 | 0.52 |
| 1:E:441:ARG:NH2 | 1:E:453:ASP:OD1 | 2.42 | 0.52 |
| 2:B:318:LEU:HD12 | 2:B:319:ASN:H | 1.75 | 0.52 |
| 1:A:348:GLU:HG3 | 1:E:115:ASN:ND2 | 2.24 | 0.52 |
| 1:G:61:ASP:CB | 1:G:86:ALA:HB2 | 2.39 | 0.51 |
| 2:B:132:ASP:HA | 2:B:157:MET:HE2 | 1.92 | 0.51 |
| 1:A:175:HIS:HD2 | 1:A:512:GLN:O | 1.93 | 0.51 |
| 1:G:527:GLN:OE1 | 1:G:527:GLN:HA | 2.10 | 0.51 |
| 1:G:264:ASN:H | 1:G:264:ASN:ND2 | 2.09 | 0.51 |
| 2:B:343:CYS:O | 2:B:347:SER:HB3 | 2.10 | 0.51 |
| 1:E:163:ARG:NH1 | 1:E:165:ILE:HG12 | 2.25 | 0.51 |
| 1:A:214:TRP:CE3 | 1:A:332:MET:HB3 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:233:ARG:NH1 | 2:D:233:ARG:HG2 | 2.25 | 0.51 |
| 2:B:199:CYS:HG | 2:B:346:CYS:HG | 1.54 | 0.51 |
| 2:D:232:VAL:HG11 | 2:D:263:LYS:HB2 | 1.92 | 0.51 |
| 2:B:393:TYR:CD1 | 2:B:607:THR:HA | 2.45 | 0.51 |
| 1:G:7:LEU:O | 1:G:11:GLN:HG3 | 2.11 | 0.51 |
| 1:G:418:ASN:HD22 | 1:G:419:PRO:CD | 2.23 | 0.51 |
| 2:H:251:GLY:O | 2:H:286:LYS:HE3 | 2.10 | 0.51 |
| 2:F:349:LEU:HB3 | 2:F:350:PRO:CD | 2.40 | 0.51 |
| 1:G:39:THR:O | 1:G:43:THR:HB | 2.11 | 0.51 |
| 1:E:34:CYS:HB2 | 1:E:123:PHE:CG | 2.45 | 0.51 |
| 1:C:221:TYR:HD2 | 1:C:246:LEU:HG | 1.76 | 0.51 |
| 1:C:61:ASP:CB | 1:C:86:ALA:HB2 | 2.39 | 0.51 |
| 1:A:418:ASN:HD22 | 1:A:419:PRO:CD | 2.23 | 0.51 |
| 1:G:441:ARG:NH2 | 1:G:453:ASP:OD2 | 2.42 | 0.51 |
| 2:B:351:GLN:HA | 2:B:351:GLN:HE21 | 1.76 | 0.51 |
| 2:H:361:LEU:O | 2:H:364:VAL:CG2 | 2.57 | 0.51 |
| 1:G:481:GLU:HB2 | 2:H:30:PHE:HE1 | 1.76 | 0.51 |
| 3:I:111:LYS:O | 3:I:112:GLU:HB3 | 2.11 | 0.51 |
| 1:E:264:ASN:ND2 | 1:E:264:ASN:H | 2.09 | 0.51 |
| 2:H:49:CYS:HA | 2:H:139:HIS:HD2 | 1.74 | 0.51 |
| 1:E:235:LYS:NZ | 1:E:238:LYS:HD3 | 2.26 | 0.51 |
| 1:C:332:MET:HG2 | 1:C:339:TYR:HE1 | 1.76 | 0.51 |
| 1:G:418:ASN:C | 1:G:418:ASN:HD22 | 2.14 | 0.51 |
| 2:H:232:VAL:HA | 2:H:236:GLN:HB3 | 1.91 | 0.51 |
| 1:E:60:ILE:HD11 | 1:E:119:PHE:HE2 | 1.76 | 0.51 |
| 1:A:213:PRO:HB3 | 1:A:332:MET:CE | 2.41 | 0.51 |
| 1:E:347:ARG:HH12 | 2:F:274:ARG:CD | 2.23 | 0.51 |
| 1:G:215:ILE:HG13 | 1:G:332:MET:CE | 2.40 | 0.51 |
| 2:D:178:ILE:HD11 | 2:D:310:ILE:HD12 | 1.93 | 0.51 |
| 2:D:377:LYS:O | 2:D:378:SER:C | 2.49 | 0.51 |
| 1:A:113:LEU:O | 1:A:117:PRO:HG3 | 2.10 | 0.51 |
| 1:A:208:ASP:O | 1:A:208:ASP:OD1 | 2.29 | 0.51 |
| 1:G:84:ASN:OD1 | 1:G:86:ALA:HB3 | 2.11 | 0.51 |
| 1:C:163:ARG:NH2 | 1:C:518:ASN:HD21 | 2.09 | 0.51 |
| 2:H:280:LEU:O | 2:H:284:VAL:HG23 | 2.10 | 0.51 |
| 1:G:333:ILE:HA | 2:H:223:ARG:NH2 | 2.24 | 0.51 |
| 2:B:249:LEU:CD1 | 2:B:260:ILE:HD11 | 2.41 | 0.51 |
| 2:F:340:LYS:HB3 | 2:F:342:ASN:ND2 | 2.26 | 0.51 |
| 2:D:232:VAL:HA | 2:D:236:GLN:HB3 | 1.93 | 0.51 |
| 1:E:221:TYR:HD2 | 1:E:246:LEU:HG | 1.76 | 0.51 |
| 2:D:703:GLY:C | 2:D:705:VAL:N | 2.63 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:163:ARG:NH1 | 1:C:165:ILE:HG12 | 2.26 | 0.51 |
| 1:E:213:PRO:HB3 | 1:E:332:MET:CE | 2.41 | 0.51 |
| 1:C:447:ASN:ND2 | 2:D:26:ARG:HH21 | 2.08 | 0.51 |
| 2:D:142:VAL:HG21 | 2:D:307:VAL:HG21 | 1.92 | 0.51 |
| 3:L:102:LEU:HD11 | 3:L:114:GLU:HG2 | 1.92 | 0.51 |
| 1:C:208:ASP:O | 1:C:208:ASP:OD1 | 2.29 | 0.51 |
| 2:B:342:ASN:ND2 | 2:B:342:ASN:N | 2.41 | 0.51 |
| 2:H:703:GLY:C | 2:H:705:VAL:N | 2.64 | 0.51 |
| 1:G:307:LEU:HB3 | 1:G:383:LEU:CD2 | 2.40 | 0.51 |
| 1:C:34:CYS:HB2 | 1:C:123:PHE:CG | 2.46 | 0.51 |
| 1:G:488:ALA:C | 1:G:490:PRO:HD3 | 2.31 | 0.51 |
| 1:C:7:LEU:O | 1:C:11:GLN:HG3 | 2.11 | 0.50 |
| 1:C:488:ALA:C | 1:C:490:PRO:HD3 | 2.31 | 0.50 |
| 2:H:191:VAL:H | 2:H:320:ASN:HA | 1.76 | 0.50 |
| 1:G:221:TYR:HD2 | 1:G:246:LEU:HG | 1.76 | 0.50 |
| 2:B:142:VAL:HG21 | 2:B:307:VAL:HG21 | 1.93 | 0.50 |
| 1:E:229:THR:O | 1:E:230:ASN:CB | 2.60 | 0.50 |
| 3:K:111:LYS:O | 3:K:112:GLU:HB3 | 2.11 | 0.50 |
| 1:C:235:LYS:NZ | 1:C:238:LYS:HD3 | 2.26 | 0.50 |
| 2:H:277:THR:HG23 | 2:H:280:LEU:CB | 2.41 | 0.50 |
| 1:A:418:ASN:C | 1:A:418:ASN:HD22 | 2.15 | 0.50 |
| 1:G:19:LEU:HD12 | 2:H:292:VAL:HG13 | 1.93 | 0.50 |
| 1:A:251:ILE:O | 1:A:252:LEU:C | 2.50 | 0.50 |
| 1:E:208:ASP:OD1 | 1:E:211:HIS:HB2 | 2.10 | 0.50 |
| 1:E:61:ASP:CB | 1:E:86:ALA:HB2 | 2.40 | 0.50 |
| 1:G:163:ARG:HG3 | 1:G:519:THR:H | 1.77 | 0.50 |
| 1:E:32:HIS:HA | 1:E:56:SER:O | 2.12 | 0.50 |
| 1:A:430:ARG:HB3 | 1:A:430:ARG:HH11 | 1.77 | 0.50 |
| 1:A:87:GLU:O | 1:A:91:GLU:HG3 | 2.11 | 0.50 |
| 1:E:357:VAL:O | 1:E:361:VAL:HG23 | 2.11 | 0.50 |
| 2:B:262:GLN:NE2 | 1:E:67:GLY:N | 2.42 | 0.50 |
| 2:D:64:LEU:HB3 | 2:D:111:LEU:HD13 | 1.88 | 0.50 |
| 2:F:703:GLY:C | 2:F:705:VAL:N | 2.64 | 0.50 |
| 1:A:235:LYS:NZ | 1:A:238:LYS:HD3 | 2.26 | 0.50 |
| 1:A:441:ARG:NH2 | 1:A:453:ASP:OD1 | 2.45 | 0.50 |
| 2:B:349:LEU:HB3 | 2:B:350:PRO:CD | 2.40 | 0.50 |
| 2:D:360:LYS:HA | 2:D:700:LYS:O | 2.12 | 0.50 |
| 2:D:349:LEU:HB3 | 2:D:350:PRO:CD | 2.42 | 0.50 |
| 1:C:185:LEU:O | 1:C:188:PRO:HD3 | 2.12 | 0.50 |
| 3:K:107:THR:HG22 | 3:K:111:LYS:N | 2.08 | 0.50 |
| 2:B:64:LEU:HD11 | 2:B:77:VAL:HG21 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:241:GLN:HG3 | 2:B:245:GLU:HA | 1.93 | 0.50 |
| 1:A:163:ARG:HG2 | 1:A:163:ARG:NH1 | 2.27 | 0.50 |
| 1:E:7:LEU:O | 1:E:11:GLN:HG3 | 2.12 | 0.50 |
| 2:F:257:ILE:HD13 | 2:F:282:GLN:HG2 | 1.93 | 0.50 |
| 1:E:447:ASN:ND2 | 2:F:26:ARG:HH21 | 2.10 | 0.50 |
| 1:G:178:ASN:HD22 | 3:L:136:ILE:HG12 | 1.76 | 0.50 |
| 2:H:241:GLN:HG3 | 2:H:245:GLU:HA | 1.92 | 0.50 |
| 1:A:33:VAL:HG21 | 1:A:54:ILE:HD11 | 1.94 | 0.50 |
| 1:A:7:LEU:O | 1:A:11:GLN:HG3 | 2.11 | 0.50 |
| 1:A:418:ASN:HD22 | 1:A:419:PRO:N | 2.09 | 0.50 |
| 1:E:119:PHE:O | 1:E:122:ARG:HG3 | 2.11 | 0.50 |
| 2:B:232:VAL:HA | 2:B:236:GLN:HB3 | 1.93 | 0.50 |
| 1:G:236:THR:HG23 | 1:G:237:TYR:CD2 | 2.47 | 0.50 |
| 2:F:353:ILE:HB | 2:F:355:PHE:CZ | 2.45 | 0.50 |
| 2:B:54:ILE:HG22 | 2:B:145:LEU:CD2 | 2.42 | 0.50 |
| 1:G:418:ASN:HD22 | 1:G:419:PRO:N | 2.10 | 0.50 |
| 1:E:43:THR:HG21 | 1:E:73:ASN:OD1 | 2.12 | 0.50 |
| 1:C:236:THR:HG23 | 1:C:237:TYR:N | 2.22 | 0.50 |
| 2:F:351:GLN:HA | 2:F:351:GLN:HE21 | 1.77 | 0.50 |
| 1:C:243:PHE:O | 1:C:246:LEU:HB3 | 2.12 | 0.50 |
| 1:C:251:ILE:HG23 | 1:C:262:GLU:CB | 2.41 | 0.50 |
| 2:H:132:ASP:N | 2:H:132:ASP:OD1 | 2.45 | 0.50 |
| 2:F:46:LEU:O | 2:F:73:ARG:HB2 | 2.12 | 0.50 |
| 2:B:233:ARG:NH1 | 2:B:234:MET:HB2 | 2.26 | 0.50 |
| 2:D:233:ARG:NH1 | 2:D:234:MET:HB2 | 2.26 | 0.50 |
| 1:A:229:THR:O | 1:A:230:ASN:HB2 | 2.12 | 0.50 |
| 1:A:481:GLU:HB2 | 2:B:30:PHE:HE1 | 1.77 | 0.50 |
| 2:F:84:ASP:H | 2:F:87:ASN:ND2 | 2.10 | 0.50 |
| 2:D:199:CYS:SG | 2:D:346:CYS:SG | 3.07 | 0.49 |
| 3:J:172:ALA:C | 3:J:173:LEU:HG | 2.32 | 0.49 |
| 1:A:233:ILE:HG22 | 1:A:233:ILE:O | 2.11 | 0.49 |
| 1:C:225:TRP:NE1 | 1:C:233:ILE:HG12 | 2.27 | 0.49 |
| 1:G:229:THR:O | 1:G:230:ASN:CB | 2.60 | 0.49 |
| 2:F:197:THR:CG2 | 2:F:198:ALA:N | 2.75 | 0.49 |
| 2:D:217:THR:HG21 | 2:D:223:ARG:HH22 | 1.77 | 0.49 |
| 1:A:168:GLU:HG3 | 1:A:394:ARG:HE | 1.77 | 0.49 |
| 2:F:128:GLN:N | 2:F:128:GLN:HE21 | 2.04 | 0.49 |
| 2:B:280:LEU:O | 2:B:284:VAL:HG23 | 2.11 | 0.49 |
| 1:A:215:ILE:HG13 | 1:A:332:MET:CE | 2.42 | 0.49 |
| 2:F:217:THR:HG21 | 2:F:223:ARG:HH22 | 1.76 | 0.49 |
| 2:H:233:ARG:NH1 | 2:H:233:ARG:HG2 | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:377:LYS:O | 2:B:378:SER:C | 2.49 | 0.49 |
| 1:G:430:ARG:HB3 | 1:G:430:ARG:NH1 | 2.28 | 0.49 |
| 1:C:236:THR:HG23 | 1:C:237:TYR:CD2 | 2.47 | 0.49 |
| 1:G:155:THR:HG23 | 1:G:493:ILE:HG22 | 1.95 | 0.49 |
| 1:C:229:THR:O | 1:C:230:ASN:CB | 2.59 | 0.49 |
| 2:F:377:LYS:O | 2:F:378:SER:C | 2.50 | 0.49 |
| 1:E:19:LEU:HD12 | 2:F:292:VAL:HG13 | 1.94 | 0.49 |
| 2:H:360:LYS:HA | 2:H:700:LYS:O | 2.12 | 0.49 |
| 3:L:111:LYS:O | 3:L:112:GLU:HB3 | 2.13 | 0.49 |
| 2:B:267:ARG:HG2 | 2:B:267:ARG:NH1 | 2.25 | 0.49 |
| 2:D:251:GLY:O | 2:D:286:LYS:HE3 | 2.12 | 0.49 |
| 1:E:407:ILE:O | 1:E:407:ILE:HG23 | 2.12 | 0.49 |
| 3:J:117:ILE:HD11 | 3:J:126:ILE:HG23 | 1.94 | 0.49 |
| 2:B:46:LEU:O | 2:B:73:ARG:HB2 | 2.12 | 0.49 |
| 1:C:84:ASN:OD1 | 1:C:86:ALA:HB3 | 2.12 | 0.49 |
| 1:G:163:ARG:NH1 | 1:G:165:ILE:HG12 | 2.28 | 0.49 |
| 2:B:233:ARG:NH1 | 2:B:233:ARG:HG2 | 2.28 | 0.49 |
| 2:B:32:HIS:CD2 | 2:B:34:ASP:H | 2.30 | 0.49 |
| 3:L:107:THR:HG23 | 3:L:109:THR:N | 2.22 | 0.49 |
| 1:E:208:ASP:O | 1:E:208:ASP:OD1 | 2.31 | 0.49 |
| 1:C:186:ASP:HB2 | 1:C:232:ARG:NH2 | 2.28 | 0.49 |
| 1:G:213:PRO:HB3 | 1:G:332:MET:CE | 2.42 | 0.49 |
| 2:B:318:LEU:HD12 | 2:B:319:ASN:N | 2.27 | 0.49 |
| 3:L:117:ILE:HD11 | 3:L:126:ILE:HG23 | 1.94 | 0.49 |
| 3:I:172:ALA:C | 3:I:173:LEU:HG | 2.33 | 0.49 |
| 1:C:418:ASN:C | 1:C:418:ASN:HD22 | 2.14 | 0.49 |
| 1:E:418:ASN:HD22 | 1:E:418:ASN:C | 2.16 | 0.49 |
| 1:G:447:ASN:HD22 | 2:H:26:ARG:HH21 | 1.60 | 0.49 |
| 2:H:208:PRO:HG3 | 3:L:171:LEU:CD1 | 2.38 | 0.49 |
| 2:D:340:LYS:HB3 | 2:D:342:ASN:ND2 | 2.28 | 0.49 |
| 2:B:353:ILE:HB | 2:B:355:PHE:CZ | 2.48 | 0.49 |
| 1:C:163:ARG:HG3 | 1:C:519:THR:H | 1.76 | 0.49 |
| 1:C:418:ASN:HD22 | 1:C:419:PRO:HD2 | 1.78 | 0.49 |
| 2:F:360:LYS:HA | 2:F:700:LYS:O | 2.12 | 0.49 |
| 1:G:211:HIS:O | 1:G:338:LYS:HD2 | 2.13 | 0.48 |
| 2:D:351:GLN:HG3 | 2:D:353:ILE:CD1 | 2.40 | 0.48 |
| 2:H:603:ILE:O | 2:H:607:THR:N | 2.35 | 0.48 |
| 2:H:154:ILE:HD13 | 2:H:154:ILE:O | 2.12 | 0.48 |
| 2:B:197:THR:CG2 | 2:B:198:ALA:N | 2.76 | 0.48 |
| 1:A:488:ALA:C | 1:A:490:PRO:HD3 | 2.32 | 0.48 |
| 2:F:233:ARG:NH1 | 2:F:233:ARG:HG2 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:34:CYS:HB2 | 1:A:123:PHE:CG | 2.47 | 0.48 |
| 2:F:142:VAL:HG21 | 2:F:307:VAL:HG21 | 1.95 | 0.48 |
| 1:A:299:LYS:HA | 1:A:368:ILE:HG23 | 1.95 | 0.48 |
| 3:L:172:ALA:C | 3:L:173:LEU:HG | 2.32 | 0.48 |
| 1:G:186:ASP:HB2 | 1:G:232:ARG:NH2 | 2.27 | 0.48 |
| 1:E:78:ARG:CZ | 2:F:13:TRP:HB3 | 2.43 | 0.48 |
| 2:B:84:ASP:H | 2:B:87:ASN:ND2 | 2.10 | 0.48 |
| 1:E:185:LEU:O | 1:E:188:PRO:HD3 | 2.14 | 0.48 |
| 1:G:208:ASP:OD1 | 1:G:208:ASP:O | 2.31 | 0.48 |
| 2:H:64:LEU:HB3 | 2:H:111:LEU:HD12 | 1.91 | 0.48 |
| 1:A:236:THR:HG23 | 1:A:237:TYR:CD2 | 2.47 | 0.48 |
| 1:A:186:ASP:HB2 | 1:A:232:ARG:NH2 | 2.28 | 0.48 |
| 2:D:392:LEU:O | 2:D:606:ARG:CB | 2.62 | 0.48 |
| 1:E:252:LEU:HB2 | 1:E:260:GLU:HG2 | 1.95 | 0.48 |
| 2:D:351:GLN:NE2 | 2:D:351:GLN:HA | 2.28 | 0.48 |
| 1:C:225:TRP:CE2 | 1:C:233:ILE:HG12 | 2.48 | 0.48 |
| 2:B:277:THR:HG23 | 2:B:280:LEU:CB | 2.43 | 0.48 |
| 2:D:249:LEU:CD1 | 2:D:260:ILE:HD11 | 2.42 | 0.48 |
| 1:C:215:ILE:HG13 | 1:C:332:MET:CE | 2.43 | 0.48 |
| 1:G:441:ARG:NH2 | 1:G:453:ASP:OD1 | 2.45 | 0.48 |
| 2:B:128:GLN:HE21 | 2:B:128:GLN:N | 2.03 | 0.48 |
| 2:B:351:GLN:HA | 2:B:351:GLN:NE2 | 2.29 | 0.48 |
| 2:D:213:PHE:CB | 2:D:218:ILE:HD11 | 2.40 | 0.48 |
| 2:D:351:GLN:CD | 2:D:353:ILE:HD11 | 2.33 | 0.48 |
| 2:D:236:GLN:HE22 | 2:D:263:LYS:HB3 | 1.78 | 0.48 |
| 3:I:101:MET:HG3 | 3:I:163:GLY:H | 1.79 | 0.48 |
| 1:A:232:ARG:C | 1:A:233:ILE:HG13 | 2.34 | 0.48 |
| 1:C:34:CYS:HB2 | 1:C:123:PHE:CD2 | 2.48 | 0.48 |
| 1:G:119:PHE:O | 1:G:122:ARG:HG3 | 2.13 | 0.48 |
| 2:D:393:TYR:HE1 | 2:D:607:THR:CA | 2.24 | 0.48 |
| 1:G:51:LEU:HD11 | 2:H:92:PHE:HB3 | 1.95 | 0.48 |
| 2:D:277:THR:HG23 | 2:D:280:LEU:CB | 2.42 | 0.48 |
| 1:E:418:ASN:HD22 | 1:E:419:PRO:N | 2.11 | 0.48 |
| 1:A:447:ASN:HD22 | 2:B:26:ARG:NH2 | 2.11 | 0.48 |
| 2:B:191:VAL:H | 2:B:320:ASN:HA | 1.78 | 0.48 |
| 2:H:158:LEU:CD1 | 2:H:177:LEU:HB2 | 2.44 | 0.48 |
| 1:E:236:THR:HG23 | 1:E:237:TYR:CD2 | 2.48 | 0.48 |
| 2:F:353:ILE:HB | 2:F:355:PHE:HE1 | 1.77 | 0.48 |
| 1:A:163:ARG:NH1 | 1:A:165:ILE:HG12 | 2.29 | 0.48 |
| 2:F:277:THR:HG23 | 2:F:280:LEU:CB | 2.43 | 0.48 |
| 1:E:481:GLU:OE2 | 2:F:315:TYR:HE2 | 1.97 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:236:GLN:HE22 | 2:B:263:LYS:HB3 | 1.79 | 0.48 |
| 1:G:155:THR:HG23 | 1:G:493:ILE:CG2 | 2.44 | 0.48 |
| 1:G:175:HIS:HD2 | 1:G:512:GLN:O | 1.96 | 0.48 |
| 1:A:307:LEU:HB3 | 1:A:383:LEU:CD2 | 2.42 | 0.48 |
| 1:E:186:ASP:HB2 | 1:E:232:ARG:NH2 | 2.28 | 0.48 |
| 1:C:213:PRO:HB3 | 1:C:332:MET:CE | 2.42 | 0.48 |
| 2:D:197:THR:CG2 | 2:D:198:ALA:N | 2.77 | 0.48 |
| 1:E:418:ASN:HD22 | 1:E:419:PRO:HD2 | 1.79 | 0.48 |
| 2:F:191:VAL:H | 2:F:320:ASN:HA | 1.79 | 0.48 |
| 2:B:360:LYS:HA | 2:B:700:LYS:O | 2.14 | 0.48 |
| 2:H:267:ARG:HG2 | 2:H:267:ARG:NH1 | 2.27 | 0.48 |
| 2:F:16:ARG:HH22 | 2:F:116:PRO:HB2 | 1.77 | 0.48 |
| 1:E:34:CYS:HB2 | 1:E:123:PHE:CD2 | 2.49 | 0.48 |
| 2:F:75:ILE:O | 2:F:120:VAL:HA | 2.13 | 0.48 |
| 2:D:32:HIS:CD2 | 2:D:34:ASP:H | 2.32 | 0.48 |
| 1:A:211:HIS:O | 1:A:338:LYS:HD2 | 2.14 | 0.48 |
| 1:G:299:LYS:HA | 1:G:368:ILE:HG23 | 1.96 | 0.48 |
| 1:C:299:LYS:HA | 1:C:368:ILE:HG23 | 1.96 | 0.48 |
| 2:B:351:GLN:HG3 | 2:B:353:ILE:CD1 | 2.44 | 0.48 |
| 1:C:43:THR:HG21 | 1:C:73:ASN:OD1 | 2.14 | 0.48 |
| 1:C:447:ASN:HD22 | 2:D:26:ARG:HH21 | 1.62 | 0.48 |
| 2:H:75:ILE:O | 2:H:120:VAL:HA | 2.14 | 0.48 |
| 1:G:407:ILE:HG23 | 1:G:407:ILE:O | 2.13 | 0.48 |
| 2:D:191:VAL:H | 2:D:320:ASN:HA | 1.79 | 0.48 |
| 2:H:89:ASN:OD1 | 2:H:90:ARG:NH1 | 2.46 | 0.48 |
| 1:C:51:LEU:HD11 | 2:D:92:PHE:HB3 | 1.96 | 0.47 |
| 3:K:172:ALA:C | 3:K:173:LEU:HG | 2.34 | 0.47 |
| 2:F:220:SER:HB2 | 2:F:221:MET:HE3 | 1.96 | 0.47 |
| 2:D:357:PRO:O | 2:D:358:SER:CB | 2.62 | 0.47 |
| 1:A:348:GLU:HG3 | 1:E:115:ASN:CG | 2.34 | 0.47 |
| 1:E:229:THR:O | 1:E:230:ASN:HB2 | 2.14 | 0.47 |
| 1:C:19:LEU:HD12 | 2:D:292:VAL:HG13 | 1.96 | 0.47 |
| 2:H:377:LYS:O | 2:H:378:SER:C | 2.52 | 0.47 |
| 1:E:146:SER:O | 1:E:147:GLN:HB2 | 2.13 | 0.47 |
| 1:E:211:HIS:O | 1:E:338:LYS:HD2 | 2.14 | 0.47 |
| 3:I:107:THR:HG23 | 3:I:109:THR:N | 2.23 | 0.47 |
| 2:F:158:LEU:CD1 | 2:F:177:LEU:HB2 | 2.44 | 0.47 |
| 2:B:703:GLY:C | 2:B:705:VAL:N | 2.65 | 0.47 |
| 2:B:338:GLU:HG3 | 3:I:148:LYS:HD3 | 1.97 | 0.47 |
| 1:A:185:LEU:O | 1:A:188:PRO:HD3 | 2.14 | 0.47 |
| 1:A:347:ARG:HH22 | 2:B:274:ARG:HD2 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:221:TYR:HD2 | 1:A:246:LEU:HG | 1.78 | 0.47 |
| 2:D:13:TRP:HZ3 | 2:D:116:PRO:HG2 | 1.79 | 0.47 |
| 1:A:36:ILE:HG21 | 1:A:131:LEU:HD21 | 1.96 | 0.47 |
| 1:G:437:LYS:HA | 1:G:437:LYS:HD2 | 1.75 | 0.47 |
| 1:G:236:THR:HG23 | 1:G:237:TYR:N | 2.22 | 0.47 |
| 2:D:240:GLU:O | 2:D:241:GLN:C | 2.53 | 0.47 |
| 3:L:101:MET:HG3 | 3:L:163:GLY:H | 1.79 | 0.47 |
| 1:A:225:TRP:NE1 | 1:A:233:ILE:HG12 | 2.28 | 0.47 |
| 3:J:101:MET:HG3 | 3:J:163:GLY:H | 1.79 | 0.47 |
| 1:C:229:THR:O | 1:C:230:ASN:HB2 | 2.14 | 0.47 |
| 3:K:107:THR:CG2 | 3:K:109:THR:H | 2.24 | 0.47 |
| 2:B:361:LEU:O | 2:B:362:GLN:C | 2.52 | 0.47 |
| 2:B:240:GLU:O | 2:B:241:GLN:C | 2.53 | 0.47 |
| 1:A:243:PHE:O | 1:A:246:LEU:HB3 | 2.14 | 0.47 |
| 1:G:233:ILE:HG22 | 1:G:233:ILE:O | 2.15 | 0.47 |
| 1:G:307:LEU:HD22 | 1:G:383:LEU:HD22 | 1.97 | 0.47 |
| 2:H:197:THR:CG2 | 2:H:198:ALA:N | 2.78 | 0.47 |
| 2:F:233:ARG:HH12 | 2:F:234:MET:HB2 | 1.78 | 0.47 |
| 2:D:320:ASN:HD21 | 2:D:336:GLU:HG3 | 1.79 | 0.47 |
| 2:H:155:ASN:CG | 2:H:200:ILE:HB | 2.35 | 0.47 |
| 3:K:106:LYS:HA | 3:K:112:GLU:HA | 1.97 | 0.47 |
| 2:D:342:ASN:ND2 | 2:D:342:ASN:N | 2.42 | 0.47 |
| 2:D:14:GLU:HG3 | 2:H:258:GLN:CG | 2.40 | 0.47 |
| 2:B:158:LEU:HD12 | 2:B:177:LEU:HD22 | 1.96 | 0.47 |
| 2:H:351:GLN:HA | 2:H:351:GLN:NE2 | 2.28 | 0.47 |
| 2:H:240:GLU:O | 2:H:241:GLN:C | 2.53 | 0.47 |
| 2:F:154:ILE:HD13 | 2:F:154:ILE:O | 2.13 | 0.47 |
| 2:D:233:ARG:HG2 | 2:D:233:ARG:HH11 | 1.78 | 0.47 |
| 2:D:132:ASP:OD1 | 2:D:132:ASP:N | 2.48 | 0.47 |
| 3:J:107:THR:HG23 | 3:J:109:THR:N | 2.24 | 0.47 |
| 1:G:243:PHE:O | 1:G:246:LEU:HB3 | 2.14 | 0.47 |
| 1:A:163:ARG:HG3 | 1:A:519:THR:H | 1.80 | 0.47 |
| 1:A:186:ASP:OD2 | 1:A:279:THR:HB | 2.15 | 0.47 |
| 1:G:225:TRP:NE1 | 1:G:233:ILE:HG12 | 2.29 | 0.47 |
| 1:C:215:ILE:H | 1:C:332:MET:HE3 | 1.80 | 0.47 |
| 2:F:357:PRO:O | 2:F:358:SER:CB | 2.62 | 0.47 |
| 1:C:430:ARG:HH11 | 1:C:430:ARG:HB3 | 1.79 | 0.47 |
| 2:H:46:LEU:O | 2:H:73:ARG:HB2 | 2.14 | 0.47 |
| 2:D:75:ILE:O | 2:D:120:VAL:HA | 2.15 | 0.47 |
| 1:G:362:ALA:O | 1:G:366:GLN:HG3 | 2.14 | 0.47 |
| 1:A:341:LYS:HE3 | 1:E:114:ASP:OD1 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:128:GLN:N | 2:H:128:GLN:NE2 | 2.59 | 0.47 |
| 1:E:233:ILE:O | 1:E:233:ILE:HG22 | 2.15 | 0.47 |
| 1:E:234:PRO:O | 1:E:235:LYS:C | 2.53 | 0.47 |
| 1:G:238:LYS:O | 1:G:241:GLU:N | 2.48 | 0.47 |
| 2:B:13:TRP:HZ3 | 2:B:116:PRO:HG2 | 1.78 | 0.47 |
| 2:H:16:ARG:HH22 | 2:H:116:PRO:HB2 | 1.77 | 0.47 |
| 1:G:34:CYS:HB2 | 1:G:123:PHE:CD2 | 2.50 | 0.47 |
| 1:G:481:GLU:OE2 | 2:H:315:TYR:HE2 | 1.98 | 0.47 |
| 2:H:233:ARG:HG2 | 2:H:233:ARG:HH11 | 1.78 | 0.47 |
| 2:H:249:LEU:HD11 | 2:H:260:ILE:HD11 | 1.96 | 0.47 |
| 1:G:268:ALA:O | 1:G:272:VAL:HG23 | 2.15 | 0.47 |
| 1:C:357:VAL:O | 1:C:361:VAL:HG23 | 2.15 | 0.47 |
| 2:F:351:GLN:HA | 2:F:351:GLN:NE2 | 2.30 | 0.47 |
| 2:D:236:GLN:NE2 | 2:D:263:LYS:HB3 | 2.30 | 0.47 |
| 3:K:101:MET:HG3 | 3:K:163:GLY:H | 1.80 | 0.47 |
| 1:E:215:ILE:HG13 | 1:E:332:MET:HE3 | 1.97 | 0.47 |
| 2:D:280:LEU:O | 2:D:284:VAL:HG23 | 2.14 | 0.47 |
| 1:G:229:THR:O | 1:G:230:ASN:HB2 | 2.15 | 0.47 |
| 1:E:430:ARG:NH1 | 1:E:430:ARG:HB3 | 2.30 | 0.47 |
| 2:D:64:LEU:HB3 | 2:D:111:LEU:HD12 | 1.93 | 0.46 |
| 2:F:351:GLN:CD | 2:F:353:ILE:HD11 | 2.36 | 0.46 |
| 1:E:243:PHE:O | 1:E:246:LEU:HB3 | 2.15 | 0.46 |
| 1:C:252:LEU:HB2 | 1:C:260:GLU:HG2 | 1.96 | 0.46 |
| 1:E:184:ARG:HB3 | 1:E:279:THR:OG1 | 2.15 | 0.46 |
| 1:A:43:THR:HG21 | 1:A:73:ASN:OD1 | 2.15 | 0.46 |
| 1:E:299:LYS:HA | 1:E:368:ILE:HG23 | 1.97 | 0.46 |
| 2:F:703:GLY:HA2 | 2:F:706:ASP:CB | 2.45 | 0.46 |
| 3:I:101:MET:CG | 3:I:163:GLY:H | 2.28 | 0.46 |
| 2:F:233:ARG:NH1 | 2:F:234:MET:HB2 | 2.30 | 0.46 |
| 2:H:38:SER:HB3 | 2:H:41:SER:OG | 2.15 | 0.46 |
| 1:E:155:THR:HG23 | 1:E:493:ILE:HG22 | 1.98 | 0.46 |
| 2:D:158:LEU:CD1 | 2:D:177:LEU:HB2 | 2.44 | 0.46 |
| 2:F:128:GLN:N | 2:F:128:GLN:NE2 | 2.59 | 0.46 |
| 2:D:267:ARG:HG2 | 2:D:267:ARG:NH1 | 2.26 | 0.46 |
| 1:C:260:GLU:CG | 1:C:261:ASP:N | 2.77 | 0.46 |
| 1:G:232:ARG:C | 1:G:233:ILE:HG13 | 2.35 | 0.46 |
| 1:A:268:ALA:O | 1:A:272:VAL:HG23 | 2.14 | 0.46 |
| 2:B:351:GLN:CD | 2:B:353:ILE:HD11 | 2.36 | 0.46 |
| 3:I:117:ILE:HD11 | 3:I:126:ILE:HG23 | 1.97 | 0.46 |
| 1:E:225:TRP:NE1 | 1:E:233:ILE:HG12 | 2.30 | 0.46 |
| 2:B:901:VAL:O | 2:B:902:ALA:O | 2.32 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:233:ARG:HH12 | 2:H:234:MET:HB2 | 1.80 | 0.46 |
| 2:D:128:GLN:HE21 | 2:D:128:GLN:N | 2.06 | 0.46 |
| 3:L:103:ILE:HA | 3:L:163:GLY:O | 2.15 | 0.46 |
| 3:L:103:ILE:HG21 | 3:L:161:ILE:CG2 | 2.46 | 0.46 |
| 1:E:238:LYS:O | 1:E:241:GLU:N | 2.48 | 0.46 |
| 1:C:119:PHE:CE1 | 1:C:122:ARG:NE | 2.82 | 0.46 |
| 2:B:320:ASN:HD21 | 2:B:336:GLU:HG3 | 1.79 | 0.46 |
| 1:E:268:ALA:O | 1:E:272:VAL:HG23 | 2.16 | 0.46 |
| 1:E:168:GLU:HG3 | 1:E:394:ARG:HE | 1.80 | 0.46 |
| 2:H:28:GLY:O | 2:H:31:THR:HG22 | 2.16 | 0.46 |
| 1:G:72:ASN:HD22 | 1:G:72:ASN:H | 1.64 | 0.46 |
| 3:K:170:VAL:CG1 | 3:K:171:LEU:N | 2.79 | 0.46 |
| 1:E:232:ARG:C | 1:E:233:ILE:HG13 | 2.35 | 0.46 |
| 1:A:155:THR:HG23 | 1:A:493:ILE:HG22 | 1.98 | 0.46 |
| 2:H:381:ILE:CG2 | 2:H:902:ALA:HB1 | 2.45 | 0.46 |
| 2:B:603:ILE:O | 2:B:607:THR:N | 2.35 | 0.46 |
| 2:D:361:LEU:O | 2:D:362:GLN:C | 2.54 | 0.46 |
| 2:H:95:ARG:CG | 2:H:95:ARG:HH11 | 2.28 | 0.46 |
| 2:F:132:ASP:OD1 | 2:F:132:ASP:N | 2.48 | 0.46 |
| 1:A:32:HIS:HA | 1:A:56:SER:O | 2.15 | 0.46 |
| 3:L:106:LYS:HA | 3:L:112:GLU:HA | 1.98 | 0.46 |
| 1:C:260:GLU:HG3 | 1:C:261:ASP:H | 1.78 | 0.46 |
| 1:A:215:ILE:H | 1:A:332:MET:HE3 | 1.80 | 0.46 |
| 1:E:347:ARG:NH2 | 2:F:274:ARG:HD2 | 2.31 | 0.46 |
| 1:E:347:ARG:NH2 | 2:F:274:ARG:NH1 | 2.63 | 0.46 |
| 1:E:125:VAL:HG12 | 1:E:126:VAL:N | 2.30 | 0.46 |
| 1:C:146:SER:O | 1:C:147:GLN:HB2 | 2.16 | 0.46 |
| 2:F:338:GLU:HG3 | 3:K:148:LYS:HD3 | 1.97 | 0.46 |
| 3:K:107:THR:HG23 | 3:K:109:THR:N | 2.23 | 0.46 |
| 1:A:84:ASN:OD1 | 1:A:86:ALA:HB3 | 2.16 | 0.46 |
| 2:D:162:LEU:HD22 | 2:D:169:LEU:HD11 | 1.98 | 0.46 |
| 1:A:307:LEU:HD22 | 1:A:383:LEU:HD22 | 1.97 | 0.46 |
| 1:C:32:HIS:HA | 1:C:56:SER:O | 2.16 | 0.46 |
| 1:E:36:ILE:O | 1:E:60:ILE:O | 2.33 | 0.46 |
| 1:A:34:CYS:HB2 | 1:A:123:PHE:CD2 | 2.51 | 0.46 |
| 2:B:340:LYS:HB3 | 2:B:342:ASN:ND2 | 2.30 | 0.46 |
| 3:J:103:ILE:HG21 | 3:J:161:ILE:CG2 | 2.46 | 0.46 |
| 1:A:266:GLU:O | 1:A:270:LYS:HG3 | 2.16 | 0.46 |
| 2:D:212:ASN:HD22 | 2:D:212:ASN:HA | 1.54 | 0.46 |
| 2:B:74:GLN:HE22 | 2:B:119:ASN:HD22 | 1.64 | 0.46 |
| 1:A:407:ILE:HG23 | 1:A:407:ILE:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:236:THR:HG23 | 1:E:237:TYR:N | 2.22 | 0.45 |
| 2:B:162:LEU:HD22 | 2:B:169:LEU:HD11 | 1.98 | 0.45 |
| 1:G:234:PRO:O | 1:G:235:LYS:C | 2.54 | 0.45 |
| 1:A:418:ASN:HD22 | 1:A:419:PRO:HD2 | 1.81 | 0.45 |
| 1:G:36:ILE:O | 1:G:60:ILE:O | 2.34 | 0.45 |
| 1:C:87:GLU:O | 1:C:91:GLU:HG3 | 2.16 | 0.45 |
| 2:H:226:GLU:OE1 | 2:H:226:GLU:N | 2.48 | 0.45 |
| 2:H:351:GLN:CD | 2:H:353:ILE:HD11 | 2.36 | 0.45 |
| 2:F:197:THR:HG22 | 2:F:198:ALA:N | 2.31 | 0.45 |
| 3:K:118:GLU:C | 3:K:120:THR:H | 2.20 | 0.45 |
| 2:H:232:VAL:HG12 | 2:H:232:VAL:O | 2.16 | 0.45 |
| 2:B:236:GLN:NE2 | 2:B:263:LYS:HB3 | 2.31 | 0.45 |
| 1:G:72:ASN:C | 1:G:72:ASN:ND2 | 2.69 | 0.45 |
| 2:D:380:ALA:O | 2:D:904:VAL:HA | 2.17 | 0.45 |
| 3:J:106:LYS:HA | 3:J:112:GLU:HA | 1.97 | 0.45 |
| 2:D:232:VAL:HG12 | 2:D:232:VAL:O | 2.16 | 0.45 |
| 1:E:163:ARG:NH1 | 1:E:163:ARG:HG2 | 2.29 | 0.45 |
| 1:G:49:LEU:O | 1:G:52:PRO:HD2 | 2.17 | 0.45 |
| 1:G:32:HIS:HA | 1:G:56:SER:O | 2.17 | 0.45 |
| 1:A:185:LEU:HD12 | 1:A:275:ALA:HB1 | 1.99 | 0.45 |
| 1:G:266:GLU:O | 1:G:270:LYS:HG3 | 2.17 | 0.45 |
| 2:B:158:LEU:CD1 | 2:B:177:LEU:HB2 | 2.47 | 0.45 |
| 2:H:357:PRO:O | 2:H:358:SER:CB | 2.65 | 0.45 |
| 1:A:481:GLU:OE1 | 1:A:481:GLU:HA | 2.16 | 0.45 |
| 1:G:178:ASN:ND2 | 3:L:136:ILE:HG12 | 2.31 | 0.45 |
| 2:B:394:LEU:C | 2:B:396:SER:H | 2.20 | 0.45 |
| 2:H:64:LEU:HD11 | 2:H:77:VAL:HG21 | 1.99 | 0.45 |
| 2:F:240:GLU:O | 2:F:241:GLN:C | 2.55 | 0.45 |
| 2:F:213:PHE:CB | 2:F:218:ILE:HD11 | 2.43 | 0.45 |
| 2:B:50:LYS:N | 2:B:139:HIS:HD2 | 2.14 | 0.45 |
| 2:F:162:LEU:HD22 | 2:F:169:LEU:HD11 | 1.98 | 0.45 |
| 2:H:349:LEU:HB3 | 2:H:350:PRO:HD2 | 1.98 | 0.45 |
| 2:H:233:ARG:NH1 | 2:H:234:MET:HB2 | 2.32 | 0.45 |
| 1:A:13:TYR:O | 1:A:16:GLN:HG2 | 2.16 | 0.45 |
| 1:E:266:GLU:O | 1:E:270:LYS:HG3 | 2.17 | 0.45 |
| 2:D:64:LEU:HD11 | 2:D:77:VAL:HG21 | 1.98 | 0.45 |
| 2:F:365:LEU:HD11 | 2:F:395:GLN:NE2 | 2.31 | 0.45 |
| 2:F:267:ARG:NH1 | 2:F:267:ARG:HG2 | 2.28 | 0.45 |
| 1:A:238:LYS:O | 1:A:241:GLU:N | 2.49 | 0.45 |
| 3:K:101:MET:CG | 3:K:163:GLY:H | 2.29 | 0.45 |
| 3:J:101:MET:CG | 3:J:163:GLY:H | 2.29 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:13:TRP:HZ3 | 2:H:116:PRO:HG2 | 1.81 | 0.45 |
| 2:F:249:LEU:HD11 | 2:F:260:ILE:HD11 | 1.98 | 0.45 |
| 1:C:268:ALA:O | 1:C:272:VAL:HG23 | 2.17 | 0.45 |
| 2:F:361:LEU:O | 2:F:362:GLN:C | 2.55 | 0.45 |
| 2:B:703:GLY:HA2 | 2:B:706:ASP:CB | 2.47 | 0.45 |
| 1:C:232:ARG:C | 1:C:233:ILE:HG13 | 2.37 | 0.45 |
| 2:D:256:HIS:O | 2:D:260:ILE:HG13 | 2.16 | 0.45 |
| 1:E:178:ASN:ND2 | 3:K:136:ILE:HG23 | 2.32 | 0.45 |
| 2:F:13:TRP:HZ3 | 2:F:116:PRO:HG2 | 1.82 | 0.45 |
| 1:G:447:ASN:HD22 | 2:H:26:ARG:NH2 | 2.14 | 0.45 |
| 1:A:155:THR:HG23 | 1:A:493:ILE:CG2 | 2.46 | 0.45 |
| 3:I:106:LYS:HA | 3:I:112:GLU:HA | 1.99 | 0.45 |
| 1:E:251:ILE:HG23 | 1:E:262:GLU:CB | 2.42 | 0.45 |
| 3:I:103:ILE:HA | 3:I:163:GLY:O | 2.17 | 0.45 |
| 1:C:163:ARG:HG2 | 1:C:163:ARG:NH1 | 2.28 | 0.45 |
| 1:C:186:ASP:OD2 | 1:C:279:THR:HB | 2.17 | 0.45 |
| 1:G:184:ARG:HB3 | 1:G:279:THR:OG1 | 2.17 | 0.45 |
| 1:E:336:SER:HB2 | 2:F:221:MET:HA | 1.99 | 0.45 |
| 1:G:481:GLU:HA | 1:G:481:GLU:OE1 | 2.16 | 0.45 |
| 2:B:256:HIS:O | 2:B:260:ILE:HG13 | 2.17 | 0.45 |
| 2:F:226:GLU:OE1 | 2:F:226:GLU:N | 2.49 | 0.45 |
| 2:B:274:ARG:NH1 | 1:E:106:GLU:O | 2.49 | 0.45 |
| 2:H:267:ARG:CG | 2:H:267:ARG:HH11 | 2.28 | 0.45 |
| 2:H:361:LEU:O | 2:H:362:GLN:C | 2.56 | 0.45 |
| 3:L:101:MET:CG | 3:L:163:GLY:H | 2.30 | 0.45 |
| 2:D:249:LEU:HD11 | 2:D:260:ILE:HD11 | 1.98 | 0.45 |
| 2:H:236:GLN:HE22 | 2:H:263:LYS:HB3 | 1.81 | 0.45 |
| 2:B:233:ARG:HH11 | 2:B:233:ARG:HG2 | 1.81 | 0.45 |
| 2:H:320:ASN:HD21 | 2:H:336:GLU:HG3 | 1.81 | 0.45 |
| 2:B:142:VAL:CG2 | 2:B:307:VAL:HG21 | 2.47 | 0.45 |
| 1:E:447:ASN:HD22 | 2:F:26:ARG:NH2 | 2.14 | 0.45 |
| 1:G:146:SER:O | 1:G:147:GLN:HB2 | 2.16 | 0.45 |
| 1:E:302:PRO:HG2 | 1:E:305:TRP:HD1 | 1.82 | 0.45 |
| 1:C:13:TYR:O | 1:C:16:GLN:HG2 | 2.17 | 0.45 |
| 1:C:437:LYS:HD2 | 1:C:437:LYS:HA | 1.75 | 0.45 |
| 1:A:236:THR:HG23 | 1:A:237:TYR:N | 2.22 | 0.45 |
| 1:C:251:ILE:HG23 | 1:C:262:GLU:HG2 | 1.98 | 0.45 |
| 2:H:162:LEU:HD22 | 2:H:169:LEU:HD11 | 1.99 | 0.45 |
| 1:E:84:ASN:OD1 | 1:E:86:ALA:HB3 | 2.17 | 0.45 |
| 1:A:225:TRP:CE2 | 1:A:233:ILE:HG12 | 2.52 | 0.45 |
| 1:C:234:PRO:O | 1:C:235:LYS:C | 2.55 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:235:LYS:HB2 | 1:C:239:GLU:OE2 | 2.17 | 0.45 |
| 1:E:235:LYS:HB3 | 1:E:239:GLU:HG3 | 1.98 | 0.45 |
| 1:E:347:ARG:HH22 | 2:F:274:ARG:CD | 2.29 | 0.45 |
| 2:H:197:THR:HG22 | 2:H:198:ALA:N | 2.32 | 0.45 |
| 1:C:33:VAL:HG21 | 1:C:54:ILE:HD11 | 1.98 | 0.45 |
| 2:H:236:GLN:NE2 | 2:H:263:LYS:HB3 | 2.32 | 0.45 |
| 1:E:119:PHE:CE1 | 1:E:122:ARG:NE | 2.83 | 0.45 |
| 1:C:441:ARG:NH2 | 1:C:453:ASP:CG | 2.70 | 0.45 |
| 1:C:407:ILE:HD11 | 1:C:412:ILE:HD12 | 1.98 | 0.45 |
| 2:F:233:ARG:HG2 | 2:F:233:ARG:HH11 | 1.82 | 0.45 |
| 1:A:90:MET:O | 1:A:94:GLN:HB2 | 2.17 | 0.45 |
| 1:A:357:VAL:O | 1:A:361:VAL:HG23 | 2.17 | 0.45 |
| 1:C:90:MET:O | 1:C:94:GLN:HB2 | 2.17 | 0.45 |
| 1:G:357:VAL:O | 1:G:361:VAL:HG23 | 2.16 | 0.45 |
| 2:B:361:LEU:C | 2:B:363:GLU:N | 2.69 | 0.44 |
| 3:K:101:MET:HG3 | 3:K:163:GLY:HA2 | 1.99 | 0.44 |
| 1:G:163:ARG:NH2 | 1:G:518:ASN:HD21 | 2.13 | 0.44 |
| 1:A:119:PHE:CE1 | 1:A:122:ARG:NE | 2.84 | 0.44 |
| 1:E:155:THR:HG23 | 1:E:493:ILE:CG2 | 2.47 | 0.44 |
| 1:G:87:GLU:O | 1:G:91:GLU:HG3 | 2.18 | 0.44 |
| 2:D:603:ILE:O | 2:D:607:THR:N | 2.38 | 0.44 |
| 1:E:251:ILE:HG23 | 1:E:262:GLU:HG2 | 1.99 | 0.44 |
| 2:D:361:LEU:C | 2:D:363:GLU:N | 2.70 | 0.44 |
| 2:D:164:TYR:CE2 | 2:D:348:GLN:HG2 | 2.52 | 0.44 |
| 1:A:235:LYS:HB2 | 1:A:239:GLU:OE2 | 2.17 | 0.44 |
| 2:F:95:ARG:HH11 | 2:F:95:ARG:CG | 2.29 | 0.44 |
| 1:A:49:LEU:O | 1:A:52:PRO:HD2 | 2.18 | 0.44 |
| 1:G:510:THR:O | 1:G:511:LYS:HB2 | 2.18 | 0.44 |
| 2:F:236:GLN:NE2 | 2:F:263:LYS:HB3 | 2.32 | 0.44 |
| 1:G:430:ARG:HB3 | 1:G:430:ARG:HH11 | 1.83 | 0.44 |
| 1:G:442:TYR:O | 1:G:445:VAL:HG23 | 2.17 | 0.44 |
| 2:B:64:LEU:HB3 | 2:B:111:LEU:HD12 | 1.97 | 0.44 |
| 2:F:604:GLU:HA | 2:F:607:THR:CB | 2.47 | 0.44 |
| 2:D:703:GLY:HA2 | 2:D:706:ASP:CB | 2.48 | 0.44 |
| 3:K:103:ILE:HG21 | 3:K:161:ILE:CG2 | 2.47 | 0.44 |
| 3:K:103:ILE:HA | 3:K:163:GLY:O | 2.17 | 0.44 |
| 1:E:481:GLU:OE1 | 1:E:481:GLU:HA | 2.17 | 0.44 |
| 2:F:236:GLN:HE22 | 2:F:263:LYS:HB3 | 1.81 | 0.44 |
| 1:C:447:ASN:HD22 | 2:D:26:ARG:NH2 | 2.14 | 0.44 |
| 2:F:351:GLN:HG3 | 2:F:353:ILE:CD1 | 2.43 | 0.44 |
| 1:C:238:LYS:O | 1:C:241:GLU:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:54:ILE:HG22 | 2:D:145:LEU:CD2 | 2.46 | 0.44 |
| 2:B:13:TRP:CZ3 | 2:B:116:PRO:HG2 | 2.52 | 0.44 |
| 1:C:419:PRO:CB | 1:C:475:LYS:HE3 | 2.47 | 0.44 |
| 2:B:132:ASP:OD1 | 2:B:132:ASP:N | 2.48 | 0.44 |
| 1:G:168:GLU:HG3 | 1:G:394:ARG:HE | 1.82 | 0.44 |
| 1:G:251:ILE:HG23 | 1:G:262:GLU:HG2 | 2.00 | 0.44 |
| 2:H:703:GLY:HA2 | 2:H:706:ASP:CB | 2.47 | 0.44 |
| 2:F:54:ILE:HG22 | 2:F:145:LEU:CD2 | 2.44 | 0.44 |
| 1:C:177:ASP:O | 1:C:178:ASN:HB2 | 2.17 | 0.44 |
| 2:B:197:THR:HG22 | 2:B:198:ALA:N | 2.32 | 0.44 |
| 1:E:407:ILE:HD11 | 1:E:412:ILE:HD12 | 1.99 | 0.44 |
| 1:E:46:LEU:O | 1:E:50:VAL:HG23 | 2.18 | 0.44 |
| 1:A:442:TYR:O | 1:A:445:VAL:HG23 | 2.17 | 0.44 |
| 2:F:56:ALA:HA | 2:F:60:GLY:HA3 | 2.00 | 0.44 |
| 1:A:281:ILE:HA | 1:A:282:PRO:HD3 | 1.86 | 0.44 |
| 1:C:266:GLU:O | 1:C:270:LYS:HG3 | 2.16 | 0.44 |
| 1:E:426:TYR:HB2 | 1:E:521:ILE:HD11 | 1.99 | 0.44 |
| 2:D:199:CYS:HG | 2:D:346:CYS:HG | 1.63 | 0.44 |
| 1:G:163:ARG:NH1 | 1:G:163:ARG:HG2 | 2.29 | 0.44 |
| 1:E:51:LEU:HD11 | 2:F:92:PHE:HB3 | 1.99 | 0.44 |
| 1:C:347:ARG:NH2 | 2:D:274:ARG:NH1 | 2.66 | 0.44 |
| 2:H:132:ASP:HA | 2:H:157:MET:CE | 2.48 | 0.44 |
| 1:E:441:ARG:NH2 | 1:E:453:ASP:CG | 2.70 | 0.44 |
| 1:E:419:PRO:CB | 1:E:475:LYS:HE3 | 2.48 | 0.44 |
| 2:B:155:ASN:CG | 2:B:200:ILE:HB | 2.38 | 0.44 |
| 2:D:226:GLU:OE1 | 2:D:226:GLU:N | 2.48 | 0.44 |
| 2:B:353:ILE:N | 2:B:353:ILE:HD13 | 2.33 | 0.44 |
| 1:C:235:LYS:HB3 | 1:C:239:GLU:HG3 | 1.97 | 0.44 |
| 1:G:347:ARG:HH12 | 2:H:274:ARG:HD2 | 1.83 | 0.44 |
| 1:G:225:TRP:CE2 | 1:G:233:ILE:HG12 | 2.52 | 0.44 |
| 2:H:220:SER:HB2 | 2:H:221:MET:HE3 | 1.98 | 0.44 |
| 3:L:136:ILE:O | 3:L:141:GLN:NE2 | 2.49 | 0.44 |
| 2:H:361:LEU:C | 2:H:363:GLU:N | 2.71 | 0.44 |
| 1:G:235:LYS:HB3 | 1:G:239:GLU:HG3 | 2.00 | 0.44 |
| 2:H:95:ARG:HD3 | 2:H:95:ARG:HA | 1.74 | 0.44 |
| 1:E:185:LEU:HD12 | 1:E:275:ALA:HB1 | 1.99 | 0.44 |
| 2:D:64:LEU:HD21 | 2:D:77:VAL:HG21 | 2.00 | 0.44 |
| 3:L:118:GLU:C | 3:L:120:THR:H | 2.22 | 0.44 |
| 2:B:178:ILE:N | 2:B:178:ILE:HD12 | 2.33 | 0.44 |
| 1:C:185:LEU:HD12 | 1:C:275:ALA:HB1 | 1.99 | 0.44 |
| 2:B:28:GLY:O | 2:B:31:THR:HG22 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:489:GLU:O | 1:C:489:GLU:HG2 | 2.18 | 0.44 |
| 2:H:322:LEU:CD1 | 2:H:322:LEU:C | 2.85 | 0.43 |
| 2:F:361:LEU:C | 2:F:363:GLU:N | 2.71 | 0.43 |
| 2:F:393:TYR:CD1 | 2:F:607:THR:HA | 2.52 | 0.43 |
| 3:I:103:ILE:HG21 | 3:I:161:ILE:CG2 | 2.48 | 0.43 |
| 1:E:87:GLU:O | 1:E:91:GLU:HG3 | 2.18 | 0.43 |
| 2:B:380:ALA:O | 2:B:904:VAL:HA | 2.18 | 0.43 |
| 1:A:252:LEU:HB2 | 1:A:260:GLU:HG2 | 1.99 | 0.43 |
| 2:B:323:VAL:O | 2:B:332:THR:HA | 2.18 | 0.43 |
| 1:E:517:ASN:C | 1:E:517:ASN:ND2 | 2.70 | 0.43 |
| 2:F:50:LYS:N | 2:F:139:HIS:HD2 | 2.15 | 0.43 |
| 2:B:901:VAL:O | 2:B:902:ALA:C | 2.53 | 0.43 |
| 1:E:347:ARG:HH22 | 2:F:274:ARG:NH1 | 2.17 | 0.43 |
| 3:I:118:GLU:C | 3:I:120:THR:H | 2.22 | 0.43 |
| 1:C:36:ILE:HG21 | 1:C:131:LEU:HD21 | 1.99 | 0.43 |
| 2:H:134:PHE:O | 2:H:137:GLN:HG3 | 2.18 | 0.43 |
| 2:D:56:ALA:HA | 2:D:60:GLY:HA3 | 2.00 | 0.43 |
| 1:E:437:LYS:HD2 | 1:E:437:LYS:HA | 1.75 | 0.43 |
| 1:G:251:ILE:HG23 | 1:G:262:GLU:CB | 2.43 | 0.43 |
| 2:H:213:PHE:CB | 2:H:218:ILE:HD11 | 2.43 | 0.43 |
| 1:E:264:ASN:ND2 | 1:E:265:PHE:H | 2.16 | 0.43 |
| 1:A:234:PRO:O | 1:A:235:LYS:C | 2.55 | 0.43 |
| 1:G:131:LEU:HA | 1:G:132:PRO:HD3 | 1.81 | 0.43 |
| 2:H:222:PRO:HD2 | 2:H:271:TYR:CD2 | 2.54 | 0.43 |
| 2:D:74:GLN:HE22 | 2:D:119:ASN:HD22 | 1.65 | 0.43 |
| 2:H:56:ALA:HA | 2:H:60:GLY:HA3 | 2.01 | 0.43 |
| 2:D:89:ASN:OD1 | 2:D:90:ARG:NH1 | 2.49 | 0.43 |
| 2:H:74:GLN:HE22 | 2:H:119:ASN:HD22 | 1.67 | 0.43 |
| 1:G:260:GLU:HG3 | 1:G:261:ASP:N | 2.33 | 0.43 |
| 1:A:518:ASN:O | 1:A:519:THR:O | 2.37 | 0.43 |
| 1:G:517:ASN:C | 1:G:517:ASN:ND2 | 2.71 | 0.43 |
| 1:G:186:ASP:HB2 | 1:G:232:ARG:CZ | 2.49 | 0.43 |
| 1:A:36:ILE:HG23 | 1:A:109:PRO:HG3 | 2.00 | 0.43 |
| 1:A:348:GLU:HG3 | 1:E:115:ASN:CB | 2.47 | 0.43 |
| 2:H:250:ASP:HB3 | 2:H:253:ASP:HB2 | 1.99 | 0.43 |
| 1:A:362:ALA:O | 1:A:366:GLN:HG3 | 2.19 | 0.43 |
| 2:H:228:CYS:SG | 2:H:268:ALA:HA | 2.59 | 0.43 |
| 1:G:302:PRO:HG2 | 1:G:305:TRP:HD1 | 1.84 | 0.43 |
| 2:H:158:LEU:HD22 | 2:H:175:VAL:HB | 2.01 | 0.43 |
| 1:C:238:LYS:O | 1:C:239:GLU:C | 2.56 | 0.43 |
| 1:C:307:LEU:HB3 | 1:C:383:LEU:CD2 | 2.46 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:VAL:HG21 | 1:A:54:ILE:CD1 | 2.48 | 0.43 |
| 2:F:132:ASP:HA | 2:F:157:MET:CE | 2.49 | 0.43 |
| 1:G:128:ALA:HB1 | 1:G:131:LEU:HD11 | 2.01 | 0.43 |
| 2:D:220:SER:HB2 | 2:D:221:MET:HE3 | 2.01 | 0.43 |
| 2:B:249:LEU:HD11 | 2:B:260:ILE:HD11 | 2.00 | 0.43 |
| 2:H:320:ASN:O | 2:H:321:TYR:HB2 | 2.18 | 0.43 |
| 1:C:168:GLU:HG3 | 1:C:394:ARG:HE | 1.84 | 0.43 |
| 2:F:394:LEU:C | 2:F:396:SER:H | 2.21 | 0.43 |
| 1:C:72:ASN:HD22 | 1:C:72:ASN:H | 1.67 | 0.43 |
| 2:D:28:GLY:O | 2:D:31:THR:HG22 | 2.18 | 0.43 |
| 2:H:323:VAL:O | 2:H:332:THR:HA | 2.18 | 0.43 |
| 2:F:323:VAL:O | 2:F:332:THR:HA | 2.19 | 0.43 |
| 1:E:186:ASP:HB2 | 1:E:232:ARG:CZ | 2.49 | 0.43 |
| 1:E:347:ARG:HH22 | 2:F:274:ARG:HH11 | 1.66 | 0.43 |
| 1:G:418:ASN:HD22 | 1:G:419:PRO:HD2 | 1.81 | 0.43 |
| 1:E:131:LEU:HA | 1:E:132:PRO:HD3 | 1.85 | 0.43 |
| 1:G:185:LEU:HD12 | 1:G:275:ALA:HB1 | 2.00 | 0.43 |
| 1:C:481:GLU:OE2 | 2:D:315:TYR:HE2 | 2.01 | 0.43 |
| 2:D:394:LEU:C | 2:D:396:SER:H | 2.21 | 0.43 |
| 1:C:426:TYR:HB2 | 1:C:521:ILE:HD11 | 2.01 | 0.43 |
| 2:B:75:ILE:O | 2:B:120:VAL:HA | 2.18 | 0.43 |
| 1:A:251:ILE:HG23 | 1:A:262:GLU:CB | 2.45 | 0.43 |
| 1:C:208:ASP:CG | 1:C:211:HIS:HB2 | 2.39 | 0.43 |
| 1:C:211:HIS:O | 1:C:338:LYS:HD2 | 2.19 | 0.43 |
| 2:B:361:LEU:O | 2:B:364:VAL:CG2 | 2.65 | 0.43 |
| 2:D:353:ILE:HD13 | 2:D:353:ILE:N | 2.33 | 0.43 |
| 1:C:186:ASP:HB2 | 1:C:232:ARG:CZ | 2.49 | 0.43 |
| 1:E:235:LYS:HB2 | 1:E:239:GLU:OE2 | 2.19 | 0.43 |
| 1:G:33:VAL:HG21 | 1:G:54:ILE:HD11 | 2.00 | 0.43 |
| 1:A:419:PRO:CB | 1:A:475:LYS:HE3 | 2.49 | 0.43 |
| 1:A:146:SER:O | 1:A:147:GLN:HB2 | 2.18 | 0.43 |
| 1:E:90:MET:O | 1:E:94:GLN:HB2 | 2.18 | 0.43 |
| 1:G:90:MET:O | 1:G:94:GLN:HB2 | 2.18 | 0.43 |
| 2:H:351:GLN:HG3 | 2:H:353:ILE:CD1 | 2.43 | 0.43 |
| 2:B:357:PRO:O | 2:B:358:SER:CB | 2.65 | 0.43 |
| 3:I:115:ILE:HD13 | 3:I:129:ARG:HB2 | 2.01 | 0.43 |
| 2:D:322:LEU:C | 2:D:322:LEU:CD1 | 2.86 | 0.43 |
| 2:F:158:LEU:HD12 | 2:F:177:LEU:HD22 | 2.01 | 0.43 |
| 2:B:213:PHE:CB | 2:B:218:ILE:HD11 | 2.41 | 0.43 |
| 2:B:54:ILE:CD1 | 2:B:154:ILE:HG13 | 2.49 | 0.43 |
| 2:B:154:ILE:HD13 | 2:B:154:ILE:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:101:MET:HG3 | 3:J:163:GLY:HA2 | 2.01 | 0.43 |
| 2:F:303:CYS:O | 2:F:307:VAL:HG23 | 2.19 | 0.43 |
| 1:E:281:ILE:HA | 1:E:282:PRO:HD3 | 1.87 | 0.43 |
| 3:K:119:PRO:O | 3:K:157:ALA:HB2 | 2.19 | 0.43 |
| 3:I:107:THR:CG2 | 3:I:109:THR:H | 2.23 | 0.43 |
| 3:J:103:ILE:HA | 3:J:163:GLY:O | 2.18 | 0.43 |
| 1:E:186:ASP:OD2 | 1:E:279:THR:HB | 2.18 | 0.43 |
| 2:D:13:TRP:CZ3 | 2:D:116:PRO:HG2 | 2.53 | 0.43 |
| 2:D:197:THR:HG22 | 2:D:198:ALA:N | 2.33 | 0.43 |
| 2:D:284:VAL:O | 2:D:287:ARG:NH1 | 2.52 | 0.43 |
| 1:E:311:LEU:HD12 | 1:E:311:LEU:HA | 1.85 | 0.43 |
| 3:J:118:GLU:C | 3:J:120:THR:H | 2.22 | 0.43 |
| 1:A:441:ARG:NH2 | 1:A:453:ASP:CG | 2.72 | 0.43 |
| 1:C:333:ILE:HA | 2:D:223:ARG:NH2 | 2.33 | 0.43 |
| 2:B:349:LEU:HB3 | 2:B:350:PRO:HD2 | 1.99 | 0.43 |
| 1:C:324:PRO:HB3 | 1:C:353:ASP:HB3 | 2.01 | 0.43 |
| 2:F:155:ASN:CG | 2:F:200:ILE:HB | 2.39 | 0.43 |
| 2:B:353:ILE:HB | 2:B:355:PHE:HE1 | 1.80 | 0.42 |
| 2:F:353:ILE:HD13 | 2:F:353:ILE:N | 2.34 | 0.42 |
| 2:H:50:LYS:N | 2:H:139:HIS:HD2 | 2.15 | 0.42 |
| 1:A:238:LYS:O | 1:A:239:GLU:C | 2.57 | 0.42 |
| 1:A:235:LYS:HB3 | 1:A:239:GLU:HG3 | 2.00 | 0.42 |
| 1:E:33:VAL:HG21 | 1:E:54:ILE:HD11 | 2.01 | 0.42 |
| 1:A:229:THR:O | 1:A:230:ASN:ND2 | 2.52 | 0.42 |
| 1:G:43:THR:HG21 | 1:G:73:ASN:OD1 | 2.19 | 0.42 |
| 2:D:349:LEU:HB3 | 2:D:350:PRO:HD2 | 2.00 | 0.42 |
| 2:F:250:ASP:HB3 | 2:F:253:ASP:HB2 | 2.01 | 0.42 |
| 1:G:426:TYR:HB2 | 1:G:521:ILE:HD11 | 2.00 | 0.42 |
| 2:B:250:ASP:HB3 | 2:B:253:ASP:HB2 | 2.01 | 0.42 |
| 2:H:365:LEU:HD11 | 2:H:395:GLN:NE2 | 2.34 | 0.42 |
| 1:E:72:ASN:ND2 | 1:E:72:ASN:C | 2.72 | 0.42 |
| 2:D:162:LEU:HD21 | 2:D:194:PRO:O | 2.19 | 0.42 |
| 2:F:164:TYR:CE2 | 2:F:348:GLN:HG2 | 2.54 | 0.42 |
| 2:H:54:ILE:HG22 | 2:H:145:LEU:CD2 | 2.47 | 0.42 |
| 1:E:307:LEU:HD22 | 1:E:383:LEU:HD22 | 2.02 | 0.42 |
| 2:H:201:GLU:HB3 | 2:H:343:CYS:SG | 2.59 | 0.42 |
| 2:F:74:GLN:HE22 | 2:F:119:ASN:HD22 | 1.68 | 0.42 |
| 1:E:497:LEU:HD12 | 1:E:497:LEU:HA | 1.91 | 0.42 |
| 2:D:158:LEU:HD22 | 2:D:175:VAL:HB | 2.02 | 0.42 |
| 1:A:396:ARG:HD2 | 1:A:534:LEU:HD21 | 2.01 | 0.42 |
| 1:E:163:ARG:NH2 | 1:E:518:ASN:HD21 | 2.16 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:238:LYS:O | 1:E:239:GLU:C | 2.57 | 0.42 |
| 2:H:284:VAL:O | 2:H:287:ARG:NH1 | 2.51 | 0.42 |
| 1:A:347:ARG:HH22 | 2:B:274:ARG:NH1 | 2.17 | 0.42 |
| 1:A:208:ASP:CG | 1:A:211:HIS:HB2 | 2.39 | 0.42 |
| 2:F:322:LEU:C | 2:F:322:LEU:CD1 | 2.86 | 0.42 |
| 1:E:225:TRP:CE2 | 1:E:233:ILE:HG12 | 2.54 | 0.42 |
| 2:D:154:ILE:HD13 | 2:D:154:ILE:O | 2.19 | 0.42 |
| 1:G:235:LYS:HB2 | 1:G:239:GLU:OE2 | 2.20 | 0.42 |
| 2:B:284:VAL:O | 2:B:287:ARG:NH1 | 2.52 | 0.42 |
| 2:H:216:ALA:O | 2:H:220:SER:HB2 | 2.20 | 0.42 |
| 1:G:311:LEU:HA | 1:G:311:LEU:HD12 | 1.83 | 0.42 |
| 1:C:426:TYR:HB2 | 1:C:521:ILE:CD1 | 2.49 | 0.42 |
| 1:C:155:THR:HG23 | 1:C:493:ILE:CG2 | 2.49 | 0.42 |
| 2:D:250:ASP:HB3 | 2:D:253:ASP:HB2 | 2.01 | 0.42 |
| 2:D:323:VAL:O | 2:D:332:THR:HA | 2.19 | 0.42 |
| 2:F:158:LEU:HD22 | 2:F:175:VAL:HB | 2.02 | 0.42 |
| 2:B:393:TYR:CZ | 2:B:395:GLN:HG2 | 2.54 | 0.42 |
| 2:B:267:ARG:CG | 2:B:267:ARG:HH11 | 2.24 | 0.42 |
| 3:I:101:MET:HG3 | 3:I:163:GLY:HA2 | 2.01 | 0.42 |
| 2:B:164:TYR:CE2 | 2:B:348:GLN:HG2 | 2.55 | 0.42 |
| 1:C:454:ILE:HD13 | 1:C:480:HIS:CE1 | 2.55 | 0.42 |
| 2:H:257:ILE:HG22 | 2:H:278:TYR:CE1 | 2.55 | 0.42 |
| 2:D:132:ASP:HA | 2:D:157:MET:CE | 2.50 | 0.42 |
| 2:B:232:VAL:O | 2:B:232:VAL:HG12 | 2.19 | 0.42 |
| 1:G:441:ARG:NH2 | 1:G:453:ASP:CG | 2.73 | 0.42 |
| 2:D:155:ASN:CG | 2:D:200:ILE:HB | 2.39 | 0.42 |
| 3:I:145:TYR:O | 3:I:146:SER:C | 2.58 | 0.42 |
| 2:F:145:LEU:O | 3:K:176:GLY:HA3 | 2.20 | 0.42 |
| 2:F:320:ASN:HD21 | 2:F:336:GLU:HG3 | 1.84 | 0.42 |
| 1:E:362:ALA:O | 1:E:366:GLN:HG3 | 2.18 | 0.42 |
| 2:F:380:ALA:O | 2:F:904:VAL:HA | 2.19 | 0.42 |
| 2:B:64:LEU:HD21 | 2:B:77:VAL:HG21 | 2.00 | 0.42 |
| 1:E:234:PRO:HB2 | 1:E:235:LYS:H | 1.71 | 0.42 |
| 1:C:347:ARG:HH22 | 2:D:274:ARG:NH1 | 2.16 | 0.42 |
| 1:C:347:ARG:HH12 | 2:D:274:ARG:HD2 | 1.85 | 0.42 |
| 2:F:178:ILE:N | 2:F:178:ILE:HD12 | 2.35 | 0.42 |
| 1:E:426:TYR:HB2 | 1:E:521:ILE:CD1 | 2.49 | 0.42 |
| 2:D:74:GLN:NE2 | 2:D:119:ASN:HD22 | 2.17 | 0.42 |
| 2:B:89:ASN:OD1 | 2:B:90:ARG:NH1 | 2.48 | 0.42 |
| 2:B:83:ILE:HD13 | 2:B:94:PHE:HB3 | 2.02 | 0.42 |
| 1:A:426:TYR:HB2 | 1:A:521:ILE:CD1 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:281:ILE:HA | 1:G:282:PRO:HD3 | 1.87 | 0.42 |
| 2:H:368:LEU:HA | 2:H:374:LEU:HD12 | 2.01 | 0.42 |
| 3:L:101:MET:HG3 | 3:L:163:GLY:HA2 | 2.02 | 0.42 |
| 2:F:183:GLU:HB2 | 3:K:173:LEU:HB3 | 2.02 | 0.42 |
| 2:F:284:VAL:O | 2:F:287:ARG:NH1 | 2.53 | 0.42 |
| 1:E:33:VAL:CG2 | 1:E:54:ILE:CD1 | 2.98 | 0.42 |
| 2:B:74:GLN:NE2 | 2:B:119:ASN:HD22 | 2.17 | 0.42 |
| 1:C:155:THR:HG23 | 1:C:493:ILE:HG22 | 2.02 | 0.42 |
| 2:B:134:PHE:O | 2:B:137:GLN:HG3 | 2.19 | 0.42 |
| 2:D:83:ILE:HD13 | 2:D:94:PHE:HB3 | 2.01 | 0.42 |
| 2:B:368:LEU:HA | 2:B:374:LEU:HD12 | 2.00 | 0.42 |
| 2:F:83:ILE:HD13 | 2:F:94:PHE:HB3 | 2.01 | 0.42 |
| 1:G:251:ILE:O | 1:G:252:LEU:C | 2.59 | 0.42 |
| 1:G:297:ILE:HG21 | 1:G:368:ILE:HD11 | 2.00 | 0.42 |
| 2:D:199:CYS:HG | 2:D:343:CYS:HG | 1.61 | 0.42 |
| 2:F:241:GLN:CG | 2:F:245:GLU:HA | 2.49 | 0.42 |
| 2:F:257:ILE:HG22 | 2:F:278:TYR:CE1 | 2.55 | 0.42 |
| 1:G:412:ILE:HA | 1:G:423:ILE:HD13 | 2.02 | 0.42 |
| 1:A:407:ILE:HD11 | 1:A:412:ILE:HD12 | 2.02 | 0.42 |
| 1:G:426:TYR:HB2 | 1:G:521:ILE:CD1 | 2.49 | 0.42 |
| 2:H:394:LEU:C | 2:H:396:SER:H | 2.22 | 0.42 |
| 1:A:72:ASN:ND2 | 1:A:72:ASN:C | 2.73 | 0.42 |
| 2:D:241:GLN:CG | 2:D:245:GLU:HA | 2.49 | 0.42 |
| 2:F:235:LEU:C | 2:F:238:PRO:HD2 | 2.40 | 0.42 |
| 1:C:33:VAL:HG21 | 1:C:54:ILE:CD1 | 2.50 | 0.42 |
| 1:C:125:VAL:HG12 | 1:C:126:VAL:N | 2.34 | 0.42 |
| 2:D:222:PRO:HD2 | 2:D:271:TYR:CD2 | 2.55 | 0.42 |
| 1:G:264:ASN:ND2 | 1:G:265:PHE:H | 2.17 | 0.41 |
| 2:H:340:LYS:HB3 | 2:H:342:ASN:HD21 | 1.85 | 0.41 |
| 1:C:518:ASN:O | 1:C:519:THR:O | 2.38 | 0.41 |
| 2:D:54:ILE:CD1 | 2:D:154:ILE:HG13 | 2.50 | 0.41 |
| 1:G:332:MET:HG2 | 1:G:339:TYR:CE1 | 2.53 | 0.41 |
| 2:B:132:ASP:HA | 2:B:157:MET:CE | 2.49 | 0.41 |
| 1:G:208:ASP:CG | 1:G:211:HIS:HB2 | 2.39 | 0.41 |
| 2:B:365:LEU:HD11 | 2:B:395:GLN:NE2 | 2.35 | 0.41 |
| 2:F:381:ILE:CG2 | 2:F:902:ALA:HB1 | 2.50 | 0.41 |
| 1:C:233:ILE:O | 1:C:233:ILE:HG22 | 2.20 | 0.41 |
| 2:H:54:ILE:CD1 | 2:H:154:ILE:HG13 | 2.50 | 0.41 |
| 1:G:238:LYS:O | 1:G:239:GLU:C | 2.58 | 0.41 |
| 1:A:33:VAL:CG2 | 1:A:54:ILE:CD1 | 2.97 | 0.41 |
| 2:F:95:ARG:HD3 | 2:F:95:ARG:HA | 1.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:178:ILE:HD12 | 2:H:178:ILE:N | 2.36 | 0.41 |
| 2:F:236:GLN:HE22 | 2:F:263:LYS:HD2 | 1.85 | 0.41 |
| 2:H:142:VAL:CG2 | 2:H:307:VAL:HG21 | 2.50 | 0.41 |
| 2:F:349:LEU:HB3 | 2:F:350:PRO:HD2 | 2.00 | 0.41 |
| 1:G:407:ILE:HD11 | 1:G:412:ILE:HD12 | 2.01 | 0.41 |
| 1:G:180:LEU:HD23 | 3:L:135:GLY:CA | 2.49 | 0.41 |
| 1:G:193:ARG:O | 1:G:197:GLN:HG3 | 2.20 | 0.41 |
| 3:I:170:VAL:CG1 | 3:I:171:LEU:N | 2.82 | 0.41 |
| 2:D:50:LYS:N | 2:D:139:HIS:HD2 | 2.14 | 0.41 |
| 1:G:186:ASP:OD2 | 1:G:279:THR:HB | 2.20 | 0.41 |
| 1:C:307:LEU:HD22 | 1:C:383:LEU:HD22 | 2.01 | 0.41 |
| 2:B:95:ARG:HD3 | 2:B:95:ARG:HA | 1.73 | 0.41 |
| 2:F:201:GLU:HB3 | 2:F:343:CYS:SG | 2.61 | 0.41 |
| 1:G:418:ASN:C | 1:G:418:ASN:ND2 | 2.73 | 0.41 |
| 1:G:419:PRO:CB | 1:G:475:LYS:HE3 | 2.50 | 0.41 |
| 1:G:119:PHE:CE1 | 1:G:122:ARG:NE | 2.85 | 0.41 |
| 1:C:226:TYR:O | 1:C:230:ASN:N | 2.53 | 0.41 |
| 1:E:72:ASN:HD22 | 1:E:72:ASN:H | 1.68 | 0.41 |
| 2:D:368:LEU:HA | 2:D:374:LEU:HD12 | 2.02 | 0.41 |
| 2:H:335:PHE:CZ | 3:L:144:ILE:CD1 | 3.02 | 0.41 |
| 1:G:454:ILE:HD13 | 1:G:480:HIS:CE1 | 2.55 | 0.41 |
| 1:A:131:LEU:HA | 1:A:132:PRO:HD3 | 1.84 | 0.41 |
| 2:H:13:TRP:CZ3 | 2:H:116:PRO:HG2 | 2.55 | 0.41 |
| 1:A:227:SER:C | 1:A:229:THR:H | 2.22 | 0.41 |
| 1:C:302:PRO:HG2 | 1:C:305:TRP:HD1 | 1.84 | 0.41 |
| 1:A:19:LEU:HD12 | 2:B:292:VAL:HG13 | 2.01 | 0.41 |
| 1:E:396:ARG:HD2 | 1:E:534:LEU:HD21 | 2.02 | 0.41 |
| 1:A:186:ASP:HB2 | 1:A:232:ARG:CZ | 2.51 | 0.41 |
| 1:C:184:ARG:HB3 | 1:C:279:THR:OG1 | 2.19 | 0.41 |
| 1:C:281:ILE:HA | 1:C:282:PRO:HD3 | 1.86 | 0.41 |
| 2:F:222:PRO:HD2 | 2:F:271:TYR:CD2 | 2.55 | 0.41 |
| 1:E:418:ASN:ND2 | 1:E:418:ASN:C | 2.74 | 0.41 |
| 2:D:320:ASN:O | 2:D:321:TYR:HB2 | 2.19 | 0.41 |
| 1:A:426:TYR:HB2 | 1:A:521:ILE:HD11 | 2.02 | 0.41 |
| 2:D:209:PRO:HD3 | 3:J:142:ARG:HH21 | 1.86 | 0.41 |
| 2:B:38:SER:HB3 | 2:B:41:SER:OG | 2.19 | 0.41 |
| 2:H:353:ILE:N | 2:H:353:ILE:HD13 | 2.36 | 0.41 |
| 2:B:267:ARG:O | 2:B:270:GLN:HB2 | 2.21 | 0.41 |
| 2:F:393:TYR:CZ | 2:F:395:GLN:HG2 | 2.56 | 0.41 |
| 3:L:115:ILE:HD13 | 3:L:129:ARG:HB2 | 2.02 | 0.41 |
| 2:B:217:THR:CG2 | 2:B:223:ARG:HH22 | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:13:TRP:CZ3 | 2:F:116:PRO:HG2 | 2.56 | 0.41 |
| 1:A:412:ILE:HA | 1:A:423:ILE:HD13 | 2.02 | 0.41 |
| 1:C:72:ASN:C | 1:C:72:ASN:ND2 | 2.71 | 0.41 |
| 1:C:481:GLU:HA | 1:C:481:GLU:OE1 | 2.20 | 0.41 |
| 1:A:424:VAL:HG11 | 1:A:478:TYR:CD1 | 2.55 | 0.41 |
| 1:C:65:VAL:CG2 | 1:C:85:ARG:HA | 2.51 | 0.41 |
| 1:A:518:ASN:O | 1:A:519:THR:C | 2.59 | 0.41 |
| 2:F:54:ILE:CD1 | 2:F:154:ILE:HG13 | 2.50 | 0.41 |
| 1:E:336:SER:OG | 2:F:271:TYR:HD2 | 2.04 | 0.41 |
| 2:F:232:VAL:HG12 | 2:F:232:VAL:O | 2.19 | 0.41 |
| 1:E:226:TYR:O | 1:E:230:ASN:N | 2.54 | 0.41 |
| 2:B:192:ILE:CD1 | 2:B:200:ILE:HG12 | 2.50 | 0.41 |
| 2:D:192:ILE:CD1 | 2:D:200:ILE:HG12 | 2.51 | 0.41 |
| 1:A:434:ARG:HD3 | 1:A:460:CYS:HB3 | 2.03 | 0.41 |
| 1:A:46:LEU:HD23 | 1:A:93:LEU:HD13 | 2.02 | 0.41 |
| 1:C:434:ARG:HD3 | 1:C:460:CYS:HB3 | 2.03 | 0.41 |
| 1:G:396:ARG:HD2 | 1:G:534:LEU:HD21 | 2.03 | 0.41 |
| 2:H:380:ALA:O | 2:H:904:VAL:HA | 2.19 | 0.41 |
| 1:E:489:GLU:O | 1:E:489:GLU:HG2 | 2.20 | 0.41 |
| 1:G:252:LEU:HD12 | 1:G:260:GLU:HG2 | 2.02 | 0.41 |
| 3:L:170:VAL:CG1 | 3:L:171:LEU:N | 2.84 | 0.41 |
| 2:H:64:LEU:HD21 | 2:H:77:VAL:HG21 | 2.01 | 0.41 |
| 1:A:65:VAL:CG2 | 1:A:85:ARG:HA | 2.51 | 0.41 |
| 2:H:164:TYR:CE2 | 2:H:348:GLN:HG2 | 2.56 | 0.41 |
| 1:C:396:ARG:HD2 | 1:C:534:LEU:HD21 | 2.02 | 0.41 |
| 1:C:162:MET:O | 1:C:519:THR:HA | 2.21 | 0.41 |
| 1:G:347:ARG:NH2 | 2:H:274:ARG:HD2 | 2.30 | 0.41 |
| 2:D:235:LEU:C | 2:D:238:PRO:HD2 | 2.40 | 0.41 |
| 2:D:237:TRP:CZ2 | 2:D:249:LEU:HA | 2.56 | 0.41 |
| 1:G:125:VAL:HG12 | 1:G:126:VAL:N | 2.36 | 0.41 |
| 1:E:33:VAL:HG21 | 1:E:54:ILE:CD1 | 2.51 | 0.41 |
| 1:A:418:ASN:C | 1:A:418:ASN:ND2 | 2.74 | 0.41 |
| 1:A:226:TYR:O | 1:A:230:ASN:N | 2.54 | 0.41 |
| 1:C:412:ILE:HA | 1:C:423:ILE:HD13 | 2.03 | 0.41 |
| 2:F:74:GLN:NE2 | 2:F:74:GLN:HA | 2.36 | 0.41 |
| 3:J:105:VAL:HG11 | 3:J:130:VAL:HG22 | 2.02 | 0.41 |
| 1:C:9:LYS:HE2 | 1:C:99:ASP:OD1 | 2.21 | 0.41 |
| 3:L:105:VAL:HG11 | 3:L:130:VAL:HG22 | 2.03 | 0.41 |
| 3:L:119:PRO:O | 3:L:157:ALA:HB2 | 2.21 | 0.41 |
| 2:H:367:TYR:O | 2:H:371:SER:HB2 | 2.21 | 0.41 |
| 1:A:437:LYS:HA | 1:A:437:LYS:HD2 | 1.75 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:301:THR:HG22 | 1:G:306:ILE:HG13 | 2.03 | 0.41 |
| 3:I:107:THR:HG22 | 3:I:111:LYS:N | 2.10 | 0.41 |
| 1:E:297:ILE:HG21 | 1:E:368:ILE:HD11 | 2.02 | 0.41 |
| 1:C:234:PRO:HB2 | 1:C:235:LYS:H | 1.73 | 0.41 |
| 1:C:33:VAL:CG2 | 1:C:54:ILE:CD1 | 2.99 | 0.41 |
| 3:K:118:GLU:C | 3:K:120:THR:N | 2.73 | 0.41 |
| 1:A:263:GLU:OE1 | 1:A:333:ILE:HD13 | 2.21 | 0.41 |
| 2:B:257:ILE:HG22 | 2:B:278:TYR:CE1 | 2.55 | 0.41 |
| 1:G:36:ILE:HG23 | 1:G:109:PRO:HG3 | 2.03 | 0.41 |
| 1:G:72:ASN:HD22 | 1:G:72:ASN:N | 2.19 | 0.41 |
| 3:I:105:VAL:HG11 | 3:I:130:VAL:HG22 | 2.03 | 0.41 |
| 2:B:267:ARG:CG | 2:B:267:ARG:NH1 | 2.83 | 0.40 |
| 1:C:282:PRO:HD2 | 1:C:285:ILE:HD12 | 2.03 | 0.40 |
| 2:B:221:MET:HG2 | 2:B:221:MET:H | 1.80 | 0.40 |
| 2:D:216:ALA:O | 2:D:220:SER:HB2 | 2.21 | 0.40 |
| 1:E:193:ARG:O | 1:E:197:GLN:HG3 | 2.22 | 0.40 |
| 2:B:56:ALA:HA | 2:B:60:GLY:HA3 | 2.03 | 0.40 |
| 1:A:264:ASN:ND2 | 1:A:265:PHE:H | 2.19 | 0.40 |
| 2:B:235:LEU:C | 2:B:238:PRO:HD2 | 2.40 | 0.40 |
| 1:C:33:VAL:CG1 | 1:C:34:CYS:N | 2.85 | 0.40 |
| 1:A:333:ILE:HA | 2:B:223:ARG:NH2 | 2.36 | 0.40 |
| 2:B:247:VAL:HA | 2:B:248:PRO:HD3 | 1.77 | 0.40 |
| 2:B:320:ASN:O | 2:B:321:TYR:HB2 | 2.20 | 0.40 |
| 2:D:74:GLN:NE2 | 2:D:74:GLN:HA | 2.35 | 0.40 |
| 2:H:83:ILE:HD13 | 2:H:94:PHE:HB3 | 2.03 | 0.40 |
| 1:C:193:ARG:O | 1:C:197:GLN:HG3 | 2.21 | 0.40 |
| 2:D:166:ASP:C | 2:D:168:VAL:H | 2.25 | 0.40 |
| 2:F:241:GLN:CB | 2:F:245:GLU:HA | 2.52 | 0.40 |
| 2:D:95:ARG:HA | 2:D:95:ARG:HD3 | 1.76 | 0.40 |
| 1:G:507:LYS:O | 1:G:511:LYS:N | 2.52 | 0.40 |
| 1:C:407:ILE:O | 1:C:407:ILE:CG2 | 2.69 | 0.40 |
| 1:A:302:PRO:HG2 | 1:A:305:TRP:HD1 | 1.86 | 0.40 |
| 1:C:301:THR:HG22 | 1:C:306:ILE:HG13 | 2.04 | 0.40 |
| 2:B:166:ASP:C | 2:B:168:VAL:H | 2.24 | 0.40 |
| 1:E:13:TYR:O | 1:E:16:GLN:HG2 | 2.20 | 0.40 |
| 2:D:365:LEU:HD11 | 2:D:395:GLN:NE2 | 2.36 | 0.40 |
| 3:J:107:THR:CG2 | 3:J:109:THR:H | 2.26 | 0.40 |
| 1:C:262:GLU:HG3 | 1:C:265:PHE:CD1 | 2.56 | 0.40 |
| 2:D:356:SER:HA | 2:D:357:PRO:HD3 | 1.93 | 0.40 |
| 1:G:215:ILE:HG13 | 1:G:332:MET:HE3 | 2.04 | 0.40 |
| 1:G:33:VAL:HG21 | 1:G:54:ILE:CD1 | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:128:ALA:HB1 | 1:A:131:LEU:HD11 | 2.02 | 0.40 |
| 2:H:247:VAL:HA | 2:H:248:PRO:HD3 | 1.81 | 0.40 |
| 3:J:102:LEU:CD1 | 3:J:114:GLU:HG2 | 2.52 | 0.40 |
| 1:E:128:ALA:HB1 | 1:E:131:LEU:HD11 | 2.04 | 0.40 |
| 1:G:227:SER:C | 1:G:229:THR:H | 2.24 | 0.40 |
| 2:H:74:GLN:NE2 | 2:H:74:GLN:HA | 2.36 | 0.40 |
| 2:D:38:SER:HB3 | 2:D:41:SER:OG | 2.21 | 0.40 |
| 1:G:13:TYR:O | 1:G:16:GLN:HG2 | 2.21 | 0.40 |
| 2:F:28:GLY:O | 2:F:31:THR:HG22 | 2.21 | 0.40 |
| 2:D:236:GLN:O | 2:D:240:GLU:HG2 | 2.22 | 0.40 |
| 1:E:332:MET:HG2 | 1:E:339:TYR:CE1 | 2.54 | 0.40 |
| 2:H:343:CYS:O | 2:H:347:SER:CB | 2.70 | 0.40 |
| 1:C:418:ASN:C | 1:C:418:ASN:ND2 | 2.74 | 0.40 |
| 1:E:229:THR:O | 1:E:230:ASN:ND2 | 2.55 | 0.40 |
| 2:H:192:ILE:CD1 | 2:H:200:ILE:HG12 | 2.52 | 0.40 |
| 1:E:74:PHE:CD1 | 2:F:65:LYS:HG3 | 2.57 | 0.40 |
| 2:F:134:PHE:O | 2:F:137:GLN:HG3 | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | A | 512/529 (97%) | 459 (90%) | 34 (7%) | 19 (4%) | 4 | 23 |
| 1 | C | 512/529 (97%) | 458 (90%) | 38 (7%) | 16 (3%) | 5 | 28 |
| 1 | E | 512/529 (97%) | 459 (90%) | 36 (7%) | 17 (3%) | 5 | 26 |
| 1 | G | 512/529 (97%) | 460 (90%) | 32 (6%) | 20 (4%) | 4 | 21 |
| 2 | B | 408/431 (95%) | 342 (84%) | 52 (13%) | 14 (3%) | 5 | 25 |
| 2 | D | 408/431 (95%) | 341 (84%) | 55 (14%) | 12 (3%) | 6 | 29 |
| 2 | F | 408/431 (95%) | 342 (84%) | 54 (13%) | 12 (3%) | 6 | 29 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 2 | H | 408/431 (95%) | 345 (85%) | 51 (12%) | 12 (3%) | 6 | 29 |
| 3 | I | 74/76 (97%) | 63 (85%) | 9 (12%) | 2 (3%) | 6 | 32 |
| 3 | J | 74/76 (97%) | 64 (86%) | 8 (11%) | 2 (3%) | 6 | 32 |
| 3 | K | 74/76 (97%) | 64 (86%) | 8 (11%) | 2 (3%) | 6 | 32 |
| 3 | L | 74/76 (97%) | 64 (86%) | 8 (11%) | 2 (3%) | 6 | 32 |
| All | All | 3976/4144 (96%) | 3461 (87%) | 385 (10%) | 130 (3%) | 5 | 26 |

All (130) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 234 | PRO |
| 1 | A | 235 | LYS |
| 1 | A | 236 | THR |
| 1 | A | 259 | PRO |
| 1 | A | 261 | ASP |
| 1 | A | 519 | THR |
| 2 | B | 116 | PRO |
| 2 | B | 358 | SER |
| 2 | B | 362 | GLN |
| 2 | B | 901 | VAL |
| 1 | C | 234 | PRO |
| 1 | C | 235 | LYS |
| 1 | C | 236 | THR |
| 1 | C | 253 | LYS |
| 1 | C | 261 | ASP |
| 1 | C | 519 | THR |
| 2 | D | 116 | PRO |
| 2 | D | 358 | SER |
| 2 | D | 362 | GLN |
| 2 | D | 901 | VAL |
| 2 | D | 902 | ALA |
| 1 | E | 234 | PRO |
| 1 | E | 235 | LYS |
| 1 | E | 236 | THR |
| 1 | E | 253 | LYS |
| 1 | E | 259 | PRO |
| 1 | E | 261 | ASP |
| 1 | E | 519 | THR |
| 2 | F | 116 | PRO |
| 2 | F | 358 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 362 | GLN |
| 2 | F | 901 | VAL |
| 1 | G | 234 | PRO |
| 1 | G | 235 | LYS |
| 1 | G | 236 | THR |
| 1 | G | 259 | PRO |
| 1 | G | 261 | ASP |
| 1 | G | 519 | THR |
| 2 | H | 116 | PRO |
| 2 | H | 358 | SER |
| 2 | H | 362 | GLN |
| 2 | H | 901 | VAL |
| 2 | H | 902 | ALA |
| 1 | A | 237 | TYR |
| 1 | A | 533 | GLN |
| 2 | B | 902 | ALA |
| 3 | I | 163 | GLY |
| 1 | C | 237 | TYR |
| 1 | C | 259 | PRO |
| 1 | C | 275 | ALA |
| 1 | C | 533 | GLN |
| 2 | D | 604 | GLU |
| 3 | J | 163 | GLY |
| 1 | E | 237 | TYR |
| 1 | E | 275 | ALA |
| 1 | E | 533 | GLN |
| 3 | K | 163 | GLY |
| 1 | G | 237 | TYR |
| 1 | G | 275 | ALA |
| 1 | G | 533 | GLN |
| 3 | L | 163 | GLY |
| 1 | A | 252 | LEU |
| 1 | A | 253 | LYS |
| 1 | A | 275 | ALA |
| 1 | A | 276 | LEU |
| 2 | B | 320 | ASN |
| 2 | B | 604 | GLU |
| 3 | I | 119 | PRO |
| 1 | C | 36 | ILE |
| 1 | C | 276 | LEU |
| 2 | D | 320 | ASN |
| 3 | J | 119 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 276 | LEU |
| 2 | F | 320 | ASN |
| 2 | F | 604 | GLU |
| 3 | K | 119 | PRO |
| 1 | G | 252 | LEU |
| 1 | G | 276 | LEU |
| 2 | H | 320 | ASN |
| 2 | H | 604 | GLU |
| 3 | L | 119 | PRO |
| 1 | A | 36 | ILE |
| 1 | A | 178 | ASN |
| 1 | A | 233 | ILE |
| 1 | A | 262 | GLU |
| 1 | A | 317 | LYS |
| 1 | A | 422 | GLU |
| 2 | B | 359 | ALA |
| 2 | B | 907 | PRO |
| 2 | B | 908 | GLN |
| 2 | D | 359 | ALA |
| 2 | D | 907 | PRO |
| 2 | D | 908 | GLN |
| 1 | E | 317 | LYS |
| 2 | F | 359 | ALA |
| 2 | F | 907 | PRO |
| 1 | G | 36 | ILE |
| 1 | G | 253 | LYS |
| 2 | H | 359 | ALA |
| 2 | H | 705 | VAL |
| 2 | H | 907 | PRO |
| 2 | B | 239 | LYS |
| 2 | B | 241 | GLN |
| 2 | B | 705 | VAL |
| 1 | C | 233 | ILE |
| 1 | C | 262 | GLU |
| 1 | C | 317 | LYS |
| 2 | D | 241 | GLN |
| 2 | D | 705 | VAL |
| 1 | E | 36 | ILE |
| 1 | E | 178 | ASN |
| 1 | E | 233 | ILE |
| 1 | E | 262 | GLU |
| 2 | F | 239 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 241 | GLN |
| 2 | F | 705 | VAL |
| 1 | G | 233 | ILE |
| 1 | G | 262 | GLU |
| 1 | G | 317 | LYS |
| 1 | G | 422 | GLU |
| 2 | H | 239 | LYS |
| 2 | H | 241 | GLN |
| 2 | B | 363 | GLU |
| 2 | F | 132 | ASP |
| 1 | G | 178 | ASN |
| 1 | E | 190 | PRO |
| 1 | G | 190 | PRO |
| 1 | C | 190 | PRO |
| 1 | G | 21 | GLY |
| 1 | A | 190 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 450/461 (98%) | 430 (96%) | 20 (4%) | 35 | 74 |
| 1 | C | 450/461 (98%) | 432 (96%) | 18 (4%) | 38 | 77 |
| 1 | E | 450/461 (98%) | 430 (96%) | 20 (4%) | 35 | 74 |
| 1 | G | 450/461 (98%) | 430 (96%) | 20 (4%) | 35 | 74 |
| 2 | B | 334/379 (88%) | 311 (93%) | 23 (7%) | 19 | 56 |
| 2 | D | 334/379 (88%) | 311 (93%) | 23 (7%) | 19 | 56 |
| 2 | F | 334/379 (88%) | 311 (93%) | 23 (7%) | 19 | 56 |
| 2 | H | 334/379 (88%) | 311 (93%) | 23 (7%) | 19 | 56 |
| 3 | I | 66/66 (100%) | 64 (97%) | 2 (3%) | 48 | 83 |
| 3 | J | 66/66 (100%) | 64 (97%) | 2 (3%) | 48 | 83 |
| 3 | K | 66/66 (100%) | 64 (97%) | 2 (3%) | 48 | 83 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 3 | L | 66/66 (100%) | 64 (97%) | 2 (3%) | 48 | 83 |
| All | All | 3400/3624 (94%) | 3222 (95%) | 178 (5%) | 29 | 68 |

All (178) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 43 | THR |
| 1 | A | 72 | ASN |
| 1 | A | 90 | MET |
| 1 | A | 214 | TRP |
| 1 | A | 245 | ASP |
| 1 | A | 253 | LYS |
| 1 | A | 259 | PRO |
| 1 | A | 260 | GLU |
| 1 | A | 262 | GLU |
| 1 | A | 264 | ASN |
| 1 | A | 277 | ASN |
| 1 | A | 292 | ASP |
| 1 | A | 293 | ARG |
| 1 | A | 309 | ARG |
| 1 | A | 311 | LEU |
| 1 | A | 407 | ILE |
| 1 | A | 410 | ASP |
| 1 | A | 418 | ASN |
| 1 | A | 422 | GLU |
| 1 | A | 517 | ASN |
| 2 | B | 82 | THR |
| 2 | B | 111 | LEU |
| 2 | B | 114 | ARG |
| 2 | B | 116 | PRO |
| 2 | B | 128 | GLN |
| 2 | B | 132 | ASP |
| 2 | B | 154 | ILE |
| 2 | B | 182 | THR |
| 2 | B | 190 | ARG |
| 2 | B | 212 | ASN |
| 2 | B | 277 | THR |
| 2 | B | 306 | GLU |
| 2 | B | 316 | ILE |
| 2 | B | 322 | LEU |
| 2 | B | 325 | ASN |
| 2 | B | 327 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 342 | ASN |
| 2 | B | 348 | GLN |
| 2 | B | 353 | ILE |
| 2 | B | 358 | SER |
| 2 | B | 362 | GLN |
| 2 | B | 364 | VAL |
| 2 | B | 382 | THR |
| 3 | I | 107 | THR |
| 3 | I | 170 | VAL |
| 1 | C | 43 | THR |
| 1 | C | 72 | ASN |
| 1 | C | 214 | TRP |
| 1 | C | 245 | ASP |
| 1 | C | 253 | LYS |
| 1 | C | 260 | GLU |
| 1 | C | 262 | GLU |
| 1 | C | 264 | ASN |
| 1 | C | 277 | ASN |
| 1 | C | 292 | ASP |
| 1 | C | 293 | ARG |
| 1 | C | 309 | ARG |
| 1 | C | 311 | LEU |
| 1 | C | 407 | ILE |
| 1 | C | 410 | ASP |
| 1 | C | 418 | ASN |
| 1 | C | 422 | GLU |
| 1 | C | 517 | ASN |
| 2 | D | 82 | THR |
| 2 | D | 111 | LEU |
| 2 | D | 114 | ARG |
| 2 | D | 116 | PRO |
| 2 | D | 128 | GLN |
| 2 | D | 132 | ASP |
| 2 | D | 154 | ILE |
| 2 | D | 182 | THR |
| 2 | D | 190 | ARG |
| 2 | D | 212 | ASN |
| 2 | D | 277 | THR |
| 2 | D | 306 | GLU |
| 2 | D | 316 | ILE |
| 2 | D | 322 | LEU |
| 2 | D | 325 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 327 | VAL |
| 2 | D | 342 | ASN |
| 2 | D | 348 | GLN |
| 2 | D | 353 | ILE |
| 2 | D | 358 | SER |
| 2 | D | 362 | GLN |
| 2 | D | 364 | VAL |
| 2 | D | 382 | THR |
| 3 | J | 107 | THR |
| 3 | J | 170 | VAL |
| 1 | E | 43 | THR |
| 1 | E | 72 | ASN |
| 1 | E | 90 | MET |
| 1 | E | 214 | TRP |
| 1 | E | 245 | ASP |
| 1 | E | 253 | LYS |
| 1 | E | 259 | PRO |
| 1 | E | 260 | GLU |
| 1 | E | 262 | GLU |
| 1 | E | 264 | ASN |
| 1 | E | 277 | ASN |
| 1 | E | 292 | ASP |
| 1 | E | 293 | ARG |
| 1 | E | 309 | ARG |
| 1 | E | 311 | LEU |
| 1 | E | 407 | ILE |
| 1 | E | 410 | ASP |
| 1 | E | 418 | ASN |
| 1 | E | 422 | GLU |
| 1 | E | 517 | ASN |
| 2 | F | 82 | THR |
| 2 | F | 111 | LEU |
| 2 | F | 114 | ARG |
| 2 | F | 116 | PRO |
| 2 | F | 128 | GLN |
| 2 | F | 132 | ASP |
| 2 | F | 154 | ILE |
| 2 | F | 182 | THR |
| 2 | F | 190 | ARG |
| 2 | F | 212 | ASN |
| 2 | F | 277 | THR |
| 2 | F | 306 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 316 | ILE |
| 2 | F | 322 | LEU |
| 2 | F | 325 | ASN |
| 2 | F | 327 | VAL |
| 2 | F | 342 | ASN |
| 2 | F | 348 | GLN |
| 2 | F | 353 | ILE |
| 2 | F | 358 | SER |
| 2 | F | 362 | GLN |
| 2 | F | 364 | VAL |
| 2 | F | 382 | THR |
| 3 | K | 107 | THR |
| 3 | K | 170 | VAL |
| 1 | G | 43 | THR |
| 1 | G | 72 | ASN |
| 1 | G | 90 | MET |
| 1 | G | 214 | TRP |
| 1 | G | 245 | ASP |
| 1 | G | 259 | PRO |
| 1 | G | 260 | GLU |
| 1 | G | 262 | GLU |
| 1 | G | 264 | ASN |
| 1 | G | 277 | ASN |
| 1 | G | 292 | ASP |
| 1 | G | 293 | ARG |
| 1 | G | 309 | ARG |
| 1 | G | 311 | LEU |
| 1 | G | 364 | LEU |
| 1 | G | 407 | ILE |
| 1 | G | 410 | ASP |
| 1 | G | 418 | ASN |
| 1 | G | 422 | GLU |
| 1 | G | 517 | ASN |
| 2 | H | 82 | THR |
| 2 | H | 111 | LEU |
| 2 | H | 114 | ARG |
| 2 | H | 116 | PRO |
| 2 | H | 128 | GLN |
| 2 | H | 132 | ASP |
| 2 | H | 154 | ILE |
| 2 | H | 182 | THR |
| 2 | H | 190 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | H | 212 | ASN |
| 2 | H | 277 | THR |
| 2 | H | 306 | GLU |
| 2 | H | 316 | ILE |
| 2 | H | 322 | LEU |
| 2 | H | 325 | ASN |
| 2 | H | 327 | VAL |
| 2 | H | 342 | ASN |
| 2 | H | 348 | GLN |
| 2 | H | 353 | ILE |
| 2 | H | 358 | SER |
| 2 | H | 362 | GLN |
| 2 | H | 364 | VAL |
| 2 | H | 382 | THR |
| 3 | L | 107 | THR |
| 3 | L | 170 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 37 | ASN |
| 1 | A | 72 | ASN |
| 1 | A | 77 | GLN |
| 1 | A | 178 | ASN |
| 1 | A | 197 | GLN |
| 1 | A | 209 | HIS |
| 1 | A | 224 | GLN |
| 1 | A | 264 | ASN |
| 1 | A | 271 | ASN |
| 1 | A | 277 | ASN |
| 1 | A | 320 | GLN |
| 1 | A | 344 | ASN |
| 1 | A | 359 | ASN |
| 1 | A | 418 | ASN |
| 1 | A | 439 | GLN |
| 1 | A | 447 | ASN |
| 1 | A | 517 | ASN |
| 1 | A | 533 | GLN |
| 2 | B | 74 | GLN |
| 2 | B | 87 | ASN |
| 2 | B | 128 | GLN |
| 2 | B | 139 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 212 | ASN |
| 2 | B | 236 | GLN |
| 2 | B | 241 | GLN |
| 2 | B | 262 | GLN |
| 2 | B | 325 | ASN |
| 2 | B | 342 | ASN |
| 2 | B | 348 | GLN |
| 2 | B | 351 | GLN |
| 2 | B | 370 | ASN |
| 2 | B | 395 | GLN |
| 1 | C | 37 | ASN |
| 1 | C | 72 | ASN |
| 1 | C | 77 | GLN |
| 1 | C | 178 | ASN |
| 1 | C | 197 | GLN |
| 1 | C | 209 | HIS |
| 1 | C | 224 | GLN |
| 1 | C | 230 | ASN |
| 1 | C | 264 | ASN |
| 1 | C | 271 | ASN |
| 1 | C | 277 | ASN |
| 1 | C | 320 | GLN |
| 1 | C | 359 | ASN |
| 1 | C | 418 | ASN |
| 1 | C | 439 | GLN |
| 1 | C | 447 | ASN |
| 1 | C | 517 | ASN |
| 1 | C | 533 | GLN |
| 2 | D | 74 | GLN |
| 2 | D | 87 | ASN |
| 2 | D | 128 | GLN |
| 2 | D | 139 | HIS |
| 2 | D | 212 | ASN |
| 2 | D | 236 | GLN |
| 2 | D | 241 | GLN |
| 2 | D | 325 | ASN |
| 2 | D | 342 | ASN |
| 2 | D | 348 | GLN |
| 2 | D | 351 | GLN |
| 2 | D | 370 | ASN |
| 2 | D | 395 | GLN |
| 1 | E | 37 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 72 | ASN |
| 1 | E | 77 | GLN |
| 1 | E | 115 | ASN |
| 1 | E | 178 | ASN |
| 1 | E | 197 | GLN |
| 1 | E | 209 | HIS |
| 1 | E | 224 | GLN |
| 1 | E | 230 | ASN |
| 1 | E | 264 | ASN |
| 1 | E | 271 | ASN |
| 1 | E | 277 | ASN |
| 1 | E | 320 | GLN |
| 1 | E | 359 | ASN |
| 1 | E | 418 | ASN |
| 1 | E | 439 | GLN |
| 1 | E | 447 | ASN |
| 1 | E | 517 | ASN |
| 2 | F | 74 | GLN |
| 2 | F | 87 | ASN |
| 2 | F | 125 | ASN |
| 2 | F | 128 | GLN |
| 2 | F | 139 | HIS |
| 2 | F | 212 | ASN |
| 2 | F | 236 | GLN |
| 2 | F | 241 | GLN |
| 2 | F | 325 | ASN |
| 2 | F | 342 | ASN |
| 2 | F | 348 | GLN |
| 2 | F | 351 | GLN |
| 2 | F | 370 | ASN |
| 2 | F | 395 | GLN |
| 1 | G | 37 | ASN |
| 1 | G | 72 | ASN |
| 1 | G | 77 | GLN |
| 1 | G | 178 | ASN |
| 1 | G | 197 | GLN |
| 1 | G | 209 | HIS |
| 1 | G | 224 | GLN |
| 1 | G | 264 | ASN |
| 1 | G | 271 | ASN |
| 1 | G | 277 | ASN |
| 1 | G | 320 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 359 | ASN |
| 1 | G | 418 | ASN |
| 1 | G | 439 | GLN |
| 1 | G | 447 | ASN |
| 1 | G | 517 | ASN |
| 1 | G | 533 | GLN |
| 2 | H | 74 | GLN |
| 2 | H | 87 | ASN |
| 2 | H | 128 | GLN |
| 2 | H | 139 | HIS |
| 2 | H | 212 | ASN |
| 2 | H | 236 | GLN |
| 2 | H | 241 | GLN |
| 2 | H | 325 | ASN |
| 2 | H | 342 | ASN |
| 2 | H | 348 | GLN |
| 2 | H | 351 | GLN |
| 2 | H | 370 | ASN |
| 2 | H | 395 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.