



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2016 – 06:34 PM EDT

PDB ID : 5FOA
Title : Crystal Structure of Human Complement C3b in complex with DAF (CCP2-4)
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.
Deposited on : 2015-11-18
Resolution : 4.19 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

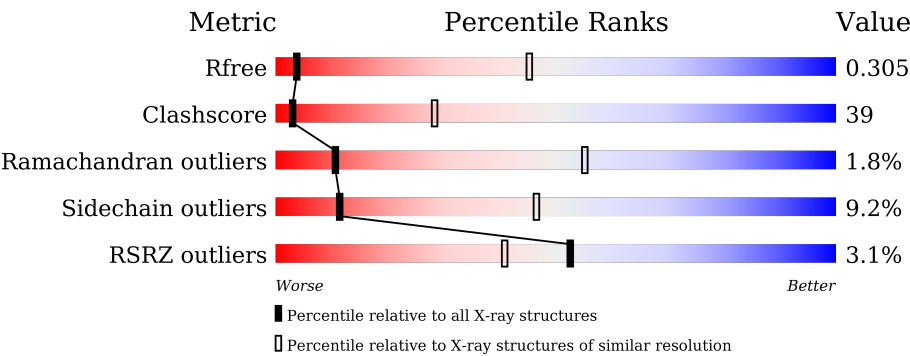
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1030 (4.76-3.60) |
| Clashscore | 102246 | 1130 (4.76-3.60) |
| Ramachandran outliers | 100387 | 1076 (4.76-3.60) |
| Sidechain outliers | 100360 | 1061 (4.76-3.60) |
| RSRZ outliers | 91569 | 1034 (4.76-3.60) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 645 | <div><div>3%</div><div><div></div><div>48%</div><div>45%</div><div>6%</div><div>.</div></div></div> |
| 1 | C | 645 | <div><div>2%</div><div><div></div><div>52%</div><div>41%</div><div>5%</div><div>.</div></div></div> |
| 2 | B | 915 | <div><div>3%</div><div><div></div><div>43%</div><div>44%</div><div>10%</div><div>..</div></div></div> |
| 2 | D | 915 | <div><div>2%</div><div><div></div><div>43%</div><div>44%</div><div>10%</div><div>..</div></div></div> |
| 3 | E | 194 | <div><div>6%</div><div><div></div><div>41%</div><div>43%</div><div>10%</div><div>..</div></div></div> |
| 3 | F | 194 | <div><div>11%</div><div><div></div><div>41%</div><div>40%</div><div>14%</div><div>..</div></div></div> |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27275 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 COMPLEMENT C3 BETA CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 642 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5002 | 3185 | 848 | 954 | 15 | | | |
| 1 | C | 642 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5002 | 3185 | 848 | 954 | 15 | | | |

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | B | 902 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7177 | 4550 | 1205 | 1384 | 38 | | | |
| 2 | D | 902 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7164 | 4543 | 1204 | 1380 | 37 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 1013 | GLU | GLN | SEE REMARK 999 | UNP P01024 |
| D | 1013 | GLU | GLN | SEE REMARK 999 | UNP P01024 |

- Molecule 3 is a protein called DECAY ACCELERATING FACTOR, CD55.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3 | E | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1465 | 920 | 249 | 283 | 13 | | | |
| 3 | F | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1465 | 920 | 249 | 283 | 13 | | | |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| E | 95 | GLY | - | EXPRESSION TAG | UNP P08174 |
| E | 96 | SER | - | EXPRESSION TAG | UNP P08174 |

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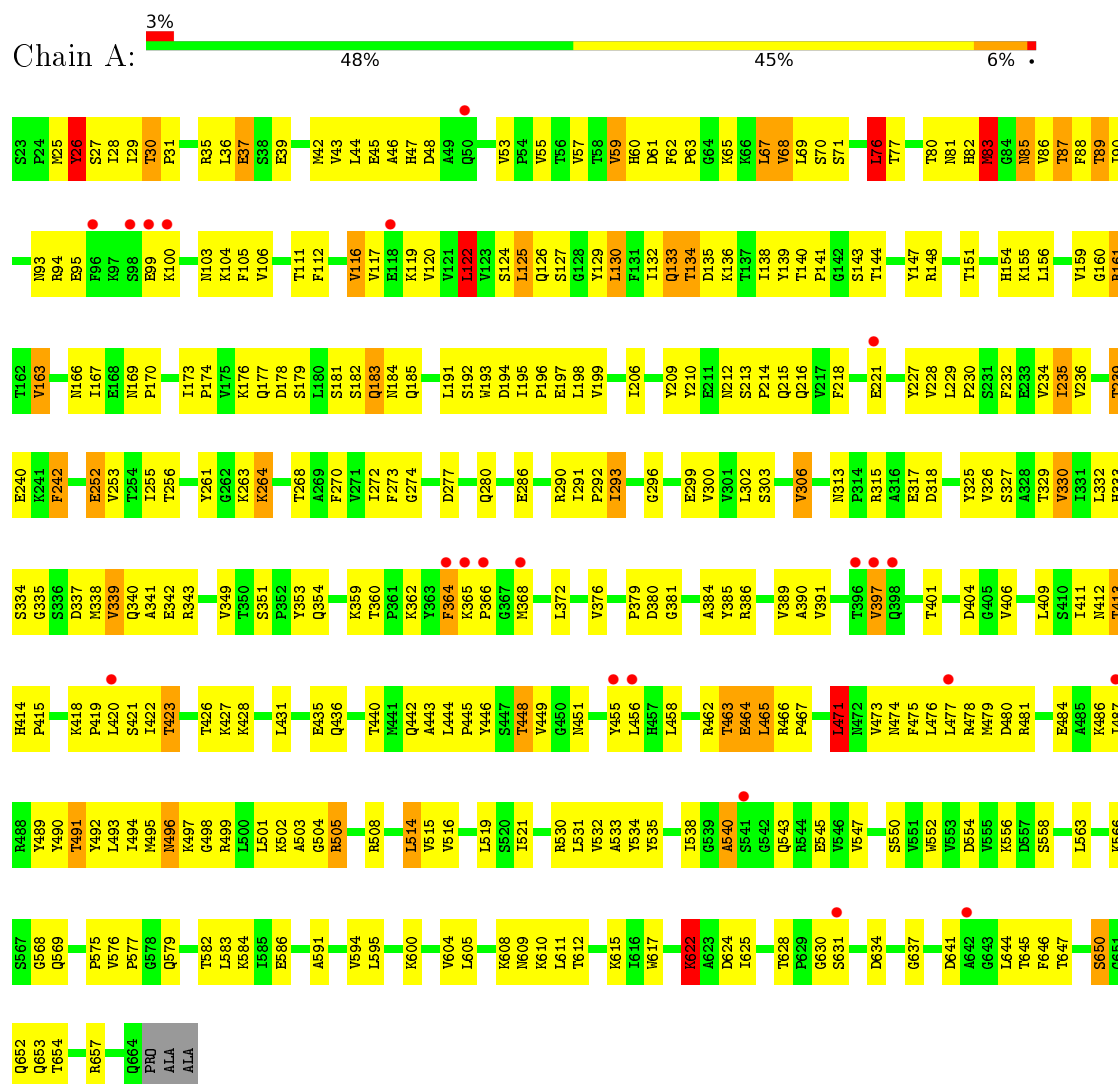
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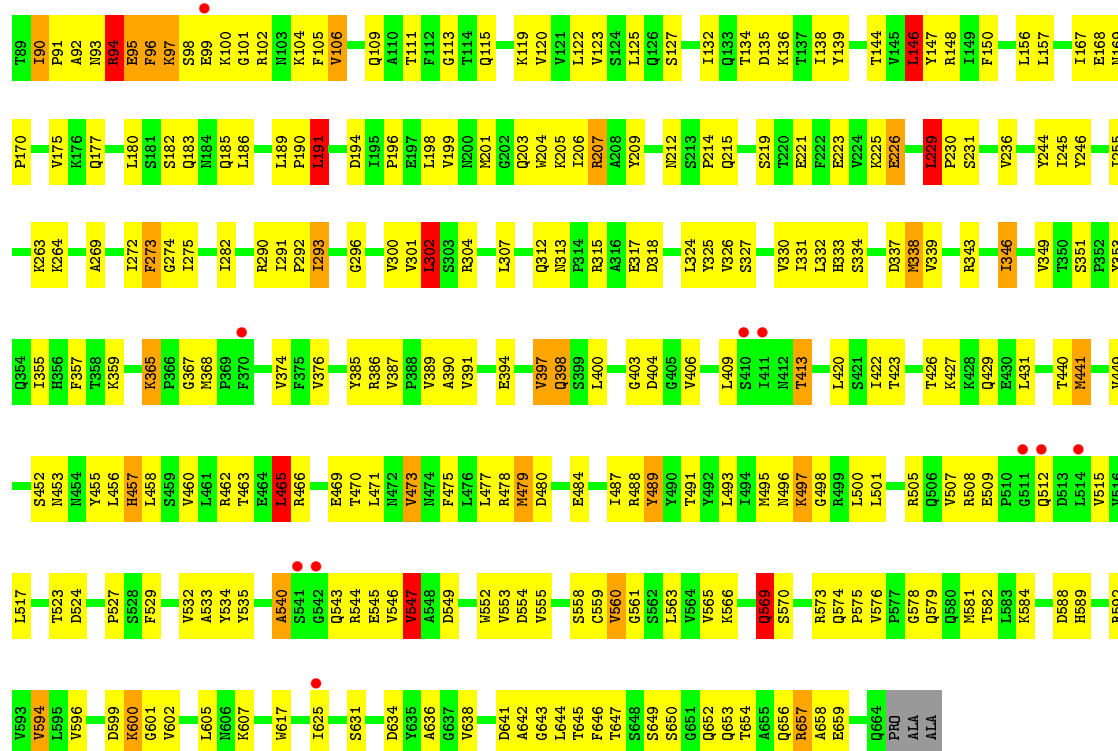
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| E | 286 | ALA | - | EXPRESSION TAG | UNP P08174 |
| E | 287 | ALA | - | EXPRESSION TAG | UNP P08174 |
| E | 288 | ALA | - | EXPRESSION TAG | UNP P08174 |
| F | 95 | GLY | - | EXPRESSION TAG | UNP P08174 |
| F | 96 | SER | - | EXPRESSION TAG | UNP P08174 |
| F | 286 | ALA | - | EXPRESSION TAG | UNP P08174 |
| F | 287 | ALA | - | EXPRESSION TAG | UNP P08174 |
| F | 288 | ALA | - | EXPRESSION TAG | UNP P08174 |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

• Molecule 1: COMPLEMENT C3 BETA CHAIN

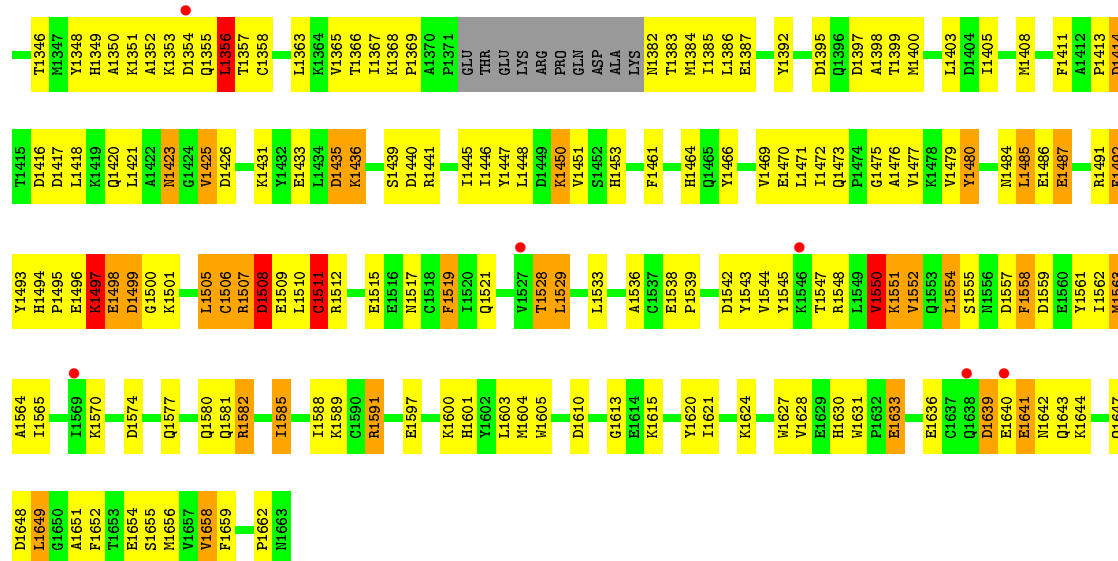




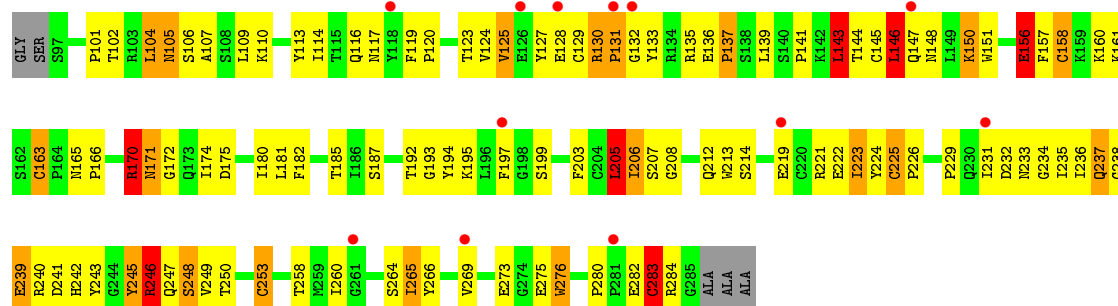
• Molecule 2: COMPLEMENT C3B ALPHA CHAIN



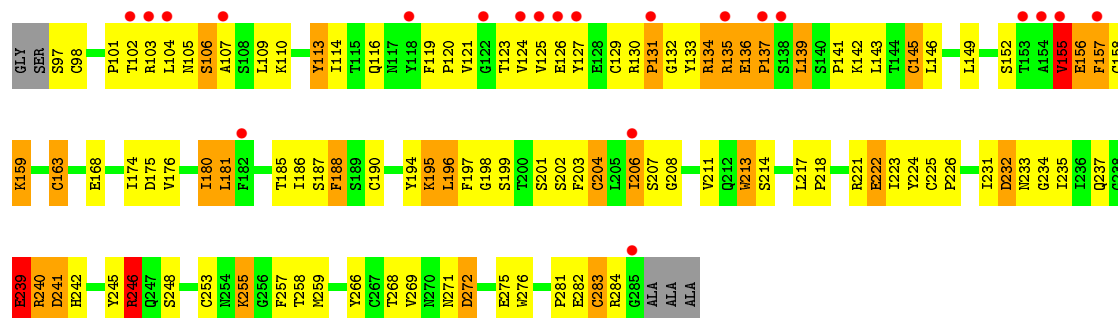
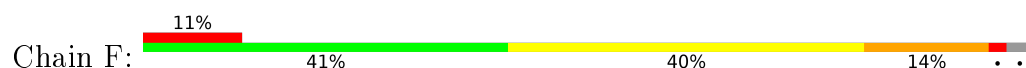




• Molecule 3: DECAY ACCELERATING FACTOR, CD55



• Molecule 3: DECAY ACCELERATING FACTOR, CD55



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 2 ₁ 2 ₁ 2 ₁ | Depositor |
| Cell constants a, b, c, α , β , γ | 117.43 Å 142.38 Å 323.70 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 110.39 – 4.19 110.39 – 4.19 | Depositor EDS |
| % Data completeness (in resolution range) | 95.5 (110.39-4.19) 89.6 (110.39-4.19) | Depositor EDS |
| R_{merge} | 0.15 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.37 (at 4.15 Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE) | Depositor |
| R, R_{free} | 0.270 , 0.307 0.267 , 0.305 | Depositor DCC |
| R_{free} test set | 1836 reflections (5.03%) | DCC |
| Wilson B-factor (Å ²) | 125.0 | Xtriage |
| Anisotropy | 0.372 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 115.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.82 | EDS |
| Total number of atoms | 27275 | wwPDB-VP |
| Average B, all atoms (Å ²) | 124.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.58 | 2/5103 (0.0%) | 0.90 | 16/6934 (0.2%) |
| 1 | C | 0.63 | 5/5103 (0.1%) | 0.95 | 21/6934 (0.3%) |
| 2 | B | 0.71 | 16/7319 (0.2%) | 1.07 | 55/9912 (0.6%) |
| 2 | D | 0.71 | 10/7306 (0.1%) | 1.09 | 49/9896 (0.5%) |
| 3 | E | 0.82 | 5/1506 (0.3%) | 1.07 | 11/2048 (0.5%) |
| 3 | F | 0.68 | 1/1506 (0.1%) | 1.00 | 11/2048 (0.5%) |
| All | All | 0.68 | 39/27843 (0.1%) | 1.02 | 163/37772 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 2 | B | 0 | 4 |
| 2 | D | 0 | 4 |
| 3 | F | 0 | 2 |
| All | All | 0 | 12 |

All (39) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2 | B | 1313 | TRP | CE3-CZ3 | -15.41 | 1.12 | 1.38 |
| 3 | E | 276 | TRP | CB-CG | -9.69 | 1.32 | 1.50 |
| 2 | D | 813 | LYS | CD-CE | -8.91 | 1.28 | 1.51 |
| 1 | A | 37 | GLU | CG-CD | -8.84 | 1.38 | 1.51 |
| 3 | E | 158 | CYS | CB-SG | -8.41 | 1.68 | 1.82 |
| 2 | B | 1358 | CYS | CB-SG | -8.33 | 1.68 | 1.82 |
| 2 | D | 841 | ARG | CB-CG | -7.26 | 1.32 | 1.52 |
| 1 | C | 67 | LEU | CG-CD2 | 7.15 | 1.78 | 1.51 |
| 2 | D | 1036 | LYS | CE-NZ | -6.97 | 1.31 | 1.49 |
| 2 | D | 1641 | GLU | CD-OE2 | 6.70 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | B | 1506 | CYS | CB-SG | -6.52 | 1.71 | 1.82 |
| 3 | E | 125 | VAL | CB-CG2 | -6.44 | 1.39 | 1.52 |
| 2 | D | 1249 | VAL | CA-CB | 6.25 | 1.67 | 1.54 |
| 1 | C | 569 | GLN | CG-CD | -6.21 | 1.36 | 1.51 |
| 2 | B | 1313 | TRP | CZ2-CH2 | -6.20 | 1.25 | 1.37 |
| 3 | E | 283 | CYS | CB-SG | -6.03 | 1.72 | 1.82 |
| 2 | D | 1550 | VAL | CB-CG2 | -5.99 | 1.40 | 1.52 |
| 1 | C | 66 | LYS | CD-CE | -5.96 | 1.36 | 1.51 |
| 3 | F | 213 | TRP | CB-CG | -5.96 | 1.39 | 1.50 |
| 2 | B | 1303 | ARG | CB-CG | -5.89 | 1.36 | 1.52 |
| 2 | D | 1554 | LEU | CG-CD1 | -5.81 | 1.30 | 1.51 |
| 2 | D | 1036 | LYS | CD-CE | -5.81 | 1.36 | 1.51 |
| 2 | B | 960 | GLU | CB-CG | -5.78 | 1.41 | 1.52 |
| 2 | B | 1511 | CYS | CB-SG | 5.67 | 1.91 | 1.82 |
| 2 | B | 1035 | GLU | CG-CD | -5.54 | 1.43 | 1.51 |
| 1 | A | 464 | GLU | CD-OE2 | -5.44 | 1.19 | 1.25 |
| 2 | B | 1580 | GLN | CG-CD | -5.40 | 1.38 | 1.51 |
| 1 | C | 547 | VAL | CB-CG1 | -5.35 | 1.41 | 1.52 |
| 1 | C | 594 | VAL | CB-CG2 | -5.34 | 1.41 | 1.52 |
| 2 | B | 1292 | LEU | CA-CB | 5.34 | 1.66 | 1.53 |
| 2 | B | 1313 | TRP | CB-CG | -5.31 | 1.40 | 1.50 |
| 2 | D | 813 | LYS | CB-CG | -5.24 | 1.38 | 1.52 |
| 3 | E | 253 | CYS | CB-SG | -5.24 | 1.73 | 1.81 |
| 2 | B | 1035 | GLU | CB-CG | -5.23 | 1.42 | 1.52 |
| 2 | B | 960 | GLU | CG-CD | -5.19 | 1.44 | 1.51 |
| 2 | D | 913 | LYS | CE-NZ | -5.15 | 1.36 | 1.49 |
| 2 | B | 1111 | LYS | CD-CE | -5.13 | 1.38 | 1.51 |
| 2 | B | 1580 | GLN | CB-CG | -5.08 | 1.38 | 1.52 |
| 2 | B | 1591 | ARG | CB-CG | -5.04 | 1.39 | 1.52 |

All (163) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 2 | D | 1554 | LEU | CB-CG-CD1 | -12.82 | 89.20 | 111.00 |
| 1 | A | 83 | MET | CG-SD-CE | -12.34 | 80.46 | 100.20 |
| 2 | D | 1649 | LEU | CB-CG-CD2 | -12.30 | 90.09 | 111.00 |
| 2 | B | 1292 | LEU | CA-CB-CG | 12.19 | 143.33 | 115.30 |
| 2 | B | 1300 | LEU | CB-CG-CD1 | -11.78 | 90.98 | 111.00 |
| 2 | B | 1292 | LEU | CB-CG-CD1 | 11.53 | 130.60 | 111.00 |
| 2 | B | 1292 | LEU | CD1-CG-CD2 | -10.99 | 77.54 | 110.50 |
| 2 | B | 1303 | ARG | NE-CZ-NH1 | -10.85 | 114.88 | 120.30 |
| 1 | A | 364 | PHE | CB-CG-CD2 | -10.77 | 113.26 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 3 | E | 143 | LEU | CB-CG-CD1 | -10.53 | 93.09 | 111.00 |
| 2 | D | 1554 | LEU | CB-CG-CD2 | 10.50 | 128.85 | 111.00 |
| 1 | A | 364 | PHE | CB-CG-CD1 | 10.08 | 127.86 | 120.80 |
| 3 | E | 146 | LEU | CA-CB-CG | 9.91 | 138.09 | 115.30 |
| 2 | D | 1639 | ASP | CB-CG-OD2 | -9.82 | 109.46 | 118.30 |
| 3 | E | 143 | LEU | CB-CG-CD2 | 9.57 | 127.27 | 111.00 |
| 2 | D | 796 | LYS | CD-CE-NZ | -9.48 | 89.89 | 111.70 |
| 2 | D | 813 | LYS | CD-CE-NZ | -9.42 | 90.04 | 111.70 |
| 1 | C | 94 | ARG | NE-CZ-NH2 | -9.37 | 115.61 | 120.30 |
| 3 | E | 143 | LEU | CA-CB-CG | 9.28 | 136.65 | 115.30 |
| 3 | E | 246 | ARG | NE-CZ-NH1 | 9.16 | 124.88 | 120.30 |
| 2 | B | 1076 | THR | CA-CB-CG2 | -9.16 | 99.58 | 112.40 |
| 1 | C | 229 | LEU | CA-CB-CG | 9.14 | 136.33 | 115.30 |
| 2 | B | 1291 | GLU | N-CA-C | -9.06 | 86.53 | 111.00 |
| 2 | D | 1037 | PHE | CB-CG-CD2 | -8.85 | 114.60 | 120.80 |
| 2 | B | 1300 | LEU | CB-CG-CD2 | 8.80 | 125.97 | 111.00 |
| 2 | D | 1037 | PHE | CB-CG-CD1 | 8.75 | 126.92 | 120.80 |
| 2 | B | 867 | LEU | CB-CG-CD2 | -8.72 | 96.18 | 111.00 |
| 2 | D | 1148 | LEU | CA-CB-CG | 8.63 | 135.15 | 115.30 |
| 2 | D | 813 | LYS | CB-CG-CD | -8.57 | 89.31 | 111.60 |
| 1 | A | 83 | MET | CA-CB-CG | -8.56 | 98.75 | 113.30 |
| 2 | D | 1243 | LEU | CB-CG-CD2 | -8.39 | 96.73 | 111.00 |
| 2 | B | 981 | LEU | CB-CG-CD1 | -8.34 | 96.83 | 111.00 |
| 3 | F | 181 | LEU | CA-CB-CG | -8.17 | 96.51 | 115.30 |
| 1 | C | 67 | LEU | CB-CG-CD1 | -8.11 | 97.22 | 111.00 |
| 2 | B | 1646 | CYS | CA-CB-SG | 8.05 | 128.49 | 114.00 |
| 2 | B | 1497 | LYS | CD-CE-NZ | -7.96 | 93.40 | 111.70 |
| 2 | B | 1092 | LEU | CB-CG-CD2 | -7.94 | 97.50 | 111.00 |
| 2 | D | 1508 | ASP | CB-CG-OD1 | 7.87 | 125.38 | 118.30 |
| 2 | D | 1511 | CYS | CA-CB-SG | 7.86 | 128.15 | 114.00 |
| 1 | C | 67 | LEU | CA-CB-CG | 7.82 | 133.28 | 115.30 |
| 2 | D | 841 | ARG | NE-CZ-NH1 | -7.72 | 116.44 | 120.30 |
| 3 | E | 130 | ARG | C-N-CD | -7.71 | 103.63 | 120.60 |
| 2 | B | 1202 | LEU | CA-CB-CG | 7.56 | 132.68 | 115.30 |
| 1 | C | 191 | LEU | CA-CB-CG | 7.49 | 132.53 | 115.30 |
| 2 | B | 1303 | ARG | CG-CD-NE | -7.49 | 96.08 | 111.80 |
| 2 | B | 1207 | LEU | CB-CG-CD1 | -7.46 | 98.31 | 111.00 |
| 3 | E | 205 | LEU | CA-CB-CG | 7.40 | 132.33 | 115.30 |
| 2 | D | 1505 | LEU | CA-CB-CG | -7.38 | 98.33 | 115.30 |
| 2 | B | 1294 | LEU | CA-CB-CG | 7.33 | 132.15 | 115.30 |
| 3 | F | 130 | ARG | C-N-CD | -7.32 | 104.50 | 120.60 |
| 1 | C | 146 | LEU | CB-CG-CD1 | -7.29 | 98.61 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | D | 761 | ILE | CG1-CB-CG2 | -7.07 | 95.85 | 111.40 |
| 1 | A | 76 | LEU | CA-CB-CG | 7.05 | 131.52 | 115.30 |
| 2 | B | 873 | CYS | CA-CB-SG | -7.02 | 101.36 | 114.00 |
| 2 | D | 894 | LEU | CA-CB-CG | -6.97 | 99.27 | 115.30 |
| 2 | D | 1582 | ARG | NE-CZ-NH1 | -6.96 | 116.82 | 120.30 |
| 2 | D | 1356 | LEU | CA-CB-CG | 6.92 | 131.22 | 115.30 |
| 1 | C | 465 | LEU | CB-CG-CD1 | -6.89 | 99.29 | 111.00 |
| 2 | B | 1292 | LEU | CB-CG-CD2 | 6.87 | 122.68 | 111.00 |
| 2 | B | 1143 | LEU | CB-CG-CD1 | 6.80 | 122.55 | 111.00 |
| 2 | B | 1506 | CYS | CA-CB-SG | 6.79 | 126.21 | 114.00 |
| 2 | B | 795 | LEU | CA-CB-CG | 6.78 | 130.90 | 115.30 |
| 3 | F | 246 | ARG | NE-CZ-NH1 | 6.75 | 123.67 | 120.30 |
| 3 | E | 276 | TRP | CA-CB-CG | -6.74 | 100.89 | 113.70 |
| 2 | D | 1176 | LEU | CB-CG-CD1 | 6.73 | 122.45 | 111.00 |
| 2 | D | 1342 | LEU | CA-CB-CG | 6.68 | 130.67 | 115.30 |
| 2 | B | 1010 | CYS | CA-CB-SG | 6.66 | 125.98 | 114.00 |
| 2 | B | 1407 | MET | CG-SD-CE | -6.64 | 89.58 | 100.20 |
| 3 | E | 136 | GLU | C-N-CD | -6.64 | 105.99 | 120.60 |
| 2 | D | 1519 | PHE | CB-CG-CD1 | -6.52 | 116.24 | 120.80 |
| 1 | C | 479 | MET | CG-SD-CE | -6.43 | 89.90 | 100.20 |
| 1 | C | 657 | ARG | CG-CD-NE | 6.35 | 125.14 | 111.80 |
| 2 | B | 1243 | LEU | CB-CG-CD2 | -6.34 | 100.21 | 111.00 |
| 2 | D | 1436 | LYS | CD-CE-NZ | -6.31 | 97.20 | 111.70 |
| 2 | D | 1554 | LEU | CD1-CG-CD2 | -6.29 | 91.64 | 110.50 |
| 1 | C | 574 | GLN | C-N-CD | 6.28 | 141.58 | 128.40 |
| 2 | B | 1607 | LEU | CA-CB-CG | 6.26 | 129.69 | 115.30 |
| 3 | E | 170 | ARG | NE-CZ-NH1 | 6.16 | 123.38 | 120.30 |
| 2 | D | 1175 | PHE | CB-CG-CD1 | -6.15 | 116.49 | 120.80 |
| 1 | A | 471 | LEU | CA-CB-CG | 6.15 | 129.44 | 115.30 |
| 1 | C | 44 | LEU | CB-CG-CD2 | -6.13 | 100.58 | 111.00 |
| 3 | F | 269 | VAL | CG1-CB-CG2 | 6.11 | 120.67 | 110.90 |
| 2 | D | 795 | LEU | CA-CB-CG | 6.07 | 129.26 | 115.30 |
| 2 | B | 967 | LEU | CB-CG-CD2 | 6.05 | 121.28 | 111.00 |
| 2 | B | 1238 | LEU | CB-CG-CD1 | -6.03 | 100.74 | 111.00 |
| 2 | B | 1637 | CYS | CA-CB-SG | 6.03 | 124.85 | 114.00 |
| 1 | C | 30 | THR | C-N-CD | 5.99 | 140.97 | 128.40 |
| 2 | D | 1107 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 2 | B | 913 | LYS | CD-CE-NZ | -5.94 | 98.03 | 111.70 |
| 1 | C | 304 | ARG | CG-CD-NE | -5.92 | 99.36 | 111.80 |
| 2 | D | 1298 | LEU | CB-CG-CD1 | -5.89 | 100.99 | 111.00 |
| 2 | D | 1202 | LEU | CA-CB-CG | 5.89 | 128.84 | 115.30 |
| 1 | A | 264 | LYS | CD-CE-NZ | -5.86 | 98.23 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | D | 1065 | ALA | N-CA-C | -5.84 | 95.22 | 111.00 |
| 2 | B | 996 | ASP | CB-CG-OD1 | 5.83 | 123.54 | 118.30 |
| 2 | B | 867 | LEU | CB-CG-CD1 | 5.82 | 120.89 | 111.00 |
| 3 | E | 172 | GLY | N-CA-C | -5.79 | 98.61 | 113.10 |
| 2 | D | 1258 | GLU | CA-CB-CG | 5.79 | 126.15 | 113.40 |
| 1 | C | 302 | LEU | CA-CB-CG | 5.78 | 128.59 | 115.30 |
| 2 | B | 754 | ASP | CB-CG-OD1 | 5.78 | 123.50 | 118.30 |
| 1 | C | 207 | ARG | NE-CZ-NH1 | -5.77 | 117.41 | 120.30 |
| 2 | B | 1632 | PRO | CA-C-O | -5.76 | 106.39 | 120.20 |
| 2 | B | 1144 | THR | CA-CB-CG2 | -5.75 | 104.35 | 112.40 |
| 2 | B | 1015 | MET | CA-CB-CG | 5.75 | 123.07 | 113.30 |
| 2 | D | 1060 | ARG | CA-CB-CG | 5.75 | 126.04 | 113.40 |
| 2 | B | 1158 | CYS | CA-CB-SG | 5.71 | 124.28 | 114.00 |
| 1 | C | 273 | PHE | CB-CG-CD2 | -5.70 | 116.81 | 120.80 |
| 2 | B | 1287 | PRO | N-CA-CB | 5.70 | 110.13 | 103.30 |
| 1 | A | 26 | TYR | CB-CG-CD1 | 5.63 | 124.38 | 121.00 |
| 2 | D | 778 | LEU | CB-CG-CD2 | -5.60 | 101.49 | 111.00 |
| 2 | D | 1497 | LYS | CD-CE-NZ | 5.55 | 124.47 | 111.70 |
| 1 | C | 489 | TYR | CB-CG-CD2 | -5.55 | 117.67 | 121.00 |
| 2 | B | 1100 | LEU | CB-CG-CD2 | -5.53 | 101.61 | 111.00 |
| 1 | A | 161 | ARG | NE-CZ-NH1 | -5.52 | 117.54 | 120.30 |
| 1 | A | 122 | LEU | CA-CB-CG | 5.52 | 128.00 | 115.30 |
| 2 | B | 1610 | ASP | CB-CG-OD1 | -5.52 | 113.33 | 118.30 |
| 2 | B | 1176 | LEU | CB-CG-CD1 | 5.51 | 120.37 | 111.00 |
| 2 | B | 1119 | GLN | CA-C-N | 5.50 | 129.31 | 117.20 |
| 1 | A | 48 | ASP | CB-CG-OD2 | 5.49 | 123.24 | 118.30 |
| 3 | F | 136 | GLU | C-N-CD | -5.48 | 108.54 | 120.60 |
| 2 | B | 1549 | LEU | CB-CG-CD1 | 5.48 | 120.31 | 111.00 |
| 2 | D | 1240 | LEU | CB-CG-CD2 | -5.47 | 101.70 | 111.00 |
| 2 | D | 1092 | LEU | CA-CB-CG | -5.46 | 102.75 | 115.30 |
| 1 | A | 505 | ARG | NE-CZ-NH2 | 5.45 | 123.03 | 120.30 |
| 2 | B | 1300 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | C | 94 | ARG | CD-NE-CZ | 5.42 | 131.19 | 123.60 |
| 2 | B | 1139 | LYS | CD-CE-NZ | -5.40 | 99.27 | 111.70 |
| 1 | C | 559 | CYS | N-CA-C | -5.39 | 96.45 | 111.00 |
| 2 | B | 1535 | LYS | CB-CG-CD | 5.38 | 125.60 | 111.60 |
| 2 | B | 1171 | LYS | CA-CB-CG | 5.38 | 125.23 | 113.40 |
| 1 | C | 207 | ARG | CB-CG-CD | -5.38 | 97.62 | 111.60 |
| 2 | D | 1106 | TRP | CA-CB-CG | -5.37 | 103.50 | 113.70 |
| 3 | F | 139 | LEU | CB-CG-CD2 | -5.36 | 101.89 | 111.00 |
| 2 | D | 1039 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 1 | A | 514 | LEU | CA-CB-CG | 5.33 | 127.57 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | D | 1497 | LYS | CA-CB-CG | 5.33 | 125.12 | 113.40 |
| 2 | B | 1046 | LEU | CA-CB-CG | 5.31 | 127.51 | 115.30 |
| 3 | F | 134 | ARG | CG-CD-NE | -5.30 | 100.67 | 111.80 |
| 2 | B | 1580 | GLN | CA-CB-CG | -5.22 | 101.92 | 113.40 |
| 3 | F | 239 | GLU | CG-CD-OE1 | 5.22 | 128.73 | 118.30 |
| 2 | D | 813 | LYS | N-CA-CB | -5.18 | 101.27 | 110.60 |
| 2 | B | 929 | LEU | CA-CB-CG | 5.17 | 127.20 | 115.30 |
| 2 | D | 764 | ARG | NE-CZ-NH1 | -5.17 | 117.71 | 120.30 |
| 3 | F | 204 | CYS | CA-CB-SG | 5.17 | 123.30 | 114.00 |
| 3 | F | 241 | ASP | CB-CG-OD2 | 5.15 | 122.94 | 118.30 |
| 2 | B | 1078 | LEU | CB-CG-CD1 | -5.15 | 102.24 | 111.00 |
| 2 | D | 1328 | GLU | CA-CB-CG | 5.15 | 124.73 | 113.40 |
| 1 | A | 48 | ASP | CB-CG-OD1 | -5.15 | 113.67 | 118.30 |
| 2 | D | 979 | ARG | CG-CD-NE | -5.14 | 101.01 | 111.80 |
| 3 | F | 241 | ASP | CB-CG-OD1 | -5.13 | 113.68 | 118.30 |
| 1 | A | 339 | VAL | CG1-CB-CG2 | -5.13 | 102.69 | 110.90 |
| 1 | C | 94 | ARG | NE-CZ-NH1 | 5.13 | 122.86 | 120.30 |
| 2 | B | 1535 | LYS | CD-CE-NZ | 5.12 | 123.47 | 111.70 |
| 2 | D | 1078 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 1 | A | 26 | TYR | CB-CG-CD2 | -5.10 | 117.94 | 121.00 |
| 2 | B | 1519 | PHE | CB-CG-CD2 | -5.08 | 117.24 | 120.80 |
| 2 | D | 1648 | ASP | CB-CG-OD1 | 5.07 | 122.87 | 118.30 |
| 2 | B | 1292 | LEU | N-CA-C | -5.06 | 97.34 | 111.00 |
| 2 | D | 1425 | VAL | CG1-CB-CG2 | 5.05 | 118.98 | 110.90 |
| 2 | B | 1077 | TRP | CA-CB-CG | -5.03 | 104.14 | 113.70 |
| 2 | D | 947 | LEU | CB-CG-CD1 | -5.03 | 102.46 | 111.00 |
| 2 | D | 1615 | LYS | C-N-CD | 5.02 | 138.95 | 128.40 |
| 2 | D | 1591 | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 183 | GLN | Mainchain |
| 1 | A | 622 | LYS | Mainchain |
| 2 | B | 1292 | LEU | Mainchain |
| 2 | B | 1311 | ILE | Mainchain |
| 2 | B | 1632 | PRO | Mainchain |
| 2 | B | 841 | ARG | Mainchain |
| 2 | D | 1063 | SER | Mainchain |
| 2 | D | 1414 | ASP | Mainchain |
| 2 | D | 1507 | ARG | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | D | 949 | PRO | Mainchain |
| 3 | F | 232 | ASP | Mainchain |
| 3 | F | 240 | ARG | Mainchain |

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 | 5002 | 0 | 5058 | 352 | 2 |
| 1 | C | 5002 | 0 | 5058 | 343 | 1 |
| 2 | B | 7177 | 0 | 7086 | 567 | 2 |
| 2 | D | 7164 | 0 | 7066 | 667 | 1 |
| 3 | E | 1465 | 0 | 1389 | 153 | 1 |
| 3 | F | 1465 | 0 | 1389 | 142 | 0 |
| All | All | 27275 | 0 | 27046 | 2109 | 4 |

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 39.

All (2109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:67:LEU:CG | 1:C:67:LEU:CD2 | 1.78 | 1.61 |
| 1:C:32:ASN:HD21 | 1:C:657:ARG:HD3 | 1.11 | 1.16 |
| 1:A:466:ARG:HG3 | 1:A:556:LYS:HD3 | 1.28 | 1.15 |
| 2:D:978:THR:HG22 | 2:D:1346:THR:HG22 | 1.31 | 1.10 |
| 3:F:157:PHE:O | 3:F:159:LYS:NZ | 1.84 | 1.09 |
| 3:F:135:ARG:HH21 | 3:F:141:PRO:HD3 | 0.92 | 1.07 |
| 2:D:1559:ASP:OD1 | 2:D:1591:ARG:NH2 | 1.87 | 1.07 |
| 2:B:1300:LEU:HD11 | 2:B:1303:ARG:HG2 | 1.33 | 1.06 |
| 2:D:758:GLU:HA | 2:D:913:LYS:HZ3 | 1.21 | 1.04 |
| 3:E:246:ARG:NH1 | 3:E:246:ARG:O | 1.87 | 1.04 |
| 2:D:947:LEU:HD11 | 2:D:1342:LEU:HB3 | 1.38 | 1.04 |
| 3:F:135:ARG:NH2 | 3:F:141:PRO:HD3 | 1.73 | 1.03 |
| 2:B:1076:THR:HG21 | 2:B:1111:LYS:HE2 | 1.09 | 1.03 |
| 1:C:62:PHE:O | 1:C:104:LYS:NZ | 1.92 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1140:ASP:O | 2:D:1144:THR:OG1 | 1.78 | 1.02 |
| 2:B:1015:MET:SD | 2:B:1056:GLN:NE2 | 2.34 | 1.01 |
| 2:D:766:GLU:HB3 | 2:D:796:LYS:HZ1 | 1.26 | 1.00 |
| 2:B:945:ARG:NH1 | 2:B:960:GLU:OE2 | 1.94 | 1.00 |
| 1:C:508:ARG:NH1 | 1:C:512:GLN:O | 1.93 | 1.00 |
| 1:A:44:LEU:HD11 | 1:A:86:VAL:HG22 | 1.42 | 1.00 |
| 2:B:1202:LEU:HD13 | 2:B:1207:LEU:HD11 | 1.42 | 1.00 |
| 2:B:1517:ASN:ND2 | 2:B:1521:GLN:OE1 | 1.95 | 1.00 |
| 1:C:94:ARG:HE | 1:C:94:ARG:HA | 1.26 | 0.99 |
| 3:E:246:ARG:C | 3:E:246:ARG:HH11 | 1.66 | 0.98 |
| 2:B:1202:LEU:HD11 | 2:B:1243:LEU:HD21 | 1.46 | 0.97 |
| 2:B:971:VAL:HG22 | 2:B:1351:LYS:HD2 | 1.42 | 0.97 |
| 1:C:560:VAL:HG22 | 2:D:813:LYS:HZ1 | 1.26 | 0.97 |
| 1:A:406:VAL:HG11 | 1:A:462:ARG:HH11 | 1.30 | 0.96 |
| 1:C:578:GLY:H | 2:D:795:LEU:HD11 | 1.29 | 0.96 |
| 3:E:239:GLU:O | 3:E:240:ARG:NH1 | 1.98 | 0.96 |
| 3:F:180:ILE:HD11 | 3:F:213:TRP:CZ2 | 2.00 | 0.96 |
| 1:C:28:ILE:HD11 | 1:C:42:MET:HG3 | 1.46 | 0.96 |
| 1:C:138:ILE:HG22 | 1:C:223:GLU:HB3 | 1.45 | 0.95 |
| 2:B:1129:MET:O | 2:B:1270:GLN:NE2 | 1.98 | 0.95 |
| 2:D:1577:GLN:H | 2:D:1580:GLN:HE21 | 1.02 | 0.95 |
| 2:D:1105:LYS:HG2 | 2:D:1106:TRP:CD1 | 2.01 | 0.95 |
| 2:D:810:SER:HB3 | 2:D:813:LYS:HB3 | 1.47 | 0.94 |
| 1:A:181:SER:HB3 | 3:E:246:ARG:HE | 1.30 | 0.94 |
| 2:B:1635:ASP:HA | 2:B:1638:GLN:HE22 | 1.31 | 0.94 |
| 1:C:508:ARG:HG3 | 1:C:508:ARG:HH11 | 1.32 | 0.93 |
| 2:D:1369:PRO:HA | 2:D:1384:MET:HG2 | 1.50 | 0.93 |
| 1:A:406:VAL:HG11 | 1:A:462:ARG:NH1 | 1.83 | 0.93 |
| 1:C:496:ASN:HB3 | 1:C:501:LEU:HG | 1.47 | 0.93 |
| 1:C:32:ASN:ND2 | 1:C:657:ARG:HD3 | 1.81 | 0.93 |
| 2:B:1013:GLU:O | 2:B:1016:ILE:HG13 | 1.68 | 0.93 |
| 2:B:1076:THR:HG21 | 2:B:1111:LYS:CE | 1.99 | 0.92 |
| 2:B:1610:ASP:N | 2:B:1610:ASP:OD1 | 1.99 | 0.92 |
| 2:D:1506:CYS:SG | 2:D:1511:CYS:HB2 | 2.10 | 0.92 |
| 2:D:1149:ILE:HD13 | 2:D:1194:TYR:HE2 | 1.33 | 0.92 |
| 1:C:523:THR:HB | 1:C:560:VAL:HG23 | 1.52 | 0.91 |
| 2:D:757:ALA:O | 2:D:913:LYS:NZ | 2.04 | 0.91 |
| 2:B:1366:THR:OG1 | 2:B:1387:GLU:OE2 | 1.89 | 0.90 |
| 2:D:1101:CYS:SG | 2:D:1161:GLN:NE2 | 2.44 | 0.90 |
| 2:D:1202:LEU:HD11 | 2:D:1243:LEU:HD21 | 1.53 | 0.90 |
| 2:B:951:ARG:HH21 | 2:B:1339:GLN:HG3 | 1.33 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1298:LEU:O | 2:B:1303:ARG:NH2 | 2.04 | 0.90 |
| 2:D:1258:GLU:HA | 2:D:1260:ARG:NH1 | 1.87 | 0.90 |
| 1:C:66:LYS:NZ | 3:E:145:CYS:O | 2.05 | 0.89 |
| 2:D:1202:LEU:HD13 | 2:D:1207:LEU:HD13 | 1.54 | 0.89 |
| 3:E:260:ILE:HD12 | 3:E:284:ARG:HD3 | 1.55 | 0.89 |
| 2:D:1105:LYS:HE3 | 2:D:1106:TRP:HE1 | 1.36 | 0.89 |
| 1:C:349:VAL:HG12 | 1:C:351:SER:H | 1.38 | 0.88 |
| 2:B:1512:ARG:NH1 | 2:B:1609:SER:O | 2.05 | 0.88 |
| 2:B:1554:LEU:HD13 | 2:B:1591:ARG:HH12 | 1.37 | 0.88 |
| 1:A:418:LYS:HD2 | 1:A:419:PRO:HD2 | 1.54 | 0.88 |
| 3:E:170:ARG:HG3 | 3:E:170:ARG:HH11 | 1.38 | 0.88 |
| 1:C:207:ARG:NH1 | 1:C:219:SER:OG | 2.05 | 0.88 |
| 2:B:841:ARG:NH1 | 2:B:902:PRO:O | 2.06 | 0.87 |
| 1:C:98:SER:O | 1:C:101:GLY:N | 2.08 | 0.87 |
| 3:F:135:ARG:HH21 | 3:F:141:PRO:CD | 1.83 | 0.87 |
| 2:B:1295:ASP:OD1 | 2:B:1310:ARG:NE | 2.07 | 0.87 |
| 1:C:50:GLN:HE21 | 1:C:51:GLY:H | 1.16 | 0.86 |
| 2:D:1033:GLN:HB3 | 2:D:1036:LYS:NZ | 1.90 | 0.86 |
| 2:D:1298:LEU:HB3 | 2:D:1332:VAL:HG22 | 1.55 | 0.86 |
| 2:B:1136:ASN:HA | 2:B:1139:LYS:HZ1 | 1.41 | 0.86 |
| 1:C:93:ASN:OD1 | 1:C:94:ARG:N | 2.08 | 0.86 |
| 1:A:568:GLY:O | 3:F:271:ASN:ND2 | 2.07 | 0.86 |
| 3:E:135:ARG:NH2 | 3:E:137:PRO:HA | 1.90 | 0.86 |
| 1:C:69:LEU:HD21 | 1:C:91:PRO:HD2 | 1.58 | 0.86 |
| 2:D:856:GLN:HA | 2:D:891:LYS:HE2 | 1.58 | 0.86 |
| 1:A:103:ASN:ND2 | 2:B:1035:GLU:OE2 | 2.08 | 0.85 |
| 2:B:1300:LEU:CD1 | 2:B:1303:ARG:HG2 | 2.06 | 0.85 |
| 2:D:867:LEU:HD11 | 2:D:913:LYS:HE2 | 1.57 | 0.85 |
| 2:D:764:ARG:NH1 | 2:D:923:ASP:OD1 | 2.09 | 0.85 |
| 2:B:1060:ARG:NH2 | 2:B:1064:SER:OG | 2.10 | 0.84 |
| 2:D:1152:GLN:NE2 | 2:D:1198:GLN:OE1 | 2.11 | 0.83 |
| 2:D:755:ILE:HG21 | 2:D:863:ARG:HD3 | 1.58 | 0.83 |
| 1:A:264:LYS:HB3 | 1:A:296:GLY:HA3 | 1.61 | 0.83 |
| 3:F:233:ASN:ND2 | 3:F:283:CYS:O | 2.11 | 0.83 |
| 1:C:594:VAL:HG13 | 2:D:807:VAL:HG13 | 1.58 | 0.83 |
| 2:D:832:ASP:OD2 | 2:D:834:ARG:NH2 | 2.12 | 0.83 |
| 1:A:181:SER:CB | 3:E:246:ARG:HH21 | 1.91 | 0.83 |
| 2:D:1106:TRP:CD1 | 2:D:1106:TRP:N | 2.44 | 0.83 |
| 2:D:883:GLN:OE1 | 2:D:883:GLN:N | 2.12 | 0.83 |
| 1:A:229:LEU:O | 2:B:834:ARG:NH2 | 2.10 | 0.83 |
| 2:D:1577:GLN:OE1 | 2:D:1580:GLN:NE2 | 2.12 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1190:ALA:HA | 2:D:1220:TRP:HZ3 | 1.42 | 0.82 |
| 2:B:985:THR:OG1 | 2:B:1339:GLN:O | 1.96 | 0.82 |
| 3:F:135:ARG:NH2 | 3:F:139:LEU:O | 2.12 | 0.82 |
| 1:A:349:VAL:HG12 | 1:A:351:SER:H | 1.42 | 0.82 |
| 2:B:1635:ASP:HA | 2:B:1638:GLN:NE2 | 1.95 | 0.82 |
| 1:C:560:VAL:HG22 | 2:D:813:LYS:NZ | 1.93 | 0.82 |
| 1:A:134:THR:HG1 | 1:A:139:TYR:HH | 1.26 | 0.82 |
| 3:E:146:LEU:HG | 3:E:150:LYS:HB2 | 1.61 | 0.82 |
| 2:D:1492:PHE:H | 2:D:1492:PHE:HD1 | 1.24 | 0.82 |
| 2:D:755:ILE:HG22 | 2:D:756:ILE:H | 1.44 | 0.81 |
| 2:B:865:GLU:OE1 | 2:B:883:GLN:NE2 | 2.13 | 0.81 |
| 2:B:862:VAL:HG12 | 2:B:916:VAL:HG12 | 1.61 | 0.81 |
| 2:B:1118:PHE:H | 2:B:1144:THR:HG22 | 1.45 | 0.81 |
| 2:D:1105:LYS:HG2 | 2:D:1106:TRP:HD1 | 1.42 | 0.81 |
| 2:D:871:ALA:O | 2:D:903:LEU:N | 2.13 | 0.81 |
| 1:C:423:THR:HG23 | 1:C:440:THR:HG22 | 1.61 | 0.81 |
| 2:D:1106:TRP:N | 2:D:1106:TRP:HD1 | 1.77 | 0.81 |
| 3:E:223:ILE:HD11 | 3:E:269:VAL:HG22 | 1.63 | 0.81 |
| 2:B:1572:GLY:O | 2:B:1574:ASP:N | 2.13 | 0.81 |
| 1:C:535:TYR:CZ | 1:C:547:VAL:HG11 | 2.15 | 0.81 |
| 2:B:1311:ILE:O | 2:B:1313:TRP:HZ3 | 1.64 | 0.81 |
| 2:D:826:MET:HG2 | 2:D:827:GLN:H | 1.46 | 0.81 |
| 1:C:385:TYR:CE1 | 1:C:386:ARG:HG3 | 2.15 | 0.80 |
| 2:D:759:GLU:HG2 | 2:D:760:ASN:H | 1.45 | 0.80 |
| 3:E:109:LEU:HB2 | 3:E:114:ILE:HG12 | 1.63 | 0.80 |
| 1:C:264:LYS:HB3 | 1:C:296:GLY:HA3 | 1.64 | 0.80 |
| 2:B:983:GLN:OE1 | 2:B:983:GLN:N | 2.15 | 0.80 |
| 2:D:1158:CYS:HA | 2:D:1161:GLN:NE2 | 1.95 | 0.80 |
| 2:D:978:THR:OG1 | 2:D:1324:THR:HG23 | 1.82 | 0.80 |
| 3:F:136:GLU:HB2 | 3:F:159:LYS:CE | 2.12 | 0.79 |
| 2:D:766:GLU:HB3 | 2:D:796:LYS:NZ | 1.95 | 0.79 |
| 2:B:1300:LEU:HD23 | 2:B:1324:THR:HG21 | 1.64 | 0.79 |
| 1:C:168:GLU:HG3 | 1:C:205:LYS:HB3 | 1.62 | 0.79 |
| 2:D:1550:VAL:HG21 | 2:D:1581:GLN:NE2 | 1.96 | 0.79 |
| 2:B:1313:TRP:N | 2:B:1313:TRP:CE3 | 2.50 | 0.79 |
| 1:A:486:LYS:HZ3 | 1:A:538:ILE:HG12 | 1.48 | 0.79 |
| 2:D:1397:ASP:HB3 | 2:D:1450:LYS:HE2 | 1.64 | 0.79 |
| 2:D:1505:LEU:HD13 | 2:D:1585:ILE:HD11 | 1.65 | 0.79 |
| 3:F:136:GLU:HB2 | 3:F:159:LYS:HE2 | 1.63 | 0.78 |
| 3:F:223:ILE:HD13 | 3:F:272:ASP:HA | 1.65 | 0.78 |
| 3:F:224:TYR:CE1 | 3:F:242:HIS:HB3 | 2.17 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:391:VAL:HG21 | 1:A:411:ILE:HD11 | 1.63 | 0.78 |
| 1:A:486:LYS:NZ | 1:A:538:ILE:HG12 | 1.97 | 0.78 |
| 3:E:225:CYS:HB3 | 3:E:276:TRP:CZ2 | 2.19 | 0.78 |
| 2:D:1517:ASN:HD21 | 2:D:1521:GLN:HB2 | 1.49 | 0.78 |
| 2:D:1577:GLN:H | 2:D:1580:GLN:NE2 | 1.79 | 0.78 |
| 2:B:1303:ARG:HH12 | 2:B:1306:LYS:HA | 1.48 | 0.78 |
| 2:B:980:ILE:HD11 | 2:B:1322:GLU:HB2 | 1.63 | 0.78 |
| 1:A:496:ASN:HD22 | 1:A:501:LEU:HD22 | 1.47 | 0.78 |
| 1:C:205:LYS:HE2 | 1:C:207:ARG:HD3 | 1.65 | 0.78 |
| 2:D:962:ILE:HG13 | 2:D:1330:PHE:O | 1.82 | 0.78 |
| 2:D:1506:CYS:CB | 2:D:1511:CYS:HB2 | 2.13 | 0.78 |
| 2:D:756:ILE:HD13 | 2:D:761:ILE:HG13 | 1.64 | 0.78 |
| 2:B:1240:LEU:HD13 | 2:B:1249:VAL:HG22 | 1.66 | 0.77 |
| 1:C:207:ARG:HH11 | 1:C:219:SER:HG | 1.32 | 0.77 |
| 1:A:53:VAL:HB | 1:A:76:LEU:HD22 | 1.64 | 0.77 |
| 1:C:59:VAL:HG23 | 1:C:106:VAL:HG21 | 1.66 | 0.77 |
| 3:E:237:GLN:HB3 | 3:E:250:THR:HG23 | 1.65 | 0.77 |
| 2:B:1238:LEU:HD11 | 2:B:1277:GLN:HE21 | 1.47 | 0.77 |
| 1:C:578:GLY:H | 2:D:795:LEU:CD1 | 1.98 | 0.77 |
| 3:F:135:ARG:HG3 | 3:F:135:ARG:HH11 | 1.49 | 0.77 |
| 3:F:233:ASN:ND2 | 3:F:283:CYS:HB3 | 2.00 | 0.77 |
| 1:A:28:ILE:HG23 | 1:A:647:THR:OG1 | 1.85 | 0.77 |
| 2:B:1111:LYS:NZ | 2:B:1119:GLN:O | 2.16 | 0.77 |
| 1:C:578:GLY:N | 2:D:795:LEU:HD11 | 2.00 | 0.77 |
| 1:C:28:ILE:HD11 | 1:C:42:MET:CG | 2.15 | 0.77 |
| 2:B:1146:PHE:O | 2:B:1149:ILE:HG13 | 1.85 | 0.77 |
| 2:B:763:SER:HB2 | 2:B:926:ARG:HB2 | 1.67 | 0.77 |
| 3:E:240:ARG:HB2 | 3:E:243:TYR:CZ | 2.20 | 0.77 |
| 2:B:1303:ARG:HH12 | 2:B:1306:LYS:CA | 1.98 | 0.76 |
| 2:D:1104:VAL:HG13 | 2:D:1151:LEU:HD11 | 1.66 | 0.76 |
| 1:C:496:ASN:OD1 | 1:C:497:LYS:HG3 | 1.85 | 0.76 |
| 1:A:286:GLU:HG3 | 1:A:306:VAL:HG23 | 1.65 | 0.76 |
| 1:A:558:SER:O | 1:A:617:TRP:NE1 | 2.17 | 0.76 |
| 2:B:1014:ASN:HB2 | 2:B:1055:GLN:NE2 | 1.99 | 0.76 |
| 1:C:312:GLN:OE1 | 1:C:312:GLN:N | 2.17 | 0.76 |
| 1:C:576:VAL:N | 1:C:579:GLN:OE1 | 2.17 | 0.76 |
| 1:C:66:LYS:HG2 | 3:E:147:GLN:HG3 | 1.67 | 0.76 |
| 2:D:1551:LYS:HE3 | 2:D:1562:ILE:CD1 | 2.16 | 0.76 |
| 2:D:1300:LEU:HD12 | 2:D:1303:ARG:H | 1.49 | 0.76 |
| 1:A:230:PRO:HG3 | 1:A:604:VAL:HG11 | 1.67 | 0.76 |
| 1:C:291:ILE:HD13 | 1:C:300:VAL:HB | 1.66 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1233:THR:HG21 | 2:B:1256:LEU:HD11 | 1.67 | 0.76 |
| 1:C:290:ARG:NH1 | 2:D:1400:MET:SD | 2.59 | 0.76 |
| 1:C:535:TYR:CE1 | 1:C:547:VAL:HG11 | 2.21 | 0.76 |
| 1:C:136:LYS:NZ | 1:C:138:ILE:O | 2.17 | 0.76 |
| 2:B:1494:HIS:HD2 | 2:B:1495:PRO:HD2 | 1.50 | 0.75 |
| 2:D:1145:ALA:HA | 2:D:1148:LEU:HG | 1.67 | 0.75 |
| 2:B:1303:ARG:NH1 | 2:B:1307:ILE:HG12 | 2.01 | 0.75 |
| 1:C:67:LEU:HD13 | 3:E:144:THR:HG21 | 1.67 | 0.75 |
| 2:B:967:LEU:HD22 | 2:B:1348:TYR:CD2 | 2.21 | 0.75 |
| 2:B:1303:ARG:NH1 | 2:B:1305:SER:O | 2.20 | 0.75 |
| 1:C:331:ILE:HG12 | 1:C:338:MET:HB3 | 1.66 | 0.75 |
| 1:A:45:GLU:OE2 | 1:A:83:MET:HE1 | 1.87 | 0.75 |
| 1:C:214:PRO:HB2 | 2:D:1316:ALA:HB3 | 1.68 | 0.75 |
| 1:A:471:LEU:HB3 | 1:A:521:ILE:HD11 | 1.68 | 0.75 |
| 2:D:1355:GLN:N | 2:D:1356:LEU:HB3 | 2.02 | 0.75 |
| 3:E:141:PRO:HA | 3:E:157:PHE:CD2 | 2.22 | 0.75 |
| 1:A:291:ILE:HD13 | 1:A:300:VAL:HB | 1.68 | 0.74 |
| 1:A:44:LEU:HD23 | 1:A:55:VAL:HG21 | 1.69 | 0.74 |
| 1:C:67:LEU:HD12 | 1:C:68:VAL:H | 1.52 | 0.74 |
| 1:A:181:SER:HB3 | 3:E:246:ARG:NE | 2.01 | 0.74 |
| 1:C:69:LEU:HD21 | 1:C:90:ILE:HA | 1.69 | 0.74 |
| 1:A:364:PHE:HE2 | 1:A:366:PRO:HA | 1.52 | 0.74 |
| 1:C:496:ASN:ND2 | 1:C:524:ASP:O | 2.20 | 0.74 |
| 2:D:1597:GLU:HG3 | 2:D:1600:LYS:HG3 | 1.67 | 0.74 |
| 1:A:136:LYS:NZ | 1:A:138:ILE:O | 2.20 | 0.74 |
| 2:B:1311:ILE:O | 2:B:1313:TRP:CZ3 | 2.41 | 0.74 |
| 1:C:473:VAL:HG13 | 1:C:517:LEU:HB3 | 1.70 | 0.74 |
| 1:C:69:LEU:CD2 | 1:C:90:ILE:HA | 2.18 | 0.74 |
| 1:A:650:SER:OG | 1:A:652:GLN:NE2 | 2.20 | 0.74 |
| 2:B:1292:LEU:HD22 | 2:B:1338:GLY:HA2 | 1.70 | 0.74 |
| 2:D:1107:LEU:HD11 | 2:D:1147:VAL:HG13 | 1.69 | 0.73 |
| 1:C:67:LEU:HG | 1:C:67:LEU:CD2 | 2.12 | 0.73 |
| 2:D:1284:LYS:NZ | 2:D:1285:ASP:OD1 | 2.20 | 0.73 |
| 3:F:239:GLU:CD | 3:F:240:ARG:H | 1.92 | 0.73 |
| 2:B:1136:ASN:HD22 | 2:B:1139:LYS:NZ | 1.87 | 0.73 |
| 2:B:763:SER:OG | 2:B:911:GLU:OE2 | 2.06 | 0.73 |
| 2:D:1436:LYS:NZ | 2:D:1439:SER:O | 2.21 | 0.73 |
| 2:D:1631:TRP:CD1 | 2:D:1649:LEU:HD21 | 2.22 | 0.73 |
| 1:A:111:THR:HG22 | 1:A:116:VAL:HG23 | 1.70 | 0.73 |
| 2:B:1019:THR:HG1 | 2:B:1081:TYR:HH | 1.34 | 0.73 |
| 1:A:181:SER:HB3 | 3:E:246:ARG:HH21 | 1.54 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1313:TRP:HE3 | 2:B:1313:TRP:N | 1.84 | 0.73 |
| 2:B:935:GLY:HA3 | 2:B:1349:HIS:ND1 | 2.04 | 0.73 |
| 1:C:508:ARG:NH1 | 1:C:508:ARG:HG3 | 2.03 | 0.73 |
| 1:A:37:GLU:OE2 | 1:A:161:ARG:NH1 | 2.22 | 0.73 |
| 2:D:1255:TRP:HA | 2:D:1258:GLU:OE2 | 1.89 | 0.73 |
| 2:B:1240:LEU:CD1 | 2:B:1249:VAL:HG22 | 2.19 | 0.72 |
| 1:A:36:LEU:HD12 | 1:A:37:GLU:HG2 | 1.70 | 0.72 |
| 2:B:1507:ARG:HB2 | 2:B:1612:TRP:CZ2 | 2.24 | 0.72 |
| 3:F:157:PHE:C | 3:F:159:LYS:NZ | 2.43 | 0.72 |
| 1:A:449:VAL:HG21 | 1:A:545:GLU:HG3 | 1.71 | 0.72 |
| 1:A:466:ARG:CG | 1:A:556:LYS:HD3 | 2.14 | 0.72 |
| 3:E:135:ARG:HH22 | 3:E:137:PRO:HA | 1.54 | 0.72 |
| 1:A:36:LEU:HD21 | 1:A:125:LEU:HA | 1.72 | 0.72 |
| 1:A:530:ARG:NH1 | 1:A:624:ASP:OD2 | 2.21 | 0.72 |
| 2:B:1111:LYS:HE3 | 2:B:1119:GLN:O | 1.89 | 0.72 |
| 2:D:1197:ALA:HB2 | 2:D:1202:LEU:HD21 | 1.72 | 0.72 |
| 1:A:313:ASN:OD1 | 1:A:315:ARG:N | 2.22 | 0.72 |
| 1:A:431:LEU:HD11 | 1:A:436:GLN:CD | 2.09 | 0.72 |
| 1:C:313:ASN:ND2 | 1:C:315:ARG:O | 2.23 | 0.72 |
| 1:C:94:ARG:CA | 1:C:94:ARG:HE | 2.02 | 0.72 |
| 1:C:93:ASN:ND2 | 1:C:95:GLU:OE1 | 2.21 | 0.72 |
| 2:D:1113:LYS:HB2 | 2:D:1117:VAL:HG22 | 1.72 | 0.72 |
| 3:F:195:LYS:HD2 | 3:F:196:LEU:H | 1.55 | 0.72 |
| 2:D:1551:LYS:HE3 | 2:D:1562:ILE:HD11 | 1.71 | 0.72 |
| 2:D:1633:GLU:HB2 | 2:D:1636:GLU:OE1 | 1.89 | 0.72 |
| 2:D:937:ARG:HH21 | 2:D:1349:HIS:HE1 | 1.37 | 0.72 |
| 1:C:561:GLY:HA3 | 2:D:813:LYS:HE2 | 1.72 | 0.72 |
| 2:D:1035:GLU:HA | 2:D:1039:LEU:CD1 | 2.19 | 0.72 |
| 2:D:1060:ARG:HD3 | 2:D:1066:PHE:CZ | 2.24 | 0.72 |
| 2:B:1497:LYS:HZ3 | 2:B:1502:LEU:HA | 1.54 | 0.72 |
| 2:D:1367:ILE:HD11 | 2:D:1386:LEU:HD13 | 1.71 | 0.72 |
| 2:D:1574:ASP:OD2 | 2:D:1620:TYR:OH | 2.05 | 0.72 |
| 1:A:25:MET:SD | 1:A:652:GLN:NE2 | 2.63 | 0.71 |
| 1:A:423:THR:HG22 | 1:A:440:THR:HG23 | 1.71 | 0.71 |
| 2:D:1303:ARG:NH2 | 3:F:239:GLU:OE1 | 2.22 | 0.71 |
| 3:E:195:LYS:HE3 | 3:E:197:PHE:HE1 | 1.55 | 0.71 |
| 3:E:273:GLU:HG3 | 3:E:275:GLU:OE2 | 1.90 | 0.71 |
| 3:F:113:TYR:HA | 3:F:116:GLN:HG2 | 1.72 | 0.71 |
| 1:A:122:LEU:HD11 | 1:A:657:ARG:HB3 | 1.72 | 0.71 |
| 2:B:1298:LEU:HB3 | 2:B:1332:VAL:HG22 | 1.72 | 0.71 |
| 2:B:958:GLN:NE2 | 2:B:1334:ALA:HB3 | 2.05 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1405:ILE:HG12 | 2:D:1477:VAL:HG22 | 1.72 | 0.71 |
| 2:B:1249:VAL:HB | 2:B:1250:PRO:HD3 | 1.72 | 0.71 |
| 2:D:1149:ILE:HD13 | 2:D:1194:TYR:CE2 | 2.23 | 0.71 |
| 2:B:1554:LEU:HD13 | 2:B:1591:ARG:NH1 | 2.05 | 0.71 |
| 2:B:780:GLU:N | 2:B:780:GLU:OE1 | 2.24 | 0.71 |
| 2:D:1161:GLN:N | 2:D:1161:GLN:OE1 | 2.23 | 0.71 |
| 3:E:224:TYR:CD2 | 3:E:242:HIS:HB3 | 2.25 | 0.71 |
| 2:D:1512:ARG:CZ | 2:D:1621:ILE:HD13 | 2.21 | 0.71 |
| 2:B:1117:VAL:HA | 2:B:1144:THR:HG21 | 1.73 | 0.71 |
| 2:B:1174:ASP:HA | 2:B:1201:ARG:HH22 | 1.55 | 0.71 |
| 2:B:1544:VAL:HG22 | 2:B:1569:ILE:HB | 1.73 | 0.71 |
| 3:E:146:LEU:HD13 | 3:E:148:ASN:H | 1.56 | 0.71 |
| 2:D:1249:VAL:CG2 | 2:D:1250:PRO:HD3 | 2.19 | 0.71 |
| 1:A:652:GLN:N | 1:A:652:GLN:OE1 | 2.22 | 0.71 |
| 2:B:1140:ASP:O | 2:B:1144:THR:OG1 | 2.07 | 0.71 |
| 2:B:873:CYS:HB3 | 2:B:901:VAL:HG13 | 1.72 | 0.71 |
| 3:E:170:ARG:CG | 3:E:170:ARG:HH11 | 2.02 | 0.71 |
| 3:E:226:PRO:N | 3:E:276:TRP:HH2 | 1.89 | 0.71 |
| 1:A:26:TYR:HE2 | 1:A:53:VAL:HG11 | 1.55 | 0.70 |
| 2:B:1101:CYS:O | 2:B:1105:LYS:HG3 | 1.91 | 0.70 |
| 2:D:1067:ALA:HB2 | 2:D:1074:PRO:HA | 1.72 | 0.70 |
| 2:D:1003:LEU:HD11 | 2:D:1276:PHE:HE2 | 1.56 | 0.70 |
| 2:D:1574:ASP:OD2 | 2:D:1582:ARG:NH1 | 2.24 | 0.70 |
| 2:B:964:PRO:HB3 | 2:B:1327:ASN:OD1 | 1.90 | 0.70 |
| 1:C:29:ILE:HA | 1:C:645:THR:O | 1.90 | 0.70 |
| 2:D:1507:ARG:HE | 2:D:1510:LEU:HD23 | 1.56 | 0.70 |
| 3:F:246:ARG:CG | 3:F:246:ARG:HH11 | 2.03 | 0.70 |
| 1:C:659:GLU:OE1 | 1:C:659:GLU:N | 2.24 | 0.70 |
| 2:D:1311:ILE:HD11 | 2:D:1318:LEU:HD23 | 1.71 | 0.70 |
| 2:D:758:GLU:HA | 2:D:913:LYS:NZ | 2.04 | 0.70 |
| 2:D:934:GLU:N | 2:D:934:GLU:OE1 | 2.22 | 0.70 |
| 3:E:133:TYR:HB3 | 3:E:158:CYS:HB3 | 1.72 | 0.70 |
| 2:B:1111:LYS:CE | 2:B:1119:GLN:O | 2.40 | 0.70 |
| 1:C:99:GLU:CB | 1:C:102:ARG:HB2 | 2.22 | 0.70 |
| 2:D:1498:GLU:C | 2:D:1500:GLY:H | 1.94 | 0.70 |
| 1:A:481:ARG:HA | 1:A:484:GLU:OE1 | 1.92 | 0.70 |
| 2:B:1118:PHE:H | 2:B:1144:THR:CG2 | 2.04 | 0.70 |
| 1:C:390:ALA:HB2 | 1:C:398:GLN:OE1 | 1.90 | 0.69 |
| 2:D:1485:LEU:HD12 | 2:D:1486:GLU:H | 1.56 | 0.69 |
| 2:D:776:GLU:HG3 | 2:D:791:MET:SD | 2.31 | 0.69 |
| 2:D:935:GLY:HA2 | 2:D:1353:LYS:H | 1.56 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:446:TYR:HE1 | 1:A:634:ASP:HA | 1.57 | 0.69 |
| 1:C:458:LEU:HD11 | 1:C:533:ALA:HB3 | 1.73 | 0.69 |
| 2:D:1149:ILE:HA | 2:D:1152:GLN:NE2 | 2.07 | 0.69 |
| 2:D:987:VAL:HG22 | 2:D:988:ALA:H | 1.57 | 0.69 |
| 2:D:1151:LEU:HG | 2:D:1165:LEU:HD11 | 1.74 | 0.69 |
| 2:D:904:LYS:O | 2:D:908:GLN:NE2 | 2.24 | 0.69 |
| 2:B:1078:LEU:HD11 | 2:B:1124:VAL:HG23 | 1.75 | 0.69 |
| 2:D:1544:VAL:HG23 | 2:D:1570:LYS:HD3 | 1.74 | 0.69 |
| 2:D:768:PRO:HD3 | 2:D:796:LYS:HZ2 | 1.56 | 0.69 |
| 2:B:938:MET:HB3 | 2:B:940:LYS:HZ2 | 1.57 | 0.69 |
| 1:A:125:LEU:HD22 | 1:A:215:GLN:HE22 | 1.56 | 0.69 |
| 1:A:647:THR:HG22 | 1:A:653:GLN:OE1 | 1.93 | 0.69 |
| 2:B:990:MET:O | 2:B:1282:TYR:OH | 2.11 | 0.69 |
| 1:C:183:GLN:N | 1:C:183:GLN:OE1 | 2.21 | 0.69 |
| 1:A:141:PRO:HA | 1:A:195:ILE:HD12 | 1.75 | 0.69 |
| 2:B:1050:LYS:O | 2:B:1054:THR:HG23 | 1.92 | 0.69 |
| 2:B:1387:GLU:OE1 | 2:B:1387:GLU:N | 2.25 | 0.69 |
| 2:B:1472:ILE:HD11 | 2:B:1494:HIS:NE2 | 2.08 | 0.69 |
| 3:E:143:LEU:HD12 | 3:E:143:LEU:C | 2.13 | 0.69 |
| 2:B:800:THR:OG1 | 2:B:801:THR:N | 2.25 | 0.69 |
| 1:A:647:THR:HG22 | 1:A:653:GLN:NE2 | 2.07 | 0.69 |
| 2:D:1496:GLU:OE1 | 2:D:1496:GLU:N | 2.23 | 0.69 |
| 2:D:948:ASP:OD2 | 2:D:951:ARG:NH1 | 2.26 | 0.69 |
| 2:B:1396:GLN:C | 2:B:1453:HIS:HD2 | 1.97 | 0.69 |
| 1:A:83:MET:HE2 | 1:A:505:ARG:HH11 | 1.57 | 0.69 |
| 2:B:1202:LEU:CD1 | 2:B:1243:LEU:HD21 | 2.22 | 0.69 |
| 2:B:1300:LEU:HD12 | 2:B:1300:LEU:O | 1.92 | 0.69 |
| 2:D:1552:VAL:HG12 | 2:D:1561:TYR:CD1 | 2.28 | 0.69 |
| 2:B:1202:LEU:HA | 2:B:1206:LEU:HD11 | 1.74 | 0.68 |
| 1:C:646:PHE:H | 1:C:654:THR:CG2 | 2.05 | 0.68 |
| 2:D:1105:LYS:HE3 | 2:D:1106:TRP:NE1 | 2.08 | 0.68 |
| 1:A:476:LEU:HD13 | 1:A:514:LEU:HD12 | 1.75 | 0.68 |
| 1:C:201:MET:HE1 | 1:C:226:GLU:H | 1.55 | 0.68 |
| 2:D:1631:TRP:HD1 | 2:D:1649:LEU:HD21 | 1.56 | 0.68 |
| 3:E:106:SER:OG | 3:E:156:GLU:HG2 | 1.92 | 0.68 |
| 1:A:181:SER:HB2 | 3:E:246:ARG:HH21 | 1.58 | 0.68 |
| 3:F:246:ARG:HG2 | 3:F:246:ARG:HH11 | 1.58 | 0.68 |
| 1:A:494:ILE:HD13 | 1:A:531:LEU:HD13 | 1.74 | 0.68 |
| 2:B:1641:GLU:N | 2:B:1641:GLU:OE1 | 2.27 | 0.68 |
| 1:A:471:LEU:CD1 | 1:A:519:LEU:HB3 | 2.23 | 0.68 |
| 2:B:1067:ALA:HB2 | 2:B:1074:PRO:HA | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1544:VAL:HG13 | 2:B:1570:LYS:HB3 | 1.73 | 0.68 |
| 2:B:877:THR:HG23 | 2:B:879:LYS:H | 1.57 | 0.68 |
| 1:A:215:GLN:HG2 | 1:A:216:GLN:N | 2.07 | 0.68 |
| 2:D:1128:GLU:CD | 2:D:1267:GLY:HA3 | 2.14 | 0.68 |
| 2:D:1066:PHE:HB2 | 2:D:1078:LEU:HD11 | 1.76 | 0.68 |
| 2:B:1076:THR:CG2 | 2:B:1111:LYS:HE2 | 2.04 | 0.68 |
| 2:B:1126:HIS:O | 2:B:1129:MET:HG2 | 1.92 | 0.68 |
| 2:B:1299:GLN:HA | 2:B:1303:ARG:NH2 | 2.09 | 0.68 |
| 2:B:1640:GLU:O | 2:B:1643:GLN:HG2 | 1.93 | 0.68 |
| 2:B:913:LYS:HD2 | 2:B:923:ASP:O | 1.94 | 0.68 |
| 1:C:246:TYR:OH | 1:C:317:GLU:OE2 | 2.08 | 0.68 |
| 2:B:1105:LYS:HG2 | 2:B:1162:VAL:HG22 | 1.75 | 0.68 |
| 2:B:1494:HIS:ND1 | 2:B:1497:LYS:HB3 | 2.09 | 0.68 |
| 2:D:949:PRO:O | 2:D:950:GLU:HB2 | 1.94 | 0.68 |
| 2:B:1174:ASP:OD1 | 2:B:1175:PHE:N | 2.27 | 0.68 |
| 2:D:1035:GLU:HA | 2:D:1039:LEU:HD12 | 1.76 | 0.68 |
| 1:A:234:VAL:HG13 | 1:A:341:ALA:HB2 | 1.75 | 0.68 |
| 2:B:1554:LEU:HD12 | 2:B:1555:SER:N | 2.09 | 0.68 |
| 2:B:1586:SER:HB2 | 2:B:1622:ILE:HG12 | 1.76 | 0.68 |
| 1:C:94:ARG:NE | 1:C:94:ARG:HA | 2.04 | 0.67 |
| 2:D:1148:LEU:HD12 | 2:D:1149:ILE:N | 2.09 | 0.67 |
| 2:D:855:ARG:HG2 | 2:D:858:GLN:HB3 | 1.76 | 0.67 |
| 1:A:130:LEU:HD11 | 1:A:151:THR:HG22 | 1.75 | 0.67 |
| 1:C:231:SER:HB3 | 2:D:834:ARG:NH2 | 2.09 | 0.67 |
| 3:F:136:GLU:HB2 | 3:F:159:LYS:NZ | 2.09 | 0.67 |
| 1:C:98:SER:O | 1:C:100:LYS:HA | 1.95 | 0.67 |
| 2:D:1435:ASP:OD1 | 2:D:1435:ASP:N | 2.25 | 0.67 |
| 3:E:276:TRP:N | 3:E:276:TRP:CE3 | 2.62 | 0.67 |
| 2:D:1417:ASP:O | 2:D:1421:LEU:HG | 1.94 | 0.67 |
| 2:D:1492:PHE:N | 2:D:1492:PHE:HD1 | 1.92 | 0.67 |
| 2:D:979:ARG:NH1 | 2:D:1323:GLU:OE2 | 2.26 | 0.67 |
| 2:B:1263:GLY:HA3 | 2:B:1272:THR:HG22 | 1.77 | 0.67 |
| 2:D:1574:ASP:CG | 2:D:1582:ARG:HH12 | 1.98 | 0.67 |
| 1:A:464:GLU:HB3 | 1:A:556:LYS:HE3 | 1.75 | 0.67 |
| 1:A:471:LEU:CD1 | 1:A:473:VAL:HG23 | 2.25 | 0.67 |
| 2:B:1650:GLY:O | 2:B:1653:THR:HG22 | 1.94 | 0.67 |
| 2:B:991:THR:HG22 | 2:B:1282:TYR:HE2 | 1.59 | 0.67 |
| 2:D:1436:LYS:HB3 | 2:D:1441:ARG:HE | 1.60 | 0.67 |
| 1:A:566:LYS:HE3 | 1:A:584:LYS:HD2 | 1.75 | 0.67 |
| 1:A:193:TRP:CZ3 | 1:A:195:ILE:HG22 | 2.30 | 0.67 |
| 1:C:138:ILE:HD11 | 1:C:602:VAL:HG13 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1659:PHE:HZ | 2:D:1662:PRO:HA | 1.60 | 0.67 |
| 2:D:983:GLN:HB3 | 2:D:1341:THR:OG1 | 1.95 | 0.67 |
| 1:A:141:PRO:HA | 1:A:195:ILE:CD1 | 2.26 | 0.66 |
| 3:E:229:PRO:HG2 | 3:E:280:PRO:HG2 | 1.75 | 0.66 |
| 3:F:107:ALA:HB2 | 3:F:158:CYS:SG | 2.35 | 0.66 |
| 2:B:1202:LEU:CD1 | 2:B:1207:LEU:HD11 | 2.24 | 0.66 |
| 2:D:906:GLY:O | 2:D:931:VAL:HG22 | 1.95 | 0.66 |
| 3:F:186:ILE:HG13 | 3:F:188:PHE:HE1 | 1.60 | 0.66 |
| 2:D:1118:PHE:H | 2:D:1144:THR:HG23 | 1.60 | 0.66 |
| 2:B:1149:ILE:HA | 2:B:1152:GLN:HE22 | 1.61 | 0.66 |
| 2:D:1311:ILE:HD13 | 2:D:1320:ARG:HH21 | 1.61 | 0.66 |
| 2:D:872:PHE:HD1 | 2:D:902:PRO:HA | 1.60 | 0.66 |
| 2:B:867:LEU:HD21 | 2:B:911:GLU:HB3 | 1.78 | 0.66 |
| 1:C:201:MET:CE | 1:C:225:LYS:HA | 2.25 | 0.66 |
| 2:B:1010:CYS:HA | 2:B:1059:PHE:CZ | 2.30 | 0.66 |
| 2:B:1172:ALA:O | 2:B:1176:LEU:HD13 | 1.95 | 0.66 |
| 2:B:1357:THR:HA | 2:B:1359:ASN:N | 2.10 | 0.66 |
| 1:C:397:VAL:CG1 | 1:C:409:LEU:HD22 | 2.25 | 0.66 |
| 1:C:479:MET:HE1 | 1:C:487:ILE:CD1 | 2.26 | 0.66 |
| 2:D:1225:LYS:HE3 | 2:D:1227:LEU:HD11 | 1.78 | 0.66 |
| 2:D:886:VAL:HG21 | 2:D:894:LEU:HD23 | 1.78 | 0.66 |
| 1:C:168:GLU:CG | 1:C:205:LYS:HB3 | 2.25 | 0.66 |
| 1:C:59:VAL:HG23 | 1:C:106:VAL:CG2 | 2.26 | 0.66 |
| 1:C:97:LYS:HG2 | 2:D:1314:GLU:HB3 | 1.78 | 0.66 |
| 1:A:471:LEU:HD11 | 1:A:519:LEU:HB3 | 1.76 | 0.65 |
| 1:C:29:ILE:HB | 1:C:43:VAL:CG1 | 2.26 | 0.65 |
| 2:D:1077:TRP:CZ2 | 2:D:1130:ILE:HA | 2.31 | 0.65 |
| 2:D:1498:GLU:O | 2:D:1500:GLY:N | 2.29 | 0.65 |
| 1:A:376:VAL:HG13 | 1:A:384:ALA:HB3 | 1.78 | 0.65 |
| 2:D:985:THR:CG2 | 2:D:987:VAL:HG12 | 2.26 | 0.65 |
| 2:D:1508:ASP:CG | 2:D:1509:GLU:H | 1.98 | 0.65 |
| 2:D:1550:VAL:HG21 | 2:D:1581:GLN:HE22 | 1.62 | 0.65 |
| 1:A:129:TYR:HA | 1:A:218:PHE:HE2 | 1.61 | 0.65 |
| 2:B:1203:LYS:HA | 2:B:1207:LEU:HD22 | 1.78 | 0.65 |
| 2:B:1652:PHE:CE1 | 2:B:1656:MET:HE3 | 2.30 | 0.65 |
| 1:C:245:ILE:H | 1:C:245:ILE:HD12 | 1.61 | 0.65 |
| 1:C:488:ARG:NH1 | 1:C:508:ARG:O | 2.29 | 0.65 |
| 1:C:573:ARG:HE | 1:C:579:GLN:NE2 | 1.94 | 0.65 |
| 2:D:1033:GLN:HB3 | 2:D:1036:LYS:HZ2 | 1.61 | 0.65 |
| 2:D:1215:LYS:O | 2:D:1216:ASP:OD1 | 2.14 | 0.65 |
| 2:D:1363:LEU:HD21 | 2:D:1477:VAL:HG12 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1604:MET:HA | 2:B:1627:TRP:O | 1.97 | 0.65 |
| 1:C:177:GLN:O | 3:F:240:ARG:NH2 | 2.29 | 0.65 |
| 1:C:205:LYS:HE3 | 1:C:219:SER:HB3 | 1.77 | 0.65 |
| 1:A:140:THR:HG23 | 1:A:227:TYR:CE2 | 2.32 | 0.65 |
| 1:C:404:ASP:OD1 | 1:C:406:VAL:HG12 | 1.96 | 0.65 |
| 2:D:934:GLU:HG2 | 2:D:1352:ALA:C | 2.17 | 0.65 |
| 2:B:1060:ARG:HG3 | 2:B:1060:ARG:HH11 | 1.62 | 0.65 |
| 2:B:1525:ASP:N | 2:B:1525:ASP:OD1 | 2.17 | 0.65 |
| 2:D:1506:CYS:SG | 2:D:1511:CYS:CB | 2.84 | 0.65 |
| 3:E:205:LEU:HD12 | 3:E:212:GLN:O | 1.97 | 0.65 |
| 3:F:246:ARG:CB | 3:F:246:ARG:HH11 | 2.09 | 0.65 |
| 1:A:313:ASN:ND2 | 1:A:318:ASP:OD2 | 2.29 | 0.65 |
| 2:D:1102:GLY:O | 2:D:1106:TRP:CD1 | 2.50 | 0.65 |
| 2:D:755:ILE:HG22 | 2:D:756:ILE:N | 2.11 | 0.65 |
| 2:D:950:GLU:N | 2:D:953:GLY:O | 2.27 | 0.64 |
| 2:D:756:ILE:HB | 3:F:134:ARG:HH22 | 1.62 | 0.64 |
| 3:F:272:ASP:N | 3:F:272:ASP:OD1 | 2.30 | 0.64 |
| 1:A:196:PRO:HD2 | 1:A:199:VAL:HG21 | 1.78 | 0.64 |
| 1:A:446:TYR:CE1 | 1:A:634:ASP:HA | 2.32 | 0.64 |
| 1:A:93:ASN:OD1 | 1:A:94:ARG:N | 2.31 | 0.64 |
| 2:B:937:ARG:NH1 | 2:B:1347:MET:HE1 | 2.12 | 0.64 |
| 2:B:1607:LEU:HD23 | 2:B:1608:SER:H | 1.60 | 0.64 |
| 1:C:487:ILE:O | 1:C:508:ARG:HD3 | 1.98 | 0.64 |
| 2:D:1326:GLU:OE1 | 2:D:1328:GLU:HB2 | 1.98 | 0.64 |
| 3:E:110:LYS:HD3 | 3:E:128:GLU:HB3 | 1.78 | 0.64 |
| 3:F:135:ARG:HG3 | 3:F:135:ARG:NH1 | 2.12 | 0.64 |
| 1:A:35:ARG:HD3 | 1:A:154:HIS:NE2 | 2.11 | 0.64 |
| 2:B:1066:PHE:CE1 | 2:B:1082:VAL:HG11 | 2.32 | 0.64 |
| 1:A:166:ASN:HD21 | 1:A:174:PRO:HG3 | 1.62 | 0.64 |
| 2:D:880:ARG:CZ | 2:D:1471:LEU:HG | 2.27 | 0.64 |
| 1:A:197:GLU:OE1 | 1:A:198:LEU:HD12 | 1.98 | 0.64 |
| 2:B:962:ILE:HG13 | 2:B:1330:PHE:O | 1.97 | 0.64 |
| 2:B:1356:LEU:HD13 | 2:B:1357:THR:H | 1.61 | 0.64 |
| 1:A:239:THR:OG1 | 1:A:252:GLU:HG2 | 1.98 | 0.64 |
| 1:A:274:GLY:HA3 | 1:A:325:TYR:CZ | 2.32 | 0.64 |
| 2:D:766:GLU:CB | 2:D:796:LYS:HZ1 | 2.08 | 0.64 |
| 2:D:905:THR:HA | 2:D:931:VAL:HG23 | 1.79 | 0.64 |
| 3:E:223:ILE:HG13 | 3:E:223:ILE:O | 1.98 | 0.64 |
| 1:C:625:ILE:HD12 | 1:C:643:GLY:HA3 | 1.80 | 0.64 |
| 2:B:1392:TYR:CD1 | 2:B:1398:ALA:HB2 | 2.32 | 0.64 |
| 2:B:938:MET:CB | 2:B:940:LYS:HZ2 | 2.11 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1249:VAL:HG22 | 2:D:1250:PRO:HD3 | 1.79 | 0.64 |
| 1:A:216:GLN:HE21 | 1:A:218:PHE:HE1 | 1.46 | 0.64 |
| 1:A:466:ARG:HG3 | 1:A:556:LYS:CD | 2.16 | 0.64 |
| 2:B:940:LYS:HD3 | 2:B:940:LYS:N | 2.13 | 0.64 |
| 2:B:991:THR:HG22 | 2:B:1282:TYR:CE2 | 2.34 | 0.64 |
| 1:C:207:ARG:NH1 | 1:C:219:SER:HG | 1.92 | 0.64 |
| 1:C:302:LEU:HD21 | 1:C:307:LEU:HB2 | 1.79 | 0.64 |
| 2:D:971:VAL:HG12 | 2:D:1349:HIS:HB2 | 1.80 | 0.64 |
| 2:D:1423:ASN:ND2 | 2:D:1423:ASN:O | 2.26 | 0.64 |
| 1:A:404:ASP:OD1 | 1:A:406:VAL:HG12 | 1.97 | 0.63 |
| 2:B:761:ILE:HD12 | 2:B:761:ILE:O | 1.97 | 0.63 |
| 2:D:1291:GLU:OE2 | 2:D:1337:LYS:HB3 | 1.99 | 0.63 |
| 2:D:1368:LYS:HB2 | 2:D:1385:ILE:HD11 | 1.80 | 0.63 |
| 2:B:1411:PHE:CZ | 2:B:1465:GLN:HB3 | 2.33 | 0.63 |
| 2:B:1516:GLU:OE1 | 2:B:1624:LYS:HG2 | 1.98 | 0.63 |
| 2:D:1552:VAL:HG12 | 2:D:1561:TYR:HD1 | 1.63 | 0.63 |
| 2:B:1405:ILE:HG12 | 2:B:1477:VAL:HG22 | 1.80 | 0.63 |
| 3:E:146:LEU:CD1 | 3:E:150:LYS:HB2 | 2.29 | 0.63 |
| 3:E:195:LYS:HE3 | 3:E:197:PHE:CE1 | 2.34 | 0.63 |
| 1:A:456:LEU:HB2 | 1:A:535:TYR:HE2 | 1.63 | 0.63 |
| 2:B:1188:THR:HA | 2:B:1191:ILE:HD11 | 1.80 | 0.63 |
| 2:D:1292:LEU:HB2 | 2:D:1313:TRP:HB2 | 1.79 | 0.63 |
| 1:C:205:LYS:CE | 1:C:219:SER:HB3 | 2.28 | 0.63 |
| 2:D:1604:MET:HA | 2:D:1627:TRP:O | 1.99 | 0.63 |
| 1:C:148:ARG:HG3 | 2:D:773:TRP:CZ2 | 2.33 | 0.63 |
| 1:A:83:MET:CE | 1:A:505:ARG:HH11 | 2.11 | 0.63 |
| 2:D:1066:PHE:CB | 2:D:1078:LEU:HD11 | 2.29 | 0.63 |
| 2:D:853:ASN:HD22 | 2:D:888:ILE:HG23 | 1.62 | 0.63 |
| 2:B:1503:ASN:ND2 | 2:B:1589:LYS:HE3 | 2.14 | 0.63 |
| 2:D:1148:LEU:O | 2:D:1152:GLN:HG2 | 1.99 | 0.63 |
| 3:F:121:VAL:HA | 3:F:145:CYS:SG | 2.39 | 0.63 |
| 3:F:222:GLU:OE2 | 3:F:224:TYR:OH | 2.13 | 0.63 |
| 1:C:600:LYS:NZ | 2:D:822:GLU:OE2 | 2.23 | 0.63 |
| 3:F:199:SER:OG | 3:F:201:SER:O | 2.15 | 0.63 |
| 1:C:69:LEU:HD21 | 1:C:91:PRO:CD | 2.28 | 0.62 |
| 2:D:763:SER:HB3 | 2:D:926:ARG:HB2 | 1.80 | 0.62 |
| 1:A:45:GLU:OE2 | 1:A:491:THR:HG21 | 1.98 | 0.62 |
| 2:B:1174:ASP:OD1 | 2:B:1175:PHE:CD2 | 2.53 | 0.62 |
| 2:B:1187:TYR:HD1 | 2:B:1232:ALA:HB2 | 1.65 | 0.62 |
| 2:B:761:ILE:HG21 | 2:B:913:LYS:HE3 | 1.81 | 0.62 |
| 2:D:1310:ARG:HD2 | 2:D:1312:HIS:NE2 | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:181:SER:CB | 3:E:246:ARG:NH2 | 2.63 | 0.62 |
| 3:F:259:MET:SD | 3:F:281:PRO:HB2 | 2.39 | 0.62 |
| 2:B:871:ALA:O | 2:B:903:LEU:N | 2.28 | 0.62 |
| 2:B:945:ARG:HD2 | 2:B:960:GLU:CD | 2.20 | 0.62 |
| 1:C:566:LYS:HB2 | 1:C:584:LYS:HE2 | 1.81 | 0.62 |
| 2:D:1108:ILE:HD11 | 2:D:1151:LEU:HD21 | 1.81 | 0.62 |
| 2:D:996:ASP:OD1 | 2:D:1036:LYS:HE2 | 1.98 | 0.62 |
| 2:B:1136:ASN:HA | 2:B:1139:LYS:NZ | 2.14 | 0.62 |
| 2:D:1089:ALA:HA | 2:D:1092:LEU:HD13 | 1.79 | 0.62 |
| 2:D:1313:TRP:CZ3 | 2:D:1318:LEU:HD11 | 2.34 | 0.62 |
| 2:D:1420:GLN:O | 2:D:1423:ASN:ND2 | 2.31 | 0.62 |
| 2:D:1528:THR:OG1 | 2:D:1529:LEU:N | 2.32 | 0.62 |
| 1:A:647:THR:HG22 | 1:A:653:GLN:CD | 2.20 | 0.62 |
| 2:D:1496:GLU:O | 2:D:1498:GLU:N | 2.32 | 0.62 |
| 2:D:1492:PHE:HE2 | 2:D:1500:GLY:O | 1.82 | 0.62 |
| 2:D:756:ILE:HD11 | 2:D:760:ASN:OD1 | 2.00 | 0.62 |
| 2:B:1436:LYS:O | 2:B:1441:ARG:NH2 | 2.33 | 0.62 |
| 2:B:1532:ARG:NH2 | 2:B:1629:GLU:OE2 | 2.31 | 0.62 |
| 2:D:957:VAL:HG21 | 2:D:1335:GLU:HA | 1.82 | 0.62 |
| 2:B:1082:VAL:O | 2:B:1086:PHE:HD1 | 1.82 | 0.62 |
| 1:C:120:VAL:O | 1:C:656:GLN:NE2 | 2.30 | 0.62 |
| 2:D:1291:GLU:OE2 | 2:D:1338:GLY:N | 2.33 | 0.62 |
| 2:D:1659:PHE:HE2 | 2:D:1662:PRO:HD3 | 1.63 | 0.62 |
| 3:E:163:CYS:HB2 | 3:E:180:ILE:O | 2.00 | 0.62 |
| 3:F:232:ASP:O | 3:F:233:ASN:OD1 | 2.18 | 0.62 |
| 2:B:1144:THR:O | 2:B:1148:LEU:HB2 | 1.98 | 0.62 |
| 2:B:1189:VAL:HG11 | 2:B:1213:THR:HG21 | 1.82 | 0.62 |
| 2:D:1210:PHE:CE1 | 2:D:1220:TRP:HH2 | 2.18 | 0.62 |
| 2:D:886:VAL:HG21 | 2:D:894:LEU:CD2 | 2.29 | 0.62 |
| 2:D:987:VAL:HG22 | 2:D:988:ALA:N | 2.15 | 0.62 |
| 3:E:141:PRO:HA | 3:E:157:PHE:HD2 | 1.63 | 0.62 |
| 3:E:145:CYS:HB2 | 3:E:151:TRP:CZ3 | 2.35 | 0.62 |
| 1:A:502:LYS:NZ | 1:A:503:ALA:O | 2.30 | 0.62 |
| 2:B:1312:HIS:C | 2:B:1313:TRP:CE3 | 2.73 | 0.62 |
| 1:C:146:LEU:HD13 | 2:D:773:TRP:CD2 | 2.34 | 0.62 |
| 2:D:800:THR:HG22 | 2:D:801:THR:H | 1.64 | 0.62 |
| 1:A:376:VAL:CG1 | 1:A:401:THR:HG21 | 2.30 | 0.61 |
| 2:B:1303:ARG:NH1 | 2:B:1306:LYS:HA | 2.13 | 0.61 |
| 2:B:1538:GLU:O | 2:B:1541:VAL:HG12 | 2.00 | 0.61 |
| 1:C:479:MET:HE1 | 1:C:487:ILE:HD11 | 1.82 | 0.61 |
| 3:E:130:ARG:NH1 | 3:E:130:ARG:HG3 | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:160:GLY:C | 1:A:161:ARG:HG2 | 2.19 | 0.61 |
| 2:B:945:ARG:HD2 | 2:B:960:GLU:OE1 | 1.99 | 0.61 |
| 2:D:985:THR:HG22 | 2:D:987:VAL:HG12 | 1.82 | 0.61 |
| 1:A:155:LYS:HG2 | 1:A:499:ARG:HE | 1.64 | 0.61 |
| 1:A:364:PHE:CE2 | 1:A:366:PRO:HA | 2.32 | 0.61 |
| 2:B:983:GLN:HG2 | 2:B:1341:THR:HB | 1.81 | 0.61 |
| 2:D:1214:ALA:HB2 | 2:D:1220:TRP:HE1 | 1.65 | 0.61 |
| 2:D:1643:GLN:HG3 | 2:D:1644:LYS:HD2 | 1.82 | 0.61 |
| 1:A:134:THR:OG1 | 1:A:139:TYR:OH | 2.07 | 0.61 |
| 1:A:317:GLU:H | 1:A:317:GLU:CD | 2.03 | 0.61 |
| 1:A:148:ARG:CZ | 1:A:594:VAL:HB | 2.30 | 0.61 |
| 2:D:1060:ARG:HH11 | 2:D:1060:ARG:HG3 | 1.65 | 0.61 |
| 1:A:167:ILE:HG12 | 1:A:176:LYS:HB3 | 1.83 | 0.61 |
| 2:B:1469:VAL:HG13 | 2:B:1472:ILE:HG22 | 1.81 | 0.61 |
| 2:D:1202:LEU:CD1 | 2:D:1243:LEU:HD21 | 2.27 | 0.61 |
| 2:D:937:ARG:HH21 | 2:D:1349:HIS:CE1 | 2.17 | 0.61 |
| 1:A:181:SER:HB3 | 3:E:246:ARG:NH2 | 2.14 | 0.61 |
| 2:B:1554:LEU:CD1 | 2:B:1591:ARG:HH12 | 2.11 | 0.61 |
| 1:C:449:VAL:HG21 | 1:C:545:GLU:HG3 | 1.83 | 0.61 |
| 1:C:646:PHE:H | 1:C:654:THR:HG21 | 1.65 | 0.61 |
| 2:D:1301:PRO:HD2 | 2:D:1328:GLU:OE2 | 2.01 | 0.61 |
| 2:D:756:ILE:HD12 | 3:F:134:ARG:HH22 | 1.65 | 0.61 |
| 1:A:647:THR:HG22 | 1:A:653:GLN:HE22 | 1.64 | 0.61 |
| 1:A:76:LEU:HG | 1:A:82:HIS:HA | 1.83 | 0.61 |
| 2:B:1548:ARG:HD2 | 2:B:1566:GLU:OE2 | 2.01 | 0.61 |
| 2:B:1643:GLN:HG3 | 2:B:1644:LYS:N | 2.16 | 0.61 |
| 2:B:780:GLU:OE2 | 2:B:789:LYS:HD3 | 2.00 | 0.61 |
| 1:C:487:ILE:H | 1:C:487:ILE:HD12 | 1.65 | 0.61 |
| 2:D:997:ALA:H | 2:D:1036:LYS:HE2 | 1.66 | 0.61 |
| 1:A:125:LEU:H | 1:A:125:LEU:CD1 | 2.12 | 0.61 |
| 1:A:622:LYS:HD2 | 1:A:622:LYS:O | 2.01 | 0.61 |
| 2:B:1496:GLU:HG2 | 2:B:1497:LYS:H | 1.65 | 0.61 |
| 1:C:135:ASP:HB3 | 1:C:146:LEU:HD11 | 1.82 | 0.61 |
| 2:D:1507:ARG:O | 2:D:1508:ASP:OD1 | 2.18 | 0.61 |
| 3:F:157:PHE:C | 3:F:159:LYS:HZ1 | 2.05 | 0.61 |
| 1:A:42:MET:HB3 | 1:A:86:VAL:HG23 | 1.83 | 0.60 |
| 2:B:1138:GLU:HG3 | 2:B:1188:THR:HG21 | 1.83 | 0.60 |
| 1:C:479:MET:HG3 | 1:C:480:ASP:OD1 | 2.01 | 0.60 |
| 2:B:1576:VAL:CA | 2:B:1580:GLN:HE22 | 2.15 | 0.60 |
| 1:A:591:ALA:HB2 | 2:B:810:SER:HB2 | 1.82 | 0.60 |
| 2:D:1131:GLY:O | 2:D:1228:TYR:HE1 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:67:LEU:CD1 | 1:C:67:LEU:CD2 | 2.71 | 0.60 |
| 3:E:146:LEU:CG | 3:E:150:LYS:HB2 | 2.30 | 0.60 |
| 2:D:1061:GLN:HG3 | 2:D:1062:PRO:HD2 | 1.83 | 0.60 |
| 2:D:1397:ASP:CB | 2:D:1450:LYS:HE2 | 2.32 | 0.60 |
| 2:D:759:GLU:HG2 | 2:D:760:ASN:N | 2.16 | 0.60 |
| 1:C:599:ASP:OD1 | 2:D:800:THR:HG21 | 2.01 | 0.60 |
| 3:F:109:LEU:HB2 | 3:F:114:ILE:HG12 | 1.81 | 0.60 |
| 2:B:1202:LEU:O | 2:B:1202:LEU:HD12 | 2.01 | 0.60 |
| 2:B:904:LYS:HG3 | 2:B:908:GLN:OE1 | 2.00 | 0.60 |
| 1:C:365:LYS:NZ | 1:C:457:HIS:HA | 2.16 | 0.60 |
| 1:C:477:LEU:HD11 | 1:C:479:MET:HE2 | 1.82 | 0.60 |
| 2:D:778:LEU:HG | 2:D:787:SER:HB3 | 1.82 | 0.60 |
| 1:A:364:PHE:CE1 | 1:A:420:LEU:HG | 2.36 | 0.60 |
| 2:D:1148:LEU:HD11 | 2:D:1195:ALA:HB1 | 1.83 | 0.60 |
| 2:D:1187:TYR:HD1 | 2:D:1232:ALA:HB2 | 1.67 | 0.60 |
| 2:D:1487:GLU:OE1 | 2:D:1487:GLU:N | 2.35 | 0.60 |
| 3:E:226:PRO:O | 3:E:276:TRP:CZ2 | 2.54 | 0.60 |
| 1:A:83:MET:HG3 | 1:A:505:ARG:HD2 | 1.81 | 0.60 |
| 2:B:1136:ASN:O | 2:B:1185:ARG:NH1 | 2.35 | 0.60 |
| 2:D:1013:GLU:O | 2:D:1016:ILE:HG22 | 2.01 | 0.60 |
| 1:A:36:LEU:CD2 | 1:A:125:LEU:HA | 2.31 | 0.60 |
| 1:A:133:GLN:HG3 | 1:A:133:GLN:O | 2.02 | 0.60 |
| 2:B:1382:ASN:OD1 | 2:B:1383:THR:N | 2.34 | 0.60 |
| 2:B:1543:TYR:HB2 | 2:B:1545:TYR:CZ | 2.36 | 0.60 |
| 2:B:872:PHE:CD1 | 2:B:902:PRO:HA | 2.37 | 0.60 |
| 2:D:947:LEU:HD12 | 2:D:947:LEU:N | 2.17 | 0.60 |
| 2:D:990:MET:N | 2:D:991:THR:HA | 2.17 | 0.60 |
| 2:B:1274:MET:SD | 2:B:1277:GLN:NE2 | 2.75 | 0.60 |
| 2:B:1303:ARG:HH12 | 2:B:1307:ILE:N | 1.99 | 0.60 |
| 2:B:1317:SER:OG | 2:B:1320:ARG:NH2 | 2.35 | 0.60 |
| 2:D:1217:LYS:HG3 | 2:D:1248:PHE:CE2 | 2.37 | 0.60 |
| 2:D:1241:LEU:HD21 | 2:D:1285:ASP:HB2 | 1.83 | 0.60 |
| 2:D:1610:ASP:HA | 2:D:1621:ILE:HD11 | 1.83 | 0.60 |
| 3:E:106:SER:O | 3:E:130:ARG:N | 2.30 | 0.60 |
| 3:F:233:ASN:ND2 | 3:F:257:PHE:CD2 | 2.69 | 0.60 |
| 2:B:1429:ILE:HD11 | 2:B:1433:GLU:HG3 | 1.83 | 0.60 |
| 2:D:1130:ILE:HD12 | 2:D:1133:LEU:HB2 | 1.84 | 0.60 |
| 2:D:1233:THR:HG22 | 2:D:1256:LEU:HD11 | 1.84 | 0.60 |
| 2:D:899:VAL:HG23 | 2:D:1473:GLN:HE21 | 1.67 | 0.60 |
| 2:D:1652:PHE:CZ | 2:D:1656:MET:HE2 | 2.36 | 0.60 |
| 2:D:987:VAL:CG2 | 2:D:988:ALA:H | 2.13 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:186:ILE:HD13 | 3:F:213:TRP:CH2 | 2.35 | 0.60 |
| 1:A:62:PHE:CE2 | 2:B:1039:LEU:HD11 | 2.36 | 0.59 |
| 1:C:465:LEU:CD1 | 1:C:555:VAL:HG22 | 2.32 | 0.59 |
| 1:C:558:SER:O | 1:C:617:TRP:NE1 | 2.26 | 0.59 |
| 2:D:1104:VAL:O | 2:D:1108:ILE:HG12 | 2.02 | 0.59 |
| 2:D:1128:GLU:OE2 | 2:D:1267:GLY:HA3 | 2.01 | 0.59 |
| 2:D:1600:LYS:HD2 | 2:D:1633:GLU:OE2 | 2.02 | 0.59 |
| 1:A:105:PHE:HE2 | 1:A:122:LEU:HG | 1.67 | 0.59 |
| 2:B:1078:LEU:HD21 | 2:B:1124:VAL:HG21 | 1.84 | 0.59 |
| 2:B:1171:LYS:O | 2:B:1174:ASP:OD1 | 2.20 | 0.59 |
| 2:B:1197:ALA:HA | 2:B:1202:LEU:HG | 1.83 | 0.59 |
| 2:B:1636:GLU:OE2 | 2:B:1642:ASN:ND2 | 2.35 | 0.59 |
| 2:B:872:PHE:HD1 | 2:B:902:PRO:HA | 1.66 | 0.59 |
| 1:C:484:GLU:OE1 | 1:C:484:GLU:N | 2.32 | 0.59 |
| 2:D:756:ILE:CG1 | 3:F:134:ARG:HH22 | 2.15 | 0.59 |
| 2:B:1240:LEU:HA | 2:B:1243:LEU:HB2 | 1.85 | 0.59 |
| 1:C:196:PRO:HD2 | 1:C:199:VAL:HG21 | 1.83 | 0.59 |
| 1:A:227:TYR:OH | 2:B:769:GLU:OE1 | 2.18 | 0.59 |
| 1:C:455:TYR:HB2 | 1:C:478:ARG:HB3 | 1.84 | 0.59 |
| 3:F:180:ILE:HD11 | 3:F:213:TRP:CH2 | 2.36 | 0.59 |
| 2:D:1185:ARG:O | 2:D:1189:VAL:HG22 | 2.02 | 0.59 |
| 2:D:1240:LEU:HD23 | 2:D:1249:VAL:HG12 | 1.83 | 0.59 |
| 2:D:1392:TYR:CD1 | 2:D:1398:ALA:HB2 | 2.37 | 0.59 |
| 1:A:611:LEU:HG | 2:B:817:VAL:HG21 | 1.83 | 0.59 |
| 2:B:1117:VAL:HG22 | 2:B:1144:THR:HG21 | 1.83 | 0.59 |
| 2:B:1214:ALA:HB2 | 2:B:1220:TRP:CE2 | 2.38 | 0.59 |
| 2:B:1607:LEU:CD2 | 2:B:1608:SER:H | 2.15 | 0.59 |
| 2:D:1128:GLU:OE1 | 2:D:1267:GLY:HA3 | 2.03 | 0.59 |
| 2:D:1149:ILE:CD1 | 2:D:1194:TYR:HE2 | 2.12 | 0.59 |
| 1:C:100:LYS:HD3 | 2:D:1313:TRP:CZ2 | 2.37 | 0.59 |
| 2:B:1007:PRO:HB2 | 2:B:1055:GLN:NE2 | 2.18 | 0.59 |
| 2:B:1075:SER:HB3 | 2:B:1078:LEU:HD12 | 1.84 | 0.59 |
| 2:B:982:LEU:HD21 | 2:B:1296:VAL:HG21 | 1.82 | 0.59 |
| 1:C:357:PHE:CE1 | 1:C:441:MET:HE1 | 2.38 | 0.59 |
| 2:D:1506:CYS:HB3 | 2:D:1511:CYS:HB2 | 1.82 | 0.59 |
| 2:D:761:ILE:HG22 | 2:D:762:VAL:N | 2.18 | 0.59 |
| 2:D:877:THR:HG23 | 2:D:879:LYS:H | 1.68 | 0.59 |
| 1:A:471:LEU:HD13 | 1:A:473:VAL:HG23 | 1.85 | 0.59 |
| 2:D:877:THR:OG1 | 2:D:878:THR:N | 2.34 | 0.59 |
| 2:D:1515:GLU:HA | 2:D:1589:LYS:NZ | 2.18 | 0.59 |
| 2:D:755:ILE:CG2 | 2:D:756:ILE:H | 2.15 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1582:ARG:HD2 | 2:B:1620:TYR:HE1 | 1.68 | 0.59 |
| 2:D:1397:ASP:OD1 | 2:D:1453:HIS:ND1 | 2.36 | 0.59 |
| 3:E:113:TYR:CD1 | 3:E:125:VAL:HG12 | 2.38 | 0.59 |
| 3:E:107:ALA:C | 3:E:130:ARG:NH1 | 2.55 | 0.59 |
| 3:E:171:ASN:ND2 | 3:E:194:TYR:CZ | 2.69 | 0.59 |
| 1:A:81:ASN:O | 1:A:82:HIS:CG | 2.56 | 0.58 |
| 2:D:1562:ILE:O | 2:D:1562:ILE:HG13 | 2.02 | 0.58 |
| 2:D:1148:LEU:HD11 | 2:D:1195:ALA:CB | 2.32 | 0.58 |
| 2:D:1253:VAL:HA | 2:D:1256:LEU:HD22 | 1.85 | 0.58 |
| 1:A:140:THR:O | 1:A:195:ILE:HD11 | 2.03 | 0.58 |
| 1:A:389:VAL:HG12 | 1:A:426:THR:HG22 | 1.85 | 0.58 |
| 2:B:1015:MET:HG2 | 2:B:1056:GLN:HE22 | 1.69 | 0.58 |
| 1:C:28:ILE:HD12 | 1:C:29:ILE:H | 1.68 | 0.58 |
| 1:C:449:VAL:O | 1:C:452:SER:OG | 2.22 | 0.58 |
| 2:D:1311:ILE:HD11 | 2:D:1318:LEU:HA | 1.85 | 0.58 |
| 1:A:628:THR:CG2 | 1:A:641:ASP:HB3 | 2.33 | 0.58 |
| 2:B:1130:ILE:HG13 | 2:B:1133:LEU:HB2 | 1.84 | 0.58 |
| 1:A:340:GLN:OE1 | 1:A:340:GLN:HA | 2.04 | 0.58 |
| 2:B:971:VAL:HB | 2:B:1349:HIS:NE2 | 2.18 | 0.58 |
| 2:B:1587:PRO:HG2 | 2:B:1590:CYS:SG | 2.44 | 0.58 |
| 2:B:1639:ASP:HB3 | 2:B:1641:GLU:OE1 | 2.04 | 0.58 |
| 1:C:28:ILE:HD12 | 1:C:29:ILE:N | 2.18 | 0.58 |
| 2:D:937:ARG:NH2 | 2:D:1349:HIS:HE1 | 2.00 | 0.58 |
| 2:D:756:ILE:CD1 | 3:F:134:ARG:HH12 | 2.16 | 0.58 |
| 2:B:1112:GLN:HA | 2:B:1112:GLN:OE1 | 2.03 | 0.58 |
| 2:B:1631:TRP:CD1 | 2:B:1649:LEU:HD13 | 2.38 | 0.58 |
| 1:C:135:ASP:OD1 | 1:C:139:TYR:OH | 2.17 | 0.58 |
| 1:C:337:ASP:OD2 | 2:D:834:ARG:NE | 2.37 | 0.58 |
| 1:C:30:THR:HG23 | 1:C:645:THR:OG1 | 2.03 | 0.58 |
| 2:D:757:ALA:O | 2:D:761:ILE:HD13 | 2.03 | 0.58 |
| 2:D:780:GLU:N | 2:D:780:GLU:OE1 | 2.36 | 0.58 |
| 1:A:169:ASN:HB2 | 1:A:170:PRO:HD2 | 1.86 | 0.58 |
| 1:A:252:GLU:OE1 | 1:A:252:GLU:N | 2.25 | 0.58 |
| 2:B:1152:GLN:NE2 | 2:B:1198:GLN:HE22 | 2.02 | 0.58 |
| 2:B:1202:LEU:CA | 2:B:1206:LEU:HD11 | 2.33 | 0.58 |
| 1:C:47:HIS:ND1 | 1:C:489:TYR:OH | 2.34 | 0.58 |
| 1:C:72:GLU:HB2 | 1:C:86:VAL:HG21 | 1.85 | 0.58 |
| 2:D:1600:LYS:HE3 | 2:D:1630:HIS:NE2 | 2.19 | 0.58 |
| 2:D:1631:TRP:CD1 | 2:D:1649:LEU:CD2 | 2.86 | 0.58 |
| 1:A:122:LEU:HD21 | 1:A:657:ARG:HG2 | 1.85 | 0.58 |
| 1:A:332:LEU:HD12 | 1:A:337:ASP:HB2 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:359:LYS:HD2 | 1:A:552:TRP:CZ3 | 2.38 | 0.58 |
| 1:A:45:GLU:OE1 | 1:A:534:TYR:OH | 2.22 | 0.58 |
| 2:B:1049:ILE:HG22 | 2:B:1093:ILE:HD13 | 1.84 | 0.58 |
| 2:B:1592:GLU:O | 2:B:1595:LYS:NZ | 2.28 | 0.58 |
| 1:C:324:LEU:HB2 | 1:C:346:ILE:CG1 | 2.34 | 0.58 |
| 1:C:39:GLU:OE1 | 1:C:39:GLU:N | 2.24 | 0.58 |
| 3:F:186:ILE:HD11 | 3:F:202:SER:HB2 | 1.84 | 0.58 |
| 2:B:958:GLN:OE1 | 2:B:958:GLN:N | 2.37 | 0.58 |
| 2:D:1067:ALA:HA | 2:D:1078:LEU:HD21 | 1.86 | 0.58 |
| 2:D:1096:ASP:OD2 | 2:D:1098:GLN:NE2 | 2.37 | 0.58 |
| 2:D:1255:TRP:HE3 | 2:D:1256:LEU:HD12 | 1.67 | 0.58 |
| 2:D:1550:VAL:CG2 | 2:D:1581:GLN:NE2 | 2.67 | 0.58 |
| 3:E:197:PHE:HE2 | 3:E:221:ARG:HD2 | 1.67 | 0.58 |
| 1:A:104:LYS:CG | 1:A:105:PHE:N | 2.66 | 0.58 |
| 1:A:563:LEU:HD22 | 2:B:808:SER:HB3 | 1.85 | 0.58 |
| 1:C:552:TRP:CH2 | 1:C:554:ASP:HB2 | 2.38 | 0.58 |
| 2:D:1105:LYS:CE | 2:D:1106:TRP:HE1 | 2.12 | 0.58 |
| 2:D:1416:ASP:OD1 | 2:D:1417:ASP:N | 2.37 | 0.58 |
| 1:C:119:LYS:NZ | 1:C:654:THR:O | 2.36 | 0.57 |
| 2:D:1494:HIS:CD2 | 2:D:1497:LYS:HD2 | 2.39 | 0.57 |
| 3:E:224:TYR:HD2 | 3:E:242:HIS:HB3 | 1.67 | 0.57 |
| 3:F:135:ARG:HE | 3:F:141:PRO:HB3 | 1.68 | 0.57 |
| 1:A:338:MET:CE | 2:B:1485:LEU:HB2 | 2.34 | 0.57 |
| 2:B:1554:LEU:HD12 | 2:B:1555:SER:H | 1.69 | 0.57 |
| 1:C:125:LEU:HB2 | 1:C:215:GLN:NE2 | 2.19 | 0.57 |
| 2:D:1240:LEU:HD11 | 2:D:1248:PHE:HB3 | 1.85 | 0.57 |
| 2:D:1475:GLY:HA3 | 2:D:1493:TYR:CZ | 2.39 | 0.57 |
| 2:D:1035:GLU:HA | 2:D:1039:LEU:HD11 | 1.86 | 0.57 |
| 2:D:794:PHE:CE2 | 3:F:176:VAL:HB | 2.39 | 0.57 |
| 1:A:135:ASP:OD1 | 1:A:139:TYR:OH | 2.22 | 0.57 |
| 1:A:57:VAL:HG21 | 1:A:86:VAL:HG21 | 1.86 | 0.57 |
| 2:B:1043:GLN:O | 2:B:1046:LEU:HG | 2.04 | 0.57 |
| 2:B:1496:GLU:HG2 | 2:B:1497:LYS:N | 2.20 | 0.57 |
| 2:D:835:LEU:HD23 | 2:D:929:LEU:HB3 | 1.86 | 0.57 |
| 1:A:272:ILE:HG22 | 1:A:327:SER:HB3 | 1.87 | 0.57 |
| 2:B:1084:LYS:HE2 | 2:B:1273:PHE:CE2 | 2.40 | 0.57 |
| 2:B:1549:LEU:HD13 | 2:B:1563:MET:CE | 2.33 | 0.57 |
| 2:B:846:GLU:OE2 | 2:B:897:PRO:HB3 | 2.05 | 0.57 |
| 2:D:1597:GLU:HG3 | 2:D:1600:LYS:CG | 2.34 | 0.57 |
| 2:D:763:SER:OG | 2:D:911:GLU:OE2 | 2.14 | 0.57 |
| 2:B:939:ASN:C | 2:B:940:LYS:HD3 | 2.25 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:560:VAL:HG13 | 2:D:813:LYS:HE3 | 1.85 | 0.57 |
| 2:D:1027:TYR:CZ | 2:D:1031:THR:HG21 | 2.40 | 0.57 |
| 2:D:1217:LYS:HG2 | 2:D:1217:LYS:O | 2.05 | 0.57 |
| 2:D:1190:ALA:HB2 | 2:D:1220:TRP:HE3 | 1.70 | 0.57 |
| 2:D:1382:ASN:OD1 | 2:D:1383:THR:N | 2.38 | 0.57 |
| 2:D:1644:LYS:HA | 2:D:1647:GLN:OE1 | 2.04 | 0.57 |
| 2:D:951:ARG:O | 2:D:952:LEU:HG | 2.05 | 0.57 |
| 2:D:975:GLU:N | 2:D:975:GLU:OE1 | 2.26 | 0.57 |
| 1:C:508:ARG:HH22 | 1:C:512:GLN:N | 2.03 | 0.57 |
| 1:C:66:LYS:HE3 | 3:E:147:GLN:N | 2.20 | 0.57 |
| 2:D:1547:THR:HB | 2:D:1563:MET:HG3 | 1.87 | 0.57 |
| 2:D:1577:GLN:N | 2:D:1580:GLN:HE21 | 1.86 | 0.57 |
| 2:B:1015:MET:CG | 2:B:1056:GLN:HE22 | 2.18 | 0.57 |
| 2:B:801:THR:OG1 | 2:B:824:THR:HG22 | 2.05 | 0.57 |
| 1:C:422:ILE:HB | 1:C:441:MET:HE3 | 1.87 | 0.57 |
| 2:D:1149:ILE:HD11 | 2:D:1153:GLU:OE2 | 2.04 | 0.57 |
| 1:C:146:LEU:HD13 | 2:D:773:TRP:CE3 | 2.39 | 0.57 |
| 1:A:209:TYR:CD2 | 1:A:214:PRO:HA | 2.39 | 0.57 |
| 2:B:1292:LEU:O | 2:B:1313:TRP:CE3 | 2.57 | 0.57 |
| 3:E:224:TYR:CE2 | 3:E:242:HIS:HB3 | 2.40 | 0.57 |
| 2:D:962:ILE:HD11 | 2:D:1330:PHE:CD2 | 2.40 | 0.56 |
| 3:E:282:GLU:OE2 | 3:E:284:ARG:HG2 | 2.04 | 0.56 |
| 3:F:188:PHE:CD2 | 3:F:218:PRO:HD2 | 2.39 | 0.56 |
| 1:A:125:LEU:H | 1:A:125:LEU:HD12 | 1.69 | 0.56 |
| 1:C:26:TYR:O | 1:C:649:SER:N | 2.38 | 0.56 |
| 2:D:1065:ALA:HB3 | 2:D:1074:PRO:HB3 | 1.87 | 0.56 |
| 1:A:28:ILE:HD12 | 1:A:43:VAL:O | 2.05 | 0.56 |
| 1:A:372:LEU:HD11 | 1:A:422:ILE:HG12 | 1.87 | 0.56 |
| 1:A:495:MET:HE1 | 1:A:625:ILE:HD11 | 1.87 | 0.56 |
| 2:B:1237:LEU:O | 2:B:1241:LEU:HG | 2.05 | 0.56 |
| 2:B:879:LYS:NZ | 2:B:1521:GLN:HE22 | 2.03 | 0.56 |
| 2:B:904:LYS:HE3 | 2:B:908:GLN:HE22 | 1.69 | 0.56 |
| 2:D:1117:VAL:HA | 2:D:1144:THR:HG21 | 1.86 | 0.56 |
| 2:D:1148:LEU:HD21 | 2:D:1195:ALA:HB1 | 1.85 | 0.56 |
| 2:D:1217:LYS:HG3 | 2:D:1248:PHE:CZ | 2.39 | 0.56 |
| 2:D:1298:LEU:CD1 | 2:D:1307:ILE:HB | 2.35 | 0.56 |
| 1:C:599:ASP:HB2 | 2:D:802:TRP:CZ3 | 2.40 | 0.56 |
| 3:F:239:GLU:OE1 | 3:F:240:ARG:O | 2.23 | 0.56 |
| 1:A:30:THR:HG22 | 1:A:645:THR:OG1 | 2.06 | 0.56 |
| 2:B:949:PRO:HG3 | 2:B:958:GLN:HE22 | 1.70 | 0.56 |
| 2:D:1216:ASP:OD2 | 2:D:1219:ARG:NH1 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1551:LYS:HE3 | 2:D:1562:ILE:HD13 | 1.86 | 0.56 |
| 2:D:756:ILE:HB | 3:F:134:ARG:NH2 | 2.19 | 0.56 |
| 1:C:263:LYS:HD2 | 2:D:854:TYR:CE1 | 2.40 | 0.56 |
| 1:A:390:ALA:HB3 | 1:A:427:LYS:HE3 | 1.86 | 0.56 |
| 1:A:366:PRO:HD2 | 1:A:455:TYR:CE1 | 2.41 | 0.56 |
| 1:C:196:PRO:HD2 | 1:C:199:VAL:CG2 | 2.36 | 0.56 |
| 2:D:1654:GLU:O | 2:D:1658:VAL:HG13 | 2.05 | 0.56 |
| 3:E:203:PHE:HB3 | 3:E:214:SER:HB3 | 1.87 | 0.56 |
| 3:E:248:SER:OG | 3:E:266:TYR:HB3 | 2.05 | 0.56 |
| 3:F:186:ILE:HG13 | 3:F:188:PHE:CE1 | 2.41 | 0.56 |
| 2:D:1433:GLU:CD | 2:D:1445:ILE:H | 2.08 | 0.56 |
| 2:D:826:MET:HG2 | 2:D:827:GLN:N | 2.19 | 0.56 |
| 2:D:912:VAL:HG13 | 2:D:925:VAL:HG23 | 1.87 | 0.56 |
| 2:D:1241:LEU:HD11 | 2:D:1285:ASP:HB3 | 1.85 | 0.56 |
| 2:D:904:LYS:HG3 | 2:D:908:GLN:NE2 | 2.21 | 0.56 |
| 1:A:178:ASP:OD2 | 3:E:247:GLN:NE2 | 2.39 | 0.56 |
| 3:F:157:PHE:C | 3:F:159:LYS:HZ2 | 2.05 | 0.56 |
| 3:F:186:ILE:HD13 | 3:F:213:TRP:CZ3 | 2.41 | 0.56 |
| 1:A:235:ILE:HD11 | 1:A:256:THR:HB | 1.88 | 0.56 |
| 2:B:1367:ILE:HD11 | 2:B:1384:MET:HB2 | 1.88 | 0.56 |
| 1:C:523:THR:CB | 1:C:560:VAL:HG23 | 2.31 | 0.56 |
| 2:D:945:ARG:HB2 | 2:D:1342:LEU:HD23 | 1.88 | 0.56 |
| 2:D:856:GLN:OE1 | 2:D:856:GLN:N | 2.35 | 0.56 |
| 3:F:124:VAL:HA | 3:F:143:LEU:O | 2.05 | 0.56 |
| 2:B:1086:PHE:O | 2:B:1095:ILE:HD12 | 2.06 | 0.56 |
| 2:D:1004:ILE:O | 2:D:1004:ILE:HG13 | 2.05 | 0.56 |
| 2:D:1210:PHE:CD1 | 2:D:1220:TRP:HH2 | 2.23 | 0.56 |
| 3:F:190:CYS:SG | 3:F:196:LEU:HD12 | 2.45 | 0.56 |
| 2:B:1303:ARG:NH1 | 2:B:1306:LYS:CA | 2.69 | 0.56 |
| 2:D:1255:TRP:CE3 | 2:D:1256:LEU:HD12 | 2.40 | 0.56 |
| 3:E:116:GLN:HG2 | 3:E:119:PHE:CE1 | 2.40 | 0.56 |
| 2:B:1607:LEU:HD22 | 2:B:1609:SER:H | 1.71 | 0.56 |
| 1:C:182:SER:O | 1:C:185:GLN:HB2 | 2.06 | 0.56 |
| 1:C:397:VAL:HG13 | 1:C:409:LEU:HD22 | 1.87 | 0.56 |
| 1:C:650:SER:OG | 1:C:652:GLN:OE1 | 2.10 | 0.56 |
| 1:A:140:THR:HG23 | 1:A:227:TYR:CZ | 2.40 | 0.55 |
| 1:A:496:ASN:O | 1:A:498:GLY:N | 2.39 | 0.55 |
| 1:C:365:LYS:NZ | 1:C:456:LEU:O | 2.36 | 0.55 |
| 2:D:945:ARG:HB2 | 2:D:1342:LEU:CD2 | 2.36 | 0.55 |
| 2:D:802:TRP:HB2 | 2:D:823:VAL:HG23 | 1.86 | 0.55 |
| 2:D:937:ARG:NH2 | 2:D:1349:HIS:CE1 | 2.73 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:157:PHE:H | 3:F:157:PHE:HD1 | 1.53 | 0.55 |
| 2:B:1507:ARG:NH1 | 2:B:1508:ASP:OD1 | 2.39 | 0.55 |
| 1:C:35:ARG:NH2 | 1:C:498:GLY:O | 2.38 | 0.55 |
| 1:A:166:ASN:OD1 | 1:A:167:ILE:N | 2.40 | 0.55 |
| 1:A:332:LEU:CD1 | 1:A:337:ASP:HB2 | 2.36 | 0.55 |
| 1:C:397:VAL:HG12 | 1:C:409:LEU:HD22 | 1.88 | 0.55 |
| 1:C:496:ASN:C | 1:C:498:GLY:H | 2.08 | 0.55 |
| 1:C:57:VAL:O | 1:C:71:SER:HA | 2.06 | 0.55 |
| 2:D:1218:ASN:HB2 | 2:D:1251:PRO:O | 2.07 | 0.55 |
| 1:A:31:PRO:HA | 1:A:644:LEU:HD23 | 1.89 | 0.55 |
| 2:B:1521:GLN:H | 2:B:1521:GLN:CD | 2.08 | 0.55 |
| 2:B:757:ALA:N | 2:B:760:ASN:HD21 | 2.03 | 0.55 |
| 2:D:1016:ILE:HD12 | 2:D:1016:ILE:O | 2.07 | 0.55 |
| 3:E:233:ASN:HB2 | 3:E:283:CYS:SG | 2.46 | 0.55 |
| 2:B:1052:GLY:O | 2:B:1056:GLN:HG2 | 2.07 | 0.55 |
| 2:B:1014:ASN:HD22 | 2:B:1055:GLN:HG3 | 1.72 | 0.55 |
| 2:B:761:ILE:HG21 | 2:B:913:LYS:CE | 2.37 | 0.55 |
| 2:D:1636:GLU:N | 2:D:1636:GLU:OE1 | 2.39 | 0.55 |
| 3:E:273:GLU:CG | 3:E:275:GLU:OE2 | 2.54 | 0.55 |
| 1:C:190:PRO:HD2 | 3:F:246:ARG:NH2 | 2.22 | 0.55 |
| 1:A:263:LYS:HG3 | 2:B:854:TYR:CE1 | 2.42 | 0.55 |
| 2:B:1203:LYS:O | 2:B:1206:LEU:HG | 2.07 | 0.55 |
| 2:B:1507:ARG:HD2 | 2:B:1508:ASP:OD1 | 2.06 | 0.55 |
| 2:B:1544:VAL:HG13 | 2:B:1570:LYS:CB | 2.37 | 0.55 |
| 2:B:1608:SER:O | 2:B:1611:PHE:HD2 | 1.89 | 0.55 |
| 1:C:394:GLU:HB3 | 1:C:397:VAL:HG23 | 1.87 | 0.55 |
| 1:C:488:ARG:NH2 | 1:C:509:GLU:OE2 | 2.39 | 0.55 |
| 2:D:1118:PHE:N | 2:D:1144:THR:HG23 | 2.21 | 0.55 |
| 2:D:1564:ALA:HB2 | 2:D:1581:GLN:HE22 | 1.71 | 0.55 |
| 3:E:197:PHE:CE2 | 3:E:221:ARG:HD2 | 2.41 | 0.55 |
| 2:B:1012:GLU:OE2 | 2:B:1068:ALA:HB2 | 2.06 | 0.55 |
| 2:B:1085:VAL:HG12 | 2:B:1086:PHE:CD1 | 2.41 | 0.55 |
| 2:D:1233:THR:CG2 | 2:D:1256:LEU:HD11 | 2.36 | 0.55 |
| 2:D:768:PRO:HD3 | 2:D:796:LYS:NZ | 2.21 | 0.55 |
| 1:A:196:PRO:HD2 | 1:A:199:VAL:CG2 | 2.35 | 0.55 |
| 2:B:1263:GLY:CA | 2:B:1272:THR:HG22 | 2.36 | 0.55 |
| 1:C:95:GLU:O | 1:C:97:LYS:N | 2.40 | 0.55 |
| 2:D:846:GLU:OE2 | 2:D:897:PRO:HB3 | 2.07 | 0.55 |
| 2:B:1300:LEU:CD1 | 2:B:1303:ARG:HE | 2.20 | 0.55 |
| 1:C:157:LEU:HD11 | 2:D:811:ASP:C | 2.27 | 0.55 |
| 1:A:628:THR:HG21 | 1:A:641:ASP:HB3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:962:ILE:HG12 | 2:B:1330:PHE:CE1 | 2.42 | 0.55 |
| 2:B:967:LEU:CD1 | 2:B:1327:ASN:HD22 | 2.19 | 0.55 |
| 2:D:1132:GLY:HA2 | 2:D:1228:TYR:CE1 | 2.42 | 0.55 |
| 2:D:1597:GLU:OE2 | 2:D:1600:LYS:HE2 | 2.07 | 0.55 |
| 2:B:1497:LYS:NZ | 2:B:1501:LYS:O | 2.35 | 0.54 |
| 1:C:540:ALA:HB3 | 1:C:543:GLN:HG2 | 1.89 | 0.54 |
| 2:D:1355:GLN:HA | 2:D:1357:THR:HG23 | 1.89 | 0.54 |
| 2:D:761:ILE:CG2 | 2:D:762:VAL:N | 2.70 | 0.54 |
| 3:E:276:TRP:H | 3:E:276:TRP:HE3 | 1.54 | 0.54 |
| 3:F:106:SER:HA | 3:F:133:TYR:CD2 | 2.42 | 0.54 |
| 1:A:566:LYS:HE3 | 1:A:584:LYS:CD | 2.37 | 0.54 |
| 2:B:1136:ASN:HD22 | 2:B:1139:LYS:HZ3 | 1.55 | 0.54 |
| 2:B:1558:PHE:CD1 | 2:B:1587:PRO:HA | 2.41 | 0.54 |
| 1:C:54:PRO:HG2 | 1:C:113:GLY:HA2 | 1.89 | 0.54 |
| 2:D:766:GLU:CB | 2:D:796:LYS:NZ | 2.66 | 0.54 |
| 2:D:905:THR:HA | 2:D:931:VAL:CG2 | 2.36 | 0.54 |
| 3:E:109:LEU:O | 3:E:114:ILE:HD11 | 2.08 | 0.54 |
| 3:E:130:ARG:HH11 | 3:E:130:ARG:HG3 | 1.72 | 0.54 |
| 1:A:471:LEU:HD21 | 1:A:519:LEU:HD23 | 1.89 | 0.54 |
| 1:C:508:ARG:HH12 | 1:C:512:GLN:C | 2.06 | 0.54 |
| 2:D:1135:ASN:O | 2:D:1136:ASN:HB2 | 2.07 | 0.54 |
| 2:D:1517:ASN:ND2 | 2:D:1521:GLN:HB2 | 2.20 | 0.54 |
| 3:F:180:ILE:HD12 | 3:F:180:ILE:C | 2.28 | 0.54 |
| 1:A:60:HIS:ND1 | 1:A:67:LEU:O | 2.34 | 0.54 |
| 2:D:1194:TYR:OH | 2:D:1198:GLN:NE2 | 2.40 | 0.54 |
| 1:A:462:ARG:NH2 | 1:A:463:THR:O | 2.30 | 0.54 |
| 2:B:1303:ARG:HH12 | 2:B:1306:LYS:C | 2.11 | 0.54 |
| 2:B:1475:GLY:HA3 | 2:B:1493:TYR:CZ | 2.43 | 0.54 |
| 2:B:1521:GLN:N | 2:B:1521:GLN:OE1 | 2.25 | 0.54 |
| 2:B:830:PHE:CE1 | 2:B:852:TYR:HD2 | 2.25 | 0.54 |
| 1:C:50:GLN:NE2 | 1:C:51:GLY:H | 1.98 | 0.54 |
| 3:E:175:ASP:HB3 | 3:E:187:SER:OG | 2.07 | 0.54 |
| 2:B:1152:GLN:HE21 | 2:B:1198:GLN:HE22 | 1.54 | 0.54 |
| 2:B:980:ILE:HG22 | 2:B:1344:VAL:HG22 | 1.89 | 0.54 |
| 1:C:368:MET:O | 1:C:413:THR:HG22 | 2.07 | 0.54 |
| 2:B:897:PRO:O | 2:B:1473:GLN:NE2 | 2.41 | 0.54 |
| 2:D:1436:LYS:O | 2:D:1441:ARG:NH2 | 2.36 | 0.54 |
| 3:E:143:LEU:HD11 | 3:E:151:TRP:CE3 | 2.43 | 0.54 |
| 1:A:221:GLU:HB2 | 1:A:609:ASN:ND2 | 2.23 | 0.54 |
| 2:B:1202:LEU:HD11 | 2:B:1243:LEU:CD2 | 2.30 | 0.54 |
| 1:C:32:ASN:HD22 | 1:C:33:ILE:HG12 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:156:GLU:OE2 | 3:E:158:CYS:O | 2.26 | 0.54 |
| 3:F:113:TYR:HA | 3:F:116:GLN:CG | 2.37 | 0.54 |
| 1:A:338:MET:HE1 | 2:B:1485:LEU:HB2 | 1.90 | 0.54 |
| 2:B:1082:VAL:HG13 | 2:B:1086:PHE:CE1 | 2.43 | 0.54 |
| 2:B:1238:LEU:CD1 | 2:B:1277:GLN:HE21 | 2.17 | 0.54 |
| 2:B:1429:ILE:HD11 | 2:B:1433:GLU:HB2 | 1.89 | 0.54 |
| 1:C:66:LYS:O | 1:C:66:LYS:NZ | 2.34 | 0.54 |
| 2:D:1417:ASP:OD1 | 2:D:1418:LEU:N | 2.41 | 0.54 |
| 3:E:170:ARG:HG3 | 3:E:170:ARG:NH1 | 2.16 | 0.54 |
| 1:A:412:ASN:ND2 | 3:F:101:PRO:O | 2.40 | 0.54 |
| 1:A:28:ILE:HD11 | 1:A:42:MET:CG | 2.38 | 0.54 |
| 1:A:44:LEU:N | 1:A:44:LEU:HD12 | 2.23 | 0.54 |
| 2:D:1562:ILE:HG13 | 2:D:1581:GLN:HE21 | 1.71 | 0.54 |
| 1:A:25:MET:HG3 | 1:A:650:SER:HG | 1.72 | 0.53 |
| 2:B:974:THR:HG21 | 2:B:1349:HIS:CD2 | 2.43 | 0.53 |
| 2:B:1358:CYS:HB3 | 2:B:1361:PHE:O | 2.07 | 0.53 |
| 1:C:657:ARG:NE | 1:C:659:GLU:O | 2.38 | 0.53 |
| 1:A:26:TYR:HD2 | 1:A:112:PHE:CD2 | 2.26 | 0.53 |
| 1:A:412:ASN:OD1 | 3:F:103:ARG:HB2 | 2.09 | 0.53 |
| 1:C:169:ASN:HB2 | 1:C:170:PRO:HD2 | 1.90 | 0.53 |
| 1:C:273:PHE:CE2 | 1:C:326:VAL:HG22 | 2.43 | 0.53 |
| 2:D:1192:ALA:HA | 2:D:1195:ALA:HB3 | 1.89 | 0.53 |
| 3:F:282:GLU:OE2 | 3:F:284:ARG:NH2 | 2.41 | 0.53 |
| 2:B:1357:THR:HA | 2:B:1358:CYS:C | 2.29 | 0.53 |
| 2:D:1180:TYR:CD2 | 2:D:1206:LEU:HG | 2.43 | 0.53 |
| 2:D:1352:ALA:HB3 | 2:D:1353:LYS:HA | 1.90 | 0.53 |
| 2:D:758:GLU:HG2 | 2:D:867:LEU:HG | 1.90 | 0.53 |
| 2:D:810:SER:CB | 2:D:813:LYS:HB3 | 2.30 | 0.53 |
| 3:F:187:SER:C | 3:F:188:PHE:HD1 | 2.11 | 0.53 |
| 1:A:496:ASN:C | 1:A:498:GLY:H | 2.12 | 0.53 |
| 1:C:132:ILE:HD13 | 1:C:206:ILE:HG22 | 1.91 | 0.53 |
| 2:B:1554:LEU:CD1 | 2:B:1591:ARG:HH22 | 2.21 | 0.53 |
| 2:B:929:LEU:HD12 | 2:B:930:LYS:N | 2.23 | 0.53 |
| 2:B:977:GLU:OE2 | 2:B:979:ARG:NE | 2.42 | 0.53 |
| 1:C:37:GLU:OE2 | 1:C:212:ASN:ND2 | 2.41 | 0.53 |
| 2:D:1280:ALA:O | 2:D:1283:GLN:NE2 | 2.41 | 0.53 |
| 3:F:126:GLU:HG3 | 3:F:142:LYS:HG2 | 1.90 | 0.53 |
| 3:F:233:ASN:HD21 | 3:F:283:CYS:HB3 | 1.71 | 0.53 |
| 1:A:647:THR:CB | 1:A:653:GLN:HE22 | 2.21 | 0.53 |
| 2:B:764:ARG:N | 2:B:924:GLY:O | 2.31 | 0.53 |
| 2:D:1417:ASP:OD2 | 2:D:1461:PHE:HB2 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1517:ASN:ND2 | 2:D:1519:PHE:O | 2.42 | 0.53 |
| 3:E:104:LEU:O | 3:E:130:ARG:CZ | 2.56 | 0.53 |
| 1:A:61:ASP:OD1 | 1:A:65:LYS:N | 2.42 | 0.53 |
| 2:B:1497:LYS:HZ1 | 2:B:1501:LYS:C | 2.11 | 0.53 |
| 2:B:1576:VAL:HA | 2:B:1580:GLN:HE22 | 1.74 | 0.53 |
| 2:D:1089:ALA:HA | 2:D:1092:LEU:CD1 | 2.38 | 0.53 |
| 2:D:1554:LEU:HD11 | 2:D:1591:ARG:CZ | 2.39 | 0.53 |
| 2:D:841:ARG:HH22 | 2:D:903:LEU:HA | 1.73 | 0.53 |
| 1:A:126:GLN:HE21 | 1:A:154:HIS:CD2 | 2.26 | 0.53 |
| 2:B:1105:LYS:HG2 | 2:B:1162:VAL:CG2 | 2.37 | 0.53 |
| 2:B:874:SER:HB3 | 2:B:900:ILE:HG22 | 1.89 | 0.53 |
| 1:C:565:VAL:HG13 | 2:D:821:PHE:HB2 | 1.90 | 0.53 |
| 2:D:1061:GLN:C | 2:D:1063:SER:N | 2.61 | 0.53 |
| 2:D:1252:VAL:O | 2:D:1256:LEU:HD13 | 2.09 | 0.53 |
| 1:A:181:SER:CB | 3:E:246:ARG:HE | 2.15 | 0.53 |
| 1:A:125:LEU:CD2 | 1:A:215:GLN:HE22 | 2.22 | 0.53 |
| 1:A:235:ILE:CD1 | 1:A:256:THR:HB | 2.38 | 0.53 |
| 1:A:242:PHE:CD2 | 1:A:379:PRO:HG2 | 2.44 | 0.53 |
| 2:B:1255:TRP:O | 2:B:1259:GLN:HG2 | 2.09 | 0.53 |
| 2:D:1047:GLU:HG3 | 2:D:1051:LYS:NZ | 2.23 | 0.53 |
| 2:D:1298:LEU:HD12 | 2:D:1307:ILE:HB | 1.90 | 0.53 |
| 2:D:1414:ASP:O | 2:D:1417:ASP:OD1 | 2.27 | 0.53 |
| 2:D:1533:LEU:HA | 2:D:1652:PHE:HE1 | 1.73 | 0.53 |
| 2:D:841:ARG:HH12 | 2:D:903:LEU:C | 2.12 | 0.53 |
| 2:D:1001:LYS:O | 2:D:1004:ILE:HG12 | 2.09 | 0.53 |
| 3:F:133:TYR:O | 3:F:134:ARG:HD2 | 2.09 | 0.53 |
| 1:A:130:LEU:HD21 | 1:A:163:VAL:CG1 | 2.38 | 0.52 |
| 2:B:1045:ALA:O | 2:B:1049:ILE:HD12 | 2.09 | 0.52 |
| 2:B:957:VAL:HG21 | 2:B:1335:GLU:HG3 | 1.91 | 0.52 |
| 2:B:886:VAL:HG11 | 2:B:894:LEU:HD22 | 1.90 | 0.52 |
| 1:C:573:ARG:HE | 1:C:579:GLN:HE21 | 1.58 | 0.52 |
| 2:D:1172:ALA:O | 2:D:1176:LEU:HD13 | 2.08 | 0.52 |
| 2:D:831:ILE:HG13 | 2:D:923:ASP:OD2 | 2.09 | 0.52 |
| 3:F:233:ASN:HD21 | 3:F:283:CYS:C | 2.08 | 0.52 |
| 1:A:35:ARG:HG2 | 1:A:124:SER:HB3 | 1.91 | 0.52 |
| 2:B:1112:GLN:HE22 | 2:B:1117:VAL:N | 2.08 | 0.52 |
| 2:B:907:LEU:O | 2:B:907:LEU:HD12 | 2.09 | 0.52 |
| 1:C:43:VAL:HG11 | 1:C:493:LEU:HD21 | 1.91 | 0.52 |
| 2:D:1313:TRP:HA | 2:D:1313:TRP:CE3 | 2.44 | 0.52 |
| 2:D:1494:HIS:CE1 | 2:D:1496:GLU:OE1 | 2.62 | 0.52 |
| 3:F:246:ARG:HB3 | 3:F:246:ARG:HH11 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:978:THR:OG1 | 2:B:1346:THR:HG22 | 2.10 | 0.52 |
| 2:B:1508:ASP:N | 2:B:1508:ASP:OD1 | 2.40 | 0.52 |
| 2:B:1561:TYR:HB3 | 2:B:1563:MET:HE3 | 1.91 | 0.52 |
| 2:D:1077:TRP:CD2 | 2:D:1130:ILE:HG22 | 2.44 | 0.52 |
| 1:A:326:VAL:CG2 | 1:A:343:ARG:HB3 | 2.39 | 0.52 |
| 2:B:1174:ASP:HA | 2:B:1201:ARG:NH2 | 2.21 | 0.52 |
| 2:B:1291:GLU:OE1 | 2:B:1291:GLU:N | 2.43 | 0.52 |
| 1:A:261:TYR:CD2 | 2:B:826:MET:SD | 3.03 | 0.52 |
| 1:C:230:PRO:HB2 | 1:C:339:VAL:CG2 | 2.40 | 0.52 |
| 2:D:1495:PRO:HG2 | 2:D:1496:GLU:OE1 | 2.10 | 0.52 |
| 2:D:872:PHE:CD1 | 2:D:902:PRO:HA | 2.44 | 0.52 |
| 3:E:116:GLN:O | 3:E:117:ASN:ND2 | 2.42 | 0.52 |
| 3:E:156:GLU:OE2 | 3:E:158:CYS:N | 2.43 | 0.52 |
| 2:B:1576:VAL:CG1 | 2:B:1582:ARG:HE | 2.22 | 0.52 |
| 2:D:1132:GLY:HA2 | 2:D:1228:TYR:CD1 | 2.45 | 0.52 |
| 2:D:764:ARG:HB3 | 2:D:767:PHE:CZ | 2.44 | 0.52 |
| 2:D:957:VAL:CG2 | 2:D:1335:GLU:HA | 2.39 | 0.52 |
| 2:D:980:ILE:HD11 | 2:D:1322:GLU:HB2 | 1.90 | 0.52 |
| 2:B:761:ILE:CG2 | 2:B:913:LYS:HE3 | 2.39 | 0.52 |
| 1:C:183:GLN:HG3 | 3:F:266:TYR:CZ | 2.45 | 0.52 |
| 1:C:496:ASN:O | 1:C:498:GLY:N | 2.42 | 0.52 |
| 2:D:1310:ARG:NH2 | 3:F:235:ILE:HG12 | 2.24 | 0.52 |
| 3:F:188:PHE:CD1 | 3:F:188:PHE:N | 2.78 | 0.52 |
| 1:A:376:VAL:HG11 | 1:A:401:THR:HG21 | 1.90 | 0.52 |
| 2:B:1149:ILE:CA | 2:B:1152:GLN:HE22 | 2.23 | 0.52 |
| 1:C:36:LEU:HD12 | 1:C:90:ILE:O | 2.10 | 0.52 |
| 2:D:1190:ALA:HB2 | 2:D:1220:TRP:CE3 | 2.45 | 0.52 |
| 2:B:1577:GLN:N | 2:B:1580:GLN:HE22 | 2.08 | 0.52 |
| 2:B:865:GLU:CD | 2:B:883:GLN:HE21 | 2.13 | 0.52 |
| 1:C:175:VAL:HB | 2:D:979:ARG:CZ | 2.40 | 0.52 |
| 1:C:96:PHE:HD1 | 1:C:104:LYS:HG2 | 1.74 | 0.52 |
| 2:D:1102:GLY:HA2 | 2:D:1105:LYS:HE2 | 1.92 | 0.52 |
| 2:D:1197:ALA:HB2 | 2:D:1202:LEU:CD2 | 2.38 | 0.52 |
| 1:C:148:ARG:NH2 | 2:D:773:TRP:CZ3 | 2.78 | 0.52 |
| 3:E:194:TYR:CD1 | 3:E:222:GLU:HA | 2.45 | 0.52 |
| 1:A:129:TYR:HA | 1:A:218:PHE:CE2 | 2.44 | 0.52 |
| 1:A:181:SER:HB3 | 3:E:246:ARG:CZ | 2.40 | 0.52 |
| 2:B:1202:LEU:HB2 | 2:B:1206:LEU:HD11 | 1.91 | 0.52 |
| 2:B:1240:LEU:HD12 | 2:B:1240:LEU:C | 2.30 | 0.52 |
| 2:D:1174:ASP:HA | 2:D:1177:GLU:HG2 | 1.90 | 0.52 |
| 2:D:1254:ARG:O | 2:D:1258:GLU:OE1 | 2.27 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:596:VAL:O | 2:D:804:ILE:HA | 2.10 | 0.52 |
| 2:B:1112:GLN:NE2 | 2:B:1116:GLY:C | 2.63 | 0.52 |
| 2:B:1549:LEU:HD12 | 2:B:1550:VAL:N | 2.25 | 0.52 |
| 2:B:760:ASN:OD1 | 2:B:761:ILE:HG23 | 2.10 | 0.52 |
| 2:B:811:ASP:OD1 | 2:B:811:ASP:N | 2.42 | 0.52 |
| 1:C:491:THR:HG22 | 1:C:505:ARG:NE | 2.25 | 0.52 |
| 2:D:1544:VAL:HG23 | 2:D:1570:LYS:HG2 | 1.91 | 0.52 |
| 2:D:979:ARG:HG3 | 2:D:1323:GLU:HG3 | 1.91 | 0.52 |
| 3:F:139:LEU:HD11 | 3:F:155:VAL:HG21 | 1.92 | 0.52 |
| 1:A:474:ASN:OD1 | 1:A:516:VAL:HG12 | 2.10 | 0.51 |
| 2:B:1312:HIS:HA | 2:B:1313:TRP:CE3 | 2.46 | 0.51 |
| 2:B:1577:GLN:N | 2:B:1580:GLN:NE2 | 2.59 | 0.51 |
| 2:B:935:GLY:HA3 | 2:B:1349:HIS:CE1 | 2.45 | 0.51 |
| 3:F:116:GLN:HG3 | 3:F:119:PHE:CE1 | 2.45 | 0.51 |
| 3:F:135:ARG:HH12 | 3:F:137:PRO:HA | 1.75 | 0.51 |
| 1:A:103:ASN:OD1 | 1:A:103:ASN:N | 2.40 | 0.51 |
| 1:A:448:THR:HG23 | 1:A:451:ASN:HA | 1.92 | 0.51 |
| 2:B:1516:GLU:CD | 2:B:1624:LYS:HG2 | 2.31 | 0.51 |
| 1:C:391:VAL:CG2 | 1:C:394:GLU:HB2 | 2.40 | 0.51 |
| 2:D:1063:SER:O | 2:D:1065:ALA:N | 2.43 | 0.51 |
| 2:D:1145:ALA:O | 2:D:1149:ILE:HG22 | 2.10 | 0.51 |
| 3:E:235:ILE:HG22 | 3:E:236:ILE:H | 1.74 | 0.51 |
| 2:B:1084:LYS:HE3 | 2:B:1149:ILE:HD13 | 1.91 | 0.51 |
| 2:B:1248:PHE:O | 2:B:1251:PRO:HD2 | 2.10 | 0.51 |
| 2:B:1317:SER:O | 2:B:1319:LEU:HG | 2.10 | 0.51 |
| 2:B:764:ARG:HD2 | 2:B:797:ASP:O | 2.09 | 0.51 |
| 2:D:1149:ILE:HA | 2:D:1152:GLN:HE21 | 1.75 | 0.51 |
| 2:D:1159:GLU:OE2 | 2:D:1165:LEU:HD23 | 2.11 | 0.51 |
| 3:E:107:ALA:N | 3:E:130:ARG:NH1 | 2.58 | 0.51 |
| 3:E:235:ILE:HG22 | 3:E:236:ILE:N | 2.26 | 0.51 |
| 2:D:756:ILE:CD1 | 3:F:134:ARG:HH22 | 2.23 | 0.51 |
| 1:A:540:ALA:HB3 | 1:A:543:GLN:HG2 | 1.91 | 0.51 |
| 2:B:1226:GLN:O | 2:B:1230:VAL:HG23 | 2.11 | 0.51 |
| 2:D:1065:ALA:CB | 2:D:1074:PRO:HB3 | 2.41 | 0.51 |
| 2:D:1313:TRP:HZ3 | 2:D:1318:LEU:HD11 | 1.73 | 0.51 |
| 2:D:1423:ASN:O | 2:D:1425:VAL:HG12 | 2.10 | 0.51 |
| 2:D:1547:THR:HG22 | 2:D:1565:ILE:HD13 | 1.93 | 0.51 |
| 2:B:1192:ALA:O | 2:B:1196:LEU:HG | 2.10 | 0.51 |
| 2:B:1261:TYR:OH | 2:B:1268:SER:HB2 | 2.11 | 0.51 |
| 1:C:148:ARG:CZ | 1:C:594:VAL:CG2 | 2.88 | 0.51 |
| 1:C:489:TYR:CD2 | 1:C:505:ARG:HD2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1255:TRP:HA | 2:D:1258:GLU:CD | 2.30 | 0.51 |
| 2:D:756:ILE:CB | 3:F:134:ARG:HH22 | 2.24 | 0.51 |
| 3:E:232:ASP:O | 3:E:283:CYS:SG | 2.69 | 0.51 |
| 3:F:203:PHE:O | 3:F:214:SER:N | 2.36 | 0.51 |
| 1:C:508:ARG:HH12 | 1:C:512:GLN:HB2 | 1.76 | 0.51 |
| 2:D:1216:ASP:OD1 | 2:D:1218:ASN:OD1 | 2.29 | 0.51 |
| 2:D:1639:ASP:OD2 | 2:D:1642:ASN:HB2 | 2.11 | 0.51 |
| 2:D:841:ARG:HH12 | 2:D:903:LEU:CA | 2.23 | 0.51 |
| 3:E:107:ALA:HB1 | 3:E:127:TYR:HB3 | 1.91 | 0.51 |
| 1:A:368:MET:O | 1:A:413:THR:HG22 | 2.09 | 0.51 |
| 2:B:1313:TRP:O | 2:B:1314:GLU:HB2 | 2.11 | 0.51 |
| 2:B:1549:LEU:HD13 | 2:B:1563:MET:HE1 | 1.92 | 0.51 |
| 2:B:1541:VAL:HG13 | 2:B:1570:LYS:HZ1 | 1.76 | 0.51 |
| 2:B:1634:GLU:OE2 | 2:B:1638:GLN:NE2 | 2.44 | 0.51 |
| 1:A:610:LYS:O | 1:A:615:LYS:NZ | 2.43 | 0.51 |
| 1:A:646:PHE:H | 1:A:654:THR:HG21 | 1.76 | 0.51 |
| 2:B:1149:ILE:HA | 2:B:1152:GLN:NE2 | 2.24 | 0.51 |
| 1:C:201:MET:HE3 | 1:C:225:LYS:HA | 1.92 | 0.51 |
| 1:C:42:MET:HB3 | 1:C:86:VAL:HG12 | 1.91 | 0.51 |
| 1:C:41:THR:HG22 | 1:C:500:LEU:HB2 | 1.92 | 0.51 |
| 2:D:1400:MET:CE | 2:D:1447:TYR:HB3 | 2.40 | 0.51 |
| 1:A:236:VAL:HG22 | 1:A:255:ILE:HD13 | 1.93 | 0.51 |
| 2:B:1118:PHE:HZ | 2:B:1151:LEU:HD11 | 1.76 | 0.51 |
| 2:B:1435:ASP:OD1 | 2:B:1435:ASP:N | 2.43 | 0.51 |
| 1:C:355:ILE:HG12 | 1:C:376:VAL:HG22 | 1.91 | 0.51 |
| 1:C:365:LYS:HZ1 | 1:C:549:ASP:CG | 2.13 | 0.51 |
| 2:D:1588:ILE:HG22 | 2:D:1591:ARG:HH21 | 1.75 | 0.51 |
| 3:E:276:TRP:N | 3:E:276:TRP:CD2 | 2.77 | 0.51 |
| 3:F:107:ALA:HB1 | 3:F:127:TYR:HB3 | 1.93 | 0.51 |
| 3:F:258:THR:O | 3:F:283:CYS:HA | 2.11 | 0.51 |
| 1:A:37:GLU:CD | 1:A:161:ARG:NH1 | 2.63 | 0.51 |
| 2:B:1060:ARG:NH2 | 2:B:1099:VAL:HA | 2.26 | 0.51 |
| 2:B:1407:MET:SD | 2:B:1413:PRO:HD3 | 2.51 | 0.51 |
| 2:B:1559:ASP:OD1 | 2:B:1586:SER:O | 2.29 | 0.51 |
| 2:B:967:LEU:HD22 | 2:B:1348:TYR:HD2 | 1.71 | 0.51 |
| 2:D:1547:THR:HB | 2:D:1563:MET:CG | 2.41 | 0.51 |
| 2:D:1505:LEU:CD1 | 2:D:1585:ILE:HD11 | 2.39 | 0.51 |
| 2:D:1631:TRP:HZ3 | 2:D:1633:GLU:HA | 1.75 | 0.51 |
| 2:D:996:ASP:O | 2:D:999:ARG:HB2 | 2.11 | 0.51 |
| 3:F:195:LYS:HD2 | 3:F:196:LEU:N | 2.24 | 0.51 |
| 2:D:1156:ASP:OD1 | 2:D:1157:ILE:HG13 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:129:CYS:HB3 | 3:F:133:TYR:HB2 | 1.91 | 0.50 |
| 1:A:376:VAL:HG12 | 1:A:401:THR:HG21 | 1.93 | 0.50 |
| 1:A:39:GLU:HG3 | 1:A:87:THR:HG22 | 1.93 | 0.50 |
| 1:A:462:ARG:HH21 | 1:A:463:THR:C | 2.13 | 0.50 |
| 2:B:1191:ILE:HG22 | 2:B:1235:TYR:CD1 | 2.47 | 0.50 |
| 1:C:465:LEU:HD11 | 1:C:555:VAL:HG22 | 1.93 | 0.50 |
| 2:D:1252:VAL:O | 2:D:1255:TRP:HB3 | 2.11 | 0.50 |
| 2:D:1533:LEU:HD21 | 2:D:1655:SER:OG | 2.11 | 0.50 |
| 1:A:397:VAL:HG12 | 1:A:409:LEU:HD23 | 1.93 | 0.50 |
| 1:A:362:LYS:NZ | 1:A:442:GLN:O | 2.30 | 0.50 |
| 2:B:1116:GLY:HA2 | 2:B:1171:LYS:HG2 | 1.94 | 0.50 |
| 2:B:841:ARG:NH2 | 2:B:903:LEU:HA | 2.26 | 0.50 |
| 1:C:104:LYS:O | 1:C:122:LEU:HD12 | 2.10 | 0.50 |
| 1:C:167:ILE:O | 1:C:175:VAL:HG22 | 2.11 | 0.50 |
| 1:C:198:LEU:HD11 | 2:D:1349:HIS:NE2 | 2.27 | 0.50 |
| 1:C:460:VAL:HG13 | 1:C:462:ARG:HD3 | 1.92 | 0.50 |
| 2:D:979:ARG:HG3 | 2:D:1323:GLU:CG | 2.42 | 0.50 |
| 2:D:1392:TYR:CE1 | 2:D:1398:ALA:HB2 | 2.47 | 0.50 |
| 2:D:798:SER:HB2 | 2:D:802:TRP:CZ2 | 2.47 | 0.50 |
| 2:D:758:GLU:CA | 2:D:913:LYS:HZ3 | 2.09 | 0.50 |
| 3:E:107:ALA:C | 3:E:130:ARG:HH12 | 2.15 | 0.50 |
| 3:E:245:TYR:C | 3:E:245:TYR:CD1 | 2.84 | 0.50 |
| 1:A:647:THR:CG2 | 1:A:653:GLN:HE22 | 2.24 | 0.50 |
| 2:B:870:PRO:O | 2:B:903:LEU:HD12 | 2.12 | 0.50 |
| 2:D:1133:LEU:O | 2:D:1139:LYS:HE3 | 2.11 | 0.50 |
| 2:D:1210:PHE:O | 2:D:1213:THR:HG22 | 2.11 | 0.50 |
| 2:D:1128:GLU:OE1 | 2:D:1267:GLY:CA | 2.59 | 0.50 |
| 3:F:241:ASP:N | 3:F:241:ASP:OD1 | 2.43 | 0.50 |
| 1:A:36:LEU:O | 1:A:37:GLU:HG2 | 2.12 | 0.50 |
| 1:A:39:GLU:OE1 | 1:A:89:THR:HG23 | 2.12 | 0.50 |
| 2:B:1281:GLN:OE1 | 2:B:1284:LYS:HE2 | 2.11 | 0.50 |
| 2:B:831:ILE:HD12 | 2:B:925:VAL:HG23 | 1.92 | 0.50 |
| 1:C:456:LEU:HB2 | 1:C:535:TYR:HE2 | 1.77 | 0.50 |
| 1:A:59:VAL:HG13 | 1:A:106:VAL:HG21 | 1.94 | 0.50 |
| 1:A:612:THR:HG23 | 1:A:615:LYS:HZ3 | 1.76 | 0.50 |
| 2:B:967:LEU:HD22 | 2:B:1348:TYR:CE2 | 2.47 | 0.50 |
| 2:B:1608:SER:HA | 2:B:1611:PHE:CE2 | 2.46 | 0.50 |
| 1:C:508:ARG:CG | 1:C:508:ARG:NH1 | 2.68 | 0.50 |
| 2:D:1060:ARG:NH2 | 2:D:1099:VAL:HA | 2.27 | 0.50 |
| 3:F:204:CYS:SG | 3:F:211:VAL:HG21 | 2.51 | 0.50 |
| 1:A:166:ASN:HD21 | 1:A:174:PRO:CG | 2.25 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:232:PHE:HE2 | 1:A:330:VAL:CG2 | 2.25 | 0.50 |
| 2:B:1643:GLN:HG3 | 2:B:1644:LYS:H | 1.75 | 0.50 |
| 2:B:826:MET:HG3 | 2:B:827:GLN:H | 1.77 | 0.50 |
| 2:D:757:ALA:O | 2:D:761:ILE:CD1 | 2.59 | 0.50 |
| 1:C:313:ASN:ND2 | 1:C:318:ASP:HB2 | 2.27 | 0.50 |
| 1:C:365:LYS:HZ3 | 1:C:457:HIS:HA | 1.75 | 0.50 |
| 1:C:460:VAL:CG2 | 1:C:471:LEU:HD21 | 2.41 | 0.50 |
| 1:C:97:LYS:CG | 2:D:1314:GLU:HB3 | 2.42 | 0.50 |
| 2:D:1348:TYR:HE1 | 2:D:1350:ALA:HB2 | 1.76 | 0.50 |
| 2:D:761:ILE:HD13 | 2:D:913:LYS:NZ | 2.27 | 0.50 |
| 3:E:171:ASN:ND2 | 3:E:194:TYR:CE1 | 2.80 | 0.50 |
| 3:F:116:GLN:HG3 | 3:F:119:PHE:CZ | 2.46 | 0.50 |
| 1:A:380:ASP:OD1 | 1:A:381:GLY:N | 2.45 | 0.50 |
| 1:A:35:ARG:HH22 | 1:A:498:GLY:HA3 | 1.76 | 0.50 |
| 1:A:63:PRO:HD3 | 2:B:1034:TRP:CZ3 | 2.46 | 0.50 |
| 2:B:1141:MET:HA | 2:B:1141:MET:HE2 | 1.94 | 0.50 |
| 2:B:1497:LYS:NZ | 2:B:1502:LEU:HA | 2.26 | 0.50 |
| 2:B:1551:LYS:HD2 | 2:B:1552:VAL:H | 1.76 | 0.50 |
| 2:B:752:ASP:HB3 | 2:B:753:GLU:OE1 | 2.12 | 0.50 |
| 1:C:475:PHE:HB2 | 1:C:515:VAL:HG13 | 1.94 | 0.50 |
| 2:D:1210:PHE:CE1 | 2:D:1220:TRP:CH2 | 3.00 | 0.50 |
| 2:D:1313:TRP:CE3 | 2:D:1318:LEU:HD21 | 2.47 | 0.50 |
| 2:D:1492:PHE:HE2 | 2:D:1500:GLY:C | 2.16 | 0.50 |
| 2:D:811:ASP:OD1 | 2:D:811:ASP:N | 2.44 | 0.50 |
| 3:E:101:PRO:HB3 | 3:E:143:LEU:HD21 | 1.94 | 0.50 |
| 1:A:329:THR:HA | 1:A:340:GLN:OE1 | 2.12 | 0.49 |
| 2:B:1032:GLU:HA | 2:B:1034:TRP:CE3 | 2.47 | 0.49 |
| 2:D:1472:ILE:HD11 | 2:D:1494:HIS:NE2 | 2.27 | 0.49 |
| 3:E:133:TYR:O | 3:E:161:LYS:HE3 | 2.12 | 0.49 |
| 3:F:246:ARG:CB | 3:F:246:ARG:NH1 | 2.74 | 0.49 |
| 1:A:484:GLU:O | 1:A:487:ILE:HG22 | 2.12 | 0.49 |
| 1:A:489:TYR:CD2 | 1:A:505:ARG:NH2 | 2.80 | 0.49 |
| 2:B:1300:LEU:HD11 | 2:B:1303:ARG:CG | 2.23 | 0.49 |
| 2:B:755:ILE:HD12 | 2:B:756:ILE:O | 2.12 | 0.49 |
| 2:D:1037:PHE:O | 2:D:1041:LYS:HD2 | 2.13 | 0.49 |
| 3:E:222:GLU:HG2 | 3:E:224:TYR:CE1 | 2.47 | 0.49 |
| 1:A:122:LEU:H | 1:A:122:LEU:HD12 | 1.77 | 0.49 |
| 2:B:795:LEU:HD11 | 2:B:825:VAL:HB | 1.93 | 0.49 |
| 2:B:764:ARG:HB3 | 2:B:797:ASP:HB3 | 1.95 | 0.49 |
| 1:C:72:GLU:HB2 | 1:C:86:VAL:CG2 | 2.42 | 0.49 |
| 2:D:1294:LEU:HB3 | 2:D:1311:ILE:CG2 | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:972:PRO:HD3 | 2:D:1351:LYS:HE3 | 1.93 | 0.49 |
| 2:D:763:SER:CB | 2:D:926:ARG:HB2 | 2.43 | 0.49 |
| 2:D:971:VAL:HA | 2:D:1351:LYS:HE3 | 1.94 | 0.49 |
| 2:D:996:ASP:OD1 | 2:D:1036:LYS:CE | 2.60 | 0.49 |
| 3:E:132:GLY:HA2 | 3:E:161:LYS:NZ | 2.27 | 0.49 |
| 2:B:1299:GLN:HA | 2:B:1303:ARG:HH21 | 1.76 | 0.49 |
| 1:C:453:ASN:OD1 | 1:C:455:TYR:HE2 | 1.95 | 0.49 |
| 2:D:1029:ASP:OD1 | 2:D:1034:TRP:NE1 | 2.32 | 0.49 |
| 2:D:1060:ARG:HD2 | 2:D:1064:SER:HA | 1.94 | 0.49 |
| 2:D:898:TYR:HA | 2:D:1473:GLN:HE22 | 1.78 | 0.49 |
| 3:F:157:PHE:CD1 | 3:F:157:PHE:N | 2.81 | 0.49 |
| 3:F:224:TYR:CD1 | 3:F:242:HIS:HB3 | 2.47 | 0.49 |
| 1:A:326:VAL:O | 1:A:342:GLU:HA | 2.12 | 0.49 |
| 2:B:1159:GLU:OE2 | 2:B:1166:PRO:HG3 | 2.12 | 0.49 |
| 2:B:1249:VAL:HB | 2:B:1250:PRO:CD | 2.42 | 0.49 |
| 2:B:1512:ARG:NH1 | 2:B:1621:ILE:HD11 | 2.28 | 0.49 |
| 1:C:355:ILE:HG23 | 1:C:374:VAL:HG13 | 1.94 | 0.49 |
| 1:C:625:ILE:CD1 | 1:C:643:GLY:HA3 | 2.42 | 0.49 |
| 2:D:1047:GLU:O | 2:D:1050:LYS:HG2 | 2.12 | 0.49 |
| 2:D:1249:VAL:HG23 | 2:D:1250:PRO:HD3 | 1.92 | 0.49 |
| 2:D:1249:VAL:O | 2:D:1252:VAL:HG12 | 2.13 | 0.49 |
| 2:D:1295:ASP:HB2 | 2:D:1335:GLU:HB3 | 1.94 | 0.49 |
| 2:D:1506:CYS:HG | 2:D:1511:CYS:CB | 2.25 | 0.49 |
| 2:D:1601:HIS:HB2 | 2:D:1631:TRP:HB3 | 1.94 | 0.49 |
| 2:B:1027:TYR:CZ | 2:B:1031:THR:HG21 | 2.46 | 0.49 |
| 2:B:1082:VAL:O | 2:B:1086:PHE:CD1 | 2.65 | 0.49 |
| 2:B:1420:GLN:O | 2:B:1423:ASN:OD1 | 2.31 | 0.49 |
| 1:C:36:LEU:HD11 | 1:C:91:PRO:C | 2.33 | 0.49 |
| 1:C:67:LEU:CD2 | 1:C:67:LEU:CB | 2.82 | 0.49 |
| 1:C:59:VAL:CG1 | 1:C:70:SER:H | 2.25 | 0.49 |
| 2:D:1063:SER:HA | 2:D:1106:TRP:HZ3 | 1.78 | 0.49 |
| 1:A:105:PHE:CE2 | 1:A:122:LEU:HG | 2.46 | 0.49 |
| 2:B:1022:VAL:HG22 | 2:B:1049:ILE:HG12 | 1.94 | 0.49 |
| 2:B:1259:GLN:C | 2:B:1260:ARG:HG3 | 2.33 | 0.49 |
| 2:B:1601:HIS:HB2 | 2:B:1631:TRP:HB3 | 1.95 | 0.49 |
| 1:C:367:GLY:H | 1:C:413:THR:HG23 | 1.77 | 0.49 |
| 2:D:1303:ARG:NH2 | 3:F:241:ASP:HA | 2.27 | 0.49 |
| 1:A:586:GLU:HG2 | 2:B:788:THR:HG23 | 1.95 | 0.49 |
| 2:B:1554:LEU:HD13 | 2:B:1591:ARG:HH22 | 1.78 | 0.49 |
| 2:B:1638:GLN:OE1 | 2:B:1638:GLN:N | 2.38 | 0.49 |
| 1:C:95:GLU:C | 1:C:97:LYS:H | 2.16 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:778:LEU:CG | 2:D:787:SER:HB3 | 2.42 | 0.49 |
| 2:D:802:TRP:HB2 | 2:D:823:VAL:CG2 | 2.43 | 0.49 |
| 3:F:180:ILE:HD12 | 3:F:180:ILE:O | 2.13 | 0.49 |
| 1:A:126:GLN:HG2 | 1:A:154:HIS:NE2 | 2.27 | 0.49 |
| 1:A:130:LEU:HD13 | 1:A:210:TYR:CZ | 2.48 | 0.49 |
| 1:A:431:LEU:HD11 | 1:A:436:GLN:NE2 | 2.27 | 0.49 |
| 2:B:1012:GLU:CD | 2:B:1124:VAL:HG22 | 2.33 | 0.49 |
| 2:B:1053:TYR:HD2 | 2:B:1086:PHE:CE2 | 2.30 | 0.49 |
| 2:B:1130:ILE:HG23 | 2:B:1133:LEU:HB2 | 1.95 | 0.49 |
| 2:B:846:GLU:OE1 | 2:B:1476:ALA:HB3 | 2.13 | 0.49 |
| 2:B:753:GLU:O | 2:B:754:ASP:OD1 | 2.30 | 0.49 |
| 1:C:236:VAL:HG22 | 1:C:255:ILE:HD13 | 1.93 | 0.49 |
| 2:D:1063:SER:O | 2:D:1063:SER:OG | 2.18 | 0.49 |
| 2:D:936:ILE:HG13 | 2:D:937:ARG:N | 2.27 | 0.49 |
| 3:E:105:ASN:OD1 | 3:E:105:ASN:N | 2.41 | 0.49 |
| 1:A:181:SER:N | 3:E:246:ARG:CZ | 2.75 | 0.49 |
| 2:B:1238:LEU:HD21 | 2:B:1278:ALA:HA | 1.94 | 0.49 |
| 1:C:230:PRO:HB2 | 1:C:339:VAL:HG22 | 1.95 | 0.49 |
| 1:C:272:ILE:HG22 | 1:C:327:SER:HB3 | 1.94 | 0.49 |
| 1:C:385:TYR:CD1 | 1:C:386:ARG:HG3 | 2.47 | 0.49 |
| 1:C:45:GLU:OE1 | 1:C:534:TYR:OH | 2.27 | 0.49 |
| 1:C:78:PRO:HA | 1:C:82:HIS:CE1 | 2.48 | 0.49 |
| 1:A:59:VAL:HG13 | 1:A:106:VAL:CG2 | 2.42 | 0.48 |
| 1:A:37:GLU:OE1 | 1:A:161:ARG:NH1 | 2.45 | 0.48 |
| 2:B:800:THR:H | 2:B:825:VAL:HG13 | 1.77 | 0.48 |
| 1:C:183:GLN:H | 1:C:183:GLN:CD | 2.14 | 0.48 |
| 1:C:489:TYR:HD2 | 1:C:505:ARG:HD2 | 1.78 | 0.48 |
| 2:D:1158:CYS:HA | 2:D:1161:GLN:HE22 | 1.75 | 0.48 |
| 2:D:758:GLU:H | 2:D:881:ARG:HH12 | 1.61 | 0.48 |
| 1:A:130:LEU:HD21 | 1:A:163:VAL:HG12 | 1.94 | 0.48 |
| 1:A:119:LYS:HB2 | 1:A:647:THR:HG21 | 1.95 | 0.48 |
| 2:B:1136:ASN:HD22 | 2:B:1139:LYS:HZ1 | 1.57 | 0.48 |
| 2:B:1149:ILE:O | 2:B:1152:GLN:NE2 | 2.46 | 0.48 |
| 2:B:1115:ASP:O | 2:B:1175:PHE:CD2 | 2.66 | 0.48 |
| 2:B:1084:LYS:HE2 | 2:B:1273:PHE:HE2 | 1.77 | 0.48 |
| 1:A:335:GLY:HA3 | 2:B:1404:ASP:OD2 | 2.14 | 0.48 |
| 2:B:877:THR:HG23 | 2:B:879:LYS:N | 2.28 | 0.48 |
| 1:C:355:ILE:HD11 | 1:C:426:THR:HG23 | 1.95 | 0.48 |
| 3:F:188:PHE:HD1 | 3:F:188:PHE:N | 2.11 | 0.48 |
| 3:F:194:TYR:CE1 | 3:F:222:GLU:HB3 | 2.48 | 0.48 |
| 1:A:365:LYS:N | 1:A:365:LYS:HD3 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:484:GLU:OE1 | 1:A:484:GLU:N | 2.41 | 0.48 |
| 2:B:1554:LEU:HD12 | 2:B:1555:SER:O | 2.13 | 0.48 |
| 2:B:1607:LEU:HD13 | 2:B:1609:SER:OG | 2.14 | 0.48 |
| 1:C:183:GLN:O | 1:C:185:GLN:HG2 | 2.13 | 0.48 |
| 1:C:29:ILE:HB | 1:C:43:VAL:HG13 | 1.94 | 0.48 |
| 1:C:50:GLN:HE21 | 1:C:51:GLY:N | 1.95 | 0.48 |
| 1:C:634:ASP:O | 1:C:638:VAL:HG23 | 2.13 | 0.48 |
| 2:D:1157:ILE:O | 2:D:1161:GLN:NE2 | 2.35 | 0.48 |
| 2:D:1543:TYR:HB2 | 2:D:1545:TYR:CZ | 2.48 | 0.48 |
| 2:D:1512:ARG:NH1 | 2:D:1621:ILE:HD13 | 2.29 | 0.48 |
| 2:D:761:ILE:HD13 | 2:D:913:LYS:HZ1 | 1.78 | 0.48 |
| 3:E:170:ARG:NH1 | 3:E:170:ARG:CG | 2.71 | 0.48 |
| 1:A:85:ASN:N | 1:A:85:ASN:OD1 | 2.46 | 0.48 |
| 2:B:826:MET:CG | 2:B:827:GLN:H | 2.27 | 0.48 |
| 2:B:868:HIS:CD2 | 2:B:877:THR:HA | 2.48 | 0.48 |
| 2:B:913:LYS:HD2 | 2:B:914:ALA:H | 1.79 | 0.48 |
| 1:C:175:VAL:HB | 2:D:979:ARG:NH1 | 2.27 | 0.48 |
| 1:C:385:TYR:HD2 | 1:C:403:GLY:HA2 | 1.77 | 0.48 |
| 2:B:1061:GLN:OE1 | 2:B:1074:PRO:HG3 | 2.13 | 0.48 |
| 2:B:1411:PHE:C | 2:B:1466:TYR:HE1 | 2.17 | 0.48 |
| 2:B:1436:LYS:HB3 | 2:B:1441:ARG:HE | 1.79 | 0.48 |
| 2:B:1496:GLU:O | 2:B:1497:LYS:C | 2.52 | 0.48 |
| 2:B:1505:LEU:HG | 2:B:1612:TRP:CH2 | 2.49 | 0.48 |
| 2:B:1557:ASP:O | 2:B:1588:ILE:HG23 | 2.12 | 0.48 |
| 1:C:77:THR:O | 1:C:80:THR:HG22 | 2.14 | 0.48 |
| 2:D:1246:PHE:CE1 | 2:D:1286:ALA:HB3 | 2.48 | 0.48 |
| 2:D:934:GLU:HG2 | 2:D:1352:ALA:O | 2.14 | 0.48 |
| 2:D:756:ILE:CD1 | 2:D:761:ILE:HG13 | 2.39 | 0.48 |
| 3:E:146:LEU:N | 3:E:150:LYS:O | 2.41 | 0.48 |
| 1:A:487:ILE:CD1 | 1:A:535:TYR:HB2 | 2.42 | 0.48 |
| 2:B:996:ASP:OD1 | 2:B:999:ARG:HB2 | 2.13 | 0.48 |
| 1:C:209:TYR:CD2 | 1:C:214:PRO:HA | 2.48 | 0.48 |
| 1:C:479:MET:HG3 | 1:C:480:ASP:N | 2.29 | 0.48 |
| 2:D:1643:GLN:HE21 | 2:D:1644:LYS:NZ | 2.12 | 0.48 |
| 1:A:471:LEU:O | 1:A:471:LEU:HD12 | 2.14 | 0.48 |
| 1:A:628:THR:HG23 | 1:A:630:GLY:H | 1.79 | 0.48 |
| 2:B:1507:ARG:CZ | 2:B:1508:ASP:OD1 | 2.62 | 0.48 |
| 2:B:1544:VAL:CG1 | 2:B:1570:LYS:HB3 | 2.42 | 0.48 |
| 2:B:1574:ASP:O | 2:B:1576:VAL:HG22 | 2.14 | 0.48 |
| 2:D:1202:LEU:O | 2:D:1207:LEU:HB2 | 2.14 | 0.48 |
| 2:D:978:THR:HG1 | 2:D:1324:THR:HG23 | 1.76 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:796:LYS:HG3 | 2:D:797:ASP:H | 1.78 | 0.48 |
| 2:B:1032:GLU:HA | 2:B:1034:TRP:CZ3 | 2.49 | 0.48 |
| 2:B:971:VAL:HG21 | 2:B:1349:HIS:CE1 | 2.48 | 0.48 |
| 2:B:1576:VAL:HG11 | 2:B:1582:ARG:HE | 1.78 | 0.48 |
| 1:C:189:LEU:CD1 | 3:F:246:ARG:HH12 | 2.26 | 0.48 |
| 1:C:527:PRO:O | 1:C:555:VAL:N | 2.34 | 0.48 |
| 1:C:115:GLN:HG2 | 1:C:649:SER:HB2 | 1.94 | 0.48 |
| 2:D:1470:GLU:HG3 | 2:D:1471:LEU:HD22 | 1.94 | 0.48 |
| 2:D:796:LYS:HA | 2:D:796:LYS:HD2 | 1.57 | 0.48 |
| 2:D:888:ILE:HD12 | 2:D:889:PRO:HD2 | 1.96 | 0.48 |
| 3:E:222:GLU:HB3 | 3:E:224:TYR:HE1 | 1.78 | 0.48 |
| 1:A:119:LYS:CB | 1:A:647:THR:HG21 | 2.43 | 0.48 |
| 1:A:130:LEU:CB | 1:A:218:PHE:HD2 | 2.26 | 0.48 |
| 2:B:965:ALA:H | 2:B:1327:ASN:HD21 | 1.60 | 0.48 |
| 1:C:28:ILE:HD13 | 1:C:44:LEU:HD23 | 1.94 | 0.48 |
| 1:C:508:ARG:NH1 | 1:C:512:GLN:HB2 | 2.28 | 0.48 |
| 1:C:561:GLY:HA3 | 2:D:813:LYS:CE | 2.42 | 0.48 |
| 1:C:617:TRP:CE3 | 1:C:617:TRP:HA | 2.49 | 0.48 |
| 1:C:532:VAL:HG11 | 1:C:644:LEU:HD12 | 1.96 | 0.48 |
| 2:D:1250:PRO:O | 2:D:1254:ARG:HG2 | 2.14 | 0.48 |
| 2:D:1508:ASP:OD1 | 2:D:1509:GLU:N | 2.40 | 0.48 |
| 2:D:856:GLN:HG2 | 2:D:857:ASN:N | 2.28 | 0.48 |
| 3:E:203:PHE:O | 3:E:214:SER:N | 2.40 | 0.48 |
| 1:A:144:THR:HG23 | 1:A:194:ASP:OD1 | 2.13 | 0.48 |
| 1:A:476:LEU:HD13 | 1:A:514:LEU:CD1 | 2.44 | 0.48 |
| 1:A:502:LYS:HD2 | 1:A:503:ALA:N | 2.29 | 0.48 |
| 1:A:487:ILE:HD11 | 1:A:535:TYR:HB2 | 1.95 | 0.48 |
| 2:B:1136:ASN:HA | 2:B:1139:LYS:CE | 2.43 | 0.48 |
| 2:B:1635:ASP:CA | 2:B:1638:GLN:HE22 | 2.16 | 0.48 |
| 1:C:275:ILE:HG13 | 1:C:282:ILE:HB | 1.95 | 0.48 |
| 1:C:488:ARG:HH12 | 1:C:507:VAL:CG1 | 2.27 | 0.48 |
| 2:D:1060:ARG:NH1 | 2:D:1060:ARG:HG3 | 2.28 | 0.48 |
| 3:F:187:SER:C | 3:F:188:PHE:CD1 | 2.87 | 0.48 |
| 3:F:222:GLU:OE2 | 3:F:224:TYR:CZ | 2.67 | 0.48 |
| 1:A:132:ILE:HD13 | 1:A:206:ILE:HG22 | 1.95 | 0.47 |
| 1:A:166:ASN:HD21 | 1:A:174:PRO:HB3 | 1.79 | 0.47 |
| 2:B:1152:GLN:HE21 | 2:B:1153:GLU:HG2 | 1.79 | 0.47 |
| 2:B:1166:PRO:O | 2:B:1170:THR:OG1 | 2.30 | 0.47 |
| 2:B:1191:ILE:HG22 | 2:B:1235:TYR:CE1 | 2.48 | 0.47 |
| 2:B:974:THR:HG21 | 2:B:1349:HIS:HD2 | 1.79 | 0.47 |
| 2:B:980:ILE:HG13 | 2:B:1322:GLU:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:588:ASP:O | 2:D:778:LEU:HD23 | 2.14 | 0.47 |
| 3:E:222:GLU:HB3 | 3:E:224:TYR:CE1 | 2.49 | 0.47 |
| 3:F:188:PHE:CE2 | 3:F:218:PRO:HD2 | 2.48 | 0.47 |
| 1:A:191:LEU:HD12 | 1:A:192:SER:H | 1.79 | 0.47 |
| 1:A:481:ARG:HA | 1:A:484:GLU:CD | 2.34 | 0.47 |
| 2:B:1031:THR:HB | 2:B:1033:GLN:HE21 | 1.79 | 0.47 |
| 2:B:1044:GLY:O | 2:B:1048:LEU:HD13 | 2.14 | 0.47 |
| 1:C:23:SER:O | 1:C:544:ARG:NH2 | 2.42 | 0.47 |
| 1:C:346:ILE:HG13 | 1:C:346:ILE:O | 2.14 | 0.47 |
| 1:C:36:LEU:HD21 | 1:C:92:ALA:HA | 1.97 | 0.47 |
| 2:D:911:GLU:HB2 | 2:D:926:ARG:HG3 | 1.96 | 0.47 |
| 3:E:124:VAL:HA | 3:E:143:LEU:O | 2.14 | 0.47 |
| 3:E:260:ILE:CD1 | 3:E:284:ARG:HD3 | 2.35 | 0.47 |
| 3:F:231:ILE:HD11 | 3:F:234:GLY:HA3 | 1.96 | 0.47 |
| 1:A:36:LEU:O | 1:A:37:GLU:CG | 2.62 | 0.47 |
| 1:A:496:ASN:ND2 | 1:A:501:LEU:HD22 | 2.22 | 0.47 |
| 2:B:1152:GLN:NE2 | 2:B:1153:GLU:HG2 | 2.28 | 0.47 |
| 2:B:1233:THR:CG2 | 2:B:1256:LEU:HD11 | 2.38 | 0.47 |
| 2:B:1494:HIS:CD2 | 2:B:1495:PRO:HD2 | 2.39 | 0.47 |
| 2:D:1215:LYS:HD2 | 2:D:1215:LYS:C | 2.34 | 0.47 |
| 2:D:1538:GLU:HB3 | 2:D:1539:PRO:HD2 | 1.96 | 0.47 |
| 2:D:794:PHE:CZ | 3:F:176:VAL:HB | 2.49 | 0.47 |
| 3:F:255:LYS:HB2 | 3:F:255:LYS:HE2 | 1.58 | 0.47 |
| 2:B:1051:LYS:O | 2:B:1055:GLN:HG2 | 2.15 | 0.47 |
| 2:B:1130:ILE:HA | 2:B:1130:ILE:HD12 | 1.54 | 0.47 |
| 2:B:1431:LYS:O | 2:B:1434:LEU:HB2 | 2.13 | 0.47 |
| 1:C:275:ILE:HG22 | 1:C:324:LEU:CD2 | 2.44 | 0.47 |
| 2:D:1056:GLN:HE22 | 2:D:1082:VAL:HG22 | 1.79 | 0.47 |
| 2:D:1186:SER:HA | 2:D:1189:VAL:CG2 | 2.43 | 0.47 |
| 2:D:1002:HIS:NE2 | 2:D:1262:TYR:O | 2.40 | 0.47 |
| 2:D:1328:GLU:OE1 | 2:D:1330:PHE:HB3 | 2.14 | 0.47 |
| 2:D:1485:LEU:HD12 | 2:D:1486:GLU:N | 2.27 | 0.47 |
| 2:D:1636:GLU:O | 2:D:1639:ASP:HB3 | 2.14 | 0.47 |
| 1:A:29:ILE:HG12 | 1:A:646:PHE:HD2 | 1.79 | 0.47 |
| 2:B:1077:TRP:CD1 | 2:B:1130:ILE:HD11 | 2.50 | 0.47 |
| 2:B:949:PRO:O | 2:B:950:GLU:HG2 | 2.15 | 0.47 |
| 2:D:753:GLU:O | 2:D:753:GLU:HG2 | 2.13 | 0.47 |
| 2:D:755:ILE:CG2 | 2:D:756:ILE:N | 2.77 | 0.47 |
| 2:D:764:ARG:HB3 | 2:D:767:PHE:HZ | 1.79 | 0.47 |
| 3:F:245:TYR:CG | 3:F:245:TYR:O | 2.68 | 0.47 |
| 2:B:1157:ILE:HD12 | 2:B:1158:CYS:SG | 2.53 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1237:LEU:HD23 | 2:B:1278:ALA:HB1 | 1.96 | 0.47 |
| 2:B:1356:LEU:HD13 | 2:B:1357:THR:N | 2.27 | 0.47 |
| 2:B:833:LEU:HG | 2:B:835:LEU:HD13 | 1.97 | 0.47 |
| 2:D:1056:GLN:NE2 | 2:D:1082:VAL:HG22 | 2.29 | 0.47 |
| 2:D:1186:SER:O | 2:D:1189:VAL:HG23 | 2.13 | 0.47 |
| 2:D:1193:GLY:O | 2:D:1202:LEU:HD23 | 2.14 | 0.47 |
| 3:E:182:PHE:CE1 | 3:E:206:ILE:HG22 | 2.50 | 0.47 |
| 2:B:1312:HIS:HE1 | 3:E:237:GLN:HE22 | 1.62 | 0.47 |
| 1:A:431:LEU:HD12 | 1:A:431:LEU:C | 2.35 | 0.47 |
| 1:A:83:MET:HE2 | 1:A:505:ARG:NH1 | 2.28 | 0.47 |
| 2:B:960:GLU:HB3 | 2:B:1332:VAL:O | 2.15 | 0.47 |
| 2:B:949:PRO:HG3 | 2:B:958:GLN:OE1 | 2.15 | 0.47 |
| 1:C:508:ARG:HH12 | 1:C:512:GLN:CB | 2.27 | 0.47 |
| 1:C:105:PHE:CZ | 1:C:658:ALA:HA | 2.50 | 0.47 |
| 2:D:831:ILE:N | 2:D:923:ASP:OD2 | 2.47 | 0.47 |
| 1:A:42:MET:HE1 | 1:A:57:VAL:HG13 | 1.95 | 0.47 |
| 1:A:496:ASN:OD1 | 1:A:496:ASN:C | 2.52 | 0.47 |
| 2:B:1549:LEU:HD13 | 2:B:1563:MET:HE2 | 1.96 | 0.47 |
| 2:B:913:LYS:HZ2 | 2:B:913:LYS:HG2 | 1.31 | 0.47 |
| 1:C:203:GLN:NE2 | 1:C:223:GLU:OE1 | 2.47 | 0.47 |
| 1:C:386:ARG:HG2 | 1:C:400:LEU:HD21 | 1.96 | 0.47 |
| 1:C:465:LEU:HD12 | 1:C:555:VAL:HG22 | 1.96 | 0.47 |
| 2:D:1310:ARG:HH21 | 3:F:235:ILE:HG12 | 1.80 | 0.47 |
| 1:A:169:ASN:HD21 | 1:A:173:ILE:HB | 1.79 | 0.47 |
| 1:A:491:THR:O | 1:A:533:ALA:HA | 2.14 | 0.47 |
| 2:B:1434:LEU:HD23 | 2:B:1434:LEU:HA | 1.81 | 0.47 |
| 1:C:135:ASP:HB3 | 1:C:146:LEU:CD1 | 2.42 | 0.47 |
| 1:C:229:LEU:CD2 | 1:C:601:GLY:HA3 | 2.45 | 0.47 |
| 2:D:995:VAL:HG13 | 2:D:1027:TYR:CE2 | 2.50 | 0.47 |
| 2:D:1261:TYR:OH | 2:D:1268:SER:HB3 | 2.14 | 0.47 |
| 2:D:932:VAL:HG13 | 2:D:933:PRO:HD2 | 1.96 | 0.47 |
| 3:E:107:ALA:N | 3:E:130:ARG:HH12 | 2.13 | 0.47 |
| 3:F:105:ASN:OD1 | 3:F:106:SER:N | 2.48 | 0.47 |
| 1:A:151:THR:HG21 | 1:A:182:SER:HB3 | 1.95 | 0.47 |
| 1:C:463:THR:O | 1:C:465:LEU:N | 2.48 | 0.47 |
| 2:D:1061:GLN:CG | 2:D:1062:PRO:HD2 | 2.45 | 0.47 |
| 2:D:1102:GLY:HA2 | 2:D:1105:LYS:CE | 2.45 | 0.47 |
| 2:D:985:THR:HA | 2:D:986:PRO:HD3 | 1.83 | 0.47 |
| 2:D:987:VAL:CG2 | 2:D:988:ALA:N | 2.77 | 0.47 |
| 1:A:35:ARG:HD3 | 1:A:154:HIS:CD2 | 2.49 | 0.47 |
| 1:A:458:LEU:HD11 | 1:A:533:ALA:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:492:TYR:HB2 | 1:A:531:LEU:HD11 | 1.96 | 0.47 |
| 2:D:1136:ASN:CA | 2:D:1139:LYS:HE2 | 2.45 | 0.47 |
| 2:D:1160:GLU:OE2 | 3:E:117:ASN:HB2 | 2.15 | 0.47 |
| 2:D:772:LEU:O | 2:D:774:ASN:N | 2.47 | 0.47 |
| 3:E:104:LEU:O | 3:E:130:ARG:NH2 | 2.48 | 0.47 |
| 2:B:1039:LEU:HD12 | 2:B:1039:LEU:HA | 1.57 | 0.46 |
| 2:B:913:LYS:HG3 | 2:B:914:ALA:N | 2.30 | 0.46 |
| 2:B:970:GLN:NE2 | 2:B:974:THR:O | 2.48 | 0.46 |
| 2:B:980:ILE:HG22 | 2:B:1344:VAL:HG13 | 1.97 | 0.46 |
| 1:C:150:PHE:CZ | 2:D:807:VAL:HG21 | 2.51 | 0.46 |
| 1:C:32:ASN:HD21 | 1:C:657:ARG:CD | 2.01 | 0.46 |
| 1:C:647:THR:HG23 | 1:C:653:GLN:HB3 | 1.97 | 0.46 |
| 1:C:636:ALA:HB1 | 1:C:654:THR:HA | 1.96 | 0.46 |
| 2:D:1366:THR:OG1 | 2:D:1387:GLU:HB3 | 2.15 | 0.46 |
| 1:C:575:PRO:HG2 | 2:D:824:THR:O | 2.16 | 0.46 |
| 2:D:904:LYS:HG3 | 2:D:908:GLN:HE22 | 1.79 | 0.46 |
| 1:A:130:LEU:HB2 | 1:A:218:PHE:HD2 | 1.80 | 0.46 |
| 1:A:299:GLU:OE1 | 1:A:299:GLU:N | 2.48 | 0.46 |
| 2:B:833:LEU:HD21 | 2:B:910:VAL:HG12 | 1.96 | 0.46 |
| 2:B:861:LYS:HD3 | 2:B:887:THR:HG23 | 1.96 | 0.46 |
| 1:C:463:THR:O | 1:C:465:LEU:HD23 | 2.15 | 0.46 |
| 2:D:1217:LYS:NZ | 2:D:1251:PRO:HG2 | 2.30 | 0.46 |
| 2:D:1450:LYS:HG3 | 2:D:1451:VAL:N | 2.25 | 0.46 |
| 1:C:157:LEU:HD21 | 2:D:811:ASP:O | 2.15 | 0.46 |
| 2:D:877:THR:HG23 | 2:D:879:LYS:N | 2.30 | 0.46 |
| 2:D:894:LEU:HA | 2:D:894:LEU:HD12 | 1.72 | 0.46 |
| 3:F:226:PRO:O | 3:F:276:TRP:NE1 | 2.44 | 0.46 |
| 1:A:104:LYS:HG2 | 1:A:105:PHE:N | 2.30 | 0.46 |
| 1:A:215:GLN:HG2 | 1:A:216:GLN:H | 1.79 | 0.46 |
| 2:B:1191:ILE:HG13 | 2:B:1191:ILE:H | 1.43 | 0.46 |
| 2:B:1413:PRO:HD2 | 2:B:1441:ARG:HD2 | 1.96 | 0.46 |
| 1:C:36:LEU:HD11 | 1:C:92:ALA:N | 2.30 | 0.46 |
| 1:A:195:ILE:O | 1:A:195:ILE:HG13 | 2.15 | 0.46 |
| 1:A:456:LEU:HB2 | 1:A:535:TYR:CE2 | 2.47 | 0.46 |
| 2:B:1060:ARG:CZ | 2:B:1099:VAL:HG13 | 2.45 | 0.46 |
| 1:C:353:TYR:CE1 | 1:C:387:VAL:HG21 | 2.49 | 0.46 |
| 1:C:569:GLN:HB2 | 1:C:570:SER:H | 1.49 | 0.46 |
| 2:D:1294:LEU:HB3 | 2:D:1311:ILE:HG23 | 1.97 | 0.46 |
| 2:D:1554:LEU:HD12 | 2:D:1555:SER:N | 2.30 | 0.46 |
| 2:D:1640:GLU:O | 2:D:1643:GLN:HG2 | 2.15 | 0.46 |
| 3:F:113:TYR:HA | 3:F:116:GLN:CD | 2.36 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1174:ASP:OD1 | 2:B:1175:PHE:HD2 | 1.98 | 0.46 |
| 2:B:1265:GLY:N | 2:B:1268:SER:OG | 2.48 | 0.46 |
| 2:B:1512:ARG:HH12 | 2:B:1610:ASP:HA | 1.80 | 0.46 |
| 2:D:1066:PHE:CE1 | 2:D:1082:VAL:HG11 | 2.51 | 0.46 |
| 2:D:1152:GLN:O | 2:D:1155:LYS:HB2 | 2.16 | 0.46 |
| 2:D:1275:VAL:HG13 | 2:D:1276:PHE:CD1 | 2.51 | 0.46 |
| 2:D:974:THR:HB | 2:D:1349:HIS:HD2 | 1.80 | 0.46 |
| 2:D:1492:PHE:N | 2:D:1492:PHE:CD1 | 2.63 | 0.46 |
| 3:E:107:ALA:O | 3:E:130:ARG:NH1 | 2.49 | 0.46 |
| 2:B:1384:MET:HE3 | 2:B:1411:PHE:CZ | 2.50 | 0.46 |
| 2:B:1541:VAL:HG13 | 2:B:1570:LYS:NZ | 2.30 | 0.46 |
| 2:B:878:THR:HG21 | 2:B:1624:LYS:NZ | 2.30 | 0.46 |
| 1:C:484:GLU:HA | 1:C:487:ILE:CD1 | 2.46 | 0.46 |
| 3:F:136:GLU:CB | 3:F:159:LYS:HE2 | 2.39 | 0.46 |
| 1:A:303:SER:OG | 1:A:306:VAL:HG12 | 2.16 | 0.46 |
| 2:B:1243:LEU:HA | 2:B:1243:LEU:HD23 | 1.50 | 0.46 |
| 2:B:1311:ILE:HD11 | 2:B:1320:ARG:HD2 | 1.98 | 0.46 |
| 1:C:599:ASP:O | 1:C:601:GLY:N | 2.48 | 0.46 |
| 2:D:1207:LEU:HA | 2:D:1207:LEU:HD12 | 1.52 | 0.46 |
| 2:D:1469:VAL:HG13 | 2:D:1472:ILE:HG22 | 1.97 | 0.46 |
| 2:D:764:ARG:HH12 | 2:D:923:ASP:CG | 2.12 | 0.46 |
| 1:A:167:ILE:HD12 | 1:A:193:TRP:CE2 | 2.51 | 0.46 |
| 1:A:273:PHE:CE1 | 1:A:326:VAL:HG12 | 2.51 | 0.46 |
| 2:B:1136:ASN:CA | 2:B:1139:LYS:HZ1 | 2.20 | 0.46 |
| 2:B:1189:VAL:CG1 | 2:B:1213:THR:HG21 | 2.43 | 0.46 |
| 2:B:1268:SER:O | 2:B:1272:THR:HG23 | 2.16 | 0.46 |
| 1:C:429:GLN:C | 1:C:431:LEU:H | 2.20 | 0.46 |
| 1:C:631:SER:O | 1:C:641:ASP:OD2 | 2.33 | 0.46 |
| 2:D:1413:PRO:HD2 | 2:D:1441:ARG:HD2 | 1.97 | 0.46 |
| 2:D:841:ARG:NH1 | 2:D:902:PRO:O | 2.49 | 0.46 |
| 1:C:175:VAL:O | 2:D:979:ARG:NH1 | 2.48 | 0.46 |
| 3:F:175:ASP:HB3 | 3:F:187:SER:OG | 2.16 | 0.46 |
| 1:A:104:LYS:HG3 | 1:A:105:PHE:H | 1.81 | 0.46 |
| 1:A:492:TYR:CZ | 1:A:504:GLY:HA3 | 2.51 | 0.46 |
| 2:B:999:ARG:NH1 | 2:B:1262:TYR:CZ | 2.84 | 0.46 |
| 2:D:1025:VAL:HG23 | 2:D:1026:HIS:N | 2.30 | 0.46 |
| 2:D:1472:ILE:HD11 | 2:D:1494:HIS:CD2 | 2.51 | 0.46 |
| 3:F:245:TYR:CD1 | 3:F:245:TYR:N | 2.84 | 0.46 |
| 2:B:977:GLU:HG2 | 2:B:1347:MET:HG2 | 1.98 | 0.46 |
| 2:D:1400:MET:HE1 | 2:D:1448:LEU:N | 2.31 | 0.46 |
| 2:D:1492:PHE:CE2 | 2:D:1500:GLY:HA3 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:979:ARG:NH1 | 2:D:979:ARG:HG3 | 2.31 | 0.46 |
| 3:E:131:PRO:HA | 3:E:132:GLY:HA2 | 1.45 | 0.46 |
| 2:B:1312:HIS:CE1 | 3:E:237:GLN:HE22 | 2.34 | 0.46 |
| 3:F:149:LEU:HD12 | 3:F:149:LEU:HA | 1.48 | 0.46 |
| 1:A:478:ARG:NH1 | 1:A:479:MET:O | 2.49 | 0.45 |
| 1:A:467:PRO:HA | 1:A:521:ILE:HG22 | 1.97 | 0.45 |
| 1:A:67:LEU:CD2 | 1:A:68:VAL:H | 2.29 | 0.45 |
| 2:B:1264:GLY:H | 2:B:1272:THR:HG21 | 1.81 | 0.45 |
| 2:B:1478:LYS:HA | 2:B:1489:CYS:O | 2.16 | 0.45 |
| 2:B:1594:LEU:HB3 | 2:B:1596:LEU:HG | 1.98 | 0.45 |
| 2:B:949:PRO:HG3 | 2:B:958:GLN:NE2 | 2.30 | 0.45 |
| 2:D:1190:ALA:HA | 2:D:1220:TRP:CZ3 | 2.34 | 0.45 |
| 3:E:207:SER:OG | 3:E:208:GLY:N | 2.47 | 0.45 |
| 2:B:1524:ASP:HA | 2:B:1527:VAL:CG2 | 2.46 | 0.45 |
| 1:C:135:ASP:OD1 | 1:C:135:ASP:N | 2.47 | 0.45 |
| 2:D:1215:LYS:HD2 | 2:D:1216:ASP:N | 2.31 | 0.45 |
| 3:E:156:GLU:C | 3:E:156:GLU:OE2 | 2.55 | 0.45 |
| 2:B:1206:LEU:C | 2:B:1206:LEU:HD12 | 2.36 | 0.45 |
| 1:C:148:ARG:NH2 | 2:D:773:TRP:CE3 | 2.84 | 0.45 |
| 3:F:163:CYS:HB2 | 3:F:180:ILE:O | 2.16 | 0.45 |
| 2:B:1014:ASN:ND2 | 2:B:1055:GLN:HG3 | 2.31 | 0.45 |
| 2:B:1326:GLU:OE1 | 2:B:1326:GLU:N | 2.49 | 0.45 |
| 2:B:1532:ARG:HH21 | 2:B:1629:GLU:CD | 2.20 | 0.45 |
| 2:B:982:LEU:HG | 2:B:1311:ILE:HD13 | 1.98 | 0.45 |
| 1:C:466:ARG:H | 1:C:469:GLU:CD | 2.19 | 0.45 |
| 2:D:1317:SER:OG | 2:D:1320:ARG:NH2 | 2.50 | 0.45 |
| 2:D:1397:ASP:OD1 | 2:D:1453:HIS:N | 2.49 | 0.45 |
| 3:E:245:TYR:CD1 | 3:E:246:ARG:HB2 | 2.51 | 0.45 |
| 3:F:197:PHE:CB | 3:F:221:ARG:NH1 | 2.79 | 0.45 |
| 1:A:169:ASN:HB2 | 1:A:170:PRO:CD | 2.46 | 0.45 |
| 1:A:240:GLU:HB3 | 1:A:242:PHE:CE1 | 2.52 | 0.45 |
| 1:A:25:MET:HE2 | 1:A:47:HIS:HD2 | 1.82 | 0.45 |
| 1:A:35:ARG:NH2 | 1:A:498:GLY:HA3 | 2.32 | 0.45 |
| 1:A:575:PRO:HA | 1:A:579:GLN:OE1 | 2.17 | 0.45 |
| 2:B:1209:LYS:O | 2:B:1213:THR:OG1 | 2.18 | 0.45 |
| 2:B:1367:ILE:HD12 | 2:B:1385:ILE:O | 2.17 | 0.45 |
| 2:B:1429:ILE:HD13 | 2:B:1445:ILE:O | 2.17 | 0.45 |
| 2:B:772:LEU:O | 2:B:774:ASN:N | 2.49 | 0.45 |
| 1:C:427:LYS:HE3 | 1:C:427:LYS:HB3 | 1.74 | 0.45 |
| 1:C:573:ARG:NE | 1:C:579:GLN:HE21 | 2.15 | 0.45 |
| 2:D:1554:LEU:CD1 | 2:D:1591:ARG:CZ | 2.95 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:143:SER:H | 1:A:195:ILE:HD11 | 1.81 | 0.45 |
| 2:B:1407:MET:HE1 | 2:B:1463:VAL:CG1 | 2.47 | 0.45 |
| 2:D:1108:ILE:HD12 | 2:D:1168:SER:CB | 2.46 | 0.45 |
| 2:D:1105:LYS:HB2 | 2:D:1162:VAL:HG21 | 1.97 | 0.45 |
| 3:E:203:PHE:CD2 | 3:E:205:LEU:HB3 | 2.52 | 0.45 |
| 2:B:1308:THR:O | 3:E:238:GLY:HA2 | 2.17 | 0.45 |
| 3:F:198:GLY:HA3 | 3:F:218:PRO:HB3 | 1.99 | 0.45 |
| 1:A:93:ASN:ND2 | 1:A:95:GLU:HG2 | 2.31 | 0.45 |
| 2:B:1534:ASP:OD1 | 2:B:1535:LYS:N | 2.50 | 0.45 |
| 2:D:1554:LEU:HD12 | 2:D:1555:SER:H | 1.81 | 0.45 |
| 2:D:1577:GLN:N | 2:D:1577:GLN:OE1 | 2.49 | 0.45 |
| 3:E:132:GLY:O | 3:E:161:LYS:HB2 | 2.16 | 0.45 |
| 1:A:76:LEU:HG | 1:A:82:HIS:CA | 2.46 | 0.45 |
| 2:B:1300:LEU:HD23 | 2:B:1324:THR:CG2 | 2.39 | 0.45 |
| 2:B:1544:VAL:HB | 2:B:1605:TRP:HB3 | 1.97 | 0.45 |
| 2:B:949:PRO:HD3 | 2:B:958:GLN:HE22 | 1.81 | 0.45 |
| 2:D:1542:ASP:O | 2:D:1570:LYS:HE2 | 2.17 | 0.45 |
| 2:D:1544:VAL:HG22 | 2:D:1605:TRP:CB | 2.46 | 0.45 |
| 2:D:781:PRO:HA | 2:D:782:PRO:HD3 | 1.78 | 0.45 |
| 1:A:293:ILE:HG13 | 1:A:293:ILE:O | 2.17 | 0.45 |
| 2:B:1117:VAL:CA | 2:B:1144:THR:HG21 | 2.45 | 0.45 |
| 2:B:1180:TYR:CZ | 2:B:1189:VAL:HG22 | 2.52 | 0.45 |
| 2:B:1245:ASP:O | 2:B:1249:VAL:HG23 | 2.17 | 0.45 |
| 2:B:1403:LEU:HB2 | 2:B:1446:ILE:O | 2.17 | 0.45 |
| 2:B:1489:CYS:SG | 2:B:1491:ARG:NH1 | 2.90 | 0.45 |
| 1:A:595:LEU:HD11 | 2:B:791:MET:HE1 | 1.98 | 0.45 |
| 1:C:225:LYS:HG2 | 1:C:226:GLU:N | 2.31 | 0.45 |
| 1:C:579:GLN:H | 2:D:795:LEU:HD11 | 1.82 | 0.45 |
| 1:C:569:GLN:N | 1:C:582:THR:OG1 | 2.50 | 0.45 |
| 2:D:1138:GLU:OE2 | 2:D:1185:ARG:HD2 | 2.17 | 0.45 |
| 2:D:841:ARG:NH1 | 2:D:903:LEU:C | 2.70 | 0.45 |
| 2:D:983:GLN:HB3 | 2:D:1341:THR:HG1 | 1.81 | 0.45 |
| 3:E:226:PRO:CD | 3:E:276:TRP:HH2 | 2.29 | 0.45 |
| 1:A:462:ARG:NH2 | 1:A:463:THR:C | 2.69 | 0.45 |
| 1:A:569:GLN:N | 1:A:582:THR:OG1 | 2.49 | 0.45 |
| 1:A:70:SER:OG | 1:A:88:PHE:HB2 | 2.17 | 0.45 |
| 2:B:1053:TYR:CD2 | 2:B:1086:PHE:HE2 | 2.35 | 0.45 |
| 2:B:1202:LEU:CB | 2:B:1206:LEU:HD11 | 2.46 | 0.45 |
| 2:B:1207:LEU:HD12 | 2:B:1207:LEU:HA | 1.42 | 0.45 |
| 2:B:1415:THR:HG23 | 2:B:1416:ASP:N | 2.32 | 0.45 |
| 2:B:1549:LEU:O | 2:B:1599:LYS:N | 2.37 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:480:ASP:OD1 | 1:C:480:ASP:N | 2.50 | 0.45 |
| 2:D:1497:LYS:O | 2:D:1500:GLY:N | 2.50 | 0.45 |
| 2:D:1558:PHE:N | 2:D:1558:PHE:CD1 | 2.85 | 0.45 |
| 2:D:1550:VAL:CG2 | 2:D:1581:GLN:HE22 | 2.29 | 0.45 |
| 2:D:1564:ALA:HB2 | 2:D:1581:GLN:NE2 | 2.31 | 0.45 |
| 2:D:810:SER:O | 2:D:814:GLY:N | 2.46 | 0.45 |
| 3:E:195:LYS:CE | 3:E:197:PHE:HE1 | 2.27 | 0.45 |
| 3:F:156:GLU:OE2 | 3:F:158:CYS:O | 2.35 | 0.45 |
| 1:A:125:LEU:HD12 | 1:A:125:LEU:N | 2.31 | 0.44 |
| 2:B:1577:GLN:O | 2:B:1580:GLN:NE2 | 2.50 | 0.44 |
| 2:B:1662:PRO:O | 2:B:1663:ASN:HB2 | 2.16 | 0.44 |
| 2:B:945:ARG:HD2 | 2:B:960:GLU:OE2 | 2.16 | 0.44 |
| 1:C:76:LEU:HD13 | 1:C:82:HIS:O | 2.17 | 0.44 |
| 2:D:1536:ALA:HB2 | 2:D:1605:TRP:CZ3 | 2.52 | 0.44 |
| 3:E:226:PRO:N | 3:E:276:TRP:CH2 | 2.78 | 0.44 |
| 3:F:246:ARG:NH1 | 3:F:246:ARG:HG2 | 2.29 | 0.44 |
| 1:A:167:ILE:CG1 | 1:A:176:LYS:HB3 | 2.47 | 0.44 |
| 1:A:185:GLN:NE2 | 3:E:245:TYR:CE1 | 2.86 | 0.44 |
| 2:B:1418:LEU:HA | 2:B:1421:LEU:HD22 | 2.00 | 0.44 |
| 2:B:1494:HIS:ND1 | 2:B:1497:LYS:CB | 2.79 | 0.44 |
| 1:C:106:VAL:HG12 | 1:C:123:VAL:HG23 | 1.99 | 0.44 |
| 2:D:999:ARG:NH1 | 2:D:999:ARG:HG3 | 2.31 | 0.44 |
| 1:A:646:PHE:H | 1:A:654:THR:CG2 | 2.30 | 0.44 |
| 2:B:1060:ARG:HG3 | 2:B:1060:ARG:NH1 | 2.30 | 0.44 |
| 2:B:1086:PHE:O | 2:B:1090:VAL:HG13 | 2.16 | 0.44 |
| 2:B:1561:TYR:HB3 | 2:B:1563:MET:CE | 2.47 | 0.44 |
| 2:B:1576:VAL:HB | 2:B:1580:GLN:NE2 | 2.33 | 0.44 |
| 2:B:1607:LEU:C | 2:B:1610:ASP:OD1 | 2.56 | 0.44 |
| 1:C:324:LEU:HB2 | 1:C:346:ILE:HG13 | 1.99 | 0.44 |
| 1:C:389:VAL:HG12 | 1:C:426:THR:HG22 | 1.98 | 0.44 |
| 2:D:1328:GLU:OE1 | 2:D:1330:PHE:HD2 | 1.99 | 0.44 |
| 2:D:1365:VAL:HG13 | 2:D:1386:LEU:HD11 | 1.99 | 0.44 |
| 2:D:812:LYS:HD2 | 2:D:812:LYS:HA | 1.69 | 0.44 |
| 3:E:231:ILE:HD11 | 3:E:234:GLY:HA3 | 1.98 | 0.44 |
| 3:E:236:ILE:HB | 3:E:239:GLU:HG2 | 1.99 | 0.44 |
| 1:A:386:ARG:HH11 | 1:A:386:ARG:HG3 | 1.82 | 0.44 |
| 2:B:1076:THR:H | 2:B:1076:THR:HG23 | 1.39 | 0.44 |
| 1:C:186:LEU:HA | 1:C:186:LEU:HD13 | 1.69 | 0.44 |
| 2:D:994:ALA:HB1 | 2:D:1027:TYR:OH | 2.18 | 0.44 |
| 2:D:1492:PHE:CZ | 2:D:1499:ASP:O | 2.71 | 0.44 |
| 2:D:911:GLU:HA | 2:D:925:VAL:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1015:MET:CG | 2:B:1056:GLN:NE2 | 2.80 | 0.44 |
| 2:B:948:ASP:OD2 | 2:B:951:ARG:NE | 2.51 | 0.44 |
| 1:C:496:ASN:C | 1:C:498:GLY:N | 2.70 | 0.44 |
| 2:D:1153:GLU:N | 2:D:1153:GLU:OE1 | 2.50 | 0.44 |
| 2:D:1651:ALA:O | 2:D:1655:SER:HB3 | 2.18 | 0.44 |
| 1:A:268:THR:HB | 2:B:1447:TYR:OH | 2.18 | 0.44 |
| 2:B:1312:HIS:CA | 2:B:1313:TRP:CE3 | 3.00 | 0.44 |
| 2:B:1407:MET:CE | 2:B:1463:VAL:HB | 2.48 | 0.44 |
| 2:B:951:ARG:HH21 | 2:B:1339:GLN:CG | 2.17 | 0.44 |
| 1:C:398:GLN:CD | 1:C:427:LYS:HE2 | 2.38 | 0.44 |
| 2:D:1067:ALA:CA | 2:D:1078:LEU:HD21 | 2.47 | 0.44 |
| 2:D:1190:ALA:CA | 2:D:1220:TRP:HZ3 | 2.22 | 0.44 |
| 1:C:561:GLY:N | 2:D:813:LYS:CE | 2.80 | 0.44 |
| 1:A:169:ASN:ND2 | 1:A:173:ILE:HB | 2.33 | 0.44 |
| 2:B:992:GLU:HA | 2:B:992:GLU:OE1 | 2.18 | 0.44 |
| 1:C:479:MET:HB3 | 1:C:479:MET:HE2 | 1.67 | 0.44 |
| 2:D:997:ALA:O | 2:D:1037:PHE:HE2 | 2.00 | 0.44 |
| 2:D:833:LEU:HG | 2:D:835:LEU:HD13 | 1.98 | 0.44 |
| 3:E:165:ASN:OD1 | 3:E:166:PRO:HD2 | 2.18 | 0.44 |
| 1:A:161:ARG:HH22 | 1:A:212:ASN:ND2 | 2.16 | 0.44 |
| 1:A:479:MET:CG | 1:A:484:GLU:HG3 | 2.48 | 0.44 |
| 1:A:465:LEU:HD11 | 1:A:521:ILE:HD13 | 1.99 | 0.44 |
| 2:B:1136:ASN:HA | 2:B:1139:LYS:HE3 | 1.99 | 0.44 |
| 2:B:1230:VAL:HG12 | 2:B:1275:VAL:CG2 | 2.47 | 0.44 |
| 2:B:1312:HIS:HA | 2:B:1313:TRP:HE3 | 1.81 | 0.44 |
| 2:B:1363:LEU:HD21 | 2:B:1477:VAL:HG12 | 1.98 | 0.44 |
| 2:B:879:LYS:HZ1 | 2:B:1521:GLN:HE22 | 1.65 | 0.44 |
| 2:B:1652:PHE:HE1 | 2:B:1656:MET:HE3 | 1.82 | 0.44 |
| 1:C:55:VAL:HA | 1:C:111:THR:O | 2.18 | 0.44 |
| 1:C:291:ILE:HA | 1:C:292:PRO:HD3 | 1.70 | 0.44 |
| 1:C:385:TYR:CD2 | 1:C:403:GLY:HA2 | 2.52 | 0.44 |
| 1:C:496:ASN:CB | 1:C:501:LEU:HG | 2.34 | 0.44 |
| 1:C:67:LEU:HD12 | 1:C:68:VAL:N | 2.27 | 0.44 |
| 2:D:793:ILE:HD12 | 2:D:794:PHE:H | 1.83 | 0.44 |
| 2:D:947:LEU:HD12 | 2:D:947:LEU:H | 1.80 | 0.44 |
| 3:E:146:LEU:HD12 | 3:E:150:LYS:H | 1.83 | 0.44 |
| 3:E:282:GLU:OE2 | 3:E:284:ARG:CG | 2.66 | 0.44 |
| 1:A:351:SER:OG | 1:A:353:TYR:O | 2.36 | 0.44 |
| 1:A:242:PHE:HD2 | 1:A:379:PRO:HG2 | 1.81 | 0.44 |
| 2:B:1077:TRP:CE2 | 2:B:1130:ILE:CD1 | 3.00 | 0.44 |
| 2:B:1444:LEU:HG | 2:B:1445:ILE:N | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1554:LEU:HD13 | 2:B:1591:ARG:CZ | 2.48 | 0.44 |
| 1:C:106:VAL:HG12 | 1:C:123:VAL:CG2 | 2.48 | 0.44 |
| 1:C:198:LEU:HD13 | 2:D:975:GLU:OE2 | 2.18 | 0.44 |
| 1:C:26:TYR:HB2 | 1:C:649:SER:HB3 | 1.99 | 0.44 |
| 2:D:1061:GLN:O | 2:D:1062:PRO:C | 2.55 | 0.44 |
| 2:D:1300:LEU:O | 2:D:1300:LEU:HD12 | 2.18 | 0.44 |
| 2:D:771:TRP:CE3 | 2:D:772:LEU:HB2 | 2.53 | 0.44 |
| 3:F:110:LYS:O | 3:F:114:ILE:HG13 | 2.18 | 0.44 |
| 2:B:1479:VAL:HG12 | 2:B:1480:TYR:N | 2.33 | 0.43 |
| 2:B:838:SER:HB2 | 2:B:932:VAL:CG2 | 2.47 | 0.43 |
| 1:C:169:ASN:HB2 | 1:C:170:PRO:CD | 2.48 | 0.43 |
| 1:C:420:LEU:HD11 | 1:C:422:ILE:HD11 | 2.00 | 0.43 |
| 2:D:1063:SER:HA | 2:D:1106:TRP:CZ3 | 2.53 | 0.43 |
| 2:D:1641:GLU:OE1 | 2:D:1641:GLU:N | 2.50 | 0.43 |
| 3:E:212:GLN:HG3 | 3:E:213:TRP:N | 2.33 | 0.43 |
| 1:A:270:PHE:CE1 | 1:A:290:ARG:HD3 | 2.53 | 0.43 |
| 2:B:1264:GLY:H | 2:B:1272:THR:CG2 | 2.31 | 0.43 |
| 2:B:1634:GLU:CD | 2:B:1634:GLU:C | 2.77 | 0.43 |
| 2:B:943:ALA:O | 2:B:1343:SER:HA | 2.19 | 0.43 |
| 1:C:563:LEU:HB3 | 2:D:818:ALA:HB2 | 1.98 | 0.43 |
| 2:D:1078:LEU:HD12 | 2:D:1078:LEU:C | 2.38 | 0.43 |
| 2:D:1554:LEU:HD12 | 2:D:1554:LEU:HA | 1.48 | 0.43 |
| 2:D:813:LYS:HA | 2:D:813:LYS:HD2 | 1.80 | 0.43 |
| 1:A:77:THR:OG1 | 1:A:80:THR:HG23 | 2.17 | 0.43 |
| 2:B:1077:TRP:NE1 | 2:B:1146:PHE:CZ | 2.86 | 0.43 |
| 2:B:1358:CYS:CB | 2:B:1361:PHE:O | 2.66 | 0.43 |
| 2:B:1368:LYS:O | 2:B:1385:ILE:HG22 | 2.18 | 0.43 |
| 2:B:1429:ILE:HD11 | 2:B:1433:GLU:CB | 2.48 | 0.43 |
| 2:B:1558:PHE:HD1 | 2:B:1587:PRO:HA | 1.81 | 0.43 |
| 1:C:60:HIS:NE2 | 1:C:109:GLN:HB2 | 2.33 | 0.43 |
| 1:C:332:LEU:C | 1:C:334:SER:H | 2.21 | 0.43 |
| 1:C:77:THR:H | 1:C:80:THR:HG22 | 1.83 | 0.43 |
| 2:D:942:VAL:HG21 | 2:D:1346:THR:HG23 | 2.00 | 0.43 |
| 2:D:1498:GLU:C | 2:D:1500:GLY:N | 2.64 | 0.43 |
| 2:D:997:ALA:H | 2:D:1036:LYS:CE | 2.30 | 0.43 |
| 1:A:552:TRP:CH2 | 1:A:554:ASP:HB2 | 2.54 | 0.43 |
| 2:B:1238:LEU:HD11 | 2:B:1277:GLN:NE2 | 2.25 | 0.43 |
| 2:B:1465:GLN:HG2 | 2:B:1465:GLN:O | 2.18 | 0.43 |
| 2:B:1506:CYS:HA | 2:B:1511:CYS:HA | 2.00 | 0.43 |
| 2:B:1503:ASN:OD1 | 2:B:1515:GLU:HG2 | 2.18 | 0.43 |
| 1:C:90:ILE:HG13 | 1:C:90:ILE:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1303:ARG:NH1 | 3:F:241:ASP:OD1 | 2.52 | 0.43 |
| 1:A:130:LEU:HD13 | 1:A:210:TYR:OH | 2.18 | 0.43 |
| 2:B:792:ASN:ND2 | 2:B:792:ASN:O | 2.26 | 0.43 |
| 2:B:884:GLN:HG3 | 2:B:885:THR:N | 2.33 | 0.43 |
| 1:C:263:LYS:HE3 | 1:C:263:LYS:HB2 | 1.63 | 0.43 |
| 2:D:1317:SER:OG | 2:D:1318:LEU:N | 2.51 | 0.43 |
| 2:D:1515:GLU:HA | 2:D:1589:LYS:HZ3 | 1.84 | 0.43 |
| 3:E:170:ARG:C | 3:E:171:ASN:OD1 | 2.56 | 0.43 |
| 3:F:106:SER:HB3 | 3:F:158:CYS:HB2 | 1.99 | 0.43 |
| 2:B:1300:LEU:CD1 | 2:B:1300:LEU:O | 2.63 | 0.43 |
| 2:B:1348:TYR:HD1 | 2:B:1349:HIS:C | 2.22 | 0.43 |
| 2:B:1360:LYS:HG3 | 2:B:1487:GLU:HB3 | 2.01 | 0.43 |
| 2:B:1502:LEU:HA | 2:B:1502:LEU:HD12 | 1.79 | 0.43 |
| 2:B:1559:ASP:OD1 | 2:B:1586:SER:N | 2.51 | 0.43 |
| 2:B:932:VAL:HG12 | 2:B:933:PRO:HD2 | 2.00 | 0.43 |
| 1:C:599:ASP:C | 1:C:601:GLY:N | 2.70 | 0.43 |
| 2:D:1214:ALA:HB2 | 2:D:1220:TRP:NE1 | 2.31 | 0.43 |
| 2:D:756:ILE:HG12 | 2:D:761:ILE:HD11 | 2.00 | 0.43 |
| 2:D:856:GLN:HG2 | 2:D:857:ASN:H | 1.83 | 0.43 |
| 2:D:899:VAL:HG23 | 2:D:1473:GLN:NE2 | 2.32 | 0.43 |
| 2:D:971:VAL:HG12 | 2:D:1349:HIS:CB | 2.48 | 0.43 |
| 3:E:223:ILE:HD11 | 3:E:269:VAL:CG2 | 2.42 | 0.43 |
| 3:E:226:PRO:O | 3:E:276:TRP:CH2 | 2.71 | 0.43 |
| 3:F:116:GLN:NE2 | 3:F:119:PHE:HE1 | 2.15 | 0.43 |
| 2:B:1083:VAL:HG13 | 2:B:1100:LEU:HD11 | 2.00 | 0.43 |
| 2:B:1214:ALA:HB2 | 2:B:1220:TRP:CD2 | 2.54 | 0.43 |
| 2:B:1360:LYS:HA | 2:B:1360:LYS:HE2 | 2.01 | 0.43 |
| 2:B:831:ILE:CD1 | 2:B:925:VAL:HG23 | 2.48 | 0.43 |
| 1:C:58:THR:OG1 | 1:C:60:HIS:HE1 | 2.02 | 0.43 |
| 2:D:1015:MET:HA | 2:D:1015:MET:CE | 2.49 | 0.43 |
| 2:D:1536:ALA:HB3 | 2:D:1652:PHE:HZ | 1.83 | 0.43 |
| 3:E:197:PHE:HB2 | 3:E:219:GLU:HG2 | 2.01 | 0.43 |
| 1:A:99:GLU:HA | 1:A:100:LYS:HA | 1.72 | 0.43 |
| 1:A:166:ASN:HD21 | 1:A:174:PRO:CB | 2.31 | 0.43 |
| 1:A:181:SER:H | 3:E:246:ARG:NE | 2.17 | 0.43 |
| 1:A:338:MET:HE2 | 2:B:1485:LEU:HB2 | 2.00 | 0.43 |
| 1:A:27:SER:OG | 1:A:45:GLU:HB2 | 2.19 | 0.43 |
| 1:A:471:LEU:CB | 1:A:521:ILE:HD11 | 2.43 | 0.43 |
| 1:A:634:ASP:OD1 | 1:A:637:GLY:N | 2.51 | 0.43 |
| 2:B:753:GLU:O | 2:B:755:ILE:HG23 | 2.18 | 0.43 |
| 1:C:120:VAL:HB | 1:C:656:GLN:NE2 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1207:LEU:O | 2:D:1210:PHE:HB3 | 2.18 | 0.43 |
| 2:D:1464:HIS:HB2 | 2:D:1466:TYR:CZ | 2.53 | 0.43 |
| 2:D:1652:PHE:CE1 | 2:D:1656:MET:HE2 | 2.53 | 0.43 |
| 3:E:146:LEU:HG | 3:E:150:LYS:CB | 2.40 | 0.43 |
| 3:E:193:GLY:O | 3:E:223:ILE:HG23 | 2.19 | 0.43 |
| 3:E:236:ILE:CG2 | 3:E:239:GLU:HG2 | 2.49 | 0.43 |
| 1:A:30:THR:HG22 | 1:A:645:THR:HG1 | 1.84 | 0.43 |
| 2:B:1060:ARG:NH1 | 2:B:1099:VAL:HG13 | 2.34 | 0.43 |
| 2:B:1154:ALA:O | 2:B:1157:ILE:HG13 | 2.19 | 0.43 |
| 2:B:1206:LEU:HD12 | 2:B:1207:LEU:N | 2.34 | 0.43 |
| 2:B:1425:VAL:O | 2:B:1426:ASP:HB2 | 2.18 | 0.43 |
| 2:B:807:VAL:HG22 | 2:B:817:VAL:HG22 | 2.01 | 0.43 |
| 2:B:949:PRO:CG | 2:B:958:GLN:HE22 | 2.31 | 0.43 |
| 1:C:175:VAL:HB | 2:D:979:ARG:NH2 | 2.34 | 0.43 |
| 1:C:205:LYS:HD2 | 1:C:221:GLU:HG2 | 2.01 | 0.43 |
| 2:D:1507:ARG:HG3 | 2:D:1507:ARG:O | 2.19 | 0.43 |
| 2:D:759:GLU:O | 2:D:760:ASN:ND2 | 2.52 | 0.43 |
| 2:D:813:LYS:O | 2:D:813:LYS:HG3 | 2.18 | 0.43 |
| 3:E:224:TYR:CD1 | 3:E:224:TYR:N | 2.87 | 0.43 |
| 3:F:245:TYR:H | 3:F:245:TYR:HD1 | 1.65 | 0.43 |
| 1:A:26:TYR:CD1 | 1:A:26:TYR:N | 2.87 | 0.43 |
| 1:A:550:SER:OG | 1:A:631:SER:N | 2.52 | 0.43 |
| 2:B:1576:VAL:HG12 | 2:B:1582:ARG:HH21 | 1.82 | 0.43 |
| 1:C:312:GLN:H | 1:C:312:GLN:CD | 2.16 | 0.43 |
| 2:D:1237:LEU:HD22 | 2:D:1256:LEU:CD2 | 2.48 | 0.43 |
| 2:D:1496:GLU:HG2 | 2:D:1497:LYS:N | 2.34 | 0.43 |
| 2:D:872:PHE:HE1 | 2:D:902:PRO:HB3 | 1.84 | 0.43 |
| 2:D:962:ILE:HG12 | 2:D:1330:PHE:CE1 | 2.53 | 0.43 |
| 3:E:120:PRO:HG2 | 3:E:123:THR:CG2 | 2.49 | 0.43 |
| 1:A:161:ARG:O | 1:A:181:SER:HA | 2.19 | 0.42 |
| 1:A:490:TYR:OH | 1:A:508:ARG:HD2 | 2.19 | 0.42 |
| 2:B:781:PRO:HA | 2:B:782:PRO:HD3 | 1.87 | 0.42 |
| 1:C:66:LYS:HD3 | 3:E:147:GLN:HG2 | 2.00 | 0.42 |
| 1:C:70:SER:OG | 1:C:88:PHE:HB2 | 2.19 | 0.42 |
| 2:D:1023:ILE:HD12 | 2:D:1023:ILE:HA | 1.91 | 0.42 |
| 2:D:1310:ARG:CD | 2:D:1312:HIS:NE2 | 2.82 | 0.42 |
| 2:D:1400:MET:HE1 | 2:D:1447:TYR:HB3 | 2.01 | 0.42 |
| 2:D:1400:MET:HE2 | 2:D:1447:TYR:HB3 | 2.00 | 0.42 |
| 2:D:851:LEU:HD23 | 2:D:862:VAL:HG21 | 2.01 | 0.42 |
| 3:E:125:VAL:HG23 | 3:E:143:LEU:HG | 2.01 | 0.42 |
| 3:E:132:GLY:HA2 | 3:E:161:LYS:HZ3 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:111:THR:CG2 | 1:A:116:VAL:HG23 | 2.42 | 0.42 |
| 1:A:277:ASP:O | 1:A:280:GLN:HG2 | 2.18 | 0.42 |
| 1:A:420:LEU:O | 1:A:443:ALA:N | 2.48 | 0.42 |
| 1:A:637:GLY:O | 1:A:641:ASP:HB2 | 2.19 | 0.42 |
| 2:B:1115:ASP:O | 2:B:1175:PHE:CG | 2.71 | 0.42 |
| 2:B:1118:PHE:N | 2:B:1144:THR:CG2 | 2.79 | 0.42 |
| 2:B:1429:ILE:HD11 | 2:B:1433:GLU:CG | 2.48 | 0.42 |
| 2:B:1559:ASP:OD2 | 2:B:1561:TYR:CZ | 2.71 | 0.42 |
| 2:B:783:LYS:HE3 | 3:F:197:PHE:CD1 | 2.55 | 0.42 |
| 1:C:449:VAL:HG23 | 1:C:449:VAL:O | 2.19 | 0.42 |
| 2:D:1208:ASN:O | 2:D:1211:LEU:HG | 2.18 | 0.42 |
| 2:D:1225:LYS:HE3 | 2:D:1227:LEU:CD1 | 2.48 | 0.42 |
| 2:D:1659:PHE:CE2 | 2:D:1662:PRO:HD3 | 2.49 | 0.42 |
| 2:D:874:SER:HB3 | 2:D:900:ILE:HG22 | 2.01 | 0.42 |
| 2:D:916:VAL:HG22 | 2:D:921:ILE:O | 2.19 | 0.42 |
| 3:F:97:SER:OG | 3:F:98:CYS:O | 2.36 | 0.42 |
| 1:A:366:PRO:HD2 | 1:A:455:TYR:CZ | 2.54 | 0.42 |
| 1:A:532:VAL:HG11 | 1:A:644:LEU:HD12 | 2.01 | 0.42 |
| 1:A:46:ALA:HB3 | 1:A:76:LEU:HD11 | 2.01 | 0.42 |
| 2:B:1128:GLU:HG3 | 2:B:1267:GLY:HA2 | 2.00 | 0.42 |
| 2:B:982:LEU:HD22 | 2:B:1296:VAL:HG11 | 2.00 | 0.42 |
| 2:B:1303:ARG:CZ | 2:B:1307:ILE:HG12 | 2.49 | 0.42 |
| 2:B:1347:MET:HE3 | 2:B:1347:MET:HB2 | 1.81 | 0.42 |
| 1:C:641:ASP:OD1 | 1:C:642:ALA:N | 2.53 | 0.42 |
| 2:D:1047:GLU:HG3 | 2:D:1051:LYS:HZ2 | 1.84 | 0.42 |
| 2:D:1061:GLN:OE1 | 2:D:1061:GLN:HA | 2.20 | 0.42 |
| 2:D:1494:HIS:ND1 | 2:D:1496:GLU:OE1 | 2.52 | 0.42 |
| 2:D:1507:ARG:NH1 | 2:D:1613:GLY:HA2 | 2.34 | 0.42 |
| 2:D:752:ASP:CG | 2:D:753:GLU:H | 2.23 | 0.42 |
| 2:D:759:GLU:O | 2:D:760:ASN:CG | 2.57 | 0.42 |
| 2:D:839:VAL:HG22 | 2:D:929:LEU:CD1 | 2.49 | 0.42 |
| 2:D:756:ILE:HD11 | 3:F:134:ARG:HH12 | 1.82 | 0.42 |
| 1:A:444:LEU:HG | 1:A:445:PRO:HD2 | 2.00 | 0.42 |
| 2:B:1010:CYS:O | 2:B:1012:GLU:N | 2.53 | 0.42 |
| 2:B:1408:MET:HG3 | 2:B:1411:PHE:HB2 | 2.01 | 0.42 |
| 2:B:896:VAL:HA | 2:B:897:PRO:HD3 | 1.76 | 0.42 |
| 1:C:488:ARG:O | 1:C:508:ARG:N | 2.48 | 0.42 |
| 1:C:495:MET:CE | 1:C:625:ILE:HD11 | 2.49 | 0.42 |
| 2:D:1258:GLU:OE1 | 2:D:1258:GLU:N | 2.49 | 0.42 |
| 3:F:131:PRO:HA | 3:F:132:GLY:HA2 | 1.35 | 0.42 |
| 1:A:120:VAL:HG11 | 2:B:1039:LEU:HD23 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:147:TYR:CZ | 1:A:191:LEU:HG | 2.54 | 0.42 |
| 1:A:385:TYR:C | 1:A:386:ARG:HG2 | 2.40 | 0.42 |
| 2:B:1117:VAL:HA | 2:B:1144:THR:CG2 | 2.47 | 0.42 |
| 1:C:508:ARG:HG2 | 1:C:509:GLU:N | 2.34 | 0.42 |
| 2:D:1368:LYS:O | 2:D:1385:ILE:HG13 | 2.19 | 0.42 |
| 2:D:1501:LYS:HD2 | 2:D:1557:ASP:OD2 | 2.19 | 0.42 |
| 2:D:1603:LEU:HD22 | 2:D:1649:LEU:CD1 | 2.49 | 0.42 |
| 2:D:948:ASP:OD2 | 2:D:951:ARG:CZ | 2.67 | 0.42 |
| 2:D:959:LYS:HE3 | 2:D:961:ASP:OD1 | 2.20 | 0.42 |
| 3:E:157:PHE:N | 3:E:157:PHE:CD1 | 2.84 | 0.42 |
| 3:E:258:THR:O | 3:E:283:CYS:HA | 2.19 | 0.42 |
| 1:A:354:GLN:O | 1:A:376:VAL:HA | 2.18 | 0.42 |
| 1:A:428:LYS:O | 1:A:431:LEU:HG | 2.20 | 0.42 |
| 1:C:65:LYS:HB3 | 1:C:65:LYS:HE3 | 1.48 | 0.42 |
| 2:D:1118:PHE:HD2 | 2:D:1144:THR:CG2 | 2.32 | 0.42 |
| 2:D:985:THR:HB | 2:D:1339:GLN:O | 2.19 | 0.42 |
| 2:D:1544:VAL:CG2 | 2:D:1570:LYS:HD3 | 2.46 | 0.42 |
| 3:E:143:LEU:CD1 | 3:E:151:TRP:CE3 | 3.03 | 0.42 |
| 1:A:43:VAL:HG21 | 1:A:493:LEU:HD23 | 2.00 | 0.42 |
| 2:B:1167:GLY:O | 2:B:1171:LYS:HB2 | 2.20 | 0.42 |
| 1:C:422:ILE:HD12 | 1:C:422:ILE:HG23 | 1.67 | 0.42 |
| 1:C:529:PHE:CZ | 1:C:553:VAL:HG11 | 2.55 | 0.42 |
| 2:D:1237:LEU:HD22 | 2:D:1256:LEU:HD21 | 2.02 | 0.42 |
| 2:D:1470:GLU:C | 2:D:1471:LEU:HD22 | 2.40 | 0.42 |
| 2:D:1562:ILE:CG1 | 2:D:1562:ILE:O | 2.67 | 0.42 |
| 1:A:28:ILE:HA | 1:A:28:ILE:HD12 | 1.75 | 0.42 |
| 1:A:253:VAL:CG1 | 1:A:300:VAL:HG13 | 2.50 | 0.42 |
| 1:A:232:PHE:CE1 | 1:A:339:VAL:HG23 | 2.55 | 0.42 |
| 1:A:46:ALA:O | 1:A:82:HIS:CG | 2.72 | 0.42 |
| 2:B:1084:LYS:HE3 | 2:B:1149:ILE:CD1 | 2.49 | 0.42 |
| 2:B:1141:MET:HG3 | 2:B:1183:LEU:HD11 | 2.02 | 0.42 |
| 1:C:391:VAL:HG13 | 1:C:397:VAL:HG11 | 2.02 | 0.42 |
| 1:C:35:ARG:NH1 | 1:C:40:GLU:OE2 | 2.37 | 0.42 |
| 2:D:1300:LEU:HD11 | 2:D:1303:ARG:HB2 | 2.00 | 0.42 |
| 2:D:1403:LEU:HB2 | 2:D:1446:ILE:O | 2.19 | 0.42 |
| 3:E:157:PHE:H | 3:E:157:PHE:HD1 | 1.65 | 0.42 |
| 3:F:245:TYR:O | 3:F:246:ARG:HB2 | 2.19 | 0.42 |
| 1:A:37:GLU:OE2 | 1:A:127:SER:HB3 | 2.19 | 0.42 |
| 1:A:88:PHE:HE2 | 1:A:90:ILE:HD11 | 1.85 | 0.42 |
| 2:B:1149:ILE:HA | 2:B:1152:GLN:OE1 | 2.19 | 0.42 |
| 2:B:1144:THR:HB | 2:B:1176:LEU:HD11 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1554:LEU:HD13 | 2:B:1591:ARG:NH2 | 2.34 | 0.42 |
| 1:C:473:VAL:HG11 | 1:C:517:LEU:HD23 | 2.01 | 0.42 |
| 1:C:102:ARG:NH2 | 2:D:1035:GLU:HB3 | 2.35 | 0.42 |
| 2:D:1225:LYS:HE2 | 2:D:1228:TYR:CZ | 2.55 | 0.42 |
| 2:D:1508:ASP:CG | 2:D:1509:GLU:N | 2.70 | 0.42 |
| 2:D:877:THR:HG23 | 2:D:880:ARG:H | 1.85 | 0.42 |
| 3:E:135:ARG:CZ | 3:E:137:PRO:HA | 2.49 | 0.42 |
| 3:E:237:GLN:HB3 | 3:E:250:THR:CG2 | 2.42 | 0.42 |
| 3:F:156:GLU:O | 3:F:159:LYS:HE3 | 2.19 | 0.42 |
| 1:A:28:ILE:HD11 | 1:A:42:MET:HG3 | 2.01 | 0.42 |
| 1:A:449:VAL:O | 1:A:449:VAL:HG23 | 2.20 | 0.42 |
| 2:B:981:LEU:HD11 | 2:B:1343:SER:OG | 2.19 | 0.42 |
| 2:B:1502:LEU:HD11 | 2:B:1515:GLU:HG3 | 2.02 | 0.42 |
| 2:B:960:GLU:O | 2:B:960:GLU:HG3 | 2.20 | 0.42 |
| 1:C:324:LEU:HB2 | 1:C:346:ILE:HD11 | 2.02 | 0.42 |
| 1:C:659:GLU:N | 1:C:659:GLU:CD | 2.72 | 0.42 |
| 2:D:1313:TRP:HE3 | 2:D:1318:LEU:HD21 | 1.83 | 0.42 |
| 2:D:962:ILE:HD11 | 2:D:1330:PHE:CE2 | 2.54 | 0.42 |
| 2:D:1408:MET:HB2 | 2:D:1411:PHE:CD1 | 2.55 | 0.42 |
| 2:D:1544:VAL:HG23 | 2:D:1570:LYS:CD | 2.45 | 0.42 |
| 3:E:246:ARG:CZ | 3:E:266:TYR:HB2 | 2.50 | 0.42 |
| 3:F:113:TYR:CA | 3:F:116:GLN:HG2 | 2.47 | 0.42 |
| 3:F:109:LEU:HD22 | 3:F:125:VAL:CG1 | 2.50 | 0.42 |
| 1:A:471:LEU:C | 1:A:471:LEU:HD12 | 2.41 | 0.41 |
| 2:B:911:GLU:HA | 2:B:925:VAL:O | 2.19 | 0.41 |
| 1:C:293:ILE:HG13 | 1:C:293:ILE:O | 2.20 | 0.41 |
| 1:C:55:VAL:HG23 | 1:C:74:THR:HG22 | 2.02 | 0.41 |
| 2:D:1027:TYR:CE2 | 2:D:1031:THR:HG21 | 2.54 | 0.41 |
| 2:D:1310:ARG:HH21 | 3:F:235:ILE:CG1 | 2.33 | 0.41 |
| 2:D:1471:LEU:HD13 | 2:D:1471:LEU:HA | 1.58 | 0.41 |
| 2:D:1479:VAL:O | 2:D:1480:TYR:HB3 | 2.19 | 0.41 |
| 2:D:948:ASP:OD2 | 2:D:951:ARG:NH2 | 2.53 | 0.41 |
| 3:E:243:TYR:CZ | 3:E:249:VAL:HG12 | 2.55 | 0.41 |
| 2:B:1111:LYS:HA | 2:B:1111:LYS:HD2 | 1.64 | 0.41 |
| 2:B:1549:LEU:HD11 | 2:B:1551:LYS:O | 2.20 | 0.41 |
| 2:B:752:ASP:HB3 | 2:B:753:GLU:H | 1.54 | 0.41 |
| 1:C:244:TYR:CE2 | 1:C:246:TYR:HB2 | 2.56 | 0.41 |
| 2:D:1077:TRP:CE2 | 2:D:1130:ILE:HG22 | 2.55 | 0.41 |
| 2:D:1216:ASP:OD1 | 2:D:1216:ASP:C | 2.57 | 0.41 |
| 2:D:1220:TRP:CE3 | 2:D:1236:ALA:HB2 | 2.56 | 0.41 |
| 2:D:1131:GLY:C | 2:D:1228:TYR:HE1 | 2.22 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:951:ARG:HH22 | 2:D:1339:GLN:HB3 | 1.84 | 0.41 |
| 3:F:103:ARG:O | 3:F:104:LEU:HD23 | 2.20 | 0.41 |
| 3:F:206:ILE:O | 3:F:206:ILE:HG13 | 2.20 | 0.41 |
| 3:F:207:SER:OG | 3:F:208:GLY:N | 2.51 | 0.41 |
| 1:A:65:LYS:HB2 | 1:A:65:LYS:HE3 | 1.69 | 0.41 |
| 1:A:67:LEU:HD23 | 1:A:68:VAL:H | 1.85 | 0.41 |
| 2:B:1023:ILE:HG13 | 2:B:1276:PHE:HB2 | 2.03 | 0.41 |
| 2:B:1348:TYR:HE1 | 2:B:1350:ALA:HB2 | 1.85 | 0.41 |
| 2:B:1592:GLU:O | 2:B:1595:LYS:HD2 | 2.20 | 0.41 |
| 2:B:1505:LEU:HD23 | 2:B:1621:ILE:HG21 | 2.03 | 0.41 |
| 3:E:224:TYR:CD2 | 3:E:242:HIS:CD2 | 3.08 | 0.41 |
| 1:A:185:GLN:NE2 | 3:E:245:TYR:HE1 | 2.18 | 0.41 |
| 1:A:475:PHE:HB2 | 1:A:515:VAL:HG23 | 2.02 | 0.41 |
| 1:A:535:TYR:CZ | 1:A:547:VAL:HB | 2.56 | 0.41 |
| 2:B:875:LEU:HD23 | 2:B:875:LEU:HA | 1.74 | 0.41 |
| 1:C:230:PRO:CB | 1:C:339:VAL:HG22 | 2.50 | 0.41 |
| 2:D:1136:ASN:O | 2:D:1137:ASN:HB2 | 2.20 | 0.41 |
| 2:D:798:SER:HB2 | 2:D:802:TRP:HZ2 | 1.85 | 0.41 |
| 3:F:194:TYR:HE1 | 3:F:222:GLU:HB3 | 1.85 | 0.41 |
| 1:A:332:LEU:C | 1:A:334:SER:H | 2.24 | 0.41 |
| 1:A:414:HIS:HA | 1:A:415:PRO:HD3 | 1.93 | 0.41 |
| 1:A:487:ILE:HA | 1:A:487:ILE:HD12 | 1.83 | 0.41 |
| 1:A:608:LYS:HB3 | 1:A:608:LYS:HE2 | 1.84 | 0.41 |
| 2:B:1187:TYR:CD1 | 2:B:1232:ALA:HB2 | 2.50 | 0.41 |
| 2:B:1403:LEU:HD12 | 2:B:1448:LEU:HD11 | 2.02 | 0.41 |
| 1:C:457:HIS:ND1 | 1:C:457:HIS:C | 2.73 | 0.41 |
| 1:C:599:ASP:HB2 | 2:D:802:TRP:HZ3 | 1.83 | 0.41 |
| 2:D:1117:VAL:HG12 | 2:D:1175:PHE:CD2 | 2.55 | 0.41 |
| 2:D:983:GLN:OE1 | 2:D:1319:LEU:HD21 | 2.20 | 0.41 |
| 3:E:139:LEU:HA | 3:E:139:LEU:HD12 | 1.81 | 0.41 |
| 3:E:206:ILE:O | 3:E:206:ILE:HG13 | 2.16 | 0.41 |
| 2:B:783:LYS:NZ | 3:F:197:PHE:HD1 | 2.18 | 0.41 |
| 3:F:268:THR:HG22 | 3:F:275:GLU:O | 2.20 | 0.41 |
| 3:F:98:CYS:HA | 3:F:149:LEU:HD11 | 2.02 | 0.41 |
| 1:A:125:LEU:HD12 | 1:A:126:GLN:H | 1.86 | 0.41 |
| 1:A:159:VAL:O | 1:A:182:SER:OG | 2.38 | 0.41 |
| 1:A:273:PHE:CD1 | 1:A:326:VAL:HG12 | 2.55 | 0.41 |
| 2:B:1128:GLU:HA | 2:B:1134:ARG:CZ | 2.50 | 0.41 |
| 1:C:144:THR:HG22 | 1:C:194:ASP:OD1 | 2.20 | 0.41 |
| 1:C:368:MET:O | 1:C:413:THR:CG2 | 2.68 | 0.41 |
| 1:C:100:LYS:HD3 | 2:D:1313:TRP:CH2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1425:VAL:O | 2:D:1426:ASP:HB2 | 2.20 | 0.41 |
| 2:D:1545:TYR:CG | 2:D:1565:ILE:HD12 | 2.55 | 0.41 |
| 2:D:1643:GLN:HE21 | 2:D:1644:LYS:HZ3 | 1.69 | 0.41 |
| 2:D:888:ILE:HA | 2:D:889:PRO:HD3 | 1.89 | 0.41 |
| 2:D:909:GLU:OE2 | 2:D:926:ARG:HD2 | 2.20 | 0.41 |
| 2:D:833:LEU:HD13 | 2:D:912:VAL:HG11 | 2.03 | 0.41 |
| 2:D:863:ARG:HG2 | 2:D:915:ALA:O | 2.21 | 0.41 |
| 2:B:841:ARG:O | 2:B:842:ASN:OD1 | 2.39 | 0.41 |
| 2:B:981:LEU:O | 2:B:1342:LEU:HD12 | 2.20 | 0.41 |
| 1:C:275:ILE:CG1 | 1:C:282:ILE:HB | 2.51 | 0.41 |
| 2:D:860:LEU:O | 2:D:888:ILE:HG22 | 2.20 | 0.41 |
| 2:D:880:ARG:HD3 | 2:D:880:ARG:HH11 | 1.72 | 0.41 |
| 2:D:913:LYS:HE3 | 2:D:913:LYS:HB2 | 1.60 | 0.41 |
| 3:E:120:PRO:HD2 | 3:E:123:THR:HG21 | 2.03 | 0.41 |
| 3:E:250:THR:HA | 3:E:264:SER:HB2 | 2.01 | 0.41 |
| 1:A:178:ASP:OD1 | 1:A:179:SER:N | 2.53 | 0.41 |
| 1:A:161:ARG:NH2 | 1:A:212:ASN:ND2 | 2.69 | 0.41 |
| 1:A:273:PHE:CG | 1:A:302:LEU:HD22 | 2.55 | 0.41 |
| 1:A:232:PHE:CZ | 1:A:339:VAL:HG23 | 2.55 | 0.41 |
| 1:C:134:THR:HG22 | 1:C:147:TYR:HB3 | 2.02 | 0.41 |
| 1:C:156:LEU:HA | 1:C:156:LEU:HD23 | 1.77 | 0.41 |
| 1:C:491:THR:HG22 | 1:C:505:ARG:CD | 2.50 | 0.41 |
| 2:D:1476:ALA:HA | 2:D:1492:PHE:HA | 2.02 | 0.41 |
| 3:E:109:LEU:CB | 3:E:114:ILE:HG12 | 2.43 | 0.41 |
| 3:F:110:LYS:HG3 | 3:F:126:GLU:O | 2.20 | 0.41 |
| 3:F:120:PRO:HG2 | 3:F:123:THR:OG1 | 2.21 | 0.41 |
| 1:A:104:LYS:CG | 1:A:105:PHE:H | 2.33 | 0.41 |
| 1:A:473:VAL:HG21 | 1:A:531:LEU:CD2 | 2.51 | 0.41 |
| 1:A:59:VAL:HG12 | 1:A:69:LEU:HB2 | 2.03 | 0.41 |
| 2:D:1062:PRO:O | 2:D:1106:TRP:CZ3 | 2.74 | 0.41 |
| 2:D:1311:ILE:CD1 | 2:D:1318:LEU:HA | 2.50 | 0.41 |
| 2:D:1631:TRP:CZ3 | 2:D:1633:GLU:HA | 2.54 | 0.41 |
| 3:E:146:LEU:HD12 | 3:E:150:LYS:N | 2.35 | 0.41 |
| 1:A:104:LYS:HE3 | 1:A:104:LYS:HB2 | 1.70 | 0.41 |
| 1:A:253:VAL:HG12 | 1:A:300:VAL:HG13 | 2.03 | 0.41 |
| 1:A:617:TRP:CE3 | 1:A:617:TRP:HA | 2.56 | 0.41 |
| 2:B:1076:THR:OG1 | 2:B:1120:GLU:OE1 | 2.27 | 0.41 |
| 2:B:1256:LEU:N | 2:B:1256:LEU:HD13 | 2.36 | 0.41 |
| 2:B:1453:HIS:ND1 | 2:B:1453:HIS:C | 2.74 | 0.41 |
| 2:B:1559:ASP:OD2 | 2:B:1561:TYR:CE2 | 2.74 | 0.41 |
| 1:C:170:PRO:HD3 | 1:C:204:TRP:CE2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1197:ALA:HA | 2:D:1202:LEU:HG | 2.02 | 0.41 |
| 2:D:1313:TRP:CG | 2:D:1314:GLU:N | 2.88 | 0.41 |
| 2:D:1550:VAL:HG23 | 2:D:1562:ILE:HG13 | 2.02 | 0.41 |
| 3:F:181:LEU:HA | 3:F:181:LEU:HD23 | 1.60 | 0.41 |
| 1:A:291:ILE:HA | 1:A:292:PRO:HD3 | 1.71 | 0.41 |
| 1:A:360:THR:HG21 | 1:A:372:LEU:HD23 | 2.02 | 0.41 |
| 2:B:1325:LYS:HE2 | 2:B:1325:LYS:HB3 | 1.81 | 0.41 |
| 2:B:1418:LEU:HA | 2:B:1418:LEU:HD23 | 2.00 | 0.41 |
| 2:B:1417:ASP:O | 2:B:1421:LEU:HD22 | 2.21 | 0.41 |
| 2:B:1471:LEU:HA | 2:B:1471:LEU:HD13 | 1.95 | 0.41 |
| 2:B:1636:GLU:O | 2:B:1639:ASP:HB2 | 2.21 | 0.41 |
| 1:C:351:SER:C | 1:C:353:TYR:H | 2.23 | 0.41 |
| 1:C:569:GLN:OE1 | 1:C:581:MET:SD | 2.79 | 0.41 |
| 2:D:1124:VAL:O | 2:D:1127:GLN:HG2 | 2.21 | 0.41 |
| 2:D:1505:LEU:HA | 2:D:1505:LEU:HD23 | 1.67 | 0.41 |
| 1:C:592:ARG:HB2 | 2:D:777:ASP:OD1 | 2.21 | 0.41 |
| 3:E:249:VAL:CG2 | 3:E:265:ILE:HG22 | 2.50 | 0.41 |
| 3:F:116:GLN:NE2 | 3:F:119:PHE:CE1 | 2.89 | 0.41 |
| 3:F:143:LEU:HD23 | 3:F:143:LEU:HA | 1.76 | 0.41 |
| 1:A:449:VAL:HG21 | 1:A:545:GLU:CG | 2.45 | 0.40 |
| 1:A:576:VAL:HG13 | 1:A:577:PRO:HD2 | 2.03 | 0.40 |
| 2:B:1403:LEU:HD23 | 2:B:1479:VAL:HG22 | 2.03 | 0.40 |
| 2:B:753:GLU:N | 2:B:753:GLU:OE1 | 2.45 | 0.40 |
| 1:A:261:TYR:HD2 | 2:B:826:MET:SD | 2.45 | 0.40 |
| 2:B:996:ASP:OD1 | 2:B:999:ARG:N | 2.54 | 0.40 |
| 1:C:646:PHE:H | 1:C:654:THR:HG23 | 1.80 | 0.40 |
| 1:C:55:VAL:CG2 | 1:C:74:THR:HG22 | 2.50 | 0.40 |
| 2:D:1171:LYS:O | 2:D:1174:ASP:HB2 | 2.21 | 0.40 |
| 2:D:1240:LEU:CD1 | 2:D:1248:PHE:HB3 | 2.51 | 0.40 |
| 2:D:934:GLU:HB2 | 2:D:1354:ASP:O | 2.22 | 0.40 |
| 2:D:1496:GLU:HG2 | 2:D:1497:LYS:H | 1.86 | 0.40 |
| 2:D:762:VAL:O | 2:D:924:GLY:HA3 | 2.21 | 0.40 |
| 2:D:967:LEU:HD22 | 2:D:1348:TYR:CD2 | 2.56 | 0.40 |
| 3:E:229:PRO:HG2 | 3:E:280:PRO:CG | 2.46 | 0.40 |
| 2:B:1382:ASN:OD1 | 2:B:1383:THR:HG22 | 2.21 | 0.40 |
| 1:C:180:LEU:HD22 | 1:C:191:LEU:HD11 | 2.04 | 0.40 |
| 1:C:449:VAL:HG21 | 1:C:545:GLU:CG | 2.50 | 0.40 |
| 1:C:607:LYS:O | 1:C:607:LYS:HG3 | 2.21 | 0.40 |
| 2:D:1149:ILE:CD1 | 2:D:1153:GLU:OE2 | 2.69 | 0.40 |
| 2:D:1494:HIS:CE1 | 2:D:1497:LYS:HG3 | 2.56 | 0.40 |
| 2:D:796:LYS:HE2 | 3:F:168:GLU:OE2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:945:ARG:NH1 | 2:B:962:ILE:HG22 | 2.37 | 0.40 |
| 1:C:135:ASP:OD2 | 1:C:136:LYS:HG3 | 2.21 | 0.40 |
| 1:C:274:GLY:HA3 | 1:C:325:TYR:CZ | 2.56 | 0.40 |
| 1:C:229:LEU:HD21 | 1:C:601:GLY:HA3 | 2.04 | 0.40 |
| 2:D:1066:PHE:HB2 | 2:D:1078:LEU:CD1 | 2.47 | 0.40 |
| 2:D:1175:PHE:CE1 | 2:D:1179:ASN:ND2 | 2.90 | 0.40 |
| 2:D:1258:GLU:HA | 2:D:1260:ARG:HH11 | 1.76 | 0.40 |
| 2:D:1310:ARG:HD2 | 2:D:1312:HIS:CD2 | 2.56 | 0.40 |
| 2:D:935:GLY:CA | 2:D:1353:LYS:H | 2.30 | 0.40 |
| 2:D:1367:ILE:HD12 | 2:D:1367:ILE:HG23 | 1.83 | 0.40 |
| 2:D:1494:HIS:CE1 | 2:D:1496:GLU:CD | 2.94 | 0.40 |
| 2:D:756:ILE:HD12 | 3:F:134:ARG:NH2 | 2.34 | 0.40 |
| 3:F:127:TYR:HE2 | 3:F:143:LEU:HD12 | 1.87 | 0.40 |
| 1:A:183:GLN:O | 1:A:184:ASN:OD1 | 2.40 | 0.40 |
| 1:A:477:LEU:HD11 | 1:A:487:ILE:HG21 | 2.04 | 0.40 |
| 2:B:1130:ILE:CG2 | 2:B:1134:ARG:H | 2.35 | 0.40 |
| 2:B:1135:ASN:HB2 | 2:B:1185:ARG:NH2 | 2.37 | 0.40 |
| 2:B:1253:VAL:HG23 | 2:B:1253:VAL:H | 1.57 | 0.40 |
| 1:C:104:LYS:HD2 | 1:C:104:LYS:HA | 1.81 | 0.40 |
| 1:C:229:LEU:HD22 | 1:C:231:SER:H | 1.86 | 0.40 |
| 1:C:269:ALA:HB2 | 1:C:330:VAL:HG22 | 2.03 | 0.40 |
| 1:C:456:LEU:HB2 | 1:C:535:TYR:CE2 | 2.57 | 0.40 |
| 1:C:589:HIS:HB2 | 2:D:782:PRO:HB3 | 2.02 | 0.40 |
| 2:D:1132:GLY:HA3 | 2:D:1187:TYR:CZ | 2.57 | 0.40 |
| 2:D:1352:ALA:N | 2:D:1353:LYS:HA | 2.36 | 0.40 |
| 2:D:898:TYR:CA | 2:D:1473:GLN:HE22 | 2.34 | 0.40 |
| 2:D:1484:ASN:HB3 | 2:D:1487:GLU:CD | 2.42 | 0.40 |
| 2:D:1544:VAL:HG22 | 2:D:1605:TRP:HB2 | 2.04 | 0.40 |
| 2:D:778:LEU:HA | 2:D:778:LEU:HD12 | 1.83 | 0.40 |
| 3:E:133:TYR:CB | 3:E:158:CYS:HB3 | 2.47 | 0.40 |
| 1:A:156:LEU:HA | 1:A:156:LEU:HD23 | 1.88 | 0.40 |
| 1:A:480:ASP:O | 1:A:484:GLU:OE1 | 2.38 | 0.40 |
| 1:A:464:GLU:CB | 1:A:556:LYS:HE3 | 2.49 | 0.40 |
| 1:A:615:LYS:HE2 | 1:A:615:LYS:HB2 | 1.69 | 0.40 |
| 2:B:1249:VAL:O | 2:B:1253:VAL:HG23 | 2.21 | 0.40 |
| 2:B:1422:ALA:CB | 2:B:1429:ILE:HG22 | 2.52 | 0.40 |
| 2:B:1653:THR:HG23 | 2:B:1654:GLU:HG2 | 2.03 | 0.40 |
| 1:C:27:SER:OG | 1:C:45:GLU:HB2 | 2.21 | 0.40 |
| 1:C:67:LEU:HD21 | 1:C:69:LEU:HD12 | 2.03 | 0.40 |
| 2:D:1066:PHE:HB3 | 2:D:1078:LEU:HD11 | 2.02 | 0.40 |
| 2:D:1137:ASN:HB2 | 2:D:1185:ARG:HE | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:1241:LEU:HA | 2:D:1241:LEU:HD12 | 1.64 | 0.40 |
| 2:D:1217:LYS:O | 2:D:1251:PRO:HB2 | 2.21 | 0.40 |
| 3:F:143:LEU:HD22 | 3:F:152:SER:O | 2.22 | 0.40 |
| 3:F:106:SER:CB | 3:F:158:CYS:HB2 | 2.52 | 0.40 |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------------|--------------------------|-------------------|
| 1:A:77:THR:OG1 | 2:B:954:ARG:NH2[3_455] | 2.06 | 0.14 |
| 1:C:413:THR:O | 1:C:512:GLN:NE2[2_755] | 2.15 | 0.05 |
| 2:B:1577:GLN:NE2 | 3:E:133:TYR:OH[3_565] | 2.15 | 0.05 |
| 1:A:435:GLU:OE2 | 2:D:1431:LYS:NZ[2_755] | 2.19 | 0.01 |

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 | 640/645 (99%) | 598 (93%) | 37 (6%) | 5 (1%) | 24 | 70 |
| 1 | C | 640/645 (99%) | 599 (94%) | 34 (5%) | 7 (1%) | 17 | 64 |
| 2 | B | 898/915 (98%) | 822 (92%) | 58 (6%) | 18 (2%) | 9 | 54 |
| 2 | D | 898/915 (98%) | 818 (91%) | 57 (6%) | 23 (3%) | 7 | 48 |
| 3 | E | 187/194 (96%) | 165 (88%) | 17 (9%) | 5 (3%) | 6 | 47 |
| 3 | F | 187/194 (96%) | 165 (88%) | 17 (9%) | 5 (3%) | 6 | 47 |
| All | All | 3450/3508 (98%) | 3167 (92%) | 220 (6%) | 63 (2%) | 11 | 55 |

All (63) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 950 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1137 | ASN |
| 2 | B | 1286 | ALA |
| 2 | B | 1287 | PRO |
| 2 | B | 1573 | SER |
| 1 | C | 397 | VAL |
| 1 | C | 497 | LYS |
| 2 | D | 950 | GLU |
| 2 | D | 988 | ALA |
| 2 | D | 1497 | LYS |
| 3 | E | 239 | GLU |
| 3 | F | 239 | GLU |
| 1 | A | 397 | VAL |
| 1 | A | 497 | LYS |
| 1 | A | 540 | ALA |
| 2 | B | 957 | VAL |
| 2 | B | 992 | GLU |
| 2 | B | 1011 | GLY |
| 2 | B | 1264 | GLY |
| 2 | B | 1301 | PRO |
| 1 | C | 96 | PHE |
| 1 | C | 540 | ALA |
| 2 | D | 757 | ALA |
| 2 | D | 957 | VAL |
| 2 | D | 989 | GLN |
| 2 | D | 1011 | GLY |
| 2 | D | 1264 | GLY |
| 2 | D | 1289 | HIS |
| 2 | D | 1301 | PRO |
| 2 | D | 1358 | CYS |
| 1 | A | 600 | LYS |
| 2 | B | 1135 | ASN |
| 1 | C | 333 | HIS |
| 2 | D | 1498 | GLU |
| 2 | D | 1633 | GLU |
| 3 | E | 131 | PRO |
| 3 | F | 131 | PRO |
| 2 | B | 1317 | SER |
| 2 | B | 1354 | ASP |
| 2 | B | 1480 | TYR |
| 1 | C | 569 | GLN |
| 1 | C | 600 | LYS |
| 2 | D | 760 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 1064 | SER |
| 2 | D | 1480 | TYR |
| 2 | D | 1499 | ASP |
| 3 | E | 156 | GLU |
| 3 | E | 237 | GLN |
| 3 | F | 237 | GLN |
| 2 | B | 796 | LYS |
| 2 | B | 935 | GLY |
| 2 | B | 1508 | ASP |
| 2 | D | 1136 | ASN |
| 2 | D | 1286 | ALA |
| 2 | D | 1287 | PRO |
| 2 | D | 1317 | SER |
| 2 | D | 1508 | ASP |
| 1 | A | 333 | HIS |
| 2 | D | 1399 | THR |
| 3 | F | 137 | PRO |
| 3 | F | 155 | VAL |
| 3 | E | 137 | PRO |
| 2 | B | 1520 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 564/567 (100%) | 522 (93%) | 42 (7%) | 17 | 57 |
| 1 | C | 564/567 (100%) | 527 (93%) | 37 (7%) | 21 | 61 |
| 2 | B | 791/810 (98%) | 719 (91%) | 72 (9%) | 12 | 47 |
| 2 | D | 787/810 (97%) | 715 (91%) | 72 (9%) | 12 | 47 |
| 3 | E | 166/167 (99%) | 138 (83%) | 28 (17%) | 2 | 20 |
| 3 | F | 166/167 (99%) | 138 (83%) | 28 (17%) | 2 | 20 |
| All | All | 3038/3088 (98%) | 2759 (91%) | 279 (9%) | 11 | 46 |

All (279) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 26 | TYR |
| 1 | A | 30 | THR |
| 1 | A | 59 | VAL |
| 1 | A | 67 | LEU |
| 1 | A | 68 | VAL |
| 1 | A | 71 | SER |
| 1 | A | 76 | LEU |
| 1 | A | 83 | MET |
| 1 | A | 85 | ASN |
| 1 | A | 87 | THR |
| 1 | A | 89 | THR |
| 1 | A | 116 | VAL |
| 1 | A | 117 | VAL |
| 1 | A | 122 | LEU |
| 1 | A | 125 | LEU |
| 1 | A | 130 | LEU |
| 1 | A | 133 | GLN |
| 1 | A | 134 | THR |
| 1 | A | 163 | VAL |
| 1 | A | 177 | GLN |
| 1 | A | 213 | SER |
| 1 | A | 228 | VAL |
| 1 | A | 235 | ILE |
| 1 | A | 239 | THR |
| 1 | A | 242 | PHE |
| 1 | A | 252 | GLU |
| 1 | A | 293 | ILE |
| 1 | A | 306 | VAL |
| 1 | A | 330 | VAL |
| 1 | A | 413 | THR |
| 1 | A | 421 | SER |
| 1 | A | 423 | THR |
| 1 | A | 448 | THR |
| 1 | A | 463 | THR |
| 1 | A | 465 | LEU |
| 1 | A | 471 | LEU |
| 1 | A | 491 | THR |
| 1 | A | 496 | ASN |
| 1 | A | 583 | LEU |
| 1 | A | 605 | LEU |
| 1 | A | 622 | LYS |
| 1 | A | 650 | SER |
| 2 | B | 755 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 759 | GLU |
| 2 | B | 763 | SER |
| 2 | B | 774 | ASN |
| 2 | B | 792 | ASN |
| 2 | B | 826 | MET |
| 2 | B | 831 | ILE |
| 2 | B | 842 | ASN |
| 2 | B | 907 | LEU |
| 2 | B | 929 | LEU |
| 2 | B | 932 | VAL |
| 2 | B | 939 | ASN |
| 2 | B | 940 | LYS |
| 2 | B | 946 | THR |
| 2 | B | 952 | LEU |
| 2 | B | 957 | VAL |
| 2 | B | 962 | ILE |
| 2 | B | 981 | LEU |
| 2 | B | 982 | LEU |
| 2 | B | 983 | GLN |
| 2 | B | 991 | THR |
| 2 | B | 995 | VAL |
| 2 | B | 996 | ASP |
| 2 | B | 1048 | LEU |
| 2 | B | 1051 | LYS |
| 2 | B | 1070 | VAL |
| 2 | B | 1072 | ARG |
| 2 | B | 1085 | VAL |
| 2 | B | 1117 | VAL |
| 2 | B | 1130 | ILE |
| 2 | B | 1157 | ILE |
| 2 | B | 1170 | THR |
| 2 | B | 1189 | VAL |
| 2 | B | 1191 | ILE |
| 2 | B | 1206 | LEU |
| 2 | B | 1244 | LYS |
| 2 | B | 1250 | PRO |
| 2 | B | 1256 | LEU |
| 2 | B | 1260 | ARG |
| 2 | B | 1269 | THR |
| 2 | B | 1291 | GLU |
| 2 | B | 1292 | LEU |
| 2 | B | 1298 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1300 | LEU |
| 2 | B | 1311 | ILE |
| 2 | B | 1319 | LEU |
| 2 | B | 1320 | ARG |
| 2 | B | 1349 | HIS |
| 2 | B | 1356 | LEU |
| 2 | B | 1357 | THR |
| 2 | B | 1366 | THR |
| 2 | B | 1384 | MET |
| 2 | B | 1407 | MET |
| 2 | B | 1414 | ASP |
| 2 | B | 1421 | LEU |
| 2 | B | 1453 | HIS |
| 2 | B | 1499 | ASP |
| 2 | B | 1503 | ASN |
| 2 | B | 1504 | LYS |
| 2 | B | 1507 | ARG |
| 2 | B | 1508 | ASP |
| 2 | B | 1511 | CYS |
| 2 | B | 1522 | LYS |
| 2 | B | 1525 | ASP |
| 2 | B | 1544 | VAL |
| 2 | B | 1550 | VAL |
| 2 | B | 1610 | ASP |
| 2 | B | 1624 | LYS |
| 2 | B | 1628 | VAL |
| 2 | B | 1633 | GLU |
| 2 | B | 1634 | GLU |
| 2 | B | 1637 | CYS |
| 1 | C | 30 | THR |
| 1 | C | 35 | ARG |
| 1 | C | 41 | THR |
| 1 | C | 60 | HIS |
| 1 | C | 67 | LEU |
| 1 | C | 71 | SER |
| 1 | C | 77 | THR |
| 1 | C | 86 | VAL |
| 1 | C | 90 | ILE |
| 1 | C | 94 | ARG |
| 1 | C | 95 | GLU |
| 1 | C | 97 | LYS |
| 1 | C | 106 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 127 | SER |
| 1 | C | 146 | LEU |
| 1 | C | 191 | LEU |
| 1 | C | 226 | GLU |
| 1 | C | 229 | LEU |
| 1 | C | 293 | ILE |
| 1 | C | 301 | VAL |
| 1 | C | 302 | LEU |
| 1 | C | 338 | MET |
| 1 | C | 343 | ARG |
| 1 | C | 346 | ILE |
| 1 | C | 359 | LYS |
| 1 | C | 365 | LYS |
| 1 | C | 398 | GLN |
| 1 | C | 413 | THR |
| 1 | C | 441 | MET |
| 1 | C | 457 | HIS |
| 1 | C | 465 | LEU |
| 1 | C | 470 | THR |
| 1 | C | 473 | VAL |
| 1 | C | 546 | VAL |
| 1 | C | 547 | VAL |
| 1 | C | 560 | VAL |
| 1 | C | 605 | LEU |
| 2 | D | 756 | ILE |
| 2 | D | 762 | VAL |
| 2 | D | 795 | LEU |
| 2 | D | 796 | LYS |
| 2 | D | 807 | VAL |
| 2 | D | 824 | THR |
| 2 | D | 862 | VAL |
| 2 | D | 883 | GLN |
| 2 | D | 885 | THR |
| 2 | D | 886 | VAL |
| 2 | D | 904 | LYS |
| 2 | D | 907 | LEU |
| 2 | D | 912 | VAL |
| 2 | D | 936 | ILE |
| 2 | D | 937 | ARG |
| 2 | D | 939 | ASN |
| 2 | D | 946 | THR |
| 2 | D | 995 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 1016 | ILE |
| 2 | D | 1021 | THR |
| 2 | D | 1039 | LEU |
| 2 | D | 1050 | LYS |
| 2 | D | 1078 | LEU |
| 2 | D | 1107 | LEU |
| 2 | D | 1109 | LEU |
| 2 | D | 1117 | VAL |
| 2 | D | 1144 | THR |
| 2 | D | 1148 | LEU |
| 2 | D | 1149 | ILE |
| 2 | D | 1151 | LEU |
| 2 | D | 1152 | GLN |
| 2 | D | 1159 | GLU |
| 2 | D | 1161 | GLN |
| 2 | D | 1189 | VAL |
| 2 | D | 1191 | ILE |
| 2 | D | 1202 | LEU |
| 2 | D | 1215 | LYS |
| 2 | D | 1244 | LYS |
| 2 | D | 1256 | LEU |
| 2 | D | 1297 | SER |
| 2 | D | 1298 | LEU |
| 2 | D | 1302 | SER |
| 2 | D | 1315 | SER |
| 2 | D | 1320 | ARG |
| 2 | D | 1324 | THR |
| 2 | D | 1331 | THR |
| 2 | D | 1341 | THR |
| 2 | D | 1342 | LEU |
| 2 | D | 1356 | LEU |
| 2 | D | 1395 | ASP |
| 2 | D | 1423 | ASN |
| 2 | D | 1435 | ASP |
| 2 | D | 1440 | ASP |
| 2 | D | 1450 | LYS |
| 2 | D | 1485 | LEU |
| 2 | D | 1487 | GLU |
| 2 | D | 1491 | ARG |
| 2 | D | 1492 | PHE |
| 2 | D | 1506 | CYS |
| 2 | D | 1511 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 1528 | THR |
| 2 | D | 1529 | LEU |
| 2 | D | 1548 | ARG |
| 2 | D | 1550 | VAL |
| 2 | D | 1551 | LYS |
| 2 | D | 1552 | VAL |
| 2 | D | 1558 | PHE |
| 2 | D | 1563 | MET |
| 2 | D | 1585 | ILE |
| 2 | D | 1624 | LYS |
| 2 | D | 1628 | VAL |
| 2 | D | 1658 | VAL |
| 3 | E | 102 | THR |
| 3 | E | 104 | LEU |
| 3 | E | 105 | ASN |
| 3 | E | 129 | CYS |
| 3 | E | 143 | LEU |
| 3 | E | 146 | LEU |
| 3 | E | 150 | LYS |
| 3 | E | 156 | GLU |
| 3 | E | 160 | LYS |
| 3 | E | 163 | CYS |
| 3 | E | 170 | ARG |
| 3 | E | 171 | ASN |
| 3 | E | 174 | ILE |
| 3 | E | 181 | LEU |
| 3 | E | 185 | THR |
| 3 | E | 192 | THR |
| 3 | E | 199 | SER |
| 3 | E | 205 | LEU |
| 3 | E | 206 | ILE |
| 3 | E | 223 | ILE |
| 3 | E | 225 | CYS |
| 3 | E | 241 | ASP |
| 3 | E | 245 | TYR |
| 3 | E | 246 | ARG |
| 3 | E | 248 | SER |
| 3 | E | 253 | CYS |
| 3 | E | 265 | ILE |
| 3 | E | 283 | CYS |
| 3 | F | 102 | THR |
| 3 | F | 106 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | F | 113 | TYR |
| 3 | F | 135 | ARG |
| 3 | F | 145 | CYS |
| 3 | F | 146 | LEU |
| 3 | F | 155 | VAL |
| 3 | F | 156 | GLU |
| 3 | F | 157 | PHE |
| 3 | F | 159 | LYS |
| 3 | F | 163 | CYS |
| 3 | F | 174 | ILE |
| 3 | F | 180 | ILE |
| 3 | F | 185 | THR |
| 3 | F | 188 | PHE |
| 3 | F | 195 | LYS |
| 3 | F | 196 | LEU |
| 3 | F | 206 | ILE |
| 3 | F | 217 | LEU |
| 3 | F | 222 | GLU |
| 3 | F | 225 | CYS |
| 3 | F | 239 | GLU |
| 3 | F | 246 | ARG |
| 3 | F | 248 | SER |
| 3 | F | 253 | CYS |
| 3 | F | 255 | LYS |
| 3 | F | 272 | ASP |
| 3 | F | 283 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 81 | ASN |
| 1 | A | 126 | GLN |
| 1 | A | 184 | ASN |
| 1 | A | 212 | ASN |
| 1 | A | 216 | GLN |
| 1 | A | 453 | ASN |
| 1 | A | 609 | ASN |
| 2 | B | 774 | ASN |
| 2 | B | 842 | ASN |
| 2 | B | 1055 | GLN |
| 2 | B | 1056 | GLN |
| 2 | B | 1136 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1152 | GLN |
| 2 | B | 1277 | GLN |
| 2 | B | 1453 | HIS |
| 2 | B | 1580 | GLN |
| 2 | B | 1642 | ASN |
| 1 | C | 32 | ASN |
| 1 | C | 50 | GLN |
| 1 | C | 60 | HIS |
| 1 | C | 126 | GLN |
| 1 | C | 185 | GLN |
| 1 | C | 215 | GLN |
| 1 | C | 589 | HIS |
| 1 | C | 656 | GLN |
| 2 | D | 1112 | GLN |
| 2 | D | 1152 | GLN |
| 2 | D | 1198 | GLN |
| 2 | D | 1349 | HIS |
| 2 | D | 1473 | GLN |
| 2 | D | 1503 | ASN |
| 2 | D | 1517 | ASN |
| 2 | D | 1580 | GLN |
| 2 | D | 1581 | GLN |
| 2 | D | 1643 | GLN |
| 3 | E | 117 | ASN |
| 3 | E | 237 | GLN |
| 3 | E | 242 | HIS |
| 3 | E | 254 | ASN |
| 3 | F | 173 | 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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| 1 | A | 642/645 (99%) | 0.15 | 22 (3%) | 49 | 38 | 19, 107, 194, 287 | 0 |
| 1 | C | 642/645 (99%) | 0.14 | 11 (1%) | 73 | 63 | 16, 91, 178, 269 | 0 |
| 2 | B | 902/915 (98%) | 0.22 | 23 (2%) | 61 | 50 | 21, 143, 235, 308 | 0 |
| 2 | D | 902/915 (98%) | 0.20 | 17 (1%) | 70 | 60 | 16, 124, 224, 358 | 0 |
| 3 | E | 189/194 (97%) | 0.39 | 12 (6%) | 23 | 16 | 45, 129, 218, 254 | 0 |
| 3 | F | 189/194 (97%) | 0.45 | 21 (11%) | 7 | 6 | 38, 139, 231, 279 | 0 |
| All | All | 3466/3508 (98%) | 0.21 | 106 (3%) | 52 | 41 | 16, 118, 221, 358 | 0 |

All (106) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 985 | THR | 6.6 |
| 3 | F | 154 | ALA | 6.3 |
| 1 | A | 99 | GLU | 5.8 |
| 2 | B | 1438 | PHE | 4.7 |
| 1 | A | 396 | THR | 4.7 |
| 2 | D | 760 | ASN | 4.6 |
| 1 | C | 66 | LYS | 4.6 |
| 3 | F | 138 | SER | 4.3 |
| 2 | D | 1640 | GLU | 4.2 |
| 1 | A | 397 | VAL | 4.2 |
| 2 | B | 984 | GLY | 4.1 |
| 1 | C | 99 | GLU | 4.1 |
| 1 | A | 100 | LYS | 3.8 |
| 2 | B | 1066 | PHE | 3.7 |
| 2 | B | 1441 | ARG | 3.7 |
| 2 | D | 752 | ASP | 3.5 |
| 2 | D | 759 | GLU | 3.4 |
| 2 | B | 1119 | GLN | 3.4 |
| 1 | C | 410 | SER | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 1065 | ALA | 3.3 |
| 2 | B | 1466 | TYR | 3.3 |
| 3 | F | 102 | THR | 3.2 |
| 2 | D | 993 | ASP | 3.2 |
| 3 | F | 107 | ALA | 3.1 |
| 2 | D | 1546 | LYS | 3.0 |
| 1 | A | 365 | LYS | 3.0 |
| 2 | B | 990 | MET | 3.0 |
| 2 | B | 986 | PRO | 2.9 |
| 1 | A | 98 | SER | 2.9 |
| 1 | A | 398 | GLN | 2.9 |
| 2 | B | 1437 | ALA | 2.9 |
| 1 | A | 96 | PHE | 2.9 |
| 3 | F | 135 | ARG | 2.9 |
| 1 | A | 366 | PRO | 2.9 |
| 2 | D | 1638 | GLN | 2.8 |
| 1 | C | 411 | ILE | 2.8 |
| 3 | F | 155 | VAL | 2.8 |
| 1 | C | 514 | LEU | 2.7 |
| 3 | E | 269 | VAL | 2.7 |
| 2 | D | 1134 | ARG | 2.7 |
| 2 | B | 947 | LEU | 2.7 |
| 3 | F | 127 | TYR | 2.7 |
| 2 | D | 915 | ALA | 2.6 |
| 3 | E | 231 | ILE | 2.6 |
| 2 | B | 1266 | TYR | 2.6 |
| 3 | F | 103 | ARG | 2.6 |
| 2 | B | 1287 | PRO | 2.6 |
| 3 | F | 118 | TYR | 2.5 |
| 2 | B | 1314 | GLU | 2.5 |
| 3 | F | 153 | THR | 2.5 |
| 2 | B | 1337 | LYS | 2.5 |
| 3 | E | 281 | PRO | 2.5 |
| 3 | E | 147 | GLN | 2.4 |
| 1 | C | 541 | SER | 2.4 |
| 3 | F | 125 | VAL | 2.4 |
| 1 | A | 364 | PHE | 2.4 |
| 1 | A | 50 | GLN | 2.4 |
| 3 | E | 219 | GLU | 2.4 |
| 1 | A | 118 | GLU | 2.4 |
| 3 | E | 131 | PRO | 2.4 |
| 3 | F | 157 | PHE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 642 | ALA | 2.4 |
| 1 | C | 542 | GLY | 2.3 |
| 2 | D | 1116 | GLY | 2.3 |
| 2 | D | 1354 | ASP | 2.3 |
| 3 | F | 122 | GLY | 2.3 |
| 3 | F | 182 | PHE | 2.3 |
| 3 | E | 126 | GLU | 2.3 |
| 3 | E | 132 | GLY | 2.3 |
| 1 | C | 625 | ILE | 2.3 |
| 1 | A | 631 | SER | 2.3 |
| 1 | A | 455 | TYR | 2.3 |
| 2 | D | 1008 | SER | 2.3 |
| 2 | B | 1223 | PRO | 2.3 |
| 3 | F | 285 | GLY | 2.2 |
| 3 | F | 131 | PRO | 2.2 |
| 1 | A | 541 | SER | 2.2 |
| 2 | D | 1119 | GLN | 2.2 |
| 2 | B | 1110 | GLU | 2.2 |
| 2 | B | 756 | ILE | 2.2 |
| 2 | B | 975 | GLU | 2.2 |
| 2 | D | 1527 | VAL | 2.2 |
| 3 | F | 126 | GLU | 2.2 |
| 1 | A | 477 | LEU | 2.2 |
| 1 | A | 221 | GLU | 2.2 |
| 1 | A | 420 | LEU | 2.2 |
| 3 | E | 261 | GLY | 2.2 |
| 1 | C | 512 | GLN | 2.2 |
| 2 | D | 1133 | LEU | 2.1 |
| 3 | F | 104 | LEU | 2.1 |
| 2 | D | 1113 | LYS | 2.1 |
| 3 | F | 124 | VAL | 2.1 |
| 1 | A | 368 | MET | 2.1 |
| 3 | E | 128 | GLU | 2.1 |
| 2 | D | 1569 | ILE | 2.1 |
| 2 | B | 1509 | GLU | 2.1 |
| 3 | E | 197 | PHE | 2.1 |
| 3 | E | 118 | TYR | 2.1 |
| 1 | C | 370 | PHE | 2.1 |
| 1 | A | 487 | ILE | 2.1 |
| 2 | B | 1305 | SER | 2.0 |
| 2 | B | 1296 | VAL | 2.0 |
| 3 | F | 137 | PRO | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 511 | GLY | 2.0 |
| 3 | F | 206 | ILE | 2.0 |
| 1 | A | 456 | LEU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.