# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:09 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 3DHW |
| Title | : | Crystal structure of methionine importer MetNI |
| Authors | : | Rees, D.C.; Kaiser, J.T.; Kadaba, N.S.; Johnson, E.; Lee, A.T. |
| Deposited on | : | 2008-06-18 |
| Resolution | : | 3.70 Å(reported) |

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

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

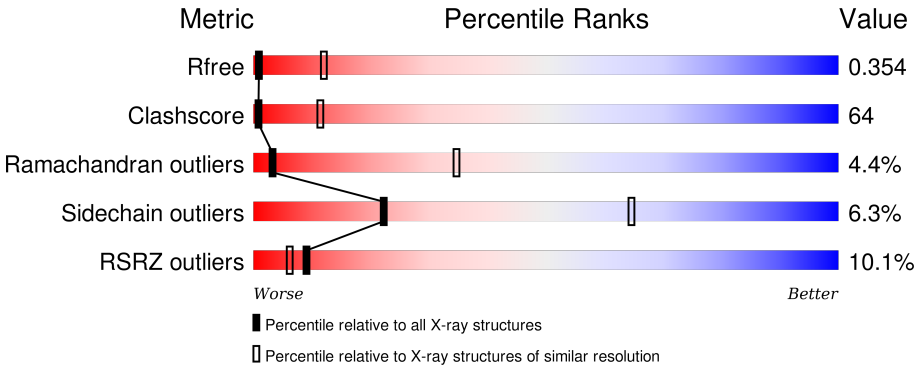
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 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 3.70 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.



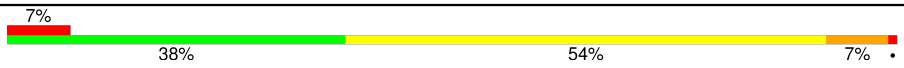
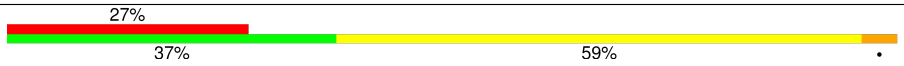
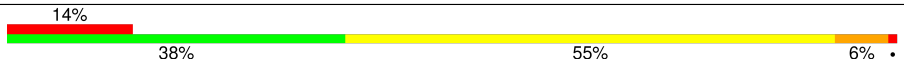

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 1101 (3.90-3.50) |
| Clashscore | 102246 | 1224 (3.90-3.50) |
| Ramachandran outliers | 100387 | 1172 (3.90-3.50) |
| Sidechain outliers | 100360 | 1170 (3.90-3.50) |
| RSRZ outliers | 91569 | 1108 (3.90-3.50) |

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 <=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 | 217 | 3% 18% 60% 12% • 6% |
| 1 | B | 217 | 7% 25% 57% 10% • 6% |
| 1 | E | 217 | 7% 24% 59% 10% 6% |
| 1 | F | 217 | 2% 21% 59% 12% • 6% |
| 2 | C | 343 | 3% 28% 56% 15% • |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | D | 343 |   |
| 2 | G | 343 |   |
| 2 | H | 343 |   |

# 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16688 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 D-methionine transport system permease protein metI.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1520 | 1014 | 244 | 254 | 8 | | | |
| 1 | B | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1520 | 1014 | 244 | 254 | 8 | | | |
| 1 | E | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1520 | 1014 | 244 | 254 | 8 | | | |
| 1 | F | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1520 | 1014 | 244 | 254 | 8 | | | |

- Molecule 2 is a protein called Methionine import ATP-binding protein metN.

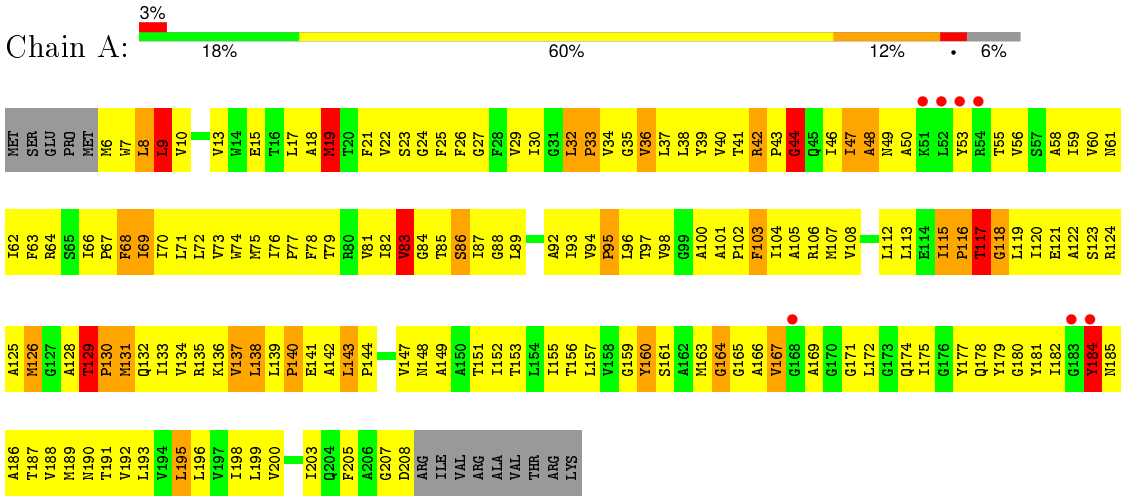
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 343 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2652 | 1664 | 467 | 509 | 12 | | | |
| 2 | D | 343 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2652 | 1664 | 467 | 509 | 12 | | | |
| 2 | G | 343 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2652 | 1664 | 467 | 509 | 12 | | | |
| 2 | H | 343 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2652 | 1664 | 467 | 509 | 12 | | | |

# 3 Residue-property plots (i)

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

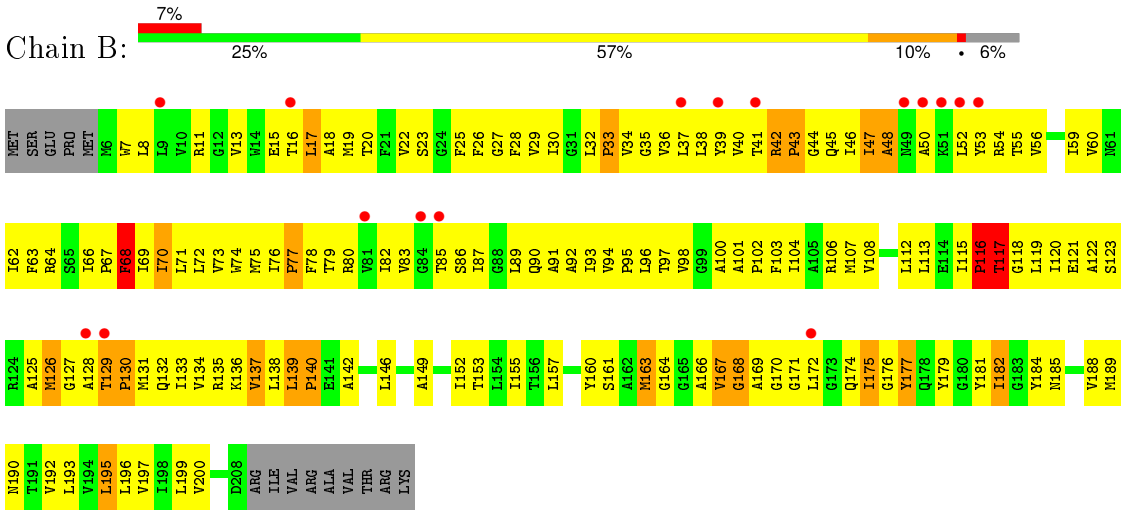
- Molecule 1: D-methionine transport system permease protein metI

Chain A:



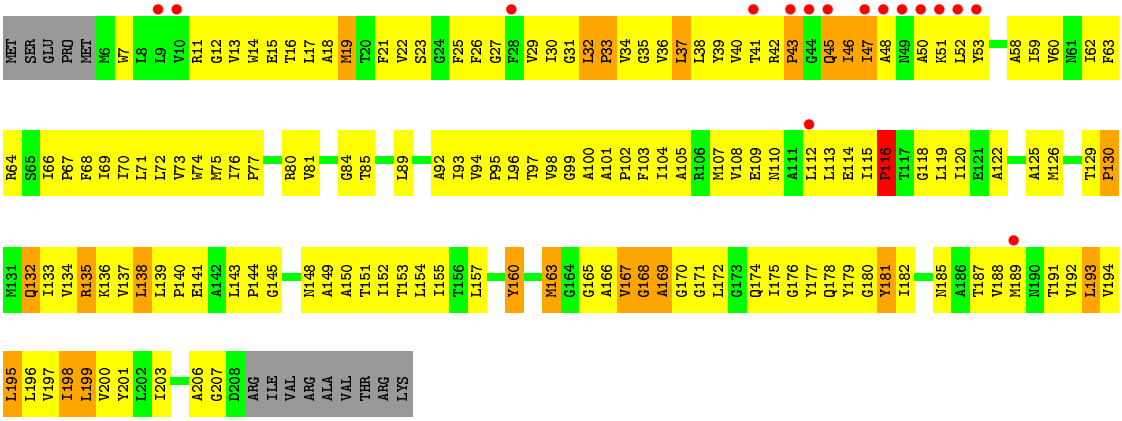

- Molecule 1: D-methionine transport system permease protein metI

Chain B:



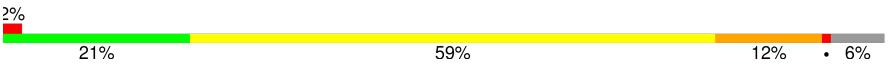

- Molecule 1: D-methionine transport system permease protein metI

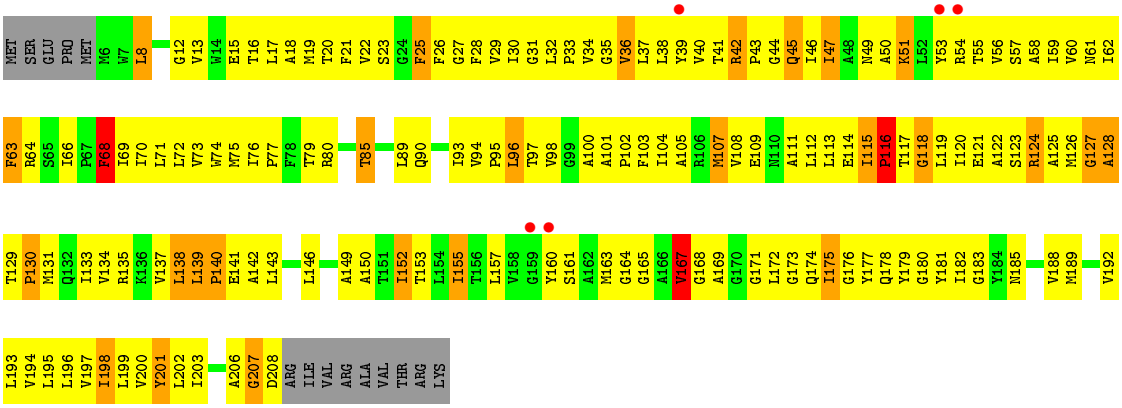
Chain E:




• Molecule 1: D-methionine transport system permease protein metI

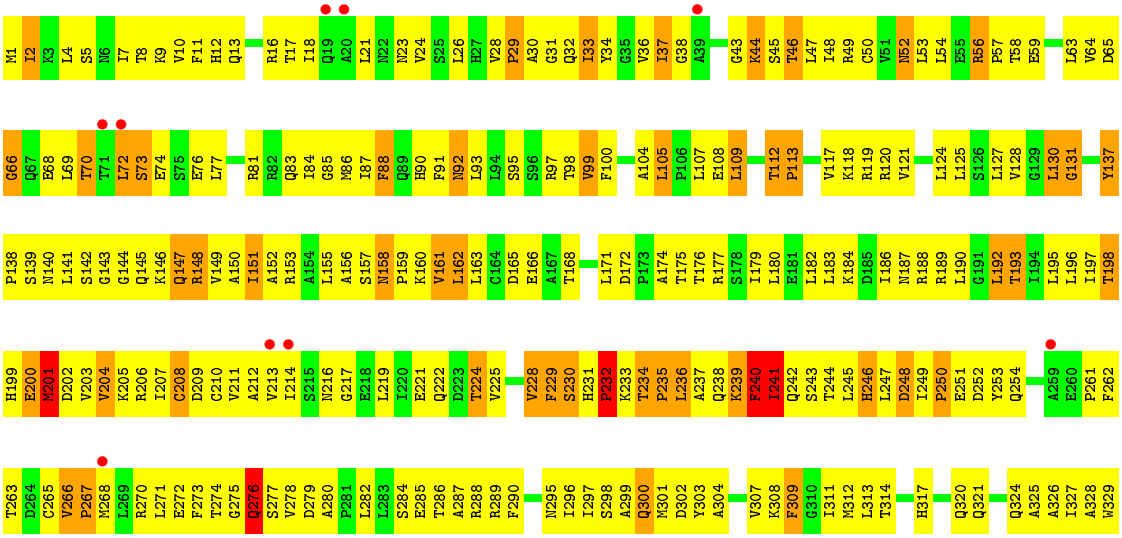
Chain F:

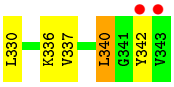



• Molecule 2: Methionine import ATP-binding protein metN

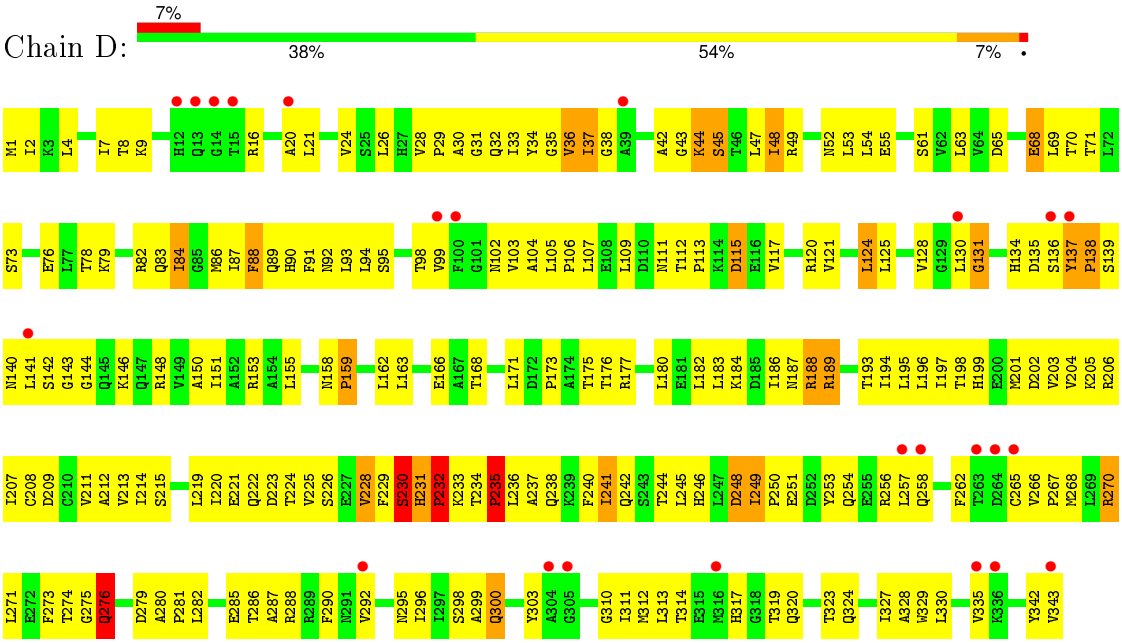
Chain C:



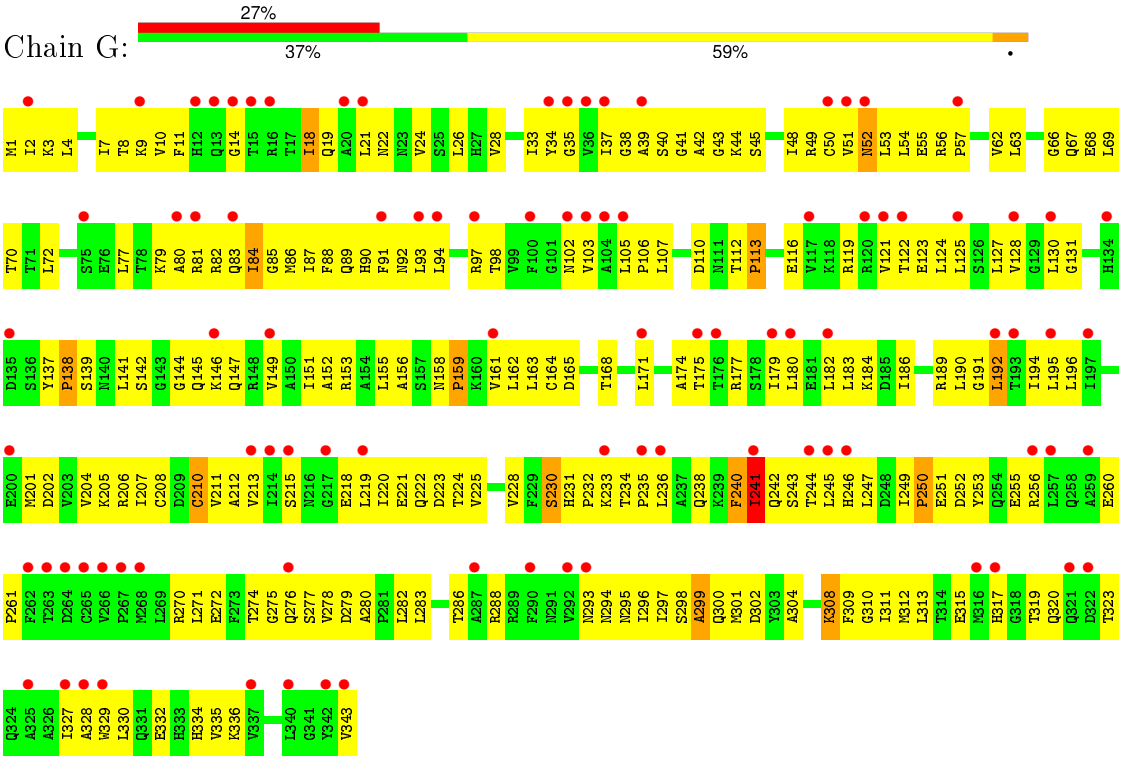

• Molecule 2: Methionine import ATP-binding protein metN

Chain D:



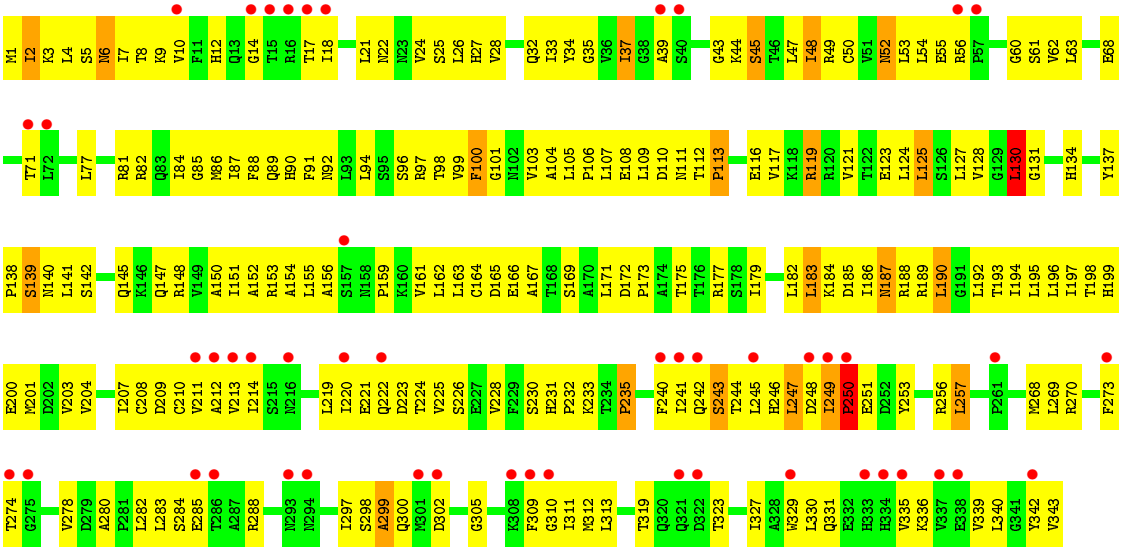

• Molecule 2: Methionine import ATP-binding protein metN

Chain G:




• Molecule 2: Methionine import ATP-binding protein metN

Chain H:


M1 I2 K3 L4 S5 W6 I7 T8 K9 V10 F11 H12 Q13 G14 T15 R16 T17 I18 L21 N22 N23 V24 S25 L26 H27 V28 Q32 I33 Y34 G35 V36 I37 G38 A39 S40 G43 K44 S45 T46 L47 I48 R49 C50 V51 N52 L53 L54 E55 R56 P57 G60 S61 V62 L63 E68
T71 L72 L77 R81 R82 Q83 I84 G85 M86 I87 F88 Q89 H90 F91 N92 L93 L94 S95 S96 R97 T98 V99 F100 G101 N102 V103 A104 L105 P106 L107 E108 L109 D110 N111 T112 P113 E116 V117 K118 R119 R120 V121 T122 E123 L124 L125 S126 L127 V128 G129 L130 G131 H134 Y137
P138 S139 N140 L141 S142 Q145 K146 Q147 R148 V149 A150 I151 A152 R153 A154 L155 A156 S157 N158 P159 K160 V161 L162 L163 C164 D165 E166 A167 T168 S169 A170 L171 D172 P173 A174 T175 T176 R177 S178 I179 L182 L183 K184 D185 I186 N187 R188 R189 L190 G191 L192 T193 I194 L195 L196 I197 T198 H199
E200 M201 D202 V203 V204 I207 C208 D209 C210 V211 A212 V213 I214 S215 N216 L219 I220 E221 Q222 D223 T224 V225 S226 E227 V228 F229 S230 H231 P232 K233 T234 P235 F240 I241 Q242 S243 T244 L245 H246 L247 D248 I249 P250 E251 D252 Y253 R256 L257 P261 M268 L269 R270 F273
T274 G275 V278 D279 A280 P281 L282 L283 S284 E285 T286 A287 R288 N293 N294 I297 S298 A299 Q300 M301 D302 G305 K308 F309 G310 I311 M312 L313 T319 Q320 Q321 D322 T323 I327 A328 W329 L330 Q331 E332 H333 H334 V335 K336 V337 E338 V339 L340 G341 Y342 V343

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 97.70Å 165.40Å 289.02Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 39.90 – 3.70<br>43.57 – 3.70 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.6 (39.90-3.70)<br>99.6 (43.57-3.70) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.69 (at 3.66Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, $R_{free}$ | 0.310 , 0.347<br>0.319 , 0.354 | Depositor<br>DCC |
| $R_{free}$ test set | 5070 reflections (10.01%) | DCC |
| Wilson B-factor (Å$^2$) | 153.5 | Xtriage |
| Anisotropy | 0.575 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.23 , 95.3 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.44$, $< L^2 > = 0.26$ | Xtriage |
| Outliers | 0 of 50643 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.89 | EDS |
| Total number of atoms | 16688 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 179.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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 | 1.08 | 2/1552 (0.1%) | 1.33 | 16/2122 (0.8%) |
| 1 | B | 0.88 | 0/1552 | 1.21 | 7/2122 (0.3%) |
| 1 | E | 0.79 | 0/1552 | 1.22 | 9/2122 (0.4%) |
| 1 | F | 1.12 | 1/1552 (0.1%) | 1.36 | 10/2122 (0.5%) |
| 2 | C | 1.40 | 13/2691 (0.5%) | 1.50 | 35/3647 (1.0%) |
| 2 | D | 1.01 | 1/2691 (0.0%) | 1.27 | 18/3647 (0.5%) |
| 2 | G | 0.70 | 0/2691 | 1.08 | 7/3647 (0.2%) |
| 2 | H | 0.93 | 0/2691 | 1.24 | 13/3647 (0.4%) |
| All | All | 1.02 | 17/16972 (0.1%) | 1.28 | 115/23076 (0.5%) |

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 | 3 |
| 1 | B | 0 | 1 |
| 1 | E | 0 | 2 |
| 2 | C | 0 | 2 |
| All | All | 0 | 8 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 309 | PHE | CD2-CE2 | 12.45 | 1.64 | 1.39 |
| 2 | C | 309 | PHE | CD1-CE1 | 12.23 | 1.63 | 1.39 |
| 2 | C | 229 | PHE | CG-CD2 | 9.48 | 1.52 | 1.38 |
| 2 | C | 228 | VAL | C-O | 9.44 | 1.41 | 1.23 |
| 2 | D | 205 | LYS | CD-CE | 7.57 | 1.70 | 1.51 |
| 2 | C | 204 | VAL | CB-CG2 | -7.19 | 1.37 | 1.52 |
| 2 | C | 201 | MET | SD-CE | 6.46 | 2.14 | 1.77 |
| 2 | C | 229 | PHE | CE1-CZ | 6.21 | 1.49 | 1.37 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 19 | MET | CG-SD | 6.12 | 1.97 | 1.81 |
| 1 | F | 201 | TYR | CE2-CZ | 5.90 | 1.46 | 1.38 |
| 1 | A | 68 | PHE | CG-CD1 | 5.78 | 1.47 | 1.38 |
| 2 | C | 50 | CYS | CB-SG | 5.68 | 1.92 | 1.82 |
| 2 | C | 213 | VAL | CB-CG2 | -5.61 | 1.41 | 1.52 |
| 2 | C | 309 | PHE | CE1-CZ | 5.42 | 1.47 | 1.37 |
| 2 | C | 161 | VAL | CA-CB | -5.42 | 1.43 | 1.54 |
| 2 | C | 74 | GLU | CG-CD | 5.29 | 1.59 | 1.51 |
| 2 | C | 240 | PHE | N-CA | -5.25 | 1.35 | 1.46 |

All (115) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 116 | PRO | N-CA-C | 9.67 | 137.25 | 112.10 |
| 2 | D | 205 | LYS | CD-CE-NZ | 9.19 | 132.83 | 111.70 |
| 2 | H | 125 | LEU | CB-CG-CD2 | -9.11 | 95.52 | 111.00 |
| 1 | F | 115 | ILE | C-N-CD | -9.07 | 100.66 | 120.60 |
| 2 | C | 239 | LYS | CA-C-N | -8.79 | 97.87 | 117.20 |
| 2 | C | 230 | SER | N-CA-C | 8.49 | 133.93 | 111.00 |
| 1 | E | 195 | LEU | CA-CB-CG | 8.43 | 134.68 | 115.30 |
| 1 | F | 138 | LEU | CA-CB-CG | -7.96 | 96.98 | 115.30 |
| 1 | E | 163 | MET | CB-CG-SD | -7.80 | 88.99 | 112.40 |
| 2 | C | 99 | VAL | CG1-CB-CG2 | -7.13 | 99.50 | 110.90 |
| 2 | D | 89 | GLN | N-CA-CB | -7.12 | 97.78 | 110.60 |
| 1 | E | 129 | THR | N-CA-C | -7.07 | 91.92 | 111.00 |
| 2 | D | 70 | THR | N-CA-C | -7.06 | 91.94 | 111.00 |
| 1 | A | 8 | LEU | CB-CG-CD1 | 7.00 | 122.91 | 111.00 |
| 2 | H | 130 | LEU | N-CA-C | -6.99 | 92.13 | 111.00 |
| 2 | C | 236 | LEU | CA-CB-CG | 6.97 | 131.34 | 115.30 |
| 2 | C | 239 | LYS | CA-C-O | 6.87 | 134.52 | 120.10 |
| 1 | F | 115 | ILE | N-CA-C | 6.81 | 129.38 | 111.00 |
| 2 | C | 241 | ILE | N-CA-C | -6.71 | 92.89 | 111.00 |
| 1 | A | 143 | LEU | C-N-CD | 6.69 | 142.45 | 128.40 |
| 1 | E | 199 | LEU | CA-CB-CG | 6.67 | 130.64 | 115.30 |
| 1 | B | 50 | ALA | N-CA-C | 6.65 | 128.96 | 111.00 |
| 1 | B | 117 | THR | N-CA-C | 6.64 | 128.93 | 111.00 |
| 2 | D | 36 | VAL | N-CA-C | -6.58 | 93.23 | 111.00 |
| 2 | G | 230 | SER | N-CA-C | 6.57 | 128.74 | 111.00 |
| 2 | C | 228 | VAL | O-C-N | 6.53 | 133.15 | 122.70 |
| 2 | H | 119 | ARG | CB-CA-C | -6.49 | 97.41 | 110.40 |
| 2 | C | 183 | LEU | CB-CG-CD2 | -6.48 | 99.99 | 111.00 |
| 2 | G | 250 | PRO | N-CA-C | -6.47 | 95.28 | 112.10 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 8 | LEU | CB-CG-CD2 | -6.43 | 100.07 | 111.00 |
| 2 | D | 88 | PHE | N-CA-C | 6.38 | 128.23 | 111.00 |
| 1 | A | 44 | GLY | N-CA-C | -6.37 | 97.19 | 113.10 |
| 1 | A | 7 | TRP | CB-CA-C | -6.29 | 97.83 | 110.40 |
| 2 | C | 148 | ARG | NE-CZ-NH1 | -6.23 | 117.19 | 120.30 |
| 1 | F | 167 | VAL | N-CA-C | 6.21 | 127.78 | 111.00 |
| 2 | C | 228 | VAL | C-N-CA | 6.12 | 137.01 | 121.70 |
| 2 | G | 320 | GLN | N-CA-C | 6.11 | 127.49 | 111.00 |
| 2 | C | 188 | ARG | CB-CG-CD | -6.10 | 95.74 | 111.60 |
| 2 | C | 336 | LYS | CA-CB-CG | 6.08 | 126.78 | 113.40 |
| 2 | C | 289 | ARG | N-CA-C | 6.08 | 127.41 | 111.00 |
| 2 | G | 192 | LEU | N-CA-C | -6.07 | 94.62 | 111.00 |
| 2 | C | 88 | PHE | N-CA-C | 6.03 | 127.29 | 111.00 |
| 2 | C | 340 | LEU | CB-CG-CD2 | -6.03 | 100.75 | 111.00 |
| 2 | H | 193 | THR | N-CA-C | -6.01 | 94.77 | 111.00 |
| 1 | F | 146 | LEU | CB-CG-CD2 | -6.01 | 100.78 | 111.00 |
| 1 | A | 68 | PHE | CB-CA-C | -5.95 | 98.49 | 110.40 |
| 1 | A | 32 | LEU | CA-CB-CG | -5.94 | 101.64 | 115.30 |
| 1 | F | 124 | ARG | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 1 | F | 63 | PHE | CB-CG-CD2 | -5.86 | 116.70 | 120.80 |
| 2 | H | 100 | PHE | CB-CG-CD2 | -5.86 | 116.70 | 120.80 |
| 1 | A | 10 | VAL | N-CA-C | 5.84 | 126.77 | 111.00 |
| 2 | C | 228 | VAL | CA-C-N | -5.80 | 104.44 | 117.20 |
| 2 | C | 44 | LYS | N-CA-C | -5.80 | 95.34 | 111.00 |
| 1 | A | 195 | LEU | CA-CB-CG | 5.76 | 128.54 | 115.30 |
| 1 | A | 208 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |
| 2 | C | 208 | CYS | CA-CB-SG | -5.71 | 103.72 | 114.00 |
| 2 | C | 234 | THR | N-CA-C | -5.71 | 95.59 | 111.00 |
| 1 | F | 127 | GLY | N-CA-C | -5.67 | 98.92 | 113.10 |
| 2 | C | 33 | ILE | CB-CA-C | -5.64 | 100.32 | 111.60 |
| 2 | C | 119 | ARG | NE-CZ-NH1 | -5.63 | 117.49 | 120.30 |
| 1 | E | 37 | LEU | CA-CB-CG | 5.63 | 128.25 | 115.30 |
| 1 | A | 138 | LEU | CB-CG-CD2 | -5.61 | 101.47 | 111.00 |
| 2 | D | 276 | GLN | CB-CA-C | -5.60 | 99.20 | 110.40 |
| 2 | G | 251 | GLU | N-CA-C | 5.60 | 126.12 | 111.00 |
| 2 | D | 251 | GLU | N-CA-C | 5.59 | 126.11 | 111.00 |
| 2 | C | 248 | ASP | N-CA-CB | -5.59 | 100.54 | 110.60 |
| 2 | D | 90 | HIS | N-CA-C | -5.57 | 95.97 | 111.00 |
| 2 | D | 188 | ARG | CB-CA-C | -5.56 | 99.28 | 110.40 |
| 2 | G | 168 | THR | N-CA-C | 5.55 | 125.98 | 111.00 |
| 2 | C | 250 | PRO | N-CA-C | -5.54 | 97.69 | 112.10 |
| 1 | F | 107 | MET | CA-CB-CG | 5.53 | 122.70 | 113.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 90 | HIS | N-CA-C | -5.50 | 96.16 | 111.00 |
| 2 | C | 235 | PRO | N-CA-C | -5.49 | 97.82 | 112.10 |
| 2 | D | 136 | SER | N-CA-C | 5.49 | 125.83 | 111.00 |
| 2 | C | 202 | ASP | CB-CG-OD1 | -5.49 | 113.36 | 118.30 |
| 2 | D | 295 | ASN | N-CA-C | -5.49 | 96.18 | 111.00 |
| 2 | C | 309 | PHE | N-CA-C | -5.47 | 96.22 | 111.00 |
| 2 | D | 270 | ARG | N-CA-C | -5.44 | 96.32 | 111.00 |
| 2 | C | 188 | ARG | CA-CB-CG | 5.43 | 125.35 | 113.40 |
| 2 | H | 100 | PHE | CB-CG-CD1 | 5.40 | 124.58 | 120.80 |
| 1 | A | 9 | LEU | N-CA-C | 5.39 | 125.56 | 111.00 |
| 1 | A | 126 | MET | CG-SD-CE | 5.38 | 108.81 | 100.20 |
| 2 | C | 240 | PHE | N-CA-CB | -5.35 | 100.97 | 110.60 |
| 2 | C | 92 | ASN | N-CA-C | 5.34 | 125.41 | 111.00 |
| 2 | D | 230 | SER | N-CA-C | 5.30 | 125.31 | 111.00 |
| 2 | D | 248 | ASP | CB-CA-C | -5.30 | 99.80 | 110.40 |
| 2 | H | 188 | ARG | CB-CA-C | -5.29 | 99.82 | 110.40 |
| 1 | E | 32 | LEU | CA-CB-CG | -5.29 | 103.14 | 115.30 |
| 1 | B | 163 | MET | CA-CB-CG | -5.28 | 104.33 | 113.30 |
| 2 | D | 68 | GLU | N-CA-CB | 5.27 | 120.08 | 110.60 |
| 2 | C | 295 | ASN | N-CA-C | -5.25 | 96.81 | 111.00 |
| 2 | G | 308 | LYS | N-CA-C | 5.24 | 125.14 | 111.00 |
| 2 | C | 192 | LEU | CB-CG-CD2 | -5.23 | 102.10 | 111.00 |
| 2 | H | 45 | SER | N-CA-CB | -5.23 | 102.66 | 110.50 |
| 2 | H | 125 | LEU | CB-CG-CD1 | 5.22 | 119.87 | 111.00 |
| 2 | D | 189 | ARG | NE-CZ-NH2 | 5.20 | 122.90 | 120.30 |
| 1 | B | 17 | LEU | CA-CB-CG | -5.18 | 103.39 | 115.30 |
| 1 | B | 44 | GLY | N-CA-C | -5.17 | 100.16 | 113.10 |
| 1 | B | 54 | ARG | CB-CA-C | -5.17 | 100.06 | 110.40 |
| 2 | H | 247 | LEU | CA-CB-CG | 5.16 | 127.16 | 115.30 |
| 2 | D | 115 | ASP | N-CA-C | 5.13 | 124.85 | 111.00 |
| 2 | C | 66 | GLY | N-CA-C | 5.12 | 125.89 | 113.10 |
| 1 | E | 138 | LEU | CA-CB-CG | -5.11 | 103.54 | 115.30 |
| 1 | B | 195 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 2 | C | 216 | ASN | N-CA-C | 5.10 | 124.76 | 111.00 |
| 2 | H | 1 | MET | N-CA-C | 5.09 | 124.76 | 111.00 |
| 1 | A | 137 | VAL | CG1-CB-CG2 | 5.09 | 119.05 | 110.90 |
| 1 | A | 24 | GLY | N-CA-C | -5.08 | 100.40 | 113.10 |
| 2 | C | 189 | ARG | N-CA-C | 5.07 | 124.69 | 111.00 |
| 1 | E | 45 | GLN | N-CA-C | 5.07 | 124.69 | 111.00 |
| 2 | H | 187 | ASN | N-CA-C | 5.05 | 124.65 | 111.00 |
| 1 | E | 193 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |
| 1 | A | 6 | MET | CG-SD-CE | 5.02 | 108.23 | 100.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 276 | GLN | N-CA-C | -5.01 | 97.46 | 111.00 |
| 2 | D | 232 | PRO | N-CA-C | 5.01 | 125.11 | 112.10 |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 179 | TYR | Sidechain |
| 1 | A | 184 | TYR | Sidechain |
| 1 | A | 205 | PHE | Sidechain |
| 1 | B | 177 | TYR | Sidechain |
| 2 | C | 198 | THR | Mainchain |
| 2 | C | 309 | PHE | Sidechain |
| 1 | E | 179 | TYR | Sidechain |
| 1 | E | 181 | TYR | Sidechain |

## 5.2 Too-close contacts (i)

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 | 1520 | 0 | 1622 | 240 | 0 |
| 1 | B | 1520 | 0 | 1622 | 259 | 0 |
| 1 | E | 1520 | 0 | 1622 | 258 | 0 |
| 1 | F | 1520 | 0 | 1622 | 301 | 0 |
| 2 | C | 2652 | 0 | 2705 | 375 | 0 |
| 2 | D | 2652 | 0 | 2705 | 310 | 0 |
| 2 | G | 2652 | 0 | 2705 | 280 | 0 |
| 2 | H | 2652 | 0 | 2705 | 344 | 0 |
| All | All | 16688 | 0 | 17308 | 2189 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (2189) 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) |
|---|---|---|---|
| 2:C:201:MET:SD | 2:C:201:MET:CE | 2.14 | 1.34 |
| 1:E:94:VAL:HG23 | 1:E:95:PRO:HD3 | 1.22 | 1.15 |
| 1:F:126:MET:SD | 1:F:129:THR:HA | 1.87 | 1.13 |
| 2:D:31:GLY:H | 2:D:193:THR:HG22 | 1.08 | 1.12 |
| 1:B:72:LEU:HD22 | 1:B:95:PRO:HB2 | 1.28 | 1.08 |
| 1:E:75:MET:HG2 | 1:E:95:PRO:HB3 | 1.15 | 1.08 |
| 2:H:52:ASN:HD21 | 2:H:54:LEU:HG | 1.12 | 1.08 |
| 2:H:223:ASP:HB3 | 2:H:228:VAL:HG22 | 1.34 | 1.08 |
| 2:D:33:ILE:HG12 | 2:D:194:ILE:HD11 | 1.31 | 1.07 |
| 2:D:36:VAL:HG12 | 2:D:214:ILE:HD11 | 1.36 | 1.06 |
| 1:F:94:VAL:HG23 | 1:F:95:PRO:HD3 | 1.33 | 1.04 |
| 2:C:44:LYS:HB2 | 2:C:197:ILE:HD11 | 1.34 | 1.04 |
| 2:C:200:GLU:HB3 | 2:C:239:LYS:HE2 | 1.39 | 1.03 |
| 2:C:247:LEU:HD21 | 2:C:298:SER:HB2 | 1.40 | 1.03 |
| 2:C:64:VAL:HG11 | 2:C:84:ILE:HD12 | 1.41 | 1.03 |
| 2:D:48:ILE:HD13 | 2:D:48:ILE:N | 1.72 | 1.01 |
| 2:D:168:THR:HB | 2:D:176:THR:HG23 | 1.38 | 1.01 |
| 2:D:240:PHE:O | 2:D:242:GLN:N | 1.92 | 1.01 |
| 2:D:48:ILE:CD1 | 2:D:197:ILE:HG12 | 1.92 | 1.00 |
| 1:E:180:GLY:HA3 | 1:F:73:VAL:HG13 | 1.41 | 1.00 |
| 1:B:69:ILE:HD11 | 1:B:163:MET:HB3 | 1.38 | 1.00 |
| 1:A:126:MET:HE1 | 2:C:153:ARG:HD2 | 1.44 | 0.99 |
| 2:D:36:VAL:HG12 | 2:D:214:ILE:CD1 | 1.91 | 0.99 |
| 1:F:164:GLY:HA2 | 1:F:169:ALA:HB3 | 1.43 | 0.99 |
| 2:C:87:ILE:HG22 | 2:C:88:PHE:H | 1.22 | 0.99 |
| 2:H:63:LEU:HB2 | 2:H:68:GLU:HG2 | 1.45 | 0.98 |
| 1:A:71:LEU:HG | 1:A:75:MET:HE2 | 1.45 | 0.98 |
| 1:F:100:ALA:O | 1:F:104:ILE:HG13 | 1.64 | 0.98 |
| 1:A:185:ASN:HB2 | 1:A:188:VAL:HG22 | 1.45 | 0.98 |
| 2:H:171:LEU:HD22 | 2:H:175:THR:HG21 | 1.44 | 0.98 |
| 2:G:300:GLN:HA | 2:H:297:ILE:O | 1.63 | 0.97 |
| 1:E:193:LEU:HD23 | 1:F:70:ILE:HG13 | 1.46 | 0.97 |
| 1:F:19:MET:HB3 | 1:F:157:LEU:HD11 | 1.45 | 0.97 |
| 1:E:38:LEU:HB2 | 1:E:112:LEU:HD13 | 1.44 | 0.97 |
| 1:A:130:PRO:HG2 | 1:A:131:MET:H | 1.30 | 0.95 |
| 1:A:126:MET:CE | 2:C:153:ARG:HD2 | 1.96 | 0.95 |
| 1:F:101:ALA:HA | 1:F:104:ILE:HD11 | 1.48 | 0.95 |
| 2:D:48:ILE:HD12 | 2:D:197:ILE:HG12 | 1.46 | 0.95 |
| 2:D:48:ILE:HD13 | 2:D:48:ILE:H | 1.23 | 0.94 |
| 2:C:214:ILE:HD11 | 2:C:219:LEU:HD23 | 1.48 | 0.94 |
| 1:B:74:TRP:O | 1:B:77:PRO:HD2 | 1.65 | 0.94 |
| 1:E:40:VAL:HA | 1:E:47:ILE:HD11 | 1.49 | 0.94 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:77:LEU:HD21 | 2:H:81:ARG:HH21 | 1.29 | 0.93 |
| 2:D:43:GLY:H | 2:D:44:LYS:NZ | 1.64 | 0.93 |
| 1:B:127:GLY:HA3 | 2:D:109:LEU:HD12 | 1.51 | 0.93 |
| 2:D:128:VAL:HG23 | 2:D:130:LEU:H | 1.33 | 0.93 |
| 1:F:188:VAL:O | 1:F:192:VAL:HG23 | 1.69 | 0.93 |
| 2:H:245:LEU:HD23 | 2:H:313:LEU:HG | 1.50 | 0.92 |
| 2:C:241:ILE:HG13 | 2:C:300:GLN:HB2 | 1.50 | 0.92 |
| 2:D:4:LEU:HD22 | 2:D:7:ILE:HD11 | 1.51 | 0.92 |
| 1:B:172:LEU:HD11 | 1:B:195:LEU:HD21 | 1.51 | 0.92 |
| 2:C:246:HIS:HA | 2:C:249:ILE:HG12 | 1.51 | 0.92 |
| 1:A:69:ILE:HG21 | 1:B:163:MET:SD | 2.09 | 0.92 |
| 2:G:241:ILE:HD11 | 2:H:248:ASP:HB2 | 1.49 | 0.92 |
| 1:E:140:PRO:HA | 1:E:143:LEU:HD12 | 1.51 | 0.92 |
| 1:B:35:GLY:HA3 | 1:B:108:VAL:HG11 | 1.52 | 0.91 |
| 2:D:166:GLU:OE2 | 2:D:199:HIS:HB2 | 1.70 | 0.91 |
| 2:D:131:GLY:O | 2:D:135:ASP:HB2 | 1.70 | 0.91 |
| 2:D:213:VAL:HG11 | 2:D:233:LYS:HD2 | 1.52 | 0.91 |
| 2:C:247:LEU:HD11 | 2:C:298:SER:HB2 | 1.53 | 0.91 |
| 2:D:2:ILE:HG23 | 2:D:28:VAL:HB | 1.49 | 0.91 |
| 1:A:75:MET:HE3 | 1:A:95:PRO:HB3 | 1.53 | 0.91 |
| 1:F:104:ILE:HG22 | 1:F:153:THR:HG21 | 1.53 | 0.91 |
| 1:B:175:ILE:HG13 | 1:B:176:GLY:N | 1.82 | 0.90 |
| 2:D:43:GLY:H | 2:D:44:LYS:HZ2 | 1.12 | 0.90 |
| 2:C:87:ILE:HG22 | 2:C:88:PHE:N | 1.83 | 0.90 |
| 2:H:52:ASN:ND2 | 2:H:54:LEU:HG | 1.87 | 0.90 |
| 1:B:22:VAL:HG11 | 1:B:93:ILE:HB | 1.52 | 0.90 |
| 2:C:247:LEU:HD11 | 2:C:298:SER:CB | 2.02 | 0.89 |
| 1:E:116:PRO:HB2 | 1:E:120:ILE:HG12 | 1.54 | 0.89 |
| 2:H:108:GLU:O | 2:H:112:THR:HG22 | 1.72 | 0.89 |
| 2:C:247:LEU:CD2 | 2:C:298:SER:HB2 | 2.01 | 0.89 |
| 2:C:147:GLN:HE21 | 2:C:147:GLN:HA | 1.38 | 0.89 |
| 2:G:52:ASN:HB3 | 2:G:84:ILE:HD12 | 1.52 | 0.89 |
| 2:H:299:ALA:HB2 | 2:H:312:MET:HG3 | 1.55 | 0.89 |
| 2:C:161:VAL:HG22 | 2:C:193:THR:HG22 | 1.52 | 0.89 |
| 1:B:167:VAL:HG13 | 1:B:168:GLY:H | 1.38 | 0.89 |
| 2:D:83:GLN:O | 2:D:159:PRO:HB2 | 1.72 | 0.89 |
| 1:A:193:LEU:HD23 | 1:B:70:ILE:HD11 | 1.55 | 0.89 |
| 2:C:4:LEU:HB3 | 2:C:7:ILE:HD12 | 1.51 | 0.89 |
| 1:E:63:PHE:HA | 1:E:66:ILE:HD12 | 1.55 | 0.88 |
| 1:E:122:ALA:HB1 | 2:G:88:PHE:CE2 | 2.08 | 0.88 |
| 2:G:224:THR:O | 2:G:228:VAL:HG23 | 1.74 | 0.88 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:92:ALA:HB2 | 1:E:169:ALA:HB3 | 1.55 | 0.88 |
| 1:B:172:LEU:HD21 | 1:B:195:LEU:HD23 | 1.55 | 0.88 |
| 2:G:3:LYS:HB3 | 2:G:63:LEU:HB3 | 1.54 | 0.87 |
| 2:D:31:GLY:N | 2:D:193:THR:HG22 | 1.90 | 0.87 |
| 2:D:189:ARG:HG3 | 2:D:189:ARG:HH21 | 1.39 | 0.87 |
| 2:H:196:LEU:HD21 | 2:H:203:VAL:HG12 | 1.56 | 0.87 |
| 1:B:125:ALA:HB2 | 2:D:54:LEU:HD21 | 1.55 | 0.87 |
| 2:H:172:ASP:HB2 | 2:H:173:PRO:HD2 | 1.56 | 0.87 |
| 1:E:149:ALA:O | 1:E:153:THR:HG23 | 1.74 | 0.87 |
| 1:F:124:ARG:NH2 | 2:H:85:GLY:HA2 | 1.89 | 0.87 |
| 2:C:234:THR:HA | 2:C:237:ALA:HB3 | 1.55 | 0.87 |
| 1:F:193:LEU:O | 1:F:197:VAL:HG23 | 1.75 | 0.86 |
| 1:A:193:LEU:HD11 | 1:B:74:TRP:CD1 | 2.10 | 0.86 |
| 2:G:128:VAL:HG11 | 2:G:152:ALA:HB2 | 1.55 | 0.86 |
| 2:G:49:ARG:HG2 | 2:G:54:LEU:HD12 | 1.54 | 0.86 |
| 1:F:124:ARG:CZ | 1:F:124:ARG:HB3 | 2.06 | 0.86 |
| 2:G:128:VAL:HG23 | 2:G:130:LEU:H | 1.39 | 0.86 |
| 1:E:75:MET:CG | 1:E:95:PRO:HB3 | 2.04 | 0.86 |
| 1:A:117:THR:C | 1:A:119:LEU:H | 1.79 | 0.86 |
| 2:H:34:TYR:OH | 2:H:212:ALA:HB2 | 1.76 | 0.86 |
| 2:H:223:ASP:HB3 | 2:H:228:VAL:CG2 | 2.06 | 0.86 |
| 2:C:105:LEU:O | 2:C:109:LEU:HG | 1.74 | 0.85 |
| 2:C:171:LEU:HD22 | 2:C:175:THR:HG21 | 1.56 | 0.85 |
| 1:E:58:ALA:O | 1:E:62:ILE:HG23 | 1.77 | 0.85 |
| 1:E:16:THR:HG21 | 1:E:199:LEU:HD11 | 1.59 | 0.85 |
| 1:F:194:VAL:O | 1:F:198:ILE:HG23 | 1.76 | 0.85 |
| 2:C:34:TYR:CD2 | 2:C:210:CYS:HB2 | 2.12 | 0.84 |
| 1:F:103:PHE:O | 1:F:107:MET:HG2 | 1.77 | 0.84 |
| 2:H:249:ILE:HG23 | 2:H:250:PRO:HD3 | 1.59 | 0.84 |
| 2:C:125:LEU:HB3 | 2:C:131:GLY:HA3 | 1.59 | 0.84 |
| 1:E:188:VAL:O | 1:E:192:VAL:HG23 | 1.77 | 0.84 |
| 2:G:98:THR:HG22 | 2:G:138:PRO:HB3 | 1.56 | 0.84 |
| 1:F:33:PRO:O | 1:F:36:VAL:HB | 1.78 | 0.84 |
| 1:E:174:GLN:HA | 1:E:177:TYR:HB3 | 1.57 | 0.84 |
| 2:C:37:ILE:HD13 | 2:C:201:MET:HG2 | 1.60 | 0.83 |
| 1:E:69:ILE:HD12 | 1:E:163:MET:HE2 | 1.58 | 0.83 |
| 2:H:240:PHE:H | 2:H:243:SER:HB3 | 1.40 | 0.83 |
| 2:D:36:VAL:CG1 | 2:D:214:ILE:HD11 | 2.08 | 0.83 |
| 2:H:52:ASN:HD21 | 2:H:54:LEU:CG | 1.92 | 0.83 |
| 1:E:119:LEU:O | 1:E:122:ALA:HB3 | 1.78 | 0.83 |
| 1:E:22:VAL:HG12 | 1:E:26:PHE:HE2 | 1.44 | 0.83 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:89:LEU:HA | 1:B:169:ALA:HB1 | 1.58 | 0.83 |
| 2:C:36:VAL:HG13 | 2:C:214:ILE:HD13 | 1.61 | 0.83 |
| 2:D:240:PHE:C | 2:D:242:GLN:H | 1.81 | 0.83 |
| 2:G:83:GLN:O | 2:G:159:PRO:HB2 | 1.77 | 0.83 |
| 2:D:44:LYS:HE2 | 2:D:45:SER:OG | 1.79 | 0.83 |
| 2:D:208:CYS:O | 2:D:225:VAL:HG21 | 1.78 | 0.82 |
| 2:C:231:HIS:HB3 | 2:C:232:PRO:HD2 | 1.60 | 0.82 |
| 2:G:8:THR:HG23 | 2:G:21:LEU:O | 1.79 | 0.82 |
| 2:C:236:LEU:HA | 2:C:239:LYS:HB2 | 1.61 | 0.82 |
| 2:G:162:LEU:O | 2:G:194:ILE:HA | 1.79 | 0.82 |
| 2:D:180:LEU:HA | 2:D:183:LEU:HD12 | 1.59 | 0.82 |
| 2:G:37:ILE:HD11 | 2:G:236:LEU:HD23 | 1.62 | 0.82 |
| 1:A:118:GLY:HA2 | 1:A:121:GLU:HG2 | 1.62 | 0.82 |
| 1:B:72:LEU:CD2 | 1:B:95:PRO:HB2 | 2.09 | 0.82 |
| 2:H:241:ILE:HD12 | 2:H:242:GLN:N | 1.94 | 0.82 |
| 1:E:22:VAL:HG22 | 1:E:93:ILE:HB | 1.62 | 0.82 |
| 1:B:179:TYR:HB3 | 1:B:185:ASN:HD22 | 1.43 | 0.82 |
| 2:G:184:LYS:HG3 | 2:G:207:ILE:HG22 | 1.62 | 0.82 |
| 1:F:38:LEU:HD22 | 1:F:112:LEU:HB3 | 1.61 | 0.82 |
| 2:D:201:MET:HG3 | 2:D:236:LEU:O | 1.79 | 0.82 |
| 1:B:119:LEU:HB3 | 2:D:92:ASN:CG | 1.99 | 0.81 |
| 1:A:119:LEU:HB3 | 2:C:92:ASN:OD1 | 1.80 | 0.81 |
| 2:C:247:LEU:CG | 2:C:298:SER:HB2 | 2.10 | 0.81 |
| 2:H:77:LEU:HD21 | 2:H:81:ARG:NH2 | 1.94 | 0.81 |
| 1:E:46:ILE:HG23 | 1:E:47:ILE:HG12 | 1.60 | 0.81 |
| 1:F:26:PHE:CD1 | 1:F:97:THR:HA | 2.14 | 0.81 |
| 1:F:124:ARG:NH1 | 2:H:86:MET:HB3 | 1.96 | 0.81 |
| 2:H:48:ILE:CG2 | 2:H:197:ILE:HD11 | 2.10 | 0.81 |
| 1:B:167:VAL:HG13 | 1:B:168:GLY:N | 1.96 | 0.81 |
| 2:C:303:TYR:HA | 2:C:307:VAL:O | 1.80 | 0.81 |
| 2:H:105:LEU:O | 2:H:108:GLU:HB3 | 1.81 | 0.81 |
| 1:F:126:MET:HA | 2:H:109:LEU:HD13 | 1.63 | 0.81 |
| 2:H:240:PHE:N | 2:H:243:SER:HB3 | 1.96 | 0.81 |
| 1:A:163:MET:SD | 1:B:163:MET:HG3 | 2.20 | 0.81 |
| 2:D:37:ILE:HD13 | 2:D:236:LEU:HD13 | 1.63 | 0.81 |
| 1:A:46:ILE:HG13 | 1:A:135:ARG:HH22 | 1.46 | 0.80 |
| 1:A:103:PHE:O | 1:A:107:MET:HG2 | 1.81 | 0.80 |
| 2:D:235:PRO:O | 2:D:238:GLN:HB2 | 1.79 | 0.80 |
| 2:C:201:MET:HB3 | 2:C:201:MET:HE3 | 1.63 | 0.80 |
| 2:H:106:PRO:HA | 2:H:109:LEU:HD12 | 1.62 | 0.80 |
| 2:C:161:VAL:HG22 | 2:C:193:THR:CG2 | 2.11 | 0.80 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:117:THR:O | 1:A:119:LEU:N | 2.14 | 0.80 |
| 2:G:299:ALA:HB2 | 2:G:312:MET:HA | 1.62 | 0.80 |
| 2:H:242:GLN:NE2 | 2:H:311:ILE:HD13 | 1.96 | 0.80 |
| 2:H:241:ILE:HG12 | 2:H:302:ASP:HB2 | 1.61 | 0.80 |
| 1:E:38:LEU:HD22 | 1:E:112:LEU:HB3 | 1.61 | 0.80 |
| 1:F:126:MET:HG2 | 2:H:109:LEU:HD13 | 1.61 | 0.80 |
| 1:E:199:LEU:O | 1:E:203:ILE:HG12 | 1.82 | 0.80 |
| 1:F:26:PHE:CD2 | 1:F:97:THR:HG22 | 2.16 | 0.80 |
| 2:H:101:GLY:O | 2:H:104:ALA:HB3 | 1.82 | 0.80 |
| 2:C:247:LEU:CD1 | 2:C:298:SER:HB2 | 2.10 | 0.80 |
| 2:C:127:LEU:HD21 | 2:C:190:LEU:HD11 | 1.64 | 0.80 |
| 2:H:33:ILE:HD12 | 2:H:207:ILE:O | 1.81 | 0.79 |
| 2:D:241:ILE:HG23 | 2:D:244:THR:OG1 | 1.82 | 0.79 |
| 2:D:98:THR:HA | 2:D:138:PRO:HB3 | 1.64 | 0.79 |
| 2:C:247:LEU:HD21 | 2:C:298:SER:CB | 2.11 | 0.79 |
| 1:F:26:PHE:CE1 | 1:F:97:THR:HA | 2.17 | 0.79 |
| 2:D:33:ILE:HG12 | 2:D:194:ILE:CD1 | 2.12 | 0.79 |
| 2:D:220:ILE:HG22 | 2:D:221:GLU:HG3 | 1.63 | 0.79 |
| 2:G:299:ALA:O | 2:H:298:SER:HA | 1.83 | 0.79 |
| 2:C:214:ILE:CD1 | 2:C:219:LEU:HD23 | 2.12 | 0.79 |
| 1:E:22:VAL:HG12 | 1:E:26:PHE:CE2 | 2.17 | 0.79 |
| 2:H:33:ILE:HG23 | 2:H:194:ILE:HD11 | 1.64 | 0.79 |
| 2:D:33:ILE:HA | 2:D:194:ILE:HG13 | 1.65 | 0.79 |
| 1:B:22:VAL:HG21 | 1:B:93:ILE:HG21 | 1.65 | 0.79 |
| 2:H:48:ILE:H | 2:H:48:ILE:CD1 | 1.96 | 0.78 |
| 1:B:69:ILE:CD1 | 1:B:163:MET:HB3 | 2.13 | 0.78 |
| 2:C:151:ILE:HG13 | 2:C:152:ALA:N | 1.95 | 0.78 |
| 2:D:241:ILE:O | 2:D:241:ILE:HG22 | 1.82 | 0.78 |
| 1:E:36:VAL:HG12 | 1:E:40:VAL:HG23 | 1.65 | 0.78 |
| 2:D:327:ILE:HG13 | 2:D:328:ALA:N | 1.97 | 0.78 |
| 2:C:196:LEU:HD12 | 2:C:197:ILE:H | 1.48 | 0.78 |
| 2:C:234:THR:CA | 2:C:237:ALA:HB3 | 2.14 | 0.78 |
| 1:A:67:PRO:O | 1:A:70:ILE:HG22 | 1.83 | 0.78 |
| 2:C:130:LEU:HD13 | 2:C:148:ARG:HH11 | 1.47 | 0.78 |
| 2:D:95:SER:HA | 2:D:139:SER:OG | 1.84 | 0.78 |
| 2:C:44:LYS:HB2 | 2:C:197:ILE:CD1 | 2.13 | 0.77 |
| 2:D:120:ARG:O | 2:D:124:LEU:HD13 | 1.83 | 0.77 |
| 2:G:125:LEU:HB3 | 2:G:131:GLY:HA3 | 1.66 | 0.77 |
| 1:F:46:ILE:HG22 | 1:F:47:ILE:HG23 | 1.65 | 0.77 |
| 2:C:196:LEU:HD12 | 2:C:197:ILE:N | 1.99 | 0.77 |
| 2:H:48:ILE:HD13 | 2:H:48:ILE:N | 2.00 | 0.77 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:198:THR:HG21 | 2:D:203:VAL:HB | 1.64 | 0.77 |
| 1:E:75:MET:HG2 | 1:E:95:PRO:CB | 2.08 | 0.77 |
| 2:H:128:VAL:HG11 | 2:H:152:ALA:HB2 | 1.66 | 0.77 |
| 2:H:241:ILE:HB | 2:H:300:GLN:HB3 | 1.65 | 0.77 |
| 2:H:245:LEU:HG | 2:H:298:SER:OG | 1.83 | 0.77 |
| 1:F:51:LYS:HB2 | 1:F:54:ARG:HD2 | 1.66 | 0.77 |
| 2:G:276:GLN:HE22 | 2:G:282:LEU:HD11 | 1.50 | 0.77 |
| 2:H:91:PHE:HZ | 2:H:171:LEU:HD21 | 1.49 | 0.77 |
| 1:E:119:LEU:HD13 | 2:G:90:HIS:HB2 | 1.65 | 0.77 |
| 1:B:27:GLY:O | 1:B:104:ILE:HD12 | 1.84 | 0.77 |
| 2:G:2:ILE:HG23 | 2:G:28:VAL:HB | 1.65 | 0.77 |
| 2:D:103:VAL:O | 2:D:106:PRO:HD2 | 1.84 | 0.77 |
| 2:C:238:GLN:O | 2:C:240:PHE:N | 2.16 | 0.77 |
| 1:E:60:VAL:HG13 | 1:E:102:PRO:HB2 | 1.67 | 0.77 |
| 2:C:247:LEU:HD22 | 2:C:297:ILE:HG22 | 1.64 | 0.77 |
| 1:E:37:LEU:O | 1:E:41:THR:HG23 | 1.85 | 0.76 |
| 1:F:42:ARG:HD3 | 1:F:49:ASN:HA | 1.65 | 0.76 |
| 2:D:37:ILE:HG12 | 2:D:38:GLY:N | 2.01 | 0.76 |
| 1:B:167:VAL:HG22 | 1:B:168:GLY:N | 2.00 | 0.76 |
| 2:D:1:MET:HG3 | 2:D:30:ALA:HB2 | 1.66 | 0.76 |
| 1:E:69:ILE:HG13 | 1:F:163:MET:SD | 2.25 | 0.76 |
| 1:E:165:GLY:HA2 | 1:E:169:ALA:O | 1.86 | 0.76 |
| 2:C:296:ILE:HA | 2:C:314:THR:HG22 | 1.67 | 0.76 |
| 1:E:180:GLY:CA | 1:F:73:VAL:HG13 | 2.15 | 0.76 |
| 1:A:132:GLN:O | 1:A:136:LYS:HB3 | 1.85 | 0.76 |
| 1:B:133:ILE:CG2 | 2:D:109:LEU:HD22 | 2.15 | 0.76 |
| 1:A:94:VAL:HB | 1:A:95:PRO:HD3 | 1.68 | 0.76 |
| 1:E:43:PRO:HA | 1:E:48:ALA:HB3 | 1.65 | 0.76 |
| 1:E:71:LEU:HD11 | 1:E:99:GLY:HA2 | 1.67 | 0.76 |
| 1:B:193:LEU:O | 1:B:197:VAL:HG23 | 1.86 | 0.76 |
| 2:D:241:ILE:HG22 | 2:D:245:LEU:HD13 | 1.68 | 0.76 |
| 2:G:180:LEU:O | 2:G:207:ILE:HG21 | 1.85 | 0.75 |
| 1:B:134:VAL:O | 1:B:137:VAL:HG22 | 1.85 | 0.75 |
| 2:G:1:MET:HE1 | 2:G:161:VAL:HG22 | 1.66 | 0.75 |
| 2:C:214:ILE:HD11 | 2:C:219:LEU:CD2 | 2.17 | 0.75 |
| 2:C:36:VAL:O | 2:C:197:ILE:HD12 | 1.87 | 0.75 |
| 1:F:23:SER:HA | 1:F:26:PHE:CZ | 2.22 | 0.75 |
| 2:C:87:ILE:CG2 | 2:C:88:PHE:H | 1.98 | 0.75 |
| 2:G:77:LEU:HD21 | 2:G:81:ARG:NH2 | 2.01 | 0.75 |
| 1:F:118:GLY:HA2 | 1:F:121:GLU:OE2 | 1.85 | 0.75 |
| 1:B:172:LEU:HD23 | 1:B:192:VAL:HG13 | 1.67 | 0.75 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:9:LYS:O | 2:D:20:ALA:HB3 | 1.86 | 0.75 |
| 2:D:31:GLY:H | 2:D:193:THR:CG2 | 1.95 | 0.75 |
| 1:B:172:LEU:CD2 | 1:B:192:VAL:HG13 | 2.17 | 0.75 |
| 2:D:44:LYS:H | 2:D:44:LYS:HD3 | 1.52 | 0.74 |
| 1:B:134:VAL:HA | 1:B:137:VAL:HG13 | 1.67 | 0.74 |
| 2:D:125:LEU:HB3 | 2:D:131:GLY:HA3 | 1.67 | 0.74 |
| 2:H:249:ILE:CG1 | 2:H:250:PRO:HD3 | 2.17 | 0.74 |
| 2:G:79:LYS:O | 2:G:83:GLN:HG2 | 1.87 | 0.74 |
| 2:C:270:ARG:HG2 | 2:C:313:LEU:HD21 | 1.69 | 0.74 |
| 2:D:234:THR:CG2 | 2:D:238:GLN:HE21 | 2.01 | 0.74 |
| 2:G:298:SER:HA | 2:H:299:ALA:O | 1.88 | 0.74 |
| 1:E:174:GLN:O | 1:E:178:GLN:HB2 | 1.87 | 0.74 |
| 2:C:2:ILE:HG23 | 2:C:28:VAL:HB | 1.69 | 0.74 |
| 2:H:26:LEU:HD11 | 2:H:34:TYR:CE1 | 2.23 | 0.74 |
| 1:B:119:LEU:HB3 | 2:D:92:ASN:ND2 | 2.03 | 0.74 |
| 2:H:49:ARG:HB3 | 2:H:54:LEU:HB2 | 1.69 | 0.74 |
| 2:G:183:LEU:HD23 | 2:G:194:ILE:HD12 | 1.70 | 0.74 |
| 1:E:62:ILE:HG13 | 1:E:63:PHE:N | 2.01 | 0.73 |
| 1:E:36:VAL:O | 1:E:40:VAL:HG23 | 1.87 | 0.73 |
| 1:E:38:LEU:HD22 | 1:E:112:LEU:HD22 | 1.70 | 0.73 |
| 1:F:124:ARG:HD2 | 2:H:52:ASN:OD1 | 1.88 | 0.73 |
| 1:F:34:VAL:O | 1:F:37:LEU:HG | 1.87 | 0.73 |
| 1:A:22:VAL:HG12 | 1:A:26:PHE:CE2 | 2.23 | 0.73 |
| 2:C:278:VAL:HA | 2:C:308:LYS:HE2 | 1.70 | 0.73 |
| 2:C:107:LEU:HD22 | 2:C:120:ARG:HH11 | 1.54 | 0.73 |
| 2:C:186:ILE:HB | 2:C:190:LEU:HD12 | 1.70 | 0.73 |
| 1:B:177:TYR:O | 1:B:181:TYR:HB3 | 1.87 | 0.73 |
| 1:F:69:ILE:HG23 | 1:F:163:MET:HE2 | 1.69 | 0.73 |
| 2:H:48:ILE:HG21 | 2:H:197:ILE:HD11 | 1.70 | 0.73 |
| 2:G:82:ARG:HH21 | 2:G:110:ASP:HB3 | 1.54 | 0.73 |
| 1:F:44:GLY:O | 1:F:45:GLN:O | 2.06 | 0.73 |
| 2:C:201:MET:N | 2:C:239:LYS:HD3 | 2.03 | 0.72 |
| 2:C:241:ILE:HG21 | 2:C:300:GLN:HG3 | 1.71 | 0.72 |
| 2:C:165:ASP:HA | 2:C:197:ILE:HG22 | 1.72 | 0.72 |
| 1:E:19:MET:O | 1:E:22:VAL:HB | 1.88 | 0.72 |
| 1:B:115:ILE:HG13 | 1:B:116:PRO:HD2 | 1.69 | 0.72 |
| 2:C:130:LEU:HD22 | 2:C:148:ARG:HB2 | 1.70 | 0.72 |
| 2:H:150:ALA:O | 2:H:153:ARG:HB3 | 1.88 | 0.72 |
| 2:C:266:VAL:HG21 | 2:C:317:HIS:HA | 1.71 | 0.72 |
| 1:A:68:PHE:HD2 | 1:A:163:MET:HG3 | 1.54 | 0.72 |
| 1:E:189:MET:SD | 1:F:73:VAL:HG12 | 2.28 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:214:ILE:HG12 | 2:H:219:LEU:HD23 | 1.70 | 0.72 |
| 1:E:193:LEU:O | 1:E:197:VAL:HG23 | 1.88 | 0.72 |
| 2:C:270:ARG:HA | 2:C:313:LEU:HD23 | 1.71 | 0.72 |
| 1:E:102:PRO:O | 1:E:105:ALA:HB3 | 1.90 | 0.72 |
| 1:E:196:LEU:HD23 | 1:E:199:LEU:HD23 | 1.71 | 0.72 |
| 1:E:32:LEU:O | 1:E:35:GLY:N | 2.19 | 0.72 |
| 1:E:60:VAL:HG13 | 1:E:102:PRO:CB | 2.20 | 0.72 |
| 2:H:283:LEU:HD21 | 2:H:312:MET:SD | 2.29 | 0.72 |
| 2:C:241:ILE:HG13 | 2:C:300:GLN:CB | 2.20 | 0.72 |
| 1:B:92:ALA:HB2 | 1:B:169:ALA:HB2 | 1.69 | 0.72 |
| 2:G:302:ASP:OD2 | 2:H:251:GLU:HG3 | 1.90 | 0.72 |
| 2:D:98:THR:HA | 2:D:138:PRO:CB | 2.19 | 0.72 |
| 2:C:201:MET:CE | 2:C:201:MET:HB3 | 2.19 | 0.72 |
| 1:E:94:VAL:CG2 | 1:E:95:PRO:HD3 | 2.12 | 0.72 |
| 2:G:223:ASP:HB2 | 2:G:228:VAL:HG22 | 1.71 | 0.72 |
| 1:F:179:TYR:O | 1:F:185:ASN:HB2 | 1.90 | 0.71 |
| 1:F:42:ARG:C | 1:F:44:GLY:H | 1.94 | 0.71 |
| 2:G:77:LEU:HD21 | 2:G:81:ARG:CZ | 2.20 | 0.71 |
| 1:B:37:LEU:HD21 | 1:B:56:VAL:CG1 | 2.19 | 0.71 |
| 1:F:12:GLY:C | 1:F:172:LEU:HD11 | 2.10 | 0.71 |
| 1:E:70:ILE:HD12 | 1:F:192:VAL:HG12 | 1.72 | 0.71 |
| 2:D:162:LEU:HB3 | 2:D:194:ILE:HG22 | 1.71 | 0.71 |
| 2:H:249:ILE:CG2 | 2:H:250:PRO:HD3 | 2.19 | 0.71 |
| 2:H:245:LEU:CD2 | 2:H:311:ILE:HG22 | 2.19 | 0.71 |
| 2:H:273:PHE:HB2 | 2:H:310:GLY:O | 1.89 | 0.71 |
| 1:F:37:LEU:HD21 | 1:F:56:VAL:HG11 | 1.72 | 0.71 |
| 2:H:249:ILE:CB | 2:H:250:PRO:HD3 | 2.20 | 0.71 |
| 2:G:4:LEU:HD23 | 2:G:62:VAL:HG13 | 1.70 | 0.71 |
| 2:D:43:GLY:N | 2:D:44:LYS:HZ2 | 1.88 | 0.71 |
| 2:H:245:LEU:HD22 | 2:H:311:ILE:HG22 | 1.71 | 0.71 |
| 1:A:42:ARG:HA | 1:A:42:ARG:CZ | 2.20 | 0.71 |
| 2:H:268:MET:O | 2:H:339:VAL:HG13 | 1.90 | 0.71 |
| 2:C:248:ASP:HB3 | 2:C:254:GLN:CG | 2.20 | 0.71 |
| 1:A:180:GLY:HA3 | 1:B:73:VAL:HG11 | 1.73 | 0.71 |
| 2:C:196:LEU:HD22 | 2:C:207:ILE:HD11 | 1.72 | 0.71 |
| 1:E:198:ILE:HG13 | 1:E:199:LEU:N | 2.04 | 0.71 |
| 1:E:172:LEU:O | 1:E:175:ILE:HG12 | 1.90 | 0.71 |
| 1:A:69:ILE:CG2 | 1:B:163:MET:SD | 2.77 | 0.71 |
| 1:F:45:GLN:HE21 | 1:F:46:ILE:HG12 | 1.56 | 0.71 |
| 1:E:80:ARG:HG3 | 1:E:85:THR:HG23 | 1.71 | 0.71 |
| 1:F:63:PHE:HA | 1:F:66:ILE:HD12 | 1.71 | 0.71 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:234:THR:HG23 | 2:C:272:GLU:OE1 | 1.91 | 0.71 |
| 2:D:124:LEU:O | 2:D:128:VAL:HG13 | 1.89 | 0.71 |
| 2:C:130:LEU:HD21 | 2:C:145:GLN:HA | 1.73 | 0.71 |
| 2:C:288:ARG:HG2 | 2:D:288:ARG:HA | 1.73 | 0.71 |
| 2:C:238:GLN:HG2 | 2:C:238:GLN:O | 1.90 | 0.70 |
| 1:E:46:ILE:O | 1:E:47:ILE:HG23 | 1.90 | 0.70 |
| 2:H:48:ILE:CD1 | 2:H:48:ILE:N | 2.53 | 0.70 |
| 2:D:99:VAL:HG23 | 2:D:137:TYR:O | 1.92 | 0.70 |
| 2:H:84:ILE:HD11 | 2:H:163:LEU:HD11 | 1.73 | 0.70 |
| 2:C:214:ILE:CG1 | 2:C:219:LEU:HD23 | 2.21 | 0.70 |
| 2:G:283:LEU:HD11 | 2:G:312:MET:SD | 2.31 | 0.70 |
| 2:D:163:LEU:HD23 | 2:D:195:LEU:HB3 | 1.72 | 0.70 |
| 1:B:22:VAL:HG21 | 1:B:93:ILE:CG2 | 2.22 | 0.70 |
| 1:F:124:ARG:HH22 | 2:H:85:GLY:HA2 | 1.57 | 0.70 |
| 1:F:164:GLY:CA | 1:F:169:ALA:HB3 | 2.21 | 0.70 |
| 2:G:288:ARG:HA | 2:H:288:ARG:HG2 | 1.72 | 0.70 |
| 2:G:70:THR:O | 2:G:72:LEU:HG | 1.92 | 0.70 |
| 1:E:171:GLY:O | 1:E:175:ILE:HG23 | 1.90 | 0.70 |
| 1:F:19:MET:HB3 | 1:F:157:LEU:CD1 | 2.21 | 0.70 |
| 1:A:124:ARG:HA | 1:A:128:ALA:HB3 | 1.72 | 0.70 |
| 2:D:144:GLY:HA2 | 2:D:175:THR:HG21 | 1.73 | 0.70 |
| 2:H:87:ILE:HG23 | 2:H:147:GLN:NE2 | 2.06 | 0.70 |
| 2:H:241:ILE:HG12 | 2:H:302:ASP:CB | 2.22 | 0.70 |
| 2:C:201:MET:H | 2:C:239:LYS:HD3 | 1.55 | 0.70 |
| 2:D:48:ILE:N | 2:D:48:ILE:CD1 | 2.45 | 0.70 |
| 2:D:234:THR:O | 2:D:237:ALA:N | 2.25 | 0.70 |
| 1:B:8:LEU:H | 1:B:8:LEU:HD12 | 1.57 | 0.70 |
| 1:A:132:GLN:O | 1:A:136:LYS:CB | 2.39 | 0.70 |
| 1:B:20:THR:O | 1:B:23:SER:HB2 | 1.91 | 0.70 |
| 2:H:269:LEU:CD2 | 2:H:339:VAL:HG22 | 2.21 | 0.70 |
| 2:C:244:THR:O | 2:C:247:LEU:HG | 1.92 | 0.70 |
| 2:G:215:SER:HB3 | 2:G:220:ILE:HD11 | 1.74 | 0.70 |
| 2:C:63:LEU:HB2 | 2:C:68:GLU:HG2 | 1.74 | 0.70 |
| 2:H:26:LEU:HD11 | 2:H:34:TYR:CZ | 2.26 | 0.69 |
| 1:F:120:ILE:O | 1:F:123:SER:HB2 | 1.93 | 0.69 |
| 1:E:11:ARG:O | 1:E:14:TRP:HB3 | 1.91 | 0.69 |
| 2:C:238:GLN:C | 2:C:240:PHE:H | 1.96 | 0.69 |
| 1:B:89:LEU:HA | 1:B:169:ALA:CB | 2.23 | 0.69 |
| 1:A:131:MET:O | 1:A:135:ARG:HG2 | 1.92 | 0.69 |
| 2:H:249:ILE:HG12 | 2:H:250:PRO:CD | 2.22 | 0.69 |
| 2:D:37:ILE:HD11 | 2:D:236:LEU:HD22 | 1.74 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:290:PHE:CE2 | 2:C:329:TRP:HB2 | 2.27 | 0.69 |
| 1:E:31:GLY:O | 1:E:34:VAL:HG22 | 1.93 | 0.69 |
| 1:E:12:GLY:O | 1:E:15:GLU:HB2 | 1.91 | 0.69 |
| 2:D:171:LEU:HD22 | 2:D:175:THR:HG21 | 1.75 | 0.69 |
| 1:E:194:VAL:O | 1:E:198:ILE:HG23 | 1.93 | 0.69 |
| 1:E:59:ILE:O | 1:E:62:ILE:HG12 | 1.93 | 0.69 |
| 1:E:119:LEU:CD1 | 2:G:90:HIS:HB2 | 2.22 | 0.69 |
| 2:G:37:ILE:HD11 | 2:G:236:LEU:CD2 | 2.22 | 0.69 |
| 2:D:9:LYS:HE2 | 2:D:55:GLU:OE1 | 1.92 | 0.69 |
| 2:H:84:ILE:HD11 | 2:H:163:LEU:CD1 | 2.23 | 0.69 |
| 1:E:50:ALA:O | 1:E:51:LYS:HG2 | 1.92 | 0.69 |
| 1:A:75:MET:CE | 1:A:95:PRO:HB3 | 2.23 | 0.69 |
| 2:H:47:LEU:O | 2:H:50:CYS:HB2 | 1.91 | 0.69 |
| 2:G:208:CYS:O | 2:G:225:VAL:HG21 | 1.93 | 0.68 |
| 2:D:26:LEU:HD11 | 2:D:34:TYR:CZ | 2.27 | 0.68 |
| 2:C:77:LEU:HD21 | 2:C:81:ARG:NH2 | 2.07 | 0.68 |
| 1:E:64:ARG:HH12 | 1:E:103:PHE:HD1 | 1.38 | 0.68 |
| 1:A:40:VAL:HA | 1:A:49:ASN:CB | 2.23 | 0.68 |
| 1:B:139:LEU:HB2 | 1:B:140:PRO:HD3 | 1.75 | 0.68 |
| 2:H:121:VAL:HG12 | 2:H:125:LEU:HD12 | 1.75 | 0.68 |
| 2:H:199:HIS:ND1 | 2:H:200:GLU:HG3 | 2.07 | 0.68 |
| 2:H:242:GLN:HE21 | 2:H:311:ILE:HD13 | 1.57 | 0.68 |
| 1:F:130:PRO:HD2 | 1:F:133:ILE:HB | 1.73 | 0.68 |
| 1:A:165:GLY:HA2 | 1:A:174:GLN:CG | 2.23 | 0.68 |
| 1:A:38:LEU:HD22 | 1:A:112:LEU:HB3 | 1.75 | 0.68 |
| 1:B:118:GLY:O | 1:B:121:GLU:HB2 | 1.92 | 0.68 |
| 2:D:197:ILE:N | 2:D:197:ILE:HD12 | 2.08 | 0.68 |
| 1:B:85:THR:HG22 | 1:B:87:ILE:HG12 | 1.74 | 0.68 |
| 2:D:26:LEU:HD11 | 2:D:34:TYR:OH | 1.93 | 0.68 |
| 2:H:249:ILE:HG12 | 2:H:250:PRO:HD3 | 1.74 | 0.68 |
| 2:G:38:GLY:HA3 | 2:G:44:LYS:HD3 | 1.75 | 0.68 |
| 2:C:273:PHE:HD1 | 2:C:276:GLN:NE2 | 1.91 | 0.68 |
| 1:F:172:LEU:HD12 | 1:F:172:LEU:N | 2.09 | 0.68 |
| 1:F:124:ARG:HG3 | 2:H:54:LEU:HD21 | 1.76 | 0.68 |
| 1:B:177:TYR:O | 1:B:181:TYR:CB | 2.41 | 0.68 |
| 1:E:85:THR:O | 1:E:85:THR:HG22 | 1.94 | 0.68 |
| 2:H:37:ILE:HB | 2:H:204:VAL:HG21 | 1.75 | 0.68 |
| 2:C:270:ARG:CG | 2:C:313:LEU:HD21 | 2.23 | 0.68 |
| 1:F:69:ILE:HD12 | 1:F:70:ILE:H | 1.59 | 0.68 |
| 1:A:165:GLY:HA2 | 1:A:174:GLN:HG3 | 1.75 | 0.68 |
| 1:A:139:LEU:HB2 | 1:A:140:PRO:HD3 | 1.76 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:266:VAL:HG22 | 2:C:267:PRO:HD2 | 1.74 | 0.67 |
| 2:C:44:LYS:NZ | 2:C:198:THR:O | 2.25 | 0.67 |
| 2:G:144:GLY:HA2 | 2:G:171:LEU:HD22 | 1.76 | 0.67 |
| 2:H:85:GLY:O | 2:H:162:LEU:HA | 1.94 | 0.67 |
| 1:B:69:ILE:HD11 | 1:B:163:MET:CE | 2.24 | 0.67 |
| 1:A:115:ILE:HD13 | 1:A:115:ILE:O | 1.94 | 0.67 |
| 2:C:48:ILE:HD11 | 2:C:163:LEU:HB3 | 1.76 | 0.67 |
| 1:F:45:GLN:NE2 | 1:F:46:ILE:HG12 | 2.09 | 0.67 |
| 1:F:128:ALA:O | 1:F:130:PRO:HD3 | 1.95 | 0.67 |
| 1:B:104:ILE:O | 1:B:107:MET:HB2 | 1.94 | 0.67 |
| 1:B:60:VAL:HG13 | 1:B:102:PRO:HA | 1.76 | 0.67 |
| 2:D:143:GLY:HA2 | 2:D:146:LYS:CD | 2.23 | 0.67 |
| 1:F:68:PHE:H | 1:F:68:PHE:HD1 | 1.41 | 0.67 |
| 1:E:163:MET:SD | 1:F:69:ILE:HG12 | 2.34 | 0.67 |
| 1:A:189:MET:HE2 | 1:B:74:TRP:N | 2.09 | 0.67 |
| 1:E:135:ARG:HD2 | 1:E:135:ARG:N | 2.08 | 0.67 |
| 2:D:330:LEU:HB3 | 2:D:335:VAL:HB | 1.77 | 0.67 |
| 2:D:36:VAL:HG11 | 2:D:47:LEU:HD23 | 1.77 | 0.67 |
| 1:F:30:ILE:HD11 | 1:F:101:ALA:CB | 2.25 | 0.67 |
| 2:D:267:PRO:HB3 | 2:D:342:TYR:CE2 | 2.30 | 0.67 |
| 2:G:121:VAL:O | 2:G:125:LEU:HG | 1.94 | 0.67 |
| 1:A:116:PRO:O | 1:A:117:THR:O | 2.13 | 0.67 |
| 1:F:198:ILE:HG13 | 1:F:199:LEU:N | 2.08 | 0.67 |
| 1:B:63:PHE:HB3 | 1:B:102:PRO:HG3 | 1.76 | 0.67 |
| 2:C:274:THR:O | 2:C:276:GLN:HG3 | 1.94 | 0.67 |
| 1:F:115:ILE:N | 1:F:116:PRO:HD2 | 2.10 | 0.67 |
| 2:C:166:GLU:OE2 | 2:C:198:THR:HA | 1.95 | 0.67 |
| 2:C:200:GLU:HB3 | 2:C:239:LYS:CE | 2.22 | 0.67 |
| 2:D:36:VAL:HG12 | 2:D:214:ILE:HD13 | 1.77 | 0.67 |
| 2:D:266:VAL:HG21 | 2:D:317:HIS:HA | 1.77 | 0.67 |
| 1:B:185:ASN:HB2 | 1:B:188:VAL:HG22 | 1.77 | 0.67 |
| 2:D:98:THR:HG22 | 2:D:138:PRO:HD3 | 1.77 | 0.67 |
| 1:A:39:TYR:CD2 | 1:A:48:ALA:HB3 | 2.30 | 0.67 |
| 1:E:38:LEU:CB | 1:E:112:LEU:HD13 | 2.24 | 0.66 |
| 1:A:121:GLU:HA | 1:A:121:GLU:OE2 | 1.95 | 0.66 |
| 2:C:127:LEU:CD2 | 2:C:190:LEU:HD11 | 2.24 | 0.66 |
| 2:G:276:GLN:NE2 | 2:G:282:LEU:HD11 | 2.10 | 0.66 |
| 1:E:66:ILE:HG12 | 1:F:193:LEU:HD21 | 1.76 | 0.66 |
| 1:F:22:VAL:HG23 | 1:F:23:SER:N | 2.09 | 0.66 |
| 2:H:299:ALA:CB | 2:H:312:MET:HG3 | 2.24 | 0.66 |
| 1:E:155:ILE:HB | 1:E:200:VAL:HG13 | 1.77 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:4:LEU:HD23 | 2:H:62:VAL:HG13 | 1.78 | 0.66 |
| 1:A:42:ARG:NE | 1:A:42:ARG:HA | 2.11 | 0.66 |
| 1:A:87:ILE:HG12 | 1:A:167:VAL:O | 1.94 | 0.66 |
| 2:C:246:HIS:HA | 2:C:249:ILE:CG1 | 2.24 | 0.66 |
| 2:D:189:ARG:CG | 2:D:189:ARG:HH21 | 2.07 | 0.66 |
| 1:F:36:VAL:O | 1:F:36:VAL:HG12 | 1.96 | 0.66 |
| 2:G:213:VAL:HG21 | 2:G:233:LYS:HD2 | 1.78 | 0.66 |
| 2:D:98:THR:HA | 2:D:138:PRO:HA | 1.78 | 0.66 |
| 2:G:241:ILE:CD1 | 2:H:248:ASP:HB2 | 2.24 | 0.66 |
| 2:G:63:LEU:HD12 | 2:G:68:GLU:HG2 | 1.77 | 0.66 |
| 1:E:81:VAL:HG23 | 1:E:84:GLY:H | 1.60 | 0.66 |
| 2:H:246:HIS:CE1 | 2:H:247:LEU:HD12 | 2.30 | 0.66 |
| 2:D:248:ASP:C | 2:D:249:ILE:O | 2.34 | 0.66 |
| 1:A:35:GLY:HA3 | 1:A:108:VAL:HG11 | 1.78 | 0.66 |
| 1:F:19:MET:CB | 1:F:157:LEU:HD11 | 2.24 | 0.66 |
| 1:F:139:LEU:N | 1:F:140:PRO:CD | 2.59 | 0.66 |
| 1:B:127:GLY:HA3 | 2:D:109:LEU:CD1 | 2.25 | 0.66 |
| 1:E:174:GLN:HA | 1:E:177:TYR:CB | 2.26 | 0.66 |
| 2:G:63:LEU:HA | 2:G:67:GLN:O | 1.96 | 0.66 |
| 2:H:84:ILE:HD11 | 2:H:163:LEU:CG | 2.26 | 0.66 |
| 2:C:53:LEU:HD22 | 2:C:69:LEU:HB3 | 1.77 | 0.66 |
| 1:E:30:ILE:C | 1:E:33:PRO:HD2 | 2.16 | 0.65 |
| 2:H:125:LEU:HB3 | 2:H:131:GLY:HA3 | 1.76 | 0.65 |
| 1:A:59:ILE:HA | 1:A:62:ILE:HG12 | 1.77 | 0.65 |
| 2:G:205:LYS:NZ | 2:G:304:ALA:HB2 | 2.10 | 0.65 |
| 2:G:295:ASN:HD21 | 2:G:317:HIS:CD2 | 2.14 | 0.65 |
| 2:H:171:LEU:HD13 | 2:H:179:ILE:HD12 | 1.78 | 0.65 |
| 2:D:7:ILE:O | 2:D:24:VAL:HG22 | 1.97 | 0.65 |
| 1:F:196:LEU:O | 1:F:199:LEU:HB3 | 1.96 | 0.65 |
| 1:A:15:GLU:OE1 | 1:A:171:GLY:HA2 | 1.95 | 0.65 |
| 2:D:98:THR:HA | 2:D:138:PRO:CA | 2.27 | 0.65 |
| 2:H:112:THR:N | 2:H:113:PRO:HD3 | 2.12 | 0.65 |
| 2:C:100:PHE:HZ | 2:C:118:LYS:HA | 1.62 | 0.65 |
| 2:C:299:ALA:O | 2:C:300:GLN:HG2 | 1.97 | 0.65 |
| 1:F:20:THR:N | 1:F:157:LEU:HD21 | 2.10 | 0.65 |
| 1:F:139:LEU:HG | 1:F:140:PRO:HD3 | 1.78 | 0.65 |
| 1:F:90:GLN:O | 1:F:93:ILE:HG12 | 1.95 | 0.65 |
| 2:G:137:TYR:HB3 | 2:G:141:LEU:HD11 | 1.77 | 0.65 |
| 1:A:64:ARG:NH1 | 1:A:106:ARG:HD2 | 2.12 | 0.65 |
| 2:H:98:THR:HA | 2:H:138:PRO:HA | 1.77 | 0.65 |
| 1:B:93:ILE:O | 1:B:96:LEU:HB3 | 1.97 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:97:ARG:NH1 | 2:G:105:LEU:HD21 | 2.12 | 0.65 |
| 1:F:171:GLY:O | 1:F:174:GLN:HB3 | 1.97 | 0.65 |
| 2:C:241:ILE:HG21 | 2:C:300:GLN:CG | 2.27 | 0.65 |
| 2:H:164:CYS:HB3 | 2:H:167:ALA:HB2 | 1.79 | 0.65 |
| 1:A:181:TYR:CE2 | 1:B:167:VAL:HG23 | 2.32 | 0.65 |
| 2:D:250:PRO:HG2 | 2:D:253:TYR:CG | 2.32 | 0.65 |
| 2:H:119:ARG:O | 2:H:123:GLU:N | 2.26 | 0.65 |
| 2:D:33:ILE:HD13 | 2:D:207:ILE:HB | 1.77 | 0.65 |
| 1:A:139:LEU:HA | 1:A:142:ALA:HB3 | 1.79 | 0.65 |
| 2:G:231:HIS:O | 2:G:233:LYS:N | 2.28 | 0.65 |
| 2:G:125:LEU:HB3 | 2:G:131:GLY:CA | 2.27 | 0.65 |
| 2:G:164:CYS:SG | 2:G:183:LEU:HD21 | 2.36 | 0.65 |
| 2:C:4:LEU:HB2 | 2:C:26:LEU:HB3 | 1.78 | 0.65 |
| 2:C:36:VAL:CG1 | 2:C:214:ILE:HD13 | 2.27 | 0.65 |
| 1:F:185:ASN:ND2 | 1:F:188:VAL:HG22 | 2.12 | 0.65 |
| 1:B:131:MET:HG3 | 1:B:132:GLN:H | 1.62 | 0.65 |
| 1:F:139:LEU:O | 1:F:142:ALA:N | 2.29 | 0.64 |
| 1:F:35:GLY:C | 1:F:37:LEU:H | 2.00 | 0.64 |
| 1:F:42:ARG:C | 1:F:44:GLY:N | 2.49 | 0.64 |
| 1:B:126:MET:SD | 2:D:153:ARG:HD2 | 2.37 | 0.64 |
| 2:C:12:HIS:HD2 | 2:C:17:THR:HG23 | 1.61 | 0.64 |
| 1:A:172:LEU:HD23 | 1:A:172:LEU:O | 1.97 | 0.64 |
| 2:H:2:ILE:HG23 | 2:H:28:VAL:HB | 1.79 | 0.64 |
| 1:B:41:THR:C | 1:B:43:PRO:HD3 | 2.18 | 0.64 |
| 1:F:137:VAL:HG23 | 1:F:138:LEU:HG | 1.79 | 0.64 |
| 1:B:167:VAL:HG22 | 1:B:168:GLY:H | 1.61 | 0.64 |
| 2:D:7:ILE:HB | 2:D:24:VAL:HG23 | 1.78 | 0.64 |
| 2:G:52:ASN:HD21 | 2:G:54:LEU:HG | 1.63 | 0.64 |
| 2:H:24:VAL:HG12 | 2:H:219:LEU:HG | 1.78 | 0.64 |
| 1:F:22:VAL:HG11 | 1:F:93:ILE:HG21 | 1.80 | 0.64 |
| 2:G:93:LEU:HD22 | 2:G:102:ASN:ND2 | 2.12 | 0.64 |
| 1:A:38:LEU:HA | 1:A:41:THR:HG23 | 1.80 | 0.64 |
| 1:A:58:ALA:O | 1:A:62:ILE:HG23 | 1.98 | 0.64 |
| 1:E:201:TYR:OH | 1:F:62:ILE:HG22 | 1.96 | 0.64 |
| 2:C:201:MET:H | 2:C:239:LYS:CD | 2.10 | 0.64 |
| 2:C:247:LEU:HD11 | 2:C:298:SER:HB3 | 1.77 | 0.64 |
| 2:H:220:ILE:CG2 | 2:H:233:LYS:HD3 | 2.27 | 0.64 |
| 2:C:234:THR:N | 2:C:235:PRO:HD2 | 2.13 | 0.64 |
| 1:F:123:SER:HA | 1:F:129:THR:HG21 | 1.80 | 0.64 |
| 1:A:181:TYR:CZ | 1:B:167:VAL:HG23 | 2.32 | 0.64 |
| 2:D:184:LYS:O | 2:D:187:ASN:HB3 | 1.98 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:80:ALA:O | 2:G:83:GLN:HB2 | 1.97 | 0.64 |
| 1:F:115:ILE:HG22 | 1:F:116:PRO:N | 2.13 | 0.64 |
| 1:B:155:ILE:CG2 | 1:B:200:VAL:HG13 | 2.27 | 0.64 |
| 2:D:279:ASP:O | 2:D:280:ALA:C | 2.36 | 0.64 |
| 2:G:252:ASP:HA | 2:G:255:GLU:HG2 | 1.78 | 0.64 |
| 1:F:129:THR:O | 1:F:129:THR:HG23 | 1.97 | 0.64 |
| 1:F:59:ILE:HA | 1:F:62:ILE:HG12 | 1.78 | 0.64 |
| 2:H:87:ILE:HG22 | 2:H:88:PHE:N | 2.11 | 0.64 |
| 2:D:151:ILE:HD11 | 2:D:182:LEU:HD21 | 1.80 | 0.64 |
| 2:G:93:LEU:HD11 | 2:G:149:VAL:HB | 1.79 | 0.64 |
| 2:G:4:LEU:HB3 | 2:G:7:ILE:HG12 | 1.80 | 0.64 |
| 1:B:68:PHE:HB3 | 1:B:160:TYR:CE2 | 2.31 | 0.64 |
| 2:C:233:LYS:O | 2:C:237:ALA:HB2 | 1.98 | 0.63 |
| 1:F:74:TRP:O | 1:F:77:PRO:HD2 | 1.97 | 0.63 |
| 2:G:37:ILE:HD11 | 2:G:236:LEU:HB3 | 1.79 | 0.63 |
| 2:D:273:PHE:CE1 | 2:D:335:VAL:HG13 | 2.32 | 0.63 |
| 2:C:157:SER:O | 2:C:158:ASN:HB2 | 1.98 | 0.63 |
| 2:C:2:ILE:CG2 | 2:C:28:VAL:HB | 2.29 | 0.63 |
| 1:E:76:ILE:HB | 1:E:77:PRO:HD3 | 1.80 | 0.63 |
| 1:F:152:ILE:HA | 1:F:155:ILE:HG23 | 1.80 | 0.63 |
| 2:H:84:ILE:HD11 | 2:H:163:LEU:HG | 1.80 | 0.63 |
| 2:C:44:LYS:NZ | 2:C:199:HIS:HA | 2.13 | 0.63 |
| 2:H:91:PHE:CZ | 2:H:171:LEU:HD21 | 2.31 | 0.63 |
| 1:A:69:ILE:HG21 | 1:B:163:MET:CE | 2.27 | 0.63 |
| 1:F:16:THR:OG1 | 1:F:172:LEU:HD13 | 1.98 | 0.63 |
| 1:E:163:MET:SD | 1:F:163:MET:HE1 | 2.38 | 0.63 |
| 2:H:221:GLU:OE1 | 2:H:230:SER:HB2 | 1.96 | 0.63 |
| 2:C:158:ASN:H | 2:C:159:PRO:HD3 | 1.64 | 0.63 |
| 1:F:55:THR:O | 1:F:58:ALA:HB3 | 1.97 | 0.63 |
| 1:B:89:LEU:HD13 | 1:B:170:GLY:O | 1.98 | 0.63 |
| 2:G:151:ILE:O | 2:G:155:LEU:HG | 1.98 | 0.63 |
| 1:E:26:PHE:HB3 | 1:E:97:THR:HB | 1.79 | 0.63 |
| 1:E:67:PRO:O | 1:E:71:LEU:HB2 | 1.98 | 0.63 |
| 2:H:63:LEU:HD13 | 2:H:68:GLU:HG3 | 1.79 | 0.63 |
| 1:F:30:ILE:HD11 | 1:F:101:ALA:HB1 | 1.81 | 0.63 |
| 2:G:3:LYS:HD3 | 2:G:63:LEU:HD13 | 1.79 | 0.63 |
| 1:B:94:VAL:HA | 1:B:97:THR:HG23 | 1.79 | 0.63 |
| 2:D:324:GLN:O | 2:D:327:ILE:HG12 | 1.99 | 0.63 |
| 2:D:265:CYS:HB2 | 2:D:343:VAL:OXT | 1.98 | 0.63 |
| 2:C:168:THR:HG21 | 2:C:176:THR:HG23 | 1.81 | 0.63 |
| 1:E:93:ILE:O | 1:E:96:LEU:HB3 | 1.98 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:124:ARG:NH1 | 1:F:124:ARG:HB3 | 2.13 | 0.63 |
| 1:E:115:ILE:HG23 | 1:E:116:PRO:HD2 | 1.79 | 0.63 |
| 2:C:249:ILE:CG2 | 2:D:206:ARG:NH1 | 2.62 | 0.62 |
| 1:F:93:ILE:HG13 | 1:F:94:VAL:N | 2.14 | 0.62 |
| 1:B:64:ARG:HG3 | 1:B:102:PRO:HB2 | 1.81 | 0.62 |
| 1:E:64:ARG:NH1 | 1:E:103:PHE:HD1 | 1.97 | 0.62 |
| 1:E:73:VAL:HG21 | 1:F:180:GLY:HA3 | 1.80 | 0.62 |
| 1:F:59:ILE:O | 1:F:62:ILE:HG12 | 1.99 | 0.62 |
| 1:F:104:ILE:HD12 | 1:F:105:ALA:N | 2.14 | 0.62 |
| 1:B:177:TYR:O | 1:B:181:TYR:N | 2.31 | 0.62 |
| 1:A:40:VAL:HA | 1:A:49:ASN:HB3 | 1.82 | 0.62 |
| 2:C:29:PRO:HG3 | 2:C:32:GLN:OE1 | 1.99 | 0.62 |
| 1:B:90:GLN:O | 1:B:93:ILE:HG12 | 2.00 | 0.62 |
| 2:G:98:THR:HA | 2:G:138:PRO:HA | 1.80 | 0.62 |
| 1:E:22:VAL:HG21 | 1:E:96:LEU:HD23 | 1.80 | 0.62 |
| 2:G:22:ASN:HB2 | 2:G:218:GLU:HG2 | 1.81 | 0.62 |
| 2:C:36:VAL:HB | 2:C:197:ILE:HD13 | 1.80 | 0.62 |
| 1:F:25:PHE:O | 1:F:29:VAL:HG23 | 2.00 | 0.62 |
| 1:B:163:MET:O | 1:B:167:VAL:HG12 | 2.00 | 0.62 |
| 1:B:93:ILE:HG13 | 1:B:94:VAL:N | 2.12 | 0.62 |
| 2:C:171:LEU:HD13 | 2:C:179:ILE:HD12 | 1.80 | 0.62 |
| 2:C:288:ARG:NH1 | 2:D:287:ALA:HB1 | 2.15 | 0.62 |
| 1:E:25:PHE:O | 1:E:29:VAL:HB | 1.98 | 0.62 |
| 1:F:89:LEU:O | 1:F:93:ILE:HG23 | 2.00 | 0.62 |
| 1:B:69:ILE:HD11 | 1:B:163:MET:HE3 | 1.79 | 0.62 |
| 2:D:36:VAL:HG11 | 2:D:47:LEU:CD2 | 2.30 | 0.62 |
| 2:D:250:PRO:O | 2:D:253:TYR:HB3 | 2.00 | 0.62 |
| 2:G:174:ALA:HA | 2:G:177:ARG:NH1 | 2.13 | 0.62 |
| 2:D:196:LEU:HD21 | 2:D:203:VAL:HG12 | 1.81 | 0.62 |
| 1:A:26:PHE:CZ | 1:A:157:LEU:HD11 | 2.34 | 0.62 |
| 2:C:168:THR:CG2 | 2:C:176:THR:HG23 | 2.30 | 0.62 |
| 1:F:107:MET:HE2 | 1:F:149:ALA:CB | 2.30 | 0.62 |
| 2:C:201:MET:HG3 | 2:C:236:LEU:O | 1.99 | 0.62 |
| 2:C:4:LEU:HD12 | 2:C:26:LEU:HD23 | 1.82 | 0.62 |
| 1:B:23:SER:HA | 1:B:26:PHE:CZ | 2.35 | 0.62 |
| 2:D:241:ILE:O | 2:D:245:LEU:HD13 | 2.00 | 0.62 |
| 2:C:44:LYS:HZ1 | 2:C:199:HIS:HA | 1.65 | 0.61 |
| 1:E:73:VAL:CG2 | 1:F:180:GLY:HA3 | 2.30 | 0.61 |
| 1:A:68:PHE:CD2 | 1:A:163:MET:HG3 | 2.34 | 0.61 |
| 1:A:128:ALA:O | 1:A:129:THR:HG23 | 2.00 | 0.61 |
| 2:C:303:TYR:CA | 2:C:307:VAL:O | 2.48 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:15:GLU:O | 1:E:18:ALA:HB3 | 2.00 | 0.61 |
| 1:A:76:ILE:HG21 | 1:B:184:TYR:CE1 | 2.35 | 0.61 |
| 1:A:22:VAL:HG12 | 1:A:26:PHE:CD2 | 2.35 | 0.61 |
| 1:A:22:VAL:HG22 | 1:A:93:ILE:HG22 | 1.82 | 0.61 |
| 1:A:40:VAL:HG22 | 1:A:48:ALA:O | 2.00 | 0.61 |
| 2:H:82:ARG:HD3 | 2:H:110:ASP:CG | 2.21 | 0.61 |
| 2:C:201:MET:HB2 | 2:C:239:LYS:HB3 | 1.82 | 0.61 |
| 2:C:7:ILE:HB | 2:C:24:VAL:CG2 | 2.30 | 0.61 |
| 1:A:130:PRO:O | 1:A:131:MET:O | 2.18 | 0.61 |
| 2:G:288:ARG:HG2 | 2:H:288:ARG:HA | 1.82 | 0.61 |
| 1:E:23:SER:HA | 1:E:26:PHE:CE2 | 2.36 | 0.61 |
| 1:B:15:GLU:HB3 | 1:B:89:LEU:HD21 | 1.81 | 0.61 |
| 2:D:48:ILE:HD11 | 2:D:197:ILE:HG12 | 1.81 | 0.61 |
| 1:F:104:ILE:CG2 | 1:F:153:THR:HG21 | 2.29 | 0.61 |
| 2:G:33:ILE:HG12 | 2:G:194:ILE:CG1 | 2.30 | 0.61 |
| 2:D:93:LEU:HD11 | 2:D:146:LYS:O | 2.01 | 0.61 |
| 2:D:234:THR:HG22 | 2:D:238:GLN:HE21 | 1.64 | 0.61 |
| 2:D:143:GLY:HA2 | 2:D:146:LYS:HE3 | 1.82 | 0.61 |
| 2:C:168:THR:HB | 2:C:176:THR:HG23 | 1.83 | 0.61 |
| 1:A:75:MET:O | 1:A:79:THR:N | 2.30 | 0.61 |
| 1:A:126:MET:HE2 | 2:C:153:ARG:HD2 | 1.80 | 0.61 |
| 1:A:130:PRO:CG | 1:A:131:MET:H | 2.07 | 0.61 |
| 2:D:125:LEU:O | 2:D:128:VAL:HG22 | 2.01 | 0.61 |
| 2:C:91:PHE:CE2 | 2:C:146:LYS:HD2 | 2.36 | 0.61 |
| 2:C:1:MET:HE1 | 2:C:161:VAL:HG23 | 1.81 | 0.61 |
| 2:H:173:PRO:O | 2:H:177:ARG:HG3 | 2.01 | 0.61 |
| 2:G:122:THR:HA | 2:G:125:LEU:HD12 | 1.81 | 0.61 |
| 2:D:91:PHE:CE1 | 2:D:171:LEU:HD21 | 2.35 | 0.61 |
| 1:B:85:THR:CG2 | 1:B:87:ILE:HG12 | 2.29 | 0.61 |
| 2:C:273:PHE:HB3 | 2:C:276:GLN:NE2 | 2.15 | 0.61 |
| 2:C:238:GLN:C | 2:C:240:PHE:N | 2.51 | 0.61 |
| 2:H:106:PRO:CA | 2:H:109:LEU:HD12 | 2.30 | 0.61 |
| 2:C:104:ALA:O | 2:C:107:LEU:N | 2.33 | 0.61 |
| 2:D:91:PHE:HE1 | 2:D:171:LEU:HD21 | 1.64 | 0.61 |
| 2:H:189:ARG:O | 2:H:190:LEU:O | 2.19 | 0.61 |
| 2:D:29:PRO:HG2 | 2:D:32:GLN:CD | 2.20 | 0.61 |
| 2:C:196:LEU:HD21 | 2:C:203:VAL:HG12 | 1.83 | 0.61 |
| 1:A:34:VAL:O | 1:A:37:LEU:HG | 2.01 | 0.61 |
| 2:G:26:LEU:HD11 | 2:G:34:TYR:CE1 | 2.35 | 0.60 |
| 1:B:75:MET:SD | 1:B:95:PRO:HA | 2.41 | 0.60 |
| 2:D:233:LYS:C | 2:D:235:PRO:HD2 | 2.21 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:150:ALA:O | 1:E:154:LEU:HG | 2.00 | 0.60 |
| 1:E:70:ILE:CD1 | 1:F:193:LEU:HA | 2.31 | 0.60 |
| 1:F:94:VAL:HA | 1:F:97:THR:HG23 | 1.83 | 0.60 |
| 1:E:38:LEU:HB2 | 1:E:112:LEU:CD1 | 2.25 | 0.60 |
| 1:E:109:GLU:O | 1:E:113:LEU:HG | 2.01 | 0.60 |
| 1:E:38:LEU:HD13 | 1:E:112:LEU:HB3 | 1.83 | 0.60 |
| 1:A:112:LEU:O | 1:A:115:ILE:HG23 | 2.00 | 0.60 |
| 1:B:11:ARG:NH1 | 1:B:11:ARG:HB3 | 2.16 | 0.60 |
| 1:B:83:VAL:HG11 | 1:B:91:ALA:HB1 | 1.83 | 0.60 |
| 1:F:123:SER:HA | 1:F:129:THR:CB | 2.31 | 0.60 |
| 1:F:59:ILE:O | 1:F:62:ILE:CG1 | 2.50 | 0.60 |
| 1:B:172:LEU:HD11 | 1:B:195:LEU:CD2 | 2.27 | 0.60 |
| 2:G:247:LEU:HG | 2:H:300:GLN:HG3 | 1.83 | 0.60 |
| 1:B:80:ARG:HB2 | 1:B:86:SER:HB3 | 1.83 | 0.60 |
| 1:B:26:PHE:CD2 | 1:B:97:THR:HG22 | 2.37 | 0.60 |
| 1:E:122:ALA:HB1 | 2:G:88:PHE:CZ | 2.36 | 0.60 |
| 1:E:174:GLN:CA | 1:E:177:TYR:HB3 | 2.29 | 0.60 |
| 2:D:241:ILE:CG2 | 2:D:244:THR:OG1 | 2.49 | 0.60 |
| 1:B:149:ALA:O | 1:B:153:THR:HG23 | 2.01 | 0.60 |
| 2:H:12:HIS:NE2 | 2:H:14:GLY:HA2 | 2.16 | 0.60 |
| 2:C:231:HIS:CB | 2:C:232:PRO:HD2 | 2.32 | 0.60 |
| 1:E:71:LEU:O | 1:E:75:MET:HB2 | 2.01 | 0.60 |
| 1:F:76:ILE:HB | 1:F:77:PRO:HD3 | 1.82 | 0.60 |
| 1:B:92:ALA:CB | 1:B:169:ALA:HB2 | 2.32 | 0.60 |
| 2:D:125:LEU:HB3 | 2:D:131:GLY:CA | 2.31 | 0.60 |
| 1:E:135:ARG:H | 1:E:135:ARG:HD2 | 1.64 | 0.60 |
| 2:C:13:GLN:HB2 | 2:C:16:ARG:HG2 | 1.83 | 0.60 |
| 2:C:252:ASP:OD2 | 2:C:253:TYR:N | 2.34 | 0.60 |
| 1:A:130:PRO:HG2 | 1:A:131:MET:N | 2.10 | 0.60 |
| 1:B:16:THR:HG21 | 1:B:199:LEU:HD21 | 1.84 | 0.60 |
| 2:H:241:ILE:O | 2:H:300:GLN:HG3 | 2.02 | 0.60 |
| 2:G:86:MET:SD | 2:G:88:PHE:CZ | 2.95 | 0.60 |
| 1:A:149:ALA:O | 1:A:152:ILE:HG12 | 2.02 | 0.60 |
| 2:G:107:LEU:HB3 | 2:G:113:PRO:HG3 | 1.83 | 0.60 |
| 2:C:186:ILE:HD12 | 2:C:192:LEU:HD23 | 1.83 | 0.60 |
| 2:C:248:ASP:HB3 | 2:C:254:GLN:HG3 | 1.83 | 0.60 |
| 2:C:234:THR:O | 2:C:238:GLN:N | 2.35 | 0.60 |
| 1:A:117:THR:C | 1:A:119:LEU:N | 2.46 | 0.60 |
| 1:A:104:ILE:HG22 | 1:A:153:THR:HG21 | 1.84 | 0.60 |
| 2:H:8:THR:HG23 | 2:H:22:ASN:HA | 1.84 | 0.60 |
| 2:C:233:LYS:HA | 2:C:235:PRO:HD2 | 1.83 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:201:MET:HG3 | 2:C:236:LEU:HB2 | 1.84 | 0.59 |
| 1:F:71:LEU:O | 1:F:75:MET:HB2 | 2.01 | 0.59 |
| 2:H:204:VAL:HA | 2:H:208:CYS:SG | 2.41 | 0.59 |
| 1:E:116:PRO:HB2 | 1:E:120:ILE:CG1 | 2.30 | 0.59 |
| 1:A:42:ARG:HB3 | 1:A:43:PRO:HD3 | 1.83 | 0.59 |
| 2:C:234:THR:O | 2:C:237:ALA:N | 2.34 | 0.59 |
| 1:F:16:THR:O | 1:F:19:MET:HB2 | 2.02 | 0.59 |
| 1:F:41:THR:HG22 | 1:F:53:TYR:CE2 | 2.37 | 0.59 |
| 2:H:182:LEU:O | 2:H:186:ILE:HG23 | 2.02 | 0.59 |
| 1:B:112:LEU:O | 1:B:115:ILE:HG22 | 2.02 | 0.59 |
| 2:H:28:VAL:HG22 | 2:H:34:TYR:CD2 | 2.37 | 0.59 |
| 2:C:97:ARG:NH2 | 2:C:108:GLU:OE2 | 2.27 | 0.59 |
| 1:A:55:THR:O | 1:A:59:ILE:HG23 | 2.01 | 0.59 |
| 2:C:138:PRO:O | 2:C:140:ASN:N | 2.35 | 0.59 |
| 2:C:262:PHE:O | 2:C:265:CYS:SG | 2.60 | 0.59 |
| 2:C:231:HIS:O | 2:C:233:LYS:N | 2.35 | 0.59 |
| 1:E:46:ILE:HD13 | 1:E:47:ILE:HG23 | 1.83 | 0.59 |
| 2:C:290:PHE:CD1 | 2:C:325:ALA:HB1 | 2.37 | 0.59 |
| 2:C:165:ASP:HA | 2:C:197:ILE:CG2 | 2.32 | 0.59 |
| 2:C:26:LEU:HD11 | 2:C:34:TYR:CZ | 2.38 | 0.59 |
| 1:E:32:LEU:C | 1:E:34:VAL:H | 2.05 | 0.59 |
| 2:H:53:LEU:HD23 | 2:H:77:LEU:CD2 | 2.31 | 0.59 |
| 1:A:78:PHE:O | 1:A:81:VAL:HG22 | 2.03 | 0.59 |
| 2:D:233:LYS:O | 2:D:233:LYS:HG3 | 2.02 | 0.59 |
| 1:E:125:ALA:CA | 2:G:54:LEU:HD21 | 2.32 | 0.59 |
| 2:G:97:ARG:CD | 2:G:105:LEU:HD11 | 2.32 | 0.59 |
| 2:H:84:ILE:CD1 | 2:H:163:LEU:HD11 | 2.32 | 0.59 |
| 1:F:165:GLY:HA2 | 1:F:174:GLN:HA | 1.84 | 0.59 |
| 2:H:209:ASP:O | 2:H:224:THR:HG23 | 2.02 | 0.59 |
| 1:B:129:THR:HA | 1:B:133:ILE:HB | 1.85 | 0.59 |
| 2:C:273:PHE:CD1 | 2:C:276:GLN:NE2 | 2.71 | 0.59 |
| 2:H:198:THR:HG21 | 2:H:204:VAL:HG23 | 1.85 | 0.59 |
| 2:D:234:THR:HG21 | 2:D:238:GLN:HE21 | 1.66 | 0.59 |
| 1:B:131:MET:HG3 | 1:B:132:GLN:N | 2.17 | 0.59 |
| 1:A:22:VAL:HG22 | 1:A:93:ILE:CG2 | 2.33 | 0.59 |
| 1:A:23:SER:HA | 1:A:26:PHE:CE2 | 2.38 | 0.59 |
| 2:G:295:ASN:HB2 | 2:G:315:GLU:HB2 | 1.85 | 0.59 |
| 2:C:296:ILE:HG23 | 2:C:314:THR:HG22 | 1.83 | 0.59 |
| 1:E:175:ILE:HG13 | 1:E:176:GLY:N | 2.17 | 0.59 |
| 1:E:203:ILE:O | 1:E:206:ALA:HB3 | 2.03 | 0.59 |
| 1:E:69:ILE:N | 1:E:69:ILE:HD13 | 2.17 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:82:ILE:O | 1:A:84:GLY:N | 2.36 | 0.59 |
| 2:H:213:VAL:HB | 2:H:233:LYS:HD2 | 1.84 | 0.59 |
| 2:C:128:VAL:HG11 | 2:C:152:ALA:HB2 | 1.85 | 0.59 |
| 1:A:59:ILE:HG13 | 1:A:60:VAL:N | 2.17 | 0.59 |
| 1:F:206:ALA:O | 1:F:207:GLY:O | 2.21 | 0.59 |
| 2:D:155:LEU:HD21 | 2:D:186:ILE:HD12 | 1.84 | 0.59 |
| 1:E:70:ILE:HD13 | 1:F:193:LEU:HA | 1.84 | 0.59 |
| 1:A:71:LEU:HG | 1:A:75:MET:CE | 2.29 | 0.59 |
| 2:H:4:LEU:CD2 | 2:H:62:VAL:HG13 | 2.32 | 0.59 |
| 1:A:132:GLN:HB3 | 1:A:136:LYS:HD2 | 1.85 | 0.59 |
| 1:E:139:LEU:HB2 | 1:E:140:PRO:HD3 | 1.85 | 0.59 |
| 2:C:12:HIS:CD2 | 2:C:17:THR:HG23 | 2.37 | 0.59 |
| 2:D:274:THR:C | 2:D:276:GLN:H | 2.05 | 0.59 |
| 1:B:47:ILE:O | 1:B:48:ALA:HB3 | 2.03 | 0.59 |
| 2:C:7:ILE:HB | 2:C:24:VAL:HG23 | 1.85 | 0.59 |
| 1:B:179:TYR:HB3 | 1:B:185:ASN:ND2 | 2.18 | 0.59 |
| 1:A:64:ARG:HH11 | 1:A:106:ARG:HD2 | 1.67 | 0.59 |
| 2:G:228:VAL:CG1 | 2:G:233:LYS:HE3 | 2.33 | 0.58 |
| 1:F:126:MET:SD | 1:F:129:THR:CA | 2.79 | 0.58 |
| 1:F:69:ILE:HD12 | 1:F:70:ILE:N | 2.18 | 0.58 |
| 1:F:69:ILE:O | 1:F:73:VAL:HG23 | 2.03 | 0.58 |
| 1:A:26:PHE:HE1 | 1:A:104:ILE:HG21 | 1.68 | 0.58 |
| 2:C:36:VAL:HG13 | 2:C:214:ILE:CD1 | 2.33 | 0.58 |
| 2:C:43:GLY:C | 2:C:45:SER:N | 2.51 | 0.58 |
| 1:A:134:VAL:O | 1:A:138:LEU:HG | 2.03 | 0.58 |
| 2:C:142:SER:O | 2:C:145:GLN:HB2 | 2.03 | 0.58 |
| 1:A:19:MET:O | 1:A:22:VAL:HB | 2.03 | 0.58 |
| 2:D:103:VAL:HG12 | 2:D:121:VAL:HG22 | 1.86 | 0.58 |
| 1:B:42:ARG:N | 1:B:43:PRO:HD3 | 2.19 | 0.58 |
| 2:C:234:THR:CG2 | 2:C:272:GLU:OE1 | 2.51 | 0.58 |
| 1:A:70:ILE:HG13 | 1:B:193:LEU:HD23 | 1.86 | 0.58 |
| 2:G:9:LYS:HB2 | 2:G:57:PRO:HB3 | 1.86 | 0.58 |
| 1:E:36:VAL:HG12 | 1:E:40:VAL:CG2 | 2.33 | 0.58 |
| 1:E:72:LEU:CD2 | 1:E:95:PRO:HB2 | 2.33 | 0.58 |
| 1:F:36:VAL:HG13 | 1:F:39:TYR:CD1 | 2.38 | 0.58 |
| 2:G:127:LEU:HD11 | 2:G:186:ILE:HG22 | 1.85 | 0.58 |
| 2:G:158:ASN:N | 2:G:159:PRO:HD3 | 2.18 | 0.58 |
| 2:G:51:VAL:CG1 | 2:G:163:LEU:HD11 | 2.34 | 0.58 |
| 2:D:93:LEU:HD22 | 2:D:102:ASN:HD22 | 1.69 | 0.58 |
| 2:H:285:GLU:HG2 | 2:H:329:TRP:CH2 | 2.39 | 0.58 |
| 1:F:72:LEU:CD2 | 1:F:95:PRO:HB2 | 2.33 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:181:TYR:HD1 | 1:B:182:ILE:HG12 | 1.69 | 0.58 |
| 2:D:143:GLY:HA2 | 2:D:146:LYS:CE | 2.34 | 0.58 |
| 1:F:133:ILE:O | 1:F:137:VAL:HG22 | 2.03 | 0.58 |
| 1:A:193:LEU:HD23 | 1:B:70:ILE:CD1 | 2.32 | 0.58 |
| 2:D:7:ILE:HB | 2:D:24:VAL:CG2 | 2.34 | 0.58 |
| 2:G:18:ILE:HD13 | 2:G:19:GLN:N | 2.19 | 0.58 |
| 2:G:22:ASN:HB2 | 2:G:218:GLU:CG | 2.34 | 0.58 |
| 1:F:72:LEU:HD23 | 1:F:95:PRO:CB | 2.34 | 0.58 |
| 2:C:196:LEU:HD23 | 2:C:208:CYS:SG | 2.44 | 0.58 |
| 1:E:104:ILE:HG22 | 1:E:153:THR:CG2 | 2.33 | 0.58 |
| 2:C:124:LEU:CD2 | 2:C:156:ALA:HA | 2.33 | 0.58 |
| 2:G:246:HIS:O | 2:H:241:ILE:HG22 | 2.04 | 0.58 |
| 2:G:300:GLN:HE22 | 2:H:244:THR:HB | 1.68 | 0.58 |
| 2:C:144:GLY:O | 2:C:147:GLN:HB3 | 2.04 | 0.58 |
| 1:A:15:GLU:HB3 | 1:A:89:LEU:HD11 | 1.85 | 0.58 |
| 2:G:26:LEU:HD12 | 2:G:222:GLN:NE2 | 2.19 | 0.58 |
| 1:A:60:VAL:O | 1:A:64:ARG:HG3 | 2.04 | 0.58 |
| 2:D:73:SER:HB2 | 2:D:76:GLU:HG2 | 1.86 | 0.58 |
| 1:B:119:LEU:O | 1:B:122:ALA:HB3 | 2.04 | 0.57 |
| 1:F:31:GLY:CA | 1:F:104:ILE:HD13 | 2.34 | 0.57 |
| 2:C:7:ILE:O | 2:C:24:VAL:HG22 | 2.04 | 0.57 |
| 1:F:122:ALA:HB1 | 1:F:126:MET:HE2 | 1.87 | 0.57 |
| 1:B:69:ILE:CD1 | 1:B:163:MET:HE3 | 2.33 | 0.57 |
| 2:C:121:VAL:O | 2:C:125:LEU:HG | 2.04 | 0.57 |
| 2:G:97:ARG:HD2 | 2:G:105:LEU:HD11 | 1.86 | 0.57 |
| 2:G:77:LEU:HD21 | 2:G:81:ARG:NH1 | 2.19 | 0.57 |
| 1:A:74:TRP:O | 1:A:77:PRO:HD2 | 2.03 | 0.57 |
| 2:D:45:SER:O | 2:D:49:ARG:NH1 | 2.37 | 0.57 |
| 1:B:67:PRO:O | 1:B:70:ILE:HG23 | 2.04 | 0.57 |
| 1:B:35:GLY:CA | 1:B:108:VAL:HG11 | 2.31 | 0.57 |
| 1:B:32:LEU:O | 1:B:35:GLY:N | 2.33 | 0.57 |
| 2:C:303:TYR:O | 2:C:304:ALA:C | 2.40 | 0.57 |
| 1:F:94:VAL:CG2 | 1:F:95:PRO:HD3 | 2.22 | 0.57 |
| 2:D:180:LEU:O | 2:D:183:LEU:HB2 | 2.04 | 0.57 |
| 2:D:268:MET:CE | 2:D:313:LEU:HB3 | 2.34 | 0.57 |
| 2:G:282:LEU:HD13 | 2:G:330:LEU:HD22 | 1.85 | 0.57 |
| 2:G:220:ILE:HD12 | 2:G:220:ILE:H | 1.70 | 0.57 |
| 1:E:32:LEU:O | 1:E:34:VAL:N | 2.37 | 0.57 |
| 1:F:179:TYR:O | 1:F:183:GLY:O | 2.22 | 0.57 |
| 1:B:60:VAL:O | 1:B:102:PRO:HB2 | 2.05 | 0.57 |
| 2:H:179:ILE:O | 2:H:183:LEU:HD22 | 2.04 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:300:GLN:HE22 | 2:H:244:THR:CB | 2.17 | 0.57 |
| 2:H:274:THR:HG21 | 2:H:336:LYS:HE2 | 1.87 | 0.57 |
| 2:C:214:ILE:HG13 | 2:C:219:LEU:HA | 1.86 | 0.57 |
| 2:H:86:MET:HG2 | 2:H:87:ILE:N | 2.19 | 0.57 |
| 2:G:97:ARG:HH11 | 2:G:105:LEU:HD21 | 1.68 | 0.57 |
| 1:B:185:ASN:CB | 1:B:188:VAL:HG22 | 2.34 | 0.57 |
| 2:C:230:SER:HG | 2:C:231:HIS:CE1 | 2.22 | 0.57 |
| 2:C:240:PHE:C | 2:C:241:ILE:HD13 | 2.24 | 0.57 |
| 1:F:175:ILE:HD11 | 1:F:192:VAL:CG2 | 2.35 | 0.57 |
| 2:H:257:LEU:HA | 2:H:342:TYR:O | 2.05 | 0.57 |
| 1:A:178:GLN:O | 1:A:182:ILE:O | 2.22 | 0.57 |
| 1:E:74:TRP:O | 1:E:77:PRO:HD2 | 2.05 | 0.57 |
| 1:F:72:LEU:HD11 | 1:F:160:TYR:CE1 | 2.40 | 0.57 |
| 1:F:42:ARG:NH2 | 1:F:51:LYS:HA | 2.19 | 0.57 |
| 2:G:106:PRO:HD3 | 2:G:153:ARG:HG3 | 1.87 | 0.57 |
| 2:C:168:THR:CB | 2:C:176:THR:HG23 | 2.34 | 0.57 |
| 1:F:137:VAL:C | 1:F:138:LEU:HG | 2.24 | 0.56 |
| 1:A:128:ALA:C | 1:A:129:THR:HG23 | 2.26 | 0.56 |
| 2:D:4:LEU:HB3 | 2:D:7:ILE:CD1 | 2.36 | 0.56 |
| 1:B:23:SER:HA | 1:B:26:PHE:CE2 | 2.40 | 0.56 |
| 2:H:240:PHE:H | 2:H:243:SER:CB | 2.15 | 0.56 |
| 2:C:303:TYR:HH | 2:D:253:TYR:HD2 | 1.53 | 0.56 |
| 2:D:63:LEU:HD13 | 2:D:68:GLU:HG3 | 1.88 | 0.56 |
| 2:C:221:GLU:OE2 | 2:C:231:HIS:HB2 | 2.05 | 0.56 |
| 1:F:126:MET:HG2 | 2:H:109:LEU:CD1 | 2.31 | 0.56 |
| 2:H:87:ILE:HD12 | 2:H:164:CYS:SG | 2.45 | 0.56 |
| 1:A:191:THR:O | 1:A:195:LEU:HB2 | 2.05 | 0.56 |
| 2:C:52:ASN:HD22 | 2:C:52:ASN:H | 1.51 | 0.56 |
| 1:E:47:ILE:O | 1:E:48:ALA:HB3 | 2.05 | 0.56 |
| 1:E:19:MET:HA | 1:E:22:VAL:HG23 | 1.88 | 0.56 |
| 1:E:42:ARG:CD | 1:E:45:GLN:HB3 | 2.35 | 0.56 |
| 2:H:52:ASN:O | 2:H:53:LEU:HB3 | 2.04 | 0.56 |
| 1:E:192:VAL:O | 1:E:195:LEU:HB3 | 2.04 | 0.56 |
| 1:B:16:THR:O | 1:B:19:MET:HB2 | 2.04 | 0.56 |
| 2:G:247:LEU:HG | 2:H:300:GLN:CD | 2.26 | 0.56 |
| 2:G:206:ARG:HH22 | 2:G:242:GLN:NE2 | 2.03 | 0.56 |
| 1:A:137:VAL:C | 1:A:140:PRO:HD2 | 2.25 | 0.56 |
| 1:A:129:THR:OG1 | 1:A:133:ILE:HD12 | 2.06 | 0.56 |
| 2:D:282:LEU:HD13 | 2:D:335:VAL:HG21 | 1.88 | 0.56 |
| 2:C:228:VAL:O | 2:C:229:PHE:CD2 | 2.59 | 0.56 |
| 1:A:128:ALA:HB1 | 1:A:134:VAL:CG2 | 2.35 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:151:ILE:HD11 | 2:D:182:LEU:CD2 | 2.35 | 0.56 |
| 2:G:63:LEU:HD21 | 2:G:66:GLY:HA2 | 1.88 | 0.56 |
| 2:D:241:ILE:CG2 | 2:D:241:ILE:O | 2.53 | 0.56 |
| 1:A:152:ILE:HG13 | 1:A:153:THR:N | 2.20 | 0.56 |
| 1:B:83:VAL:HG11 | 1:B:91:ALA:CB | 2.36 | 0.56 |
| 2:H:184:LYS:O | 2:H:187:ASN:HB3 | 2.06 | 0.56 |
| 2:C:33:ILE:HD13 | 2:C:207:ILE:O | 2.06 | 0.56 |
| 1:F:72:LEU:HD23 | 1:F:95:PRO:HB2 | 1.86 | 0.56 |
| 1:A:94:VAL:CB | 1:A:95:PRO:HD3 | 2.34 | 0.56 |
| 1:A:26:PHE:CD1 | 1:A:104:ILE:HD13 | 2.41 | 0.56 |
| 2:H:256:ARG:O | 2:H:343:VAL:HG12 | 2.05 | 0.56 |
| 1:F:175:ILE:HG13 | 1:F:176:GLY:N | 2.20 | 0.56 |
| 2:D:148:ARG:HA | 2:D:151:ILE:HG12 | 1.87 | 0.56 |
| 1:B:22:VAL:CG1 | 1:B:93:ILE:HD12 | 2.35 | 0.56 |
| 2:C:302:ASP:O | 2:C:308:LYS:HA | 2.05 | 0.56 |
| 1:A:167:VAL:HG11 | 1:B:181:TYR:O | 2.04 | 0.56 |
| 2:H:33:ILE:HD13 | 2:H:207:ILE:HB | 1.88 | 0.56 |
| 2:C:11:PHE:HB2 | 2:C:18:ILE:HG23 | 1.88 | 0.56 |
| 1:E:27:GLY:HA2 | 1:E:104:ILE:HD12 | 1.86 | 0.56 |
| 1:E:41:THR:HG22 | 1:E:53:TYR:CE2 | 2.41 | 0.56 |
| 1:B:69:ILE:HG13 | 1:B:163:MET:HE2 | 1.87 | 0.56 |
| 2:D:198:THR:OG1 | 2:D:203:VAL:HG21 | 2.05 | 0.56 |
| 1:A:193:LEU:HD11 | 1:B:74:TRP:NE1 | 2.21 | 0.56 |
| 1:B:107:MET:CE | 1:B:152:ILE:HD11 | 2.36 | 0.56 |
| 1:B:59:ILE:HG13 | 1:B:60:VAL:N | 2.21 | 0.56 |
| 1:F:32:LEU:HD23 | 1:F:108:VAL:HG21 | 1.88 | 0.56 |
| 2:H:48:ILE:HD13 | 2:H:49:ARG:H | 1.71 | 0.56 |
| 2:G:144:GLY:CA | 2:G:175:THR:HG21 | 2.36 | 0.56 |
| 2:C:244:THR:HA | 2:C:298:SER:OG | 2.06 | 0.56 |
| 1:E:71:LEU:HD22 | 1:E:160:TYR:OH | 2.06 | 0.56 |
| 1:F:124:ARG:NH2 | 2:H:85:GLY:CA | 2.67 | 0.56 |
| 2:H:242:GLN:NE2 | 2:H:311:ILE:CD1 | 2.68 | 0.56 |
| 2:H:299:ALA:HA | 2:H:312:MET:HA | 1.86 | 0.56 |
| 1:B:41:THR:C | 1:B:42:ARG:HG3 | 2.26 | 0.56 |
| 1:B:68:PHE:N | 1:B:68:PHE:CD1 | 2.73 | 0.56 |
| 1:E:40:VAL:HG12 | 1:E:53:TYR:HD2 | 1.72 | 0.55 |
| 2:H:151:ILE:HD11 | 2:H:182:LEU:HD21 | 1.87 | 0.55 |
| 2:H:183:LEU:O | 2:H:186:ILE:HG12 | 2.06 | 0.55 |
| 2:H:186:ILE:HB | 2:H:192:LEU:HD12 | 1.87 | 0.55 |
| 2:G:299:ALA:CB | 2:G:312:MET:HG3 | 2.36 | 0.55 |
| 2:H:28:VAL:HG22 | 2:H:34:TYR:CG | 2.41 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:69:ILE:CG2 | 1:F:163:MET:HE2 | 2.35 | 0.55 |
| 1:B:167:VAL:CG1 | 1:B:168:GLY:H | 2.07 | 0.55 |
| 1:E:118:GLY:C | 1:E:119:LEU:HG | 2.26 | 0.55 |
| 2:D:37:ILE:CD1 | 2:D:236:LEU:HD13 | 2.35 | 0.55 |
| 1:B:89:LEU:CA | 1:B:169:ALA:HB1 | 2.33 | 0.55 |
| 1:F:101:ALA:HA | 1:F:104:ILE:CD1 | 2.30 | 0.55 |
| 1:B:101:ALA:HA | 1:B:104:ILE:HG12 | 1.88 | 0.55 |
| 1:A:87:ILE:HG22 | 1:A:88:GLY:N | 2.22 | 0.55 |
| 2:G:288:ARG:HA | 2:H:288:ARG:CG | 2.36 | 0.55 |
| 2:G:171:LEU:HD13 | 2:G:179:ILE:HG13 | 1.88 | 0.55 |
| 1:B:128:ALA:HB1 | 2:D:78:THR:HG23 | 1.87 | 0.55 |
| 1:F:173:GLY:O | 1:F:177:TYR:N | 2.29 | 0.55 |
| 1:B:130:PRO:O | 1:B:134:VAL:HG12 | 2.07 | 0.55 |
| 2:D:249:ILE:HG22 | 2:D:313:LEU:HD12 | 1.88 | 0.55 |
| 2:D:150:ALA:O | 2:D:153:ARG:HB3 | 2.06 | 0.55 |
| 2:D:299:ALA:HB1 | 2:D:312:MET:HG2 | 1.87 | 0.55 |
| 1:E:104:ILE:HG22 | 1:E:153:THR:HG21 | 1.89 | 0.55 |
| 2:H:124:LEU:HD22 | 2:H:152:ALA:O | 2.07 | 0.55 |
| 1:F:178:GLN:O | 1:F:182:ILE:O | 2.24 | 0.55 |
| 2:G:299:ALA:HB2 | 2:G:312:MET:HG3 | 1.87 | 0.55 |
| 2:C:137:TYR:OH | 2:C:140:ASN:HB3 | 2.07 | 0.55 |
| 1:B:69:ILE:HD11 | 1:B:163:MET:CB | 2.25 | 0.55 |
| 2:H:138:PRO:O | 2:H:140:ASN:N | 2.40 | 0.55 |
| 2:C:300:GLN:NE2 | 2:D:298:SER:HB2 | 2.21 | 0.55 |
| 1:F:176:GLY:O | 1:F:180:GLY:HA3 | 2.07 | 0.55 |
| 1:E:192:VAL:HA | 1:E:195:LEU:HD22 | 1.87 | 0.55 |
| 2:H:224:THR:O | 2:H:228:VAL:HG23 | 2.06 | 0.55 |
| 2:D:52:ASN:ND2 | 2:D:86:MET:HE3 | 2.22 | 0.55 |
| 2:D:221:GLU:OE1 | 2:D:231:HIS:O | 2.25 | 0.55 |
| 2:C:241:ILE:HD11 | 2:C:311:ILE:HD11 | 1.89 | 0.55 |
| 2:G:246:HIS:HB3 | 2:H:241:ILE:HG23 | 1.87 | 0.55 |
| 1:B:22:VAL:HG12 | 1:B:26:PHE:CE2 | 2.42 | 0.55 |
| 1:E:122:ALA:HB1 | 2:G:88:PHE:CD2 | 2.42 | 0.55 |
| 2:D:248:ASP:O | 2:D:249:ILE:CG1 | 2.55 | 0.55 |
| 2:G:82:ARG:NH2 | 2:G:110:ASP:HB3 | 2.20 | 0.55 |
| 2:H:319:THR:O | 2:H:323:THR:HG23 | 2.07 | 0.55 |
| 1:E:13:VAL:CG2 | 1:E:195:LEU:HD11 | 2.36 | 0.55 |
| 1:F:93:ILE:O | 1:F:96:LEU:HB2 | 2.07 | 0.55 |
| 2:H:48:ILE:HG13 | 2:H:197:ILE:HD11 | 1.88 | 0.55 |
| 2:H:220:ILE:HB | 2:H:233:LYS:HD3 | 1.88 | 0.55 |
| 2:D:208:CYS:O | 2:D:225:VAL:CG2 | 2.52 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:125:ALA:HA | 2:G:54:LEU:HD21 | 1.88 | 0.55 |
| 2:D:103:VAL:CG1 | 2:D:121:VAL:HG22 | 2.36 | 0.55 |
| 1:E:16:THR:HA | 1:E:19:MET:HG2 | 1.88 | 0.55 |
| 1:E:73:VAL:HG13 | 1:E:74:TRP:N | 2.22 | 0.55 |
| 2:H:77:LEU:HG | 2:H:81:ARG:HE | 1.71 | 0.55 |
| 2:D:196:LEU:C | 2:D:197:ILE:HD12 | 2.27 | 0.55 |
| 1:B:76:ILE:O | 1:B:77:PRO:C | 2.44 | 0.55 |
| 1:E:119:LEU:HD13 | 2:G:90:HIS:CB | 2.36 | 0.55 |
| 2:D:83:GLN:C | 2:D:159:PRO:HB2 | 2.27 | 0.55 |
| 2:G:301:MET:HG2 | 2:G:310:GLY:HA3 | 1.88 | 0.55 |
| 1:E:12:GLY:O | 1:E:172:LEU:HD21 | 2.07 | 0.54 |
| 2:H:241:ILE:HD13 | 2:H:300:GLN:C | 2.28 | 0.54 |
| 2:C:99:VAL:HG22 | 2:C:149:VAL:CG2 | 2.36 | 0.54 |
| 2:G:84:ILE:HA | 2:G:161:VAL:O | 2.06 | 0.54 |
| 2:D:250:PRO:HG2 | 2:D:253:TYR:CD2 | 2.42 | 0.54 |
| 1:B:118:GLY:HA2 | 1:B:121:GLU:CD | 2.27 | 0.54 |
| 1:F:139:LEU:CG | 1:F:140:PRO:HD3 | 2.36 | 0.54 |
| 1:F:36:VAL:HG13 | 1:F:39:TYR:CE1 | 2.43 | 0.54 |
| 2:H:87:ILE:HG23 | 2:H:147:GLN:HE22 | 1.69 | 0.54 |
| 1:A:185:ASN:CB | 1:A:188:VAL:HG22 | 2.30 | 0.54 |
| 2:D:82:ARG:O | 2:D:159:PRO:HB3 | 2.06 | 0.54 |
| 2:G:63:LEU:HD12 | 2:G:68:GLU:CG | 2.36 | 0.54 |
| 1:A:40:VAL:HG12 | 1:A:53:TYR:HB2 | 1.87 | 0.54 |
| 1:A:9:LEU:O | 1:A:13:VAL:HG23 | 2.07 | 0.54 |
| 2:H:43:GLY:C | 2:H:45:SER:N | 2.56 | 0.54 |
| 2:C:249:ILE:N | 2:C:250:PRO:HD2 | 2.23 | 0.54 |
| 2:H:103:VAL:HB | 2:H:121:VAL:HG13 | 1.89 | 0.54 |
| 2:D:173:PRO:O | 2:D:177:ARG:HG3 | 2.07 | 0.54 |
| 1:A:132:GLN:O | 1:A:136:LYS:N | 2.34 | 0.54 |
| 1:F:119:LEU:N | 1:F:119:LEU:HD12 | 2.23 | 0.54 |
| 1:F:139:LEU:N | 1:F:140:PRO:HD2 | 2.22 | 0.54 |
| 2:C:153:ARG:O | 2:C:156:ALA:HB3 | 2.07 | 0.54 |
| 1:E:38:LEU:CD2 | 1:E:112:LEU:HB3 | 2.36 | 0.54 |
| 1:E:32:LEU:C | 1:E:34:VAL:N | 2.61 | 0.54 |
| 1:E:42:ARG:HD2 | 1:E:45:GLN:HB3 | 1.88 | 0.54 |
| 1:E:189:MET:HE1 | 1:F:74:TRP:HA | 1.89 | 0.54 |
| 2:H:105:LEU:HD22 | 2:H:109:LEU:HD11 | 1.90 | 0.54 |
| 2:G:189:ARG:O | 2:G:191:GLY:N | 2.41 | 0.54 |
| 2:D:254:GLN:O | 2:D:257:LEU:HB3 | 2.07 | 0.54 |
| 1:E:101:ALA:HB3 | 1:E:102:PRO:CD | 2.37 | 0.54 |
| 2:D:87:ILE:HG22 | 2:D:88:PHE:N | 2.22 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:155:ILE:HG13 | 1:A:156:THR:N | 2.23 | 0.54 |
| 2:D:276:GLN:OE1 | 2:D:280:ALA:HB2 | 2.07 | 0.54 |
| 1:F:35:GLY:HA3 | 1:F:108:VAL:CG1 | 2.37 | 0.54 |
| 2:H:105:LEU:CB | 2:H:106:PRO:CD | 2.86 | 0.54 |
| 1:B:15:GLU:O | 1:B:19:MET:HG2 | 2.08 | 0.54 |
| 2:G:241:ILE:C | 2:G:241:ILE:HD13 | 2.28 | 0.54 |
| 1:A:141:GLU:O | 1:A:144:PRO:HD2 | 2.08 | 0.54 |
| 1:B:37:LEU:HD21 | 1:B:56:VAL:HB | 1.88 | 0.54 |
| 2:C:33:ILE:HD12 | 2:C:209:ASP:OD2 | 2.08 | 0.54 |
| 2:C:249:ILE:HG22 | 2:D:206:ARG:NH1 | 2.22 | 0.54 |
| 1:F:123:SER:HA | 1:F:129:THR:CG2 | 2.37 | 0.54 |
| 2:D:246:HIS:ND1 | 2:D:270:ARG:NH1 | 2.56 | 0.54 |
| 2:H:3:LYS:HA | 2:H:26:LEU:O | 2.08 | 0.54 |
| 1:A:107:MET:HB3 | 1:A:149:ALA:HB1 | 1.89 | 0.54 |
| 1:B:55:THR:O | 1:B:59:ILE:HG12 | 2.07 | 0.54 |
| 2:G:112:THR:N | 2:G:113:PRO:HD3 | 2.23 | 0.54 |
| 2:H:27:HIS:H | 2:H:222:GLN:NE2 | 2.06 | 0.54 |
| 1:E:34:VAL:HB | 1:E:37:LEU:HG | 1.90 | 0.54 |
| 2:D:2:ILE:CG2 | 2:D:28:VAL:HB | 2.31 | 0.54 |
| 2:D:248:ASP:O | 2:D:249:ILE:HG13 | 2.08 | 0.54 |
| 1:B:118:GLY:HA2 | 1:B:121:GLU:OE1 | 2.08 | 0.54 |
| 2:C:158:ASN:N | 2:C:159:PRO:HD3 | 2.21 | 0.54 |
| 1:A:63:PHE:HB3 | 1:A:102:PRO:HG3 | 1.88 | 0.54 |
| 1:A:29:VAL:O | 1:A:33:PRO:HG2 | 2.07 | 0.54 |
| 1:B:78:PHE:O | 1:B:82:ILE:HG12 | 2.08 | 0.54 |
| 1:E:75:MET:HE2 | 1:E:98:VAL:HG21 | 1.90 | 0.54 |
| 1:F:58:ALA:O | 1:F:62:ILE:HG23 | 2.08 | 0.54 |
| 2:H:196:LEU:HD21 | 2:H:203:VAL:CG1 | 2.34 | 0.54 |
| 2:G:183:LEU:HD23 | 2:G:194:ILE:CD1 | 2.36 | 0.54 |
| 1:E:40:VAL:HG22 | 1:E:47:ILE:HD11 | 1.90 | 0.53 |
| 2:H:242:GLN:HG3 | 2:H:311:ILE:HB | 1.90 | 0.53 |
| 1:E:125:ALA:HB2 | 2:G:54:LEU:HD21 | 1.90 | 0.53 |
| 2:C:235:PRO:C | 2:C:237:ALA:H | 2.11 | 0.53 |
| 2:H:105:LEU:O | 2:H:109:LEU:HG | 2.07 | 0.53 |
| 1:B:179:TYR:HE2 | 1:F:182:ILE:O | 1.91 | 0.53 |
| 2:D:196:LEU:HD23 | 2:D:208:CYS:SG | 2.47 | 0.53 |
| 1:B:60:VAL:HG13 | 1:B:102:PRO:CA | 2.38 | 0.53 |
| 2:H:84:ILE:HG13 | 2:H:161:VAL:O | 2.08 | 0.53 |
| 2:H:21:LEU:HD21 | 2:H:47:LEU:HB2 | 1.90 | 0.53 |
| 1:A:40:VAL:HA | 1:A:49:ASN:HB2 | 1.89 | 0.53 |
| 2:C:271:LEU:HD23 | 2:C:337:VAL:HG13 | 1.90 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:46:THR:HG22 | 2:C:47:LEU:N | 2.22 | 0.53 |
| 2:H:48:ILE:CG1 | 2:H:197:ILE:HD11 | 2.38 | 0.53 |
| 1:A:66:ILE:HG21 | 1:A:71:LEU:HB2 | 1.89 | 0.53 |
| 2:G:206:ARG:HH22 | 2:G:242:GLN:HE22 | 1.57 | 0.53 |
| 1:E:126:MET:SD | 2:G:106:PRO:HB3 | 2.48 | 0.53 |
| 1:A:26:PHE:HD1 | 1:A:104:ILE:HD13 | 1.72 | 0.53 |
| 1:A:22:VAL:HG12 | 1:A:26:PHE:HE2 | 1.72 | 0.53 |
| 2:C:69:LEU:HD12 | 2:C:69:LEU:N | 2.23 | 0.53 |
| 2:G:260:GLU:HG2 | 2:G:261:PRO:HD2 | 1.90 | 0.53 |
| 2:C:247:LEU:HD23 | 2:D:300:GLN:OE1 | 2.09 | 0.53 |
| 1:F:19:MET:HB2 | 1:F:157:LEU:HD21 | 1.91 | 0.53 |
| 1:E:143:LEU:N | 1:E:144:PRO:HD2 | 2.24 | 0.53 |
| 2:G:282:LEU:HD13 | 2:G:330:LEU:CD2 | 2.38 | 0.53 |
| 1:B:120:ILE:HD12 | 2:D:94:LEU:CD2 | 2.38 | 0.53 |
| 2:C:224:THR:O | 2:C:228:VAL:HG23 | 2.09 | 0.53 |
| 2:G:201:MET:O | 2:G:202:ASP:C | 2.45 | 0.53 |
| 2:C:241:ILE:HB | 2:C:243:SER:HB3 | 1.90 | 0.53 |
| 1:B:185:ASN:HB2 | 1:B:188:VAL:CG2 | 2.38 | 0.53 |
| 1:F:182:ILE:HG13 | 1:F:182:ILE:O | 2.09 | 0.53 |
| 2:H:241:ILE:HD12 | 2:H:242:GLN:H | 1.72 | 0.53 |
| 2:D:98:THR:HG22 | 2:D:138:PRO:CD | 2.39 | 0.53 |
| 1:B:56:VAL:O | 1:B:60:VAL:HG23 | 2.08 | 0.53 |
| 2:C:162:LEU:HD23 | 2:C:163:LEU:N | 2.24 | 0.53 |
| 2:C:247:LEU:HD13 | 2:C:297:ILE:CG2 | 2.38 | 0.53 |
| 1:E:34:VAL:HG21 | 1:E:105:ALA:HA | 1.91 | 0.53 |
| 1:E:97:THR:O | 1:E:101:ALA:N | 2.42 | 0.53 |
| 1:F:126:MET:CE | 1:F:129:THR:OG1 | 2.57 | 0.53 |
| 2:H:91:PHE:HE1 | 2:H:147:GLN:HB2 | 1.72 | 0.53 |
| 2:D:163:LEU:CD2 | 2:D:195:LEU:HB3 | 2.37 | 0.53 |
| 2:H:105:LEU:HD22 | 2:H:109:LEU:HD21 | 1.91 | 0.53 |
| 1:B:28:PHE:HB3 | 1:B:32:LEU:CD1 | 2.38 | 0.53 |
| 2:G:86:MET:SD | 2:G:88:PHE:CE2 | 3.02 | 0.53 |
| 2:G:158:ASN:N | 2:G:159:PRO:CD | 2.71 | 0.53 |
| 2:D:282:LEU:HD13 | 2:D:335:VAL:CG2 | 2.38 | 0.53 |
| 2:D:299:ALA:CB | 2:D:312:MET:HG2 | 2.39 | 0.53 |
| 2:C:48:ILE:HD13 | 2:C:165:ASP:HB2 | 1.91 | 0.53 |
| 2:C:44:LYS:CB | 2:C:197:ILE:HD11 | 2.24 | 0.53 |
| 2:C:270:ARG:HG2 | 2:C:313:LEU:CD2 | 2.36 | 0.53 |
| 2:D:94:LEU:H | 2:D:102:ASN:HD21 | 1.55 | 0.53 |
| 2:C:300:GLN:HE21 | 2:C:301:MET:H | 1.57 | 0.53 |
| 1:F:126:MET:HB3 | 1:F:128:ALA:C | 2.28 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:33:ILE:CD1 | 2:H:207:ILE:HB | 2.39 | 0.53 |
| 2:H:241:ILE:HG21 | 2:H:302:ASP:HB2 | 1.91 | 0.53 |
| 1:E:22:VAL:O | 1:E:26:PHE:CD2 | 2.62 | 0.53 |
| 1:E:75:MET:CE | 1:E:98:VAL:HG21 | 2.39 | 0.53 |
| 1:F:12:GLY:C | 1:F:172:LEU:CD1 | 2.78 | 0.53 |
| 2:H:124:LEU:CD2 | 2:H:152:ALA:O | 2.57 | 0.53 |
| 2:G:247:LEU:HG | 2:H:300:GLN:CG | 2.39 | 0.53 |
| 2:D:148:ARG:O | 2:D:151:ILE:HG12 | 2.09 | 0.53 |
| 1:A:23:SER:HA | 1:A:26:PHE:CD2 | 2.43 | 0.53 |
| 1:E:68:PHE:CB | 1:E:69:ILE:HD13 | 2.38 | 0.52 |
| 2:G:276:GLN:O | 2:G:308:LYS:HD3 | 2.08 | 0.52 |
| 1:A:13:VAL:HG21 | 1:A:195:LEU:HD11 | 1.91 | 0.52 |
| 2:H:100:PHE:CD2 | 2:H:100:PHE:C | 2.81 | 0.52 |
| 1:E:27:GLY:HA2 | 1:E:104:ILE:CD1 | 2.40 | 0.52 |
| 1:B:125:ALA:CB | 2:D:54:LEU:HD21 | 2.33 | 0.52 |
| 2:H:269:LEU:HD23 | 2:H:339:VAL:HG22 | 1.91 | 0.52 |
| 2:C:253:TYR:HD2 | 2:D:303:TYR:HE1 | 1.57 | 0.52 |
| 1:E:157:LEU:O | 1:E:160:TYR:HB3 | 2.09 | 0.52 |
| 1:F:42:ARG:HH21 | 1:F:50:ALA:C | 2.12 | 0.52 |
| 2:H:33:ILE:HG23 | 2:H:194:ILE:CD1 | 2.38 | 0.52 |
| 1:A:135:ARG:HA | 1:A:138:LEU:HD12 | 1.91 | 0.52 |
| 1:E:110:ASN:O | 1:E:114:GLU:HG2 | 2.09 | 0.52 |
| 1:F:59:ILE:CA | 1:F:62:ILE:HG12 | 2.39 | 0.52 |
| 1:B:69:ILE:CD1 | 1:B:163:MET:CE | 2.87 | 0.52 |
| 2:G:204:VAL:O | 2:G:208:CYS:HB2 | 2.09 | 0.52 |
| 2:H:249:ILE:HG23 | 2:H:250:PRO:CD | 2.36 | 0.52 |
| 1:F:111:ALA:O | 1:F:114:GLU:HB3 | 2.08 | 0.52 |
| 1:E:16:THR:O | 1:E:19:MET:HB2 | 2.09 | 0.52 |
| 1:E:40:VAL:CA | 1:E:47:ILE:HD11 | 2.33 | 0.52 |
| 1:A:69:ILE:HG21 | 1:B:163:MET:HE1 | 1.91 | 0.52 |
| 2:D:130:LEU:HD11 | 2:D:134:HIS:HB2 | 1.90 | 0.52 |
| 1:B:38:LEU:HD22 | 1:B:112:LEU:HB3 | 1.91 | 0.52 |
| 2:H:116:GLU:HA | 2:H:119:ARG:HH11 | 1.73 | 0.52 |
| 2:H:97:ARG:NH2 | 2:H:108:GLU:OE1 | 2.39 | 0.52 |
| 1:B:69:ILE:CG1 | 1:B:163:MET:HE2 | 2.39 | 0.52 |
| 2:D:158:ASN:N | 2:D:159:PRO:HD3 | 2.23 | 0.52 |
| 1:A:41:THR:O | 1:A:42:ARG:HB2 | 2.10 | 0.52 |
| 2:G:38:GLY:CA | 2:G:44:LYS:HD3 | 2.40 | 0.52 |
| 1:F:177:TYR:O | 1:F:181:TYR:N | 2.42 | 0.52 |
| 1:A:122:ALA:HB1 | 2:C:88:PHE:CZ | 2.45 | 0.52 |
| 2:C:86:MET:HE3 | 2:C:163:LEU:HD12 | 1.90 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:107:MET:HE2 | 1:F:149:ALA:HB1 | 1.90 | 0.52 |
| 1:F:42:ARG:HE | 1:F:49:ASN:C | 2.13 | 0.52 |
| 2:H:49:ARG:O | 2:H:54:LEU:N | 2.38 | 0.52 |
| 2:D:44:LYS:CE | 2:D:45:SER:OG | 2.55 | 0.52 |
| 1:B:133:ILE:HG21 | 2:D:109:LEU:HD22 | 1.91 | 0.52 |
| 2:D:273:PHE:N | 2:D:310:GLY:O | 2.34 | 0.52 |
| 2:C:137:TYR:HD2 | 2:C:138:PRO:N | 2.08 | 0.52 |
| 2:H:165:ASP:O | 2:H:166:GLU:C | 2.47 | 0.52 |
| 2:H:53:LEU:HD23 | 2:H:77:LEU:HD21 | 1.92 | 0.52 |
| 2:G:298:SER:HB2 | 2:H:300:GLN:OE1 | 2.10 | 0.52 |
| 1:B:40:VAL:O | 1:B:40:VAL:HG12 | 2.10 | 0.52 |
| 2:C:278:VAL:CA | 2:C:308:LYS:HE2 | 2.39 | 0.52 |
| 1:B:64:ARG:NE | 1:B:103:PHE:HA | 2.25 | 0.52 |
| 1:A:26:PHE:HZ | 1:A:157:LEU:HD11 | 1.75 | 0.52 |
| 2:C:288:ARG:HH11 | 2:D:287:ALA:HB1 | 1.75 | 0.52 |
| 1:A:61:ASN:HB2 | 1:A:106:ARG:HH22 | 1.75 | 0.52 |
| 1:A:36:VAL:O | 1:A:36:VAL:HG13 | 2.09 | 0.52 |
| 1:F:107:MET:CE | 1:F:152:ILE:HD11 | 2.40 | 0.52 |
| 1:F:36:VAL:O | 1:F:36:VAL:CG1 | 2.58 | 0.52 |
| 2:H:87:ILE:CG2 | 2:H:88:PHE:N | 2.73 | 0.52 |
| 2:H:141:LEU:HG | 2:H:145:GLN:CB | 2.39 | 0.52 |
| 2:C:247:LEU:HD13 | 2:C:297:ILE:HG22 | 1.91 | 0.51 |
| 2:C:4:LEU:HD22 | 2:C:7:ILE:CD1 | 2.40 | 0.51 |
| 2:D:212:ALA:HB1 | 2:D:219:LEU:HD11 | 1.91 | 0.51 |
| 2:D:238:GLN:HA | 2:D:242:GLN:HB2 | 1.91 | 0.51 |
| 2:C:142:SER:N | 2:C:145:GLN:OE1 | 2.35 | 0.51 |
| 2:C:151:ILE:CG1 | 2:C:152:ALA:N | 2.69 | 0.51 |
| 1:A:100:ALA:O | 1:A:104:ILE:HG12 | 2.10 | 0.51 |
| 2:H:214:ILE:CG1 | 2:H:219:LEU:HD23 | 2.38 | 0.51 |
| 1:B:123:SER:HB2 | 1:B:126:MET:CE | 2.39 | 0.51 |
| 2:G:41:GLY:HA2 | 2:G:45:SER:OG | 2.10 | 0.51 |
| 2:C:235:PRO:O | 2:C:236:LEU:HG | 2.10 | 0.51 |
| 1:E:70:ILE:CD1 | 1:F:192:VAL:HG12 | 2.39 | 0.51 |
| 2:H:33:ILE:HB | 2:H:208:CYS:HA | 1.92 | 0.51 |
| 2:D:52:ASN:OD1 | 2:D:54:LEU:HG | 2.11 | 0.51 |
| 2:G:184:LYS:CG | 2:G:207:ILE:HG22 | 2.35 | 0.51 |
| 1:F:196:LEU:HD23 | 1:F:199:LEU:HD23 | 1.91 | 0.51 |
| 1:B:100:ALA:O | 1:B:104:ILE:HG12 | 2.10 | 0.51 |
| 1:E:18:ALA:O | 1:E:22:VAL:HG23 | 2.11 | 0.51 |
| 2:G:247:LEU:HD11 | 2:H:244:THR:CG2 | 2.39 | 0.51 |
| 1:B:131:MET:O | 1:B:135:ARG:HG2 | 2.10 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:40:VAL:HG11 | 1:B:52:LEU:HB2 | 1.92 | 0.51 |
| 1:B:40:VAL:HG12 | 1:B:53:TYR:HB2 | 1.92 | 0.51 |
| 2:C:93:LEU:HD11 | 2:C:149:VAL:HB | 1.92 | 0.51 |
| 1:A:100:ALA:HB2 | 1:A:157:LEU:HD21 | 1.93 | 0.51 |
| 2:G:205:LYS:HZ3 | 2:G:304:ALA:HB2 | 1.75 | 0.51 |
| 1:A:122:ALA:O | 1:A:125:ALA:HB3 | 2.11 | 0.51 |
| 1:E:67:PRO:HB2 | 1:E:70:ILE:HG22 | 1.92 | 0.51 |
| 1:F:126:MET:HE1 | 1:F:134:VAL:HB | 1.93 | 0.51 |
| 2:H:105:LEU:CD2 | 2:H:109:LEU:HD21 | 2.41 | 0.51 |
| 2:H:49:ARG:HG2 | 2:H:54:LEU:HD12 | 1.93 | 0.51 |
| 1:B:115:ILE:HG13 | 1:B:116:PRO:CD | 2.39 | 0.51 |
| 2:G:271:LEU:HD22 | 2:G:335:VAL:HG12 | 1.92 | 0.51 |
| 1:A:148:ASN:O | 1:A:151:THR:HG22 | 2.10 | 0.51 |
| 2:C:52:ASN:HD22 | 2:C:52:ASN:N | 2.06 | 0.51 |
| 2:D:206:ARG:HH11 | 2:D:206:ARG:HG3 | 1.75 | 0.51 |
| 1:E:19:MET:HA | 1:E:22:VAL:CG2 | 2.40 | 0.51 |
| 1:F:70:ILE:HG23 | 1:F:71:LEU:N | 2.25 | 0.51 |
| 2:H:213:VAL:CB | 2:H:233:LYS:HD2 | 2.40 | 0.51 |
| 2:C:113:PRO:HD2 | 2:C:117:VAL:HG23 | 1.91 | 0.51 |
| 2:C:125:LEU:HB3 | 2:C:131:GLY:CA | 2.36 | 0.51 |
| 2:G:241:ILE:O | 2:G:241:ILE:HD13 | 2.09 | 0.51 |
| 2:D:266:VAL:CG2 | 2:D:317:HIS:HA | 2.39 | 0.51 |
| 1:B:155:ILE:HB | 1:B:200:VAL:HG13 | 1.93 | 0.51 |
| 1:F:79:THR:HG22 | 1:F:85:THR:O | 2.10 | 0.51 |
| 1:E:187:THR:O | 1:E:191:THR:HG23 | 2.10 | 0.51 |
| 2:H:113:PRO:O | 2:H:117:VAL:HG23 | 2.10 | 0.51 |
| 2:D:234:THR:HG22 | 2:D:238:GLN:HG2 | 1.92 | 0.51 |
| 1:A:185:ASN:HD22 | 1:A:188:VAL:CG2 | 2.22 | 0.51 |
| 1:A:131:MET:O | 1:A:135:ARG:CG | 2.57 | 0.51 |
| 1:B:134:VAL:HA | 1:B:137:VAL:CG1 | 2.36 | 0.51 |
| 1:E:196:LEU:O | 1:E:199:LEU:HB3 | 2.10 | 0.51 |
| 1:F:35:GLY:HA3 | 1:F:108:VAL:HB | 1.93 | 0.51 |
| 2:D:204:VAL:HG13 | 2:D:208:CYS:HB2 | 1.93 | 0.51 |
| 2:G:241:ILE:O | 2:G:241:ILE:HG23 | 2.11 | 0.51 |
| 2:C:91:PHE:CD2 | 2:C:146:LYS:HD2 | 2.46 | 0.51 |
| 2:C:69:LEU:O | 2:C:70:THR:HG23 | 2.11 | 0.51 |
| 1:B:128:ALA:HB1 | 2:D:78:THR:CG2 | 2.41 | 0.51 |
| 1:E:192:VAL:HA | 1:E:195:LEU:CD2 | 2.41 | 0.51 |
| 1:F:41:THR:C | 1:F:43:PRO:HD3 | 2.30 | 0.51 |
| 1:F:59:ILE:HG13 | 1:F:60:VAL:N | 2.26 | 0.51 |
| 2:H:105:LEU:HB3 | 2:H:106:PRO:CD | 2.41 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:141:GLU:OE2 | 2:C:95:SER:N | 2.44 | 0.51 |
| 1:B:18:ALA:O | 1:B:22:VAL:HG23 | 2.10 | 0.51 |
| 2:G:159:PRO:HG2 | 2:G:192:LEU:HD22 | 1.93 | 0.51 |
| 2:D:248:ASP:O | 2:D:249:ILE:C | 2.49 | 0.51 |
| 2:C:278:VAL:C | 2:C:280:ALA:H | 2.13 | 0.51 |
| 1:A:180:GLY:CA | 1:B:73:VAL:HG11 | 2.39 | 0.51 |
| 1:A:56:VAL:O | 1:A:59:ILE:HG12 | 2.10 | 0.51 |
| 2:C:196:LEU:HD21 | 2:C:203:VAL:CG1 | 2.41 | 0.51 |
| 1:F:126:MET:CG | 2:H:109:LEU:HD13 | 2.38 | 0.51 |
| 1:A:81:VAL:HG23 | 1:A:82:ILE:HG13 | 1.92 | 0.51 |
| 1:F:30:ILE:HD11 | 1:F:101:ALA:CA | 2.41 | 0.51 |
| 2:D:83:GLN:NE2 | 2:D:159:PRO:HA | 2.26 | 0.51 |
| 2:D:84:ILE:HD11 | 2:D:163:LEU:CD1 | 2.41 | 0.51 |
| 2:C:30:ALA:HA | 2:C:193:THR:OG1 | 2.10 | 0.51 |
| 1:A:19:MET:HA | 1:A:22:VAL:HG23 | 1.92 | 0.51 |
| 2:G:220:ILE:N | 2:G:220:ILE:HD12 | 2.25 | 0.51 |
| 2:G:113:PRO:HB2 | 2:G:116:GLU:HB2 | 1.91 | 0.51 |
| 1:E:26:PHE:CD1 | 1:E:104:ILE:HD13 | 2.46 | 0.50 |
| 2:H:91:PHE:CE1 | 2:H:147:GLN:HB2 | 2.46 | 0.50 |
| 2:H:128:VAL:CG1 | 2:H:152:ALA:HB2 | 2.38 | 0.50 |
| 1:E:120:ILE:HD12 | 2:G:94:LEU:HD23 | 1.93 | 0.50 |
| 1:A:18:ALA:O | 1:A:22:VAL:HG23 | 2.11 | 0.50 |
| 2:H:141:LEU:HG | 2:H:145:GLN:HB3 | 1.91 | 0.50 |
| 1:E:181:TYR:HD2 | 1:F:167:VAL:HG13 | 1.76 | 0.50 |
| 2:C:239:LYS:O | 2:C:240:PHE:O | 2.30 | 0.50 |
| 1:E:39:TYR:HE2 | 1:E:46:ILE:HG13 | 1.76 | 0.50 |
| 1:E:70:ILE:HA | 1:E:73:VAL:HG12 | 1.93 | 0.50 |
| 1:F:172:LEU:HD12 | 1:F:172:LEU:H | 1.74 | 0.50 |
| 2:H:37:ILE:HG23 | 2:H:213:VAL:HG22 | 1.92 | 0.50 |
| 2:D:209:ASP:O | 2:D:225:VAL:HG23 | 2.10 | 0.50 |
| 2:D:26:LEU:HD11 | 2:D:34:TYR:CE1 | 2.47 | 0.50 |
| 1:B:107:MET:HE2 | 1:B:152:ILE:HD11 | 1.93 | 0.50 |
| 2:D:273:PHE:HE1 | 2:D:335:VAL:HG13 | 1.74 | 0.50 |
| 2:D:265:CYS:SG | 2:D:342:TYR:HB3 | 2.51 | 0.50 |
| 2:G:205:LYS:HZ1 | 2:G:304:ALA:HB2 | 1.74 | 0.50 |
| 2:C:234:THR:N | 2:C:235:PRO:CD | 2.74 | 0.50 |
| 1:E:98:VAL:O | 1:E:102:PRO:HD2 | 2.10 | 0.50 |
| 1:B:33:PRO:O | 1:B:36:VAL:HB | 2.12 | 0.50 |
| 2:C:91:PHE:HE1 | 2:C:147:GLN:HB2 | 1.76 | 0.50 |
| 2:C:274:THR:O | 2:C:276:GLN:N | 2.44 | 0.50 |
| 1:B:39:TYR:O | 1:B:48:ALA:HB2 | 2.11 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:39:TYR:CE2 | 1:E:46:ILE:HG13 | 2.47 | 0.50 |
| 2:D:234:THR:N | 2:D:235:PRO:HD2 | 2.27 | 0.50 |
| 2:C:107:LEU:HD12 | 2:C:121:VAL:CG2 | 2.41 | 0.50 |
| 2:H:270:ARG:HA | 2:H:313:LEU:CD2 | 2.41 | 0.50 |
| 2:G:249:ILE:HD11 | 2:H:177:ARG:HH21 | 1.76 | 0.50 |
| 2:G:97:ARG:HH11 | 2:G:105:LEU:HD11 | 1.76 | 0.50 |
| 1:B:37:LEU:HD21 | 1:B:56:VAL:CB | 2.41 | 0.50 |
| 2:G:10:VAL:O | 2:G:10:VAL:HG13 | 2.11 | 0.50 |
| 1:F:130:PRO:HD2 | 1:F:133:ILE:CB | 2.41 | 0.50 |
| 2:H:52:ASN:O | 2:H:81:ARG:NH1 | 2.45 | 0.50 |
| 1:E:108:VAL:HG12 | 1:E:112:LEU:HD11 | 1.92 | 0.50 |
| 2:C:205:LYS:HD2 | 2:C:304:ALA:HB2 | 1.92 | 0.50 |
| 2:G:35:GLY:O | 2:G:212:ALA:N | 2.38 | 0.50 |
| 2:G:89:GLN:HG3 | 2:G:165:ASP:CG | 2.32 | 0.50 |
| 1:A:198:ILE:HG13 | 1:A:199:LEU:N | 2.26 | 0.50 |
| 1:F:15:GLU:O | 1:F:18:ALA:HB3 | 2.11 | 0.50 |
| 1:E:160:TYR:HD1 | 1:E:160:TYR:O | 1.95 | 0.50 |
| 2:G:241:ILE:HD13 | 2:G:242:GLN:HB2 | 1.93 | 0.50 |
| 2:C:149:VAL:O | 2:C:152:ALA:HB3 | 2.11 | 0.50 |
| 1:A:115:ILE:HG12 | 1:A:116:PRO:N | 2.27 | 0.50 |
| 2:H:28:VAL:HG13 | 2:H:34:TYR:HB2 | 1.94 | 0.50 |
| 1:B:37:LEU:HD21 | 1:B:56:VAL:HG12 | 1.90 | 0.50 |
| 1:A:34:VAL:C | 1:A:36:VAL:H | 2.12 | 0.50 |
| 2:H:89:GLN:HG2 | 2:H:166:GLU:HB2 | 1.94 | 0.50 |
| 1:A:199:LEU:O | 1:A:203:ILE:HG13 | 2.11 | 0.50 |
| 1:F:57:SER:O | 1:F:61:ASN:HB2 | 2.12 | 0.50 |
| 2:C:52:ASN:ND2 | 2:C:54:LEU:HG | 2.27 | 0.50 |
| 1:F:63:PHE:O | 1:F:66:ILE:HB | 2.12 | 0.50 |
| 2:G:247:LEU:HD11 | 2:H:244:THR:HG23 | 1.93 | 0.50 |
| 1:B:22:VAL:HG11 | 1:B:93:ILE:CB | 2.34 | 0.50 |
| 1:E:92:ALA:HB2 | 1:E:169:ALA:CB | 2.34 | 0.50 |
| 1:F:165:GLY:HA2 | 1:F:174:GLN:CA | 2.41 | 0.50 |
| 1:F:173:GLY:O | 1:F:177:TYR:CB | 2.59 | 0.50 |
| 2:C:234:THR:H | 2:C:235:PRO:HD2 | 1.77 | 0.50 |
| 1:F:122:ALA:HB1 | 1:F:126:MET:CE | 2.42 | 0.50 |
| 1:A:69:ILE:HG13 | 1:B:163:MET:SD | 2.51 | 0.50 |
| 1:A:79:THR:O | 1:A:82:ILE:O | 2.29 | 0.50 |
| 1:F:30:ILE:HD11 | 1:F:101:ALA:HA | 1.94 | 0.50 |
| 2:G:243:SER:HA | 2:H:244:THR:HG21 | 1.92 | 0.50 |
| 1:B:40:VAL:CG1 | 1:B:52:LEU:HB2 | 2.42 | 0.50 |
| 1:B:26:PHE:CB | 1:B:97:THR:HB | 2.42 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:34:TYR:CZ | 2:H:212:ALA:HB2 | 2.47 | 0.50 |
| 2:D:241:ILE:HG22 | 2:D:245:LEU:CD1 | 2.38 | 0.50 |
| 2:D:249:ILE:HG22 | 2:D:313:LEU:CD1 | 2.42 | 0.50 |
| 2:D:327:ILE:CG1 | 2:D:328:ALA:N | 2.70 | 0.50 |
| 2:G:7:ILE:HD11 | 2:G:62:VAL:HG22 | 1.94 | 0.50 |
| 2:H:226:SER:OG | 2:H:305:GLY:HA3 | 2.12 | 0.50 |
| 2:C:21:LEU:HD11 | 2:C:46:THR:HG22 | 1.94 | 0.50 |
| 1:E:160:TYR:C | 1:E:160:TYR:CD1 | 2.84 | 0.50 |
| 2:H:130:LEU:HD11 | 2:H:148:ARG:HB2 | 1.93 | 0.50 |
| 2:H:245:LEU:HB3 | 2:H:313:LEU:HD11 | 1.93 | 0.50 |
| 2:D:84:ILE:HD11 | 2:D:163:LEU:HG | 1.94 | 0.50 |
| 1:B:85:THR:HG22 | 1:B:87:ILE:H | 1.77 | 0.50 |
| 2:C:2:ILE:HD11 | 2:C:195:LEU:CD2 | 2.40 | 0.49 |
| 2:C:36:VAL:HB | 2:C:197:ILE:CD1 | 2.42 | 0.49 |
| 1:E:63:PHE:HB3 | 1:E:102:PRO:HG3 | 1.94 | 0.49 |
| 1:E:71:LEU:HD13 | 1:E:160:TYR:OH | 2.11 | 0.49 |
| 1:F:124:ARG:O | 1:F:127:GLY:N | 2.45 | 0.49 |
| 2:H:125:LEU:O | 2:H:130:LEU:O | 2.29 | 0.49 |
| 2:H:87:ILE:HD12 | 2:H:162:LEU:HD21 | 1.95 | 0.49 |
| 1:B:122:ALA:HB1 | 2:D:88:PHE:CZ | 2.47 | 0.49 |
| 2:C:107:LEU:CD1 | 2:C:121:VAL:HG23 | 2.43 | 0.49 |
| 2:G:49:ARG:HH11 | 2:G:49:ARG:HG3 | 1.77 | 0.49 |
| 2:H:220:ILE:CB | 2:H:233:LYS:HD3 | 2.42 | 0.49 |
| 2:D:234:THR:N | 2:D:235:PRO:CD | 2.74 | 0.49 |
| 1:A:159:GLY:O | 1:B:68:PHE:HE1 | 1.96 | 0.49 |
| 1:B:161:SER:O | 1:B:164:GLY:N | 2.46 | 0.49 |
| 2:C:239:LYS:HG3 | 2:C:240:PHE:CE1 | 2.48 | 0.49 |
| 1:E:34:VAL:HG21 | 1:E:105:ALA:CA | 2.41 | 0.49 |
| 1:F:127:GLY:O | 1:F:128:ALA:HB2 | 2.13 | 0.49 |
| 2:H:5:SER:HB2 | 2:H:61:SER:O | 2.12 | 0.49 |
| 1:A:123:SER:O | 1:A:128:ALA:HB2 | 2.12 | 0.49 |
| 2:G:51:VAL:HG11 | 2:G:163:LEU:HD21 | 1.95 | 0.49 |
| 1:F:126:MET:C | 1:F:128:ALA:N | 2.64 | 0.49 |
| 1:F:130:PRO:CD | 1:F:133:ILE:HB | 2.42 | 0.49 |
| 2:D:184:LYS:CE | 2:D:207:ILE:HG22 | 2.42 | 0.49 |
| 2:C:145:GLN:O | 2:C:146:LYS:C | 2.51 | 0.49 |
| 2:H:12:HIS:CE1 | 2:H:14:GLY:HA2 | 2.47 | 0.49 |
| 2:D:33:ILE:HG21 | 2:D:207:ILE:HD12 | 1.94 | 0.49 |
| 2:C:147:GLN:NE2 | 2:C:147:GLN:HA | 2.19 | 0.49 |
| 2:C:147:GLN:O | 2:C:150:ALA:HB3 | 2.12 | 0.49 |
| 2:C:10:VAL:HG23 | 2:C:18:ILE:O | 2.13 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:56:VAL:O | 1:F:59:ILE:HG12 | 2.12 | 0.49 |
| 2:D:34:TYR:OH | 2:D:222:GLN:HG3 | 2.12 | 0.49 |
| 2:G:245:LEU:HD23 | 2:H:173:PRO:HG3 | 1.94 | 0.49 |
| 2:C:303:TYR:C | 2:C:307:VAL:O | 2.50 | 0.49 |
| 2:D:215:SER:HB3 | 2:D:220:ILE:CD1 | 2.42 | 0.49 |
| 2:G:147:GLN:HG2 | 2:G:171:LEU:HD11 | 1.94 | 0.49 |
| 2:D:184:LYS:HE2 | 2:D:207:ILE:HG22 | 1.94 | 0.49 |
| 2:D:52:ASN:ND2 | 2:D:86:MET:CE | 2.75 | 0.49 |
| 1:B:80:ARG:CB | 1:B:86:SER:HB3 | 2.43 | 0.49 |
| 2:C:321:GLN:O | 2:C:324:GLN:HB2 | 2.13 | 0.49 |
| 2:C:241:ILE:C | 2:C:243:SER:N | 2.64 | 0.49 |
| 1:F:68:PHE:N | 1:F:68:PHE:CD1 | 2.79 | 0.49 |
| 2:H:77:LEU:O | 2:H:81:ARG:HG3 | 2.12 | 0.49 |
| 2:H:37:ILE:C | 2:H:37:ILE:HD13 | 2.33 | 0.49 |
| 2:D:1:MET:CE | 2:D:65:ASP:HA | 2.42 | 0.49 |
| 2:G:62:VAL:O | 2:G:69:LEU:N | 2.37 | 0.49 |
| 1:E:110:ASN:OD1 | 1:E:113:LEU:HD12 | 2.13 | 0.49 |
| 2:H:44:LYS:CG | 2:H:45:SER:N | 2.75 | 0.49 |
| 2:H:280:ALA:C | 2:H:282:LEU:H | 2.16 | 0.49 |
| 1:F:98:VAL:O | 1:F:102:PRO:HD2 | 2.13 | 0.49 |
| 1:A:96:LEU:N | 1:A:96:LEU:HD12 | 2.27 | 0.49 |
| 2:D:198:THR:HG21 | 2:D:203:VAL:CB | 2.40 | 0.49 |
| 2:D:234:THR:O | 2:D:235:PRO:C | 2.50 | 0.49 |
| 1:B:28:PHE:HB3 | 1:B:32:LEU:HD12 | 1.94 | 0.49 |
| 1:E:125:ALA:CB | 2:G:54:LEU:HD21 | 2.43 | 0.49 |
| 2:G:293:ASN:HB2 | 2:G:317:HIS:HB2 | 1.94 | 0.49 |
| 1:A:98:VAL:O | 1:A:102:PRO:HD2 | 2.12 | 0.49 |
| 1:E:89:LEU:CD2 | 1:E:170:GLY:HA2 | 2.43 | 0.49 |
| 2:C:7:ILE:HA | 2:C:59:GLU:O | 2.13 | 0.49 |
| 1:E:155:ILE:CD1 | 1:F:64:ARG:HH22 | 2.26 | 0.49 |
| 1:F:126:MET:HA | 2:H:109:LEU:CD1 | 2.37 | 0.49 |
| 1:A:185:ASN:HD22 | 1:A:188:VAL:HG21 | 1.78 | 0.49 |
| 2:G:145:GLN:O | 2:G:149:VAL:HG23 | 2.12 | 0.49 |
| 2:G:7:ILE:O | 2:G:24:VAL:HG22 | 2.13 | 0.49 |
| 2:G:144:GLY:HA2 | 2:G:175:THR:HG21 | 1.94 | 0.49 |
| 1:A:172:LEU:HD23 | 1:A:172:LEU:C | 2.33 | 0.49 |
| 2:H:56:ARG:HD3 | 2:H:71:THR:HG21 | 1.94 | 0.49 |
| 2:C:298:SER:O | 2:C:299:ALA:HB2 | 2.13 | 0.48 |
| 2:C:300:GLN:HE21 | 2:C:300:GLN:HA | 1.77 | 0.48 |
| 1:E:48:ALA:HA | 1:E:53:TYR:H | 1.77 | 0.48 |
| 1:A:163:MET:O | 1:A:164:GLY:O | 2.31 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:92:ALA:O | 1:B:95:PRO:HG2 | 2.13 | 0.48 |
| 2:H:223:ASP:OD1 | 2:H:224:THR:N | 2.46 | 0.48 |
| 2:G:299:ALA:HB2 | 2:G:312:MET:CA | 2.39 | 0.48 |
| 2:D:249:ILE:HG13 | 2:D:250:PRO:O | 2.13 | 0.48 |
| 2:D:29:PRO:CG | 2:D:32:GLN:CD | 2.81 | 0.48 |
| 1:A:9:LEU:N | 1:A:9:LEU:HD23 | 2.27 | 0.48 |
| 1:E:12:GLY:C | 1:E:172:LEU:HD21 | 2.33 | 0.48 |
| 1:F:119:LEU:O | 1:F:123:SER:N | 2.46 | 0.48 |
| 2:H:183:LEU:HA | 2:H:186:ILE:HG12 | 1.95 | 0.48 |
| 1:B:13:VAL:N | 1:B:172:LEU:HD12 | 2.28 | 0.48 |
| 1:E:108:VAL:HG12 | 1:E:112:LEU:CD1 | 2.43 | 0.48 |
| 2:C:248:ASP:HB3 | 2:C:254:GLN:CD | 2.33 | 0.48 |
| 1:A:30:ILE:HD12 | 1:A:101:ALA:HB2 | 1.95 | 0.48 |
| 1:A:73:VAL:HG13 | 1:B:189:MET:SD | 2.53 | 0.48 |
| 2:G:56:ARG:NH1 | 2:G:56:ARG:HB2 | 2.28 | 0.48 |
| 1:E:74:TRP:HA | 1:F:189:MET:CE | 2.42 | 0.48 |
| 2:H:309:PHE:O | 2:H:311:ILE:HD12 | 2.14 | 0.48 |
| 2:G:213:VAL:HG21 | 2:G:233:LYS:CD | 2.43 | 0.48 |
| 2:C:290:PHE:CE2 | 2:C:329:TRP:CB | 2.96 | 0.48 |
| 2:C:290:PHE:HE2 | 2:C:329:TRP:CB | 2.26 | 0.48 |
| 2:C:77:LEU:HD21 | 2:C:81:ARG:CZ | 2.43 | 0.48 |
| 1:A:59:ILE:CA | 1:A:62:ILE:HG12 | 2.43 | 0.48 |
| 2:H:274:THR:CG2 | 2:H:336:LYS:HE2 | 2.43 | 0.48 |
| 2:C:177:ARG:CZ | 2:C:206:ARG:NH2 | 2.77 | 0.48 |
| 2:C:47:LEU:O | 2:C:48:ILE:C | 2.51 | 0.48 |
| 1:F:32:LEU:HD23 | 1:F:108:VAL:CG2 | 2.42 | 0.48 |
| 1:A:67:PRO:HD2 | 1:A:70:ILE:HG21 | 1.95 | 0.48 |
| 1:A:69:ILE:HD12 | 1:B:163:MET:SD | 2.54 | 0.48 |
| 1:B:79:THR:HG22 | 1:B:86:SER:HA | 1.94 | 0.48 |
| 1:B:36:VAL:O | 1:B:40:VAL:HG23 | 2.14 | 0.48 |
| 2:D:141:LEU:HG | 2:D:142:SER:N | 2.29 | 0.48 |
| 1:F:35:GLY:C | 1:F:37:LEU:N | 2.67 | 0.48 |
| 1:A:74:TRP:HE1 | 1:B:190:ASN:ND2 | 2.11 | 0.48 |
| 2:H:231:HIS:O | 2:H:233:LYS:N | 2.44 | 0.48 |
| 2:D:35:GLY:O | 2:D:212:ALA:N | 2.41 | 0.48 |
| 2:C:211:VAL:CG1 | 2:C:228:VAL:HG21 | 2.43 | 0.48 |
| 1:F:80:ARG:HA | 1:F:85:THR:HA | 1.95 | 0.48 |
| 1:A:85:THR:O | 1:A:86:SER:HB3 | 2.14 | 0.48 |
| 2:H:33:ILE:CG2 | 2:H:194:ILE:HD11 | 2.40 | 0.48 |
| 2:G:301:MET:HA | 2:G:309:PHE:O | 2.13 | 0.48 |
| 1:A:47:ILE:O | 1:A:47:ILE:HG23 | 2.12 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:211:VAL:CG1 | 2:H:225:VAL:HG22 | 2.44 | 0.48 |
| 1:F:124:ARG:HD3 | 2:H:86:MET:SD | 2.54 | 0.48 |
| 1:F:126:MET:CA | 2:H:109:LEU:HD13 | 2.40 | 0.48 |
| 1:F:124:ARG:HH11 | 2:H:86:MET:HB3 | 1.75 | 0.48 |
| 1:B:167:VAL:CG2 | 1:B:168:GLY:H | 2.23 | 0.48 |
| 2:D:43:GLY:H | 2:D:44:LYS:HZ3 | 1.59 | 0.48 |
| 2:C:130:LEU:CD2 | 2:C:145:GLN:HA | 2.42 | 0.48 |
| 2:D:266:VAL:HG21 | 2:D:317:HIS:CG | 2.47 | 0.48 |
| 2:G:9:LYS:HE2 | 2:G:55:GLU:HB3 | 1.95 | 0.48 |
| 2:H:331:GLN:HA | 2:H:335:VAL:O | 2.14 | 0.48 |
| 1:B:106:ARG:O | 1:B:106:ARG:HG2 | 2.11 | 0.48 |
| 2:G:124:LEU:CD1 | 2:G:156:ALA:HA | 2.44 | 0.48 |
| 1:B:92:ALA:C | 1:B:95:PRO:HD2 | 2.34 | 0.48 |
| 2:D:33:ILE:CD1 | 2:D:207:ILE:HB | 2.44 | 0.48 |
| 2:H:6:ASN:N | 2:H:25:SER:OG | 2.43 | 0.48 |
| 2:G:196:LEU:HD23 | 2:G:208:CYS:SG | 2.53 | 0.48 |
| 1:A:130:PRO:CG | 1:A:131:MET:N | 2.72 | 0.48 |
| 2:C:99:VAL:HG22 | 2:C:149:VAL:HG22 | 1.96 | 0.48 |
| 2:D:248:ASP:O | 2:D:249:ILE:O | 2.31 | 0.48 |
| 1:B:59:ILE:O | 1:B:62:ILE:HG12 | 2.14 | 0.48 |
| 2:G:51:VAL:HB | 2:G:163:LEU:HD11 | 1.94 | 0.48 |
| 2:G:4:LEU:CD2 | 2:G:62:VAL:HG13 | 2.41 | 0.48 |
| 2:H:10:VAL:HG23 | 2:H:18:ILE:O | 2.14 | 0.48 |
| 1:E:196:LEU:HD23 | 1:E:199:LEU:CD2 | 2.42 | 0.48 |
| 1:F:172:LEU:CD1 | 1:F:172:LEU:N | 2.75 | 0.48 |
| 1:F:161:SER:C | 1:F:163:MET:N | 2.65 | 0.48 |
| 1:F:37:LEU:O | 1:F:41:THR:HG23 | 2.13 | 0.48 |
| 2:H:48:ILE:HG21 | 2:H:197:ILE:CD1 | 2.40 | 0.48 |
| 1:A:165:GLY:HA2 | 1:A:174:GLN:HG2 | 1.96 | 0.48 |
| 2:H:201:MET:O | 2:H:204:VAL:N | 2.47 | 0.48 |
| 2:C:107:LEU:HD12 | 2:C:121:VAL:HG23 | 1.95 | 0.48 |
| 2:H:243:SER:HA | 2:H:246:HIS:CD2 | 2.49 | 0.48 |
| 1:A:22:VAL:O | 1:A:25:PHE:HB3 | 2.14 | 0.48 |
| 2:H:44:LYS:HG3 | 2:H:45:SER:N | 2.27 | 0.48 |
| 2:C:177:ARG:NE | 2:C:206:ARG:NH2 | 2.62 | 0.48 |
| 2:C:253:TYR:HD2 | 2:D:303:TYR:CE1 | 2.32 | 0.48 |
| 1:F:172:LEU:CD1 | 1:F:172:LEU:H | 2.27 | 0.48 |
| 1:F:22:VAL:CG2 | 1:F:23:SER:N | 2.77 | 0.48 |
| 1:B:132:GLN:O | 1:B:136:LYS:HG2 | 2.13 | 0.48 |
| 2:G:37:ILE:CD1 | 2:G:236:LEU:HB3 | 2.44 | 0.48 |
| 2:C:214:ILE:HG13 | 2:C:219:LEU:HD23 | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:121:GLU:O | 1:F:125:ALA:HB2 | 2.14 | 0.47 |
| 2:H:53:LEU:O | 2:H:53:LEU:HG | 2.13 | 0.47 |
| 1:B:22:VAL:HG13 | 1:B:93:ILE:HD12 | 1.96 | 0.47 |
| 1:B:126:MET:SD | 2:D:153:ARG:CD | 3.01 | 0.47 |
| 1:E:163:MET:O | 1:E:166:ALA:HB3 | 2.14 | 0.47 |
| 1:B:72:LEU:HD22 | 1:B:95:PRO:CB | 2.20 | 0.47 |
| 2:H:299:ALA:HA | 2:H:311:ILE:O | 2.15 | 0.47 |
| 1:B:70:ILE:O | 1:B:70:ILE:HG13 | 2.09 | 0.47 |
| 1:B:26:PHE:CD1 | 1:B:97:THR:HA | 2.48 | 0.47 |
| 2:C:1:MET:CE | 2:C:161:VAL:HG23 | 2.43 | 0.47 |
| 2:G:249:ILE:HD13 | 2:H:177:ARG:HE | 1.79 | 0.47 |
| 1:A:166:ALA:HB1 | 1:B:181:TYR:HE2 | 1.79 | 0.47 |
| 2:C:28:VAL:O | 2:C:29:PRO:O | 2.32 | 0.47 |
| 1:F:13:VAL:N | 1:F:172:LEU:HD11 | 2.29 | 0.47 |
| 1:F:71:LEU:HD21 | 1:F:98:VAL:CG1 | 2.44 | 0.47 |
| 2:H:106:PRO:HA | 2:H:109:LEU:HB2 | 1.96 | 0.47 |
| 1:A:76:ILE:HB | 1:A:77:PRO:HD3 | 1.96 | 0.47 |
| 1:B:93:ILE:O | 1:B:97:THR:HG23 | 2.14 | 0.47 |
| 1:E:174:GLN:HG2 | 1:E:177:TYR:CG | 2.49 | 0.47 |
| 1:A:104:ILE:HG13 | 1:A:105:ALA:N | 2.30 | 0.47 |
| 2:D:143:GLY:HA2 | 2:D:146:LYS:HD2 | 1.94 | 0.47 |
| 2:G:112:THR:N | 2:G:113:PRO:CD | 2.77 | 0.47 |
| 2:C:296:ILE:HD13 | 2:D:296:ILE:CD1 | 2.44 | 0.47 |
| 1:E:63:PHE:CB | 1:E:102:PRO:HG3 | 2.45 | 0.47 |
| 1:E:163:MET:CE | 1:F:163:MET:HE1 | 2.44 | 0.47 |
| 1:F:37:LEU:CD2 | 1:F:56:VAL:HG11 | 2.43 | 0.47 |
| 2:H:125:LEU:HA | 2:H:128:VAL:HG22 | 1.96 | 0.47 |
| 2:H:245:LEU:HG | 2:H:298:SER:CB | 2.44 | 0.47 |
| 2:C:31:GLY:N | 2:C:193:THR:OG1 | 2.46 | 0.47 |
| 1:A:87:ILE:CG2 | 1:A:88:GLY:N | 2.77 | 0.47 |
| 2:H:84:ILE:HG13 | 2:H:161:VAL:HB | 1.96 | 0.47 |
| 1:B:68:PHE:O | 1:B:71:LEU:HB3 | 2.14 | 0.47 |
| 2:C:234:THR:HA | 2:C:237:ALA:CB | 2.38 | 0.47 |
| 1:E:69:ILE:HD12 | 1:E:163:MET:CE | 2.36 | 0.47 |
| 1:A:161:SER:O | 1:A:164:GLY:N | 2.47 | 0.47 |
| 1:A:169:ALA:O | 1:A:174:GLN:NE2 | 2.48 | 0.47 |
| 1:A:72:LEU:HA | 1:A:75:MET:HE3 | 1.95 | 0.47 |
| 2:H:37:ILE:HG23 | 2:H:37:ILE:O | 2.14 | 0.47 |
| 1:F:31:GLY:HA3 | 1:F:104:ILE:HD13 | 1.95 | 0.47 |
| 2:G:298:SER:O | 2:G:299:ALA:HB2 | 2.14 | 0.47 |
| 1:A:139:LEU:O | 1:A:143:LEU:N | 2.46 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:101:ALA:HA | 1:B:104:ILE:CG1 | 2.45 | 0.47 |
| 1:A:180:GLY:C | 1:B:73:VAL:HG13 | 2.35 | 0.47 |
| 1:A:47:ILE:O | 1:A:48:ALA:HB2 | 2.14 | 0.47 |
| 2:C:168:THR:HB | 2:C:176:THR:CG2 | 2.44 | 0.47 |
| 1:E:132:GLN:O | 1:E:136:LYS:HB2 | 2.15 | 0.47 |
| 2:H:127:LEU:O | 2:H:127:LEU:HD12 | 2.14 | 0.47 |
| 1:E:70:ILE:HD11 | 1:F:193:LEU:CA | 2.45 | 0.47 |
| 1:F:123:SER:CA | 1:F:129:THR:HG21 | 2.44 | 0.47 |
| 2:H:121:VAL:HG12 | 2:H:125:LEU:CD1 | 2.43 | 0.47 |
| 2:D:43:GLY:N | 2:D:44:LYS:NZ | 2.48 | 0.47 |
| 2:C:124:LEU:HD21 | 2:C:156:ALA:HA | 1.96 | 0.47 |
| 2:G:246:HIS:HB3 | 2:H:241:ILE:CG2 | 2.45 | 0.47 |
| 2:H:34:TYR:CE1 | 2:H:212:ALA:HB2 | 2.50 | 0.47 |
| 2:D:98:THR:CA | 2:D:138:PRO:HB3 | 2.41 | 0.47 |
| 1:B:166:ALA:HA | 1:B:177:TYR:CD2 | 2.48 | 0.47 |
| 2:G:163:LEU:HD23 | 2:G:195:LEU:HB3 | 1.97 | 0.47 |
| 1:A:40:VAL:HG13 | 1:A:49:ASN:HA | 1.97 | 0.47 |
| 1:B:128:ALA:CB | 2:D:78:THR:HG23 | 2.45 | 0.47 |
| 2:C:2:ILE:HG23 | 2:C:28:VAL:O | 2.14 | 0.47 |
| 2:C:58:THR:O | 2:C:59:GLU:HG3 | 2.15 | 0.47 |
| 1:F:179:TYR:O | 1:F:185:ASN:CB | 2.59 | 0.47 |
| 1:F:59:ILE:C | 1:F:62:ILE:HG12 | 2.34 | 0.47 |
| 1:F:26:PHE:CE2 | 1:F:97:THR:HG22 | 2.50 | 0.47 |
| 2:H:125:LEU:HA | 2:H:128:VAL:CG2 | 2.45 | 0.47 |
| 2:H:91:PHE:O | 2:H:92:ASN:HB2 | 2.14 | 0.47 |
| 1:F:118:GLY:O | 1:F:121:GLU:HB2 | 2.15 | 0.47 |
| 1:F:39:TYR:OH | 1:F:135:ARG:HD2 | 2.15 | 0.47 |
| 2:D:162:LEU:HB3 | 2:D:194:ILE:CG2 | 2.41 | 0.47 |
| 2:D:42:ALA:N | 2:D:44:LYS:HZ2 | 2.13 | 0.47 |
| 2:H:63:LEU:HD13 | 2:H:68:GLU:CG | 2.44 | 0.47 |
| 2:G:241:ILE:HB | 2:G:302:ASP:OD1 | 2.14 | 0.47 |
| 2:D:128:VAL:HA | 2:D:182:LEU:HD11 | 1.97 | 0.47 |
| 1:A:41:THR:HG21 | 1:A:113:LEU:HD21 | 1.97 | 0.47 |
| 2:C:98:THR:HA | 2:C:138:PRO:HB3 | 1.95 | 0.47 |
| 2:C:211:VAL:HG22 | 2:C:212:ALA:N | 2.29 | 0.47 |
| 2:C:8:THR:HG23 | 2:C:21:LEU:O | 2.15 | 0.47 |
| 2:D:44:LYS:CD | 2:D:44:LYS:H | 2.21 | 0.47 |
| 2:C:104:ALA:O | 2:C:107:LEU:HB2 | 2.15 | 0.47 |
| 2:C:130:LEU:HD22 | 2:C:148:ARG:HD2 | 1.97 | 0.47 |
| 2:D:37:ILE:HD12 | 2:D:201:MET:SD | 2.55 | 0.47 |
| 2:D:53:LEU:HG | 2:D:53:LEU:O | 2.15 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:247:LEU:CD2 | 2:C:297:ILE:O | 2.62 | 0.47 |
| 2:C:249:ILE:O | 2:C:251:GLU:N | 2.48 | 0.47 |
| 1:E:153:THR:O | 1:E:157:LEU:N | 2.39 | 0.47 |
| 1:F:76:ILE:CB | 1:F:77:PRO:HD3 | 2.45 | 0.47 |
| 2:H:33:ILE:CD1 | 2:H:207:ILE:O | 2.57 | 0.47 |
| 2:G:48:ILE:HD12 | 2:G:86:MET:HE2 | 1.96 | 0.47 |
| 2:G:221:GLU:OE1 | 2:G:230:SER:HB3 | 2.14 | 0.47 |
| 2:G:103:VAL:O | 2:G:106:PRO:HD2 | 2.14 | 0.47 |
| 1:A:147:VAL:O | 1:A:151:THR:HG22 | 2.15 | 0.47 |
| 2:C:247:LEU:HD22 | 2:C:297:ILE:O | 2.14 | 0.47 |
| 1:E:104:ILE:O | 1:E:107:MET:HB2 | 2.15 | 0.47 |
| 2:G:283:LEU:HD13 | 2:G:296:ILE:HD11 | 1.97 | 0.47 |
| 2:H:283:LEU:HD11 | 2:H:312:MET:CE | 2.45 | 0.47 |
| 2:H:242:GLN:HB2 | 2:H:311:ILE:HD13 | 1.95 | 0.47 |
| 2:G:245:LEU:N | 2:G:245:LEU:HD12 | 2.29 | 0.47 |
| 1:A:180:GLY:C | 1:B:73:VAL:CG1 | 2.83 | 0.47 |
| 2:D:144:GLY:HA2 | 2:D:171:LEU:HD22 | 1.97 | 0.47 |
| 1:B:117:THR:HB | 1:B:118:GLY:H | 1.43 | 0.47 |
| 2:G:142:SER:O | 2:G:146:LYS:HG3 | 2.14 | 0.47 |
| 2:C:2:ILE:HD11 | 2:C:195:LEU:HD22 | 1.97 | 0.46 |
| 2:C:247:LEU:HD23 | 2:D:300:GLN:CD | 2.35 | 0.46 |
| 1:F:138:LEU:HD23 | 1:F:138:LEU:HA | 1.60 | 0.46 |
| 2:D:102:ASN:O | 2:D:105:LEU:HB2 | 2.15 | 0.46 |
| 2:D:285:GLU:HG2 | 2:D:329:TRP:CH2 | 2.50 | 0.46 |
| 1:A:17:LEU:HD23 | 1:A:17:LEU:N | 2.30 | 0.46 |
| 2:C:162:LEU:CD2 | 2:C:162:LEU:C | 2.83 | 0.46 |
| 1:E:30:ILE:HA | 1:E:33:PRO:HG2 | 1.97 | 0.46 |
| 1:F:60:VAL:HG13 | 1:F:102:PRO:HA | 1.96 | 0.46 |
| 1:F:40:VAL:HG12 | 1:F:53:TYR:HB2 | 1.98 | 0.46 |
| 2:C:125:LEU:CB | 2:C:131:GLY:HA3 | 2.38 | 0.46 |
| 1:F:30:ILE:CD1 | 1:F:101:ALA:HB1 | 2.43 | 0.46 |
| 2:G:300:GLN:HG2 | 2:H:298:SER:CB | 2.45 | 0.46 |
| 1:B:26:PHE:HB3 | 1:B:97:THR:HB | 1.98 | 0.46 |
| 1:E:165:GLY:O | 1:E:174:GLN:HG3 | 2.14 | 0.46 |
| 2:G:282:LEU:O | 2:G:286:THR:HG23 | 2.16 | 0.46 |
| 2:D:228:VAL:O | 2:D:229:PHE:HD2 | 1.98 | 0.46 |
| 2:C:204:VAL:HG13 | 2:C:208:CYS:HB2 | 1.96 | 0.46 |
| 2:D:206:ARG:NH1 | 2:D:206:ARG:HG3 | 2.30 | 0.46 |
| 1:F:185:ASN:CG | 1:F:188:VAL:HG22 | 2.36 | 0.46 |
| 1:E:188:VAL:HG23 | 1:E:189:MET:N | 2.31 | 0.46 |
| 2:H:147:GLN:HG2 | 2:H:179:ILE:HD13 | 1.97 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:70:ILE:CG2 | 1:A:71:LEU:N | 2.78 | 0.46 |
| 2:G:300:GLN:NE2 | 2:H:244:THR:OG1 | 2.48 | 0.46 |
| 1:A:46:ILE:HG13 | 1:A:135:ARG:NH2 | 2.22 | 0.46 |
| 2:C:130:LEU:HD22 | 2:C:148:ARG:CB | 2.43 | 0.46 |
| 2:H:243:SER:HA | 2:H:246:HIS:NE2 | 2.30 | 0.46 |
| 2:G:186:ILE:HD12 | 2:G:192:LEU:HD12 | 1.97 | 0.46 |
| 2:G:33:ILE:HG12 | 2:G:194:ILE:HD11 | 1.97 | 0.46 |
| 1:E:50:ALA:HB3 | 1:E:52:LEU:HD12 | 1.96 | 0.46 |
| 2:D:73:SER:HB2 | 2:D:76:GLU:CG | 2.44 | 0.46 |
| 2:D:61:SER:HB3 | 2:D:68:GLU:CD | 2.35 | 0.46 |
| 1:F:126:MET:HE1 | 1:F:129:THR:OG1 | 2.16 | 0.46 |
| 1:F:22:VAL:O | 1:F:25:PHE:HB2 | 2.16 | 0.46 |
| 1:F:41:THR:HA | 1:F:53:TYR:CD2 | 2.50 | 0.46 |
| 2:D:162:LEU:HD23 | 2:D:162:LEU:C | 2.35 | 0.46 |
| 2:G:221:GLU:OE1 | 2:G:231:HIS:N | 2.41 | 0.46 |
| 2:G:130:LEU:HD23 | 2:G:149:VAL:HG22 | 1.96 | 0.46 |
| 2:H:250:PRO:HG2 | 2:H:253:TYR:HB2 | 1.97 | 0.46 |
| 1:B:63:PHE:CB | 1:B:102:PRO:HG3 | 2.42 | 0.46 |
| 2:H:56:ARG:CD | 2:H:71:THR:HG21 | 2.45 | 0.46 |
| 2:G:319:THR:O | 2:G:323:THR:HG23 | 2.16 | 0.46 |
| 1:F:118:GLY:HA2 | 1:F:121:GLU:CD | 2.35 | 0.46 |
| 2:G:299:ALA:CB | 2:G:312:MET:HA | 2.39 | 0.46 |
| 2:C:130:LEU:CD2 | 2:C:148:ARG:HB2 | 2.43 | 0.46 |
| 2:G:7:ILE:HG21 | 2:G:50:CYS:SG | 2.56 | 0.46 |
| 2:D:144:GLY:HA2 | 2:D:175:THR:CG2 | 2.44 | 0.46 |
| 2:D:224:THR:O | 2:D:228:VAL:HG23 | 2.15 | 0.46 |
| 2:C:37:ILE:HD12 | 2:C:198:THR:HG23 | 1.96 | 0.46 |
| 1:E:160:TYR:HD1 | 1:E:160:TYR:C | 2.19 | 0.46 |
| 1:F:59:ILE:O | 1:F:63:PHE:HD1 | 1.99 | 0.46 |
| 2:H:48:ILE:HD13 | 2:H:48:ILE:H | 1.64 | 0.46 |
| 1:F:124:ARG:CZ | 2:H:86:MET:CB | 2.94 | 0.46 |
| 2:H:201:MET:SD | 2:H:204:VAL:HB | 2.55 | 0.46 |
| 2:D:52:ASN:HD21 | 2:D:54:LEU:HG | 1.81 | 0.46 |
| 2:C:84:ILE:HG23 | 2:C:84:ILE:O | 2.16 | 0.46 |
| 2:D:242:GLN:O | 2:D:246:HIS:HB3 | 2.15 | 0.46 |
| 2:D:28:VAL:HG22 | 2:D:34:TYR:CD2 | 2.51 | 0.46 |
| 1:E:182:ILE:O | 1:E:182:ILE:HG13 | 2.16 | 0.46 |
| 1:A:26:PHE:CE2 | 1:A:157:LEU:HD11 | 2.50 | 0.46 |
| 2:D:76:GLU:O | 2:D:79:LYS:HB2 | 2.16 | 0.46 |
| 2:G:271:LEU:HD22 | 2:G:335:VAL:CG1 | 2.45 | 0.46 |
| 1:F:152:ILE:HG13 | 1:F:152:ILE:H | 1.50 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:123:SER:HA | 1:F:129:THR:HB | 1.96 | 0.46 |
| 1:A:163:MET:C | 1:A:164:GLY:O | 2.53 | 0.46 |
| 1:B:129:THR:HA | 1:B:133:ILE:CB | 2.46 | 0.46 |
| 2:C:97:ARG:NH1 | 2:C:105:LEU:HD23 | 2.31 | 0.46 |
| 2:H:211:VAL:HB | 2:H:225:VAL:HG22 | 1.97 | 0.46 |
| 2:C:327:ILE:HG13 | 2:C:328:ALA:N | 2.31 | 0.46 |
| 2:C:234:THR:O | 2:C:237:ALA:HB3 | 2.15 | 0.46 |
| 2:D:163:LEU:HD21 | 2:D:195:LEU:HD23 | 1.98 | 0.46 |
| 1:A:118:GLY:O | 1:A:121:GLU:N | 2.49 | 0.46 |
| 2:D:201:MET:HG3 | 2:D:236:LEU:C | 2.36 | 0.46 |
| 2:D:250:PRO:HG2 | 2:D:253:TYR:CB | 2.46 | 0.46 |
| 1:F:8:LEU:H | 1:F:8:LEU:HD23 | 1.81 | 0.46 |
| 2:C:26:LEU:HG | 2:C:28:VAL:HG23 | 1.97 | 0.46 |
| 2:C:313:LEU:HA | 2:C:313:LEU:HD23 | 1.62 | 0.46 |
| 1:E:70:ILE:HD11 | 1:F:193:LEU:N | 2.30 | 0.46 |
| 1:F:71:LEU:HD11 | 1:F:98:VAL:HG12 | 1.97 | 0.46 |
| 2:H:151:ILE:HG13 | 2:H:152:ALA:N | 2.29 | 0.46 |
| 1:A:74:TRP:CG | 1:B:193:LEU:HD11 | 2.51 | 0.46 |
| 2:H:241:ILE:CG2 | 2:H:302:ASP:HB2 | 2.46 | 0.46 |
| 2:H:270:ARG:HB2 | 2:H:340:LEU:HD21 | 1.98 | 0.46 |
| 2:C:143:GLY:O | 2:C:144:GLY:C | 2.53 | 0.46 |
| 2:G:52:ASN:C | 2:G:52:ASN:HD22 | 2.18 | 0.46 |
| 2:G:83:GLN:O | 2:G:159:PRO:CB | 2.58 | 0.46 |
| 2:G:162:LEU:HB3 | 2:G:194:ILE:HG22 | 1.97 | 0.46 |
| 2:C:278:VAL:O | 2:C:280:ALA:N | 2.43 | 0.46 |
| 1:A:92:ALA:O | 1:A:95:PRO:HD2 | 2.15 | 0.46 |
| 1:A:70:ILE:HD11 | 1:B:192:VAL:HG11 | 1.97 | 0.46 |
| 2:G:283:LEU:HB3 | 2:G:294:ASN:ND2 | 2.31 | 0.46 |
| 2:D:34:TYR:HH | 2:D:222:GLN:HG3 | 1.81 | 0.46 |
| 1:A:105:ALA:O | 1:A:108:VAL:HB | 2.15 | 0.46 |
| 2:G:77:LEU:HD21 | 2:G:81:ARG:HH22 | 1.77 | 0.46 |
| 1:E:40:VAL:HA | 1:E:47:ILE:CD1 | 2.34 | 0.45 |
| 1:F:121:GLU:OE1 | 2:H:92:ASN:CG | 2.54 | 0.45 |
| 1:F:68:PHE:N | 1:F:68:PHE:HD1 | 2.11 | 0.45 |
| 2:D:86:MET:HG2 | 2:D:87:ILE:N | 2.31 | 0.45 |
| 2:D:120:ARG:O | 2:D:124:LEU:HD22 | 2.16 | 0.45 |
| 2:D:245:LEU:O | 2:D:313:LEU:HD11 | 2.16 | 0.45 |
| 2:G:28:VAL:HG22 | 2:G:34:TYR:CD2 | 2.51 | 0.45 |
| 1:B:43:PRO:HG2 | 1:B:45:GLN:HG2 | 1.98 | 0.45 |
| 1:A:30:ILE:O | 1:A:34:VAL:HG22 | 2.16 | 0.45 |
| 2:H:323:THR:O | 2:H:327:ILE:HG12 | 2.16 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:56:ARG:HA | 2:C:57:PRO:HD2 | 1.71 | 0.45 |
| 2:C:46:THR:CG2 | 2:C:47:LEU:N | 2.78 | 0.45 |
| 1:E:66:ILE:HG12 | 1:F:193:LEU:CD2 | 2.45 | 0.45 |
| 2:G:184:LYS:NZ | 2:G:206:ARG:O | 2.49 | 0.45 |
| 2:G:244:THR:HB | 2:G:247:LEU:CD1 | 2.46 | 0.45 |
| 1:E:138:LEU:O | 1:E:141:GLU:HB2 | 2.16 | 0.45 |
| 1:A:153:THR:O | 1:A:157:LEU:N | 2.36 | 0.45 |
| 1:A:93:ILE:O | 1:A:97:THR:HG23 | 2.16 | 0.45 |
| 2:G:301:MET:SD | 2:G:308:LYS:HE3 | 2.57 | 0.45 |
| 1:A:40:VAL:CG1 | 1:A:53:TYR:HB2 | 2.46 | 0.45 |
| 1:F:114:GLU:C | 1:F:116:PRO:HD2 | 2.35 | 0.45 |
| 2:G:329:TRP:O | 2:G:332:GLU:HB2 | 2.16 | 0.45 |
| 1:A:66:ILE:HD13 | 1:B:193:LEU:HD13 | 1.98 | 0.45 |
| 2:D:242:GLN:HE22 | 2:D:311:ILE:HD12 | 1.81 | 0.45 |
| 2:G:240:PHE:HD1 | 2:G:241:ILE:H | 1.64 | 0.45 |
| 1:F:196:LEU:HD23 | 1:F:199:LEU:CD2 | 2.47 | 0.45 |
| 2:H:256:ARG:O | 2:H:257:LEU:HB2 | 2.16 | 0.45 |
| 1:F:200:VAL:O | 1:F:203:ILE:HB | 2.16 | 0.45 |
| 1:E:148:ASN:O | 1:E:151:THR:HB | 2.17 | 0.45 |
| 2:C:73:SER:HB2 | 2:C:76:GLU:HB2 | 1.97 | 0.45 |
| 1:F:118:GLY:HA2 | 1:F:121:GLU:HB2 | 1.99 | 0.45 |
| 1:F:41:THR:HG22 | 1:F:53:TYR:HE2 | 1.80 | 0.45 |
| 2:C:64:VAL:CG1 | 2:C:84:ILE:HD12 | 2.28 | 0.45 |
| 1:B:108:VAL:O | 1:B:112:LEU:HG | 2.16 | 0.45 |
| 1:E:115:ILE:HD11 | 1:E:141:GLU:O | 2.16 | 0.45 |
| 1:E:138:LEU:HA | 1:E:138:LEU:HD23 | 1.68 | 0.45 |
| 2:D:158:ASN:N | 2:D:159:PRO:CD | 2.78 | 0.45 |
| 2:G:35:GLY:N | 2:G:210:CYS:O | 2.40 | 0.45 |
| 2:G:35:GLY:O | 2:G:211:VAL:HA | 2.15 | 0.45 |
| 2:C:296:ILE:HG23 | 2:C:314:THR:CG2 | 2.46 | 0.45 |
| 2:C:2:ILE:CG2 | 2:C:28:VAL:O | 2.65 | 0.45 |
| 1:F:59:ILE:O | 1:F:62:ILE:HG13 | 2.16 | 0.45 |
| 1:B:62:ILE:HG13 | 1:B:63:PHE:N | 2.30 | 0.45 |
| 2:C:288:ARG:HD3 | 2:D:287:ALA:O | 2.16 | 0.45 |
| 2:H:10:VAL:HG21 | 2:H:17:THR:HG23 | 1.98 | 0.45 |
| 2:H:37:ILE:HB | 2:H:204:VAL:CG2 | 2.46 | 0.45 |
| 2:D:240:PHE:HD2 | 2:D:242:GLN:HG2 | 1.82 | 0.45 |
| 2:G:93:LEU:HD11 | 2:G:149:VAL:CB | 2.46 | 0.45 |
| 2:D:95:SER:HA | 2:D:139:SER:HG | 1.80 | 0.45 |
| 2:C:313:LEU:HD22 | 2:C:340:LEU:HD11 | 1.99 | 0.45 |
| 1:F:188:VAL:HG23 | 1:F:189:MET:N | 2.32 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:171:LEU:HD13 | 2:H:179:ILE:CD1 | 2.46 | 0.45 |
| 2:H:221:GLU:HB2 | 2:H:233:LYS:NZ | 2.32 | 0.45 |
| 2:C:93:LEU:HD11 | 2:C:146:LYS:O | 2.16 | 0.45 |
| 2:G:128:VAL:CG1 | 2:G:152:ALA:HB2 | 2.36 | 0.45 |
| 2:G:4:LEU:HB3 | 2:G:7:ILE:CG1 | 2.46 | 0.45 |
| 1:E:72:LEU:HD23 | 1:E:95:PRO:HB2 | 1.98 | 0.45 |
| 1:A:128:ALA:HB1 | 1:A:134:VAL:HG22 | 1.99 | 0.45 |
| 1:B:28:PHE:O | 1:B:32:LEU:HB2 | 2.17 | 0.45 |
| 1:A:39:TYR:CD2 | 1:A:48:ALA:CB | 2.98 | 0.45 |
| 2:G:87:ILE:HG23 | 2:G:147:GLN:NE2 | 2.31 | 0.45 |
| 1:E:181:TYR:CD2 | 1:F:167:VAL:HG13 | 2.52 | 0.45 |
| 2:G:270:ARG:HG3 | 2:G:313:LEU:CD2 | 2.46 | 0.45 |
| 1:F:124:ARG:CZ | 2:H:86:MET:HB3 | 2.47 | 0.45 |
| 2:H:231:HIS:C | 2:H:233:LYS:H | 2.20 | 0.45 |
| 1:B:76:ILE:HA | 1:B:79:THR:HB | 1.99 | 0.45 |
| 2:C:145:GLN:O | 2:C:148:ARG:N | 2.50 | 0.45 |
| 2:D:189:ARG:NH2 | 2:D:189:ARG:HG3 | 2.20 | 0.45 |
| 2:C:97:ARG:HH11 | 2:C:105:LEU:HD23 | 1.82 | 0.45 |
| 1:B:41:THR:O | 1:B:42:ARG:HG3 | 2.16 | 0.45 |
| 1:F:167:VAL:HG12 | 1:F:168:GLY:N | 2.32 | 0.45 |
| 2:C:320:GLN:HB3 | 2:C:324:GLN:HE21 | 1.82 | 0.45 |
| 2:G:274:THR:HB | 2:G:334:HIS:HB3 | 1.99 | 0.45 |
| 1:E:68:PHE:HB3 | 1:E:69:ILE:HD13 | 1.97 | 0.45 |
| 1:F:32:LEU:HB2 | 1:F:33:PRO:HD3 | 1.99 | 0.45 |
| 2:H:162:LEU:HD21 | 2:H:164:CYS:SG | 2.56 | 0.45 |
| 2:G:196:LEU:HD22 | 2:G:207:ILE:HD11 | 1.98 | 0.45 |
| 2:G:283:LEU:CD1 | 2:G:296:ILE:HD11 | 2.47 | 0.45 |
| 1:B:66:ILE:HA | 1:B:67:PRO:HD3 | 1.57 | 0.45 |
| 1:B:137:VAL:CG2 | 1:B:138:LEU:N | 2.80 | 0.45 |
| 2:D:4:LEU:HB3 | 2:D:7:ILE:HD11 | 1.99 | 0.45 |
| 2:C:99:VAL:HG22 | 2:C:149:VAL:HG21 | 1.98 | 0.45 |
| 1:E:125:ALA:HB1 | 2:G:52:ASN:OD1 | 2.16 | 0.45 |
| 2:D:189:ARG:NH2 | 2:D:189:ARG:CG | 2.74 | 0.45 |
| 1:F:18:ALA:HA | 1:F:21:PHE:HD2 | 1.81 | 0.45 |
| 2:D:16:ARG:HG3 | 2:D:16:ARG:HH11 | 1.82 | 0.45 |
| 2:H:86:MET:CG | 2:H:87:ILE:N | 2.80 | 0.44 |
| 1:A:69:ILE:O | 1:A:72:LEU:HB3 | 2.17 | 0.44 |
| 1:A:188:VAL:O | 1:A:192:VAL:HG23 | 2.17 | 0.44 |
| 2:D:107:LEU:HD21 | 2:D:120:ARG:HD2 | 1.99 | 0.44 |
| 1:E:139:LEU:N | 1:E:140:PRO:CD | 2.80 | 0.44 |
| 1:B:97:THR:OG1 | 1:B:98:VAL:N | 2.50 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:256:ARG:HH22 | 2:H:278:VAL:HG11 | 1.82 | 0.44 |
| 1:A:27:GLY:O | 1:A:32:LEU:HD12 | 2.17 | 0.44 |
| 2:G:278:VAL:C | 2:G:280:ALA:H | 2.20 | 0.44 |
| 2:D:8:THR:HA | 2:D:21:LEU:O | 2.16 | 0.44 |
| 2:C:26:LEU:HD11 | 2:C:34:TYR:CE1 | 2.52 | 0.44 |
| 1:E:39:TYR:O | 1:E:46:ILE:HG21 | 2.18 | 0.44 |
| 1:F:189:MET:O | 1:F:192:VAL:HB | 2.18 | 0.44 |
| 1:F:124:ARG:HG3 | 2:H:54:LEU:HD11 | 1.99 | 0.44 |
| 2:H:4:LEU:O | 2:H:25:SER:HA | 2.17 | 0.44 |
| 1:A:193:LEU:HD11 | 1:B:74:TRP:CG | 2.52 | 0.44 |
| 2:H:250:PRO:CG | 2:H:253:TYR:HB2 | 2.47 | 0.44 |
| 1:B:123:SER:HB2 | 1:B:126:MET:HE3 | 1.99 | 0.44 |
| 2:C:300:GLN:NE2 | 2:C:301:MET:H | 2.15 | 0.44 |
| 2:C:47:LEU:C | 2:C:49:ARG:N | 2.70 | 0.44 |
| 1:F:72:LEU:HD11 | 1:F:160:TYR:HE1 | 1.80 | 0.44 |
| 2:H:35:GLY:HA3 | 2:H:208:CYS:SG | 2.58 | 0.44 |
| 2:D:49:ARG:HG2 | 2:D:54:LEU:HD12 | 1.98 | 0.44 |
| 2:H:298:SER:OG | 2:H:313:LEU:HB2 | 2.17 | 0.44 |
| 1:A:131:MET:HB3 | 1:A:132:GLN:H | 1.35 | 0.44 |
| 2:G:2:ILE:CG2 | 2:G:28:VAL:HB | 2.41 | 0.44 |
| 1:B:68:PHE:HA | 1:B:160:TYR:OH | 2.18 | 0.44 |
| 2:H:82:ARG:HH12 | 2:H:111:ASN:ND2 | 2.16 | 0.44 |
| 2:H:107:LEU:HD21 | 2:H:156:ALA:O | 2.17 | 0.44 |
| 2:C:172:ASP:OD2 | 2:C:174:ALA:HB3 | 2.17 | 0.44 |
| 1:F:172:LEU:HB3 | 1:F:192:VAL:HG13 | 2.00 | 0.44 |
| 2:D:87:ILE:HD12 | 2:D:162:LEU:HD21 | 1.99 | 0.44 |
| 2:H:6:ASN:H | 2:H:25:SER:HG | 1.65 | 0.44 |
| 2:G:97:ARG:HD3 | 2:G:105:LEU:HD11 | 2.00 | 0.44 |
| 2:H:2:ILE:CG2 | 2:H:28:VAL:HB | 2.47 | 0.44 |
| 2:C:97:ARG:NH1 | 2:C:105:LEU:CD2 | 2.81 | 0.44 |
| 1:B:107:MET:HE3 | 1:B:149:ALA:HB1 | 2.00 | 0.44 |
| 1:B:47:ILE:O | 1:B:48:ALA:CB | 2.65 | 0.44 |
| 1:F:17:LEU:HD23 | 1:F:17:LEU:HA | 1.53 | 0.44 |
| 1:E:41:THR:O | 1:E:43:PRO:HD3 | 2.17 | 0.44 |
| 1:E:42:ARG:HB3 | 1:E:46:ILE:HG22 | 2.00 | 0.44 |
| 2:H:103:VAL:CG2 | 2:H:152:ALA:HB3 | 2.47 | 0.44 |
| 1:B:188:VAL:O | 1:B:192:VAL:HG23 | 2.18 | 0.44 |
| 2:D:44:LYS:O | 2:D:48:ILE:CD1 | 2.66 | 0.44 |
| 2:D:249:ILE:HG13 | 2:D:250:PRO:N | 2.31 | 0.44 |
| 2:G:28:VAL:HG13 | 2:G:34:TYR:CD2 | 2.53 | 0.44 |
| 2:G:238:GLN:NE2 | 2:G:311:ILE:HD13 | 2.33 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:152:ILE:HA | 1:E:155:ILE:HG12 | 2.00 | 0.44 |
| 1:E:189:MET:CE | 1:F:74:TRP:HA | 2.48 | 0.44 |
| 2:H:155:LEU:HA | 2:H:159:PRO:HG3 | 1.98 | 0.44 |
| 1:B:130:PRO:HD2 | 1:B:133:ILE:CG1 | 2.47 | 0.44 |
| 2:C:130:LEU:HD21 | 2:C:145:GLN:HG2 | 1.98 | 0.44 |
| 2:G:102:ASN:HD22 | 2:G:149:VAL:HG11 | 1.81 | 0.44 |
| 1:B:100:ALA:O | 1:B:104:ILE:HG23 | 2.18 | 0.44 |
| 2:D:1:MET:HB3 | 2:D:1:MET:HE2 | 1.86 | 0.44 |
| 2:C:11:PHE:HB2 | 2:C:18:ILE:CG2 | 2.47 | 0.44 |
| 1:F:29:VAL:O | 1:F:33:PRO:HG2 | 2.18 | 0.44 |
| 1:A:82:ILE:O | 1:A:83:VAL:C | 2.55 | 0.44 |
| 2:H:270:ARG:HA | 2:H:313:LEU:HD23 | 1.99 | 0.44 |
| 1:B:134:VAL:CA | 1:B:137:VAL:HG13 | 2.42 | 0.44 |
| 1:E:85:THR:O | 1:E:85:THR:CG2 | 2.65 | 0.44 |
| 2:C:288:ARG:NH1 | 2:D:292:VAL:O | 2.49 | 0.44 |
| 2:D:137:TYR:HD2 | 2:D:140:ASN:O | 2.01 | 0.44 |
| 1:F:40:VAL:O | 1:F:42:ARG:HG2 | 2.18 | 0.44 |
| 1:F:69:ILE:HG13 | 1:F:69:ILE:H | 1.48 | 0.44 |
| 2:H:186:ILE:HB | 2:H:192:LEU:CD1 | 2.46 | 0.44 |
| 1:A:174:GLN:HA | 1:A:177:TYR:HB3 | 2.00 | 0.44 |
| 1:A:181:TYR:O | 1:A:184:TYR:HE1 | 2.00 | 0.44 |
| 2:C:112:THR:N | 2:C:113:PRO:HD3 | 2.33 | 0.44 |
| 2:H:241:ILE:HD13 | 2:H:300:GLN:O | 2.18 | 0.44 |
| 1:E:140:PRO:HA | 1:E:143:LEU:CD1 | 2.37 | 0.44 |
| 1:B:146:LEU:O | 1:B:149:ALA:HB3 | 2.18 | 0.44 |
| 2:C:63:LEU:HD11 | 2:C:66:GLY:CA | 2.48 | 0.44 |
| 2:G:179:ILE:O | 2:G:182:LEU:HB3 | 2.18 | 0.44 |
| 2:D:184:LYS:O | 2:D:188:ARG:HG3 | 2.18 | 0.44 |
| 1:B:133:ILE:O | 1:B:136:LYS:HB2 | 2.18 | 0.44 |
| 1:B:22:VAL:CG1 | 1:B:93:ILE:HB | 2.36 | 0.44 |
| 2:G:85:GLY:O | 2:G:162:LEU:HD12 | 2.18 | 0.44 |
| 2:C:285:GLU:HG2 | 2:C:329:TRP:CH2 | 2.53 | 0.44 |
| 2:C:43:GLY:C | 2:C:45:SER:H | 2.09 | 0.44 |
| 2:C:9:LYS:HZ2 | 2:C:56:ARG:H | 1.65 | 0.44 |
| 1:E:34:VAL:HG21 | 1:E:105:ALA:O | 2.18 | 0.43 |
| 1:E:32:LEU:N | 1:E:33:PRO:CD | 2.81 | 0.43 |
| 1:F:117:THR:O | 1:F:119:LEU:N | 2.51 | 0.43 |
| 1:F:122:ALA:O | 1:F:126:MET:HE3 | 2.18 | 0.43 |
| 1:F:126:MET:HG2 | 2:H:109:LEU:HD22 | 2.00 | 0.43 |
| 1:B:179:TYR:CD2 | 1:B:185:ASN:ND2 | 2.86 | 0.43 |
| 2:H:33:ILE:HD13 | 2:H:207:ILE:HD12 | 2.00 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:144:PRO:HG2 | 1:E:145:GLY:H | 1.82 | 0.43 |
| 1:B:32:LEU:HB2 | 1:B:33:PRO:HD3 | 2.00 | 0.43 |
| 2:C:148:ARG:O | 2:C:149:VAL:C | 2.54 | 0.43 |
| 2:C:190:LEU:HD23 | 2:C:190:LEU:HA | 1.66 | 0.43 |
| 2:G:276:GLN:OE1 | 2:G:282:LEU:HD11 | 2.18 | 0.43 |
| 1:B:104:ILE:HA | 1:B:107:MET:CG | 2.49 | 0.43 |
| 1:F:173:GLY:O | 1:F:177:TYR:HB2 | 2.18 | 0.43 |
| 2:G:41:GLY:O | 2:G:43:GLY:N | 2.50 | 0.43 |
| 2:G:119:ARG:O | 2:G:123:GLU:HG3 | 2.18 | 0.43 |
| 2:C:246:HIS:O | 2:C:250:PRO:HD2 | 2.18 | 0.43 |
| 2:C:85:GLY:O | 2:C:163:LEU:N | 2.47 | 0.43 |
| 2:H:87:ILE:HG22 | 2:H:88:PHE:H | 1.84 | 0.43 |
| 2:G:242:GLN:O | 2:H:244:THR:HG22 | 2.18 | 0.43 |
| 2:G:91:PHE:HE1 | 2:G:171:LEU:CD2 | 2.31 | 0.43 |
| 2:D:113:PRO:O | 2:D:117:VAL:HG23 | 2.18 | 0.43 |
| 2:D:290:PHE:N | 2:D:290:PHE:CD2 | 2.86 | 0.43 |
| 2:C:300:GLN:CA | 2:C:300:GLN:HE21 | 2.31 | 0.43 |
| 1:F:37:LEU:HB3 | 1:F:40:VAL:HB | 1.98 | 0.43 |
| 2:H:87:ILE:CG2 | 2:H:147:GLN:NE2 | 2.77 | 0.43 |
| 2:H:48:ILE:H | 2:H:48:ILE:HD12 | 1.78 | 0.43 |
| 2:C:130:LEU:HD21 | 2:C:145:GLN:CA | 2.46 | 0.43 |
| 2:G:63:LEU:HD21 | 2:G:66:GLY:CA | 2.48 | 0.43 |
| 2:D:94:LEU:H | 2:D:102:ASN:ND2 | 2.16 | 0.43 |
| 2:C:77:LEU:HD21 | 2:C:81:ARG:HH21 | 1.83 | 0.43 |
| 2:H:82:ARG:CD | 2:H:110:ASP:CG | 2.86 | 0.43 |
| 1:F:141:GLU:OE2 | 2:H:96:SER:N | 2.48 | 0.43 |
| 2:C:86:MET:HG2 | 2:C:87:ILE:O | 2.18 | 0.43 |
| 2:C:8:THR:O | 2:C:58:THR:HB | 2.17 | 0.43 |
| 1:E:22:VAL:O | 1:E:26:PHE:HD2 | 2.00 | 0.43 |
| 1:E:69:ILE:HG23 | 1:E:163:MET:CE | 2.48 | 0.43 |
| 2:H:125:LEU:O | 2:H:128:VAL:CG2 | 2.66 | 0.43 |
| 1:B:22:VAL:HG12 | 1:B:26:PHE:HE2 | 1.82 | 0.43 |
| 1:E:122:ALA:O | 1:E:125:ALA:HB3 | 2.19 | 0.43 |
| 2:G:130:LEU:O | 2:G:130:LEU:HG | 2.19 | 0.43 |
| 2:G:33:ILE:HG12 | 2:G:194:ILE:HG12 | 1.98 | 0.43 |
| 1:A:18:ALA:HA | 1:A:21:PHE:HD2 | 1.82 | 0.43 |
| 1:B:104:ILE:HA | 1:B:107:MET:HG2 | 1.99 | 0.43 |
| 2:G:252:ASP:O | 2:G:256:ARG:HB2 | 2.18 | 0.43 |
| 1:B:11:ARG:CZ | 1:B:11:ARG:HB3 | 2.48 | 0.43 |
| 1:A:69:ILE:CG1 | 1:B:163:MET:SD | 3.07 | 0.43 |
| 2:H:241:ILE:H | 2:H:241:ILE:HG13 | 1.58 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:133:ILE:O | 1:A:137:VAL:HG22 | 2.19 | 0.43 |
| 2:C:1:MET:HG3 | 2:C:30:ALA:HB2 | 2.01 | 0.43 |
| 2:C:10:VAL:HG21 | 2:C:17:THR:HG22 | 1.99 | 0.43 |
| 2:H:7:ILE:HD13 | 2:H:60:GLY:HA3 | 2.01 | 0.43 |
| 2:C:284:SER:O | 2:C:287:ALA:HB3 | 2.19 | 0.43 |
| 2:C:29:PRO:HG2 | 2:C:32:GLN:HB2 | 2.00 | 0.43 |
| 1:E:198:ILE:HG13 | 1:E:199:LEU:H | 1.80 | 0.43 |
| 1:E:40:VAL:HG22 | 1:E:47:ILE:CD1 | 2.48 | 0.43 |
| 1:F:20:THR:N | 1:F:157:LEU:CD2 | 2.81 | 0.43 |
| 2:H:124:LEU:HD23 | 2:H:155:LEU:HB2 | 2.01 | 0.43 |
| 1:B:38:LEU:HD22 | 1:B:112:LEU:CB | 2.49 | 0.43 |
| 1:B:96:LEU:HD11 | 1:B:157:LEU:HD11 | 2.00 | 0.43 |
| 2:C:278:VAL:HG21 | 2:D:256:ARG:HH22 | 1.83 | 0.43 |
| 2:H:163:LEU:HD23 | 2:H:195:LEU:HB3 | 2.00 | 0.43 |
| 2:C:137:TYR:CZ | 2:C:140:ASN:O | 2.72 | 0.43 |
| 2:D:224:THR:HG22 | 2:D:226:SER:H | 1.84 | 0.43 |
| 1:F:117:THR:C | 1:F:119:LEU:N | 2.72 | 0.43 |
| 1:F:41:THR:O | 1:F:43:PRO:HD3 | 2.18 | 0.43 |
| 1:F:138:LEU:HD21 | 2:H:94:LEU:CD2 | 2.49 | 0.43 |
| 2:D:48:ILE:HD12 | 2:D:197:ILE:CG1 | 2.33 | 0.43 |
| 2:C:193:THR:HG22 | 2:C:193:THR:O | 2.19 | 0.43 |
| 1:A:22:VAL:O | 1:A:26:PHE:CD2 | 2.71 | 0.43 |
| 2:C:266:VAL:HG13 | 2:C:267:PRO:N | 2.33 | 0.43 |
| 1:E:100:ALA:O | 1:E:103:PHE:HB3 | 2.18 | 0.43 |
| 2:H:142:SER:O | 2:H:145:GLN:HB2 | 2.19 | 0.43 |
| 2:C:37:ILE:HG13 | 2:C:38:GLY:N | 2.32 | 0.43 |
| 1:E:96:LEU:HD12 | 1:E:160:TYR:CD1 | 2.54 | 0.43 |
| 1:B:196:LEU:O | 1:B:199:LEU:HB3 | 2.19 | 0.43 |
| 1:B:130:PRO:HD2 | 1:B:133:ILE:HG13 | 2.00 | 0.43 |
| 1:E:137:VAL:HG12 | 2:G:97:ARG:HH22 | 1.84 | 0.43 |
| 2:D:155:LEU:HD11 | 2:D:186:ILE:CD1 | 2.48 | 0.43 |
| 1:A:191:THR:O | 1:A:195:LEU:CB | 2.66 | 0.43 |
| 2:G:277:SER:O | 2:G:280:ALA:HB3 | 2.19 | 0.43 |
| 1:E:62:ILE:HG22 | 1:F:201:TYR:OH | 2.19 | 0.43 |
| 1:F:118:GLY:C | 1:F:121:GLU:HB2 | 2.40 | 0.43 |
| 1:F:68:PHE:O | 1:F:160:TYR:OH | 2.36 | 0.43 |
| 1:F:161:SER:C | 1:F:163:MET:H | 2.21 | 0.43 |
| 2:H:245:LEU:HD22 | 2:H:311:ILE:CG2 | 2.43 | 0.43 |
| 2:H:298:SER:O | 2:H:299:ALA:HB2 | 2.17 | 0.43 |
| 2:D:24:VAL:HG23 | 2:D:24:VAL:O | 2.19 | 0.43 |
| 2:G:213:VAL:N | 2:G:221:GLU:O | 2.40 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:34:TYR:CD2 | 2:H:210:CYS:HB2 | 2.53 | 0.43 |
| 2:D:330:LEU:HB3 | 2:D:335:VAL:CB | 2.47 | 0.43 |
| 1:B:25:PHE:O | 1:B:29:VAL:HB | 2.18 | 0.43 |
| 2:C:253:TYR:HE1 | 2:C:268:MET:HE1 | 1.84 | 0.43 |
| 2:C:4:LEU:HD13 | 2:C:47:LEU:HD11 | 2.01 | 0.43 |
| 2:C:246:HIS:CE1 | 2:D:202:ASP:OD1 | 2.72 | 0.43 |
| 2:H:130:LEU:CD1 | 2:H:148:ARG:HB2 | 2.49 | 0.43 |
| 2:H:37:ILE:CG2 | 2:H:213:VAL:HG22 | 2.49 | 0.43 |
| 2:D:197:ILE:N | 2:D:197:ILE:CD1 | 2.77 | 0.43 |
| 2:H:242:GLN:O | 2:H:244:THR:N | 2.52 | 0.43 |
| 1:E:38:LEU:HD22 | 1:E:112:LEU:CB | 2.40 | 0.43 |
| 1:B:139:LEU:CB | 1:B:140:PRO:HD3 | 2.46 | 0.43 |
| 2:D:266:VAL:HG22 | 2:D:267:PRO:HD2 | 2.01 | 0.43 |
| 1:E:21:PHE:HB3 | 1:E:25:PHE:CE1 | 2.54 | 0.43 |
| 1:E:133:ILE:HA | 1:E:136:LYS:HB3 | 2.00 | 0.43 |
| 1:F:28:PHE:CZ | 1:F:150:ALA:CB | 3.02 | 0.43 |
| 2:G:250:PRO:HB2 | 2:G:253:TYR:CD2 | 2.54 | 0.43 |
| 2:C:243:SER:O | 2:D:300:GLN:OE1 | 2.36 | 0.42 |
| 2:C:312:MET:HG2 | 2:C:314:THR:HG23 | 2.00 | 0.42 |
| 2:H:155:LEU:HA | 2:H:159:PRO:CG | 2.49 | 0.42 |
| 2:H:175:THR:HG22 | 2:H:179:ILE:HD12 | 2.00 | 0.42 |
| 1:E:126:MET:HE2 | 2:G:153:ARG:HG2 | 2.01 | 0.42 |
| 1:A:19:MET:HA | 1:A:22:VAL:CG2 | 2.48 | 0.42 |
| 2:D:215:SER:HB3 | 2:D:220:ILE:HD11 | 2.01 | 0.42 |
| 2:C:63:LEU:HD11 | 2:C:66:GLY:C | 2.39 | 0.42 |
| 1:A:13:VAL:CG2 | 1:A:195:LEU:HD11 | 2.49 | 0.42 |
| 2:G:212:ALA:HB1 | 2:G:219:LEU:HD23 | 1.99 | 0.42 |
| 2:G:272:GLU:HB3 | 2:G:336:LYS:HG3 | 2.01 | 0.42 |
| 1:E:74:TRP:HA | 1:F:189:MET:HE1 | 2.01 | 0.42 |
| 2:H:52:ASN:HD21 | 2:H:54:LEU:CD2 | 2.32 | 0.42 |
| 1:A:92:ALA:O | 1:A:96:LEU:HD13 | 2.20 | 0.42 |
| 2:G:247:LEU:HA | 2:H:300:GLN:NE2 | 2.35 | 0.42 |
| 2:G:24:VAL:O | 2:G:24:VAL:HG23 | 2.20 | 0.42 |
| 2:D:16:ARG:HG3 | 2:D:16:ARG:NH1 | 2.34 | 0.42 |
| 2:G:250:PRO:HG2 | 2:G:297:ILE:CG2 | 2.49 | 0.42 |
| 2:C:238:GLN:O | 2:C:238:GLN:CG | 2.53 | 0.42 |
| 2:C:245:LEU:O | 2:C:247:LEU:N | 2.53 | 0.42 |
| 1:F:124:ARG:NH1 | 2:H:86:MET:CB | 2.75 | 0.42 |
| 1:F:62:ILE:O | 1:F:66:ILE:HG13 | 2.19 | 0.42 |
| 2:H:128:VAL:HB | 2:H:148:ARG:HB3 | 2.01 | 0.42 |
| 2:H:37:ILE:HG12 | 2:H:198:THR:HG23 | 2.00 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:107:LEU:O | 2:D:111:ASN:HB2 | 2.19 | 0.42 |
| 1:B:113:LEU:HA | 1:B:113:LEU:HD23 | 1.76 | 0.42 |
| 2:D:268:MET:HE2 | 2:D:313:LEU:HB3 | 2.02 | 0.42 |
| 1:B:8:LEU:H | 1:B:8:LEU:CD1 | 2.29 | 0.42 |
| 1:A:101:ALA:HB3 | 1:A:102:PRO:CD | 2.49 | 0.42 |
| 2:D:115:ASP:C | 2:D:117:VAL:N | 2.70 | 0.42 |
| 2:D:319:THR:HG22 | 2:D:320:GLN:N | 2.34 | 0.42 |
| 2:C:155:LEU:HD23 | 2:C:155:LEU:HA | 1.71 | 0.42 |
| 1:A:125:ALA:HA | 2:C:54:LEU:HD21 | 2.02 | 0.42 |
| 1:F:134:VAL:HG13 | 1:F:135:ARG:HG3 | 2.02 | 0.42 |
| 2:D:35:GLY:HA3 | 2:D:208:CYS:SG | 2.59 | 0.42 |
| 2:D:52:ASN:ND2 | 2:D:54:LEU:HG | 2.35 | 0.42 |
| 2:D:87:ILE:CD1 | 2:D:162:LEU:HD21 | 2.50 | 0.42 |
| 2:H:163:LEU:CD2 | 2:H:195:LEU:HB3 | 2.50 | 0.42 |
| 2:G:295:ASN:ND2 | 2:G:317:HIS:CD2 | 2.86 | 0.42 |
| 2:D:274:THR:C | 2:D:276:GLN:N | 2.71 | 0.42 |
| 2:H:139:SER:C | 2:H:141:LEU:H | 2.21 | 0.42 |
| 1:F:134:VAL:HG13 | 1:F:135:ARG:N | 2.33 | 0.42 |
| 1:F:53:TYR:HE2 | 1:F:109:GLU:OE2 | 2.02 | 0.42 |
| 2:D:36:VAL:O | 2:D:197:ILE:HA | 2.19 | 0.42 |
| 2:G:240:PHE:HD1 | 2:G:241:ILE:N | 2.16 | 0.42 |
| 2:G:49:ARG:NH1 | 2:G:49:ARG:HG3 | 2.34 | 0.42 |
| 2:G:159:PRO:O | 2:G:192:LEU:CD2 | 2.67 | 0.42 |
| 1:A:15:GLU:O | 1:A:18:ALA:HB3 | 2.19 | 0.42 |
| 2:H:43:GLY:C | 2:H:45:SER:H | 2.10 | 0.42 |
| 2:D:53:LEU:HD22 | 2:D:69:LEU:HB3 | 2.02 | 0.42 |
| 2:C:247:LEU:C | 2:C:250:PRO:HD2 | 2.39 | 0.42 |
| 1:F:172:LEU:HD23 | 1:F:195:LEU:HD23 | 2.01 | 0.42 |
| 1:F:76:ILE:HG22 | 1:F:77:PRO:N | 2.35 | 0.42 |
| 2:H:103:VAL:CG1 | 2:H:121:VAL:HG13 | 2.49 | 0.42 |
| 1:A:96:LEU:N | 1:A:96:LEU:CD1 | 2.83 | 0.42 |
| 2:G:247:LEU:HD21 | 2:H:244:THR:HG21 | 2.02 | 0.42 |
| 1:A:186:ALA:O | 1:A:190:ASN:OD1 | 2.38 | 0.42 |
| 2:C:186:ILE:CD1 | 2:C:192:LEU:HD23 | 2.49 | 0.42 |
| 2:G:53:LEU:HB3 | 2:G:81:ARG:HH21 | 1.84 | 0.42 |
| 1:A:39:TYR:CG | 1:A:48:ALA:HB3 | 2.54 | 0.42 |
| 2:C:10:VAL:HG22 | 2:C:11:PHE:N | 2.34 | 0.42 |
| 1:F:206:ALA:O | 1:F:207:GLY:C | 2.57 | 0.42 |
| 2:G:9:LYS:HE3 | 2:G:11:PHE:HB2 | 2.02 | 0.42 |
| 2:H:323:THR:O | 2:H:327:ILE:HG23 | 2.20 | 0.42 |
| 1:F:35:GLY:O | 1:F:37:LEU:N | 2.52 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:173:PRO:HA | 2:D:176:THR:HB | 2.01 | 0.42 |
| 1:B:40:VAL:HG11 | 1:B:53:TYR:N | 2.35 | 0.42 |
| 1:E:178:GLN:O | 1:E:182:ILE:O | 2.37 | 0.42 |
| 2:G:130:LEU:CD2 | 2:G:149:VAL:HG22 | 2.50 | 0.42 |
| 1:B:149:ALA:O | 1:B:152:ILE:HG12 | 2.19 | 0.42 |
| 2:G:87:ILE:CD1 | 2:G:151:ILE:HD13 | 2.50 | 0.42 |
| 1:B:171:GLY:O | 1:B:174:GLN:HB3 | 2.19 | 0.42 |
| 2:C:4:LEU:HD12 | 2:C:26:LEU:HB3 | 2.02 | 0.42 |
| 2:C:253:TYR:OH | 2:C:297:ILE:HD11 | 2.20 | 0.42 |
| 1:F:37:LEU:HD22 | 1:F:40:VAL:HG21 | 2.02 | 0.42 |
| 1:F:70:ILE:CG2 | 1:F:71:LEU:N | 2.82 | 0.42 |
| 1:F:121:GLU:OE2 | 2:H:92:ASN:HB3 | 2.20 | 0.42 |
| 1:B:119:LEU:HB3 | 2:D:92:ASN:OD1 | 2.18 | 0.42 |
| 2:C:107:LEU:HB3 | 2:C:117:VAL:HG22 | 2.02 | 0.42 |
| 1:B:132:GLN:O | 1:B:135:ARG:HB2 | 2.20 | 0.42 |
| 2:D:28:VAL:HG13 | 2:D:34:TYR:HB2 | 2.02 | 0.42 |
| 1:A:119:LEU:CB | 2:C:92:ASN:OD1 | 2.60 | 0.42 |
| 1:F:38:LEU:HB2 | 1:F:112:LEU:HD13 | 2.02 | 0.42 |
| 1:A:159:GLY:O | 1:B:68:PHE:CE1 | 2.73 | 0.42 |
| 2:H:189:ARG:C | 2:H:190:LEU:O | 2.57 | 0.42 |
| 2:C:268:MET:HA | 2:C:314:THR:O | 2.19 | 0.42 |
| 2:C:4:LEU:HA | 2:C:7:ILE:HD11 | 2.02 | 0.42 |
| 1:E:16:THR:HG21 | 1:E:199:LEU:HD21 | 2.01 | 0.42 |
| 1:E:26:PHE:HB2 | 1:E:30:ILE:CG1 | 2.49 | 0.42 |
| 1:E:163:MET:HB3 | 1:E:163:MET:HE3 | 1.68 | 0.42 |
| 1:A:70:ILE:HG23 | 1:A:71:LEU:N | 2.33 | 0.42 |
| 1:B:7:TRP:NE1 | 1:F:182:ILE:HG22 | 2.35 | 0.42 |
| 2:G:240:PHE:CE1 | 2:G:243:SER:OG | 2.72 | 0.42 |
| 2:D:2:ILE:CD1 | 2:D:195:LEU:HD22 | 2.49 | 0.42 |
| 1:A:59:ILE:O | 1:A:62:ILE:HG12 | 2.19 | 0.42 |
| 2:C:221:GLU:OE2 | 2:C:231:HIS:N | 2.51 | 0.42 |
| 1:E:101:ALA:HB3 | 1:E:102:PRO:HD3 | 2.01 | 0.42 |
| 1:F:121:GLU:O | 1:F:125:ALA:CB | 2.68 | 0.42 |
| 1:F:130:PRO:HG2 | 1:F:133:ILE:CG1 | 2.50 | 0.42 |
| 1:F:25:PHE:O | 1:F:29:VAL:CG2 | 2.66 | 0.42 |
| 1:F:26:PHE:HA | 1:F:29:VAL:HB | 2.01 | 0.42 |
| 1:E:108:VAL:O | 1:E:112:LEU:HG | 2.19 | 0.42 |
| 2:D:313:LEU:N | 2:D:313:LEU:HD23 | 2.34 | 0.42 |
| 1:A:89:LEU:HD23 | 1:A:89:LEU:HA | 1.83 | 0.42 |
| 1:B:120:ILE:HD12 | 2:D:94:LEU:HD21 | 2.01 | 0.42 |
| 2:C:168:THR:HG21 | 2:C:180:LEU:HG | 2.02 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:8:LEU:H | 1:F:8:LEU:CD2 | 2.26 | 0.42 |
| 2:C:242:GLN:HA | 2:C:242:GLN:NE2 | 2.34 | 0.42 |
| 2:G:234:THR:N | 2:G:235:PRO:HD2 | 2.35 | 0.42 |
| 2:C:238:GLN:O | 2:C:240:PHE:CD2 | 2.73 | 0.41 |
| 2:C:313:LEU:HD22 | 2:C:340:LEU:CD1 | 2.50 | 0.41 |
| 1:E:34:VAL:O | 1:E:37:LEU:HB2 | 2.19 | 0.41 |
| 1:E:47:ILE:O | 1:E:48:ALA:CB | 2.68 | 0.41 |
| 2:H:104:ALA:O | 2:H:105:LEU:C | 2.57 | 0.41 |
| 1:A:66:ILE:CG2 | 1:A:71:LEU:HB2 | 2.50 | 0.41 |
| 2:C:120:ARG:O | 2:C:124:LEU:HD13 | 2.20 | 0.41 |
| 1:A:196:LEU:HD12 | 1:B:70:ILE:HD13 | 2.01 | 0.41 |
| 2:C:147:GLN:O | 2:C:151:ILE:HG23 | 2.20 | 0.41 |
| 2:G:103:VAL:HG22 | 2:G:152:ALA:HB1 | 2.02 | 0.41 |
| 2:G:144:GLY:HA3 | 2:G:175:THR:HG21 | 2.02 | 0.41 |
| 1:A:148:ASN:HA | 1:A:151:THR:HG22 | 2.01 | 0.41 |
| 2:C:184:LYS:O | 2:C:187:ASN:HB3 | 2.20 | 0.41 |
| 1:E:189:MET:O | 1:E:192:VAL:HB | 2.19 | 0.41 |
| 2:H:87:ILE:CG2 | 2:H:88:PHE:H | 2.32 | 0.41 |
| 1:A:120:ILE:O | 1:A:123:SER:HB3 | 2.20 | 0.41 |
| 1:A:139:LEU:N | 1:A:140:PRO:CD | 2.82 | 0.41 |
| 1:A:193:LEU:HA | 1:B:70:ILE:HD11 | 2.01 | 0.41 |
| 1:B:36:VAL:CG1 | 1:B:36:VAL:O | 2.68 | 0.41 |
| 2:D:143:GLY:HA2 | 2:D:146:LYS:HG3 | 2.03 | 0.41 |
| 2:D:282:LEU:O | 2:D:286:THR:HG23 | 2.21 | 0.41 |
| 2:H:141:LEU:CG | 2:H:145:GLN:HB3 | 2.50 | 0.41 |
| 2:H:99:VAL:HB | 2:H:134:HIS:O | 2.20 | 0.41 |
| 1:F:138:LEU:C | 1:F:140:PRO:HD2 | 2.41 | 0.41 |
| 2:H:87:ILE:CD1 | 2:H:151:ILE:HG22 | 2.49 | 0.41 |
| 1:E:38:LEU:HD13 | 1:E:112:LEU:CB | 2.48 | 0.41 |
| 2:C:147:GLN:HG2 | 2:C:179:ILE:HD13 | 2.01 | 0.41 |
| 2:G:39:ALA:HB2 | 2:G:236:LEU:HD21 | 2.01 | 0.41 |
| 1:A:39:TYR:O | 1:A:49:ASN:HB3 | 2.21 | 0.41 |
| 2:D:71:THR:O | 2:D:71:THR:HG22 | 2.20 | 0.41 |
| 2:C:249:ILE:N | 2:C:250:PRO:CD | 2.83 | 0.41 |
| 1:E:37:LEU:HA | 1:E:40:VAL:HB | 2.02 | 0.41 |
| 1:B:129:THR:HA | 1:B:133:ILE:CG2 | 2.50 | 0.41 |
| 2:D:104:ALA:HA | 2:D:107:LEU:HD12 | 2.02 | 0.41 |
| 1:A:180:GLY:CA | 1:B:73:VAL:CG1 | 2.98 | 0.41 |
| 2:D:287:ALA:HA | 2:D:292:VAL:H | 1.85 | 0.41 |
| 1:A:39:TYR:O | 1:A:44:GLY:HA2 | 2.21 | 0.41 |
| 2:H:137:TYR:HE2 | 2:H:141:LEU:HA | 1.85 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:208:ASP:N | 1:F:208:ASP:OD1 | 2.54 | 0.41 |
| 2:G:327:ILE:HG13 | 2:G:328:ALA:N | 2.35 | 0.41 |
| 2:C:34:TYR:HD2 | 2:C:210:CYS:HB2 | 1.80 | 0.41 |
| 2:C:270:ARG:HA | 2:C:312:MET:O | 2.21 | 0.41 |
| 2:H:151:ILE:HA | 2:H:154:ALA:HB3 | 2.02 | 0.41 |
| 1:A:132:GLN:O | 1:A:133:ILE:C | 2.57 | 0.41 |
| 2:G:1:MET:CE | 2:G:161:VAL:HG22 | 2.43 | 0.41 |
| 1:E:168:GLY:O | 1:E:169:ALA:HB2 | 2.20 | 0.41 |
| 2:G:293:ASN:HA | 2:H:284:SER:CB | 2.51 | 0.41 |
| 2:C:86:MET:CE | 2:C:163:LEU:HD12 | 2.48 | 0.41 |
| 1:E:16:THR:OG1 | 1:E:172:LEU:CD1 | 2.68 | 0.41 |
| 1:E:155:ILE:CB | 1:E:200:VAL:HG13 | 2.48 | 0.41 |
| 1:F:69:ILE:HG23 | 1:F:163:MET:CE | 2.44 | 0.41 |
| 1:A:185:ASN:C | 1:A:187:THR:N | 2.72 | 0.41 |
| 2:D:4:LEU:CD2 | 2:D:7:ILE:HD11 | 2.36 | 0.41 |
| 1:B:93:ILE:CG1 | 1:B:94:VAL:N | 2.81 | 0.41 |
| 1:A:115:ILE:HA | 1:A:116:PRO:HD3 | 1.83 | 0.41 |
| 2:G:138:PRO:HG2 | 2:G:139:SER:H | 1.84 | 0.41 |
| 1:A:152:ILE:O | 1:A:155:ILE:HG12 | 2.20 | 0.41 |
| 1:B:17:LEU:HA | 1:B:17:LEU:HD23 | 1.75 | 0.41 |
| 2:C:208:CYS:O | 2:C:225:VAL:HG21 | 2.21 | 0.41 |
| 2:C:271:LEU:HB2 | 2:C:312:MET:HB3 | 2.03 | 0.41 |
| 2:C:247:LEU:N | 2:D:300:GLN:OE1 | 2.54 | 0.41 |
| 1:E:200:VAL:O | 1:E:203:ILE:HB | 2.20 | 0.41 |
| 1:E:66:ILE:HA | 1:E:67:PRO:HD3 | 1.91 | 0.41 |
| 1:F:179:TYR:HD2 | 1:F:185:ASN:HD22 | 1.68 | 0.41 |
| 1:F:72:LEU:HD23 | 1:F:95:PRO:HB3 | 2.01 | 0.41 |
| 1:A:169:ALA:C | 1:A:174:GLN:NE2 | 2.74 | 0.41 |
| 1:B:167:VAL:CG1 | 1:B:168:GLY:N | 2.65 | 0.41 |
| 1:B:172:LEU:CD2 | 1:B:195:LEU:HD23 | 2.37 | 0.41 |
| 2:H:32:GLN:HG2 | 2:H:209:ASP:OD1 | 2.20 | 0.41 |
| 2:D:44:LYS:HG2 | 2:D:45:SER:N | 2.35 | 0.41 |
| 2:G:243:SER:HA | 2:H:244:THR:CG2 | 2.50 | 0.41 |
| 1:A:190:ASN:HA | 1:A:193:LEU:HD12 | 2.02 | 0.41 |
| 1:B:32:LEU:HD23 | 1:B:32:LEU:HA | 1.88 | 0.41 |
| 2:G:85:GLY:C | 2:G:162:LEU:HD12 | 2.40 | 0.41 |
| 1:F:113:LEU:O | 1:F:116:PRO:CD | 2.68 | 0.41 |
| 1:B:42:ARG:N | 1:B:43:PRO:CD | 2.83 | 0.41 |
| 2:G:124:LEU:HD11 | 2:G:156:ALA:HA | 2.02 | 0.41 |
| 2:C:21:LEU:HD23 | 2:C:217:GLY:HA2 | 2.02 | 0.41 |
| 1:F:42:ARG:CD | 1:F:49:ASN:HA | 2.44 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:198:THR:HG21 | 2:H:200:GLU:O | 2.20 | 0.41 |
| 2:H:33:ILE:O | 2:H:209:ASP:N | 2.54 | 0.41 |
| 2:D:35:GLY:O | 2:D:211:VAL:HA | 2.21 | 0.41 |
| 2:H:5:SER:O | 2:H:6:ASN:C | 2.58 | 0.41 |
| 2:H:62:VAL:O | 2:H:68:GLU:HA | 2.21 | 0.41 |
| 1:E:14:TRP:CZ3 | 1:E:17:LEU:HD12 | 2.56 | 0.41 |
| 2:C:177:ARG:CZ | 2:C:206:ARG:HH21 | 2.33 | 0.41 |
| 2:C:326:ALA:O | 2:C:330:LEU:HG | 2.20 | 0.41 |
| 2:C:235:PRO:O | 2:C:236:LEU:CG | 2.69 | 0.41 |
| 2:C:5:SER:O | 2:C:7:ILE:HG13 | 2.21 | 0.41 |
| 2:C:234:THR:C | 2:C:237:ALA:HB3 | 2.40 | 0.41 |
| 1:E:97:THR:OG1 | 1:E:98:VAL:N | 2.54 | 0.41 |
| 1:E:73:VAL:O | 1:E:77:PRO:HD3 | 2.20 | 0.41 |
| 1:F:46:ILE:CG2 | 1:F:47:ILE:HG23 | 2.45 | 0.41 |
| 1:A:196:LEU:O | 1:A:200:VAL:HG23 | 2.21 | 0.41 |
| 1:B:115:ILE:CG1 | 1:B:116:PRO:HD2 | 2.45 | 0.41 |
| 2:G:52:ASN:C | 2:G:52:ASN:ND2 | 2.74 | 0.41 |
| 2:G:103:VAL:HG12 | 2:G:121:VAL:HG22 | 2.03 | 0.41 |
| 2:D:230:SER:HB3 | 2:D:231:HIS:H | 1.52 | 0.41 |
| 2:G:28:VAL:HG13 | 2:G:34:TYR:HD2 | 1.86 | 0.41 |
| 2:C:290:PHE:CZ | 2:C:329:TRP:HB2 | 2.54 | 0.41 |
| 2:G:87:ILE:HD12 | 2:G:151:ILE:HD13 | 2.03 | 0.41 |
| 2:G:91:PHE:HE1 | 2:G:171:LEU:HD21 | 1.86 | 0.41 |
| 1:E:134:VAL:HB | 1:E:135:ARG:NH2 | 2.36 | 0.41 |
| 2:G:112:THR:O | 2:G:112:THR:HG22 | 2.21 | 0.41 |
| 2:C:98:THR:HA | 2:C:138:PRO:HA | 2.01 | 0.41 |
| 1:A:32:LEU:HB2 | 1:A:33:PRO:HD3 | 2.03 | 0.41 |
| 2:G:43:GLY:C | 2:G:45:SER:N | 2.73 | 0.41 |
| 2:H:330:LEU:O | 2:H:335:VAL:HB | 2.21 | 0.41 |
| 2:D:290:PHE:N | 2:D:290:PHE:HD2 | 2.19 | 0.41 |
| 2:D:258:GLN:HG3 | 2:D:262:PHE:CD2 | 2.56 | 0.41 |
| 2:H:9:LYS:HE3 | 2:H:55:GLU:HB3 | 2.02 | 0.41 |
| 2:C:282:LEU:O | 2:C:286:THR:HG23 | 2.21 | 0.41 |
| 2:C:253:TYR:HE1 | 2:C:268:MET:CE | 2.34 | 0.41 |
| 1:E:175:ILE:HG13 | 1:E:176:GLY:H | 1.85 | 0.41 |
| 2:G:247:LEU:HD21 | 2:G:300:GLN:NE2 | 2.36 | 0.41 |
| 1:B:22:VAL:HG21 | 1:B:93:ILE:CB | 2.51 | 0.41 |
| 1:E:118:GLY:O | 1:E:119:LEU:HG | 2.21 | 0.41 |
| 1:E:119:LEU:O | 2:G:92:ASN:ND2 | 2.54 | 0.41 |
| 2:G:105:LEU:N | 2:G:106:PRO:HD2 | 2.35 | 0.41 |
| 1:A:42:ARG:HB3 | 1:A:43:PRO:CD | 2.49 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:142:ALA:O | 1:B:146:LEU:N | 2.46 | 0.41 |
| 1:B:118:GLY:HA2 | 1:B:121:GLU:HB2 | 2.03 | 0.41 |
| 2:D:271:LEU:HB3 | 2:D:273:PHE:CE1 | 2.56 | 0.41 |
| 1:A:160:TYR:HD1 | 1:A:160:TYR:O | 2.04 | 0.41 |
| 2:C:34:TYR:OH | 2:C:222:GLN:HG3 | 2.21 | 0.40 |
| 1:E:76:ILE:CB | 1:E:77:PRO:HD3 | 2.51 | 0.40 |
| 1:F:64:ARG:HD2 | 1:F:103:PHE:CZ | 2.56 | 0.40 |
| 1:F:71:LEU:O | 1:F:75:MET:HE3 | 2.21 | 0.40 |
| 1:A:177:TYR:O | 1:A:181:TYR:N | 2.42 | 0.40 |
| 2:G:298:SER:HB3 | 2:H:300:GLN:NE2 | 2.36 | 0.40 |
| 2:C:83:GLN:O | 2:C:159:PRO:CB | 2.70 | 0.40 |
| 2:C:261:PRO:HB3 | 2:C:342:TYR:CE1 | 2.55 | 0.40 |
| 1:F:143:LEU:HD23 | 1:F:143:LEU:HA | 1.84 | 0.40 |
| 2:C:249:ILE:HD13 | 2:C:249:ILE:HA | 1.97 | 0.40 |
| 2:C:247:LEU:CD2 | 2:C:297:ILE:HG22 | 2.44 | 0.40 |
| 1:F:193:LEU:C | 1:F:193:LEU:HD13 | 2.42 | 0.40 |
| 2:D:36:VAL:CG2 | 2:D:197:ILE:HG13 | 2.51 | 0.40 |
| 2:G:276:GLN:OE1 | 2:G:282:LEU:CD1 | 2.69 | 0.40 |
| 1:E:7:TRP:CE3 | 1:E:11:ARG:HD2 | 2.56 | 0.40 |
| 1:B:126:MET:HB2 | 1:B:126:MET:HE3 | 1.90 | 0.40 |
| 1:E:21:PHE:O | 1:E:25:PHE:CD1 | 2.74 | 0.40 |
| 2:H:185:ASP:OD1 | 2:H:189:ARG:NH2 | 2.54 | 0.40 |
| 2:G:41:GLY:C | 2:G:43:GLY:H | 2.24 | 0.40 |
| 2:G:343:VAL:HG12 | 2:G:343:VAL:OXT | 2.21 | 0.40 |
| 2:C:236:LEU:HA | 2:C:239:LYS:CB | 2.43 | 0.40 |
| 1:E:69:ILE:CD1 | 1:E:163:MET:HE2 | 2.38 | 0.40 |
| 1:F:26:PHE:CD1 | 1:F:27:GLY:N | 2.89 | 0.40 |
| 1:A:69:ILE:HD13 | 1:A:70:ILE:H | 1.86 | 0.40 |
| 1:A:143:LEU:O | 1:A:144:PRO:C | 2.55 | 0.40 |
| 1:B:30:ILE:C | 1:B:33:PRO:HD2 | 2.41 | 0.40 |
| 1:B:38:LEU:HD11 | 1:B:113:LEU:HD21 | 2.04 | 0.40 |
| 1:A:118:GLY:HA2 | 1:A:121:GLU:CG | 2.44 | 0.40 |
| 2:C:69:LEU:H | 2:C:69:LEU:HD12 | 1.86 | 0.40 |
| 2:C:100:PHE:CZ | 2:C:118:LYS:HA | 2.49 | 0.40 |
| 2:H:166:GLU:HB3 | 2:H:169:SER:OG | 2.22 | 0.40 |
| 1:F:107:MET:HE2 | 1:F:152:ILE:HD11 | 2.03 | 0.40 |
| 1:F:126:MET:HE1 | 1:F:134:VAL:CB | 2.50 | 0.40 |
| 1:F:127:GLY:O | 1:F:128:ALA:CB | 2.69 | 0.40 |
| 2:H:105:LEU:O | 2:H:108:GLU:CB | 2.63 | 0.40 |
| 1:B:167:VAL:O | 1:B:169:ALA:N | 2.55 | 0.40 |
| 1:A:112:LEU:HD23 | 1:A:112:LEU:HA | 1.89 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:37:ILE:HD11 | 2:G:236:LEU:CB | 2.48 | 0.40 |
| 2:D:102:ASN:HA | 2:D:105:LEU:CD1 | 2.51 | 0.40 |
| 2:D:91:PHE:CD1 | 2:D:146:LYS:HB2 | 2.56 | 0.40 |
| 1:E:50:ALA:O | 1:E:52:LEU:HG | 2.21 | 0.40 |
| 1:E:114:GLU:OE1 | 1:E:114:GLU:HA | 2.21 | 0.40 |
| 2:C:65:ASP:OD2 | 2:C:160:LYS:HD2 | 2.20 | 0.40 |
| 1:E:59:ILE:HG13 | 1:E:60:VAL:N | 2.35 | 0.40 |
| 2:H:33:ILE:HG21 | 2:H:207:ILE:HG13 | 2.02 | 0.40 |
| 2:D:2:ILE:HD13 | 2:D:195:LEU:HD22 | 2.04 | 0.40 |
| 2:C:171:LEU:HD13 | 2:C:179:ILE:CD1 | 2.49 | 0.40 |
| 1:F:196:LEU:CD2 | 1:F:199:LEU:HD23 | 2.51 | 0.40 |
| 2:G:159:PRO:O | 2:G:192:LEU:HD23 | 2.22 | 0.40 |
| 2:G:51:VAL:HA | 2:G:62:VAL:HG11 | 2.04 | 0.40 |
| 1:E:14:TRP:CE3 | 1:E:17:LEU:HD12 | 2.57 | 0.40 |
| 2:G:19:GLN:HB3 | 2:G:22:ASN:HD21 | 1.86 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 201/217 (93%) | 178 (89%) | 9 (4%) | 14 (7%) | 1 | 22 |
| 1 | B | 201/217 (93%) | 187 (93%) | 3 (2%) | 11 (6%) | 2 | 29 |
| 1 | E | 201/217 (93%) | 180 (90%) | 11 (6%) | 10 (5%) | 3 | 31 |
| 1 | F | 201/217 (93%) | 177 (88%) | 10 (5%) | 14 (7%) | 1 | 22 |
| 2 | C | 341/343 (99%) | 307 (90%) | 19 (6%) | 15 (4%) | 3 | 35 |
| 2 | D | 341/343 (99%) | 323 (95%) | 8 (2%) | 10 (3%) | 6 | 46 |
| 2 | G | 341/343 (99%) | 317 (93%) | 14 (4%) | 10 (3%) | 6 | 46 |
| 2 | H | 341/343 (99%) | 316 (93%) | 14 (4%) | 11 (3%) | 5 | 44 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 2168/2240 (97%) | 1985 (92%) | 88 (4%) | 95 (4%) | 3 35 |

All (95) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 42 | ARG |
| 1 | A | 47 | ILE |
| 1 | A | 48 | ALA |
| 1 | A | 83 | VAL |
| 1 | A | 117 | THR |
| 1 | A | 118 | GLY |
| 1 | A | 131 | MET |
| 1 | B | 43 | PRO |
| 1 | B | 47 | ILE |
| 1 | B | 48 | ALA |
| 1 | B | 68 | PHE |
| 1 | B | 117 | THR |
| 1 | B | 167 | VAL |
| 2 | C | 29 | PRO |
| 2 | C | 109 | LEU |
| 2 | C | 139 | SER |
| 2 | C | 232 | PRO |
| 2 | C | 240 | PHE |
| 2 | C | 275 | GLY |
| 2 | D | 138 | PRO |
| 2 | D | 228 | VAL |
| 2 | D | 230 | SER |
| 2 | D | 232 | PRO |
| 2 | D | 241 | ILE |
| 2 | D | 249 | ILE |
| 1 | E | 47 | ILE |
| 1 | E | 130 | PRO |
| 1 | E | 132 | GLN |
| 1 | F | 36 | VAL |
| 1 | F | 45 | GLN |
| 1 | F | 47 | ILE |
| 1 | F | 51 | LYS |
| 1 | F | 68 | PHE |
| 1 | F | 85 | THR |
| 1 | F | 116 | PRO |
| 1 | F | 128 | ALA |
| 1 | F | 130 | PRO |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 131 | MET |
| 1 | F | 207 | GLY |
| 2 | G | 138 | PRO |
| 2 | G | 190 | LEU |
| 2 | G | 232 | PRO |
| 2 | H | 139 | SER |
| 2 | H | 232 | PRO |
| 2 | H | 250 | PRO |
| 1 | A | 50 | ALA |
| 1 | A | 164 | GLY |
| 1 | A | 207 | GLY |
| 1 | B | 46 | ILE |
| 1 | B | 168 | GLY |
| 2 | C | 23 | ASN |
| 2 | C | 72 | LEU |
| 2 | C | 246 | HIS |
| 2 | C | 279 | ASP |
| 1 | E | 116 | PRO |
| 2 | G | 42 | ALA |
| 2 | H | 6 | ASN |
| 2 | H | 39 | ALA |
| 2 | H | 243 | SER |
| 1 | A | 129 | THR |
| 1 | B | 116 | PRO |
| 1 | B | 126 | MET |
| 1 | B | 130 | PRO |
| 2 | C | 277 | SER |
| 2 | D | 235 | PRO |
| 2 | D | 276 | GLN |
| 1 | E | 43 | PRO |
| 1 | E | 168 | GLY |
| 2 | G | 279 | ASP |
| 2 | G | 299 | ALA |
| 2 | H | 113 | PRO |
| 2 | H | 235 | PRO |
| 2 | H | 299 | ALA |
| 2 | C | 113 | PRO |
| 2 | D | 275 | GLY |
| 1 | E | 33 | PRO |
| 1 | E | 169 | ALA |
| 1 | F | 25 | PHE |
| 1 | F | 118 | GLY |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 257 | LEU |
| 1 | A | 130 | PRO |
| 1 | E | 167 | VAL |
| 2 | G | 275 | GLY |
| 2 | H | 190 | LEU |
| 2 | C | 2 | ILE |
| 1 | F | 167 | VAL |
| 2 | G | 241 | ILE |
| 2 | G | 113 | PRO |
| 1 | A | 116 | PRO |
| 2 | C | 158 | ASN |
| 2 | D | 131 | GLY |
| 1 | A | 44 | GLY |
| 1 | E | 207 | GLY |
| 2 | C | 131 | GLY |
| 2 | G | 14 | GLY |

### 5.3.2 Protein sidechains (i)

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 | 158/172 (92%) | 140 (89%) | 18 (11%) | 7 38 |
| 1 | B | 158/172 (92%) | 145 (92%) | 13 (8%) | 14 53 |
| 1 | E | 158/172 (92%) | 149 (94%) | 9 (6%) | 25 68 |
| 1 | F | 158/172 (92%) | 146 (92%) | 12 (8%) | 16 57 |
| 2 | C | 298/298 (100%) | 269 (90%) | 29 (10%) | 10 46 |
| 2 | D | 298/298 (100%) | 281 (94%) | 17 (6%) | 25 68 |
| 2 | G | 298/298 (100%) | 290 (97%) | 8 (3%) | 52 83 |
| 2 | H | 298/298 (100%) | 289 (97%) | 9 (3%) | 48 81 |
| All | All | 1824/1880 (97%) | 1709 (94%) | 115 (6%) | 22 64 |

All (115) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 8 | LEU |
| 1 | A | 9 | LEU |
| 1 | A | 19 | MET |
| 1 | A | 33 | PRO |
| 1 | A | 36 | VAL |
| 1 | A | 69 | ILE |
| 1 | A | 83 | VAL |
| 1 | A | 86 | SER |
| 1 | A | 95 | PRO |
| 1 | A | 103 | PHE |
| 1 | A | 115 | ILE |
| 1 | A | 117 | THR |
| 1 | A | 129 | THR |
| 1 | A | 140 | PRO |
| 1 | A | 160 | TYR |
| 1 | A | 167 | VAL |
| 1 | A | 175 | ILE |
| 1 | A | 184 | TYR |
| 1 | B | 33 | PRO |
| 1 | B | 34 | VAL |
| 1 | B | 42 | ARG |
| 1 | B | 68 | PHE |
| 1 | B | 70 | ILE |
| 1 | B | 77 | PRO |
| 1 | B | 116 | PRO |
| 1 | B | 129 | THR |
| 1 | B | 137 | VAL |
| 1 | B | 139 | LEU |
| 1 | B | 140 | PRO |
| 1 | B | 175 | ILE |
| 1 | B | 182 | ILE |
| 2 | C | 37 | ILE |
| 2 | C | 46 | THR |
| 2 | C | 52 | ASN |
| 2 | C | 56 | ARG |
| 2 | C | 70 | THR |
| 2 | C | 72 | LEU |
| 2 | C | 73 | SER |
| 2 | C | 90 | HIS |
| 2 | C | 105 | LEU |
| 2 | C | 112 | THR |
| 2 | C | 130 | LEU |
| 2 | C | 137 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 141 | LEU |
| 2 | C | 147 | GLN |
| 2 | C | 151 | ILE |
| 2 | C | 162 | LEU |
| 2 | C | 182 | LEU |
| 2 | C | 193 | THR |
| 2 | C | 200 | GLU |
| 2 | C | 201 | MET |
| 2 | C | 224 | THR |
| 2 | C | 232 | PRO |
| 2 | C | 240 | PHE |
| 2 | C | 241 | ILE |
| 2 | C | 263 | THR |
| 2 | C | 266 | VAL |
| 2 | C | 267 | PRO |
| 2 | C | 276 | GLN |
| 2 | C | 300 | GLN |
| 2 | D | 37 | ILE |
| 2 | D | 44 | LYS |
| 2 | D | 45 | SER |
| 2 | D | 48 | ILE |
| 2 | D | 84 | ILE |
| 2 | D | 112 | THR |
| 2 | D | 124 | LEU |
| 2 | D | 137 | TYR |
| 2 | D | 159 | PRO |
| 2 | D | 223 | ASP |
| 2 | D | 231 | HIS |
| 2 | D | 232 | PRO |
| 2 | D | 235 | PRO |
| 2 | D | 281 | PRO |
| 2 | D | 300 | GLN |
| 2 | D | 314 | THR |
| 2 | D | 323 | THR |
| 1 | E | 19 | MET |
| 1 | E | 46 | ILE |
| 1 | E | 116 | PRO |
| 1 | E | 130 | PRO |
| 1 | E | 135 | ARG |
| 1 | E | 160 | TYR |
| 1 | E | 167 | VAL |
| 1 | E | 185 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 198 | ILE |
| 1 | F | 8 | LEU |
| 1 | F | 42 | ARG |
| 1 | F | 68 | PHE |
| 1 | F | 96 | LEU |
| 1 | F | 116 | PRO |
| 1 | F | 139 | LEU |
| 1 | F | 140 | PRO |
| 1 | F | 152 | ILE |
| 1 | F | 155 | ILE |
| 1 | F | 175 | ILE |
| 1 | F | 198 | ILE |
| 1 | F | 202 | LEU |
| 2 | G | 18 | ILE |
| 2 | G | 40 | SER |
| 2 | G | 52 | ASN |
| 2 | G | 84 | ILE |
| 2 | G | 159 | PRO |
| 2 | G | 210 | CYS |
| 2 | G | 240 | PHE |
| 2 | G | 241 | ILE |
| 2 | H | 2 | ILE |
| 2 | H | 37 | ILE |
| 2 | H | 48 | ILE |
| 2 | H | 52 | ASN |
| 2 | H | 130 | LEU |
| 2 | H | 183 | LEU |
| 2 | H | 235 | PRO |
| 2 | H | 249 | ILE |
| 2 | H | 250 | PRO |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 185 | ASN |
| 1 | A | 190 | ASN |
| 1 | B | 178 | GLN |
| 1 | B | 185 | ASN |
| 1 | B | 190 | ASN |
| 2 | C | 12 | HIS |
| 2 | C | 52 | ASN |
| 2 | C | 147 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 187 | ASN |
| 2 | C | 199 | HIS |
| 2 | C | 242 | GLN |
| 2 | C | 246 | HIS |
| 2 | C | 295 | ASN |
| 2 | C | 300 | GLN |
| 2 | C | 320 | GLN |
| 2 | C | 324 | GLN |
| 2 | D | 111 | ASN |
| 2 | D | 134 | HIS |
| 2 | D | 140 | ASN |
| 2 | D | 147 | GLN |
| 2 | D | 187 | ASN |
| 2 | D | 216 | ASN |
| 2 | D | 238 | GLN |
| 2 | D | 242 | GLN |
| 2 | D | 320 | GLN |
| 2 | D | 334 | HIS |
| 1 | E | 174 | GLN |
| 1 | F | 45 | GLN |
| 1 | F | 110 | ASN |
| 1 | F | 190 | ASN |
| 2 | G | 22 | ASN |
| 2 | G | 52 | ASN |
| 2 | G | 67 | GLN |
| 2 | G | 92 | ASN |
| 2 | G | 102 | ASN |
| 2 | G | 111 | ASN |
| 2 | G | 147 | GLN |
| 2 | G | 242 | GLN |
| 2 | G | 246 | HIS |
| 2 | G | 294 | ASN |
| 2 | G | 295 | ASN |
| 2 | G | 300 | GLN |
| 2 | G | 320 | GLN |
| 2 | H | 52 | ASN |
| 2 | H | 67 | GLN |
| 2 | H | 111 | ASN |
| 2 | H | 147 | GLN |
| 2 | H | 158 | ASN |
| 2 | H | 222 | GLN |
| 2 | H | 242 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 300 | 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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 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, $95^{th}$ 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 | 203/217 (93%) | 0.03 | 7 (3%) 49 34 | 113, 166, 210, 234 | 0 |
| 1 | B | 203/217 (93%) | 0.26 | 16 (7%) 15 9 | 135, 195, 245, 259 | 0 |
| 1 | E | 203/217 (93%) | 0.30 | 16 (7%) 15 9 | 136, 202, 249, 260 | 0 |
| 1 | F | 203/217 (93%) | -0.03 | 5 (2%) 61 45 | 106, 166, 222, 244 | 0 |
| 2 | C | 343/343 (100%) | 0.07 | 11 (3%) 51 35 | 74, 133, 194, 241 | 0 |
| 2 | D | 343/343 (100%) | 0.30 | 24 (6%) 19 11 | 105, 170, 214, 229 | 0 |
| 2 | G | 343/343 (100%) | 1.19 | 93 (27%) 1 1 | 157, 209, 249, 265 | 0 |
| 2 | H | 343/343 (100%) | 0.67 | 49 (14%) 4 3 | 94, 186, 234, 253 | 0 |
| All | All | 2184/2240 (97%) | 0.40 | 221 (10%) 9 6 | 74, 179, 238, 265 | 0 |

All (221) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | G | 214 | ILE | 8.7 |
| 2 | H | 17 | THR | 8.4 |
| 1 | E | 44 | GLY | 6.6 |
| 2 | G | 91 | PHE | 6.5 |
| 1 | B | 52 | LEU | 6.3 |
| 2 | H | 248 | ASP | 6.3 |
| 2 | G | 13 | GLN | 6.2 |
| 2 | G | 343 | VAL | 6.2 |
| 2 | G | 292 | VAL | 6.2 |
| 2 | G | 215 | SER | 5.9 |
| 2 | H | 274 | THR | 5.9 |
| 2 | G | 179 | ILE | 5.7 |
| 2 | G | 246 | HIS | 5.7 |
| 2 | H | 286 | THR | 5.7 |
| 2 | H | 15 | THR | 5.6 |
| 2 | D | 343 | VAL | 5.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 168 | GLY | 5.6 |
| 2 | G | 266 | VAL | 5.6 |
| 2 | G | 83 | GLN | 5.5 |
| 2 | H | 261 | PRO | 5.4 |
| 2 | G | 264 | ASP | 5.3 |
| 2 | G | 121 | VAL | 5.3 |
| 2 | D | 304 | ALA | 5.2 |
| 2 | G | 217 | GLY | 5.0 |
| 2 | G | 130 | LEU | 5.0 |
| 2 | H | 212 | ALA | 4.9 |
| 1 | E | 49 | ASN | 4.8 |
| 2 | H | 333 | HIS | 4.7 |
| 2 | G | 317 | HIS | 4.7 |
| 2 | H | 16 | ARG | 4.7 |
| 2 | H | 310 | GLY | 4.7 |
| 2 | G | 267 | PRO | 4.6 |
| 2 | G | 103 | VAL | 4.6 |
| 1 | B | 51 | LYS | 4.6 |
| 1 | B | 39 | TYR | 4.6 |
| 1 | B | 50 | ALA | 4.6 |
| 2 | H | 309 | PHE | 4.6 |
| 1 | E | 28 | PHE | 4.6 |
| 2 | G | 182 | LEU | 4.6 |
| 2 | G | 263 | THR | 4.5 |
| 2 | G | 176 | THR | 4.5 |
| 2 | G | 316 | MET | 4.5 |
| 1 | A | 51 | LYS | 4.5 |
| 2 | G | 93 | LEU | 4.5 |
| 2 | G | 265 | CYS | 4.4 |
| 2 | G | 135 | ASP | 4.4 |
| 2 | D | 316 | MET | 4.3 |
| 2 | G | 161 | VAL | 4.2 |
| 2 | G | 236 | LEU | 4.2 |
| 2 | H | 293 | ASN | 4.1 |
| 2 | H | 249 | ILE | 4.1 |
| 2 | G | 259 | ALA | 4.0 |
| 2 | D | 263 | THR | 4.0 |
| 1 | A | 184 | TYR | 3.9 |
| 2 | D | 141 | LEU | 3.9 |
| 2 | H | 213 | VAL | 3.9 |
| 1 | E | 50 | ALA | 3.9 |
| 2 | H | 71 | THR | 3.9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | G | 104 | ALA | 3.9 |
| 2 | G | 235 | PRO | 3.9 |
| 2 | C | 71 | THR | 3.7 |
| 2 | G | 100 | PHE | 3.7 |
| 2 | H | 220 | ILE | 3.7 |
| 2 | D | 99 | VAL | 3.7 |
| 2 | G | 80 | ALA | 3.7 |
| 2 | D | 13 | GLN | 3.6 |
| 2 | G | 51 | VAL | 3.6 |
| 2 | H | 40 | SER | 3.5 |
| 2 | D | 39 | ALA | 3.5 |
| 2 | H | 337 | VAL | 3.5 |
| 2 | G | 244 | THR | 3.5 |
| 1 | E | 53 | TYR | 3.4 |
| 2 | G | 15 | THR | 3.4 |
| 2 | G | 122 | THR | 3.4 |
| 1 | B | 84 | GLY | 3.4 |
| 2 | H | 273 | PHE | 3.4 |
| 2 | G | 245 | LEU | 3.4 |
| 1 | E | 10 | VAL | 3.4 |
| 2 | G | 16 | ARG | 3.3 |
| 2 | D | 305 | GLY | 3.3 |
| 2 | G | 102 | ASN | 3.2 |
| 2 | H | 334 | HIS | 3.2 |
| 2 | G | 36 | VAL | 3.2 |
| 1 | E | 52 | LEU | 3.2 |
| 2 | G | 171 | LEU | 3.2 |
| 2 | G | 35 | GLY | 3.2 |
| 2 | H | 214 | ILE | 3.2 |
| 2 | G | 276 | GLN | 3.1 |
| 2 | G | 322 | ASP | 3.1 |
| 2 | D | 130 | LEU | 3.1 |
| 2 | G | 213 | VAL | 3.1 |
| 2 | G | 175 | THR | 3.1 |
| 2 | G | 97 | ARG | 3.1 |
| 2 | G | 268 | MET | 3.1 |
| 2 | H | 294 | ASN | 3.1 |
| 2 | G | 180 | LEU | 3.0 |
| 2 | G | 2 | ILE | 3.0 |
| 2 | H | 242 | GLN | 3.0 |
| 2 | C | 259 | ALA | 3.0 |
| 2 | D | 15 | THR | 3.0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | G | 14 | GLY | 3.0 |
| 1 | B | 128 | ALA | 2.9 |
| 1 | E | 48 | ALA | 2.9 |
| 2 | G | 21 | LEU | 2.9 |
| 1 | B | 49 | ASN | 2.9 |
| 2 | G | 193 | THR | 2.9 |
| 1 | B | 172 | LEU | 2.9 |
| 2 | C | 72 | LEU | 2.9 |
| 2 | D | 100 | PHE | 2.9 |
| 2 | D | 257 | LEU | 2.9 |
| 2 | G | 75 | SER | 2.9 |
| 2 | G | 293 | ASN | 2.8 |
| 1 | B | 81 | VAL | 2.8 |
| 2 | C | 214 | ILE | 2.8 |
| 2 | G | 81 | ARG | 2.8 |
| 2 | G | 146 | LYS | 2.8 |
| 2 | G | 105 | LEU | 2.8 |
| 2 | H | 301 | MET | 2.8 |
| 1 | A | 53 | TYR | 2.8 |
| 2 | G | 328 | ALA | 2.8 |
| 2 | H | 14 | GLY | 2.8 |
| 2 | G | 37 | ILE | 2.8 |
| 2 | H | 342 | TYR | 2.8 |
| 1 | E | 51 | LYS | 2.7 |
| 2 | G | 9 | LYS | 2.7 |
| 2 | H | 321 | GLN | 2.7 |
| 2 | G | 149 | VAL | 2.7 |
| 2 | H | 285 | GLU | 2.7 |
| 2 | G | 50 | CYS | 2.7 |
| 2 | G | 342 | TYR | 2.7 |
| 2 | G | 39 | ALA | 2.7 |
| 2 | G | 200 | GLU | 2.7 |
| 2 | H | 322 | ASP | 2.7 |
| 2 | H | 211 | VAL | 2.6 |
| 2 | H | 72 | LEU | 2.6 |
| 2 | H | 308 | LYS | 2.6 |
| 2 | H | 39 | ALA | 2.6 |
| 2 | C | 20 | ALA | 2.6 |
| 2 | D | 137 | TYR | 2.5 |
| 2 | G | 128 | VAL | 2.5 |
| 2 | H | 56 | ARG | 2.5 |
| 2 | G | 12 | HIS | 2.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | D | 20 | ALA | 2.5 |
| 2 | H | 275 | GLY | 2.5 |
| 1 | E | 43 | PRO | 2.5 |
| 2 | D | 14 | GLY | 2.5 |
| 2 | G | 321 | GLN | 2.5 |
| 2 | C | 268 | MET | 2.5 |
| 2 | G | 287 | ALA | 2.5 |
| 2 | H | 57 | PRO | 2.5 |
| 2 | G | 290 | PHE | 2.4 |
| 1 | B | 85 | THR | 2.4 |
| 2 | C | 19 | GLN | 2.4 |
| 2 | G | 219 | LEU | 2.4 |
| 1 | E | 45 | GLN | 2.4 |
| 2 | H | 18 | ILE | 2.4 |
| 1 | B | 53 | TYR | 2.4 |
| 2 | C | 342 | TYR | 2.4 |
| 2 | D | 265 | CYS | 2.4 |
| 2 | G | 257 | LEU | 2.4 |
| 2 | H | 222 | GLN | 2.4 |
| 2 | D | 258 | GLN | 2.4 |
| 1 | B | 129 | THR | 2.4 |
| 2 | H | 245 | LEU | 2.3 |
| 2 | H | 240 | PHE | 2.3 |
| 2 | G | 241 | ILE | 2.3 |
| 2 | H | 10 | VAL | 2.3 |
| 2 | C | 343 | VAL | 2.3 |
| 2 | G | 256 | ARG | 2.3 |
| 2 | D | 12 | HIS | 2.3 |
| 1 | A | 52 | LEU | 2.3 |
| 2 | G | 20 | ALA | 2.3 |
| 2 | G | 134 | HIS | 2.3 |
| 1 | B | 9 | LEU | 2.3 |
| 1 | E | 47 | ILE | 2.3 |
| 1 | E | 112 | LEU | 2.3 |
| 2 | G | 262 | PHE | 2.3 |
| 2 | G | 329 | TRP | 2.3 |
| 2 | G | 327 | ILE | 2.3 |
| 2 | G | 120 | ARG | 2.3 |
| 2 | G | 197 | ILE | 2.3 |
| 2 | D | 264 | ASP | 2.3 |
| 2 | G | 117 | VAL | 2.3 |
| 2 | H | 250 | PRO | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | G | 192 | LEU | 2.2 |
| 2 | H | 329 | TRP | 2.2 |
| 2 | G | 57 | PRO | 2.2 |
| 2 | G | 233 | LYS | 2.2 |
| 2 | D | 292 | VAL | 2.2 |
| 2 | H | 335 | VAL | 2.2 |
| 1 | E | 9 | LEU | 2.2 |
| 1 | F | 159 | GLY | 2.2 |
| 2 | G | 94 | LEU | 2.2 |
| 1 | E | 189 | MET | 2.2 |
| 1 | E | 41 | THR | 2.2 |
| 2 | G | 325 | ALA | 2.2 |
| 2 | G | 52 | ASN | 2.1 |
| 1 | A | 183 | GLY | 2.1 |
| 2 | C | 39 | ALA | 2.1 |
| 2 | C | 213 | VAL | 2.1 |
| 1 | F | 39 | TYR | 2.1 |
| 2 | G | 337 | VAL | 2.1 |
| 2 | H | 338 | GLU | 2.1 |
| 2 | H | 216 | ASN | 2.1 |
| 2 | G | 340 | LEU | 2.1 |
| 1 | B | 41 | THR | 2.1 |
| 2 | D | 336 | LYS | 2.1 |
| 2 | D | 136 | SER | 2.1 |
| 2 | G | 125 | LEU | 2.1 |
| 2 | H | 157 | SER | 2.1 |
| 2 | G | 195 | LEU | 2.1 |
| 2 | H | 241 | ILE | 2.1 |
| 1 | F | 53 | TYR | 2.1 |
| 1 | A | 54 | ARG | 2.1 |
| 1 | F | 160 | TYR | 2.1 |
| 2 | G | 34 | TYR | 2.1 |
| 2 | H | 302 | ASP | 2.1 |
| 1 | B | 16 | THR | 2.0 |
| 2 | D | 335 | VAL | 2.0 |
| 1 | B | 37 | LEU | 2.0 |
| 1 | F | 54 | ARG | 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

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.