# Full wwPDB EM Validation Report ⓘ

Mar 19, 2024 – 12:42 PM JST

| | | |
|---|---|---|
| PDB ID | : | 5WQ7 |
| EMDB ID | : | EMD-6675 |
| Title | : | CryoEM structure of type II secretion system secretin GspD in E.coli K12 |
| Authors | : | Yan, Z.; Yin, M.; Li, X. |
| Deposited on | : | 2016-11-23 |
| Resolution | : | 3.04 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

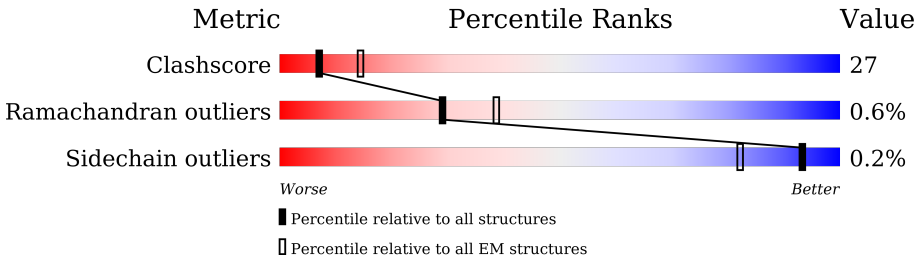
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.04 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 627 | 12% 44% 30% · 25% |
| 1 | B | 627 | 12% 45% 30% · 25% |
| 1 | C | 627 | 11% 44% 31% · 25% |
| 1 | D | 627 | 12% 44% 30% · 25% |
| 1 | E | 627 | 11% 44% 30% · 25% |
| 1 | F | 627 | 12% 44% 30% · 25% |
| 1 | G | 627 | 12% 44% 30% · 25% |
| 1 | H | 627 | 12% 45% 30% · 25% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | I | 627 | 11% 44% 30% 25% |
| 1 | J | 627 | 12% 44% 31% 25% |
| 1 | K | 627 | 12% 45% 30% 25% |
| 1 | L | 627 | 11% 45% 30% 25% |
| 1 | M | 627 | 12% 44% 30% 25% |
| 1 | N | 627 | 12% 44% 30% 25% |
| 1 | O | 627 | 12% 44% 30% 25% |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 54480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

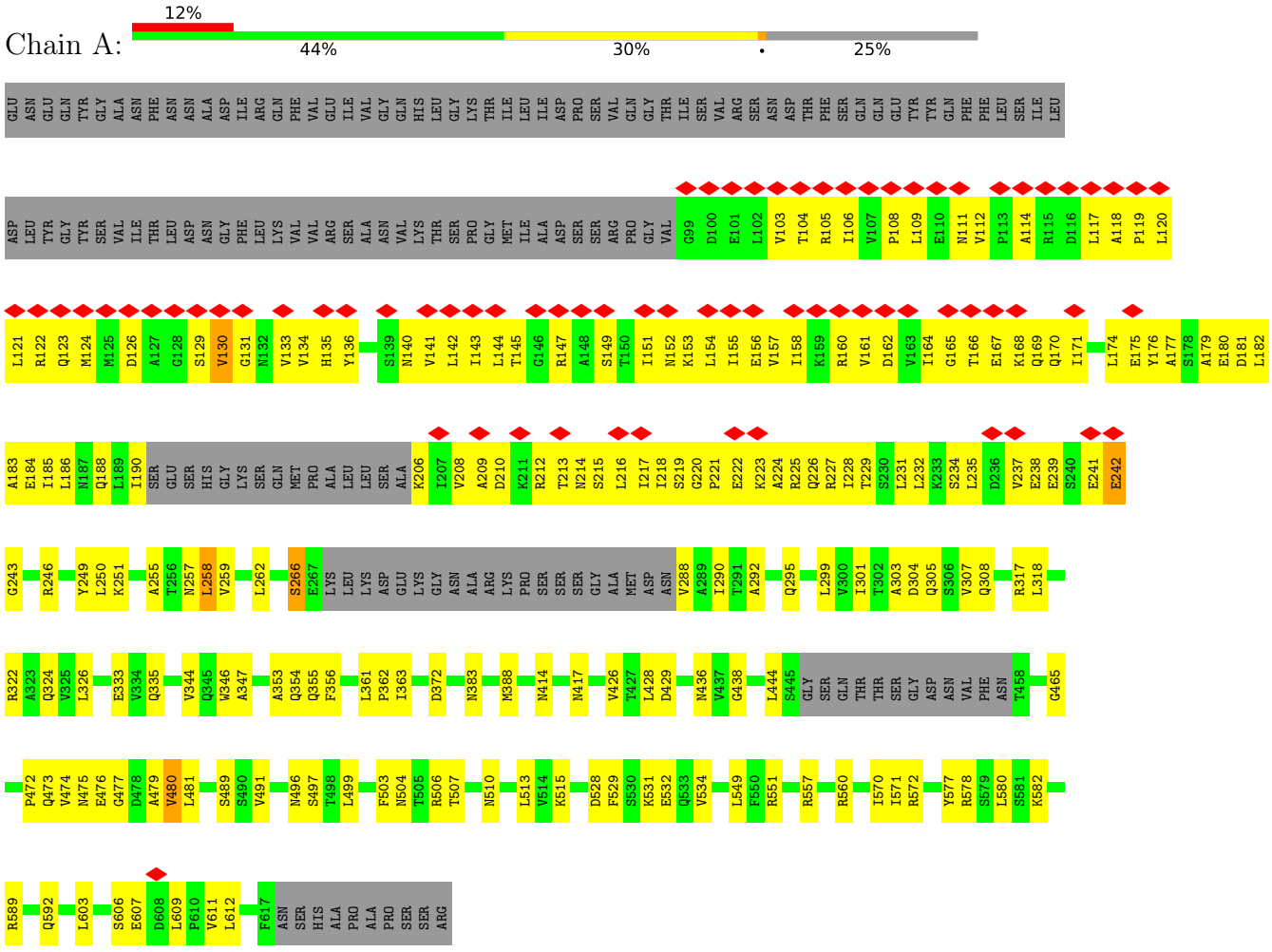
- Molecule 1 is a protein called Putative type II secretion system protein D.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | B | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | C | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | D | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | E | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | F | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | G | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | H | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | I | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | J | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | K | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | L | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | M | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | N | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |
| 1 | O | 472 | Total | C | N | O | S | 0 | 0 |
| | | | 3632 | 2279 | 628 | 720 | 5 | | |

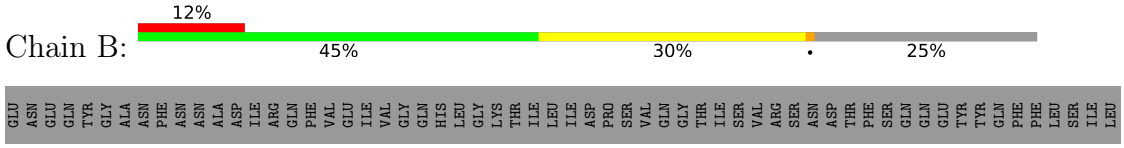
# 3 Residue-property plots (i)

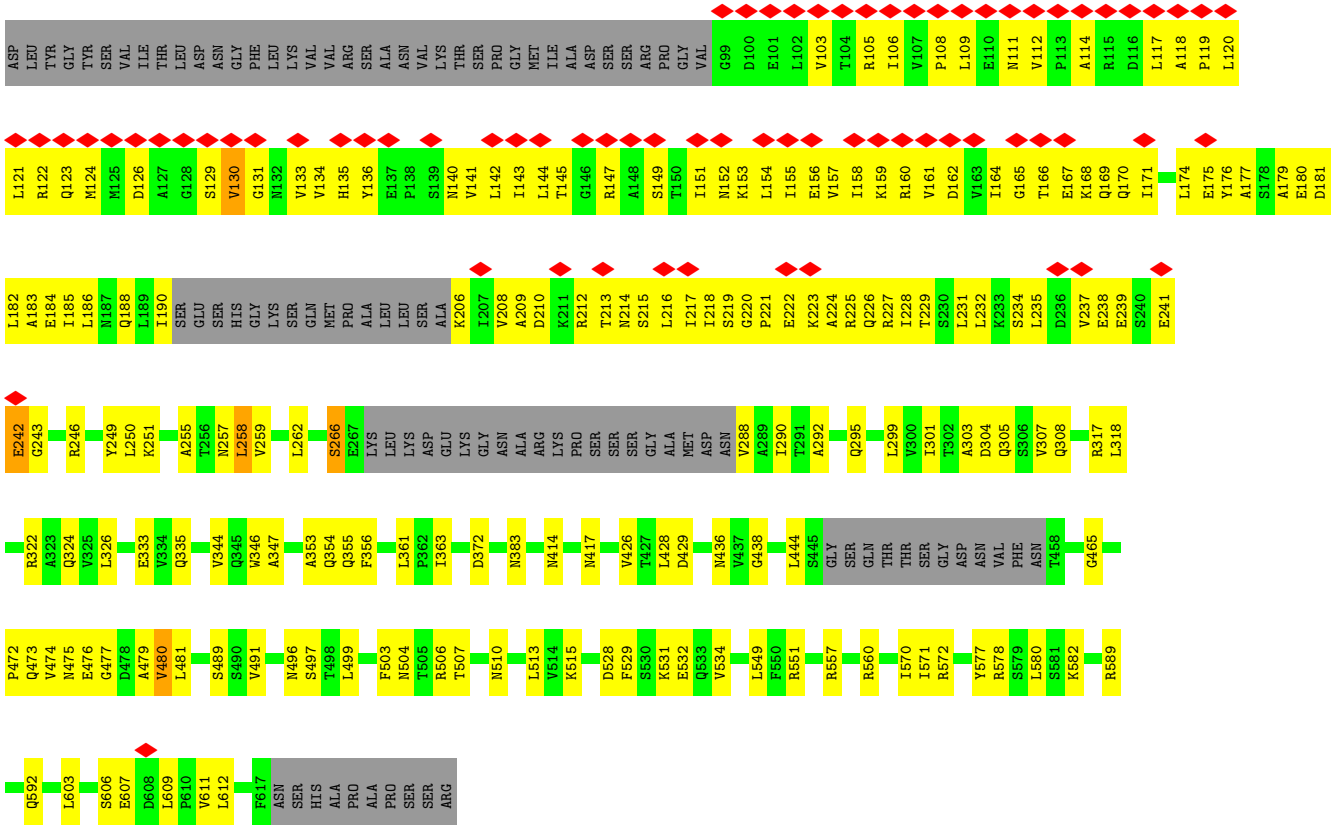
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Putative type II secretion system protein D



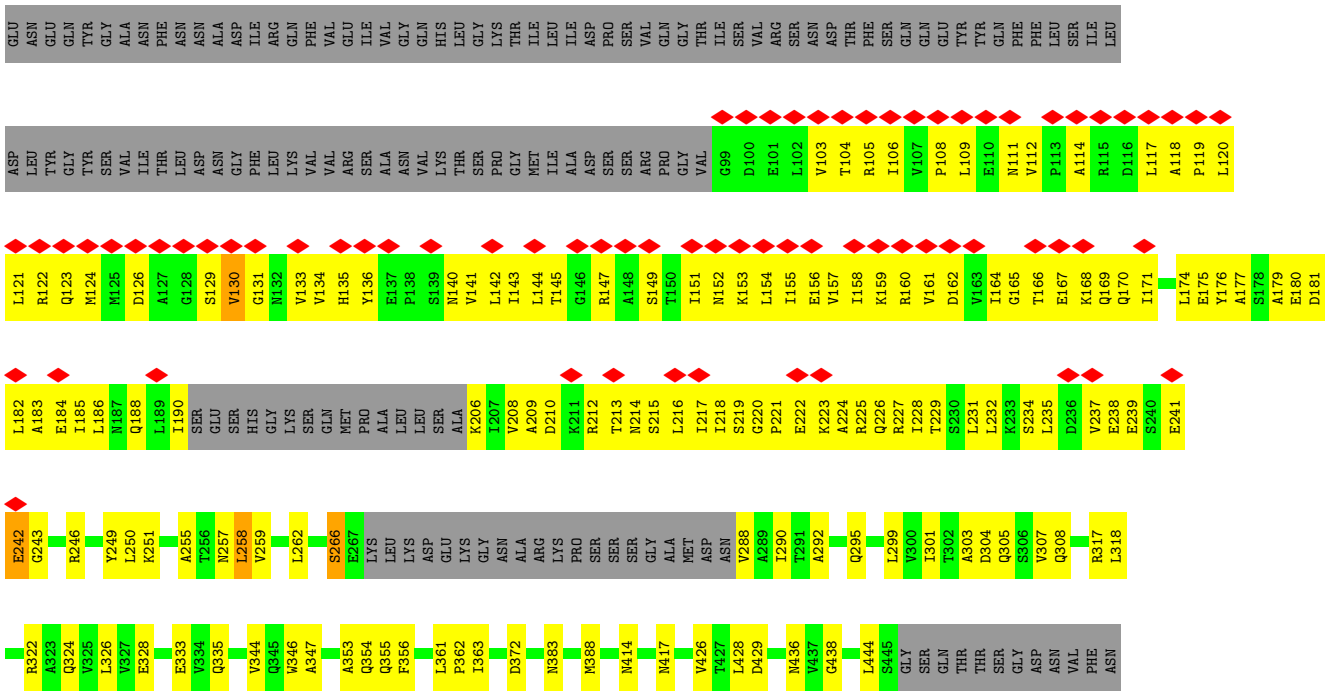

• Molecule 1: Putative type II secretion system protein D

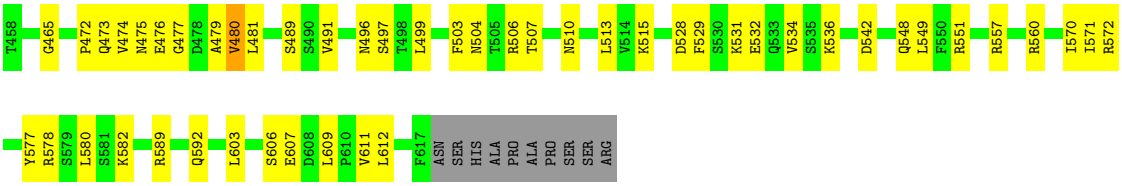




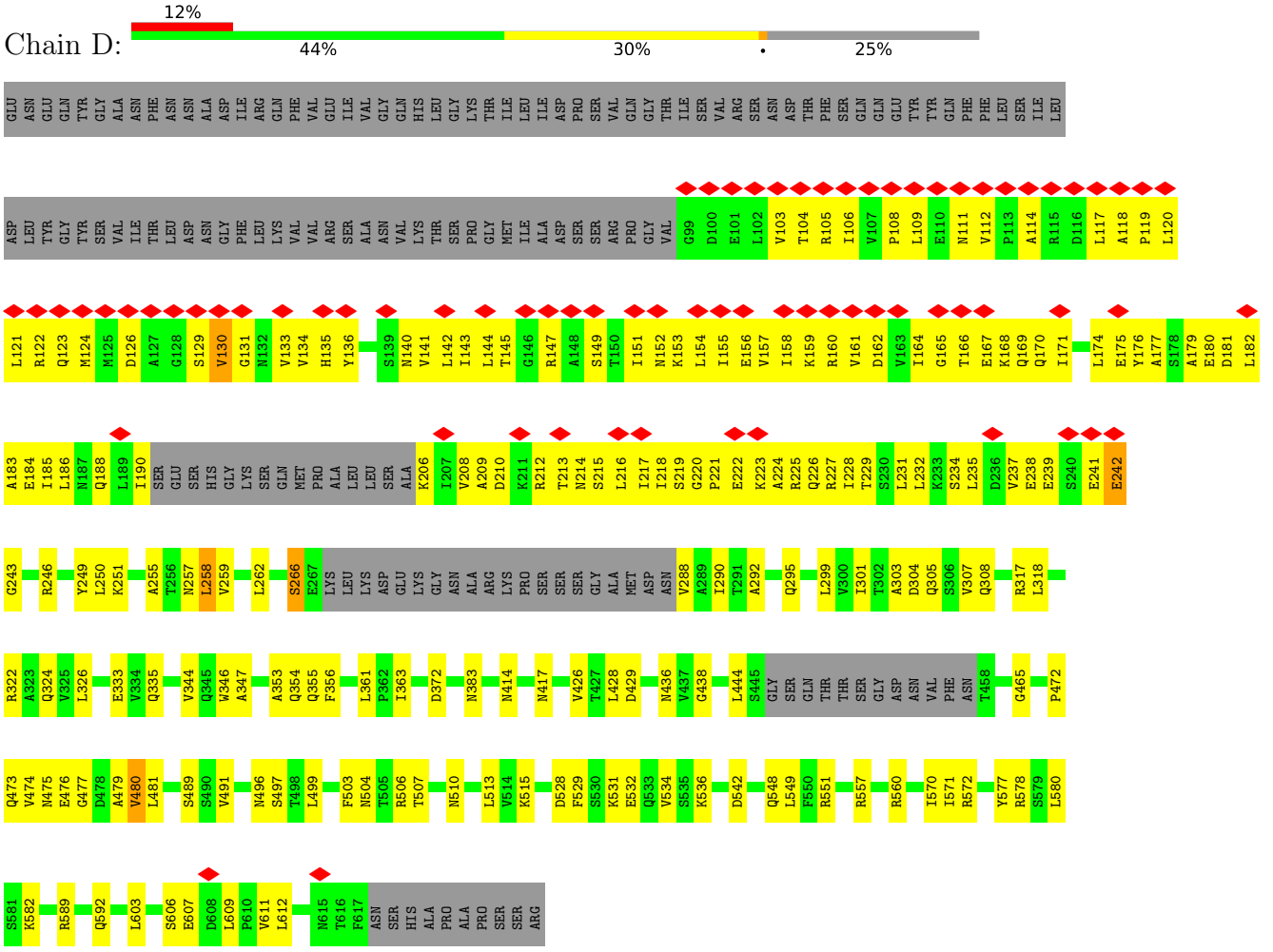
• Molecule 1: Putative type II secretion system protein D

Chain C:

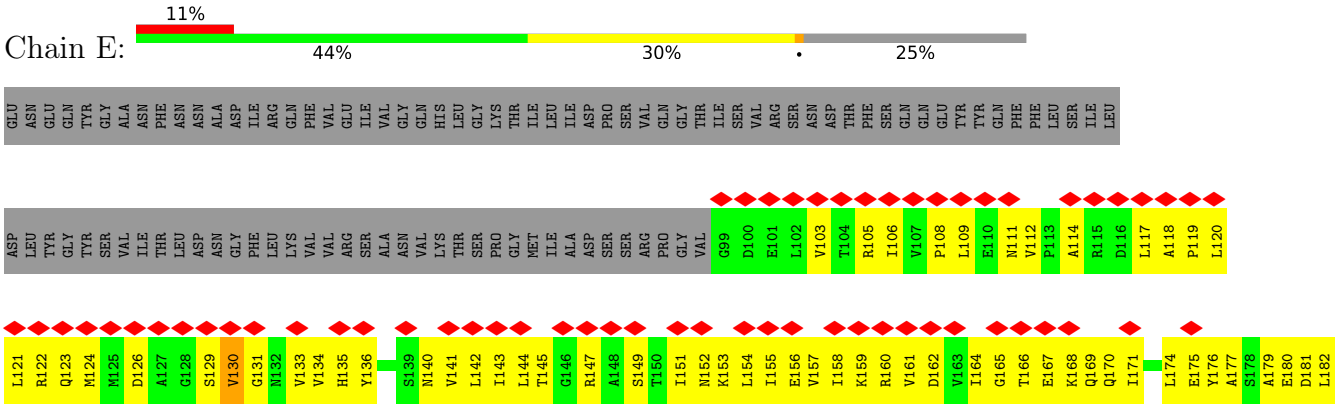



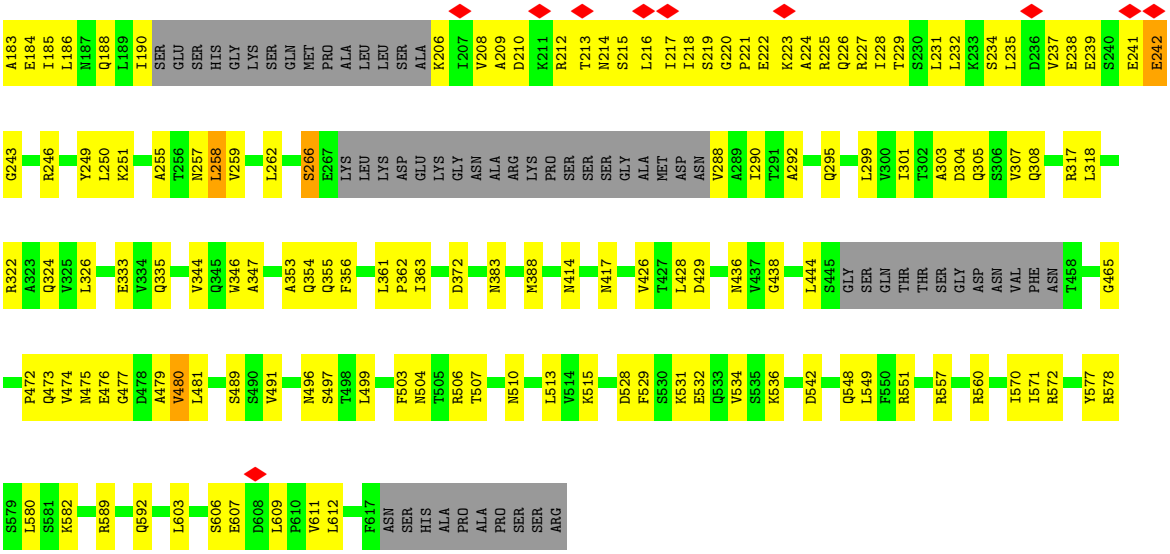



• Molecule 1: Putative type II secretion system protein D

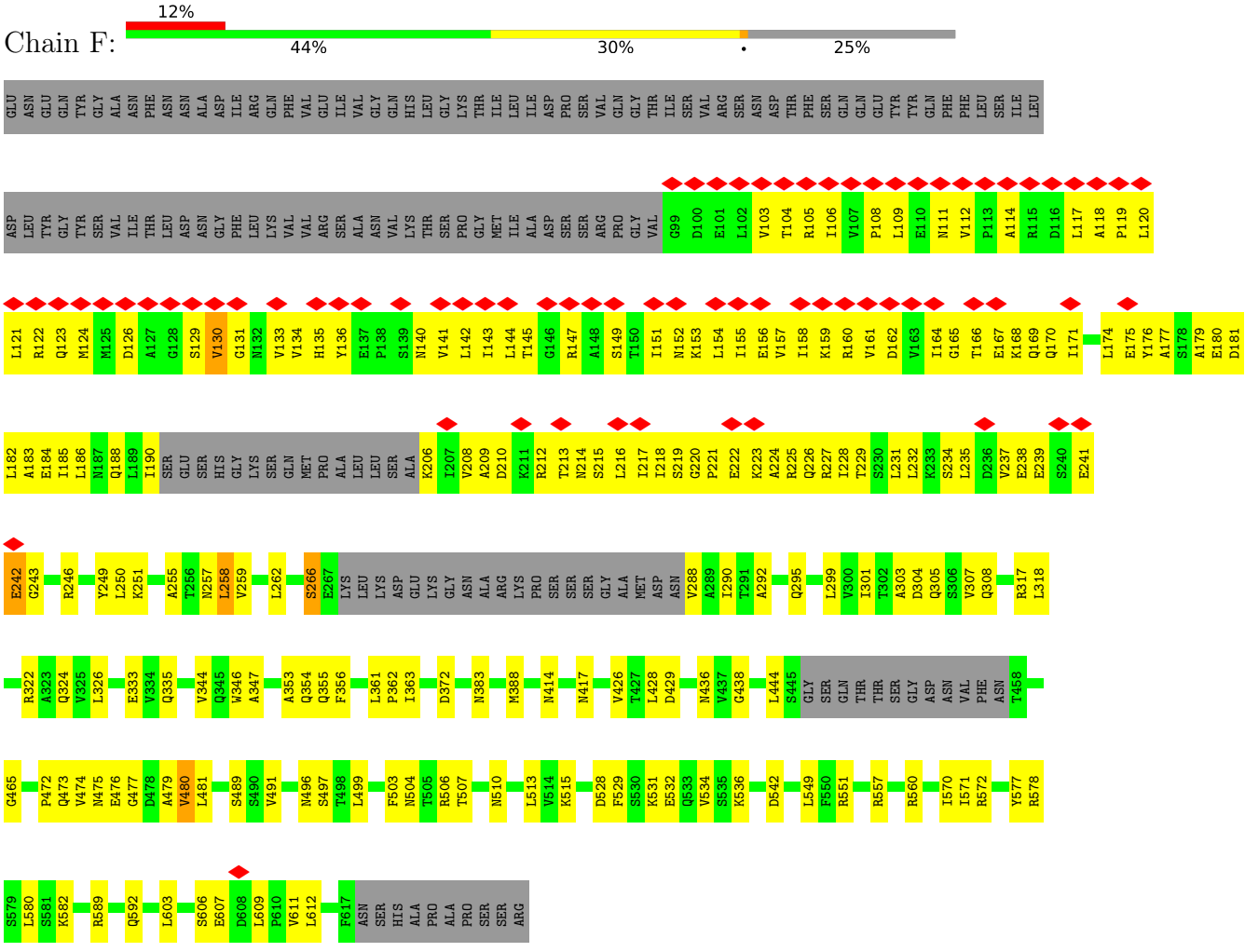



• Molecule 1: Putative type II secretion system protein D



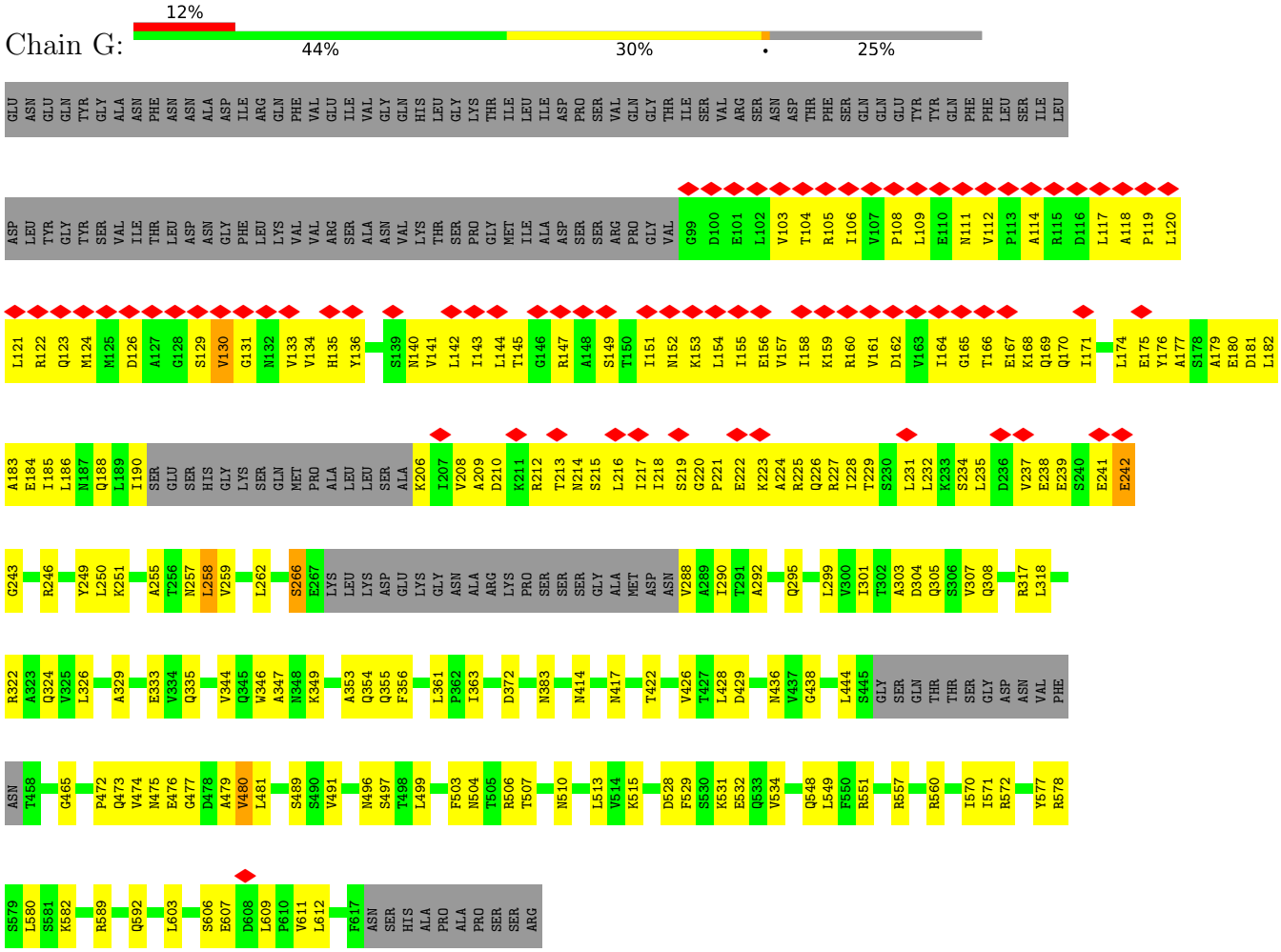


• Molecule 1: Putative type II secretion system protein D



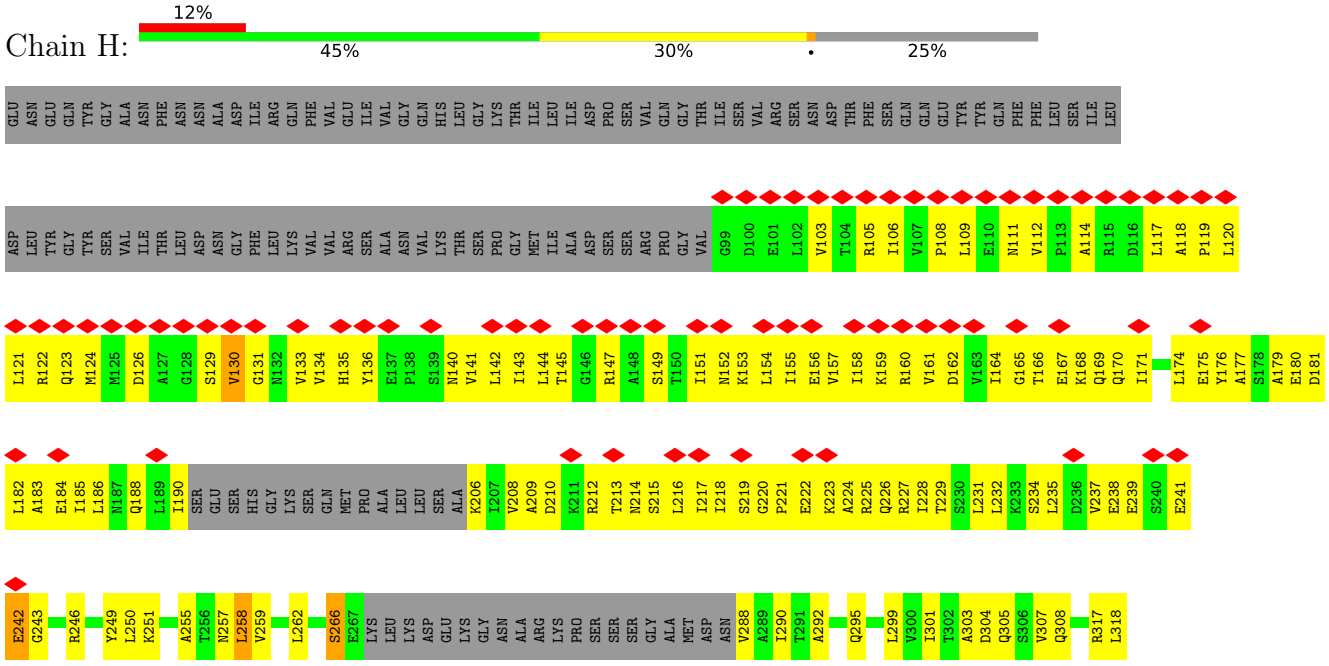

• Molecule 1: Putative type II secretion system protein D

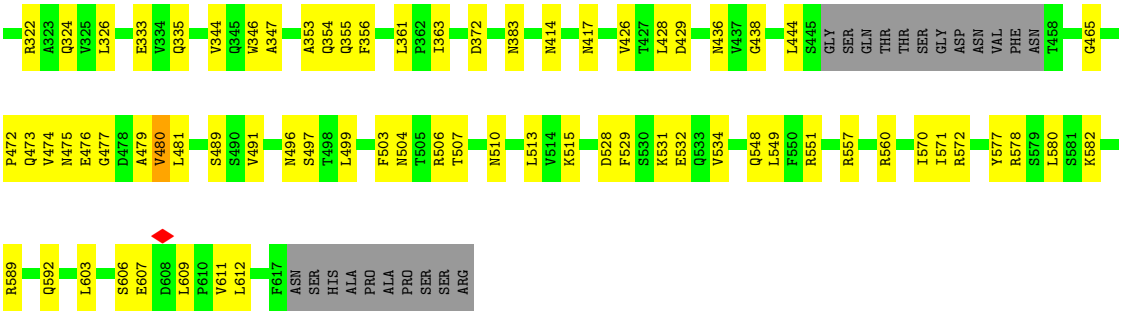
Chain G:



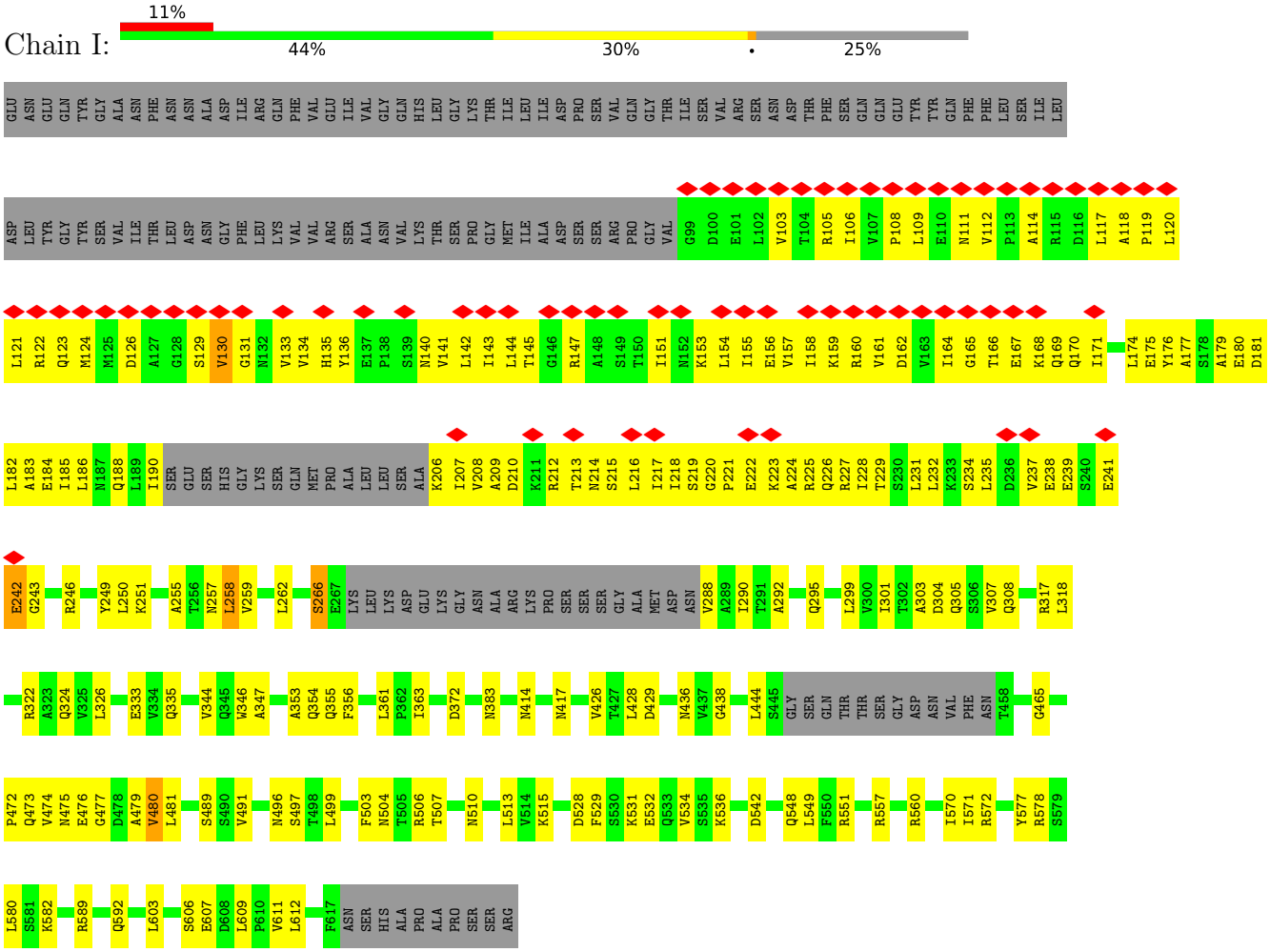

• Molecule 1: Putative type II secretion system protein D

Chain H:

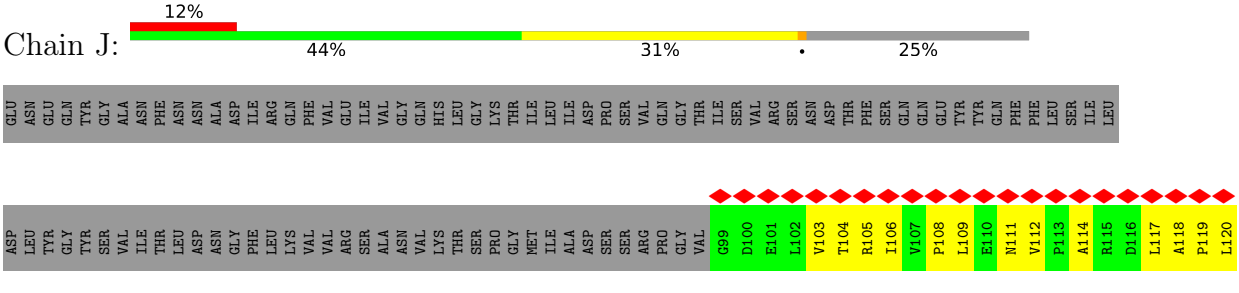


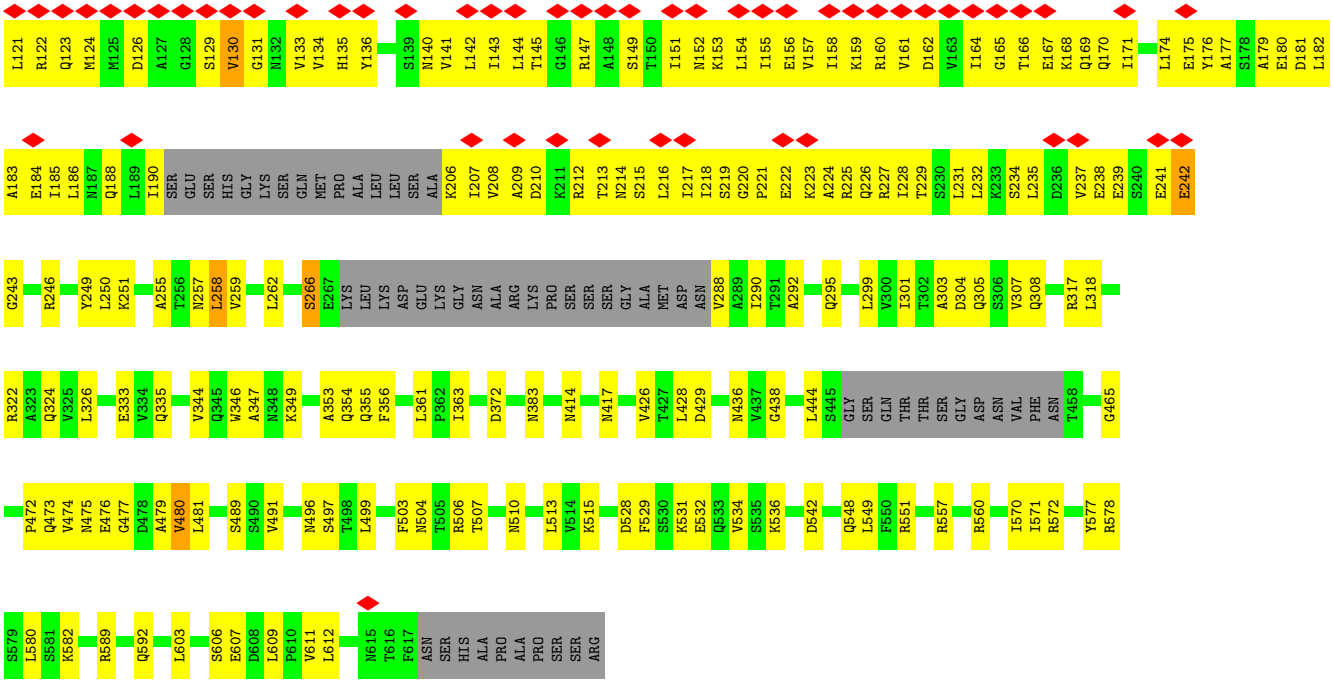


• Molecule 1: Putative type II secretion system protein D



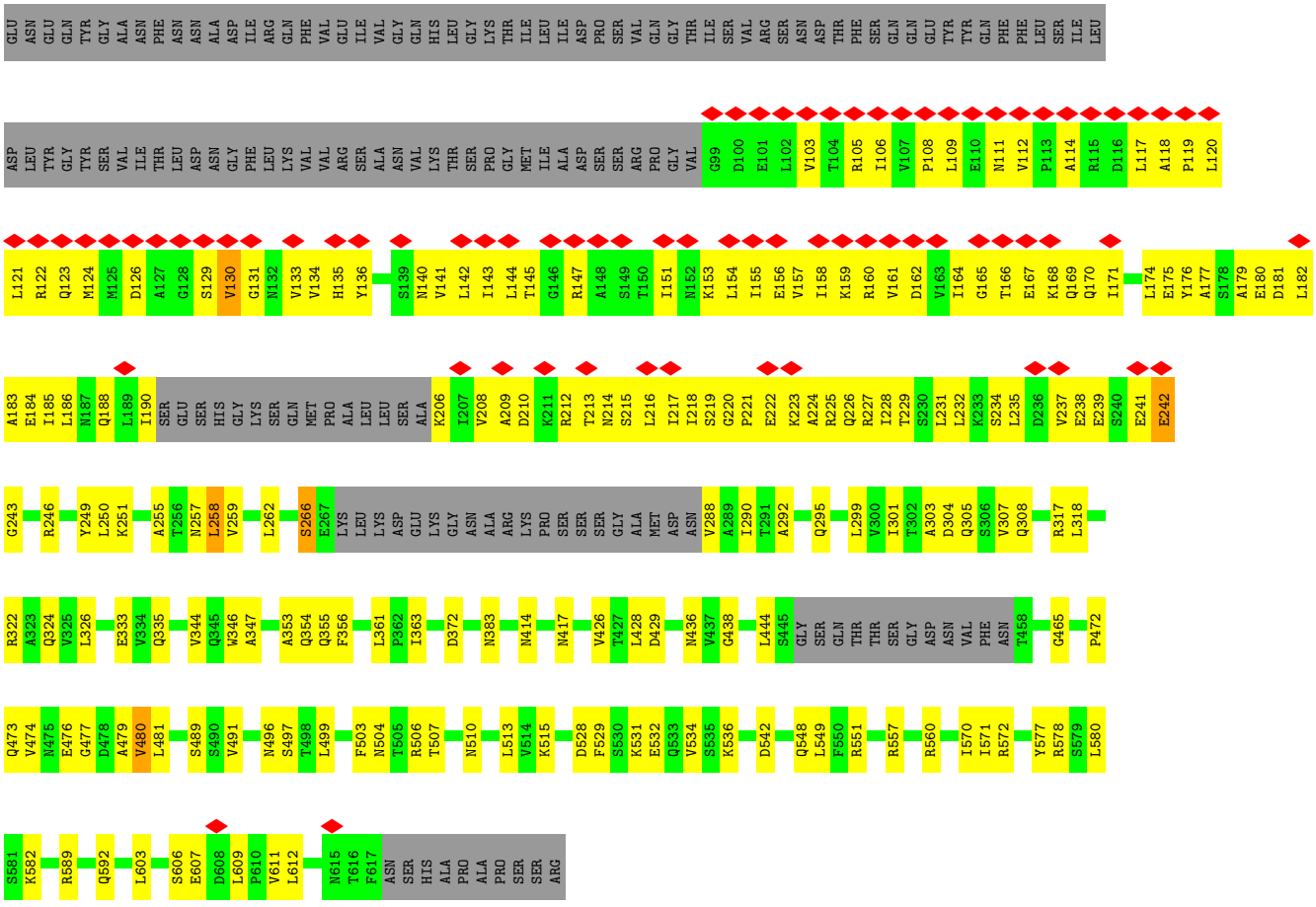

• Molecule 1: Putative type II secretion system protein D





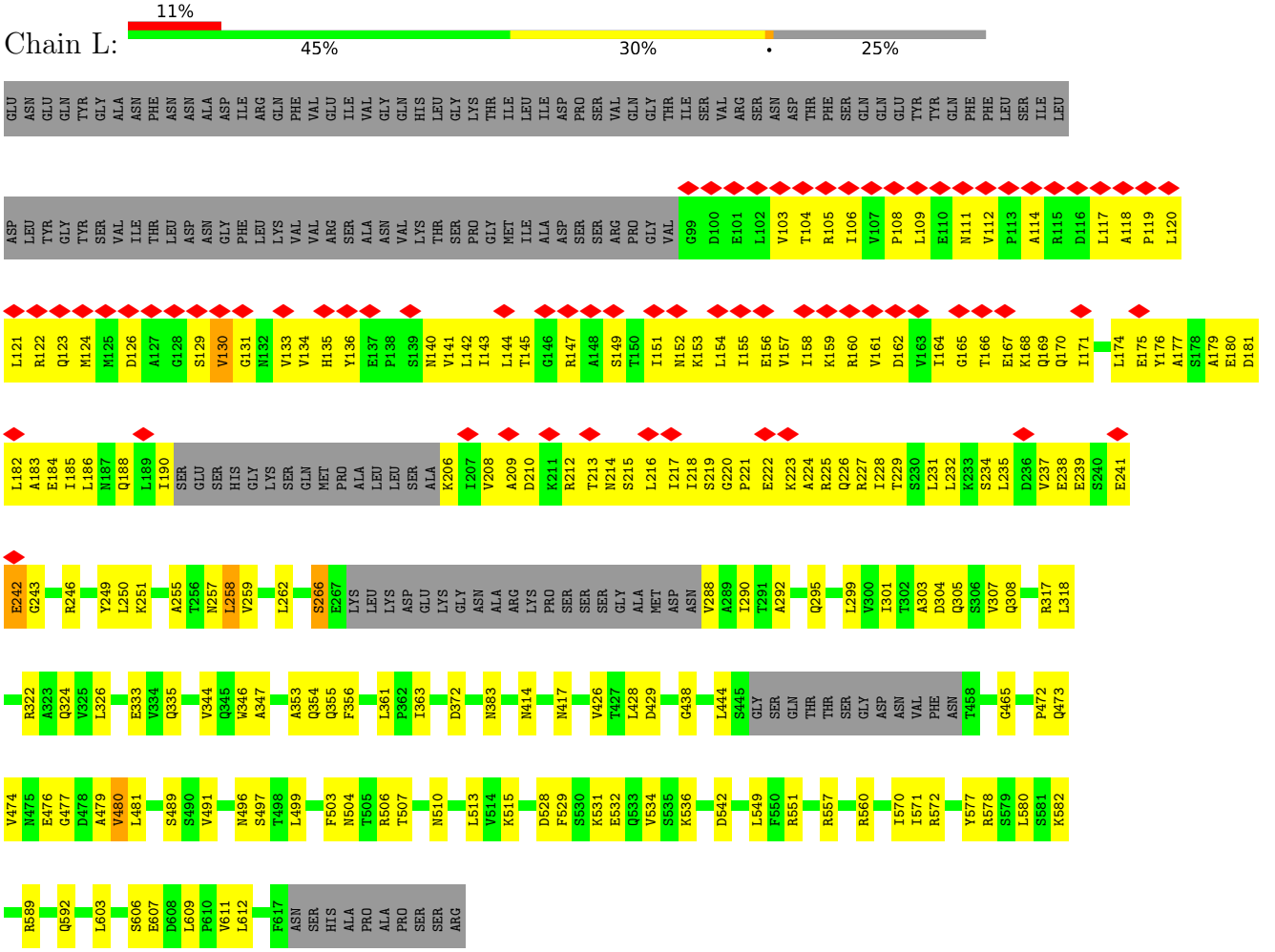

• Molecule 1: Putative type II secretion system protein D

Chain K:

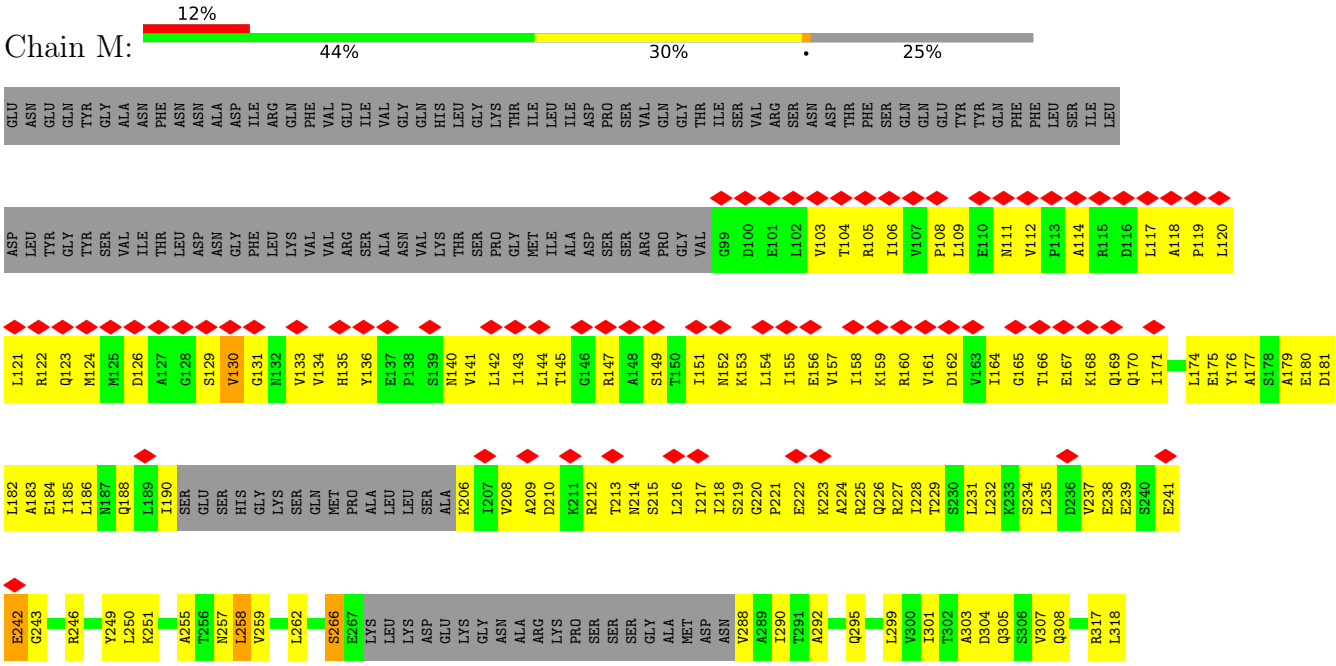
• Molecule 1: Putative type II secretion system protein D

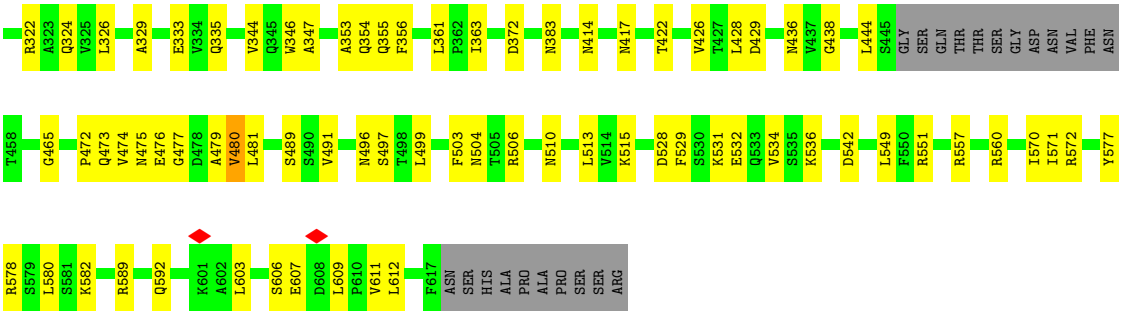
Chain L:



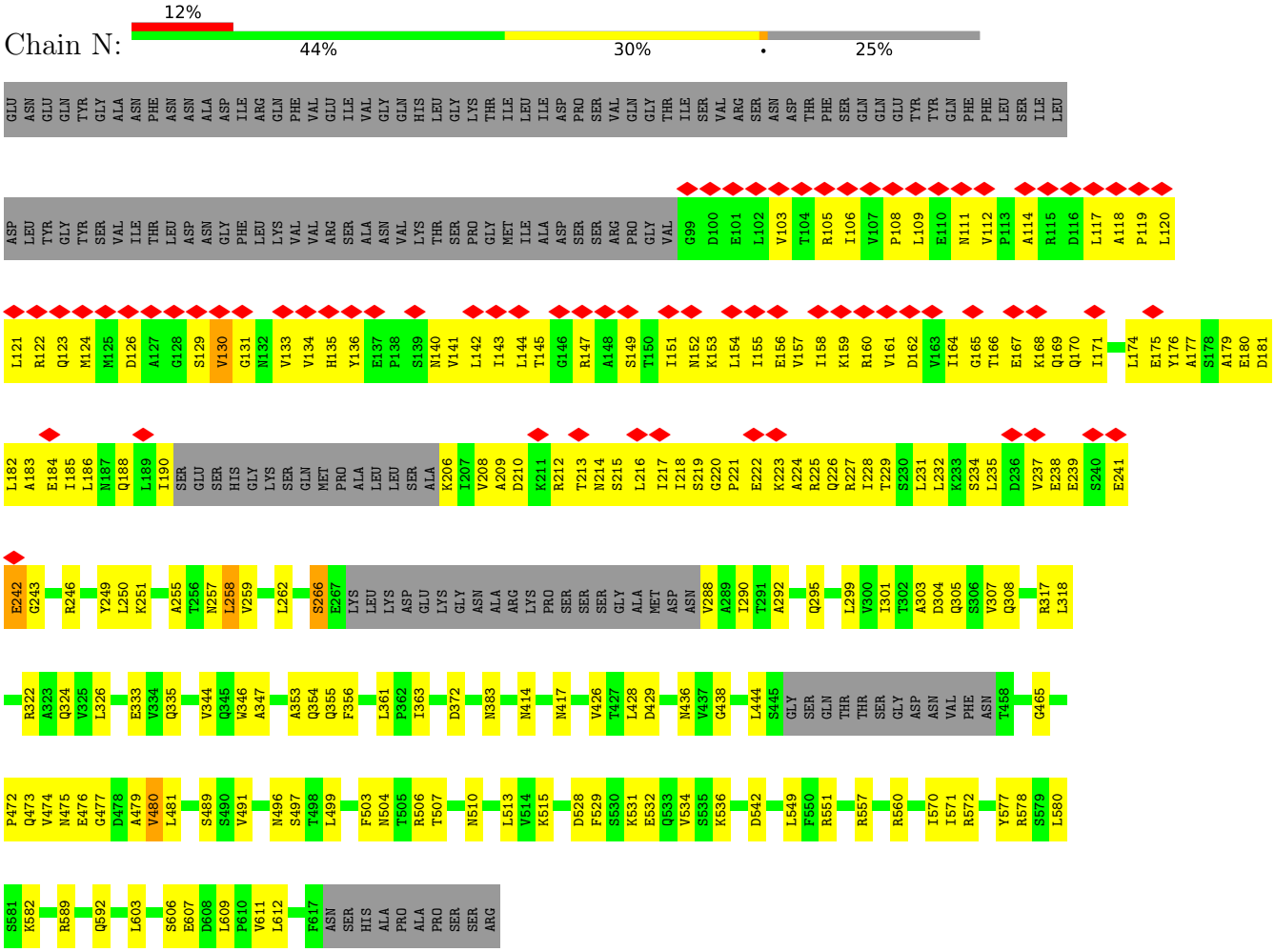

• Molecule 1: Putative type II secretion system protein D

Chain M:

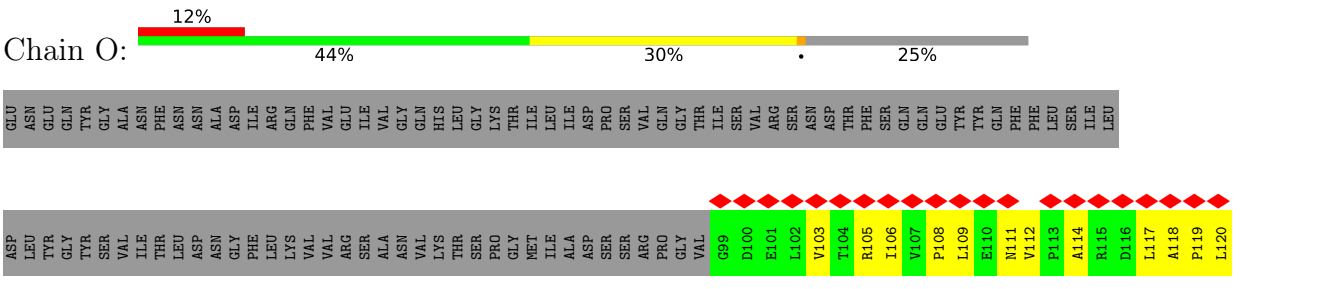


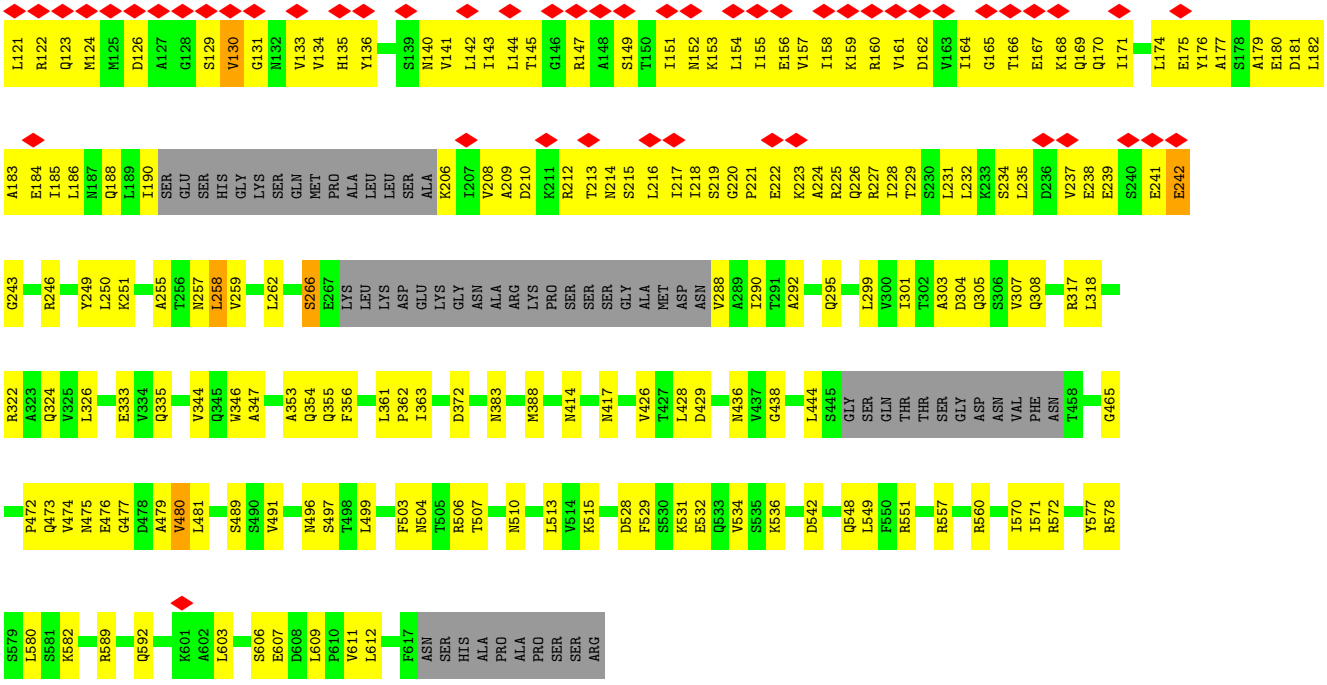


• Molecule 1: Putative type II secretion system protein D




• Molecule 1: Putative type II secretion system protein D




L121 R122 Q123 M124 M125 D126 A127 G128 S129 V130 G131 N132 V133 V134 H135 Y136 S139 N140 V141 L142 I143 L144 T145 G146 R147 A148 S149 T150 I151 N152 K153 L154 I155 E156 V157 I158 K159 R160 V161 D162 V163 I164 G165 T166 E167 K168 Q169 Q170 I171 L174 E175 Y176 A177 S178 A179 E180 D181 L182
A183 E184 I185 L186 N187 Q188 L189 T190 SER GLU SER HIS GLY LYS SER GLN MET PRO ALA LEU LEU SER ALA K206 T207 V208 A209 D210 K211 R212 T213 N214 S215 L216 I217 I218 S219 G220 P221 E222 K223 A224 R225 Q226 R227 I228 T229 S230 L231 L232 K233 S234 L235 D236 V237 E238 E239 S240 E241 E242
G243 R246 Y249 L250 K251 A255 T256 N257 L258 V259 L262 S266 E267 LYS LEU LYS ASP GLU LYS GLY ASN ALA ARG LYS PRO SER SER SER GLY ALA MET ASP ASN V288 A289 I290 T291 A292 Q295 L299 V300 I301 T302 A303 D304 Q305 S306 V307 Q308 R317 L318
R322 A323 Q324 V325 L326 E333 V334 Q335 V344 Q345 W346 A347 A353 Q354 Q355 F356 L361 P362 I363 D372 N383 M388 N414 N417 V426 T427 L428 D429 N436 V437 G438 L444 S445 GLY SER GLN THR THR SER GLY ASP ASN VAL PHE ASN T458 G465
P472 Q473 V474 N475 E476 G477 D478 A479 V480 L481 S489 S490 V491 N496 S497 T498 L499 F503 N504 T505 R506 T507 N510 L513 V514 K515 D528 F529 S530 K531 E532 Q533 V534 S535 K536 D542 Q548 L549 F550 R551 R557 R560 I570 I571 R572 Y577 R578
S579 L580 S581 K582 R589 Q592 K601 A602 L603 S606 E607 D608 L609 P610 V611 L612 F617 ASN SER HIS ALA PRO ALA PRO SER SER ARG

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C15 | Depositor |
| Number of particles used | 30659 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 1.6 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.296 | Depositor |
| Minimum map value | -0.161 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.005 | Depositor |
| Recommended contour level | 0.022 | Depositor |
| Map size (Å) | 501.6, 501.6, 501.6 | wwPDB |
| Map dimensions | 380, 380, 380 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.32, 1.32, 1.32 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | B | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | C | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | D | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | E | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | F | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | G | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | H | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | I | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | J | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | K | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | L | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | M | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | N | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| 1 | O | 0.42 | 0/3673 | 0.59 | 1/4983 (0.0%) |
| All | All | 0.42 | 0/55095 | 0.59 | 15/74745 (0.0%) |

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 | 1 |
| 1 | B | 0 | 1 |
| 1 | C | 0 | 1 |
| 1 | D | 0 | 1 |
| 1 | E | 0 | 1 |
| 1 | F | 0 | 1 |
| 1 | G | 0 | 1 |
| 1 | H | 0 | 1 |
| 1 | I | 0 | 1 |
| 1 | J | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | K | 0 | 1 |
| 1 | L | 0 | 1 |
| 1 | M | 0 | 1 |
| 1 | N | 0 | 1 |
| 1 | O | 0 | 1 |
| All | All | 0 | 15 |

There are no bond length outliers.

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | H | 266 | SER | CB-CA-C | -5.47 | 99.70 | 110.10 |
| 1 | L | 266 | SER | CB-CA-C | -5.47 | 99.70 | 110.10 |
| 1 | B | 266 | SER | CB-CA-C | -5.46 | 99.73 | 110.10 |
| 1 | D | 266 | SER | CB-CA-C | -5.46 | 99.73 | 110.10 |
| 1 | O | 266 | SER | CB-CA-C | -5.45 | 99.74 | 110.10 |
| 1 | K | 266 | SER | CB-CA-C | -5.45 | 99.74 | 110.10 |
| 1 | A | 266 | SER | CB-CA-C | -5.45 | 99.74 | 110.10 |
| 1 | N | 266 | SER | CB-CA-C | -5.45 | 99.75 | 110.10 |
| 1 | E | 266 | SER | CB-CA-C | -5.45 | 99.75 | 110.10 |
| 1 | I | 266 | SER | CB-CA-C | -5.45 | 99.75 | 110.10 |
| 1 | M | 266 | SER | CB-CA-C | -5.44 | 99.76 | 110.10 |
| 1 | F | 266 | SER | CB-CA-C | -5.44 | 99.76 | 110.10 |
| 1 | G | 266 | SER | CB-CA-C | -5.44 | 99.77 | 110.10 |
| 1 | C | 266 | SER | CB-CA-C | -5.44 | 99.77 | 110.10 |
| 1 | J | 266 | SER | CB-CA-C | -5.42 | 99.79 | 110.10 |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 166 | THR | Peptide |
| 1 | B | 166 | THR | Peptide |
| 1 | C | 166 | THR | Peptide |
| 1 | D | 166 | THR | Peptide |
| 1 | E | 166 | THR | Peptide |
| 1 | F | 166 | THR | Peptide |
| 1 | G | 166 | THR | Peptide |
| 1 | H | 166 | THR | Peptide |
| 1 | I | 166 | THR | Peptide |
| 1 | J | 166 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | K | 166 | THR | Peptide |
| 1 | L | 166 | THR | Peptide |
| 1 | M | 166 | THR | Peptide |
| 1 | N | 166 | THR | Peptide |
| 1 | O | 166 | THR | Peptide |

## 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 | 3632 | 0 | 3702 | 225 | 0 |
| 1 | B | 3632 | 0 | 3702 | 226 | 0 |
| 1 | C | 3632 | 0 | 3702 | 227 | 0 |
| 1 | D | 3632 | 0 | 3702 | 226 | 0 |
| 1 | E | 3632 | 0 | 3702 | 224 | 0 |
| 1 | F | 3632 | 0 | 3702 | 225 | 0 |
| 1 | G | 3632 | 0 | 3702 | 227 | 0 |
| 1 | H | 3632 | 0 | 3702 | 224 | 0 |
| 1 | I | 3632 | 0 | 3702 | 228 | 0 |
| 1 | J | 3632 | 0 | 3702 | 233 | 0 |
| 1 | K | 3632 | 0 | 3702 | 224 | 0 |
| 1 | L | 3632 | 0 | 3702 | 223 | 0 |
| 1 | M | 3632 | 0 | 3702 | 227 | 0 |
| 1 | N | 3632 | 0 | 3702 | 227 | 0 |
| 1 | O | 3632 | 0 | 3702 | 227 | 0 |
| All | All | 54480 | 0 | 55530 | 2956 | 0 |

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

All (2956) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:210:ASP:O | 1:B:214:ASN:HA | 1.50 | 1.11 |
| 1:E:210:ASP:O | 1:E:214:ASN:HA | 1.50 | 1.11 |
| 1:H:210:ASP:O | 1:H:214:ASN:HA | 1.50 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:210:ASP:O | 1:A:214:ASN:HA | 1.50 | 1.11 |
| 1:I:210:ASP:O | 1:I:214:ASN:HA | 1.50 | 1.11 |
| 1:C:210:ASP:O | 1:C:214:ASN:HA | 1.50 | 1.11 |
| 1:G:210:ASP:O | 1:G:214:ASN:HA | 1.50 | 1.11 |
| 1:F:210:ASP:O | 1:F:214:ASN:HA | 1.50 | 1.11 |
| 1:J:210:ASP:O | 1:J:214:ASN:HA | 1.50 | 1.10 |
| 1:O:210:ASP:O | 1:O:214:ASN:HA | 1.51 | 1.10 |
| 1:D:210:ASP:O | 1:D:214:ASN:HA | 1.50 | 1.10 |
| 1:N:210:ASP:O | 1:N:214:ASN:HA | 1.50 | 1.09 |
| 1:K:210:ASP:O | 1:K:214:ASN:HA | 1.50 | 1.09 |
| 1:M:210:ASP:O | 1:M:214:ASN:HA | 1.50 | 1.08 |
| 1:L:210:ASP:O | 1:L:214:ASN:HA | 1.50 | 1.07 |
| 1:D:333:GLU:OE1 | 1:D:506:ARG:NH1 | 1.90 | 1.05 |
| 1:H:333:GLU:OE1 | 1:H:506:ARG:NH1 | 1.90 | 1.05 |
| 1:L:333:GLU:OE1 | 1:L:506:ARG:NH1 | 1.90 | 1.05 |
| 1:M:333:GLU:OE1 | 1:M:506:ARG:NH1 | 1.90 | 1.05 |
| 1:B:333:GLU:OE1 | 1:B:506:ARG:NH1 | 1.90 | 1.04 |
| 1:I:333:GLU:OE1 | 1:I:506:ARG:NH1 | 1.90 | 1.04 |
| 1:A:333:GLU:OE1 | 1:A:506:ARG:NH1 | 1.90 | 1.04 |
| 1:C:333:GLU:OE1 | 1:C:506:ARG:NH1 | 1.90 | 1.03 |
| 1:F:333:GLU:OE1 | 1:F:506:ARG:NH1 | 1.90 | 1.03 |
| 1:E:333:GLU:OE1 | 1:E:506:ARG:NH1 | 1.90 | 1.03 |
| 1:G:333:GLU:OE1 | 1:G:506:ARG:NH1 | 1.90 | 1.03 |
| 1:J:333:GLU:OE1 | 1:J:506:ARG:NH1 | 1.90 | 1.03 |
| 1:K:333:GLU:OE1 | 1:K:506:ARG:NH1 | 1.90 | 1.03 |
| 1:N:333:GLU:OE1 | 1:N:506:ARG:NH1 | 1.90 | 1.03 |
| 1:O:333:GLU:OE1 | 1:O:506:ARG:NH1 | 1.90 | 1.03 |
| 1:D:119:PRO:O | 1:D:123:GLN:HB2 | 1.65 | 0.97 |
| 1:E:119:PRO:O | 1:E:123:GLN:HB2 | 1.65 | 0.97 |
| 1:C:119:PRO:O | 1:C:123:GLN:HB2 | 1.65 | 0.96 |
| 1:J:119:PRO:O | 1:J:123:GLN:HB2 | 1.65 | 0.96 |
| 1:I:119:PRO:O | 1:I:123:GLN:HB2 | 1.65 | 0.96 |
| 1:A:119:PRO:O | 1:A:123:GLN:HB2 | 1.65 | 0.96 |
| 1:F:119:PRO:O | 1:F:123:GLN:HB2 | 1.65 | 0.96 |
| 1:K:119:PRO:O | 1:K:123:GLN:HB2 | 1.65 | 0.95 |
| 1:O:119:PRO:O | 1:O:123:GLN:HB2 | 1.65 | 0.95 |
| 1:B:119:PRO:O | 1:B:123:GLN:HB2 | 1.65 | 0.95 |
| 1:H:119:PRO:O | 1:H:123:GLN:HB2 | 1.65 | 0.95 |
| 1:K:212:ARG:HH22 | 1:L:177:ALA:HB1 | 1.32 | 0.95 |
| 1:G:119:PRO:O | 1:G:123:GLN:HB2 | 1.65 | 0.95 |
| 1:N:119:PRO:O | 1:N:123:GLN:HB2 | 1.65 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:212:ARG:HH22 | 1:I:177:ALA:HB1 | 1.31 | 0.94 |
| 1:N:212:ARG:HH22 | 1:O:177:ALA:HB1 | 1.32 | 0.94 |
| 1:L:119:PRO:O | 1:L:123:GLN:HB2 | 1.65 | 0.94 |
| 1:M:119:PRO:O | 1:M:123:GLN:HB2 | 1.65 | 0.94 |
| 1:A:218:ILE:HG12 | 1:A:228:ILE:HG21 | 1.49 | 0.94 |
| 1:L:212:ARG:HH22 | 1:M:177:ALA:HB1 | 1.32 | 0.94 |
| 1:O:218:ILE:HG12 | 1:O:228:ILE:HG21 | 1.49 | 0.94 |
| 1:I:212:ARG:HH22 | 1:J:177:ALA:HB1 | 1.31 | 0.94 |
| 1:B:218:ILE:HG12 | 1:B:228:ILE:HG21 | 1.49 | 0.93 |
| 1:N:218:ILE:HG12 | 1:N:228:ILE:HG21 | 1.49 | 0.93 |
| 1:H:218:ILE:HG12 | 1:H:228:ILE:HG21 | 1.49 | 0.93 |
| 1:I:218:ILE:HG12 | 1:I:228:ILE:HG21 | 1.49 | 0.93 |
| 1:J:212:ARG:HH22 | 1:K:177:ALA:HB1 | 1.32 | 0.93 |
| 1:G:218:ILE:HG12 | 1:G:228:ILE:HG21 | 1.49 | 0.93 |
| 1:C:218:ILE:HG12 | 1:C:228:ILE:HG21 | 1.49 | 0.93 |
| 1:M:212:ARG:HH22 | 1:N:177:ALA:HB1 | 1.31 | 0.93 |
| 1:A:177:ALA:HB1 | 1:O:212:ARG:HH22 | 1.32 | 0.93 |
| 1:J:218:ILE:HG12 | 1:J:228:ILE:HG21 | 1.49 | 0.93 |
| 1:B:212:ARG:HH22 | 1:C:177:ALA:HB1 | 1.32 | 0.92 |
| 1:M:218:ILE:HG12 | 1:M:228:ILE:HG21 | 1.49 | 0.92 |
| 1:E:212:ARG:HH22 | 1:F:177:ALA:HB1 | 1.32 | 0.92 |
| 1:F:218:ILE:HG12 | 1:F:228:ILE:HG21 | 1.49 | 0.92 |
| 1:G:212:ARG:HH22 | 1:H:177:ALA:HB1 | 1.32 | 0.92 |
| 1:F:212:ARG:HH22 | 1:G:177:ALA:HB1 | 1.32 | 0.92 |
| 1:D:218:ILE:HG12 | 1:D:228:ILE:HG21 | 1.49 | 0.92 |
| 1:L:218:ILE:HG12 | 1:L:228:ILE:HG21 | 1.49 | 0.91 |
| 1:A:212:ARG:HH22 | 1:B:177:ALA:HB1 | 1.31 | 0.91 |
| 1:K:218:ILE:HG12 | 1:K:228:ILE:HG21 | 1.49 | 0.91 |
| 1:C:212:ARG:HH22 | 1:D:177:ALA:HB1 | 1.32 | 0.91 |
| 1:E:218:ILE:HG12 | 1:E:228:ILE:HG21 | 1.49 | 0.91 |
| 1:D:212:ARG:HH22 | 1:E:177:ALA:HB1 | 1.31 | 0.90 |
| 1:N:210:ASP:OD2 | 1:N:213:THR:OG1 | 1.91 | 0.89 |
| 1:J:210:ASP:OD2 | 1:J:213:THR:OG1 | 1.92 | 0.88 |
| 1:C:109:LEU:O | 1:C:140:ASN:ND2 | 2.07 | 0.88 |
| 1:K:210:ASP:OD2 | 1:K:213:THR:OG1 | 1.91 | 0.88 |
| 1:I:109:LEU:O | 1:I:140:ASN:ND2 | 2.07 | 0.88 |
| 1:B:109:LEU:O | 1:B:140:ASN:ND2 | 2.07 | 0.88 |
| 1:E:109:LEU:O | 1:E:140:ASN:ND2 | 2.07 | 0.88 |
| 1:G:109:LEU:O | 1:G:140:ASN:ND2 | 2.07 | 0.88 |
| 1:F:109:LEU:O | 1:F:140:ASN:ND2 | 2.07 | 0.88 |
| 1:M:210:ASP:OD2 | 1:M:213:THR:OG1 | 1.91 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:210:ASP:OD2 | 1:O:213:THR:OG1 | 1.91 | 0.88 |
| 1:A:109:LEU:O | 1:A:140:ASN:ND2 | 2.07 | 0.88 |
| 1:G:210:ASP:OD2 | 1:G:213:THR:OG1 | 1.91 | 0.88 |
| 1:J:109:LEU:O | 1:J:140:ASN:ND2 | 2.07 | 0.88 |
| 1:B:210:ASP:OD2 | 1:B:213:THR:OG1 | 1.91 | 0.87 |
| 1:H:109:LEU:O | 1:H:140:ASN:ND2 | 2.07 | 0.87 |
| 1:I:210:ASP:OD2 | 1:I:213:THR:OG1 | 1.91 | 0.87 |
| 1:C:210:ASP:OD2 | 1:C:213:THR:OG1 | 1.92 | 0.87 |
| 1:K:109:LEU:O | 1:K:140:ASN:ND2 | 2.07 | 0.87 |
| 1:M:109:LEU:O | 1:M:140:ASN:ND2 | 2.07 | 0.87 |
| 1:F:210:ASP:OD2 | 1:F:213:THR:OG1 | 1.91 | 0.87 |
| 1:D:109:LEU:O | 1:D:140:ASN:ND2 | 2.07 | 0.87 |
| 1:H:210:ASP:OD2 | 1:H:213:THR:OG1 | 1.91 | 0.87 |
| 1:N:109:LEU:O | 1:N:140:ASN:ND2 | 2.07 | 0.87 |
| 1:L:109:LEU:O | 1:L:140:ASN:ND2 | 2.07 | 0.87 |
| 1:L:210:ASP:OD2 | 1:L:213:THR:OG1 | 1.92 | 0.87 |
| 1:A:210:ASP:OD2 | 1:A:213:THR:OG1 | 1.91 | 0.86 |
| 1:O:109:LEU:O | 1:O:140:ASN:ND2 | 2.07 | 0.86 |
| 1:D:210:ASP:OD2 | 1:D:213:THR:OG1 | 1.91 | 0.86 |
| 1:O:206:LYS:N | 1:O:219:SER:HG | 1.74 | 0.86 |
| 1:L:206:LYS:N | 1:L:219:SER:HG | 1.74 | 0.86 |
| 1:F:242:GLU:CG | 1:F:243:GLY:H | 1.89 | 0.86 |
| 1:J:206:LYS:N | 1:J:219:SER:HG | 1.74 | 0.86 |
| 1:K:242:GLU:CG | 1:K:243:GLY:H | 1.89 | 0.86 |
| 1:M:242:GLU:CG | 1:M:243:GLY:H | 1.89 | 0.86 |
| 1:M:206:LYS:N | 1:M:219:SER:HG | 1.74 | 0.85 |
| 1:D:242:GLU:CG | 1:D:243:GLY:H | 1.89 | 0.85 |
| 1:E:210:ASP:OD2 | 1:E:213:THR:OG1 | 1.92 | 0.85 |
| 1:G:206:LYS:N | 1:G:219:SER:HG | 1.74 | 0.85 |
| 1:H:242:GLU:CG | 1:H:243:GLY:H | 1.89 | 0.85 |
| 1:I:206:LYS:N | 1:I:219:SER:HG | 1.74 | 0.85 |
| 1:A:206:LYS:N | 1:A:219:SER:HG | 1.75 | 0.85 |
| 1:A:242:GLU:CG | 1:A:243:GLY:H | 1.89 | 0.85 |
| 1:B:242:GLU:CG | 1:B:243:GLY:H | 1.89 | 0.85 |
| 1:C:206:LYS:N | 1:C:219:SER:HG | 1.74 | 0.85 |
| 1:N:206:LYS:N | 1:N:219:SER:HG | 1.74 | 0.85 |
| 1:B:206:LYS:N | 1:B:219:SER:HG | 1.74 | 0.85 |
| 1:F:206:LYS:N | 1:F:219:SER:HG | 1.74 | 0.85 |
| 1:I:242:GLU:CG | 1:I:243:GLY:H | 1.89 | 0.85 |
| 1:J:242:GLU:CG | 1:J:243:GLY:H | 1.89 | 0.85 |
| 1:C:242:GLU:CG | 1:C:243:GLY:H | 1.89 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:206:LYS:N | 1:E:219:SER:HG | 1.74 | 0.85 |
| 1:K:206:LYS:N | 1:K:219:SER:HG | 1.74 | 0.85 |
| 1:N:242:GLU:CG | 1:N:243:GLY:H | 1.89 | 0.85 |
| 1:G:242:GLU:CG | 1:G:243:GLY:H | 1.89 | 0.85 |
| 1:O:242:GLU:CG | 1:O:243:GLY:H | 1.89 | 0.85 |
| 1:H:206:LYS:N | 1:H:219:SER:HG | 1.74 | 0.84 |
| 1:E:242:GLU:CG | 1:E:243:GLY:H | 1.89 | 0.84 |
| 1:L:242:GLU:CG | 1:L:243:GLY:H | 1.89 | 0.84 |
| 1:D:206:LYS:N | 1:D:219:SER:HG | 1.74 | 0.83 |
| 1:B:109:LEU:HD23 | 1:B:114:ALA:HA | 1.61 | 0.83 |
| 1:L:109:LEU:HD23 | 1:L:114:ALA:HA | 1.61 | 0.83 |
| 1:K:109:LEU:HD23 | 1:K:114:ALA:HA | 1.61 | 0.83 |
| 1:N:109:LEU:HD23 | 1:N:114:ALA:HA | 1.61 | 0.83 |
| 1:C:109:LEU:HD23 | 1:C:114:ALA:HA | 1.61 | 0.83 |
| 1:D:109:LEU:HD23 | 1:D:114:ALA:HA | 1.61 | 0.83 |
| 1:E:109:LEU:HD23 | 1:E:114:ALA:HA | 1.61 | 0.83 |
| 1:I:109:LEU:HD23 | 1:I:114:ALA:HA | 1.61 | 0.83 |
| 1:A:109:LEU:HD23 | 1:A:114:ALA:HA | 1.61 | 0.82 |
| 1:O:109:LEU:HD23 | 1:O:114:ALA:HA | 1.61 | 0.82 |
| 1:H:109:LEU:HD23 | 1:H:114:ALA:HA | 1.61 | 0.82 |
| 1:J:109:LEU:HD23 | 1:J:114:ALA:HA | 1.61 | 0.82 |
| 1:M:109:LEU:HD23 | 1:M:114:ALA:HA | 1.61 | 0.82 |
| 1:F:109:LEU:HD23 | 1:F:114:ALA:HA | 1.61 | 0.82 |
| 1:G:109:LEU:HD23 | 1:G:114:ALA:HA | 1.61 | 0.82 |
| 1:L:117:LEU:HD21 | 1:L:161:VAL:HG21 | 1.62 | 0.82 |
| 1:O:117:LEU:HD21 | 1:O:161:VAL:HG21 | 1.62 | 0.81 |
| 1:J:117:LEU:HD21 | 1:J:161:VAL:HG21 | 1.63 | 0.81 |
| 1:N:117:LEU:HD21 | 1:N:161:VAL:HG21 | 1.63 | 0.81 |
| 1:K:258:LEU:HD21 | 1:K:318:LEU:HD23 | 1.63 | 0.81 |
| 1:L:258:LEU:HD21 | 1:L:318:LEU:HD23 | 1.63 | 0.81 |
| 1:M:117:LEU:HD21 | 1:M:161:VAL:HG21 | 1.62 | 0.81 |
| 1:A:117:LEU:HD21 | 1:A:161:VAL:HG21 | 1.62 | 0.81 |
| 1:I:258:LEU:HD21 | 1:I:318:LEU:HD23 | 1.63 | 0.81 |
| 1:J:258:LEU:HD21 | 1:J:318:LEU:HD23 | 1.63 | 0.81 |
| 1:B:117:LEU:HD21 | 1:B:161:VAL:HG21 | 1.63 | 0.81 |
| 1:I:117:LEU:HD21 | 1:I:161:VAL:HG21 | 1.63 | 0.81 |
| 1:K:117:LEU:HD21 | 1:K:161:VAL:HG21 | 1.63 | 0.81 |
| 1:G:258:LEU:HD21 | 1:G:318:LEU:HD23 | 1.63 | 0.81 |
| 1:N:258:LEU:HD21 | 1:N:318:LEU:HD23 | 1.63 | 0.81 |
| 1:C:117:LEU:HD21 | 1:C:161:VAL:HG21 | 1.63 | 0.80 |
| 1:H:258:LEU:HD21 | 1:H:318:LEU:HD23 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:117:LEU:HD21 | 1:G:161:VAL:HG21 | 1.62 | 0.80 |
| 1:M:258:LEU:HD21 | 1:M:318:LEU:HD23 | 1.63 | 0.80 |
| 1:H:117:LEU:HD21 | 1:H:161:VAL:HG21 | 1.62 | 0.80 |
| 1:F:117:LEU:HD21 | 1:F:161:VAL:HG21 | 1.63 | 0.80 |
| 1:F:258:LEU:HD21 | 1:F:318:LEU:HD23 | 1.63 | 0.80 |
| 1:O:258:LEU:HD21 | 1:O:318:LEU:HD23 | 1.63 | 0.80 |
| 1:E:117:LEU:HD21 | 1:E:161:VAL:HG21 | 1.63 | 0.80 |
| 1:F:242:GLU:CG | 1:F:243:GLY:N | 2.45 | 0.80 |
| 1:I:141:VAL:HG21 | 1:J:164:ILE:HD12 | 1.64 | 0.80 |
| 1:K:242:GLU:CG | 1:K:243:GLY:N | 2.45 | 0.80 |
| 1:D:117:LEU:HD21 | 1:D:161:VAL:HG21 | 1.63 | 0.80 |
| 1:H:141:VAL:HG21 | 1:I:164:ILE:HD12 | 1.64 | 0.80 |
| 1:E:242:GLU:HG2 | 1:E:243:GLY:N | 1.97 | 0.79 |
| 1:O:242:GLU:CG | 1:O:243:GLY:N | 2.45 | 0.79 |
| 1:J:242:GLU:HG2 | 1:J:243:GLY:N | 1.97 | 0.79 |
| 1:L:242:GLU:HG2 | 1:L:243:GLY:N | 1.97 | 0.79 |
| 1:G:242:GLU:HG2 | 1:G:243:GLY:N | 1.98 | 0.79 |
| 1:J:141:VAL:HG21 | 1:K:164:ILE:HD12 | 1.64 | 0.79 |
| 1:M:242:GLU:HG2 | 1:M:243:GLY:N | 1.97 | 0.79 |
| 1:D:258:LEU:HD21 | 1:D:318:LEU:HD23 | 1.63 | 0.79 |
| 1:E:242:GLU:CG | 1:E:243:GLY:N | 2.45 | 0.79 |
| 1:H:242:GLU:HG2 | 1:H:243:GLY:N | 1.97 | 0.79 |
| 1:A:258:LEU:HD21 | 1:A:318:LEU:HD23 | 1.63 | 0.79 |
| 1:B:258:LEU:HD21 | 1:B:318:LEU:HD23 | 1.63 | 0.79 |
| 1:E:258:LEU:HD21 | 1:E:318:LEU:HD23 | 1.63 | 0.79 |
| 1:F:242:GLU:HG2 | 1:F:243:GLY:N | 1.97 | 0.79 |
| 1:G:141:VAL:HG21 | 1:H:164:ILE:HD12 | 1.64 | 0.79 |
| 1:I:242:GLU:CG | 1:I:243:GLY:N | 2.45 | 0.79 |
| 1:O:242:GLU:HG2 | 1:O:243:GLY:N | 1.98 | 0.79 |
| 1:C:242:GLU:CG | 1:C:243:GLY:N | 2.45 | 0.79 |
| 1:C:258:LEU:HD21 | 1:C:318:LEU:HD23 | 1.63 | 0.79 |
| 1:G:212:ARG:NE | 1:H:181:ASP:OD2 | 2.16 | 0.79 |
| 1:I:242:GLU:HG2 | 1:I:243:GLY:N | 1.97 | 0.79 |
| 1:A:181:ASP:OD2 | 1:O:212:ARG:NE | 2.16 | 0.79 |
| 1:C:242:GLU:HG2 | 1:C:243:GLY:N | 1.97 | 0.79 |
| 1:F:212:ARG:NE | 1:G:181:ASP:OD2 | 2.16 | 0.79 |
| 1:N:212:ARG:NE | 1:O:181:ASP:OD2 | 2.16 | 0.79 |
| 1:G:242:GLU:CG | 1:G:243:GLY:N | 2.45 | 0.79 |
| 1:H:212:ARG:NE | 1:I:181:ASP:OD2 | 2.16 | 0.79 |
| 1:L:242:GLU:CG | 1:L:243:GLY:N | 2.45 | 0.78 |
| 1:M:212:ARG:NE | 1:N:181:ASP:OD2 | 2.16 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:242:GLU:CG | 1:M:243:GLY:N | 2.45 | 0.78 |
| 1:A:212:ARG:NE | 1:B:181:ASP:OD2 | 2.16 | 0.78 |
| 1:D:242:GLU:CG | 1:D:243:GLY:N | 2.45 | 0.78 |
| 1:B:242:GLU:HG2 | 1:B:243:GLY:N | 1.97 | 0.78 |
| 1:N:242:GLU:HG2 | 1:N:243:GLY:N | 1.97 | 0.78 |
| 1:K:141:VAL:HG21 | 1:L:164:ILE:HD12 | 1.64 | 0.78 |
| 1:N:141:VAL:HG21 | 1:O:164:ILE:HD12 | 1.64 | 0.78 |
| 1:J:242:GLU:CG | 1:J:243:GLY:N | 2.45 | 0.78 |
| 1:M:141:VAL:HG21 | 1:N:164:ILE:HD12 | 1.64 | 0.78 |
| 1:A:164:ILE:HD12 | 1:O:141:VAL:HG21 | 1.64 | 0.78 |
| 1:C:212:ARG:NE | 1:D:181:ASP:OD2 | 2.16 | 0.78 |
| 1:E:212:ARG:NE | 1:F:181:ASP:OD2 | 2.16 | 0.78 |
| 1:F:141:VAL:HG21 | 1:G:164:ILE:HD12 | 1.64 | 0.78 |
| 1:K:242:GLU:HG2 | 1:K:243:GLY:N | 1.97 | 0.78 |
| 1:L:212:ARG:NE | 1:M:181:ASP:OD2 | 2.16 | 0.78 |
| 1:N:242:GLU:CG | 1:N:243:GLY:N | 2.45 | 0.78 |
| 1:A:141:VAL:HG21 | 1:B:164:ILE:HD12 | 1.64 | 0.78 |
| 1:A:242:GLU:CG | 1:A:243:GLY:N | 2.45 | 0.78 |
| 1:B:212:ARG:NE | 1:C:181:ASP:OD2 | 2.16 | 0.78 |
| 1:I:212:ARG:NE | 1:J:181:ASP:OD2 | 2.16 | 0.78 |
| 1:D:212:ARG:NE | 1:E:181:ASP:OD2 | 2.16 | 0.77 |
| 1:B:141:VAL:HG21 | 1:C:164:ILE:HD12 | 1.64 | 0.77 |
| 1:C:141:VAL:HG21 | 1:D:164:ILE:HD12 | 1.64 | 0.77 |
| 1:D:141:VAL:HG21 | 1:E:164:ILE:HD12 | 1.64 | 0.77 |
| 1:L:141:VAL:HG21 | 1:M:164:ILE:HD12 | 1.64 | 0.77 |
| 1:A:242:GLU:HG2 | 1:A:243:GLY:N | 1.97 | 0.77 |
| 1:D:242:GLU:HG2 | 1:D:243:GLY:N | 1.98 | 0.77 |
| 1:K:212:ARG:NE | 1:L:181:ASP:OD2 | 2.16 | 0.77 |
| 1:E:141:VAL:HG21 | 1:F:164:ILE:HD12 | 1.64 | 0.77 |
| 1:E:295:GLN:HG2 | 1:F:257:ASN:HD21 | 1.50 | 0.77 |
| 1:G:295:GLN:HG2 | 1:H:257:ASN:HD21 | 1.50 | 0.77 |
| 1:J:295:GLN:HG2 | 1:K:257:ASN:HD21 | 1.50 | 0.76 |
| 1:B:242:GLU:CG | 1:B:243:GLY:N | 2.45 | 0.76 |
| 1:J:212:ARG:NE | 1:K:181:ASP:OD2 | 2.16 | 0.76 |
| 1:C:295:GLN:HG2 | 1:D:257:ASN:HD21 | 1.50 | 0.76 |
| 1:L:295:GLN:HG2 | 1:M:257:ASN:HD21 | 1.50 | 0.76 |
| 1:H:295:GLN:HG2 | 1:I:257:ASN:HD21 | 1.50 | 0.76 |
| 1:I:295:GLN:HG2 | 1:J:257:ASN:HD21 | 1.50 | 0.76 |
| 1:B:295:GLN:HG2 | 1:C:257:ASN:HD21 | 1.50 | 0.76 |
| 1:K:609:LEU:HG | 1:M:528:ASP:OD2 | 1.86 | 0.76 |
| 1:B:609:LEU:HG | 1:D:528:ASP:OD2 | 1.86 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:257:ASN:HD21 | 1:O:295:GLN:HG2 | 1.50 | 0.75 |
| 1:A:609:LEU:HG | 1:C:528:ASP:OD2 | 1.86 | 0.75 |
| 1:B:528:ASP:OD2 | 1:O:609:LEU:HG | 1.86 | 0.75 |
| 1:C:609:LEU:HG | 1:E:528:ASP:OD2 | 1.86 | 0.75 |
| 1:F:609:LEU:HG | 1:H:528:ASP:OD2 | 1.86 | 0.75 |
| 1:I:609:LEU:HG | 1:K:528:ASP:OD2 | 1.86 | 0.75 |
| 1:J:609:LEU:HG | 1:L:528:ASP:OD2 | 1.86 | 0.75 |
| 1:L:609:LEU:HG | 1:N:528:ASP:OD2 | 1.86 | 0.75 |
| 1:D:609:LEU:HG | 1:F:528:ASP:OD2 | 1.86 | 0.75 |
| 1:H:609:LEU:HG | 1:J:528:ASP:OD2 | 1.86 | 0.75 |
| 1:A:108:PRO:HB3 | 1:A:141:VAL:HG12 | 1.69 | 0.75 |
| 1:B:108:PRO:HB3 | 1:B:141:VAL:HG12 | 1.69 | 0.75 |
| 1:C:108:PRO:HB3 | 1:C:141:VAL:HG12 | 1.69 | 0.75 |
| 1:E:609:LEU:HG | 1:G:528:ASP:OD2 | 1.86 | 0.75 |
| 1:O:108:PRO:HB3 | 1:O:141:VAL:HG12 | 1.69 | 0.75 |
| 1:A:528:ASP:OD2 | 1:N:609:LEU:HG | 1.86 | 0.75 |
| 1:D:295:GLN:HG2 | 1:E:257:ASN:HD21 | 1.50 | 0.75 |
| 1:D:108:PRO:HB3 | 1:D:141:VAL:HG12 | 1.69 | 0.75 |
| 1:G:609:LEU:HG | 1:I:528:ASP:OD2 | 1.86 | 0.75 |
| 1:N:295:GLN:HG2 | 1:O:257:ASN:HD21 | 1.50 | 0.75 |
| 1:F:295:GLN:HG2 | 1:G:257:ASN:HD21 | 1.50 | 0.75 |
| 1:G:295:GLN:NE2 | 1:H:322:ARG:HH12 | 1.85 | 0.75 |
| 1:N:295:GLN:NE2 | 1:O:322:ARG:HH12 | 1.85 | 0.75 |
| 1:C:114:ALA:HB1 | 1:C:142:LEU:HD12 | 1.69 | 0.75 |
| 1:M:295:GLN:HG2 | 1:N:257:ASN:HD21 | 1.50 | 0.75 |
| 1:N:108:PRO:HB3 | 1:N:141:VAL:HG12 | 1.69 | 0.75 |
| 1:D:295:GLN:NE2 | 1:E:322:ARG:HH12 | 1.85 | 0.74 |
| 1:I:114:ALA:HB1 | 1:I:142:LEU:HD12 | 1.69 | 0.74 |
| 1:L:108:PRO:HB3 | 1:L:141:VAL:HG12 | 1.69 | 0.74 |
| 1:M:108:PRO:HB3 | 1:M:141:VAL:HG12 | 1.69 | 0.74 |
| 1:A:114:ALA:HB1 | 1:A:142:LEU:HD12 | 1.69 | 0.74 |
| 1:A:295:GLN:NE2 | 1:B:322:ARG:HH12 | 1.85 | 0.74 |
| 1:E:114:ALA:HB1 | 1:E:142:LEU:HD12 | 1.69 | 0.74 |
| 1:G:114:ALA:HB1 | 1:G:142:LEU:HD12 | 1.69 | 0.74 |
| 1:E:108:PRO:HB3 | 1:E:141:VAL:HG12 | 1.69 | 0.74 |
| 1:E:295:GLN:NE2 | 1:F:322:ARG:HH12 | 1.85 | 0.74 |
| 1:H:295:GLN:NE2 | 1:I:322:ARG:HH12 | 1.85 | 0.74 |
| 1:K:295:GLN:HG2 | 1:L:257:ASN:HD21 | 1.50 | 0.74 |
| 1:M:609:LEU:HG | 1:O:528:ASP:OD2 | 1.86 | 0.74 |
| 1:B:326:LEU:HD22 | 1:B:580:LEU:HD21 | 1.69 | 0.74 |
| 1:C:326:LEU:HD22 | 1:C:580:LEU:HD21 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:295:GLN:NE2 | 1:K:322:ARG:HH12 | 1.85 | 0.74 |
| 1:K:114:ALA:HB1 | 1:K:142:LEU:HD12 | 1.69 | 0.74 |
| 1:D:326:LEU:HD22 | 1:D:580:LEU:HD21 | 1.69 | 0.74 |
| 1:K:108:PRO:HB3 | 1:K:141:VAL:HG12 | 1.69 | 0.74 |
| 1:A:295:GLN:HG2 | 1:B:257:ASN:HD21 | 1.50 | 0.74 |
| 1:H:242:GLU:CG | 1:H:243:GLY:N | 2.45 | 0.74 |
| 1:M:114:ALA:HB1 | 1:M:142:LEU:HD12 | 1.69 | 0.74 |
| 1:L:295:GLN:NE2 | 1:M:322:ARG:HH12 | 1.85 | 0.74 |
| 1:B:295:GLN:NE2 | 1:C:322:ARG:HH12 | 1.85 | 0.74 |
| 1:H:111:ASN:ND2 | 1:H:162:ASP:O | 2.21 | 0.74 |
| 1:H:114:ALA:HB1 | 1:H:142:LEU:HD12 | 1.69 | 0.74 |
| 1:A:326:LEU:HD22 | 1:A:580:LEU:HD21 | 1.69 | 0.74 |
| 1:G:111:ASN:ND2 | 1:G:162:ASP:O | 2.21 | 0.74 |
| 1:K:295:GLN:NE2 | 1:L:322:ARG:HH12 | 1.85 | 0.74 |
| 1:F:108:PRO:HB3 | 1:F:141:VAL:HG12 | 1.69 | 0.73 |
| 1:F:114:ALA:HB1 | 1:F:142:LEU:HD12 | 1.69 | 0.73 |
| 1:J:108:PRO:HB3 | 1:J:141:VAL:HG12 | 1.69 | 0.73 |
| 1:O:114:ALA:HB1 | 1:O:142:LEU:HD12 | 1.69 | 0.73 |
| 1:B:114:ALA:HB1 | 1:B:142:LEU:HD12 | 1.69 | 0.73 |
| 1:E:112:VAL:O | 1:E:140:ASN:ND2 | 2.21 | 0.73 |
| 1:N:114:ALA:HB1 | 1:N:142:LEU:HD12 | 1.69 | 0.73 |
| 1:A:111:ASN:ND2 | 1:A:162:ASP:O | 2.21 | 0.73 |
| 1:D:114:ALA:HB1 | 1:D:142:LEU:HD12 | 1.69 | 0.73 |
| 1:I:295:GLN:NE2 | 1:J:322:ARG:HH12 | 1.85 | 0.73 |
| 1:L:326:LEU:HD22 | 1:L:580:LEU:HD21 | 1.69 | 0.73 |
| 1:M:295:GLN:NE2 | 1:N:322:ARG:HH12 | 1.85 | 0.73 |
| 1:M:324:GLN:NE2 | 1:N:513:LEU:H | 1.87 | 0.73 |
| 1:A:324:GLN:NE2 | 1:B:513:LEU:H | 1.87 | 0.73 |
| 1:D:324:GLN:NE2 | 1:E:513:LEU:H | 1.87 | 0.73 |
| 1:E:326:LEU:HD22 | 1:E:580:LEU:HD21 | 1.69 | 0.73 |
| 1:F:295:GLN:NE2 | 1:G:322:ARG:HH12 | 1.85 | 0.73 |
| 1:K:326:LEU:HD22 | 1:K:580:LEU:HD21 | 1.69 | 0.73 |
| 1:A:513:LEU:H | 1:O:324:GLN:NE2 | 1.87 | 0.73 |
| 1:B:111:ASN:ND2 | 1:B:162:ASP:O | 2.21 | 0.73 |
| 1:B:112:VAL:O | 1:B:140:ASN:ND2 | 2.21 | 0.73 |
| 1:G:108:PRO:HB3 | 1:G:141:VAL:HG12 | 1.69 | 0.73 |
| 1:I:108:PRO:HB3 | 1:I:141:VAL:HG12 | 1.69 | 0.73 |
| 1:B:103:VAL:HG21 | 1:B:105:ARG:HH21 | 1.54 | 0.73 |
| 1:F:111:ASN:ND2 | 1:F:162:ASP:O | 2.21 | 0.73 |
| 1:G:324:GLN:NE2 | 1:H:513:LEU:H | 1.87 | 0.73 |
| 1:H:108:PRO:HB3 | 1:H:141:VAL:HG12 | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:208:VAL:HB | 1:I:217:ILE:HB | 1.71 | 0.73 |
| 1:J:114:ALA:HB1 | 1:J:142:LEU:HD12 | 1.69 | 0.73 |
| 1:L:112:VAL:O | 1:L:140:ASN:ND2 | 2.21 | 0.73 |
| 1:B:208:VAL:HB | 1:B:217:ILE:HB | 1.71 | 0.73 |
| 1:J:324:GLN:NE2 | 1:K:513:LEU:H | 1.87 | 0.73 |
| 1:L:103:VAL:HG21 | 1:L:105:ARG:HH21 | 1.54 | 0.73 |
| 1:M:326:LEU:HD22 | 1:M:580:LEU:HD21 | 1.69 | 0.73 |
| 1:A:208:VAL:HB | 1:A:217:ILE:HB | 1.71 | 0.73 |
| 1:C:103:VAL:HG21 | 1:C:105:ARG:HH21 | 1.54 | 0.73 |
| 1:H:208:VAL:HB | 1:H:217:ILE:HB | 1.71 | 0.73 |
| 1:J:208:VAL:HB | 1:J:217:ILE:HB | 1.71 | 0.73 |
| 1:J:326:LEU:HD22 | 1:J:580:LEU:HD21 | 1.69 | 0.73 |
| 1:A:181:ASP:O | 1:A:184:GLU:N | 2.22 | 0.73 |
| 1:B:324:GLN:NE2 | 1:C:513:LEU:H | 1.87 | 0.73 |
| 1:C:208:VAL:HB | 1:C:217:ILE:HB | 1.71 | 0.73 |
| 1:C:295:GLN:NE2 | 1:D:322:ARG:HH12 | 1.85 | 0.73 |
| 1:C:324:GLN:NE2 | 1:D:513:LEU:H | 1.87 | 0.73 |
| 1:O:181:ASP:O | 1:O:184:GLU:N | 2.22 | 0.73 |
| 1:G:326:LEU:HD22 | 1:G:580:LEU:HD21 | 1.69 | 0.73 |
| 1:H:103:VAL:HG21 | 1:H:105:ARG:HH21 | 1.54 | 0.73 |
| 1:H:326:LEU:HD22 | 1:H:580:LEU:HD21 | 1.69 | 0.73 |
| 1:J:181:ASP:O | 1:J:184:GLU:N | 2.22 | 0.73 |
| 1:K:103:VAL:HG21 | 1:K:105:ARG:HH21 | 1.54 | 0.73 |
| 1:M:103:VAL:HG21 | 1:M:105:ARG:HH21 | 1.54 | 0.73 |
| 1:O:326:LEU:HD22 | 1:O:580:LEU:HD21 | 1.69 | 0.73 |
| 1:C:111:ASN:ND2 | 1:C:162:ASP:O | 2.21 | 0.72 |
| 1:F:324:GLN:NE2 | 1:G:513:LEU:H | 1.87 | 0.72 |
| 1:I:326:LEU:HD22 | 1:I:580:LEU:HD21 | 1.69 | 0.72 |
| 1:A:103:VAL:HG21 | 1:A:105:ARG:HH21 | 1.54 | 0.72 |
| 1:B:181:ASP:O | 1:B:184:GLU:N | 2.22 | 0.72 |
| 1:D:103:VAL:HG21 | 1:D:105:ARG:HH21 | 1.54 | 0.72 |
| 1:D:208:VAL:HB | 1:D:217:ILE:HB | 1.71 | 0.72 |
| 1:D:262:LEU:HD12 | 1:D:299:LEU:HD21 | 1.72 | 0.72 |
| 1:E:181:ASP:O | 1:E:184:GLU:N | 2.22 | 0.72 |
| 1:F:181:ASP:O | 1:F:184:GLU:N | 2.22 | 0.72 |
| 1:G:181:ASP:O | 1:G:184:GLU:N | 2.22 | 0.72 |
| 1:G:262:LEU:HD12 | 1:G:299:LEU:HD21 | 1.71 | 0.72 |
| 1:H:112:VAL:O | 1:H:140:ASN:ND2 | 2.21 | 0.72 |
| 1:H:262:LEU:HD12 | 1:H:299:LEU:HD21 | 1.71 | 0.72 |
| 1:K:208:VAL:HB | 1:K:217:ILE:HB | 1.71 | 0.72 |
| 1:N:181:ASP:O | 1:N:184:GLU:N | 2.22 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:324:GLN:NE2 | 1:O:513:LEU:H | 1.87 | 0.72 |
| 1:O:208:VAL:HB | 1:O:217:ILE:HB | 1.71 | 0.72 |
| 1:A:112:VAL:O | 1:A:140:ASN:ND2 | 2.21 | 0.72 |
| 1:A:262:LEU:HD12 | 1:A:299:LEU:HD21 | 1.72 | 0.72 |
| 1:C:262:LEU:HD12 | 1:C:299:LEU:HD21 | 1.72 | 0.72 |
| 1:D:181:ASP:O | 1:D:184:GLU:N | 2.22 | 0.72 |
| 1:E:262:LEU:HD12 | 1:E:299:LEU:HD21 | 1.71 | 0.72 |
| 1:F:262:LEU:HD12 | 1:F:299:LEU:HD21 | 1.71 | 0.72 |
| 1:G:208:VAL:HB | 1:G:217:ILE:HB | 1.71 | 0.72 |
| 1:H:181:ASP:O | 1:H:184:GLU:N | 2.22 | 0.72 |
| 1:I:181:ASP:O | 1:I:184:GLU:N | 2.22 | 0.72 |
| 1:L:324:GLN:NE2 | 1:M:513:LEU:H | 1.87 | 0.72 |
| 1:C:181:ASP:O | 1:C:184:GLU:N | 2.22 | 0.72 |
| 1:E:208:VAL:HB | 1:E:217:ILE:HB | 1.71 | 0.72 |
| 1:E:324:GLN:NE2 | 1:F:513:LEU:H | 1.87 | 0.72 |
| 1:I:324:GLN:NE2 | 1:J:513:LEU:H | 1.87 | 0.72 |
| 1:K:181:ASP:O | 1:K:184:GLU:N | 2.22 | 0.72 |
| 1:K:206:LYS:N | 1:K:219:SER:OG | 2.23 | 0.72 |
| 1:K:324:GLN:NE2 | 1:L:513:LEU:H | 1.87 | 0.72 |
| 1:L:114:ALA:HB1 | 1:L:142:LEU:HD12 | 1.69 | 0.72 |
| 1:N:326:LEU:HD22 | 1:N:580:LEU:HD21 | 1.69 | 0.72 |
| 1:O:262:LEU:HD12 | 1:O:299:LEU:HD21 | 1.72 | 0.72 |
| 1:F:103:VAL:HG21 | 1:F:105:ARG:HH21 | 1.54 | 0.72 |
| 1:J:206:LYS:N | 1:J:219:SER:OG | 2.23 | 0.72 |
| 1:K:210:ASP:O | 1:K:214:ASN:CA | 2.36 | 0.72 |
| 1:L:208:VAL:HB | 1:L:217:ILE:HB | 1.71 | 0.72 |
| 1:F:208:VAL:HB | 1:F:217:ILE:HB | 1.71 | 0.72 |
| 1:F:326:LEU:HD22 | 1:F:580:LEU:HD21 | 1.69 | 0.72 |
| 1:J:103:VAL:HG21 | 1:J:105:ARG:HH21 | 1.54 | 0.72 |
| 1:N:208:VAL:HB | 1:N:217:ILE:HB | 1.71 | 0.72 |
| 1:A:322:ARG:HH12 | 1:O:295:GLN:NE2 | 1.85 | 0.72 |
| 1:B:262:LEU:HD12 | 1:B:299:LEU:HD21 | 1.71 | 0.72 |
| 1:E:288:VAL:HG21 | 1:E:307:VAL:HG11 | 1.71 | 0.72 |
| 1:F:288:VAL:HG21 | 1:F:307:VAL:HG11 | 1.71 | 0.72 |
| 1:H:288:VAL:HG21 | 1:H:307:VAL:HG11 | 1.71 | 0.72 |
| 1:I:288:VAL:HG21 | 1:I:307:VAL:HG11 | 1.71 | 0.72 |
| 1:M:208:VAL:HB | 1:M:217:ILE:HB | 1.71 | 0.72 |
| 1:H:324:GLN:NE2 | 1:I:513:LEU:H | 1.87 | 0.72 |
| 1:J:262:LEU:HD12 | 1:J:299:LEU:HD21 | 1.71 | 0.72 |
| 1:M:111:ASN:ND2 | 1:M:162:ASP:O | 2.21 | 0.72 |
| 1:M:181:ASP:O | 1:M:184:GLU:N | 2.22 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:206:LYS:N | 1:B:219:SER:OG | 2.23 | 0.72 |
| 1:D:112:VAL:O | 1:D:140:ASN:ND2 | 2.21 | 0.72 |
| 1:E:111:ASN:ND2 | 1:E:162:ASP:O | 2.21 | 0.72 |
| 1:G:288:VAL:HG21 | 1:G:307:VAL:HG11 | 1.71 | 0.72 |
| 1:I:262:LEU:HD12 | 1:I:299:LEU:HD21 | 1.71 | 0.72 |
| 1:D:206:LYS:N | 1:D:219:SER:OG | 2.23 | 0.72 |
| 1:M:262:LEU:HD12 | 1:M:299:LEU:HD21 | 1.71 | 0.72 |
| 1:N:103:VAL:HG21 | 1:N:105:ARG:HH21 | 1.54 | 0.72 |
| 1:D:288:VAL:HG21 | 1:D:307:VAL:HG11 | 1.72 | 0.71 |
| 1:E:206:LYS:N | 1:E:219:SER:OG | 2.23 | 0.71 |
| 1:L:111:ASN:ND2 | 1:L:162:ASP:O | 2.21 | 0.71 |
| 1:L:206:LYS:N | 1:L:219:SER:OG | 2.23 | 0.71 |
| 1:D:111:ASN:ND2 | 1:D:162:ASP:O | 2.21 | 0.71 |
| 1:I:103:VAL:HG21 | 1:I:105:ARG:HH21 | 1.54 | 0.71 |
| 1:J:288:VAL:HG21 | 1:J:307:VAL:HG11 | 1.72 | 0.71 |
| 1:K:262:LEU:HD12 | 1:K:299:LEU:HD21 | 1.71 | 0.71 |
| 1:L:262:LEU:HD12 | 1:L:299:LEU:HD21 | 1.71 | 0.71 |
| 1:C:206:LYS:N | 1:C:219:SER:OG | 2.23 | 0.71 |
| 1:E:103:VAL:HG21 | 1:E:105:ARG:HH21 | 1.54 | 0.71 |
| 1:L:181:ASP:O | 1:L:184:GLU:N | 2.22 | 0.71 |
| 1:N:206:LYS:N | 1:N:219:SER:OG | 2.23 | 0.71 |
| 1:D:210:ASP:O | 1:D:214:ASN:CA | 2.36 | 0.71 |
| 1:K:112:VAL:O | 1:K:140:ASN:ND2 | 2.21 | 0.71 |
| 1:M:589:ARG:HB2 | 1:M:612:LEU:HD12 | 1.73 | 0.71 |
| 1:N:262:LEU:HD12 | 1:N:299:LEU:HD21 | 1.72 | 0.71 |
| 1:O:103:VAL:HG21 | 1:O:105:ARG:HH21 | 1.54 | 0.71 |
| 1:O:206:LYS:N | 1:O:219:SER:OG | 2.23 | 0.71 |
| 1:O:210:ASP:O | 1:O:214:ASN:CA | 2.36 | 0.71 |
| 1:F:206:LYS:N | 1:F:219:SER:OG | 2.23 | 0.71 |
| 1:L:589:ARG:HB2 | 1:L:612:LEU:HD12 | 1.73 | 0.71 |
| 1:C:288:VAL:HG21 | 1:C:307:VAL:HG11 | 1.71 | 0.71 |
| 1:C:589:ARG:HB2 | 1:C:612:LEU:HD12 | 1.73 | 0.71 |
| 1:D:589:ARG:HB2 | 1:D:612:LEU:HD12 | 1.73 | 0.71 |
| 1:I:206:LYS:N | 1:I:219:SER:OG | 2.23 | 0.71 |
| 1:K:111:ASN:ND2 | 1:K:162:ASP:O | 2.21 | 0.71 |
| 1:K:589:ARG:HB2 | 1:K:612:LEU:HD12 | 1.73 | 0.71 |
| 1:N:255:ALA:O | 1:N:259:VAL:HG23 | 1.91 | 0.71 |
| 1:N:589:ARG:HB2 | 1:N:612:LEU:HD12 | 1.73 | 0.71 |
| 1:B:589:ARG:HB2 | 1:B:612:LEU:HD12 | 1.73 | 0.71 |
| 1:G:206:LYS:N | 1:G:219:SER:OG | 2.23 | 0.71 |
| 1:K:288:VAL:HG21 | 1:K:307:VAL:HG11 | 1.71 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:112:VAL:O | 1:O:140:ASN:ND2 | 2.21 | 0.71 |
| 1:O:255:ALA:O | 1:O:259:VAL:HG23 | 1.91 | 0.71 |
| 1:D:255:ALA:O | 1:D:259:VAL:HG23 | 1.91 | 0.71 |
| 1:E:255:ALA:O | 1:E:259:VAL:HG23 | 1.91 | 0.71 |
| 1:O:589:ARG:HB2 | 1:O:612:LEU:HD12 | 1.73 | 0.71 |
| 1:A:589:ARG:HB2 | 1:A:612:LEU:HD12 | 1.73 | 0.71 |
| 1:E:589:ARG:HB2 | 1:E:612:LEU:HD12 | 1.73 | 0.71 |
| 1:J:111:ASN:ND2 | 1:J:162:ASP:O | 2.21 | 0.71 |
| 1:M:288:VAL:HG21 | 1:M:307:VAL:HG11 | 1.71 | 0.71 |
| 1:N:288:VAL:HG21 | 1:N:307:VAL:HG11 | 1.71 | 0.71 |
| 1:A:288:VAL:HG21 | 1:A:307:VAL:HG11 | 1.71 | 0.71 |
| 1:F:255:ALA:O | 1:F:259:VAL:HG23 | 1.91 | 0.71 |
| 1:J:589:ARG:HB2 | 1:J:612:LEU:HD12 | 1.73 | 0.71 |
| 1:M:255:ALA:O | 1:M:259:VAL:HG23 | 1.91 | 0.71 |
| 1:O:288:VAL:HG21 | 1:O:307:VAL:HG11 | 1.71 | 0.71 |
| 1:M:206:LYS:N | 1:M:219:SER:OG | 2.23 | 0.70 |
| 1:C:255:ALA:O | 1:C:259:VAL:HG23 | 1.91 | 0.70 |
| 1:G:103:VAL:HG21 | 1:G:105:ARG:HH21 | 1.54 | 0.70 |
| 1:G:112:VAL:O | 1:G:140:ASN:ND2 | 2.21 | 0.70 |
| 1:G:255:ALA:O | 1:G:259:VAL:HG23 | 1.91 | 0.70 |
| 1:H:206:LYS:N | 1:H:219:SER:OG | 2.23 | 0.70 |
| 1:F:589:ARG:HB2 | 1:F:612:LEU:HD12 | 1.73 | 0.70 |
| 1:J:210:ASP:O | 1:J:214:ASN:CA | 2.36 | 0.70 |
| 1:L:288:VAL:HG21 | 1:L:307:VAL:HG11 | 1.71 | 0.70 |
| 1:B:288:VAL:HG21 | 1:B:307:VAL:HG11 | 1.71 | 0.70 |
| 1:E:210:ASP:O | 1:E:214:ASN:CA | 2.36 | 0.70 |
| 1:H:210:ASP:O | 1:H:214:ASN:CA | 2.36 | 0.70 |
| 1:H:255:ALA:O | 1:H:259:VAL:HG23 | 1.91 | 0.70 |
| 1:I:589:ARG:HB2 | 1:I:612:LEU:HD12 | 1.73 | 0.70 |
| 1:A:255:ALA:O | 1:A:259:VAL:HG23 | 1.91 | 0.70 |
| 1:B:255:ALA:O | 1:B:259:VAL:HG23 | 1.91 | 0.70 |
| 1:G:589:ARG:HB2 | 1:G:612:LEU:HD12 | 1.73 | 0.70 |
| 1:I:255:ALA:O | 1:I:259:VAL:HG23 | 1.91 | 0.70 |
| 1:A:206:LYS:N | 1:A:219:SER:OG | 2.23 | 0.70 |
| 1:G:210:ASP:O | 1:G:214:ASN:CA | 2.36 | 0.70 |
| 1:H:170:GLN:HB3 | 1:H:225:ARG:NH1 | 2.07 | 0.70 |
| 1:J:174:LEU:O | 1:J:214:ASN:ND2 | 2.25 | 0.70 |
| 1:J:255:ALA:O | 1:J:259:VAL:HG23 | 1.91 | 0.70 |
| 1:L:255:ALA:O | 1:L:259:VAL:HG23 | 1.91 | 0.70 |
| 1:N:174:LEU:O | 1:N:214:ASN:ND2 | 2.25 | 0.70 |
| 1:C:210:ASP:O | 1:C:214:ASN:CA | 2.36 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:170:GLN:HB3 | 1:E:225:ARG:NH1 | 2.07 | 0.70 |
| 1:F:170:GLN:HB3 | 1:F:225:ARG:NH1 | 2.07 | 0.70 |
| 1:H:589:ARG:HB2 | 1:H:612:LEU:HD12 | 1.73 | 0.70 |
| 1:K:174:LEU:O | 1:K:214:ASN:ND2 | 2.25 | 0.70 |
| 1:O:174:LEU:O | 1:O:214:ASN:ND2 | 2.25 | 0.70 |
| 1:D:170:GLN:HB3 | 1:D:225:ARG:NH1 | 2.07 | 0.70 |
| 1:H:242:GLU:HG3 | 1:H:243:GLY:H | 1.57 | 0.70 |
| 1:N:111:ASN:ND2 | 1:N:162:ASP:O | 2.21 | 0.70 |
| 1:G:170:GLN:HB3 | 1:G:225:ARG:NH1 | 2.07 | 0.69 |
| 1:O:170:GLN:HB3 | 1:O:225:ARG:NH1 | 2.07 | 0.69 |
| 1:G:242:GLU:HG3 | 1:G:243:GLY:H | 1.57 | 0.69 |
| 1:I:170:GLN:HB3 | 1:I:225:ARG:NH1 | 2.07 | 0.69 |
| 1:J:242:GLU:HG3 | 1:J:243:GLY:H | 1.57 | 0.69 |
| 1:L:174:LEU:O | 1:L:214:ASN:ND2 | 2.25 | 0.69 |
| 1:A:170:GLN:HB3 | 1:A:225:ARG:NH1 | 2.07 | 0.69 |
| 1:E:242:GLU:HG3 | 1:E:243:GLY:H | 1.57 | 0.69 |
| 1:K:255:ALA:O | 1:K:259:VAL:HG23 | 1.91 | 0.69 |
| 1:M:174:LEU:O | 1:M:214:ASN:ND2 | 2.25 | 0.69 |
| 1:N:170:GLN:HB3 | 1:N:225:ARG:NH1 | 2.07 | 0.69 |
| 1:B:222:GLU:HG2 | 1:B:225:ARG:HD2 | 1.75 | 0.69 |
| 1:C:112:VAL:O | 1:C:140:ASN:ND2 | 2.21 | 0.69 |
| 1:D:174:LEU:O | 1:D:214:ASN:ND2 | 2.25 | 0.69 |
| 1:J:222:GLU:HG2 | 1:J:225:ARG:HD2 | 1.75 | 0.69 |
| 1:K:222:GLU:HG2 | 1:K:225:ARG:HD2 | 1.75 | 0.69 |
| 1:M:170:GLN:HB3 | 1:M:225:ARG:NH1 | 2.07 | 0.69 |
| 1:A:222:GLU:HG2 | 1:A:225:ARG:HD2 | 1.75 | 0.69 |
| 1:E:174:LEU:O | 1:E:214:ASN:ND2 | 2.25 | 0.69 |
| 1:F:174:LEU:O | 1:F:214:ASN:ND2 | 2.25 | 0.69 |
| 1:I:174:LEU:O | 1:I:214:ASN:ND2 | 2.25 | 0.69 |
| 1:N:210:ASP:O | 1:N:214:ASN:CA | 2.36 | 0.69 |
| 1:A:174:LEU:O | 1:A:214:ASN:ND2 | 2.25 | 0.69 |
| 1:C:174:LEU:O | 1:C:214:ASN:ND2 | 2.25 | 0.69 |
| 1:G:174:LEU:O | 1:G:214:ASN:ND2 | 2.25 | 0.69 |
| 1:G:186:LEU:HD22 | 1:G:231:LEU:HD23 | 1.75 | 0.69 |
| 1:L:170:GLN:HB3 | 1:L:225:ARG:NH1 | 2.07 | 0.69 |
| 1:B:174:LEU:O | 1:B:214:ASN:ND2 | 2.25 | 0.69 |
| 1:C:295:GLN:HG2 | 1:D:257:ASN:ND2 | 2.08 | 0.69 |
| 1:D:222:GLU:HG2 | 1:D:225:ARG:HD2 | 1.75 | 0.69 |
| 1:E:222:GLU:HG2 | 1:E:225:ARG:HD2 | 1.75 | 0.69 |
| 1:G:222:GLU:HG2 | 1:G:225:ARG:HD2 | 1.75 | 0.69 |
| 1:I:186:LEU:HD22 | 1:I:231:LEU:HD23 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:222:GLU:HG2 | 1:I:225:ARG:HD2 | 1.75 | 0.69 |
| 1:L:222:GLU:HG2 | 1:L:225:ARG:HD2 | 1.75 | 0.69 |
| 1:N:112:VAL:O | 1:N:140:ASN:ND2 | 2.21 | 0.69 |
| 1:C:222:GLU:HG2 | 1:C:225:ARG:HD2 | 1.75 | 0.69 |
| 1:D:295:GLN:HG2 | 1:E:257:ASN:ND2 | 2.08 | 0.69 |
| 1:E:186:LEU:HD22 | 1:E:231:LEU:HD23 | 1.75 | 0.69 |
| 1:H:174:LEU:O | 1:H:214:ASN:ND2 | 2.25 | 0.69 |
| 1:H:222:GLU:HG2 | 1:H:225:ARG:HD2 | 1.75 | 0.69 |
| 1:J:295:GLN:HG2 | 1:K:257:ASN:ND2 | 2.08 | 0.69 |
| 1:K:295:GLN:HG2 | 1:L:257:ASN:ND2 | 2.08 | 0.69 |
| 1:O:111:ASN:ND2 | 1:O:162:ASP:O | 2.21 | 0.69 |
| 1:O:222:GLU:HG2 | 1:O:225:ARG:HD2 | 1.75 | 0.69 |
| 1:B:170:GLN:HB3 | 1:B:225:ARG:NH1 | 2.07 | 0.69 |
| 1:B:295:GLN:HG2 | 1:C:257:ASN:ND2 | 2.08 | 0.69 |
| 1:C:170:GLN:HB3 | 1:C:225:ARG:NH1 | 2.07 | 0.69 |
| 1:F:210:ASP:O | 1:F:214:ASN:CA | 2.36 | 0.69 |
| 1:J:112:VAL:O | 1:J:140:ASN:ND2 | 2.21 | 0.69 |
| 1:L:295:GLN:HG2 | 1:M:257:ASN:ND2 | 2.08 | 0.69 |
| 1:N:222:GLU:HG2 | 1:N:225:ARG:HD2 | 1.75 | 0.69 |
| 1:A:242:GLU:HG3 | 1:A:243:GLY:H | 1.57 | 0.69 |
| 1:E:295:GLN:HG2 | 1:F:257:ASN:ND2 | 2.08 | 0.69 |
| 1:F:222:GLU:HG2 | 1:F:225:ARG:HD2 | 1.75 | 0.69 |
| 1:K:170:GLN:HB3 | 1:K:225:ARG:NH1 | 2.07 | 0.69 |
| 1:M:222:GLU:HG2 | 1:M:225:ARG:HD2 | 1.75 | 0.68 |
| 1:C:186:LEU:HD22 | 1:C:231:LEU:HD23 | 1.75 | 0.68 |
| 1:F:186:LEU:HD22 | 1:F:231:LEU:HD23 | 1.75 | 0.68 |
| 1:I:111:ASN:ND2 | 1:I:162:ASP:O | 2.21 | 0.68 |
| 1:J:170:GLN:HB3 | 1:J:225:ARG:NH1 | 2.07 | 0.68 |
| 1:O:242:GLU:HG3 | 1:O:243:GLY:H | 1.57 | 0.68 |
| 1:A:295:GLN:HG2 | 1:B:257:ASN:ND2 | 2.08 | 0.68 |
| 1:D:186:LEU:HD22 | 1:D:231:LEU:HD23 | 1.75 | 0.68 |
| 1:F:242:GLU:HG3 | 1:F:243:GLY:H | 1.57 | 0.68 |
| 1:H:186:LEU:HD22 | 1:H:231:LEU:HD23 | 1.75 | 0.68 |
| 1:I:210:ASP:O | 1:I:214:ASN:CA | 2.36 | 0.68 |
| 1:I:295:GLN:HG2 | 1:J:257:ASN:ND2 | 2.08 | 0.68 |
| 1:K:186:LEU:HD22 | 1:K:231:LEU:HD23 | 1.75 | 0.68 |
| 1:M:242:GLU:HG3 | 1:M:243:GLY:H | 1.57 | 0.68 |
| 1:M:295:GLN:HG2 | 1:N:257:ASN:ND2 | 2.08 | 0.68 |
| 1:C:242:GLU:HG3 | 1:C:243:GLY:H | 1.57 | 0.68 |
| 1:F:295:GLN:HG2 | 1:G:257:ASN:ND2 | 2.08 | 0.68 |
| 1:K:242:GLU:HG3 | 1:K:243:GLY:H | 1.57 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:186:LEU:HD22 | 1:A:231:LEU:HD23 | 1.75 | 0.68 |
| 1:J:186:LEU:HD22 | 1:J:231:LEU:HD23 | 1.75 | 0.68 |
| 1:L:242:GLU:HG3 | 1:L:243:GLY:H | 1.57 | 0.68 |
| 1:A:257:ASN:ND2 | 1:O:295:GLN:HG2 | 2.08 | 0.68 |
| 1:L:186:LEU:HD22 | 1:L:231:LEU:HD23 | 1.75 | 0.68 |
| 1:B:242:GLU:HG3 | 1:B:243:GLY:H | 1.57 | 0.67 |
| 1:C:119:PRO:O | 1:C:123:GLN:CB | 2.42 | 0.67 |
| 1:F:112:VAL:O | 1:F:140:ASN:ND2 | 2.21 | 0.67 |
| 1:H:119:PRO:O | 1:H:123:GLN:CB | 2.42 | 0.67 |
| 1:H:295:GLN:HG2 | 1:I:257:ASN:ND2 | 2.08 | 0.67 |
| 1:N:295:GLN:HG2 | 1:O:257:ASN:ND2 | 2.08 | 0.67 |
| 1:B:210:ASP:O | 1:B:214:ASN:CA | 2.36 | 0.67 |
| 1:F:135:HIS:CD2 | 1:F:136:TYR:H | 2.13 | 0.67 |
| 1:I:112:VAL:O | 1:I:140:ASN:ND2 | 2.21 | 0.67 |
| 1:G:135:HIS:CD2 | 1:G:136:TYR:H | 2.13 | 0.67 |
| 1:N:186:LEU:HD22 | 1:N:231:LEU:HD23 | 1.75 | 0.67 |
| 1:E:119:PRO:O | 1:E:123:GLN:CB | 2.42 | 0.67 |
| 1:E:135:HIS:CD2 | 1:E:136:TYR:H | 2.13 | 0.67 |
| 1:H:135:HIS:CD2 | 1:H:136:TYR:H | 2.13 | 0.67 |
| 1:I:135:HIS:CD2 | 1:I:136:TYR:H | 2.13 | 0.67 |
| 1:L:210:ASP:O | 1:L:214:ASN:CA | 2.36 | 0.67 |
| 1:N:242:GLU:HG3 | 1:N:243:GLY:H | 1.57 | 0.67 |
| 1:A:241:GLU:O | 1:A:242:GLU:HB3 | 1.95 | 0.67 |
| 1:B:186:LEU:HD22 | 1:B:231:LEU:HD23 | 1.75 | 0.67 |
| 1:B:324:GLN:HE21 | 1:C:513:LEU:H | 1.43 | 0.67 |
| 1:D:135:HIS:CD2 | 1:D:136:TYR:H | 2.13 | 0.67 |
| 1:M:606:SER:HB3 | 1:O:532:GLU:HB2 | 1.77 | 0.67 |
| 1:D:242:GLU:HG3 | 1:D:243:GLY:H | 1.57 | 0.67 |
| 1:G:295:GLN:HG2 | 1:H:257:ASN:ND2 | 2.08 | 0.67 |
| 1:A:532:GLU:HB2 | 1:N:606:SER:HB3 | 1.77 | 0.67 |
| 1:F:119:PRO:O | 1:F:123:GLN:CB | 2.42 | 0.67 |
| 1:I:242:GLU:HG3 | 1:I:243:GLY:H | 1.57 | 0.67 |
| 1:J:135:HIS:CD2 | 1:J:136:TYR:H | 2.13 | 0.67 |
| 1:L:606:SER:HB3 | 1:N:532:GLU:HB2 | 1.77 | 0.67 |
| 1:N:135:HIS:CD2 | 1:N:136:TYR:H | 2.13 | 0.67 |
| 1:O:135:HIS:CD2 | 1:O:136:TYR:H | 2.13 | 0.67 |
| 1:A:513:LEU:H | 1:O:324:GLN:HE21 | 1.43 | 0.67 |
| 1:B:241:GLU:O | 1:B:242:GLU:HB3 | 1.95 | 0.67 |
| 1:M:186:LEU:HD22 | 1:M:231:LEU:HD23 | 1.75 | 0.67 |
| 1:M:210:ASP:O | 1:M:214:ASN:CA | 2.36 | 0.67 |
| 1:O:241:GLU:O | 1:O:242:GLU:HB3 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:186:LEU:HD22 | 1:O:231:LEU:HD23 | 1.75 | 0.67 |
| 1:K:241:GLU:O | 1:K:242:GLU:HB3 | 1.95 | 0.66 |
| 1:K:606:SER:HB3 | 1:M:532:GLU:HB2 | 1.77 | 0.66 |
| 1:M:135:HIS:CD2 | 1:M:136:TYR:H | 2.13 | 0.66 |
| 1:A:135:HIS:CD2 | 1:A:136:TYR:H | 2.13 | 0.66 |
| 1:C:135:HIS:CD2 | 1:C:136:TYR:H | 2.13 | 0.66 |
| 1:D:324:GLN:HE21 | 1:E:513:LEU:H | 1.43 | 0.66 |
| 1:B:532:GLU:HB2 | 1:O:606:SER:HB3 | 1.77 | 0.66 |
| 1:J:606:SER:HB3 | 1:L:532:GLU:HB2 | 1.77 | 0.66 |
| 1:K:119:PRO:O | 1:K:123:GLN:CB | 2.42 | 0.66 |
| 1:K:135:HIS:CD2 | 1:K:136:TYR:H | 2.13 | 0.66 |
| 1:I:119:PRO:O | 1:I:123:GLN:CB | 2.42 | 0.66 |
| 1:L:241:GLU:O | 1:L:242:GLU:HB3 | 1.95 | 0.66 |
| 1:D:119:PRO:O | 1:D:123:GLN:CB | 2.42 | 0.66 |
| 1:D:606:SER:HB3 | 1:F:532:GLU:HB2 | 1.77 | 0.66 |
| 1:I:606:SER:HB3 | 1:K:532:GLU:HB2 | 1.77 | 0.66 |
| 1:J:241:GLU:O | 1:J:242:GLU:HB3 | 1.95 | 0.66 |
| 1:N:241:GLU:O | 1:N:242:GLU:HB3 | 1.95 | 0.66 |
| 1:L:135:HIS:CD2 | 1:L:136:TYR:H | 2.13 | 0.66 |
| 1:M:112:VAL:O | 1:M:140:ASN:ND2 | 2.21 | 0.66 |
| 1:E:324:GLN:HE21 | 1:F:513:LEU:H | 1.43 | 0.66 |
| 1:C:606:SER:HB3 | 1:E:532:GLU:HB2 | 1.77 | 0.66 |
| 1:A:606:SER:HB3 | 1:C:532:GLU:HB2 | 1.77 | 0.66 |
| 1:B:135:HIS:CD2 | 1:B:136:TYR:H | 2.13 | 0.66 |
| 1:E:606:SER:HB3 | 1:G:532:GLU:HB2 | 1.77 | 0.66 |
| 1:H:606:SER:HB3 | 1:J:532:GLU:HB2 | 1.77 | 0.66 |
| 1:B:119:PRO:O | 1:B:123:GLN:CB | 2.42 | 0.66 |
| 1:C:241:GLU:O | 1:C:242:GLU:HB3 | 1.95 | 0.66 |
| 1:F:241:GLU:O | 1:F:242:GLU:HB3 | 1.95 | 0.66 |
| 1:G:241:GLU:O | 1:G:242:GLU:HB3 | 1.95 | 0.66 |
| 1:E:241:GLU:O | 1:E:242:GLU:HB3 | 1.95 | 0.65 |
| 1:H:241:GLU:O | 1:H:242:GLU:HB3 | 1.95 | 0.65 |
| 1:L:114:ALA:N | 1:L:140:ASN:OD1 | 2.28 | 0.65 |
| 1:N:324:GLN:HE21 | 1:O:513:LEU:H | 1.43 | 0.65 |
| 1:O:119:PRO:O | 1:O:123:GLN:CB | 2.42 | 0.65 |
| 1:D:212:ARG:NH2 | 1:E:177:ALA:HB1 | 2.10 | 0.65 |
| 1:E:242:GLU:HG2 | 1:E:243:GLY:H | 1.60 | 0.65 |
| 1:C:324:GLN:HE21 | 1:D:513:LEU:H | 1.43 | 0.65 |
| 1:L:324:GLN:HE21 | 1:M:513:LEU:H | 1.43 | 0.65 |
| 1:M:241:GLU:O | 1:M:242:GLU:HB3 | 1.95 | 0.65 |
| 1:B:606:SER:HB3 | 1:D:532:GLU:HB2 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:212:ARG:NH2 | 1:D:177:ALA:HB1 | 2.10 | 0.65 |
| 1:E:212:ARG:NH2 | 1:F:177:ALA:HB1 | 2.10 | 0.65 |
| 1:G:324:GLN:HE21 | 1:H:513:LEU:H | 1.43 | 0.65 |
| 1:C:242:GLU:HG2 | 1:C:243:GLY:H | 1.60 | 0.65 |
| 1:G:606:SER:HB3 | 1:I:532:GLU:HB2 | 1.77 | 0.65 |
| 1:M:324:GLN:HE21 | 1:N:513:LEU:H | 1.43 | 0.65 |
| 1:O:179:ALA:HB1 | 1:O:209:ALA:HB1 | 1.79 | 0.65 |
| 1:F:606:SER:HB3 | 1:H:532:GLU:HB2 | 1.77 | 0.65 |
| 1:I:324:GLN:HE21 | 1:J:513:LEU:H | 1.43 | 0.65 |
| 1:K:114:ALA:N | 1:K:140:ASN:OD1 | 2.28 | 0.65 |
| 1:L:179:ALA:HB1 | 1:L:209:ALA:HB1 | 1.79 | 0.65 |
| 1:M:179:ALA:HB1 | 1:M:209:ALA:HB1 | 1.79 | 0.65 |
| 1:G:119:PRO:O | 1:G:123:GLN:CB | 2.42 | 0.65 |
| 1:I:241:GLU:O | 1:I:242:GLU:HB3 | 1.95 | 0.65 |
| 1:N:179:ALA:HB1 | 1:N:209:ALA:HB1 | 1.79 | 0.65 |
| 1:A:324:GLN:HE21 | 1:B:513:LEU:H | 1.43 | 0.65 |
| 1:J:114:ALA:N | 1:J:140:ASN:OD1 | 2.28 | 0.65 |
| 1:J:179:ALA:HB1 | 1:J:209:ALA:HB1 | 1.79 | 0.65 |
| 1:B:212:ARG:NH2 | 1:C:177:ALA:HB1 | 2.10 | 0.64 |
| 1:D:241:GLU:O | 1:D:242:GLU:HB3 | 1.95 | 0.64 |
| 1:E:181:ASP:O | 1:E:184:GLU:HG2 | 1.98 | 0.64 |
| 1:F:181:ASP:O | 1:F:184:GLU:HG2 | 1.98 | 0.64 |
| 1:F:212:ARG:NH2 | 1:G:177:ALA:HB1 | 2.10 | 0.64 |
| 1:F:324:GLN:HE21 | 1:G:513:LEU:H | 1.43 | 0.64 |
| 1:K:179:ALA:HB1 | 1:K:209:ALA:HB1 | 1.79 | 0.64 |
| 1:K:181:ASP:O | 1:K:184:GLU:HG2 | 1.98 | 0.64 |
| 1:A:179:ALA:HB1 | 1:A:209:ALA:HB1 | 1.79 | 0.64 |
| 1:C:114:ALA:N | 1:C:140:ASN:OD1 | 2.28 | 0.64 |
| 1:E:114:ALA:N | 1:E:140:ASN:OD1 | 2.28 | 0.64 |
| 1:F:114:ALA:N | 1:F:140:ASN:OD1 | 2.28 | 0.64 |
| 1:I:114:ALA:N | 1:I:140:ASN:OD1 | 2.28 | 0.64 |
| 1:B:179:ALA:HB1 | 1:B:209:ALA:HB1 | 1.79 | 0.64 |
| 1:D:114:ALA:N | 1:D:140:ASN:OD1 | 2.28 | 0.64 |
| 1:G:114:ALA:N | 1:G:140:ASN:OD1 | 2.28 | 0.64 |
| 1:G:181:ASP:O | 1:G:184:GLU:HG2 | 1.98 | 0.64 |
| 1:H:114:ALA:N | 1:H:140:ASN:OD1 | 2.28 | 0.64 |
| 1:J:181:ASP:O | 1:J:184:GLU:HG2 | 1.98 | 0.64 |
| 1:K:324:GLN:HE21 | 1:L:513:LEU:H | 1.43 | 0.64 |
| 1:A:206:LYS:HZ1 | 1:B:190:ILE:HB | 1.62 | 0.64 |
| 1:B:114:ALA:N | 1:B:140:ASN:OD1 | 2.28 | 0.64 |
| 1:D:181:ASP:O | 1:D:184:GLU:HG2 | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:181:ASP:O | 1:M:184:GLU:HG2 | 1.98 | 0.64 |
| 1:N:181:ASP:O | 1:N:184:GLU:HG2 | 1.97 | 0.64 |
| 1:A:210:ASP:O | 1:A:214:ASN:CA | 2.36 | 0.64 |
| 1:C:179:ALA:HB1 | 1:C:209:ALA:HB1 | 1.79 | 0.64 |
| 1:K:213:THR:HG22 | 1:L:239:GLU:HB3 | 1.79 | 0.64 |
| 1:K:259:VAL:CG2 | 1:K:292:ALA:HB2 | 2.28 | 0.64 |
| 1:L:181:ASP:O | 1:L:184:GLU:HG2 | 1.98 | 0.64 |
| 1:A:114:ALA:N | 1:A:140:ASN:OD1 | 2.28 | 0.64 |
| 1:A:181:ASP:O | 1:A:184:GLU:HG2 | 1.98 | 0.64 |
| 1:J:213:THR:HG22 | 1:K:239:GLU:HB3 | 1.79 | 0.64 |
| 1:J:324:GLN:HE21 | 1:K:513:LEU:H | 1.43 | 0.64 |
| 1:N:259:VAL:CG2 | 1:N:292:ALA:HB2 | 2.28 | 0.64 |
| 1:B:213:THR:HG22 | 1:C:239:GLU:HB3 | 1.79 | 0.64 |
| 1:E:213:THR:HG22 | 1:F:239:GLU:HB3 | 1.79 | 0.64 |
| 1:I:179:ALA:HB1 | 1:I:209:ALA:HB1 | 1.79 | 0.64 |
| 1:M:242:GLU:HG2 | 1:M:243:GLY:H | 1.60 | 0.64 |
| 1:C:170:GLN:HB3 | 1:C:225:ARG:HH12 | 1.63 | 0.64 |
| 1:C:181:ASP:O | 1:C:184:GLU:HG2 | 1.98 | 0.64 |
| 1:D:170:GLN:HB3 | 1:D:225:ARG:HH12 | 1.63 | 0.64 |
| 1:I:181:ASP:O | 1:I:184:GLU:HG2 | 1.98 | 0.64 |
| 1:J:259:VAL:CG2 | 1:J:292:ALA:HB2 | 2.28 | 0.64 |
| 1:L:213:THR:HG22 | 1:M:239:GLU:HB3 | 1.79 | 0.64 |
| 1:O:181:ASP:O | 1:O:184:GLU:HG2 | 1.98 | 0.64 |
| 1:A:190:ILE:HB | 1:O:206:LYS:HZ1 | 1.62 | 0.64 |
| 1:A:213:THR:HG22 | 1:B:239:GLU:HB3 | 1.79 | 0.64 |
| 1:B:206:LYS:HZ1 | 1:C:190:ILE:HB | 1.62 | 0.64 |
| 1:G:479:ALA:HA | 1:G:515:LYS:HA | 1.80 | 0.64 |
| 1:H:181:ASP:O | 1:H:184:GLU:HG2 | 1.98 | 0.64 |
| 1:H:259:VAL:CG2 | 1:H:292:ALA:HB2 | 2.28 | 0.64 |
| 1:I:213:THR:HG22 | 1:J:239:GLU:HB3 | 1.79 | 0.64 |
| 1:I:259:VAL:CG2 | 1:I:292:ALA:HB2 | 2.28 | 0.64 |
| 1:J:479:ALA:HA | 1:J:515:LYS:HA | 1.80 | 0.64 |
| 1:K:479:ALA:HA | 1:K:515:LYS:HA | 1.80 | 0.64 |
| 1:L:259:VAL:CG2 | 1:L:292:ALA:HB2 | 2.28 | 0.64 |
| 1:O:114:ALA:N | 1:O:140:ASN:OD1 | 2.28 | 0.64 |
| 1:D:213:THR:HG22 | 1:E:239:GLU:HB3 | 1.79 | 0.64 |
| 1:F:479:ALA:HA | 1:F:515:LYS:HA | 1.80 | 0.64 |
| 1:K:426:VAL:O | 1:L:510:ASN:ND2 | 2.27 | 0.64 |
| 1:A:212:ARG:NH2 | 1:B:177:ALA:HB1 | 2.10 | 0.63 |
| 1:C:206:LYS:HZ1 | 1:D:190:ILE:HB | 1.62 | 0.63 |
| 1:G:259:VAL:CG2 | 1:G:292:ALA:HB2 | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:206:LYS:HZ1 | 1:J:190:ILE:HB | 1.63 | 0.63 |
| 1:M:479:ALA:HA | 1:M:515:LYS:HA | 1.80 | 0.63 |
| 1:N:119:PRO:O | 1:N:123:GLN:CB | 2.42 | 0.63 |
| 1:B:181:ASP:O | 1:B:184:GLU:HG2 | 1.98 | 0.63 |
| 1:G:212:ARG:NH2 | 1:H:177:ALA:HB1 | 2.10 | 0.63 |
| 1:H:479:ALA:HA | 1:H:515:LYS:HA | 1.80 | 0.63 |
| 1:I:479:ALA:HA | 1:I:515:LYS:HA | 1.80 | 0.63 |
| 1:M:259:VAL:CG2 | 1:M:292:ALA:HB2 | 2.28 | 0.63 |
| 1:B:259:VAL:CG2 | 1:B:292:ALA:HB2 | 2.28 | 0.63 |
| 1:H:206:LYS:HZ1 | 1:I:190:ILE:HB | 1.62 | 0.63 |
| 1:L:354:GLN:HE21 | 1:L:356:PHE:HE2 | 1.47 | 0.63 |
| 1:M:213:THR:HG22 | 1:N:239:GLU:HB3 | 1.79 | 0.63 |
| 1:B:170:GLN:HB3 | 1:B:225:ARG:HH12 | 1.63 | 0.63 |
| 1:G:179:ALA:HB1 | 1:G:209:ALA:HB1 | 1.79 | 0.63 |
| 1:H:179:ALA:HB1 | 1:H:209:ALA:HB1 | 1.79 | 0.63 |
| 1:L:426:VAL:O | 1:M:510:ASN:ND2 | 2.27 | 0.63 |
| 1:N:170:GLN:HB3 | 1:N:225:ARG:HH12 | 1.63 | 0.63 |
| 1:N:479:ALA:HA | 1:N:515:LYS:HA | 1.80 | 0.63 |
| 1:O:259:VAL:CG2 | 1:O:292:ALA:HB2 | 2.28 | 0.63 |
| 1:C:213:THR:HG22 | 1:D:239:GLU:HB3 | 1.79 | 0.63 |
| 1:D:179:ALA:HB1 | 1:D:209:ALA:HB1 | 1.79 | 0.63 |
| 1:D:479:ALA:HA | 1:D:515:LYS:HA | 1.80 | 0.63 |
| 1:E:259:VAL:CG2 | 1:E:292:ALA:HB2 | 2.28 | 0.63 |
| 1:E:479:ALA:HA | 1:E:515:LYS:HA | 1.81 | 0.63 |
| 1:F:213:THR:HG22 | 1:G:239:GLU:HB3 | 1.79 | 0.63 |
| 1:G:206:LYS:HZ1 | 1:H:190:ILE:HB | 1.63 | 0.63 |
| 1:H:213:THR:HG22 | 1:I:239:GLU:HB3 | 1.79 | 0.63 |
| 1:J:242:GLU:HG2 | 1:J:243:GLY:H | 1.60 | 0.63 |
| 1:L:206:LYS:HZ1 | 1:M:190:ILE:HB | 1.62 | 0.63 |
| 1:N:354:GLN:HE21 | 1:N:356:PHE:HE2 | 1.47 | 0.63 |
| 1:D:354:GLN:HE21 | 1:D:356:PHE:HE2 | 1.47 | 0.63 |
| 1:I:354:GLN:HE21 | 1:I:356:PHE:HE2 | 1.47 | 0.63 |
| 1:K:206:LYS:HZ1 | 1:L:190:ILE:HB | 1.63 | 0.63 |
| 1:L:119:PRO:O | 1:L:123:GLN:CB | 2.42 | 0.63 |
| 1:L:479:ALA:HA | 1:L:515:LYS:HA | 1.80 | 0.63 |
| 1:N:114:ALA:N | 1:N:140:ASN:OD1 | 2.28 | 0.63 |
| 1:O:170:GLN:HB3 | 1:O:225:ARG:HH12 | 1.63 | 0.63 |
| 1:A:177:ALA:HB1 | 1:O:212:ARG:NH2 | 2.10 | 0.63 |
| 1:A:259:VAL:CG2 | 1:A:292:ALA:HB2 | 2.28 | 0.63 |
| 1:A:354:GLN:HE21 | 1:A:356:PHE:HE2 | 1.47 | 0.63 |
| 1:C:479:ALA:HA | 1:C:515:LYS:HA | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:179:ALA:HB1 | 1:E:209:ALA:HB1 | 1.79 | 0.63 |
| 1:F:179:ALA:HB1 | 1:F:209:ALA:HB1 | 1.79 | 0.63 |
| 1:F:354:GLN:HE21 | 1:F:356:PHE:HE2 | 1.47 | 0.63 |
| 1:M:170:GLN:HB3 | 1:M:225:ARG:HH12 | 1.63 | 0.63 |
| 1:A:479:ALA:HA | 1:A:515:LYS:HA | 1.80 | 0.63 |
| 1:G:117:LEU:HD22 | 1:G:120:LEU:HD13 | 1.81 | 0.63 |
| 1:I:117:LEU:HD22 | 1:I:120:LEU:HD13 | 1.81 | 0.63 |
| 1:M:119:PRO:O | 1:M:123:GLN:CB | 2.42 | 0.63 |
| 1:C:354:GLN:HE21 | 1:C:356:PHE:HE2 | 1.47 | 0.63 |
| 1:L:170:GLN:HB3 | 1:L:225:ARG:HH12 | 1.63 | 0.63 |
| 1:M:426:VAL:O | 1:N:510:ASN:ND2 | 2.27 | 0.63 |
| 1:N:212:ARG:NH2 | 1:O:177:ALA:HB1 | 2.10 | 0.63 |
| 1:N:213:THR:HG22 | 1:O:239:GLU:HB3 | 1.79 | 0.63 |
| 1:D:259:VAL:CG2 | 1:D:292:ALA:HB2 | 2.28 | 0.62 |
| 1:E:206:LYS:HZ1 | 1:F:190:ILE:HB | 1.63 | 0.62 |
| 1:H:324:GLN:HE21 | 1:I:513:LEU:H | 1.43 | 0.62 |
| 1:I:170:GLN:HB3 | 1:I:225:ARG:HH12 | 1.63 | 0.62 |
| 1:D:206:LYS:HZ1 | 1:E:190:ILE:HB | 1.62 | 0.62 |
| 1:E:117:LEU:HD22 | 1:E:120:LEU:HD13 | 1.81 | 0.62 |
| 1:G:213:THR:HG22 | 1:H:239:GLU:HB3 | 1.79 | 0.62 |
| 1:H:170:GLN:HB3 | 1:H:225:ARG:HH12 | 1.63 | 0.62 |
| 1:J:206:LYS:HZ1 | 1:K:190:ILE:HB | 1.62 | 0.62 |
| 1:O:479:ALA:HA | 1:O:515:LYS:HA | 1.80 | 0.62 |
| 1:A:170:GLN:HB3 | 1:A:225:ARG:HH12 | 1.63 | 0.62 |
| 1:A:239:GLU:HB3 | 1:O:213:THR:HG22 | 1.79 | 0.62 |
| 1:B:479:ALA:HA | 1:B:515:LYS:HA | 1.80 | 0.62 |
| 1:H:242:GLU:HG2 | 1:H:243:GLY:H | 1.60 | 0.62 |
| 1:J:119:PRO:O | 1:J:123:GLN:CB | 2.42 | 0.62 |
| 1:N:426:VAL:O | 1:O:510:ASN:ND2 | 2.27 | 0.62 |
| 1:G:354:GLN:HE21 | 1:G:356:PHE:HE2 | 1.47 | 0.62 |
| 1:J:354:GLN:HE21 | 1:J:356:PHE:HE2 | 1.47 | 0.62 |
| 1:K:170:GLN:HB3 | 1:K:225:ARG:HH12 | 1.63 | 0.62 |
| 1:M:212:ARG:NH2 | 1:N:177:ALA:HB1 | 2.10 | 0.62 |
| 1:C:259:VAL:CG2 | 1:C:292:ALA:HB2 | 2.28 | 0.62 |
| 1:K:117:LEU:HD22 | 1:K:120:LEU:HD13 | 1.81 | 0.62 |
| 1:K:168:LYS:N | 1:K:220:GLY:O | 2.30 | 0.62 |
| 1:L:153:LYS:O | 1:L:157:VAL:HG23 | 2.00 | 0.62 |
| 1:M:153:LYS:O | 1:M:157:VAL:HG23 | 2.00 | 0.62 |
| 1:B:354:GLN:HE21 | 1:B:356:PHE:HE2 | 1.47 | 0.62 |
| 1:G:266:SER:HB3 | 1:G:290:ILE:CD1 | 2.30 | 0.62 |
| 1:K:153:LYS:O | 1:K:157:VAL:HG23 | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:121:LEU:HD22 | 1:L:154:LEU:HD23 | 1.82 | 0.62 |
| 1:H:212:ARG:NH2 | 1:I:177:ALA:HB1 | 2.10 | 0.62 |
| 1:J:170:GLN:HB3 | 1:J:225:ARG:HH12 | 1.63 | 0.62 |
| 1:K:121:LEU:HD22 | 1:K:154:LEU:HD23 | 1.82 | 0.62 |
| 1:L:266:SER:HB3 | 1:L:290:ILE:CD1 | 2.30 | 0.62 |
| 1:M:114:ALA:N | 1:M:140:ASN:OD1 | 2.28 | 0.62 |
| 1:M:121:LEU:HD22 | 1:M:154:LEU:HD23 | 1.82 | 0.62 |
| 1:J:121:LEU:HD22 | 1:J:154:LEU:HD23 | 1.82 | 0.62 |
| 1:J:266:SER:HB3 | 1:J:290:ILE:CD1 | 2.30 | 0.62 |
| 1:A:317:ARG:O | 1:O:249:TYR:OH | 2.17 | 0.62 |
| 1:F:259:VAL:CG2 | 1:F:292:ALA:HB2 | 2.28 | 0.62 |
| 1:F:266:SER:HB3 | 1:F:290:ILE:CD1 | 2.30 | 0.62 |
| 1:H:266:SER:HB3 | 1:H:290:ILE:CD1 | 2.30 | 0.62 |
| 1:J:153:LYS:O | 1:J:157:VAL:HG23 | 2.00 | 0.62 |
| 1:K:354:GLN:HE21 | 1:K:356:PHE:HE2 | 1.47 | 0.62 |
| 1:L:212:ARG:NH2 | 1:M:177:ALA:HB1 | 2.10 | 0.62 |
| 1:M:266:SER:HB3 | 1:M:290:ILE:CD1 | 2.30 | 0.62 |
| 1:N:121:LEU:HD22 | 1:N:154:LEU:HD23 | 1.82 | 0.62 |
| 1:N:249:TYR:OH | 1:O:317:ARG:O | 2.17 | 0.62 |
| 1:O:354:GLN:HE21 | 1:O:356:PHE:HE2 | 1.47 | 0.62 |
| 1:C:117:LEU:HD22 | 1:C:120:LEU:HD13 | 1.81 | 0.62 |
| 1:D:153:LYS:O | 1:D:157:VAL:HG23 | 2.00 | 0.62 |
| 1:E:153:LYS:O | 1:E:157:VAL:HG23 | 2.00 | 0.62 |
| 1:F:153:LYS:O | 1:F:157:VAL:HG23 | 2.00 | 0.62 |
| 1:G:170:GLN:HB3 | 1:G:225:ARG:HH12 | 1.63 | 0.62 |
| 1:H:121:LEU:HD22 | 1:H:154:LEU:HD23 | 1.82 | 0.62 |
| 1:M:206:LYS:HZ1 | 1:N:190:ILE:HB | 1.63 | 0.62 |
| 1:N:153:LYS:O | 1:N:157:VAL:HG23 | 2.00 | 0.62 |
| 1:A:119:PRO:O | 1:A:123:GLN:CB | 2.42 | 0.61 |
| 1:B:153:LYS:O | 1:B:157:VAL:HG23 | 2.00 | 0.61 |
| 1:C:153:LYS:O | 1:C:157:VAL:HG23 | 2.00 | 0.61 |
| 1:I:121:LEU:HD22 | 1:I:154:LEU:HD23 | 1.82 | 0.61 |
| 1:K:266:SER:HB3 | 1:K:290:ILE:CD1 | 2.30 | 0.61 |
| 1:N:266:SER:HB3 | 1:N:290:ILE:CD1 | 2.30 | 0.61 |
| 1:B:176:TYR:CD1 | 1:B:238:GLU:OE1 | 2.54 | 0.61 |
| 1:F:170:GLN:HB3 | 1:F:225:ARG:HH12 | 1.63 | 0.61 |
| 1:G:121:LEU:HD22 | 1:G:154:LEU:HD23 | 1.82 | 0.61 |
| 1:H:153:LYS:O | 1:H:157:VAL:HG23 | 2.00 | 0.61 |
| 1:K:212:ARG:NH2 | 1:L:177:ALA:HB1 | 2.10 | 0.61 |
| 1:M:176:TYR:CD1 | 1:M:238:GLU:OE1 | 2.53 | 0.61 |
| 1:F:246:ARG:NH1 | 1:F:308:GLN:HG3 | 2.16 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:153:LYS:O | 1:G:157:VAL:HG23 | 2.00 | 0.61 |
| 1:H:246:ARG:NH1 | 1:H:308:GLN:HG3 | 2.16 | 0.61 |
| 1:A:153:LYS:O | 1:A:157:VAL:HG23 | 2.00 | 0.61 |
| 1:A:176:TYR:CD1 | 1:A:238:GLU:OE1 | 2.54 | 0.61 |
| 1:D:246:ARG:NH1 | 1:D:308:GLN:HG3 | 2.16 | 0.61 |
| 1:E:266:SER:HB3 | 1:E:290:ILE:CD1 | 2.30 | 0.61 |
| 1:G:246:ARG:NH1 | 1:G:308:GLN:HG3 | 2.16 | 0.61 |
| 1:I:212:ARG:NH2 | 1:J:177:ALA:HB1 | 2.10 | 0.61 |
| 1:I:249:TYR:OH | 1:J:317:ARG:O | 2.17 | 0.61 |
| 1:I:266:SER:HB3 | 1:I:290:ILE:CD1 | 2.30 | 0.61 |
| 1:J:212:ARG:NH2 | 1:K:177:ALA:HB1 | 2.10 | 0.61 |
| 1:M:354:GLN:HE21 | 1:M:356:PHE:HE2 | 1.47 | 0.61 |
| 1:E:168:LYS:N | 1:E:220:GLY:O | 2.31 | 0.61 |
| 1:E:246:ARG:NH1 | 1:E:308:GLN:HG3 | 2.16 | 0.61 |
| 1:I:153:LYS:O | 1:I:157:VAL:HG23 | 2.00 | 0.61 |
| 1:K:242:GLU:HG2 | 1:K:243:GLY:H | 1.60 | 0.61 |
| 1:N:206:LYS:HZ1 | 1:O:190:ILE:HB | 1.64 | 0.61 |
| 1:D:168:LYS:N | 1:D:220:GLY:O | 2.31 | 0.61 |
| 1:F:117:LEU:HD22 | 1:F:120:LEU:HD13 | 1.81 | 0.61 |
| 1:F:121:LEU:HD22 | 1:F:154:LEU:HD23 | 1.82 | 0.61 |
| 1:F:168:LYS:N | 1:F:220:GLY:O | 2.30 | 0.61 |
| 1:H:176:TYR:CD1 | 1:H:238:GLU:OE1 | 2.54 | 0.61 |
| 1:J:168:LYS:N | 1:J:220:GLY:O | 2.31 | 0.61 |
| 1:M:117:LEU:HD22 | 1:M:120:LEU:HD13 | 1.81 | 0.61 |
| 1:O:117:LEU:HD22 | 1:O:120:LEU:HD13 | 1.81 | 0.61 |
| 1:O:121:LEU:HD22 | 1:O:154:LEU:HD23 | 1.82 | 0.61 |
| 1:D:266:SER:HB3 | 1:D:290:ILE:CD1 | 2.30 | 0.61 |
| 1:D:426:VAL:O | 1:E:510:ASN:ND2 | 2.27 | 0.61 |
| 1:E:170:GLN:HB3 | 1:E:225:ARG:HH12 | 1.63 | 0.61 |
| 1:F:479:ALA:O | 1:F:480:VAL:HG13 | 2.01 | 0.61 |
| 1:G:176:TYR:CD1 | 1:G:238:GLU:OE1 | 2.54 | 0.61 |
| 1:I:246:ARG:NH1 | 1:I:308:GLN:HG3 | 2.16 | 0.61 |
| 1:J:246:ARG:NH1 | 1:J:308:GLN:HG3 | 2.16 | 0.61 |
| 1:L:479:ALA:O | 1:L:480:VAL:HG13 | 2.01 | 0.61 |
| 1:M:249:TYR:OH | 1:N:317:ARG:O | 2.17 | 0.61 |
| 1:A:121:LEU:HD22 | 1:A:154:LEU:HD23 | 1.82 | 0.61 |
| 1:C:176:TYR:CD1 | 1:C:238:GLU:OE1 | 2.54 | 0.61 |
| 1:H:117:LEU:HD22 | 1:H:120:LEU:HD13 | 1.81 | 0.61 |
| 1:L:176:TYR:CD1 | 1:L:238:GLU:OE1 | 2.54 | 0.61 |
| 1:N:117:LEU:HD22 | 1:N:120:LEU:HD13 | 1.81 | 0.61 |
| 1:N:176:TYR:CD1 | 1:N:238:GLU:OE1 | 2.54 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:117:LEU:HD22 | 1:A:120:LEU:HD13 | 1.81 | 0.61 |
| 1:A:266:SER:HB3 | 1:A:290:ILE:CD1 | 2.30 | 0.61 |
| 1:B:266:SER:HB3 | 1:B:290:ILE:CD1 | 2.30 | 0.61 |
| 1:D:120:LEU:HD22 | 1:D:157:VAL:HG11 | 1.83 | 0.61 |
| 1:D:479:ALA:O | 1:D:480:VAL:HG13 | 2.01 | 0.61 |
| 1:E:354:GLN:HE21 | 1:E:356:PHE:HE2 | 1.47 | 0.61 |
| 1:H:354:GLN:HE21 | 1:H:356:PHE:HE2 | 1.47 | 0.61 |
| 1:H:479:ALA:O | 1:H:480:VAL:HG13 | 2.01 | 0.61 |
| 1:J:479:ALA:O | 1:J:480:VAL:HG13 | 2.01 | 0.61 |
| 1:N:479:ALA:O | 1:N:480:VAL:HG13 | 2.01 | 0.61 |
| 1:B:246:ARG:NH1 | 1:B:308:GLN:HG3 | 2.16 | 0.61 |
| 1:B:249:TYR:OH | 1:C:317:ARG:O | 2.17 | 0.61 |
| 1:C:168:LYS:N | 1:C:220:GLY:O | 2.31 | 0.61 |
| 1:C:266:SER:HB3 | 1:C:290:ILE:CD1 | 2.30 | 0.61 |
| 1:G:168:LYS:N | 1:G:220:GLY:O | 2.31 | 0.61 |
| 1:O:266:SER:HB3 | 1:O:290:ILE:CD1 | 2.30 | 0.61 |
| 1:C:246:ARG:NH1 | 1:C:308:GLN:HG3 | 2.16 | 0.60 |
| 1:D:117:LEU:HD22 | 1:D:120:LEU:HD13 | 1.81 | 0.60 |
| 1:E:176:TYR:CD1 | 1:E:238:GLU:OE1 | 2.54 | 0.60 |
| 1:G:120:LEU:HD22 | 1:G:157:VAL:HG11 | 1.83 | 0.60 |
| 1:K:176:TYR:CD1 | 1:K:238:GLU:OE1 | 2.54 | 0.60 |
| 1:O:120:LEU:HD22 | 1:O:157:VAL:HG11 | 1.83 | 0.60 |
| 1:O:153:LYS:O | 1:O:157:VAL:HG23 | 2.00 | 0.60 |
| 1:O:176:TYR:CD1 | 1:O:238:GLU:OE1 | 2.54 | 0.60 |
| 1:B:121:LEU:HD22 | 1:B:154:LEU:HD23 | 1.82 | 0.60 |
| 1:B:479:ALA:O | 1:B:480:VAL:HG13 | 2.01 | 0.60 |
| 1:C:120:LEU:HD22 | 1:C:157:VAL:HG11 | 1.83 | 0.60 |
| 1:C:479:ALA:O | 1:C:480:VAL:HG13 | 2.01 | 0.60 |
| 1:E:121:LEU:HD22 | 1:E:154:LEU:HD23 | 1.82 | 0.60 |
| 1:H:120:LEU:HD22 | 1:H:157:VAL:HG11 | 1.83 | 0.60 |
| 1:K:246:ARG:NH1 | 1:K:308:GLN:HG3 | 2.16 | 0.60 |
| 1:A:426:VAL:O | 1:B:510:ASN:ND2 | 2.27 | 0.60 |
| 1:D:121:LEU:HD22 | 1:D:154:LEU:HD23 | 1.82 | 0.60 |
| 1:E:249:TYR:OH | 1:F:317:ARG:O | 2.17 | 0.60 |
| 1:E:295:GLN:CG | 1:F:257:ASN:ND2 | 2.65 | 0.60 |
| 1:I:295:GLN:CG | 1:J:257:ASN:ND2 | 2.65 | 0.60 |
| 1:J:117:LEU:HD22 | 1:J:120:LEU:HD13 | 1.81 | 0.60 |
| 1:J:223:LYS:HA | 1:J:226:GLN:HG2 | 1.83 | 0.60 |
| 1:A:120:LEU:HD22 | 1:A:157:VAL:HG11 | 1.83 | 0.60 |
| 1:A:295:GLN:CG | 1:B:257:ASN:ND2 | 2.65 | 0.60 |
| 1:A:479:ALA:O | 1:A:480:VAL:HG13 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:295:GLN:CG | 1:E:257:ASN:ND2 | 2.65 | 0.60 |
| 1:E:167:GLU:HA | 1:E:221:PRO:HA | 1.84 | 0.60 |
| 1:E:426:VAL:O | 1:F:510:ASN:ND2 | 2.27 | 0.60 |
| 1:F:176:TYR:CD1 | 1:F:238:GLU:OE1 | 2.54 | 0.60 |
| 1:F:223:LYS:HA | 1:F:226:GLN:HG2 | 1.83 | 0.60 |
| 1:I:176:TYR:CD1 | 1:I:238:GLU:OE1 | 2.54 | 0.60 |
| 1:I:223:LYS:HA | 1:I:226:GLN:HG2 | 1.83 | 0.60 |
| 1:J:176:TYR:CD1 | 1:J:238:GLU:OE1 | 2.54 | 0.60 |
| 1:J:295:GLN:CG | 1:K:257:ASN:ND2 | 2.65 | 0.60 |
| 1:L:117:LEU:HD22 | 1:L:120:LEU:HD13 | 1.81 | 0.60 |
| 1:D:176:TYR:CD1 | 1:D:238:GLU:OE1 | 2.54 | 0.60 |
| 1:E:223:LYS:HA | 1:E:226:GLN:HG2 | 1.83 | 0.60 |
| 1:F:167:GLU:HA | 1:F:221:PRO:HA | 1.84 | 0.60 |
| 1:F:295:GLN:CG | 1:G:257:ASN:ND2 | 2.65 | 0.60 |
| 1:K:223:LYS:HA | 1:K:226:GLN:HG2 | 1.83 | 0.60 |
| 1:M:295:GLN:CG | 1:N:257:ASN:ND2 | 2.65 | 0.60 |
| 1:A:510:ASN:ND2 | 1:O:426:VAL:O | 2.27 | 0.60 |
| 1:D:167:GLU:HA | 1:D:221:PRO:HA | 1.84 | 0.60 |
| 1:E:355:GLN:HB2 | 1:E:363:ILE:HG22 | 1.84 | 0.60 |
| 1:G:167:GLU:HA | 1:G:221:PRO:HA | 1.84 | 0.60 |
| 1:G:223:LYS:HA | 1:G:226:GLN:HG2 | 1.83 | 0.60 |
| 1:L:246:ARG:NH1 | 1:L:308:GLN:HG3 | 2.16 | 0.60 |
| 1:L:295:GLN:CG | 1:M:257:ASN:ND2 | 2.65 | 0.60 |
| 1:N:120:LEU:HD22 | 1:N:157:VAL:HG11 | 1.83 | 0.60 |
| 1:B:117:LEU:HD22 | 1:B:120:LEU:HD13 | 1.81 | 0.60 |
| 1:B:295:GLN:CG | 1:C:257:ASN:ND2 | 2.65 | 0.60 |
| 1:E:120:LEU:HD22 | 1:E:157:VAL:HG11 | 1.83 | 0.60 |
| 1:H:223:LYS:HA | 1:H:226:GLN:HG2 | 1.84 | 0.60 |
| 1:H:295:GLN:CG | 1:I:257:ASN:ND2 | 2.65 | 0.60 |
| 1:I:167:GLU:HA | 1:I:221:PRO:HA | 1.84 | 0.60 |
| 1:J:167:GLU:HA | 1:J:221:PRO:HA | 1.84 | 0.60 |
| 1:A:168:LYS:N | 1:A:220:GLY:O | 2.30 | 0.60 |
| 1:B:426:VAL:O | 1:C:510:ASN:ND2 | 2.27 | 0.60 |
| 1:C:121:LEU:HD22 | 1:C:154:LEU:HD23 | 1.82 | 0.60 |
| 1:C:167:GLU:HA | 1:C:221:PRO:HA | 1.84 | 0.60 |
| 1:I:120:LEU:HD22 | 1:I:157:VAL:HG11 | 1.83 | 0.60 |
| 1:K:295:GLN:CG | 1:L:257:ASN:ND2 | 2.65 | 0.60 |
| 1:A:246:ARG:NH1 | 1:A:308:GLN:HG3 | 2.16 | 0.60 |
| 1:B:168:LYS:N | 1:B:220:GLY:O | 2.31 | 0.60 |
| 1:D:223:LYS:HA | 1:D:226:GLN:HG2 | 1.83 | 0.60 |
| 1:H:167:GLU:HA | 1:H:221:PRO:HA | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:479:ALA:O | 1:I:480:VAL:HG13 | 2.01 | 0.60 |
| 1:K:167:GLU:HA | 1:K:221:PRO:HA | 1.84 | 0.60 |
| 1:N:246:ARG:NH1 | 1:N:308:GLN:HG3 | 2.16 | 0.60 |
| 1:O:479:ALA:O | 1:O:480:VAL:HG13 | 2.01 | 0.60 |
| 1:D:355:GLN:HB2 | 1:D:363:ILE:HG22 | 1.84 | 0.60 |
| 1:F:120:LEU:HD22 | 1:F:157:VAL:HG11 | 1.83 | 0.60 |
| 1:F:355:GLN:HB2 | 1:F:363:ILE:HG22 | 1.84 | 0.60 |
| 1:L:223:LYS:HA | 1:L:226:GLN:HG2 | 1.84 | 0.60 |
| 1:M:246:ARG:NH1 | 1:M:308:GLN:HG3 | 2.16 | 0.60 |
| 1:A:257:ASN:ND2 | 1:O:295:GLN:CG | 2.65 | 0.59 |
| 1:I:168:LYS:N | 1:I:220:GLY:O | 2.31 | 0.59 |
| 1:K:479:ALA:O | 1:K:480:VAL:HG13 | 2.01 | 0.59 |
| 1:M:479:ALA:O | 1:M:480:VAL:HG13 | 2.01 | 0.59 |
| 1:B:355:GLN:HB2 | 1:B:363:ILE:HG22 | 1.84 | 0.59 |
| 1:C:295:GLN:CG | 1:D:257:ASN:ND2 | 2.65 | 0.59 |
| 1:C:355:GLN:HB2 | 1:C:363:ILE:HG22 | 1.84 | 0.59 |
| 1:H:355:GLN:HB2 | 1:H:363:ILE:HG22 | 1.84 | 0.59 |
| 1:L:167:GLU:HA | 1:L:221:PRO:HA | 1.84 | 0.59 |
| 1:M:120:LEU:HD22 | 1:M:157:VAL:HG11 | 1.83 | 0.59 |
| 1:N:295:GLN:CG | 1:O:257:ASN:ND2 | 2.65 | 0.59 |
| 1:O:246:ARG:NH1 | 1:O:308:GLN:HG3 | 2.16 | 0.59 |
| 1:E:479:ALA:O | 1:E:480:VAL:HG13 | 2.01 | 0.59 |
| 1:F:426:VAL:O | 1:G:510:ASN:ND2 | 2.27 | 0.59 |
| 1:I:355:GLN:HB2 | 1:I:363:ILE:HG22 | 1.84 | 0.59 |
| 1:B:167:GLU:HA | 1:B:221:PRO:HA | 1.84 | 0.59 |
| 1:C:157:VAL:HG22 | 1:C:160:ARG:NH2 | 2.18 | 0.59 |
| 1:C:168:LYS:HD2 | 1:C:169:GLN:H | 1.68 | 0.59 |
| 1:G:355:GLN:HB2 | 1:G:363:ILE:HG22 | 1.84 | 0.59 |
| 1:G:479:ALA:O | 1:G:480:VAL:HG13 | 2.01 | 0.59 |
| 1:N:210:ASP:HB3 | 1:N:215:SER:H | 1.68 | 0.59 |
| 1:A:210:ASP:HB3 | 1:A:215:SER:H | 1.68 | 0.59 |
| 1:A:355:GLN:HB2 | 1:A:363:ILE:HG22 | 1.84 | 0.59 |
| 1:K:157:VAL:HG22 | 1:K:160:ARG:NH2 | 2.18 | 0.59 |
| 1:L:249:TYR:OH | 1:M:317:ARG:O | 2.17 | 0.59 |
| 1:M:167:GLU:HA | 1:M:221:PRO:HA | 1.84 | 0.59 |
| 1:O:157:VAL:HG22 | 1:O:160:ARG:NH2 | 2.18 | 0.59 |
| 1:B:120:LEU:HD22 | 1:B:157:VAL:HG11 | 1.83 | 0.59 |
| 1:B:168:LYS:HD2 | 1:B:169:GLN:H | 1.68 | 0.59 |
| 1:D:168:LYS:HD2 | 1:D:169:GLN:H | 1.68 | 0.59 |
| 1:H:157:VAL:HG22 | 1:H:160:ARG:NH2 | 2.18 | 0.59 |
| 1:J:120:LEU:HD22 | 1:J:157:VAL:HG11 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:168:LYS:HD2 | 1:L:169:GLN:H | 1.68 | 0.59 |
| 1:M:168:LYS:HD2 | 1:M:169:GLN:H | 1.68 | 0.59 |
| 1:M:210:ASP:HB3 | 1:M:215:SER:H | 1.68 | 0.59 |
| 1:O:210:ASP:HB3 | 1:O:215:SER:H | 1.68 | 0.59 |
| 1:C:223:LYS:HA | 1:C:226:GLN:HG2 | 1.83 | 0.59 |
| 1:D:372:ASP:OD2 | 1:D:383:ASN:ND2 | 2.36 | 0.59 |
| 1:E:372:ASP:OD2 | 1:E:383:ASN:ND2 | 2.36 | 0.59 |
| 1:F:157:VAL:HG22 | 1:F:160:ARG:NH2 | 2.18 | 0.59 |
| 1:G:295:GLN:CG | 1:H:257:ASN:ND2 | 2.65 | 0.59 |
| 1:I:157:VAL:HG22 | 1:I:160:ARG:NH2 | 2.18 | 0.59 |
| 1:M:223:LYS:HA | 1:M:226:GLN:HG2 | 1.83 | 0.59 |
| 1:N:157:VAL:HG22 | 1:N:160:ARG:NH2 | 2.18 | 0.59 |
| 1:B:223:LYS:HA | 1:B:226:GLN:HG2 | 1.83 | 0.59 |
| 1:K:168:LYS:HD2 | 1:K:169:GLN:H | 1.68 | 0.59 |
| 1:L:120:LEU:HD22 | 1:L:157:VAL:HG11 | 1.83 | 0.59 |
| 1:N:167:GLU:HA | 1:N:221:PRO:HA | 1.84 | 0.59 |
| 1:N:223:LYS:HA | 1:N:226:GLN:HG2 | 1.83 | 0.59 |
| 1:A:167:GLU:HA | 1:A:221:PRO:HA | 1.84 | 0.59 |
| 1:C:426:VAL:O | 1:D:510:ASN:ND2 | 2.27 | 0.59 |
| 1:F:372:ASP:OD2 | 1:F:383:ASN:ND2 | 2.36 | 0.59 |
| 1:G:157:VAL:HG22 | 1:G:160:ARG:NH2 | 2.18 | 0.59 |
| 1:H:249:TYR:OH | 1:I:317:ARG:O | 2.17 | 0.59 |
| 1:L:157:VAL:HG22 | 1:L:160:ARG:NH2 | 2.18 | 0.59 |
| 1:L:210:ASP:HB3 | 1:L:215:SER:H | 1.68 | 0.59 |
| 1:D:157:VAL:HG22 | 1:D:160:ARG:NH2 | 2.18 | 0.59 |
| 1:I:168:LYS:HD2 | 1:I:169:GLN:H | 1.68 | 0.59 |
| 1:N:168:LYS:HD2 | 1:N:169:GLN:H | 1.68 | 0.59 |
| 1:O:167:GLU:HA | 1:O:221:PRO:HA | 1.84 | 0.59 |
| 1:A:249:TYR:OH | 1:B:317:ARG:O | 2.17 | 0.58 |
| 1:B:157:VAL:HG22 | 1:B:160:ARG:NH2 | 2.18 | 0.58 |
| 1:B:210:ASP:HB3 | 1:B:215:SER:H | 1.68 | 0.58 |
| 1:C:372:ASP:OD2 | 1:C:383:ASN:ND2 | 2.36 | 0.58 |
| 1:O:168:LYS:N | 1:O:220:GLY:O | 2.31 | 0.58 |
| 1:A:157:VAL:HG22 | 1:A:160:ARG:NH2 | 2.18 | 0.58 |
| 1:F:206:LYS:HZ1 | 1:G:190:ILE:HB | 1.67 | 0.58 |
| 1:G:372:ASP:OD2 | 1:G:383:ASN:ND2 | 2.36 | 0.58 |
| 1:J:168:LYS:HD2 | 1:J:169:GLN:H | 1.68 | 0.58 |
| 1:J:355:GLN:HB2 | 1:J:363:ILE:HG22 | 1.84 | 0.58 |
| 1:K:372:ASP:OD2 | 1:K:383:ASN:ND2 | 2.36 | 0.58 |
| 1:N:372:ASP:OD2 | 1:N:383:ASN:ND2 | 2.36 | 0.58 |
| 1:O:355:GLN:HB2 | 1:O:363:ILE:HG22 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:372:ASP:OD2 | 1:O:383:ASN:ND2 | 2.36 | 0.58 |
| 1:A:223:LYS:HA | 1:A:226:GLN:HG2 | 1.83 | 0.58 |
| 1:E:168:LYS:HD2 | 1:E:169:GLN:H | 1.68 | 0.58 |
| 1:G:168:LYS:HD2 | 1:G:169:GLN:H | 1.68 | 0.58 |
| 1:J:157:VAL:HG22 | 1:J:160:ARG:NH2 | 2.18 | 0.58 |
| 1:J:372:ASP:OD2 | 1:J:383:ASN:ND2 | 2.36 | 0.58 |
| 1:K:355:GLN:HB2 | 1:K:363:ILE:HG22 | 1.84 | 0.58 |
| 1:O:223:LYS:HA | 1:O:226:GLN:HG2 | 1.83 | 0.58 |
| 1:D:210:ASP:HB3 | 1:D:215:SER:H | 1.68 | 0.58 |
| 1:K:120:LEU:HD22 | 1:K:157:VAL:HG11 | 1.83 | 0.58 |
| 1:N:355:GLN:HB2 | 1:N:363:ILE:HG22 | 1.84 | 0.58 |
| 1:A:372:ASP:OD2 | 1:A:383:ASN:ND2 | 2.36 | 0.58 |
| 1:A:479:ALA:O | 1:A:570:ILE:HD11 | 2.04 | 0.58 |
| 1:K:210:ASP:HB3 | 1:K:215:SER:H | 1.68 | 0.58 |
| 1:M:372:ASP:OD2 | 1:M:383:ASN:ND2 | 2.36 | 0.58 |
| 1:O:479:ALA:O | 1:O:570:ILE:HD11 | 2.04 | 0.58 |
| 1:A:168:LYS:HD2 | 1:A:169:GLN:H | 1.68 | 0.58 |
| 1:B:479:ALA:O | 1:B:570:ILE:HD11 | 2.04 | 0.58 |
| 1:G:426:VAL:O | 1:H:510:ASN:ND2 | 2.27 | 0.58 |
| 1:H:479:ALA:O | 1:H:570:ILE:HD11 | 2.04 | 0.58 |
| 1:I:578:ARG:O | 1:I:582:LYS:N | 2.32 | 0.58 |
| 1:L:355:GLN:HB2 | 1:L:363:ILE:HG22 | 1.84 | 0.58 |
| 1:E:157:VAL:HG22 | 1:E:160:ARG:NH2 | 2.18 | 0.58 |
| 1:J:210:ASP:HB3 | 1:J:215:SER:H | 1.68 | 0.58 |
| 1:M:355:GLN:HB2 | 1:M:363:ILE:HG22 | 1.84 | 0.58 |
| 1:N:479:ALA:O | 1:N:570:ILE:HD11 | 2.04 | 0.58 |
| 1:B:354:GLN:NE2 | 1:B:356:PHE:HE2 | 2.02 | 0.58 |
| 1:C:210:ASP:HB3 | 1:C:215:SER:H | 1.68 | 0.58 |
| 1:D:479:ALA:O | 1:D:570:ILE:HD11 | 2.04 | 0.58 |
| 1:G:578:ARG:O | 1:G:582:LYS:N | 2.32 | 0.58 |
| 1:H:372:ASP:OD2 | 1:H:383:ASN:ND2 | 2.36 | 0.58 |
| 1:I:372:ASP:OD2 | 1:I:383:ASN:ND2 | 2.36 | 0.58 |
| 1:C:354:GLN:NE2 | 1:C:356:PHE:HE2 | 2.02 | 0.58 |
| 1:C:479:ALA:O | 1:C:570:ILE:HD11 | 2.04 | 0.58 |
| 1:E:479:ALA:O | 1:E:570:ILE:HD11 | 2.04 | 0.58 |
| 1:H:168:LYS:HD2 | 1:H:169:GLN:H | 1.68 | 0.58 |
| 1:H:168:LYS:N | 1:H:220:GLY:O | 2.31 | 0.58 |
| 1:M:157:VAL:HG22 | 1:M:160:ARG:NH2 | 2.18 | 0.58 |
| 1:M:479:ALA:O | 1:M:570:ILE:HD11 | 2.04 | 0.58 |
| 1:A:578:ARG:O | 1:A:582:LYS:N | 2.32 | 0.58 |
| 1:D:354:GLN:NE2 | 1:D:356:PHE:HE2 | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:479:ALA:O | 1:I:570:ILE:HD11 | 2.04 | 0.58 |
| 1:L:372:ASP:OD2 | 1:L:383:ASN:ND2 | 2.36 | 0.58 |
| 1:O:168:LYS:HD2 | 1:O:169:GLN:H | 1.68 | 0.58 |
| 1:B:372:ASP:OD2 | 1:B:383:ASN:ND2 | 2.36 | 0.57 |
| 1:E:210:ASP:HB3 | 1:E:215:SER:H | 1.68 | 0.57 |
| 1:L:479:ALA:O | 1:L:570:ILE:HD11 | 2.04 | 0.57 |
| 1:D:249:TYR:OH | 1:E:317:ARG:O | 2.17 | 0.57 |
| 1:G:210:ASP:HB3 | 1:G:215:SER:H | 1.68 | 0.57 |
| 1:G:479:ALA:O | 1:G:570:ILE:HD11 | 2.04 | 0.57 |
| 1:K:479:ALA:O | 1:K:570:ILE:HD11 | 2.04 | 0.57 |
| 1:M:354:GLN:NE2 | 1:M:356:PHE:HE2 | 2.02 | 0.57 |
| 1:F:168:LYS:HD2 | 1:F:169:GLN:H | 1.68 | 0.57 |
| 1:J:479:ALA:O | 1:J:570:ILE:HD11 | 2.04 | 0.57 |
| 1:N:354:GLN:NE2 | 1:N:356:PHE:HE2 | 2.02 | 0.57 |
| 1:C:231:LEU:O | 1:C:234:SER:HB2 | 2.05 | 0.57 |
| 1:E:231:LEU:O | 1:E:234:SER:HB2 | 2.05 | 0.57 |
| 1:E:354:GLN:NE2 | 1:E:356:PHE:HE2 | 2.02 | 0.57 |
| 1:N:168:LYS:N | 1:N:220:GLY:O | 2.31 | 0.57 |
| 1:N:185:ILE:HG13 | 1:N:186:LEU:N | 2.20 | 0.57 |
| 1:O:185:ILE:HG13 | 1:O:186:LEU:N | 2.20 | 0.57 |
| 1:A:185:ILE:HG13 | 1:A:186:LEU:N | 2.20 | 0.57 |
| 1:A:231:LEU:O | 1:A:234:SER:HB2 | 2.05 | 0.57 |
| 1:B:231:LEU:O | 1:B:234:SER:HB2 | 2.05 | 0.57 |
| 1:D:231:LEU:O | 1:D:234:SER:HB2 | 2.05 | 0.57 |
| 1:F:231:LEU:O | 1:F:234:SER:HB2 | 2.05 | 0.57 |
| 1:H:210:ASP:HB3 | 1:H:215:SER:H | 1.68 | 0.57 |
| 1:M:231:LEU:O | 1:M:234:SER:HB2 | 2.05 | 0.57 |
| 1:L:185:ILE:HG13 | 1:L:186:LEU:N | 2.20 | 0.57 |
| 1:O:231:LEU:O | 1:O:234:SER:HB2 | 2.05 | 0.57 |
| 1:A:354:GLN:NE2 | 1:A:356:PHE:HE2 | 2.02 | 0.57 |
| 1:F:479:ALA:O | 1:F:570:ILE:HD11 | 2.04 | 0.57 |
| 1:L:354:GLN:NE2 | 1:L:356:PHE:HE2 | 2.02 | 0.57 |
| 1:I:231:LEU:O | 1:I:234:SER:HB2 | 2.05 | 0.57 |
| 1:J:185:ILE:HG13 | 1:J:186:LEU:N | 2.20 | 0.57 |
| 1:J:231:LEU:O | 1:J:234:SER:HB2 | 2.05 | 0.57 |
| 1:N:231:LEU:O | 1:N:234:SER:HB2 | 2.05 | 0.57 |
| 1:O:354:GLN:NE2 | 1:O:356:PHE:HE2 | 2.02 | 0.57 |
| 1:G:176:TYR:CE1 | 1:G:238:GLU:OE1 | 2.58 | 0.57 |
| 1:J:176:TYR:CE1 | 1:J:238:GLU:OE1 | 2.58 | 0.57 |
| 1:L:176:TYR:CE1 | 1:L:238:GLU:OE1 | 2.58 | 0.57 |
| 1:C:185:ILE:HG13 | 1:C:186:LEU:N | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:176:TYR:CE1 | 1:F:238:GLU:OE1 | 2.58 | 0.56 |
| 1:I:210:ASP:HB3 | 1:I:215:SER:H | 1.68 | 0.56 |
| 1:M:185:ILE:HG13 | 1:M:186:LEU:N | 2.20 | 0.56 |
| 1:H:354:GLN:NE2 | 1:H:356:PHE:HE2 | 2.02 | 0.56 |
| 1:H:426:VAL:O | 1:I:510:ASN:ND2 | 2.27 | 0.56 |
| 1:I:176:TYR:CE1 | 1:I:238:GLU:OE1 | 2.58 | 0.56 |
| 1:K:185:ILE:HG13 | 1:K:186:LEU:N | 2.20 | 0.56 |
| 1:K:249:TYR:OH | 1:L:317:ARG:O | 2.17 | 0.56 |
| 1:A:344:VAL:HB | 1:A:549:LEU:O | 2.06 | 0.56 |
| 1:G:231:LEU:O | 1:G:234:SER:HB2 | 2.05 | 0.56 |
| 1:H:176:TYR:CE1 | 1:H:238:GLU:OE1 | 2.58 | 0.56 |
| 1:H:185:ILE:HG13 | 1:H:186:LEU:N | 2.20 | 0.56 |
| 1:I:354:GLN:NE2 | 1:I:356:PHE:HE2 | 2.02 | 0.56 |
| 1:K:176:TYR:CE1 | 1:K:238:GLU:OE1 | 2.58 | 0.56 |
| 1:L:231:LEU:O | 1:L:234:SER:HB2 | 2.05 | 0.56 |
| 1:M:176:TYR:CE1 | 1:M:238:GLU:OE1 | 2.58 | 0.56 |
| 1:B:185:ILE:HG13 | 1:B:186:LEU:N | 2.20 | 0.56 |
| 1:F:210:ASP:HB3 | 1:F:215:SER:H | 1.68 | 0.56 |
| 1:J:344:VAL:HB | 1:J:549:LEU:O | 2.06 | 0.56 |
| 1:L:578:ARG:O | 1:L:582:LYS:N | 2.32 | 0.56 |
| 1:N:344:VAL:HB | 1:N:549:LEU:O | 2.06 | 0.56 |
| 1:O:578:ARG:O | 1:O:582:LYS:N | 2.32 | 0.56 |
| 1:D:185:ILE:HG13 | 1:D:186:LEU:N | 2.20 | 0.56 |
| 1:E:344:VAL:HB | 1:E:549:LEU:O | 2.06 | 0.56 |
| 1:F:185:ILE:HG13 | 1:F:186:LEU:N | 2.20 | 0.56 |
| 1:F:354:GLN:NE2 | 1:F:356:PHE:HE2 | 2.02 | 0.56 |
| 1:H:344:VAL:HB | 1:H:549:LEU:O | 2.06 | 0.56 |
| 1:I:344:VAL:HB | 1:I:549:LEU:O | 2.06 | 0.56 |
| 1:K:344:VAL:HB | 1:K:549:LEU:O | 2.06 | 0.56 |
| 1:L:344:VAL:HB | 1:L:549:LEU:O | 2.06 | 0.56 |
| 1:M:344:VAL:HB | 1:M:549:LEU:O | 2.06 | 0.56 |
| 1:N:176:TYR:CE1 | 1:N:238:GLU:OE1 | 2.58 | 0.56 |
| 1:O:344:VAL:HB | 1:O:549:LEU:O | 2.06 | 0.56 |
| 1:C:258:LEU:CD2 | 1:C:318:LEU:HD23 | 2.36 | 0.56 |
| 1:H:231:LEU:O | 1:H:234:SER:HB2 | 2.05 | 0.56 |
| 1:E:176:TYR:CE1 | 1:E:238:GLU:OE1 | 2.58 | 0.56 |
| 1:G:124:MET:HG2 | 1:G:154:LEU:HG | 1.88 | 0.56 |
| 1:J:124:MET:HG2 | 1:J:154:LEU:HG | 1.88 | 0.56 |
| 1:J:354:GLN:NE2 | 1:J:356:PHE:HE2 | 2.02 | 0.56 |
| 1:D:344:VAL:HB | 1:D:549:LEU:O | 2.06 | 0.56 |
| 1:E:161:VAL:HA | 1:E:164:ILE:HG12 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:182:LEU:HD21 | 1:G:216:LEU:HD22 | 1.88 | 0.56 |
| 1:G:185:ILE:HG13 | 1:G:186:LEU:N | 2.20 | 0.56 |
| 1:G:354:GLN:NE2 | 1:G:356:PHE:HE2 | 2.02 | 0.56 |
| 1:I:124:MET:HG2 | 1:I:154:LEU:HG | 1.88 | 0.56 |
| 1:I:161:VAL:HA | 1:I:164:ILE:HG12 | 1.88 | 0.56 |
| 1:I:182:LEU:HD21 | 1:I:216:LEU:HD22 | 1.88 | 0.56 |
| 1:J:182:LEU:HD21 | 1:J:216:LEU:HD22 | 1.88 | 0.56 |
| 1:K:231:LEU:O | 1:K:234:SER:HB2 | 2.05 | 0.56 |
| 1:K:354:GLN:NE2 | 1:K:356:PHE:HE2 | 2.02 | 0.56 |
| 1:M:182:LEU:HD21 | 1:M:216:LEU:HD22 | 1.88 | 0.56 |
| 1:F:161:VAL:HA | 1:F:164:ILE:HG12 | 1.88 | 0.56 |
| 1:F:182:LEU:HD21 | 1:F:216:LEU:HD22 | 1.88 | 0.56 |
| 1:G:344:VAL:HB | 1:G:549:LEU:O | 2.06 | 0.56 |
| 1:H:124:MET:HG2 | 1:H:154:LEU:HG | 1.88 | 0.56 |
| 1:H:161:VAL:HA | 1:H:164:ILE:HG12 | 1.88 | 0.56 |
| 1:I:185:ILE:HG13 | 1:I:186:LEU:N | 2.20 | 0.56 |
| 1:J:249:TYR:OH | 1:K:317:ARG:O | 2.17 | 0.56 |
| 1:L:124:MET:HG2 | 1:L:154:LEU:HG | 1.88 | 0.56 |
| 1:L:182:LEU:HD21 | 1:L:216:LEU:HD22 | 1.88 | 0.56 |
| 1:N:182:LEU:HD21 | 1:N:216:LEU:HD22 | 1.88 | 0.56 |
| 1:B:176:TYR:CE1 | 1:B:238:GLU:OE1 | 2.58 | 0.56 |
| 1:C:176:TYR:CE1 | 1:C:238:GLU:OE1 | 2.58 | 0.56 |
| 1:D:258:LEU:CD2 | 1:D:318:LEU:HD23 | 2.36 | 0.56 |
| 1:E:185:ILE:HG13 | 1:E:186:LEU:N | 2.20 | 0.56 |
| 1:F:249:TYR:OH | 1:G:317:ARG:O | 2.17 | 0.56 |
| 1:G:249:TYR:OH | 1:H:317:ARG:O | 2.17 | 0.56 |
| 1:A:182:LEU:HD21 | 1:A:216:LEU:HD22 | 1.88 | 0.55 |
| 1:B:344:VAL:HB | 1:B:549:LEU:O | 2.06 | 0.55 |
| 1:E:603:LEU:HD13 | 1:G:551:ARG:NH1 | 2.21 | 0.55 |
| 1:F:344:VAL:HB | 1:F:549:LEU:O | 2.06 | 0.55 |
| 1:H:182:LEU:HD21 | 1:H:216:LEU:HD22 | 1.88 | 0.55 |
| 1:K:124:MET:HG2 | 1:K:154:LEU:HG | 1.88 | 0.55 |
| 1:M:124:MET:HG2 | 1:M:154:LEU:HG | 1.88 | 0.55 |
| 1:A:176:TYR:CE1 | 1:A:238:GLU:OE1 | 2.58 | 0.55 |
| 1:D:161:VAL:HA | 1:D:164:ILE:HG12 | 1.88 | 0.55 |
| 1:D:182:LEU:HD21 | 1:D:216:LEU:HD22 | 1.88 | 0.55 |
| 1:J:161:VAL:HA | 1:J:164:ILE:HG12 | 1.88 | 0.55 |
| 1:K:182:LEU:HD21 | 1:K:216:LEU:HD22 | 1.88 | 0.55 |
| 1:M:168:LYS:N | 1:M:220:GLY:O | 2.31 | 0.55 |
| 1:E:124:MET:HG2 | 1:E:154:LEU:HG | 1.88 | 0.55 |
| 1:G:161:VAL:HA | 1:G:164:ILE:HG12 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:182:LEU:HD21 | 1:O:216:LEU:HD22 | 1.88 | 0.55 |
| 1:C:161:VAL:HA | 1:C:164:ILE:HG12 | 1.88 | 0.55 |
| 1:C:182:LEU:HD21 | 1:C:216:LEU:HD22 | 1.88 | 0.55 |
| 1:C:603:LEU:HD13 | 1:E:551:ARG:NH1 | 2.21 | 0.55 |
| 1:D:603:LEU:HD13 | 1:F:551:ARG:NH1 | 2.21 | 0.55 |
| 1:F:266:SER:HB3 | 1:F:290:ILE:HD11 | 1.89 | 0.55 |
| 1:G:603:LEU:HD13 | 1:I:551:ARG:NH1 | 2.21 | 0.55 |
| 1:B:161:VAL:HA | 1:B:164:ILE:HG12 | 1.88 | 0.55 |
| 1:B:182:LEU:HD21 | 1:B:216:LEU:HD22 | 1.88 | 0.55 |
| 1:D:176:TYR:CE1 | 1:D:238:GLU:OE1 | 2.58 | 0.55 |
| 1:E:182:LEU:HD21 | 1:E:216:LEU:HD22 | 1.88 | 0.55 |
| 1:E:266:SER:HB3 | 1:E:290:ILE:HD11 | 1.89 | 0.55 |
| 1:J:105:ARG:NE | 1:J:151:ILE:HD12 | 2.22 | 0.55 |
| 1:K:161:VAL:HA | 1:K:164:ILE:HG12 | 1.88 | 0.55 |
| 1:L:161:VAL:HA | 1:L:164:ILE:HG12 | 1.88 | 0.55 |
| 1:O:176:TYR:CE1 | 1:O:238:GLU:OE1 | 2.58 | 0.55 |
| 1:G:266:SER:HB3 | 1:G:290:ILE:HD11 | 1.89 | 0.55 |
| 1:M:603:LEU:HD13 | 1:O:551:ARG:NH1 | 2.21 | 0.55 |
| 1:D:124:MET:HG2 | 1:D:154:LEU:HG | 1.88 | 0.55 |
| 1:F:124:MET:HG2 | 1:F:154:LEU:HG | 1.88 | 0.55 |
| 1:J:151:ILE:O | 1:J:155:ILE:HG12 | 2.07 | 0.55 |
| 1:K:153:LYS:HA | 1:K:156:GLU:HB2 | 1.89 | 0.55 |
| 1:K:496:ASN:OD1 | 1:K:497:SER:N | 2.40 | 0.55 |
| 1:K:603:LEU:HD13 | 1:M:551:ARG:NH1 | 2.21 | 0.55 |
| 1:A:551:ARG:NH1 | 1:N:603:LEU:HD13 | 2.21 | 0.55 |
| 1:B:151:ILE:O | 1:B:155:ILE:HG12 | 2.07 | 0.55 |
| 1:B:603:LEU:HD13 | 1:D:551:ARG:NH1 | 2.21 | 0.55 |
| 1:C:344:VAL:HB | 1:C:549:LEU:O | 2.06 | 0.55 |
| 1:F:151:ILE:O | 1:F:155:ILE:HG12 | 2.07 | 0.55 |
| 1:F:603:LEU:HD13 | 1:H:551:ARG:NH1 | 2.21 | 0.55 |
| 1:K:258:LEU:CD2 | 1:K:318:LEU:HD23 | 2.36 | 0.55 |
| 1:M:258:LEU:CD2 | 1:M:318:LEU:HD23 | 2.36 | 0.55 |
| 1:M:496:ASN:OD1 | 1:M:497:SER:N | 2.40 | 0.55 |
| 1:O:266:SER:HB3 | 1:O:290:ILE:HD11 | 1.89 | 0.55 |
| 1:B:551:ARG:NH1 | 1:O:603:LEU:HD13 | 2.21 | 0.55 |
| 1:D:266:SER:HB3 | 1:D:290:ILE:HD11 | 1.89 | 0.55 |
| 1:I:426:VAL:O | 1:J:510:ASN:ND2 | 2.27 | 0.55 |
| 1:J:258:LEU:CD2 | 1:J:318:LEU:HD23 | 2.36 | 0.55 |
| 1:J:496:ASN:OD1 | 1:J:497:SER:N | 2.40 | 0.55 |
| 1:L:258:LEU:CD2 | 1:L:318:LEU:HD23 | 2.36 | 0.55 |
| 1:N:124:MET:HG2 | 1:N:154:LEU:HG | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:124:MET:HG2 | 1:O:154:LEU:HG | 1.88 | 0.55 |
| 1:B:496:ASN:OD1 | 1:B:497:SER:N | 2.40 | 0.55 |
| 1:F:496:ASN:OD1 | 1:F:497:SER:N | 2.40 | 0.55 |
| 1:H:258:LEU:CD2 | 1:H:318:LEU:HD23 | 2.36 | 0.55 |
| 1:J:153:LYS:HA | 1:J:156:GLU:HB2 | 1.89 | 0.55 |
| 1:J:426:VAL:O | 1:K:510:ASN:ND2 | 2.27 | 0.55 |
| 1:M:414:ASN:HB3 | 1:N:534:VAL:HG22 | 1.90 | 0.55 |
| 1:N:266:SER:HB3 | 1:N:290:ILE:HD11 | 1.89 | 0.55 |
| 1:A:124:MET:HG2 | 1:A:154:LEU:HG | 1.88 | 0.54 |
| 1:A:151:ILE:O | 1:A:155:ILE:HG12 | 2.07 | 0.54 |
| 1:A:266:SER:HB3 | 1:A:290:ILE:HD11 | 1.89 | 0.54 |
| 1:C:151:ILE:O | 1:C:155:ILE:HG12 | 2.07 | 0.54 |
| 1:C:496:ASN:OD1 | 1:C:497:SER:N | 2.40 | 0.54 |
| 1:E:151:ILE:O | 1:E:155:ILE:HG12 | 2.07 | 0.54 |
| 1:E:258:LEU:CD2 | 1:E:318:LEU:HD23 | 2.36 | 0.54 |
| 1:E:496:ASN:OD1 | 1:E:497:SER:N | 2.40 | 0.54 |
| 1:G:105:ARG:NE | 1:G:151:ILE:HD12 | 2.22 | 0.54 |
| 1:G:288:VAL:HG22 | 1:G:303:ALA:CB | 2.38 | 0.54 |
| 1:I:105:ARG:NE | 1:I:151:ILE:HD12 | 2.22 | 0.54 |
| 1:I:151:ILE:O | 1:I:155:ILE:HG12 | 2.07 | 0.54 |
| 1:I:496:ASN:OD1 | 1:I:497:SER:N | 2.40 | 0.54 |
| 1:K:414:ASN:HB3 | 1:L:534:VAL:HG22 | 1.90 | 0.54 |
| 1:L:603:LEU:HD13 | 1:N:551:ARG:NH1 | 2.21 | 0.54 |
| 1:N:161:VAL:HA | 1:N:164:ILE:HG12 | 1.88 | 0.54 |
| 1:O:161:VAL:HA | 1:O:164:ILE:HG12 | 1.88 | 0.54 |
| 1:A:161:VAL:HA | 1:A:164:ILE:HG12 | 1.88 | 0.54 |
| 1:E:105:ARG:NE | 1:E:151:ILE:HD12 | 2.22 | 0.54 |
| 1:E:118:ALA:HA | 1:E:136:TYR:OH | 2.07 | 0.54 |
| 1:F:105:ARG:NE | 1:F:151:ILE:HD12 | 2.22 | 0.54 |
| 1:H:414:ASN:HB3 | 1:I:534:VAL:HG22 | 1.90 | 0.54 |
| 1:I:603:LEU:HD13 | 1:K:551:ARG:NH1 | 2.21 | 0.54 |
| 1:K:105:ARG:NE | 1:K:151:ILE:HD12 | 2.22 | 0.54 |
| 1:K:151:ILE:O | 1:K:155:ILE:HG12 | 2.07 | 0.54 |
| 1:M:118:ALA:HA | 1:M:136:TYR:OH | 2.07 | 0.54 |
| 1:M:161:VAL:HA | 1:M:164:ILE:HG12 | 1.88 | 0.54 |
| 1:N:258:LEU:CD2 | 1:N:318:LEU:HD23 | 2.36 | 0.54 |
| 1:N:496:ASN:OD1 | 1:N:497:SER:N | 2.40 | 0.54 |
| 1:A:603:LEU:HD13 | 1:C:551:ARG:NH1 | 2.21 | 0.54 |
| 1:C:288:VAL:HG22 | 1:C:303:ALA:CB | 2.38 | 0.54 |
| 1:D:105:ARG:NE | 1:D:151:ILE:HD12 | 2.22 | 0.54 |
| 1:D:118:ALA:HA | 1:D:136:TYR:OH | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:414:ASN:HB3 | 1:K:534:VAL:HG22 | 1.90 | 0.54 |
| 1:N:153:LYS:HA | 1:N:156:GLU:HB2 | 1.89 | 0.54 |
| 1:N:414:ASN:HB3 | 1:O:534:VAL:HG22 | 1.90 | 0.54 |
| 1:A:288:VAL:HG22 | 1:A:303:ALA:CB | 2.38 | 0.54 |
| 1:B:124:MET:HG2 | 1:B:154:LEU:HG | 1.88 | 0.54 |
| 1:B:288:VAL:HG22 | 1:B:303:ALA:CB | 2.38 | 0.54 |
| 1:C:105:ARG:NE | 1:C:151:ILE:HD12 | 2.22 | 0.54 |
| 1:F:130:VAL:HG22 | 1:F:131:GLY:H | 1.73 | 0.54 |
| 1:G:151:ILE:O | 1:G:155:ILE:HG12 | 2.07 | 0.54 |
| 1:H:578:ARG:O | 1:H:582:LYS:N | 2.32 | 0.54 |
| 1:I:221:PRO:HG2 | 1:I:224:ALA:H | 1.73 | 0.54 |
| 1:I:414:ASN:HB3 | 1:J:534:VAL:HG22 | 1.90 | 0.54 |
| 1:L:118:ALA:HA | 1:L:136:TYR:OH | 2.07 | 0.54 |
| 1:C:124:MET:HG2 | 1:C:154:LEU:HG | 1.88 | 0.54 |
| 1:D:288:VAL:HG22 | 1:D:303:ALA:CB | 2.38 | 0.54 |
| 1:G:130:VAL:HG22 | 1:G:131:GLY:H | 1.73 | 0.54 |
| 1:G:221:PRO:HG2 | 1:G:224:ALA:H | 1.73 | 0.54 |
| 1:H:221:PRO:HG2 | 1:H:224:ALA:H | 1.73 | 0.54 |
| 1:H:266:SER:HB3 | 1:H:290:ILE:HD11 | 1.89 | 0.54 |
| 1:L:414:ASN:HB3 | 1:M:534:VAL:HG22 | 1.90 | 0.54 |
| 1:M:105:ARG:NE | 1:M:151:ILE:HD12 | 2.22 | 0.54 |
| 1:M:266:SER:HB3 | 1:M:290:ILE:HD11 | 1.89 | 0.54 |
| 1:N:118:ALA:HA | 1:N:136:TYR:OH | 2.07 | 0.54 |
| 1:O:288:VAL:HG22 | 1:O:303:ALA:CB | 2.38 | 0.54 |
| 1:O:473:GLN:HB3 | 1:O:481:LEU:HB3 | 1.90 | 0.54 |
| 1:A:414:ASN:HB3 | 1:B:534:VAL:HG22 | 1.90 | 0.54 |
| 1:B:105:ARG:NE | 1:B:151:ILE:HD12 | 2.22 | 0.54 |
| 1:B:130:VAL:HG22 | 1:B:131:GLY:H | 1.73 | 0.54 |
| 1:B:212:ARG:HH12 | 1:C:177:ALA:CB | 2.21 | 0.54 |
| 1:B:266:SER:HB3 | 1:B:290:ILE:HD11 | 1.89 | 0.54 |
| 1:C:212:ARG:HH12 | 1:D:177:ALA:CB | 2.21 | 0.54 |
| 1:D:212:ARG:HH12 | 1:E:177:ALA:CB | 2.21 | 0.54 |
| 1:E:212:ARG:HH12 | 1:F:177:ALA:CB | 2.21 | 0.54 |
| 1:E:288:VAL:HG22 | 1:E:303:ALA:CB | 2.38 | 0.54 |
| 1:H:288:VAL:HG22 | 1:H:303:ALA:CB | 2.38 | 0.54 |
| 1:M:153:LYS:HA | 1:M:156:GLU:HB2 | 1.89 | 0.54 |
| 1:N:105:ARG:NE | 1:N:151:ILE:HD12 | 2.22 | 0.54 |
| 1:O:130:VAL:HG22 | 1:O:131:GLY:H | 1.73 | 0.54 |
| 1:A:473:GLN:HB3 | 1:A:481:LEU:HB3 | 1.90 | 0.54 |
| 1:A:534:VAL:HG22 | 1:O:414:ASN:HB3 | 1.90 | 0.54 |
| 1:C:118:ALA:HA | 1:C:136:TYR:OH | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:224:ALA:HA | 1:D:227:ARG:HG2 | 1.90 | 0.54 |
| 1:E:130:VAL:HG22 | 1:E:131:GLY:H | 1.73 | 0.54 |
| 1:E:153:LYS:HA | 1:E:156:GLU:HB2 | 1.89 | 0.54 |
| 1:F:288:VAL:HG22 | 1:F:303:ALA:CB | 2.38 | 0.54 |
| 1:F:473:GLN:HB3 | 1:F:481:LEU:HB3 | 1.90 | 0.54 |
| 1:H:153:LYS:HA | 1:H:156:GLU:HB2 | 1.89 | 0.54 |
| 1:K:118:ALA:HA | 1:K:136:TYR:OH | 2.07 | 0.54 |
| 1:L:153:LYS:HA | 1:L:156:GLU:HB2 | 1.89 | 0.54 |
| 1:L:266:SER:HB3 | 1:L:290:ILE:HD11 | 1.89 | 0.54 |
| 1:L:496:ASN:OD1 | 1:L:497:SER:N | 2.40 | 0.54 |
| 1:N:130:VAL:HG22 | 1:N:131:GLY:H | 1.73 | 0.54 |
| 1:N:473:GLN:HB3 | 1:N:481:LEU:HB3 | 1.90 | 0.54 |
| 1:A:224:ALA:HA | 1:A:227:ARG:HG2 | 1.90 | 0.54 |
| 1:B:224:ALA:HA | 1:B:227:ARG:HG2 | 1.90 | 0.54 |
| 1:C:153:LYS:HA | 1:C:156:GLU:HB2 | 1.89 | 0.54 |
| 1:C:249:TYR:OH | 1:D:317:ARG:O | 2.17 | 0.54 |
| 1:D:130:VAL:HG22 | 1:D:131:GLY:H | 1.73 | 0.54 |
| 1:F:118:ALA:HA | 1:F:136:TYR:OH | 2.07 | 0.54 |
| 1:F:221:PRO:HG2 | 1:F:224:ALA:H | 1.73 | 0.54 |
| 1:G:118:ALA:HA | 1:G:136:TYR:OH | 2.07 | 0.54 |
| 1:G:153:LYS:HA | 1:G:156:GLU:HB2 | 1.89 | 0.54 |
| 1:G:414:ASN:HB3 | 1:H:534:VAL:HG22 | 1.90 | 0.54 |
| 1:H:118:ALA:HA | 1:H:136:TYR:OH | 2.07 | 0.54 |
| 1:H:603:LEU:HD13 | 1:J:551:ARG:NH1 | 2.21 | 0.54 |
| 1:I:288:VAL:HG22 | 1:I:303:ALA:CB | 2.38 | 0.54 |
| 1:L:224:ALA:HA | 1:L:227:ARG:HG2 | 1.90 | 0.54 |
| 1:N:224:ALA:HA | 1:N:227:ARG:HG2 | 1.90 | 0.54 |
| 1:O:118:ALA:HA | 1:O:136:TYR:OH | 2.07 | 0.54 |
| 1:O:151:ILE:O | 1:O:155:ILE:HG12 | 2.07 | 0.54 |
| 1:O:153:LYS:HA | 1:O:156:GLU:HB2 | 1.89 | 0.54 |
| 1:O:496:ASN:OD1 | 1:O:497:SER:N | 2.40 | 0.54 |
| 1:A:130:VAL:HG22 | 1:A:131:GLY:H | 1.73 | 0.54 |
| 1:A:496:ASN:OD1 | 1:A:497:SER:N | 2.40 | 0.54 |
| 1:C:224:ALA:HA | 1:C:227:ARG:HG2 | 1.90 | 0.54 |
| 1:C:266:SER:HB3 | 1:C:290:ILE:HD11 | 1.89 | 0.54 |
| 1:E:216:LEU:HD23 | 1:E:232:LEU:HD11 | 1.90 | 0.54 |
| 1:E:224:ALA:HA | 1:E:227:ARG:HG2 | 1.90 | 0.54 |
| 1:F:134:VAL:HG22 | 1:F:144:LEU:HD22 | 1.90 | 0.54 |
| 1:F:414:ASN:HB3 | 1:G:534:VAL:HG22 | 1.90 | 0.54 |
| 1:G:216:LEU:HD23 | 1:G:232:LEU:HD11 | 1.90 | 0.54 |
| 1:G:473:GLN:HB3 | 1:G:481:LEU:HB3 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:496:ASN:OD1 | 1:G:497:SER:N | 2.40 | 0.54 |
| 1:H:134:VAL:HG22 | 1:H:144:LEU:HD22 | 1.90 | 0.54 |
| 1:H:151:ILE:O | 1:H:155:ILE:HG12 | 2.07 | 0.54 |
| 1:I:118:ALA:HA | 1:I:136:TYR:OH | 2.07 | 0.54 |
| 1:J:221:PRO:HG2 | 1:J:224:ALA:H | 1.73 | 0.54 |
| 1:J:288:VAL:HG22 | 1:J:303:ALA:CB | 2.38 | 0.54 |
| 1:K:224:ALA:HA | 1:K:227:ARG:HG2 | 1.90 | 0.54 |
| 1:K:288:VAL:HG22 | 1:K:303:ALA:CB | 2.38 | 0.54 |
| 1:L:151:ILE:O | 1:L:155:ILE:HG12 | 2.07 | 0.54 |
| 1:A:105:ARG:NE | 1:A:151:ILE:HD12 | 2.22 | 0.54 |
| 1:A:118:ALA:HA | 1:A:136:TYR:OH | 2.07 | 0.54 |
| 1:A:134:VAL:HG22 | 1:A:144:LEU:HD22 | 1.90 | 0.54 |
| 1:B:414:ASN:HB3 | 1:C:534:VAL:HG22 | 1.90 | 0.54 |
| 1:D:216:LEU:HD23 | 1:D:232:LEU:HD11 | 1.90 | 0.54 |
| 1:D:578:ARG:O | 1:D:582:LYS:N | 2.32 | 0.54 |
| 1:E:221:PRO:HG2 | 1:E:224:ALA:H | 1.73 | 0.54 |
| 1:E:414:ASN:HB3 | 1:F:534:VAL:HG22 | 1.90 | 0.54 |
| 1:E:473:GLN:HB3 | 1:E:481:LEU:HB3 | 1.90 | 0.54 |
| 1:F:212:ARG:HH12 | 1:G:177:ALA:CB | 2.21 | 0.54 |
| 1:F:216:LEU:HD23 | 1:F:232:LEU:HD11 | 1.91 | 0.54 |
| 1:H:105:ARG:NE | 1:H:151:ILE:HD12 | 2.22 | 0.54 |
| 1:H:130:VAL:HG22 | 1:H:131:GLY:H | 1.73 | 0.54 |
| 1:K:266:SER:HB3 | 1:K:290:ILE:HD11 | 1.89 | 0.54 |
| 1:L:105:ARG:NE | 1:L:151:ILE:HD12 | 2.22 | 0.54 |
| 1:L:212:ARG:HH12 | 1:M:177:ALA:CB | 2.21 | 0.54 |
| 1:M:224:ALA:HA | 1:M:227:ARG:HG2 | 1.90 | 0.54 |
| 1:N:288:VAL:HG22 | 1:N:303:ALA:CB | 2.38 | 0.54 |
| 1:O:224:ALA:HA | 1:O:227:ARG:HG2 | 1.90 | 0.54 |
| 1:O:258:LEU:CD2 | 1:O:318:LEU:HD23 | 2.36 | 0.54 |
| 1:A:212:ARG:HH12 | 1:B:177:ALA:CB | 2.21 | 0.53 |
| 1:C:216:LEU:HD23 | 1:C:232:LEU:HD11 | 1.90 | 0.53 |
| 1:D:134:VAL:HG22 | 1:D:144:LEU:HD22 | 1.90 | 0.53 |
| 1:D:496:ASN:OD1 | 1:D:497:SER:N | 2.40 | 0.53 |
| 1:E:304:ASP:OD1 | 1:E:305:GLN:N | 2.42 | 0.53 |
| 1:K:212:ARG:HH12 | 1:L:177:ALA:CB | 2.21 | 0.53 |
| 1:K:304:ASP:OD1 | 1:K:305:GLN:N | 2.42 | 0.53 |
| 1:M:212:ARG:HH12 | 1:N:177:ALA:CB | 2.21 | 0.53 |
| 1:M:473:GLN:HB3 | 1:M:481:LEU:HB3 | 1.90 | 0.53 |
| 1:N:134:VAL:HG22 | 1:N:144:LEU:HD22 | 1.90 | 0.53 |
| 1:N:578:ARG:O | 1:N:582:LYS:N | 2.32 | 0.53 |
| 1:O:105:ARG:NE | 1:O:151:ILE:HD12 | 2.22 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:153:LYS:HA | 1:B:156:GLU:HB2 | 1.89 | 0.53 |
| 1:D:304:ASP:OD1 | 1:D:305:GLN:N | 2.42 | 0.53 |
| 1:F:258:LEU:CD2 | 1:F:318:LEU:HD23 | 2.36 | 0.53 |
| 1:F:304:ASP:OD1 | 1:F:305:GLN:N | 2.42 | 0.53 |
| 1:H:216:LEU:HD23 | 1:H:232:LEU:HD11 | 1.90 | 0.53 |
| 1:K:578:ARG:O | 1:K:582:LYS:N | 2.32 | 0.53 |
| 1:M:130:VAL:HG22 | 1:M:131:GLY:H | 1.73 | 0.53 |
| 1:O:221:PRO:HG2 | 1:O:224:ALA:H | 1.73 | 0.53 |
| 1:A:177:ALA:CB | 1:O:212:ARG:HH12 | 2.21 | 0.53 |
| 1:B:473:GLN:HB3 | 1:B:481:LEU:HB3 | 1.90 | 0.53 |
| 1:C:578:ARG:O | 1:C:582:LYS:N | 2.32 | 0.53 |
| 1:D:151:ILE:O | 1:D:155:ILE:HG12 | 2.07 | 0.53 |
| 1:D:414:ASN:HB3 | 1:E:534:VAL:HG22 | 1.90 | 0.53 |
| 1:D:473:GLN:HB3 | 1:D:481:LEU:HB3 | 1.90 | 0.53 |
| 1:E:578:ARG:O | 1:E:582:LYS:N | 2.32 | 0.53 |
| 1:H:473:GLN:HB3 | 1:H:481:LEU:HB3 | 1.90 | 0.53 |
| 1:J:212:ARG:HH12 | 1:K:177:ALA:CB | 2.21 | 0.53 |
| 1:J:603:LEU:HD13 | 1:L:551:ARG:NH1 | 2.21 | 0.53 |
| 1:L:168:LYS:N | 1:L:220:GLY:O | 2.30 | 0.53 |
| 1:M:288:VAL:HG22 | 1:M:303:ALA:CB | 2.38 | 0.53 |
| 1:N:221:PRO:HG2 | 1:N:224:ALA:H | 1.73 | 0.53 |
| 1:C:304:ASP:OD1 | 1:C:305:GLN:N | 2.42 | 0.53 |
| 1:D:153:LYS:HA | 1:D:156:GLU:HB2 | 1.89 | 0.53 |
| 1:D:221:PRO:HG2 | 1:D:224:ALA:H | 1.73 | 0.53 |
| 1:F:224:ALA:HA | 1:F:227:ARG:HG2 | 1.90 | 0.53 |
| 1:F:578:ARG:O | 1:F:582:LYS:N | 2.32 | 0.53 |
| 1:H:224:ALA:HA | 1:H:227:ARG:HG2 | 1.90 | 0.53 |
| 1:I:153:LYS:HA | 1:I:156:GLU:HB2 | 1.89 | 0.53 |
| 1:I:212:ARG:HH12 | 1:J:177:ALA:CB | 2.21 | 0.53 |
| 1:J:118:ALA:HA | 1:J:136:TYR:OH | 2.07 | 0.53 |
| 1:J:134:VAL:HG22 | 1:J:144:LEU:HD22 | 1.90 | 0.53 |
| 1:J:266:SER:HB3 | 1:J:290:ILE:HD11 | 1.89 | 0.53 |
| 1:L:304:ASP:OD1 | 1:L:305:GLN:N | 2.42 | 0.53 |
| 1:N:212:ARG:HH12 | 1:O:177:ALA:CB | 2.21 | 0.53 |
| 1:O:304:ASP:OD1 | 1:O:305:GLN:N | 2.42 | 0.53 |
| 1:B:216:LEU:HD23 | 1:B:232:LEU:HD11 | 1.90 | 0.53 |
| 1:C:134:VAL:HG22 | 1:C:144:LEU:HD22 | 1.90 | 0.53 |
| 1:F:153:LYS:HA | 1:F:156:GLU:HB2 | 1.89 | 0.53 |
| 1:G:157:VAL:HG22 | 1:G:160:ARG:HH21 | 1.74 | 0.53 |
| 1:G:224:ALA:HA | 1:G:227:ARG:HG2 | 1.90 | 0.53 |
| 1:G:304:ASP:OD1 | 1:G:305:GLN:N | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:216:LEU:HD23 | 1:I:232:LEU:HD11 | 1.90 | 0.53 |
| 1:I:224:ALA:HA | 1:I:227:ARG:HG2 | 1.90 | 0.53 |
| 1:I:266:SER:HB3 | 1:I:290:ILE:HD11 | 1.89 | 0.53 |
| 1:I:589:ARG:HG3 | 1:I:611:VAL:HG22 | 1.91 | 0.53 |
| 1:J:224:ALA:HA | 1:J:227:ARG:HG2 | 1.90 | 0.53 |
| 1:J:304:ASP:OD1 | 1:J:305:GLN:N | 2.42 | 0.53 |
| 1:J:589:ARG:HG3 | 1:J:611:VAL:HG22 | 1.91 | 0.53 |
| 1:L:134:VAL:HG22 | 1:L:144:LEU:HD22 | 1.90 | 0.53 |
| 1:L:288:VAL:HG22 | 1:L:303:ALA:CB | 2.38 | 0.53 |
| 1:N:259:VAL:HG21 | 1:N:292:ALA:HB2 | 1.90 | 0.53 |
| 1:A:174:LEU:HG | 1:A:216:LEU:N | 2.24 | 0.53 |
| 1:B:134:VAL:HG22 | 1:B:144:LEU:HD22 | 1.90 | 0.53 |
| 1:H:212:ARG:HH12 | 1:I:177:ALA:CB | 2.21 | 0.53 |
| 1:I:258:LEU:CD2 | 1:I:318:LEU:HD23 | 2.36 | 0.53 |
| 1:K:259:VAL:HG21 | 1:K:292:ALA:HB2 | 1.90 | 0.53 |
| 1:M:151:ILE:O | 1:M:155:ILE:HG12 | 2.07 | 0.53 |
| 1:N:151:ILE:O | 1:N:155:ILE:HG12 | 2.07 | 0.53 |
| 1:N:174:LEU:HG | 1:N:216:LEU:N | 2.24 | 0.53 |
| 1:A:221:PRO:HG2 | 1:A:224:ALA:H | 1.73 | 0.53 |
| 1:B:118:ALA:HA | 1:B:136:TYR:OH | 2.07 | 0.53 |
| 1:C:414:ASN:HB3 | 1:D:534:VAL:HG22 | 1.90 | 0.53 |
| 1:D:259:VAL:HG21 | 1:D:292:ALA:HB2 | 1.90 | 0.53 |
| 1:G:589:ARG:HG3 | 1:G:611:VAL:HG22 | 1.91 | 0.53 |
| 1:H:496:ASN:OD1 | 1:H:497:SER:N | 2.40 | 0.53 |
| 1:J:216:LEU:HD23 | 1:J:232:LEU:HD11 | 1.90 | 0.53 |
| 1:M:259:VAL:HG21 | 1:M:292:ALA:HB2 | 1.90 | 0.53 |
| 1:N:304:ASP:OD1 | 1:N:305:GLN:N | 2.42 | 0.53 |
| 1:O:157:VAL:HG22 | 1:O:160:ARG:HH21 | 1.74 | 0.53 |
| 1:A:153:LYS:HA | 1:A:156:GLU:HB2 | 1.89 | 0.53 |
| 1:A:216:LEU:HD23 | 1:A:232:LEU:HD11 | 1.90 | 0.53 |
| 1:A:304:ASP:OD1 | 1:A:305:GLN:N | 2.42 | 0.53 |
| 1:B:242:GLU:HG2 | 1:B:243:GLY:H | 1.60 | 0.53 |
| 1:C:174:LEU:HG | 1:C:216:LEU:N | 2.24 | 0.53 |
| 1:C:221:PRO:HG2 | 1:C:224:ALA:H | 1.73 | 0.53 |
| 1:C:473:GLN:HB3 | 1:C:481:LEU:HB3 | 1.90 | 0.53 |
| 1:D:288:VAL:HG13 | 1:D:303:ALA:HB2 | 1.91 | 0.53 |
| 1:G:212:ARG:HH12 | 1:H:177:ALA:CB | 2.21 | 0.53 |
| 1:H:174:LEU:HG | 1:H:216:LEU:N | 2.24 | 0.53 |
| 1:I:130:VAL:HG22 | 1:I:131:GLY:H | 1.72 | 0.53 |
| 1:I:174:LEU:HG | 1:I:216:LEU:N | 2.24 | 0.53 |
| 1:J:578:ARG:O | 1:J:582:LYS:N | 2.32 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:130:VAL:HG22 | 1:K:131:GLY:H | 1.73 | 0.53 |
| 1:K:221:PRO:HG2 | 1:K:224:ALA:H | 1.73 | 0.53 |
| 1:L:589:ARG:HG3 | 1:L:611:VAL:HG22 | 1.91 | 0.53 |
| 1:O:109:LEU:HG | 1:O:112:VAL:O | 2.09 | 0.53 |
| 1:A:288:VAL:HG13 | 1:A:303:ALA:HB2 | 1.91 | 0.53 |
| 1:C:130:VAL:HG22 | 1:C:131:GLY:H | 1.73 | 0.53 |
| 1:C:259:VAL:HG21 | 1:C:292:ALA:HB2 | 1.90 | 0.53 |
| 1:E:259:VAL:HG21 | 1:E:292:ALA:HB2 | 1.90 | 0.53 |
| 1:F:288:VAL:HG13 | 1:F:303:ALA:HB2 | 1.91 | 0.53 |
| 1:G:174:LEU:HG | 1:G:216:LEU:N | 2.24 | 0.53 |
| 1:G:288:VAL:HG13 | 1:G:303:ALA:HB2 | 1.91 | 0.53 |
| 1:H:304:ASP:OD1 | 1:H:305:GLN:N | 2.42 | 0.53 |
| 1:H:589:ARG:HG3 | 1:H:611:VAL:HG22 | 1.91 | 0.53 |
| 1:I:134:VAL:HG22 | 1:I:144:LEU:HD22 | 1.90 | 0.53 |
| 1:I:288:VAL:HG13 | 1:I:303:ALA:HB2 | 1.91 | 0.53 |
| 1:K:216:LEU:HD23 | 1:K:232:LEU:HD11 | 1.90 | 0.53 |
| 1:L:157:VAL:HG22 | 1:L:160:ARG:HH21 | 1.74 | 0.53 |
| 1:L:216:LEU:HD23 | 1:L:232:LEU:HD11 | 1.90 | 0.53 |
| 1:L:221:PRO:HG2 | 1:L:224:ALA:H | 1.73 | 0.53 |
| 1:L:473:GLN:HB3 | 1:L:481:LEU:HB3 | 1.90 | 0.53 |
| 1:M:221:PRO:HG2 | 1:M:224:ALA:H | 1.73 | 0.53 |
| 1:O:216:LEU:HD23 | 1:O:232:LEU:HD11 | 1.90 | 0.53 |
| 1:B:157:VAL:HG22 | 1:B:160:ARG:HH21 | 1.74 | 0.53 |
| 1:B:288:VAL:HG13 | 1:B:303:ALA:HB2 | 1.91 | 0.53 |
| 1:F:589:ARG:HG3 | 1:F:611:VAL:HG22 | 1.91 | 0.53 |
| 1:J:160:ARG:O | 1:J:164:ILE:HG12 | 2.09 | 0.53 |
| 1:J:174:LEU:HG | 1:J:216:LEU:N | 2.24 | 0.53 |
| 1:K:589:ARG:HG3 | 1:K:611:VAL:HG22 | 1.91 | 0.53 |
| 1:L:109:LEU:HG | 1:L:112:VAL:O | 2.09 | 0.53 |
| 1:L:130:VAL:HG22 | 1:L:131:GLY:H | 1.73 | 0.53 |
| 1:M:301:ILE:HG22 | 1:M:308:GLN:HE22 | 1.74 | 0.53 |
| 1:N:216:LEU:HD23 | 1:N:232:LEU:HD11 | 1.90 | 0.53 |
| 1:A:160:ARG:HG2 | 1:A:164:ILE:HD13 | 1.91 | 0.52 |
| 1:B:304:ASP:OD1 | 1:B:305:GLN:N | 2.42 | 0.52 |
| 1:C:109:LEU:HG | 1:C:112:VAL:O | 2.09 | 0.52 |
| 1:C:160:ARG:HG2 | 1:C:164:ILE:HD13 | 1.91 | 0.52 |
| 1:C:288:VAL:HG13 | 1:C:303:ALA:HB2 | 1.91 | 0.52 |
| 1:G:134:VAL:HG22 | 1:G:144:LEU:HD22 | 1.90 | 0.52 |
| 1:H:301:ILE:HG22 | 1:H:308:GLN:HE22 | 1.74 | 0.52 |
| 1:I:157:VAL:HG22 | 1:I:160:ARG:HH21 | 1.74 | 0.52 |
| 1:I:473:GLN:HB3 | 1:I:481:LEU:HB3 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:109:LEU:HG | 1:J:112:VAL:O | 2.09 | 0.52 |
| 1:J:288:VAL:HG13 | 1:J:303:ALA:HB2 | 1.91 | 0.52 |
| 1:K:160:ARG:O | 1:K:164:ILE:HG12 | 2.09 | 0.52 |
| 1:L:174:LEU:HG | 1:L:216:LEU:N | 2.24 | 0.52 |
| 1:L:242:GLU:HG2 | 1:L:243:GLY:H | 1.60 | 0.52 |
| 1:M:216:LEU:HD23 | 1:M:232:LEU:HD11 | 1.90 | 0.52 |
| 1:O:301:ILE:HG22 | 1:O:308:GLN:HE22 | 1.74 | 0.52 |
| 1:B:174:LEU:HG | 1:B:216:LEU:N | 2.24 | 0.52 |
| 1:D:157:VAL:HG22 | 1:D:160:ARG:HH21 | 1.74 | 0.52 |
| 1:E:288:VAL:HG13 | 1:E:303:ALA:HB2 | 1.91 | 0.52 |
| 1:F:174:LEU:HG | 1:F:216:LEU:N | 2.24 | 0.52 |
| 1:H:288:VAL:HG13 | 1:H:303:ALA:HB2 | 1.91 | 0.52 |
| 1:I:109:LEU:HG | 1:I:112:VAL:O | 2.09 | 0.52 |
| 1:I:160:ARG:O | 1:I:164:ILE:HG12 | 2.09 | 0.52 |
| 1:L:160:ARG:O | 1:L:164:ILE:HG12 | 2.09 | 0.52 |
| 1:L:259:VAL:HG21 | 1:L:292:ALA:HB2 | 1.90 | 0.52 |
| 1:N:160:ARG:HG2 | 1:N:164:ILE:HD13 | 1.91 | 0.52 |
| 1:O:134:VAL:HG22 | 1:O:144:LEU:HD22 | 1.90 | 0.52 |
| 1:O:288:VAL:HG13 | 1:O:303:ALA:HB2 | 1.91 | 0.52 |
| 1:A:258:LEU:CD2 | 1:A:318:LEU:HD23 | 2.36 | 0.52 |
| 1:B:221:PRO:HG2 | 1:B:224:ALA:H | 1.73 | 0.52 |
| 1:E:134:VAL:HG22 | 1:E:144:LEU:HD22 | 1.90 | 0.52 |
| 1:E:174:LEU:HG | 1:E:216:LEU:N | 2.24 | 0.52 |
| 1:F:109:LEU:HG | 1:F:112:VAL:O | 2.09 | 0.52 |
| 1:K:174:LEU:HG | 1:K:216:LEU:N | 2.24 | 0.52 |
| 1:M:160:ARG:O | 1:M:164:ILE:HG12 | 2.09 | 0.52 |
| 1:A:259:VAL:HG21 | 1:A:292:ALA:HB2 | 1.90 | 0.52 |
| 1:B:109:LEU:HG | 1:B:112:VAL:O | 2.09 | 0.52 |
| 1:B:301:ILE:HG22 | 1:B:308:GLN:HE22 | 1.74 | 0.52 |
| 1:D:160:ARG:HG2 | 1:D:164:ILE:HD13 | 1.91 | 0.52 |
| 1:E:160:ARG:HG2 | 1:E:164:ILE:HD13 | 1.92 | 0.52 |
| 1:F:301:ILE:HG22 | 1:F:308:GLN:HE22 | 1.74 | 0.52 |
| 1:G:109:LEU:HG | 1:G:112:VAL:O | 2.09 | 0.52 |
| 1:G:160:ARG:HG2 | 1:G:164:ILE:HD13 | 1.91 | 0.52 |
| 1:G:258:LEU:CD2 | 1:G:318:LEU:HD23 | 2.36 | 0.52 |
| 1:I:304:ASP:OD1 | 1:I:305:GLN:N | 2.42 | 0.52 |
| 1:K:134:VAL:HG22 | 1:K:144:LEU:HD22 | 1.90 | 0.52 |
| 1:K:288:VAL:HG13 | 1:K:303:ALA:HB2 | 1.91 | 0.52 |
| 1:M:109:LEU:HG | 1:M:112:VAL:O | 2.09 | 0.52 |
| 1:M:589:ARG:HG3 | 1:M:611:VAL:HG22 | 1.91 | 0.52 |
| 1:O:259:VAL:HG21 | 1:O:292:ALA:HB2 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:578:ARG:O | 1:B:582:LYS:N | 2.32 | 0.52 |
| 1:D:301:ILE:HG22 | 1:D:308:GLN:HE22 | 1.74 | 0.52 |
| 1:H:160:ARG:O | 1:H:164:ILE:HG12 | 2.09 | 0.52 |
| 1:J:259:VAL:HG21 | 1:J:292:ALA:HB2 | 1.90 | 0.52 |
| 1:K:301:ILE:HG22 | 1:K:308:GLN:HE22 | 1.74 | 0.52 |
| 1:M:134:VAL:HG22 | 1:M:144:LEU:HD22 | 1.90 | 0.52 |
| 1:N:288:VAL:HG13 | 1:N:303:ALA:HB2 | 1.91 | 0.52 |
| 1:A:157:VAL:HG22 | 1:A:160:ARG:HH21 | 1.74 | 0.52 |
| 1:E:301:ILE:HG22 | 1:E:308:GLN:HE22 | 1.74 | 0.52 |
| 1:F:160:ARG:HG2 | 1:F:164:ILE:HD13 | 1.91 | 0.52 |
| 1:G:477:GLY:O | 1:G:572:ARG:NH2 | 2.43 | 0.52 |
| 1:H:259:VAL:HG21 | 1:H:292:ALA:HB2 | 1.90 | 0.52 |
| 1:L:477:GLY:O | 1:L:572:ARG:NH2 | 2.43 | 0.52 |
| 1:M:304:ASP:OD1 | 1:M:305:GLN:N | 2.42 | 0.52 |
| 1:O:174:LEU:HG | 1:O:216:LEU:N | 2.24 | 0.52 |
| 1:B:160:ARG:HG2 | 1:B:164:ILE:HD13 | 1.91 | 0.52 |
| 1:B:259:VAL:HG21 | 1:B:292:ALA:HB2 | 1.90 | 0.52 |
| 1:C:157:VAL:HG22 | 1:C:160:ARG:HH21 | 1.74 | 0.52 |
| 1:J:130:VAL:HG22 | 1:J:131:GLY:H | 1.72 | 0.52 |
| 1:J:301:ILE:HG22 | 1:J:308:GLN:HE22 | 1.75 | 0.52 |
| 1:J:473:GLN:HB3 | 1:J:481:LEU:HB3 | 1.90 | 0.52 |
| 1:L:288:VAL:HG13 | 1:L:303:ALA:HB2 | 1.91 | 0.52 |
| 1:N:109:LEU:HG | 1:N:112:VAL:O | 2.09 | 0.52 |
| 1:A:109:LEU:HG | 1:A:112:VAL:O | 2.09 | 0.52 |
| 1:A:301:ILE:HG22 | 1:A:308:GLN:HE22 | 1.74 | 0.52 |
| 1:B:589:ARG:HG3 | 1:B:611:VAL:HG22 | 1.91 | 0.52 |
| 1:E:109:LEU:HG | 1:E:112:VAL:O | 2.09 | 0.52 |
| 1:F:259:VAL:HG21 | 1:F:292:ALA:HB2 | 1.90 | 0.52 |
| 1:I:160:ARG:HG2 | 1:I:164:ILE:HD13 | 1.91 | 0.52 |
| 1:I:259:VAL:HG21 | 1:I:292:ALA:HB2 | 1.90 | 0.52 |
| 1:K:473:GLN:HB3 | 1:K:481:LEU:HB3 | 1.90 | 0.52 |
| 1:M:288:VAL:HG13 | 1:M:303:ALA:HB2 | 1.91 | 0.52 |
| 1:N:160:ARG:O | 1:N:164:ILE:HG12 | 2.09 | 0.52 |
| 1:O:160:ARG:HG2 | 1:O:164:ILE:HD13 | 1.91 | 0.52 |
| 1:C:589:ARG:HG3 | 1:C:611:VAL:HG22 | 1.91 | 0.52 |
| 1:F:157:VAL:HG22 | 1:F:160:ARG:HH21 | 1.74 | 0.52 |
| 1:G:259:VAL:HG21 | 1:G:292:ALA:HB2 | 1.90 | 0.52 |
| 1:M:160:ARG:HG2 | 1:M:164:ILE:HD13 | 1.91 | 0.52 |
| 1:M:174:LEU:HG | 1:M:216:LEU:N | 2.24 | 0.52 |
| 1:O:589:ARG:HG3 | 1:O:611:VAL:HG22 | 1.91 | 0.52 |
| 1:A:242:GLU:HG2 | 1:A:243:GLY:H | 1.60 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:589:ARG:HG3 | 1:E:611:VAL:HG22 | 1.91 | 0.52 |
| 1:I:301:ILE:HG22 | 1:I:308:GLN:HE22 | 1.74 | 0.52 |
| 1:K:135:HIS:CE1 | 1:L:120:LEU:HD12 | 2.45 | 0.52 |
| 1:K:160:ARG:HG2 | 1:K:164:ILE:HD13 | 1.91 | 0.52 |
| 1:K:477:GLY:O | 1:K:572:ARG:NH2 | 2.43 | 0.52 |
| 1:L:135:HIS:CE1 | 1:M:120:LEU:HD12 | 2.45 | 0.52 |
| 1:C:135:HIS:CE1 | 1:D:120:LEU:HD12 | 2.45 | 0.51 |
| 1:C:301:ILE:HG22 | 1:C:308:GLN:HE22 | 1.74 | 0.51 |
| 1:D:135:HIS:CE1 | 1:E:120:LEU:HD12 | 2.45 | 0.51 |
| 1:D:174:LEU:HG | 1:D:216:LEU:N | 2.24 | 0.51 |
| 1:F:477:GLY:O | 1:F:572:ARG:NH2 | 2.43 | 0.51 |
| 1:G:160:ARG:O | 1:G:164:ILE:HG12 | 2.10 | 0.51 |
| 1:H:109:LEU:HG | 1:H:112:VAL:O | 2.09 | 0.51 |
| 1:I:135:HIS:CE1 | 1:J:120:LEU:HD12 | 2.45 | 0.51 |
| 1:J:135:HIS:CE1 | 1:K:120:LEU:HD12 | 2.45 | 0.51 |
| 1:J:157:VAL:HG22 | 1:J:160:ARG:HH21 | 1.74 | 0.51 |
| 1:K:157:VAL:HG22 | 1:K:160:ARG:HH21 | 1.74 | 0.51 |
| 1:L:301:ILE:HG22 | 1:L:308:GLN:HE22 | 1.74 | 0.51 |
| 1:M:135:HIS:CE1 | 1:N:120:LEU:HD12 | 2.45 | 0.51 |
| 1:N:157:VAL:HG22 | 1:N:160:ARG:HH21 | 1.74 | 0.51 |
| 1:O:242:GLU:HG2 | 1:O:243:GLY:H | 1.60 | 0.51 |
| 1:D:109:LEU:HG | 1:D:112:VAL:O | 2.09 | 0.51 |
| 1:D:589:ARG:HG3 | 1:D:611:VAL:HG22 | 1.91 | 0.51 |
| 1:F:104:THR:OG1 | 1:F:144:LEU:O | 2.21 | 0.51 |
| 1:N:589:ARG:HG3 | 1:N:611:VAL:HG22 | 1.91 | 0.51 |
| 1:B:160:ARG:O | 1:B:164:ILE:HG12 | 2.09 | 0.51 |
| 1:F:160:ARG:O | 1:F:164:ILE:HG12 | 2.09 | 0.51 |
| 1:G:301:ILE:HG22 | 1:G:308:GLN:HE22 | 1.74 | 0.51 |
| 1:H:135:HIS:CE1 | 1:I:120:LEU:HD12 | 2.45 | 0.51 |
| 1:J:262:LEU:CD1 | 1:J:299:LEU:HD21 | 2.40 | 0.51 |
| 1:K:109:LEU:HG | 1:K:112:VAL:O | 2.09 | 0.51 |
| 1:L:160:ARG:HG2 | 1:L:164:ILE:HD13 | 1.91 | 0.51 |
| 1:A:180:GLU:O | 1:A:183:ALA:HB3 | 2.11 | 0.51 |
| 1:B:135:HIS:CE1 | 1:C:120:LEU:HD12 | 2.45 | 0.51 |
| 1:E:135:HIS:CE1 | 1:F:120:LEU:HD12 | 2.45 | 0.51 |
| 1:F:180:GLU:O | 1:F:183:ALA:HB3 | 2.11 | 0.51 |
| 1:G:180:GLU:O | 1:G:183:ALA:HB3 | 2.11 | 0.51 |
| 1:A:589:ARG:HG3 | 1:A:611:VAL:HG22 | 1.91 | 0.51 |
| 1:L:117:LEU:HB3 | 1:L:121:LEU:HG | 1.92 | 0.51 |
| 1:N:135:HIS:CE1 | 1:O:120:LEU:HD12 | 2.45 | 0.51 |
| 1:A:135:HIS:CE1 | 1:B:120:LEU:HD12 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:180:GLU:O | 1:B:183:ALA:HB3 | 2.11 | 0.51 |
| 1:D:171:ILE:HG22 | 1:D:217:ILE:HG23 | 1.93 | 0.51 |
| 1:D:242:GLU:HG2 | 1:D:243:GLY:H | 1.60 | 0.51 |
| 1:E:157:VAL:HG22 | 1:E:160:ARG:HH21 | 1.74 | 0.51 |
| 1:H:180:GLU:O | 1:H:183:ALA:HB3 | 2.11 | 0.51 |
| 1:K:117:LEU:HB3 | 1:K:121:LEU:HG | 1.92 | 0.51 |
| 1:M:117:LEU:HB3 | 1:M:121:LEU:HG | 1.92 | 0.51 |
| 1:N:301:ILE:HG22 | 1:N:308:GLN:HE22 | 1.74 | 0.51 |
| 1:C:117:LEU:HB3 | 1:C:121:LEU:HG | 1.92 | 0.51 |
| 1:C:160:ARG:O | 1:C:164:ILE:HG12 | 2.10 | 0.51 |
| 1:C:171:ILE:HG22 | 1:C:217:ILE:HG23 | 1.93 | 0.51 |
| 1:H:262:LEU:CD1 | 1:H:299:LEU:HD21 | 2.40 | 0.51 |
| 1:L:335:GLN:HE21 | 1:L:560:ARG:HE | 1.59 | 0.51 |
| 1:O:160:ARG:O | 1:O:164:ILE:HG12 | 2.10 | 0.51 |
| 1:O:180:GLU:O | 1:O:183:ALA:HB3 | 2.11 | 0.51 |
| 1:B:171:ILE:HG22 | 1:B:217:ILE:HG23 | 1.93 | 0.51 |
| 1:B:262:LEU:CD1 | 1:B:299:LEU:HD21 | 2.40 | 0.51 |
| 1:D:117:LEU:HB3 | 1:D:121:LEU:HG | 1.92 | 0.51 |
| 1:E:171:ILE:HG22 | 1:E:217:ILE:HG23 | 1.93 | 0.51 |
| 1:E:180:GLU:O | 1:E:183:ALA:HB3 | 2.11 | 0.51 |
| 1:F:135:HIS:CE1 | 1:G:120:LEU:HD12 | 2.45 | 0.51 |
| 1:H:160:ARG:HG2 | 1:H:164:ILE:HD13 | 1.91 | 0.51 |
| 1:J:117:LEU:HB3 | 1:J:121:LEU:HG | 1.92 | 0.51 |
| 1:J:335:GLN:HE21 | 1:J:560:ARG:HE | 1.59 | 0.51 |
| 1:K:335:GLN:HE21 | 1:K:560:ARG:HE | 1.59 | 0.51 |
| 1:N:262:LEU:CD1 | 1:N:299:LEU:HD21 | 2.40 | 0.51 |
| 1:A:477:GLY:O | 1:A:572:ARG:NH2 | 2.43 | 0.51 |
| 1:B:117:LEU:HB3 | 1:B:121:LEU:HG | 1.92 | 0.51 |
| 1:B:258:LEU:CD2 | 1:B:318:LEU:HD23 | 2.36 | 0.51 |
| 1:G:135:HIS:CE1 | 1:H:120:LEU:HD12 | 2.45 | 0.51 |
| 1:I:180:GLU:O | 1:I:183:ALA:HB3 | 2.11 | 0.51 |
| 1:M:335:GLN:HE21 | 1:M:560:ARG:HE | 1.59 | 0.51 |
| 1:N:117:LEU:HB3 | 1:N:121:LEU:HG | 1.92 | 0.51 |
| 1:D:180:GLU:O | 1:D:183:ALA:HB3 | 2.11 | 0.51 |
| 1:E:160:ARG:O | 1:E:164:ILE:HG12 | 2.09 | 0.51 |
| 1:H:157:VAL:HG22 | 1:H:160:ARG:HH21 | 1.74 | 0.51 |
| 1:J:180:GLU:O | 1:J:183:ALA:HB3 | 2.11 | 0.51 |
| 1:J:477:GLY:O | 1:J:572:ARG:NH2 | 2.43 | 0.51 |
| 1:N:335:GLN:HE21 | 1:N:560:ARG:HE | 1.59 | 0.50 |
| 1:A:120:LEU:HD12 | 1:O:135:HIS:CE1 | 2.45 | 0.50 |
| 1:B:335:GLN:HE21 | 1:B:560:ARG:HE | 1.59 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:262:LEU:CD1 | 1:E:299:LEU:HD21 | 2.40 | 0.50 |
| 1:E:477:GLY:O | 1:E:572:ARG:NH2 | 2.43 | 0.50 |
| 1:I:335:GLN:HE21 | 1:I:560:ARG:HE | 1.59 | 0.50 |
| 1:K:180:GLU:O | 1:K:183:ALA:HB3 | 2.11 | 0.50 |
| 1:A:335:GLN:HE21 | 1:A:560:ARG:HE | 1.59 | 0.50 |
| 1:M:578:ARG:O | 1:M:582:LYS:N | 2.32 | 0.50 |
| 1:N:180:GLU:O | 1:N:183:ALA:HB3 | 2.11 | 0.50 |
| 1:O:335:GLN:HE21 | 1:O:560:ARG:HE | 1.59 | 0.50 |
| 1:A:160:ARG:O | 1:A:164:ILE:HG12 | 2.09 | 0.50 |
| 1:A:171:ILE:HG22 | 1:A:217:ILE:HG23 | 1.93 | 0.50 |
| 1:C:180:GLU:O | 1:C:183:ALA:HB3 | 2.11 | 0.50 |
| 1:F:171:ILE:HG22 | 1:F:217:ILE:HG23 | 1.93 | 0.50 |
| 1:F:242:GLU:HG2 | 1:F:243:GLY:H | 1.60 | 0.50 |
| 1:G:335:GLN:HE21 | 1:G:560:ARG:HE | 1.59 | 0.50 |
| 1:H:335:GLN:HE21 | 1:H:560:ARG:HE | 1.59 | 0.50 |
| 1:I:117:LEU:HB3 | 1:I:121:LEU:HG | 1.92 | 0.50 |
| 1:O:117:LEU:HB3 | 1:O:121:LEU:HG | 1.92 | 0.50 |
| 1:B:322:ARG:HG3 | 1:B:428:LEU:HD22 | 1.94 | 0.50 |
| 1:C:335:GLN:HE21 | 1:C:560:ARG:HE | 1.59 | 0.50 |
| 1:E:322:ARG:HG3 | 1:E:428:LEU:HD22 | 1.94 | 0.50 |
| 1:G:288:VAL:HG22 | 1:G:303:ALA:HB1 | 1.94 | 0.50 |
| 1:J:160:ARG:HG2 | 1:J:164:ILE:HD13 | 1.91 | 0.50 |
| 1:L:180:GLU:O | 1:L:183:ALA:HB3 | 2.11 | 0.50 |
| 1:E:117:LEU:HB3 | 1:E:121:LEU:HG | 1.92 | 0.50 |
| 1:F:262:LEU:CD1 | 1:F:299:LEU:HD21 | 2.40 | 0.50 |
| 1:F:288:VAL:HG22 | 1:F:303:ALA:HB1 | 1.94 | 0.50 |
| 1:A:262:LEU:CD1 | 1:A:299:LEU:HD21 | 2.40 | 0.50 |
| 1:D:160:ARG:O | 1:D:164:ILE:HG12 | 2.10 | 0.50 |
| 1:E:288:VAL:HG22 | 1:E:303:ALA:HB1 | 1.94 | 0.50 |
| 1:F:335:GLN:HE21 | 1:F:560:ARG:HE | 1.59 | 0.50 |
| 1:H:322:ARG:HG3 | 1:H:428:LEU:HD22 | 1.94 | 0.50 |
| 1:K:262:LEU:CD1 | 1:K:299:LEU:HD21 | 2.40 | 0.50 |
| 1:N:322:ARG:HG3 | 1:N:428:LEU:HD22 | 1.94 | 0.50 |
| 1:A:117:LEU:HB3 | 1:A:121:LEU:HG | 1.92 | 0.50 |
| 1:A:218:ILE:HD13 | 1:A:228:ILE:HD13 | 1.94 | 0.50 |
| 1:B:218:ILE:HD13 | 1:B:228:ILE:HD13 | 1.94 | 0.50 |
| 1:G:104:THR:OG1 | 1:G:144:LEU:O | 2.21 | 0.50 |
| 1:G:117:LEU:HB3 | 1:G:121:LEU:HG | 1.92 | 0.50 |
| 1:H:117:LEU:HB3 | 1:H:121:LEU:HG | 1.92 | 0.50 |
| 1:H:288:VAL:HG22 | 1:H:303:ALA:HB1 | 1.94 | 0.50 |
| 1:N:218:ILE:HD13 | 1:N:228:ILE:HD13 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:477:GLY:O | 1:O:572:ARG:NH2 | 2.43 | 0.50 |
| 1:E:335:GLN:HE21 | 1:E:560:ARG:HE | 1.59 | 0.50 |
| 1:M:180:GLU:O | 1:M:183:ALA:HB3 | 2.11 | 0.50 |
| 1:M:262:LEU:CD1 | 1:M:299:LEU:HD21 | 2.40 | 0.50 |
| 1:O:218:ILE:HD13 | 1:O:228:ILE:HD13 | 1.94 | 0.50 |
| 1:C:218:ILE:HD13 | 1:C:228:ILE:HD13 | 1.94 | 0.49 |
| 1:I:477:GLY:O | 1:I:572:ARG:NH2 | 2.43 | 0.49 |
| 1:M:157:VAL:HG22 | 1:M:160:ARG:HH21 | 1.74 | 0.49 |
| 1:D:218:ILE:HD13 | 1:D:228:ILE:HD13 | 1.94 | 0.49 |
| 1:D:288:VAL:HG22 | 1:D:303:ALA:HB1 | 1.94 | 0.49 |
| 1:F:322:ARG:HG3 | 1:F:428:LEU:HD22 | 1.94 | 0.49 |
| 1:I:262:LEU:CD1 | 1:I:299:LEU:HD21 | 2.40 | 0.49 |
| 1:M:218:ILE:HD13 | 1:M:228:ILE:HD13 | 1.94 | 0.49 |
| 1:O:322:ARG:HG3 | 1:O:428:LEU:HD22 | 1.94 | 0.49 |
| 1:A:322:ARG:HG3 | 1:A:428:LEU:HD22 | 1.94 | 0.49 |
| 1:D:477:GLY:O | 1:D:572:ARG:NH2 | 2.43 | 0.49 |
| 1:G:250:LEU:HD13 | 1:G:258:LEU:HD12 | 1.95 | 0.49 |
| 1:G:322:ARG:HG3 | 1:G:428:LEU:HD22 | 1.94 | 0.49 |
| 1:L:444:LEU:HB2 | 1:M:499:LEU:HD21 | 1.94 | 0.49 |
| 1:M:444:LEU:HB2 | 1:N:499:LEU:HD21 | 1.94 | 0.49 |
| 1:N:242:GLU:HG2 | 1:N:243:GLY:H | 1.60 | 0.49 |
| 1:C:322:ARG:HG3 | 1:C:428:LEU:HD22 | 1.94 | 0.49 |
| 1:G:171:ILE:HG22 | 1:G:217:ILE:HG23 | 1.93 | 0.49 |
| 1:J:322:ARG:HG3 | 1:J:428:LEU:HD22 | 1.94 | 0.49 |
| 1:K:171:ILE:HG22 | 1:K:217:ILE:HG23 | 1.93 | 0.49 |
| 1:K:218:ILE:HD13 | 1:K:228:ILE:HD13 | 1.94 | 0.49 |
| 1:L:171:ILE:HG22 | 1:L:217:ILE:HG23 | 1.93 | 0.49 |
| 1:L:322:ARG:HG3 | 1:L:428:LEU:HD22 | 1.94 | 0.49 |
| 1:N:250:LEU:HD13 | 1:N:258:LEU:HD12 | 1.95 | 0.49 |
| 1:O:171:ILE:HG22 | 1:O:217:ILE:HG23 | 1.93 | 0.49 |
| 1:C:262:LEU:CD1 | 1:C:299:LEU:HD21 | 2.41 | 0.49 |
| 1:D:322:ARG:HG3 | 1:D:428:LEU:HD22 | 1.94 | 0.49 |
| 1:D:335:GLN:HE21 | 1:D:560:ARG:HE | 1.59 | 0.49 |
| 1:F:117:LEU:HB3 | 1:F:121:LEU:HG | 1.92 | 0.49 |
| 1:L:218:ILE:HD13 | 1:L:228:ILE:HD13 | 1.94 | 0.49 |
| 1:O:250:LEU:HD13 | 1:O:258:LEU:HD12 | 1.95 | 0.49 |
| 1:A:499:LEU:HD21 | 1:O:444:LEU:HB2 | 1.94 | 0.49 |
| 1:C:477:GLY:O | 1:C:572:ARG:NH2 | 2.43 | 0.49 |
| 1:F:250:LEU:HD13 | 1:F:258:LEU:HD12 | 1.95 | 0.49 |
| 1:H:250:LEU:HD13 | 1:H:258:LEU:HD12 | 1.95 | 0.49 |
| 1:I:171:ILE:HG22 | 1:I:217:ILE:HG23 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:171:ILE:HG22 | 1:J:217:ILE:HG23 | 1.93 | 0.49 |
| 1:M:171:ILE:HG22 | 1:M:217:ILE:HG23 | 1.93 | 0.49 |
| 1:O:262:LEU:CD1 | 1:O:299:LEU:HD21 | 2.40 | 0.49 |
| 1:E:444:LEU:HB2 | 1:F:499:LEU:HD21 | 1.94 | 0.49 |
| 1:F:206:LYS:HZ3 | 1:G:190:ILE:C | 2.16 | 0.49 |
| 1:G:262:LEU:CD1 | 1:G:299:LEU:HD21 | 2.40 | 0.49 |
| 1:I:288:VAL:HG22 | 1:I:303:ALA:HB1 | 1.94 | 0.49 |
| 1:J:218:ILE:HD13 | 1:J:228:ILE:HD13 | 1.94 | 0.49 |
| 1:J:444:LEU:HB2 | 1:K:499:LEU:HD21 | 1.94 | 0.49 |
| 1:N:444:LEU:HB2 | 1:O:499:LEU:HD21 | 1.94 | 0.49 |
| 1:E:218:ILE:HD13 | 1:E:228:ILE:HD13 | 1.94 | 0.49 |
| 1:M:250:LEU:HD13 | 1:M:258:LEU:HD12 | 1.95 | 0.49 |
| 1:A:250:LEU:HD13 | 1:A:258:LEU:HD12 | 1.95 | 0.49 |
| 1:F:218:ILE:HD13 | 1:F:228:ILE:HD13 | 1.94 | 0.49 |
| 1:F:444:LEU:HB2 | 1:G:499:LEU:HD21 | 1.94 | 0.49 |
| 1:H:171:ILE:HG22 | 1:H:217:ILE:HG23 | 1.93 | 0.49 |
| 1:I:218:ILE:HD13 | 1:I:228:ILE:HD13 | 1.94 | 0.49 |
| 1:I:250:LEU:HD13 | 1:I:258:LEU:HD12 | 1.95 | 0.49 |
| 1:K:444:LEU:HB2 | 1:L:499:LEU:HD21 | 1.94 | 0.49 |
| 1:N:171:ILE:HG22 | 1:N:217:ILE:HG23 | 1.93 | 0.49 |
| 1:O:429:ASP:HA | 1:O:472:PRO:HG2 | 1.95 | 0.49 |
| 1:B:491:VAL:HG22 | 1:B:503:PHE:HE1 | 1.78 | 0.49 |
| 1:C:288:VAL:HG22 | 1:C:303:ALA:HB1 | 1.94 | 0.49 |
| 1:D:444:LEU:HB2 | 1:E:499:LEU:HD21 | 1.94 | 0.49 |
| 1:D:491:VAL:HG22 | 1:D:503:PHE:HE1 | 1.78 | 0.49 |
| 1:G:218:ILE:HD13 | 1:G:228:ILE:HD13 | 1.94 | 0.49 |
| 1:G:607:GLU:OE2 | 1:I:557:ARG:HB2 | 2.13 | 0.49 |
| 1:H:218:ILE:HD13 | 1:H:228:ILE:HD13 | 1.94 | 0.49 |
| 1:K:491:VAL:HG22 | 1:K:503:PHE:HE1 | 1.78 | 0.49 |
| 1:L:607:GLU:OE2 | 1:N:557:ARG:HB2 | 2.13 | 0.49 |
| 1:A:288:VAL:HG22 | 1:A:303:ALA:HB1 | 1.94 | 0.48 |
| 1:A:429:ASP:HA | 1:A:472:PRO:HG2 | 1.95 | 0.48 |
| 1:B:557:ARG:HB2 | 1:O:607:GLU:OE2 | 2.13 | 0.48 |
| 1:G:429:ASP:HA | 1:G:472:PRO:HG2 | 1.95 | 0.48 |
| 1:H:607:GLU:OE2 | 1:J:557:ARG:HB2 | 2.13 | 0.48 |
| 1:I:444:LEU:HB2 | 1:J:499:LEU:HD21 | 1.94 | 0.48 |
| 1:I:491:VAL:HG22 | 1:I:503:PHE:HE1 | 1.78 | 0.48 |
| 1:I:607:GLU:OE2 | 1:K:557:ARG:HB2 | 2.13 | 0.48 |
| 1:K:429:ASP:HA | 1:K:472:PRO:HG2 | 1.95 | 0.48 |
| 1:L:288:VAL:HG22 | 1:L:303:ALA:HB1 | 1.94 | 0.48 |
| 1:M:288:VAL:HG22 | 1:M:303:ALA:HB1 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:477:GLY:O | 1:N:572:ARG:NH2 | 2.43 | 0.48 |
| 1:O:288:VAL:HG22 | 1:O:303:ALA:HB1 | 1.94 | 0.48 |
| 1:C:607:GLU:OE2 | 1:E:557:ARG:HB2 | 2.13 | 0.48 |
| 1:D:104:THR:OG1 | 1:D:144:LEU:O | 2.21 | 0.48 |
| 1:F:607:GLU:OE2 | 1:H:557:ARG:HB2 | 2.13 | 0.48 |
| 1:H:429:ASP:HA | 1:H:472:PRO:HG2 | 1.95 | 0.48 |
| 1:J:607:GLU:OE2 | 1:L:557:ARG:HB2 | 2.13 | 0.48 |
| 1:L:429:ASP:HA | 1:L:472:PRO:HG2 | 1.95 | 0.48 |
| 1:M:491:VAL:HG22 | 1:M:503:PHE:HE1 | 1.78 | 0.48 |
| 1:B:477:GLY:O | 1:B:572:ARG:NH2 | 2.43 | 0.48 |
| 1:E:250:LEU:HD13 | 1:E:258:LEU:HD12 | 1.95 | 0.48 |
| 1:E:607:GLU:OE2 | 1:G:557:ARG:HB2 | 2.13 | 0.48 |
| 1:H:246:ARG:HH22 | 1:H:305:GLN:HE22 | 1.61 | 0.48 |
| 1:I:322:ARG:HG3 | 1:I:428:LEU:HD22 | 1.94 | 0.48 |
| 1:L:250:LEU:HD13 | 1:L:258:LEU:HD12 | 1.95 | 0.48 |
| 1:M:322:ARG:HG3 | 1:M:428:LEU:HD22 | 1.94 | 0.48 |
| 1:N:288:VAL:HG22 | 1:N:303:ALA:HB1 | 1.94 | 0.48 |
| 1:O:491:VAL:HG22 | 1:O:503:PHE:HE1 | 1.78 | 0.48 |
| 1:A:444:LEU:HB2 | 1:B:499:LEU:HD21 | 1.94 | 0.48 |
| 1:D:607:GLU:OE2 | 1:F:557:ARG:HB2 | 2.13 | 0.48 |
| 1:F:429:ASP:HA | 1:F:472:PRO:HG2 | 1.95 | 0.48 |
| 1:K:288:VAL:HG22 | 1:K:303:ALA:HB1 | 1.94 | 0.48 |
| 1:K:607:GLU:OE2 | 1:M:557:ARG:HB2 | 2.13 | 0.48 |
| 1:A:607:GLU:OE2 | 1:C:557:ARG:HB2 | 2.13 | 0.48 |
| 1:E:136:TYR:CE1 | 1:E:142:LEU:HG | 2.49 | 0.48 |
| 1:F:246:ARG:HH22 | 1:F:305:GLN:HE22 | 1.61 | 0.48 |
| 1:J:250:LEU:HD13 | 1:J:258:LEU:HD12 | 1.95 | 0.48 |
| 1:B:250:LEU:HD13 | 1:B:258:LEU:HD12 | 1.95 | 0.48 |
| 1:B:288:VAL:HG22 | 1:B:303:ALA:HB1 | 1.94 | 0.48 |
| 1:E:592:GLN:OE1 | 1:E:611:VAL:HG23 | 2.14 | 0.48 |
| 1:F:491:VAL:HG22 | 1:F:503:PHE:HE1 | 1.78 | 0.48 |
| 1:G:444:LEU:HB2 | 1:H:499:LEU:HD21 | 1.94 | 0.48 |
| 1:H:477:GLY:O | 1:H:572:ARG:NH2 | 2.43 | 0.48 |
| 1:H:592:GLN:OE1 | 1:H:611:VAL:HG23 | 2.14 | 0.48 |
| 1:I:592:GLN:OE1 | 1:I:611:VAL:HG23 | 2.14 | 0.48 |
| 1:K:322:ARG:HG3 | 1:K:428:LEU:HD22 | 1.94 | 0.48 |
| 1:L:212:ARG:HH21 | 1:M:181:ASP:HB2 | 1.79 | 0.48 |
| 1:N:429:ASP:HA | 1:N:472:PRO:HG2 | 1.95 | 0.48 |
| 1:B:136:TYR:CE1 | 1:B:142:LEU:HG | 2.49 | 0.48 |
| 1:C:136:TYR:CE1 | 1:C:142:LEU:HG | 2.49 | 0.48 |
| 1:D:592:GLN:OE1 | 1:D:611:VAL:HG23 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:429:ASP:HA | 1:E:472:PRO:HG2 | 1.95 | 0.48 |
| 1:F:212:ARG:HH21 | 1:G:181:ASP:HB2 | 1.79 | 0.48 |
| 1:F:491:VAL:HG22 | 1:F:503:PHE:CE1 | 2.49 | 0.48 |
| 1:G:592:GLN:OE1 | 1:G:611:VAL:HG23 | 2.14 | 0.48 |
| 1:H:491:VAL:HG22 | 1:H:503:PHE:CE1 | 2.49 | 0.48 |
| 1:J:171:ILE:HB | 1:J:217:ILE:HG13 | 1.96 | 0.48 |
| 1:K:171:ILE:HB | 1:K:217:ILE:HG13 | 1.96 | 0.48 |
| 1:N:212:ARG:HH21 | 1:O:181:ASP:HB2 | 1.79 | 0.48 |
| 1:A:104:THR:OG1 | 1:A:144:LEU:O | 2.21 | 0.48 |
| 1:B:429:ASP:HA | 1:B:472:PRO:HG2 | 1.95 | 0.48 |
| 1:B:444:LEU:HB2 | 1:C:499:LEU:HD21 | 1.94 | 0.48 |
| 1:C:491:VAL:HG22 | 1:C:503:PHE:CE1 | 2.49 | 0.48 |
| 1:F:592:GLN:OE1 | 1:F:611:VAL:HG23 | 2.14 | 0.48 |
| 1:G:491:VAL:HG22 | 1:G:503:PHE:HE1 | 1.78 | 0.48 |
| 1:I:108:PRO:HA | 1:I:141:VAL:HA | 1.96 | 0.48 |
| 1:J:108:PRO:HA | 1:J:141:VAL:HA | 1.96 | 0.48 |
| 1:J:592:GLN:OE1 | 1:J:611:VAL:HG23 | 2.14 | 0.48 |
| 1:K:491:VAL:HG22 | 1:K:503:PHE:CE1 | 2.49 | 0.48 |
| 1:L:491:VAL:HG22 | 1:L:503:PHE:CE1 | 2.49 | 0.48 |
| 1:M:491:VAL:HG22 | 1:M:503:PHE:CE1 | 2.49 | 0.48 |
| 1:A:557:ARG:HB2 | 1:N:607:GLU:OE2 | 2.13 | 0.48 |
| 1:D:109:LEU:HD13 | 1:D:162:ASP:HA | 1.96 | 0.48 |
| 1:H:109:LEU:HD13 | 1:H:162:ASP:HA | 1.96 | 0.48 |
| 1:H:136:TYR:CE1 | 1:H:142:LEU:HG | 2.49 | 0.48 |
| 1:I:120:LEU:O | 1:I:123:GLN:HB3 | 2.14 | 0.48 |
| 1:I:429:ASP:HA | 1:I:472:PRO:HG2 | 1.95 | 0.48 |
| 1:J:288:VAL:HG22 | 1:J:303:ALA:HB1 | 1.94 | 0.48 |
| 1:J:429:ASP:HA | 1:J:472:PRO:HG2 | 1.95 | 0.48 |
| 1:K:136:TYR:CE1 | 1:K:142:LEU:HG | 2.49 | 0.48 |
| 1:L:491:VAL:HG22 | 1:L:503:PHE:HE1 | 1.78 | 0.48 |
| 1:M:171:ILE:HB | 1:M:217:ILE:HG13 | 1.96 | 0.48 |
| 1:M:607:GLU:OE2 | 1:O:557:ARG:HB2 | 2.13 | 0.48 |
| 1:N:120:LEU:O | 1:N:123:GLN:HB3 | 2.14 | 0.48 |
| 1:N:171:ILE:HB | 1:N:217:ILE:HG13 | 1.96 | 0.48 |
| 1:N:491:VAL:HG22 | 1:N:503:PHE:CE1 | 2.49 | 0.48 |
| 1:A:109:LEU:HD13 | 1:A:162:ASP:HA | 1.96 | 0.48 |
| 1:A:212:ARG:HH21 | 1:B:181:ASP:HB2 | 1.79 | 0.48 |
| 1:A:491:VAL:HG22 | 1:A:503:PHE:CE1 | 2.49 | 0.48 |
| 1:C:109:LEU:HD13 | 1:C:162:ASP:HA | 1.96 | 0.48 |
| 1:F:136:TYR:CE1 | 1:F:142:LEU:HG | 2.49 | 0.48 |
| 1:G:120:LEU:O | 1:G:123:GLN:HB3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:108:PRO:HA | 1:H:141:VAL:HA | 1.96 | 0.48 |
| 1:I:171:ILE:HB | 1:I:217:ILE:HG13 | 1.96 | 0.48 |
| 1:J:212:ARG:HH21 | 1:K:181:ASP:HB2 | 1.79 | 0.48 |
| 1:J:246:ARG:HH22 | 1:J:305:GLN:HE22 | 1.61 | 0.48 |
| 1:K:250:LEU:HD13 | 1:K:258:LEU:HD12 | 1.95 | 0.48 |
| 1:L:171:ILE:HB | 1:L:217:ILE:HG13 | 1.96 | 0.48 |
| 1:O:491:VAL:HG22 | 1:O:503:PHE:CE1 | 2.49 | 0.48 |
| 1:B:109:LEU:HD13 | 1:B:162:ASP:HA | 1.96 | 0.47 |
| 1:C:212:ARG:HH21 | 1:D:181:ASP:HB2 | 1.79 | 0.47 |
| 1:C:444:LEU:HB2 | 1:D:499:LEU:HD21 | 1.94 | 0.47 |
| 1:D:212:ARG:HH21 | 1:E:181:ASP:HB2 | 1.79 | 0.47 |
| 1:D:250:LEU:HD13 | 1:D:258:LEU:HD12 | 1.95 | 0.47 |
| 1:E:491:VAL:HG22 | 1:E:503:PHE:CE1 | 2.49 | 0.47 |
| 1:F:108:PRO:HA | 1:F:141:VAL:HA | 1.96 | 0.47 |
| 1:G:109:LEU:HD13 | 1:G:162:ASP:HA | 1.96 | 0.47 |
| 1:G:171:ILE:HB | 1:G:217:ILE:HG13 | 1.96 | 0.47 |
| 1:H:171:ILE:HB | 1:H:217:ILE:HG13 | 1.96 | 0.47 |
| 1:H:444:LEU:HB2 | 1:I:499:LEU:HD21 | 1.94 | 0.47 |
| 1:J:491:VAL:HG22 | 1:J:503:PHE:CE1 | 2.49 | 0.47 |
| 1:K:108:PRO:HA | 1:K:141:VAL:HA | 1.96 | 0.47 |
| 1:B:607:GLU:OE2 | 1:D:557:ARG:HB2 | 2.13 | 0.47 |
| 1:C:106:ILE:HG22 | 1:C:143:ILE:HA | 1.96 | 0.47 |
| 1:D:429:ASP:HA | 1:D:472:PRO:HG2 | 1.95 | 0.47 |
| 1:D:491:VAL:HG22 | 1:D:503:PHE:CE1 | 2.49 | 0.47 |
| 1:E:109:LEU:HD13 | 1:E:162:ASP:HA | 1.96 | 0.47 |
| 1:G:108:PRO:HA | 1:G:141:VAL:HA | 1.96 | 0.47 |
| 1:G:136:TYR:CE1 | 1:G:142:LEU:HG | 2.49 | 0.47 |
| 1:I:212:ARG:HH21 | 1:J:181:ASP:HB2 | 1.79 | 0.47 |
| 1:J:109:LEU:HD13 | 1:J:162:ASP:HA | 1.96 | 0.47 |
| 1:K:109:LEU:HD13 | 1:K:162:ASP:HA | 1.96 | 0.47 |
| 1:K:592:GLN:OE1 | 1:K:611:VAL:HG23 | 2.14 | 0.47 |
| 1:L:120:LEU:O | 1:L:123:GLN:HB3 | 2.14 | 0.47 |
| 1:N:491:VAL:HG22 | 1:N:503:PHE:HE1 | 1.78 | 0.47 |
| 1:A:120:LEU:O | 1:A:123:GLN:HB3 | 2.14 | 0.47 |
| 1:A:592:GLN:OE1 | 1:A:611:VAL:HG23 | 2.14 | 0.47 |
| 1:B:106:ILE:HG22 | 1:B:143:ILE:HA | 1.96 | 0.47 |
| 1:C:246:ARG:HH22 | 1:C:305:GLN:HE22 | 1.61 | 0.47 |
| 1:D:108:PRO:HA | 1:D:141:VAL:HA | 1.96 | 0.47 |
| 1:D:120:LEU:O | 1:D:123:GLN:HB3 | 2.14 | 0.47 |
| 1:E:108:PRO:HA | 1:E:141:VAL:HA | 1.96 | 0.47 |
| 1:F:120:LEU:O | 1:F:123:GLN:HB3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:491:VAL:HG22 | 1:H:503:PHE:HE1 | 1.78 | 0.47 |
| 1:I:109:LEU:HD13 | 1:I:162:ASP:HA | 1.96 | 0.47 |
| 1:K:120:LEU:O | 1:K:123:GLN:HB3 | 2.14 | 0.47 |
| 1:L:104:THR:OG1 | 1:L:144:LEU:O | 2.21 | 0.47 |
| 1:L:136:TYR:CE1 | 1:L:142:LEU:HG | 2.49 | 0.47 |
| 1:L:262:LEU:CD1 | 1:L:299:LEU:HD21 | 2.40 | 0.47 |
| 1:M:429:ASP:HA | 1:M:472:PRO:HG2 | 1.95 | 0.47 |
| 1:O:136:TYR:CE1 | 1:O:142:LEU:HG | 2.49 | 0.47 |
| 1:O:171:ILE:HB | 1:O:217:ILE:HG13 | 1.96 | 0.47 |
| 1:B:491:VAL:HG22 | 1:B:503:PHE:CE1 | 2.49 | 0.47 |
| 1:C:108:PRO:HA | 1:C:141:VAL:HA | 1.96 | 0.47 |
| 1:C:120:LEU:O | 1:C:123:GLN:HB3 | 2.14 | 0.47 |
| 1:C:250:LEU:HD13 | 1:C:258:LEU:HD12 | 1.95 | 0.47 |
| 1:D:246:ARG:HH22 | 1:D:305:GLN:HE22 | 1.61 | 0.47 |
| 1:E:246:ARG:HH22 | 1:E:305:GLN:HE22 | 1.61 | 0.47 |
| 1:G:212:ARG:HH21 | 1:H:181:ASP:HB2 | 1.79 | 0.47 |
| 1:M:477:GLY:O | 1:M:572:ARG:NH2 | 2.43 | 0.47 |
| 1:O:109:LEU:HD13 | 1:O:162:ASP:HA | 1.96 | 0.47 |
| 1:A:106:ILE:HG22 | 1:A:143:ILE:HA | 1.96 | 0.47 |
| 1:B:108:PRO:HA | 1:B:141:VAL:HA | 1.96 | 0.47 |
| 1:C:592:GLN:OE1 | 1:C:611:VAL:HG23 | 2.14 | 0.47 |
| 1:D:106:ILE:HG22 | 1:D:143:ILE:HA | 1.97 | 0.47 |
| 1:D:136:TYR:CE1 | 1:D:142:LEU:HG | 2.49 | 0.47 |
| 1:F:109:LEU:HD13 | 1:F:162:ASP:HA | 1.96 | 0.47 |
| 1:F:171:ILE:HB | 1:F:217:ILE:HG13 | 1.96 | 0.47 |
| 1:L:108:PRO:HA | 1:L:141:VAL:HA | 1.96 | 0.47 |
| 1:L:592:GLN:OE1 | 1:L:611:VAL:HG23 | 2.14 | 0.47 |
| 1:M:109:LEU:HD13 | 1:M:162:ASP:HA | 1.96 | 0.47 |
| 1:N:109:LEU:HD13 | 1:N:162:ASP:HA | 1.96 | 0.47 |
| 1:A:108:PRO:HA | 1:A:141:VAL:HA | 1.96 | 0.47 |
| 1:E:120:LEU:O | 1:E:123:GLN:HB3 | 2.14 | 0.47 |
| 1:E:491:VAL:HG22 | 1:E:503:PHE:HE1 | 1.78 | 0.47 |
| 1:M:136:TYR:CE1 | 1:M:142:LEU:HG | 2.49 | 0.47 |
| 1:O:108:PRO:HA | 1:O:141:VAL:HA | 1.96 | 0.47 |
| 1:A:171:ILE:HB | 1:A:217:ILE:HG13 | 1.96 | 0.47 |
| 1:A:491:VAL:HG22 | 1:A:503:PHE:HE1 | 1.78 | 0.47 |
| 1:B:171:ILE:HB | 1:B:217:ILE:HG13 | 1.96 | 0.47 |
| 1:B:592:GLN:OE1 | 1:B:611:VAL:HG23 | 2.14 | 0.47 |
| 1:C:182:LEU:HA | 1:C:185:ILE:HG12 | 1.97 | 0.47 |
| 1:C:429:ASP:HA | 1:C:472:PRO:HG2 | 1.95 | 0.47 |
| 1:D:182:LEU:HA | 1:D:185:ILE:HG12 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:235:LEU:HD23 | 1:D:237:VAL:HG12 | 1.97 | 0.47 |
| 1:G:242:GLU:HG2 | 1:G:243:GLY:H | 1.60 | 0.47 |
| 1:G:246:ARG:HH22 | 1:G:305:GLN:HE22 | 1.61 | 0.47 |
| 1:G:491:VAL:HG22 | 1:G:503:PHE:CE1 | 2.49 | 0.47 |
| 1:H:212:ARG:HH21 | 1:I:181:ASP:HB2 | 1.79 | 0.47 |
| 1:I:129:SER:HB3 | 1:I:147:ARG:HH22 | 1.80 | 0.47 |
| 1:I:491:VAL:HG22 | 1:I:503:PHE:CE1 | 2.49 | 0.47 |
| 1:J:136:TYR:CE1 | 1:J:142:LEU:HG | 2.49 | 0.47 |
| 1:M:108:PRO:HA | 1:M:141:VAL:HA | 1.96 | 0.47 |
| 1:M:592:GLN:OE1 | 1:M:611:VAL:HG23 | 2.14 | 0.47 |
| 1:N:108:PRO:HA | 1:N:141:VAL:HA | 1.96 | 0.47 |
| 1:N:136:TYR:CE1 | 1:N:142:LEU:HG | 2.49 | 0.47 |
| 1:O:106:ILE:HG22 | 1:O:143:ILE:HA | 1.96 | 0.47 |
| 1:O:592:GLN:OE1 | 1:O:611:VAL:HG23 | 2.14 | 0.47 |
| 1:A:136:TYR:CE1 | 1:A:142:LEU:HG | 2.49 | 0.47 |
| 1:C:491:VAL:HG22 | 1:C:503:PHE:HE1 | 1.78 | 0.47 |
| 1:D:171:ILE:HB | 1:D:217:ILE:HG13 | 1.96 | 0.47 |
| 1:E:106:ILE:HG22 | 1:E:143:ILE:HA | 1.97 | 0.47 |
| 1:E:171:ILE:HB | 1:E:217:ILE:HG13 | 1.96 | 0.47 |
| 1:J:118:ALA:HB1 | 1:J:122:ARG:NH2 | 2.30 | 0.47 |
| 1:J:491:VAL:HG22 | 1:J:503:PHE:HE1 | 1.78 | 0.47 |
| 1:L:109:LEU:HD13 | 1:L:162:ASP:HA | 1.96 | 0.47 |
| 1:M:246:ARG:HH22 | 1:M:305:GLN:HE22 | 1.61 | 0.47 |
| 1:N:118:ALA:HB1 | 1:N:122:ARG:NH2 | 2.30 | 0.47 |
| 1:N:246:ARG:HH22 | 1:N:305:GLN:HE22 | 1.61 | 0.47 |
| 1:A:182:LEU:HA | 1:A:185:ILE:HG12 | 1.97 | 0.47 |
| 1:B:120:LEU:O | 1:B:123:GLN:HB3 | 2.14 | 0.47 |
| 1:B:182:LEU:HA | 1:B:185:ILE:HG12 | 1.97 | 0.47 |
| 1:C:235:LEU:HD23 | 1:C:237:VAL:HG12 | 1.97 | 0.47 |
| 1:E:212:ARG:HH21 | 1:F:181:ASP:HB2 | 1.79 | 0.47 |
| 1:E:235:LEU:HD23 | 1:E:237:VAL:HG12 | 1.97 | 0.47 |
| 1:H:235:LEU:HD23 | 1:H:237:VAL:HG12 | 1.97 | 0.47 |
| 1:I:136:TYR:CE1 | 1:I:142:LEU:HG | 2.49 | 0.47 |
| 1:J:120:LEU:O | 1:J:123:GLN:HB3 | 2.14 | 0.47 |
| 1:K:212:ARG:HH21 | 1:L:181:ASP:HB2 | 1.79 | 0.47 |
| 1:L:129:SER:HB3 | 1:L:147:ARG:HH22 | 1.80 | 0.47 |
| 1:M:118:ALA:HB1 | 1:M:122:ARG:NH2 | 2.30 | 0.47 |
| 1:M:120:LEU:O | 1:M:123:GLN:HB3 | 2.14 | 0.47 |
| 1:M:129:SER:HB3 | 1:M:147:ARG:HH22 | 1.80 | 0.47 |
| 1:C:118:ALA:HB1 | 1:C:122:ARG:NH2 | 2.30 | 0.47 |
| 1:D:118:ALA:HB1 | 1:D:122:ARG:NH2 | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:235:LEU:HD23 | 1:F:237:VAL:HG12 | 1.97 | 0.47 |
| 1:G:235:LEU:HD23 | 1:G:237:VAL:HG12 | 1.97 | 0.47 |
| 1:H:120:LEU:O | 1:H:123:GLN:HB3 | 2.14 | 0.47 |
| 1:J:129:SER:HB3 | 1:J:147:ARG:HH22 | 1.80 | 0.47 |
| 1:K:118:ALA:HB1 | 1:K:122:ARG:NH2 | 2.30 | 0.47 |
| 1:N:592:GLN:OE1 | 1:N:611:VAL:HG23 | 2.14 | 0.47 |
| 1:O:182:LEU:HA | 1:O:185:ILE:HG12 | 1.97 | 0.47 |
| 1:A:220:GLY:HA3 | 1:A:224:ALA:HB3 | 1.98 | 0.46 |
| 1:A:246:ARG:HH22 | 1:A:305:GLN:HE22 | 1.61 | 0.46 |
| 1:E:182:LEU:HA | 1:E:185:ILE:HG12 | 1.97 | 0.46 |
| 1:F:106:ILE:HG22 | 1:F:143:ILE:HA | 1.96 | 0.46 |
| 1:G:182:LEU:HA | 1:G:185:ILE:HG12 | 1.97 | 0.46 |
| 1:I:224:ALA:HA | 1:I:227:ARG:NE | 2.30 | 0.46 |
| 1:J:106:ILE:HG22 | 1:J:143:ILE:HA | 1.96 | 0.46 |
| 1:L:111:ASN:HB3 | 1:L:165:GLY:O | 2.16 | 0.46 |
| 1:M:111:ASN:HB3 | 1:M:165:GLY:O | 2.16 | 0.46 |
| 1:A:181:ASP:HB2 | 1:O:212:ARG:HH21 | 1.79 | 0.46 |
| 1:B:220:GLY:HA3 | 1:B:224:ALA:HB3 | 1.98 | 0.46 |
| 1:D:129:SER:HB3 | 1:D:147:ARG:HH22 | 1.80 | 0.46 |
| 1:E:111:ASN:HB3 | 1:E:165:GLY:O | 2.16 | 0.46 |
| 1:E:118:ALA:HB1 | 1:E:122:ARG:NH2 | 2.30 | 0.46 |
| 1:F:182:LEU:HA | 1:F:185:ILE:HG12 | 1.97 | 0.46 |
| 1:G:106:ILE:HG22 | 1:G:143:ILE:HA | 1.96 | 0.46 |
| 1:G:224:ALA:HA | 1:G:227:ARG:NE | 2.31 | 0.46 |
| 1:I:242:GLU:HG2 | 1:I:243:GLY:H | 1.60 | 0.46 |
| 1:K:106:ILE:HG22 | 1:K:143:ILE:HA | 1.96 | 0.46 |
| 1:L:118:ALA:HB1 | 1:L:122:ARG:NH2 | 2.30 | 0.46 |
| 1:M:212:ARG:HH21 | 1:N:181:ASP:HB2 | 1.79 | 0.46 |
| 1:M:220:GLY:HA3 | 1:M:224:ALA:HB3 | 1.98 | 0.46 |
| 1:N:220:GLY:HA3 | 1:N:224:ALA:HB3 | 1.98 | 0.46 |
| 1:O:118:ALA:HB1 | 1:O:122:ARG:NH2 | 2.30 | 0.46 |
| 1:A:111:ASN:HB3 | 1:A:165:GLY:O | 2.16 | 0.46 |
| 1:A:235:LEU:HD23 | 1:A:237:VAL:HG12 | 1.97 | 0.46 |
| 1:B:111:ASN:HB3 | 1:B:165:GLY:O | 2.16 | 0.46 |
| 1:B:118:ALA:HB1 | 1:B:122:ARG:NH2 | 2.30 | 0.46 |
| 1:C:171:ILE:HB | 1:C:217:ILE:HG13 | 1.96 | 0.46 |
| 1:D:133:VAL:HB | 1:D:145:THR:HB | 1.98 | 0.46 |
| 1:D:262:LEU:CD1 | 1:D:299:LEU:HD21 | 2.40 | 0.46 |
| 1:E:133:VAL:HB | 1:E:145:THR:HB | 1.98 | 0.46 |
| 1:F:129:SER:HB3 | 1:F:147:ARG:HH22 | 1.80 | 0.46 |
| 1:K:111:ASN:HB3 | 1:K:165:GLY:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:224:ALA:HA | 1:K:227:ARG:NE | 2.30 | 0.46 |
| 1:K:251:LYS:HB3 | 1:L:476:GLU:HB2 | 1.98 | 0.46 |
| 1:M:251:LYS:HB3 | 1:N:476:GLU:HB2 | 1.98 | 0.46 |
| 1:N:111:ASN:HB3 | 1:N:165:GLY:O | 2.16 | 0.46 |
| 1:N:224:ALA:HA | 1:N:227:ARG:NE | 2.30 | 0.46 |
| 1:O:220:GLY:HA3 | 1:O:224:ALA:HB3 | 1.98 | 0.46 |
| 1:O:224:ALA:HA | 1:O:227:ARG:NE | 2.30 | 0.46 |
| 1:A:476:GLU:HB2 | 1:O:251:LYS:HB3 | 1.98 | 0.46 |
| 1:B:129:SER:HB3 | 1:B:147:ARG:HH22 | 1.80 | 0.46 |
| 1:B:235:LEU:HD23 | 1:B:237:VAL:HG12 | 1.97 | 0.46 |
| 1:B:246:ARG:HH22 | 1:B:305:GLN:HE22 | 1.61 | 0.46 |
| 1:C:220:GLY:HA3 | 1:C:224:ALA:HB3 | 1.98 | 0.46 |
| 1:I:118:ALA:HB1 | 1:I:122:ARG:NH2 | 2.30 | 0.46 |
| 1:I:235:LEU:HD23 | 1:I:237:VAL:HG12 | 1.97 | 0.46 |
| 1:I:251:LYS:HB3 | 1:J:476:GLU:HB2 | 1.98 | 0.46 |
| 1:J:111:ASN:HB3 | 1:J:165:GLY:O | 2.16 | 0.46 |
| 1:K:246:ARG:HH22 | 1:K:305:GLN:HE22 | 1.61 | 0.46 |
| 1:N:106:ILE:HG22 | 1:N:143:ILE:HA | 1.97 | 0.46 |
| 1:N:182:LEU:HA | 1:N:185:ILE:HG12 | 1.97 | 0.46 |
| 1:A:224:ALA:HA | 1:A:227:ARG:NE | 2.30 | 0.46 |
| 1:C:133:VAL:HB | 1:C:145:THR:HB | 1.98 | 0.46 |
| 1:E:259:VAL:HG22 | 1:E:299:LEU:CD1 | 2.46 | 0.46 |
| 1:F:111:ASN:HB3 | 1:F:165:GLY:O | 2.16 | 0.46 |
| 1:F:118:ALA:HB1 | 1:F:122:ARG:NH2 | 2.30 | 0.46 |
| 1:F:259:VAL:HG22 | 1:F:299:LEU:CD1 | 2.46 | 0.46 |
| 1:G:489:SER:HA | 1:G:504:ASN:O | 2.16 | 0.46 |
| 1:L:220:GLY:HA3 | 1:L:224:ALA:HB3 | 1.98 | 0.46 |
| 1:L:259:VAL:HG22 | 1:L:299:LEU:CD1 | 2.46 | 0.46 |
| 1:M:224:ALA:HA | 1:M:227:ARG:NE | 2.31 | 0.46 |
| 1:O:111:ASN:HB3 | 1:O:165:GLY:O | 2.16 | 0.46 |
| 1:O:259:VAL:HG22 | 1:O:299:LEU:CD1 | 2.46 | 0.46 |
| 1:B:259:VAL:HG22 | 1:B:299:LEU:CD1 | 2.46 | 0.46 |
| 1:D:220:GLY:HA3 | 1:D:224:ALA:HB3 | 1.97 | 0.46 |
| 1:E:224:ALA:HA | 1:E:227:ARG:NE | 2.30 | 0.46 |
| 1:F:133:VAL:HB | 1:F:145:THR:HB | 1.98 | 0.46 |
| 1:F:489:SER:HA | 1:F:504:ASN:O | 2.16 | 0.46 |
| 1:H:106:ILE:HG22 | 1:H:143:ILE:HA | 1.96 | 0.46 |
| 1:I:106:ILE:HG22 | 1:I:143:ILE:HA | 1.97 | 0.46 |
| 1:I:111:ASN:HB3 | 1:I:165:GLY:O | 2.16 | 0.46 |
| 1:I:259:VAL:HG22 | 1:I:299:LEU:CD1 | 2.46 | 0.46 |
| 1:L:106:ILE:HG22 | 1:L:143:ILE:HA | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:224:ALA:HA | 1:L:227:ARG:NE | 2.30 | 0.46 |
| 1:O:120:LEU:O | 1:O:123:GLN:HB3 | 2.14 | 0.46 |
| 1:A:489:SER:HA | 1:A:504:ASN:O | 2.16 | 0.46 |
| 1:B:212:ARG:HH21 | 1:C:181:ASP:HB2 | 1.79 | 0.46 |
| 1:B:224:ALA:HA | 1:B:227:ARG:NE | 2.31 | 0.46 |
| 1:D:259:VAL:HG22 | 1:D:299:LEU:CD1 | 2.46 | 0.46 |
| 1:E:220:GLY:HA3 | 1:E:224:ALA:HB3 | 1.98 | 0.46 |
| 1:G:111:ASN:HB3 | 1:G:165:GLY:O | 2.16 | 0.46 |
| 1:G:129:SER:HB3 | 1:G:147:ARG:HH22 | 1.80 | 0.46 |
| 1:H:111:ASN:HB3 | 1:H:165:GLY:O | 2.16 | 0.46 |
| 1:I:220:GLY:HA3 | 1:I:224:ALA:HB3 | 1.98 | 0.46 |
| 1:K:220:GLY:HA3 | 1:K:224:ALA:HB3 | 1.98 | 0.46 |
| 1:O:235:LEU:HD23 | 1:O:237:VAL:HG12 | 1.97 | 0.46 |
| 1:A:129:SER:HB3 | 1:A:147:ARG:HH22 | 1.80 | 0.46 |
| 1:B:170:GLN:HG3 | 1:B:218:ILE:HG23 | 1.98 | 0.46 |
| 1:C:170:GLN:HG3 | 1:C:218:ILE:HG23 | 1.98 | 0.46 |
| 1:C:224:ALA:HA | 1:C:227:ARG:NE | 2.30 | 0.46 |
| 1:C:259:VAL:HG22 | 1:C:299:LEU:CD1 | 2.46 | 0.46 |
| 1:F:224:ALA:HA | 1:F:227:ARG:NE | 2.30 | 0.46 |
| 1:G:118:ALA:HB1 | 1:G:122:ARG:NH2 | 2.30 | 0.46 |
| 1:G:220:GLY:HA3 | 1:G:224:ALA:HB3 | 1.98 | 0.46 |
| 1:G:259:VAL:HG22 | 1:G:299:LEU:CD1 | 2.46 | 0.46 |
| 1:H:220:GLY:HA3 | 1:H:224:ALA:HB3 | 1.98 | 0.46 |
| 1:J:220:GLY:HA3 | 1:J:224:ALA:HB3 | 1.98 | 0.46 |
| 1:J:235:LEU:HD23 | 1:J:237:VAL:HG12 | 1.97 | 0.46 |
| 1:J:438:GLY:HA3 | 1:J:465:GLY:HA3 | 1.98 | 0.46 |
| 1:K:259:VAL:HG22 | 1:K:299:LEU:CD1 | 2.46 | 0.46 |
| 1:N:147:ARG:O | 1:N:151:ILE:HG12 | 2.16 | 0.46 |
| 1:N:259:VAL:HG22 | 1:N:299:LEU:CD1 | 2.46 | 0.46 |
| 1:O:129:SER:HB3 | 1:O:147:ARG:HH22 | 1.80 | 0.46 |
| 1:O:489:SER:HA | 1:O:504:ASN:O | 2.16 | 0.46 |
| 1:D:170:GLN:HG3 | 1:D:218:ILE:HG23 | 1.98 | 0.46 |
| 1:F:220:GLY:HA3 | 1:F:224:ALA:HB3 | 1.98 | 0.46 |
| 1:G:133:VAL:HB | 1:G:145:THR:HB | 1.98 | 0.46 |
| 1:G:474:VAL:HG22 | 1:G:480:VAL:HG12 | 1.98 | 0.46 |
| 1:H:118:ALA:HB1 | 1:H:122:ARG:NH2 | 2.30 | 0.46 |
| 1:H:129:SER:HB3 | 1:H:147:ARG:HH22 | 1.80 | 0.46 |
| 1:H:182:LEU:HA | 1:H:185:ILE:HG12 | 1.97 | 0.46 |
| 1:H:224:ALA:HA | 1:H:227:ARG:NE | 2.30 | 0.46 |
| 1:I:246:ARG:HH22 | 1:I:305:GLN:HE22 | 1.61 | 0.46 |
| 1:I:438:GLY:HA3 | 1:I:465:GLY:HA3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:224:ALA:HA | 1:J:227:ARG:NE | 2.30 | 0.46 |
| 1:K:129:SER:HB3 | 1:K:147:ARG:HH22 | 1.80 | 0.46 |
| 1:K:235:LEU:HD23 | 1:K:237:VAL:HG12 | 1.97 | 0.46 |
| 1:L:147:ARG:O | 1:L:151:ILE:HG12 | 2.16 | 0.46 |
| 1:L:246:ARG:HH22 | 1:L:305:GLN:HE22 | 1.61 | 0.46 |
| 1:M:182:LEU:HA | 1:M:185:ILE:HG12 | 1.97 | 0.46 |
| 1:A:118:ALA:HB1 | 1:A:122:ARG:NH2 | 2.30 | 0.46 |
| 1:B:133:VAL:HB | 1:B:145:THR:HB | 1.98 | 0.46 |
| 1:B:474:VAL:HG22 | 1:B:480:VAL:HG12 | 1.98 | 0.46 |
| 1:B:489:SER:HA | 1:B:504:ASN:O | 2.16 | 0.46 |
| 1:D:111:ASN:HB3 | 1:D:165:GLY:O | 2.16 | 0.46 |
| 1:D:224:ALA:HA | 1:D:227:ARG:NE | 2.31 | 0.46 |
| 1:H:489:SER:HA | 1:H:504:ASN:O | 2.16 | 0.46 |
| 1:K:438:GLY:HA3 | 1:K:465:GLY:HA3 | 1.98 | 0.46 |
| 1:M:106:ILE:HG22 | 1:M:143:ILE:HA | 1.96 | 0.46 |
| 1:N:474:VAL:HG22 | 1:N:480:VAL:HG12 | 1.98 | 0.46 |
| 1:O:474:VAL:HG22 | 1:O:480:VAL:HG12 | 1.98 | 0.46 |
| 1:A:170:GLN:HG3 | 1:A:218:ILE:HG23 | 1.98 | 0.45 |
| 1:B:251:LYS:HB3 | 1:C:476:GLU:HB2 | 1.98 | 0.45 |
| 1:C:111:ASN:HB3 | 1:C:165:GLY:O | 2.16 | 0.45 |
| 1:D:474:VAL:HG22 | 1:D:480:VAL:HG12 | 1.98 | 0.45 |
| 1:E:170:GLN:HG3 | 1:E:218:ILE:HG23 | 1.98 | 0.45 |
| 1:E:489:SER:HA | 1:E:504:ASN:O | 2.16 | 0.45 |
| 1:G:251:LYS:HB3 | 1:H:476:GLU:HB2 | 1.98 | 0.45 |
| 1:H:259:VAL:HG22 | 1:H:299:LEU:CD1 | 2.46 | 0.45 |
| 1:H:474:VAL:HG22 | 1:H:480:VAL:HG12 | 1.98 | 0.45 |
| 1:I:182:LEU:HA | 1:I:185:ILE:HG12 | 1.97 | 0.45 |
| 1:K:489:SER:HA | 1:K:504:ASN:O | 2.16 | 0.45 |
| 1:L:182:LEU:HA | 1:L:185:ILE:HG12 | 1.97 | 0.45 |
| 1:N:129:SER:HB3 | 1:N:147:ARG:HH22 | 1.80 | 0.45 |
| 1:O:246:ARG:HH22 | 1:O:305:GLN:HE22 | 1.61 | 0.45 |
| 1:A:147:ARG:O | 1:A:151:ILE:HG12 | 2.16 | 0.45 |
| 1:A:474:VAL:HG22 | 1:A:480:VAL:HG12 | 1.98 | 0.45 |
| 1:C:129:SER:HB3 | 1:C:147:ARG:HH22 | 1.80 | 0.45 |
| 1:C:438:GLY:HA3 | 1:C:465:GLY:HA3 | 1.98 | 0.45 |
| 1:D:438:GLY:HA3 | 1:D:465:GLY:HA3 | 1.98 | 0.45 |
| 1:E:474:VAL:HG22 | 1:E:480:VAL:HG12 | 1.98 | 0.45 |
| 1:F:474:VAL:HG22 | 1:F:480:VAL:HG12 | 1.98 | 0.45 |
| 1:G:222:GLU:O | 1:G:225:ARG:HB2 | 2.17 | 0.45 |
| 1:H:133:VAL:HB | 1:H:145:THR:HB | 1.98 | 0.45 |
| 1:I:118:ALA:HB3 | 1:I:119:PRO:HD3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:475:ASN:HA | 1:I:476:GLU:HA | 1.78 | 0.45 |
| 1:J:118:ALA:HB3 | 1:J:119:PRO:HD3 | 1.98 | 0.45 |
| 1:J:182:LEU:HA | 1:J:185:ILE:HG12 | 1.97 | 0.45 |
| 1:J:474:VAL:HG22 | 1:J:480:VAL:HG12 | 1.98 | 0.45 |
| 1:K:222:GLU:O | 1:K:225:ARG:HB2 | 2.17 | 0.45 |
| 1:K:474:VAL:HG22 | 1:K:480:VAL:HG12 | 1.98 | 0.45 |
| 1:L:347:ALA:HA | 1:L:353:ALA:HA | 1.99 | 0.45 |
| 1:L:489:SER:HA | 1:L:504:ASN:O | 2.16 | 0.45 |
| 1:M:235:LEU:HD23 | 1:M:237:VAL:HG12 | 1.97 | 0.45 |
| 1:M:347:ALA:HA | 1:M:353:ALA:HA | 1.99 | 0.45 |
| 1:N:235:LEU:HD23 | 1:N:237:VAL:HG12 | 1.97 | 0.45 |
| 1:N:489:SER:HA | 1:N:504:ASN:O | 2.16 | 0.45 |
| 1:C:222:GLU:O | 1:C:225:ARG:HB2 | 2.17 | 0.45 |
| 1:D:222:GLU:O | 1:D:225:ARG:HB2 | 2.17 | 0.45 |
| 1:I:133:VAL:HB | 1:I:145:THR:HB | 1.98 | 0.45 |
| 1:J:347:ALA:HA | 1:J:353:ALA:HA | 1.99 | 0.45 |
| 1:K:182:LEU:HA | 1:K:185:ILE:HG12 | 1.97 | 0.45 |
| 1:A:133:VAL:HB | 1:A:145:THR:HB | 1.98 | 0.45 |
| 1:B:161:VAL:HA | 1:B:164:ILE:CG1 | 2.47 | 0.45 |
| 1:F:170:GLN:HG3 | 1:F:218:ILE:HG23 | 1.98 | 0.45 |
| 1:H:118:ALA:HB3 | 1:H:119:PRO:HD3 | 1.98 | 0.45 |
| 1:H:222:GLU:O | 1:H:225:ARG:HB2 | 2.17 | 0.45 |
| 1:H:438:GLY:HA3 | 1:H:465:GLY:HA3 | 1.98 | 0.45 |
| 1:I:474:VAL:HG22 | 1:I:480:VAL:HG12 | 1.98 | 0.45 |
| 1:J:147:ARG:O | 1:J:151:ILE:HG12 | 2.16 | 0.45 |
| 1:J:259:VAL:HG22 | 1:J:299:LEU:CD1 | 2.46 | 0.45 |
| 1:K:109:LEU:HD21 | 1:K:112:VAL:HB | 1.99 | 0.45 |
| 1:M:474:VAL:HG22 | 1:M:480:VAL:HG12 | 1.98 | 0.45 |
| 1:B:222:GLU:O | 1:B:225:ARG:HB2 | 2.17 | 0.45 |
| 1:C:474:VAL:HG22 | 1:C:480:VAL:HG12 | 1.98 | 0.45 |
| 1:D:489:SER:HA | 1:D:504:ASN:O | 2.16 | 0.45 |
| 1:D:529:PHE:HZ | 1:D:531:LYS:HE3 | 1.82 | 0.45 |
| 1:E:222:GLU:O | 1:E:225:ARG:HB2 | 2.17 | 0.45 |
| 1:E:438:GLY:HA3 | 1:E:465:GLY:HA3 | 1.98 | 0.45 |
| 1:I:489:SER:HA | 1:I:504:ASN:O | 2.16 | 0.45 |
| 1:K:347:ALA:HA | 1:K:353:ALA:HA | 1.99 | 0.45 |
| 1:L:133:VAL:HB | 1:L:145:THR:HB | 1.98 | 0.45 |
| 1:L:438:GLY:HA3 | 1:L:465:GLY:HA3 | 1.98 | 0.45 |
| 1:L:474:VAL:HG22 | 1:L:480:VAL:HG12 | 1.98 | 0.45 |
| 1:M:133:VAL:HB | 1:M:145:THR:HB | 1.98 | 0.45 |
| 1:N:161:VAL:HA | 1:N:164:ILE:CG1 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:206:LYS:HZ3 | 1:O:190:ILE:C | 2.20 | 0.45 |
| 1:O:347:ALA:HA | 1:O:353:ALA:HA | 1.99 | 0.45 |
| 1:A:161:VAL:HA | 1:A:164:ILE:CG1 | 2.47 | 0.45 |
| 1:A:222:GLU:O | 1:A:225:ARG:HB2 | 2.17 | 0.45 |
| 1:A:529:PHE:HZ | 1:A:531:LYS:HE3 | 1.82 | 0.45 |
| 1:B:438:GLY:HA3 | 1:B:465:GLY:HA3 | 1.98 | 0.45 |
| 1:G:170:GLN:HG3 | 1:G:218:ILE:HG23 | 1.98 | 0.45 |
| 1:I:147:ARG:O | 1:I:151:ILE:HG12 | 2.16 | 0.45 |
| 1:J:222:GLU:O | 1:J:225:ARG:HB2 | 2.17 | 0.45 |
| 1:K:133:VAL:HB | 1:K:145:THR:HB | 1.98 | 0.45 |
| 1:L:222:GLU:O | 1:L:225:ARG:HB2 | 2.17 | 0.45 |
| 1:L:235:LEU:HD23 | 1:L:237:VAL:HG12 | 1.97 | 0.45 |
| 1:M:220:GLY:HA3 | 1:M:224:ALA:CB | 2.47 | 0.45 |
| 1:M:529:PHE:HZ | 1:M:531:LYS:HE3 | 1.82 | 0.45 |
| 1:N:251:LYS:HB3 | 1:O:476:GLU:HB2 | 1.98 | 0.45 |
| 1:N:347:ALA:HA | 1:N:353:ALA:HA | 1.99 | 0.45 |
| 1:O:161:VAL:HA | 1:O:164:ILE:CG1 | 2.47 | 0.45 |
| 1:O:170:GLN:HG3 | 1:O:218:ILE:HG23 | 1.98 | 0.45 |
| 1:B:529:PHE:HZ | 1:B:531:LYS:HE3 | 1.82 | 0.45 |
| 1:D:147:ARG:O | 1:D:151:ILE:HG12 | 2.16 | 0.45 |
| 1:D:220:GLY:HA3 | 1:D:224:ALA:CB | 2.47 | 0.45 |
| 1:G:109:LEU:HD21 | 1:G:112:VAL:HB | 1.99 | 0.45 |
| 1:H:109:LEU:HD21 | 1:H:112:VAL:HB | 1.99 | 0.45 |
| 1:H:161:VAL:HA | 1:H:164:ILE:CG1 | 2.46 | 0.45 |
| 1:H:220:GLY:HA3 | 1:H:224:ALA:CB | 2.47 | 0.45 |
| 1:I:161:VAL:HA | 1:I:164:ILE:CG1 | 2.46 | 0.45 |
| 1:J:133:VAL:HB | 1:J:145:THR:HB | 1.98 | 0.45 |
| 1:K:170:GLN:HG3 | 1:K:218:ILE:HG23 | 1.98 | 0.45 |
| 1:K:220:GLY:HA3 | 1:K:224:ALA:CB | 2.47 | 0.45 |
| 1:K:529:PHE:HZ | 1:K:531:LYS:HE3 | 1.82 | 0.45 |
| 1:L:220:GLY:HA3 | 1:L:224:ALA:CB | 2.47 | 0.45 |
| 1:L:251:LYS:HB3 | 1:M:476:GLU:HB2 | 1.98 | 0.45 |
| 1:M:161:VAL:HA | 1:M:164:ILE:CG1 | 2.47 | 0.45 |
| 1:N:109:LEU:HD11 | 1:N:112:VAL:HB | 1.99 | 0.45 |
| 1:N:529:PHE:HZ | 1:N:531:LYS:HE3 | 1.82 | 0.45 |
| 1:O:109:LEU:HD21 | 1:O:112:VAL:HB | 1.99 | 0.45 |
| 1:A:438:GLY:HA3 | 1:A:465:GLY:HA3 | 1.98 | 0.45 |
| 1:B:346:TRP:O | 1:B:346:TRP:CE3 | 2.70 | 0.45 |
| 1:C:489:SER:HA | 1:C:504:ASN:O | 2.16 | 0.45 |
| 1:D:251:LYS:HB3 | 1:E:476:GLU:HB2 | 1.98 | 0.45 |
| 1:F:222:GLU:O | 1:F:225:ARG:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:118:ALA:HB3 | 1:G:119:PRO:HD3 | 1.98 | 0.45 |
| 1:G:147:ARG:O | 1:G:151:ILE:HG12 | 2.16 | 0.45 |
| 1:G:220:GLY:HA3 | 1:G:224:ALA:CB | 2.47 | 0.45 |
| 1:I:220:GLY:HA3 | 1:I:224:ALA:CB | 2.47 | 0.45 |
| 1:I:347:ALA:HA | 1:I:353:ALA:HA | 1.99 | 0.45 |
| 1:J:109:LEU:HD21 | 1:J:112:VAL:HB | 1.99 | 0.45 |
| 1:J:170:GLN:HG3 | 1:J:218:ILE:HG23 | 1.98 | 0.45 |
| 1:J:220:GLY:HA3 | 1:J:224:ALA:CB | 2.47 | 0.45 |
| 1:J:251:LYS:HB3 | 1:K:476:GLU:HB2 | 1.98 | 0.45 |
| 1:K:118:ALA:HB3 | 1:K:119:PRO:HD3 | 1.98 | 0.45 |
| 1:K:147:ARG:O | 1:K:151:ILE:HG12 | 2.16 | 0.45 |
| 1:M:109:LEU:HD11 | 1:M:112:VAL:HB | 1.99 | 0.45 |
| 1:M:259:VAL:HG22 | 1:M:299:LEU:CD1 | 2.46 | 0.45 |
| 1:N:109:LEU:HD21 | 1:N:112:VAL:HB | 1.99 | 0.45 |
| 1:O:109:LEU:HD11 | 1:O:112:VAL:HB | 1.99 | 0.45 |
| 1:A:259:VAL:HG22 | 1:A:299:LEU:CD1 | 2.46 | 0.45 |
| 1:A:347:ALA:HA | 1:A:353:ALA:HA | 1.99 | 0.45 |
| 1:E:147:ARG:O | 1:E:151:ILE:HG12 | 2.16 | 0.45 |
| 1:F:438:GLY:HA3 | 1:F:465:GLY:HA3 | 1.98 | 0.45 |
| 1:F:529:PHE:HZ | 1:F:531:LYS:HE3 | 1.82 | 0.45 |
| 1:H:346:TRP:O | 1:H:346:TRP:CE3 | 2.70 | 0.45 |
| 1:I:346:TRP:CE3 | 1:I:346:TRP:O | 2.70 | 0.45 |
| 1:J:489:SER:HA | 1:J:504:ASN:O | 2.16 | 0.45 |
| 1:J:529:PHE:HZ | 1:J:531:LYS:HE3 | 1.82 | 0.45 |
| 1:L:109:LEU:HD11 | 1:L:112:VAL:HB | 1.99 | 0.45 |
| 1:M:104:THR:OG1 | 1:M:144:LEU:O | 2.21 | 0.45 |
| 1:O:222:GLU:O | 1:O:225:ARG:HB2 | 2.17 | 0.45 |
| 1:A:118:ALA:HB3 | 1:A:119:PRO:HD3 | 1.98 | 0.45 |
| 1:C:346:TRP:O | 1:C:346:TRP:CE3 | 2.70 | 0.45 |
| 1:E:129:SER:HB3 | 1:E:147:ARG:HH22 | 1.80 | 0.45 |
| 1:E:251:LYS:HB3 | 1:F:476:GLU:HB2 | 1.98 | 0.45 |
| 1:H:170:GLN:HG3 | 1:H:218:ILE:HG23 | 1.98 | 0.45 |
| 1:I:109:LEU:HD11 | 1:I:112:VAL:HB | 1.99 | 0.45 |
| 1:L:109:LEU:HD21 | 1:L:112:VAL:HB | 1.99 | 0.45 |
| 1:L:170:GLN:HG3 | 1:L:218:ILE:HG23 | 1.98 | 0.45 |
| 1:N:133:VAL:HB | 1:N:145:THR:HB | 1.98 | 0.45 |
| 1:N:220:GLY:HA3 | 1:N:224:ALA:CB | 2.47 | 0.45 |
| 1:N:414:ASN:HB3 | 1:O:534:VAL:CG2 | 2.47 | 0.45 |
| 1:O:438:GLY:HA3 | 1:O:465:GLY:HA3 | 1.98 | 0.45 |
| 1:A:109:LEU:HD11 | 1:A:112:VAL:HB | 1.99 | 0.44 |
| 1:B:147:ARG:O | 1:B:151:ILE:HG12 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:151:ILE:HA | 1:B:154:LEU:HB2 | 2.00 | 0.44 |
| 1:C:414:ASN:HB3 | 1:D:534:VAL:CG2 | 2.47 | 0.44 |
| 1:E:346:TRP:O | 1:E:346:TRP:CE3 | 2.70 | 0.44 |
| 1:E:414:ASN:HB3 | 1:F:534:VAL:CG2 | 2.47 | 0.44 |
| 1:F:346:TRP:CE3 | 1:F:346:TRP:O | 2.70 | 0.44 |
| 1:H:347:ALA:HA | 1:H:353:ALA:HA | 1.99 | 0.44 |
| 1:H:529:PHE:HZ | 1:H:531:LYS:HE3 | 1.82 | 0.44 |
| 1:I:170:GLN:HG3 | 1:I:218:ILE:HG23 | 1.98 | 0.44 |
| 1:J:109:LEU:HD11 | 1:J:112:VAL:HB | 1.99 | 0.44 |
| 1:J:414:ASN:HB3 | 1:K:534:VAL:CG2 | 2.47 | 0.44 |
| 1:K:109:LEU:HD11 | 1:K:112:VAL:HB | 1.99 | 0.44 |
| 1:M:147:ARG:O | 1:M:151:ILE:HG12 | 2.16 | 0.44 |
| 1:M:346:TRP:O | 1:M:346:TRP:CE3 | 2.70 | 0.44 |
| 1:M:489:SER:HA | 1:M:504:ASN:O | 2.16 | 0.44 |
| 1:O:118:ALA:HB3 | 1:O:119:PRO:HD3 | 1.98 | 0.44 |
| 1:O:133:VAL:HB | 1:O:145:THR:HB | 1.98 | 0.44 |
| 1:A:109:LEU:HD21 | 1:A:112:VAL:HB | 1.99 | 0.44 |
| 1:A:534:VAL:CG2 | 1:O:414:ASN:HB3 | 2.47 | 0.44 |
| 1:E:151:ILE:HA | 1:E:154:LEU:HB2 | 2.00 | 0.44 |
| 1:E:220:GLY:HA3 | 1:E:224:ALA:CB | 2.47 | 0.44 |
| 1:F:109:LEU:HD21 | 1:F:112:VAL:HB | 1.99 | 0.44 |
| 1:F:251:LYS:HB3 | 1:G:476:GLU:HB2 | 1.98 | 0.44 |
| 1:H:109:LEU:HD11 | 1:H:112:VAL:HB | 1.99 | 0.44 |
| 1:H:147:ARG:O | 1:H:151:ILE:HG12 | 2.16 | 0.44 |
| 1:H:251:LYS:HB3 | 1:I:476:GLU:HB2 | 1.98 | 0.44 |
| 1:I:225:ARG:O | 1:I:229:THR:HG23 | 2.18 | 0.44 |
| 1:J:161:VAL:HA | 1:J:164:ILE:CG1 | 2.47 | 0.44 |
| 1:J:346:TRP:O | 1:J:346:TRP:CE3 | 2.70 | 0.44 |
| 1:J:475:ASN:HA | 1:J:476:GLU:HA | 1.78 | 0.44 |
| 1:M:414:ASN:HB3 | 1:N:534:VAL:CG2 | 2.47 | 0.44 |
| 1:M:438:GLY:HA3 | 1:M:465:GLY:HA3 | 1.98 | 0.44 |
| 1:N:170:GLN:HG3 | 1:N:218:ILE:HG23 | 1.98 | 0.44 |
| 1:B:118:ALA:HB3 | 1:B:119:PRO:HD3 | 1.98 | 0.44 |
| 1:B:347:ALA:HA | 1:B:353:ALA:HA | 1.99 | 0.44 |
| 1:C:118:ALA:HB3 | 1:C:119:PRO:HD3 | 1.98 | 0.44 |
| 1:C:220:GLY:HA3 | 1:C:224:ALA:CB | 2.47 | 0.44 |
| 1:D:151:ILE:HA | 1:D:154:LEU:HB2 | 2.00 | 0.44 |
| 1:E:161:VAL:HA | 1:E:164:ILE:CG1 | 2.46 | 0.44 |
| 1:F:220:GLY:HA3 | 1:F:224:ALA:CB | 2.47 | 0.44 |
| 1:G:161:VAL:HA | 1:G:164:ILE:CG1 | 2.46 | 0.44 |
| 1:G:346:TRP:O | 1:G:346:TRP:CE3 | 2.70 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:347:ALA:HA | 1:G:353:ALA:HA | 1.99 | 0.44 |
| 1:J:225:ARG:O | 1:J:229:THR:HG23 | 2.18 | 0.44 |
| 1:K:414:ASN:HB3 | 1:L:534:VAL:CG2 | 2.47 | 0.44 |
| 1:L:414:ASN:HB3 | 1:M:534:VAL:CG2 | 2.47 | 0.44 |
| 1:N:222:GLU:O | 1:N:225:ARG:HB2 | 2.17 | 0.44 |
| 1:N:346:TRP:CE3 | 1:N:346:TRP:O | 2.70 | 0.44 |
| 1:O:220:GLY:HA3 | 1:O:224:ALA:CB | 2.47 | 0.44 |
| 1:A:220:GLY:HA3 | 1:A:224:ALA:CB | 2.47 | 0.44 |
| 1:A:251:LYS:HB3 | 1:B:476:GLU:HB2 | 1.98 | 0.44 |
| 1:C:151:ILE:HA | 1:C:154:LEU:HB2 | 2.00 | 0.44 |
| 1:D:118:ALA:HB3 | 1:D:119:PRO:HD3 | 1.98 | 0.44 |
| 1:D:161:VAL:HA | 1:D:164:ILE:CG1 | 2.47 | 0.44 |
| 1:G:151:ILE:HA | 1:G:154:LEU:HB2 | 2.00 | 0.44 |
| 1:G:324:GLN:HB2 | 1:G:571:ILE:HB | 1.99 | 0.44 |
| 1:G:438:GLY:HA3 | 1:G:465:GLY:HA3 | 1.98 | 0.44 |
| 1:I:529:PHE:HZ | 1:I:531:LYS:HE3 | 1.82 | 0.44 |
| 1:K:161:VAL:HA | 1:K:164:ILE:CG1 | 2.47 | 0.44 |
| 1:N:118:ALA:HB3 | 1:N:119:PRO:HD3 | 1.98 | 0.44 |
| 1:O:151:ILE:HA | 1:O:154:LEU:HB2 | 2.00 | 0.44 |
| 1:O:346:TRP:CE3 | 1:O:346:TRP:O | 2.70 | 0.44 |
| 1:B:220:GLY:HA3 | 1:B:224:ALA:CB | 2.47 | 0.44 |
| 1:C:347:ALA:HA | 1:C:353:ALA:HA | 1.99 | 0.44 |
| 1:E:225:ARG:O | 1:E:229:THR:HG23 | 2.18 | 0.44 |
| 1:E:529:PHE:HZ | 1:E:531:LYS:HE3 | 1.82 | 0.44 |
| 1:G:109:LEU:HD11 | 1:G:112:VAL:HB | 1.99 | 0.44 |
| 1:H:324:GLN:HB2 | 1:H:571:ILE:HB | 1.99 | 0.44 |
| 1:K:225:ARG:O | 1:K:229:THR:HG23 | 2.18 | 0.44 |
| 1:L:118:ALA:HB3 | 1:L:119:PRO:HD3 | 1.98 | 0.44 |
| 1:L:346:TRP:CE3 | 1:L:346:TRP:O | 2.70 | 0.44 |
| 1:N:324:GLN:HB2 | 1:N:571:ILE:HB | 1.99 | 0.44 |
| 1:N:438:GLY:HA3 | 1:N:465:GLY:HA3 | 1.98 | 0.44 |
| 1:A:151:ILE:HA | 1:A:154:LEU:HB2 | 2.00 | 0.44 |
| 1:B:109:LEU:HD11 | 1:B:112:VAL:HB | 1.99 | 0.44 |
| 1:C:104:THR:OG1 | 1:C:144:LEU:O | 2.21 | 0.44 |
| 1:C:147:ARG:O | 1:C:151:ILE:HG12 | 2.16 | 0.44 |
| 1:C:251:LYS:HB3 | 1:D:476:GLU:HB2 | 1.98 | 0.44 |
| 1:F:147:ARG:O | 1:F:151:ILE:HG12 | 2.16 | 0.44 |
| 1:F:225:ARG:O | 1:F:229:THR:HG23 | 2.18 | 0.44 |
| 1:G:529:PHE:HZ | 1:G:531:LYS:HE3 | 1.82 | 0.44 |
| 1:I:109:LEU:HD21 | 1:I:112:VAL:HB | 1.99 | 0.44 |
| 1:K:335:GLN:HB2 | 1:K:417:ASN:HB3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:170:GLN:HG3 | 1:M:218:ILE:HG23 | 1.98 | 0.44 |
| 1:M:324:GLN:HB2 | 1:M:571:ILE:HB | 1.99 | 0.44 |
| 1:N:151:ILE:HA | 1:N:154:LEU:HB2 | 2.00 | 0.44 |
| 1:O:147:ARG:O | 1:O:151:ILE:HG12 | 2.16 | 0.44 |
| 1:A:346:TRP:CE3 | 1:A:346:TRP:O | 2.70 | 0.44 |
| 1:A:414:ASN:HB3 | 1:B:534:VAL:CG2 | 2.47 | 0.44 |
| 1:D:221:PRO:O | 1:D:225:ARG:HG3 | 2.18 | 0.44 |
| 1:D:225:ARG:O | 1:D:229:THR:HG23 | 2.18 | 0.44 |
| 1:F:118:ALA:HB3 | 1:F:119:PRO:HD3 | 1.98 | 0.44 |
| 1:F:151:ILE:HA | 1:F:154:LEU:HB2 | 2.00 | 0.44 |
| 1:F:324:GLN:HB2 | 1:F:571:ILE:HB | 1.99 | 0.44 |
| 1:F:414:ASN:HB3 | 1:G:534:VAL:CG2 | 2.47 | 0.44 |
| 1:H:151:ILE:HA | 1:H:154:LEU:HB2 | 2.00 | 0.44 |
| 1:H:225:ARG:O | 1:H:229:THR:HG23 | 2.18 | 0.44 |
| 1:I:222:GLU:O | 1:I:225:ARG:HB2 | 2.17 | 0.44 |
| 1:L:221:PRO:O | 1:L:225:ARG:HG3 | 2.18 | 0.44 |
| 1:M:109:LEU:HD21 | 1:M:112:VAL:HB | 1.99 | 0.44 |
| 1:M:222:GLU:O | 1:M:225:ARG:HB2 | 2.17 | 0.44 |
| 1:N:259:VAL:HG22 | 1:N:299:LEU:HD11 | 2.00 | 0.44 |
| 1:O:225:ARG:O | 1:O:229:THR:HG23 | 2.18 | 0.44 |
| 1:B:259:VAL:HG22 | 1:B:299:LEU:HD11 | 2.00 | 0.44 |
| 1:B:414:ASN:HB3 | 1:C:534:VAL:CG2 | 2.47 | 0.44 |
| 1:F:109:LEU:HD11 | 1:F:112:VAL:HB | 1.99 | 0.44 |
| 1:F:347:ALA:HA | 1:F:353:ALA:HA | 1.99 | 0.44 |
| 1:H:210:ASP:OD1 | 1:H:212:ARG:N | 2.51 | 0.44 |
| 1:I:324:GLN:HB2 | 1:I:571:ILE:HB | 1.99 | 0.44 |
| 1:J:221:PRO:O | 1:J:225:ARG:HG3 | 2.18 | 0.44 |
| 1:M:259:VAL:HG22 | 1:M:299:LEU:HD11 | 2.00 | 0.44 |
| 1:M:335:GLN:HB2 | 1:M:417:ASN:HB3 | 2.00 | 0.44 |
| 1:O:324:GLN:HB2 | 1:O:571:ILE:HB | 1.99 | 0.44 |
| 1:A:225:ARG:O | 1:A:229:THR:HG23 | 2.18 | 0.44 |
| 1:A:361:LEU:HD12 | 1:A:361:LEU:O | 2.18 | 0.44 |
| 1:C:259:VAL:HG22 | 1:C:299:LEU:HD11 | 2.00 | 0.44 |
| 1:C:529:PHE:HZ | 1:C:531:LYS:HE3 | 1.82 | 0.44 |
| 1:D:347:ALA:HA | 1:D:353:ALA:HA | 1.99 | 0.44 |
| 1:E:109:LEU:HD21 | 1:E:112:VAL:HB | 1.99 | 0.44 |
| 1:E:118:ALA:HB3 | 1:E:119:PRO:HD3 | 1.98 | 0.44 |
| 1:E:206:LYS:O | 1:E:218:ILE:HD12 | 2.18 | 0.44 |
| 1:G:414:ASN:HB3 | 1:H:534:VAL:CG2 | 2.47 | 0.44 |
| 1:I:361:LEU:HD12 | 1:I:361:LEU:O | 2.18 | 0.44 |
| 1:K:210:ASP:OD1 | 1:K:212:ARG:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:259:VAL:HG22 | 1:K:299:LEU:HD11 | 2.00 | 0.44 |
| 1:K:346:TRP:O | 1:K:346:TRP:CE3 | 2.70 | 0.44 |
| 1:L:225:ARG:O | 1:L:229:THR:HG23 | 2.18 | 0.44 |
| 1:L:324:GLN:HB2 | 1:L:571:ILE:HB | 1.99 | 0.44 |
| 1:L:335:GLN:HB2 | 1:L:417:ASN:HB3 | 2.00 | 0.44 |
| 1:M:118:ALA:HB3 | 1:M:119:PRO:HD3 | 1.98 | 0.44 |
| 1:N:221:PRO:O | 1:N:225:ARG:HG3 | 2.18 | 0.44 |
| 1:O:259:VAL:HG22 | 1:O:299:LEU:HD11 | 2.00 | 0.44 |
| 1:A:210:ASP:OD1 | 1:A:212:ARG:N | 2.51 | 0.43 |
| 1:B:109:LEU:HD21 | 1:B:112:VAL:HB | 1.99 | 0.43 |
| 1:C:210:ASP:OD1 | 1:C:212:ARG:N | 2.51 | 0.43 |
| 1:E:324:GLN:HB2 | 1:E:571:ILE:HB | 1.99 | 0.43 |
| 1:E:347:ALA:HA | 1:E:353:ALA:HA | 1.99 | 0.43 |
| 1:F:221:PRO:O | 1:F:225:ARG:HG3 | 2.18 | 0.43 |
| 1:H:414:ASN:HB3 | 1:I:534:VAL:CG2 | 2.47 | 0.43 |
| 1:H:475:ASN:HA | 1:H:476:GLU:HA | 1.78 | 0.43 |
| 1:I:335:GLN:HB2 | 1:I:417:ASN:HB3 | 2.00 | 0.43 |
| 1:J:259:VAL:HG22 | 1:J:299:LEU:HD11 | 2.00 | 0.43 |
| 1:J:335:GLN:HB2 | 1:J:417:ASN:HB3 | 2.00 | 0.43 |
| 1:K:361:LEU:HD12 | 1:K:361:LEU:O | 2.18 | 0.43 |
| 1:L:161:VAL:HA | 1:L:164:ILE:CG1 | 2.46 | 0.43 |
| 1:L:259:VAL:HG22 | 1:L:299:LEU:HD11 | 2.00 | 0.43 |
| 1:N:335:GLN:HB2 | 1:N:417:ASN:HB3 | 2.00 | 0.43 |
| 1:O:221:PRO:HD2 | 1:O:224:ALA:HB2 | 2.00 | 0.43 |
| 1:A:221:PRO:HD2 | 1:A:224:ALA:HB2 | 2.00 | 0.43 |
| 1:B:221:PRO:HD2 | 1:B:224:ALA:HB2 | 2.00 | 0.43 |
| 1:B:221:PRO:O | 1:B:225:ARG:HG3 | 2.18 | 0.43 |
| 1:C:109:LEU:HD11 | 1:C:112:VAL:HB | 1.99 | 0.43 |
| 1:C:225:ARG:O | 1:C:229:THR:HG23 | 2.18 | 0.43 |
| 1:C:361:LEU:HD12 | 1:C:361:LEU:O | 2.18 | 0.43 |
| 1:D:206:LYS:O | 1:D:218:ILE:HD12 | 2.18 | 0.43 |
| 1:D:346:TRP:CE3 | 1:D:346:TRP:O | 2.70 | 0.43 |
| 1:G:225:ARG:O | 1:G:229:THR:HG23 | 2.18 | 0.43 |
| 1:I:221:PRO:O | 1:I:225:ARG:HG3 | 2.18 | 0.43 |
| 1:J:324:GLN:HB2 | 1:J:571:ILE:HB | 1.99 | 0.43 |
| 1:L:529:PHE:HZ | 1:L:531:LYS:HE3 | 1.82 | 0.43 |
| 1:N:225:ARG:O | 1:N:229:THR:HG23 | 2.18 | 0.43 |
| 1:O:221:PRO:O | 1:O:225:ARG:HG3 | 2.18 | 0.43 |
| 1:A:259:VAL:HG22 | 1:A:299:LEU:HD11 | 2.00 | 0.43 |
| 1:C:221:PRO:HD2 | 1:C:224:ALA:HB2 | 2.00 | 0.43 |
| 1:D:106:ILE:HG13 | 1:D:106:ILE:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:361:LEU:HD12 | 1:G:361:LEU:O | 2.18 | 0.43 |
| 1:H:335:GLN:HB2 | 1:H:417:ASN:HB3 | 2.00 | 0.43 |
| 1:I:206:LYS:O | 1:I:218:ILE:HD12 | 2.18 | 0.43 |
| 1:I:210:ASP:OD1 | 1:I:212:ARG:N | 2.51 | 0.43 |
| 1:L:151:ILE:HA | 1:L:154:LEU:HB2 | 2.00 | 0.43 |
| 1:L:210:ASP:OD1 | 1:L:212:ARG:N | 2.51 | 0.43 |
| 1:M:151:ILE:HA | 1:M:154:LEU:HB2 | 2.00 | 0.43 |
| 1:N:106:ILE:O | 1:N:106:ILE:HG13 | 2.19 | 0.43 |
| 1:N:361:LEU:HD12 | 1:N:361:LEU:O | 2.18 | 0.43 |
| 1:O:106:ILE:HG13 | 1:O:106:ILE:O | 2.19 | 0.43 |
| 1:O:529:PHE:HZ | 1:O:531:LYS:HE3 | 1.82 | 0.43 |
| 1:A:106:ILE:O | 1:A:106:ILE:HG13 | 2.19 | 0.43 |
| 1:D:109:LEU:HD11 | 1:D:112:VAL:HB | 1.99 | 0.43 |
| 1:D:414:ASN:HB3 | 1:E:534:VAL:CG2 | 2.47 | 0.43 |
| 1:E:109:LEU:HD11 | 1:E:112:VAL:HB | 1.99 | 0.43 |
| 1:F:161:VAL:HA | 1:F:164:ILE:CG1 | 2.47 | 0.43 |
| 1:F:206:LYS:O | 1:F:218:ILE:HD12 | 2.18 | 0.43 |
| 1:G:221:PRO:O | 1:G:225:ARG:HG3 | 2.18 | 0.43 |
| 1:I:414:ASN:HB3 | 1:J:534:VAL:CG2 | 2.47 | 0.43 |
| 1:J:151:ILE:HA | 1:J:154:LEU:HB2 | 2.00 | 0.43 |
| 1:K:151:ILE:HA | 1:K:154:LEU:HB2 | 2.00 | 0.43 |
| 1:M:106:ILE:HG13 | 1:M:106:ILE:O | 2.19 | 0.43 |
| 1:N:221:PRO:HD2 | 1:N:224:ALA:HB2 | 2.00 | 0.43 |
| 1:B:106:ILE:HG13 | 1:B:106:ILE:O | 2.19 | 0.43 |
| 1:C:161:VAL:HA | 1:C:164:ILE:CG1 | 2.47 | 0.43 |
| 1:C:324:GLN:HB2 | 1:C:571:ILE:HB | 1.99 | 0.43 |
| 1:D:335:GLN:HB2 | 1:D:417:ASN:HB3 | 2.00 | 0.43 |
| 1:D:361:LEU:HD12 | 1:D:361:LEU:O | 2.18 | 0.43 |
| 1:E:335:GLN:HB2 | 1:E:417:ASN:HB3 | 2.00 | 0.43 |
| 1:E:361:LEU:HD12 | 1:E:361:LEU:O | 2.18 | 0.43 |
| 1:G:210:ASP:OD1 | 1:G:212:ARG:N | 2.51 | 0.43 |
| 1:H:206:LYS:O | 1:H:218:ILE:HD12 | 2.18 | 0.43 |
| 1:H:221:PRO:O | 1:H:225:ARG:HG3 | 2.18 | 0.43 |
| 1:H:259:VAL:HG22 | 1:H:299:LEU:HD11 | 2.00 | 0.43 |
| 1:K:324:GLN:HB2 | 1:K:571:ILE:HB | 1.99 | 0.43 |
| 1:M:221:PRO:HD2 | 1:M:224:ALA:HB2 | 2.00 | 0.43 |
| 1:A:221:PRO:O | 1:A:225:ARG:HG3 | 2.18 | 0.43 |
| 1:A:324:GLN:HB2 | 1:A:571:ILE:HB | 1.99 | 0.43 |
| 1:C:109:LEU:HD21 | 1:C:112:VAL:HB | 1.99 | 0.43 |
| 1:E:259:VAL:HG22 | 1:E:299:LEU:HD11 | 2.00 | 0.43 |
| 1:G:221:PRO:HD2 | 1:G:224:ALA:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:151:ILE:HA | 1:I:154:LEU:HB2 | 2.00 | 0.43 |
| 1:I:259:VAL:HG22 | 1:I:299:LEU:HD11 | 2.00 | 0.43 |
| 1:L:106:ILE:HG13 | 1:L:106:ILE:O | 2.19 | 0.43 |
| 1:N:262:LEU:HD23 | 1:N:262:LEU:HA | 1.83 | 0.43 |
| 1:O:124:MET:HB3 | 1:O:154:LEU:HD21 | 2.01 | 0.43 |
| 1:B:124:MET:HB3 | 1:B:154:LEU:HD21 | 2.01 | 0.43 |
| 1:C:106:ILE:O | 1:C:106:ILE:HG13 | 2.19 | 0.43 |
| 1:C:124:MET:HB3 | 1:C:154:LEU:HD21 | 2.01 | 0.43 |
| 1:D:109:LEU:HD21 | 1:D:112:VAL:HB | 1.99 | 0.43 |
| 1:D:124:MET:HB3 | 1:D:154:LEU:HD21 | 2.01 | 0.43 |
| 1:D:259:VAL:HG22 | 1:D:299:LEU:HD11 | 2.00 | 0.43 |
| 1:D:324:GLN:HB2 | 1:D:571:ILE:HB | 1.99 | 0.43 |
| 1:F:361:LEU:HD12 | 1:F:361:LEU:O | 2.18 | 0.43 |
| 1:H:117:LEU:HD13 | 1:H:157:VAL:HG12 | 2.01 | 0.43 |
| 1:H:221:PRO:HD2 | 1:H:224:ALA:HB2 | 2.00 | 0.43 |
| 1:I:117:LEU:HD13 | 1:I:157:VAL:HG12 | 2.01 | 0.43 |
| 1:I:232:LEU:HD23 | 1:I:232:LEU:HA | 1.90 | 0.43 |
| 1:J:206:LYS:O | 1:J:218:ILE:HD12 | 2.18 | 0.43 |
| 1:J:210:ASP:OD1 | 1:J:212:ARG:N | 2.51 | 0.43 |
| 1:J:221:PRO:HD2 | 1:J:224:ALA:HB2 | 2.00 | 0.43 |
| 1:K:106:ILE:O | 1:K:106:ILE:HG13 | 2.19 | 0.43 |
| 1:M:221:PRO:O | 1:M:225:ARG:HG3 | 2.18 | 0.43 |
| 1:M:347:ALA:HB2 | 1:M:363:ILE:HG12 | 2.01 | 0.43 |
| 1:M:361:LEU:HD12 | 1:M:361:LEU:O | 2.18 | 0.43 |
| 1:O:335:GLN:HB2 | 1:O:417:ASN:HB3 | 2.00 | 0.43 |
| 1:C:221:PRO:O | 1:C:225:ARG:HG3 | 2.18 | 0.43 |
| 1:E:210:ASP:OD1 | 1:E:212:ARG:N | 2.51 | 0.43 |
| 1:F:259:VAL:HG22 | 1:F:299:LEU:HD11 | 2.00 | 0.43 |
| 1:G:117:LEU:HD13 | 1:G:157:VAL:HG12 | 2.01 | 0.43 |
| 1:I:221:PRO:HD2 | 1:I:224:ALA:HB2 | 2.00 | 0.43 |
| 1:J:117:LEU:HD13 | 1:J:157:VAL:HG12 | 2.01 | 0.43 |
| 1:N:124:MET:HB3 | 1:N:154:LEU:HD21 | 2.01 | 0.43 |
| 1:N:210:ASP:OD1 | 1:N:212:ARG:N | 2.51 | 0.43 |
| 1:O:206:LYS:O | 1:O:218:ILE:HD12 | 2.18 | 0.43 |
| 1:A:124:MET:HB3 | 1:A:154:LEU:HD21 | 2.01 | 0.43 |
| 1:A:206:LYS:O | 1:A:218:ILE:HD12 | 2.18 | 0.43 |
| 1:A:335:GLN:HB2 | 1:A:417:ASN:HB3 | 2.00 | 0.43 |
| 1:A:475:ASN:HA | 1:A:476:GLU:HA | 1.78 | 0.43 |
| 1:B:225:ARG:O | 1:B:229:THR:HG23 | 2.18 | 0.43 |
| 1:B:324:GLN:HB2 | 1:B:571:ILE:HB | 1.99 | 0.43 |
| 1:C:206:LYS:O | 1:C:218:ILE:HD12 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:221:PRO:O | 1:E:225:ARG:HG3 | 2.18 | 0.43 |
| 1:G:259:VAL:HG22 | 1:G:299:LEU:HD11 | 2.00 | 0.43 |
| 1:I:171:ILE:HD11 | 1:J:234:SER:HB3 | 2.01 | 0.43 |
| 1:K:221:PRO:O | 1:K:225:ARG:HG3 | 2.18 | 0.43 |
| 1:L:221:PRO:HD2 | 1:L:224:ALA:HB2 | 2.00 | 0.43 |
| 1:L:347:ALA:HB2 | 1:L:363:ILE:HG12 | 2.01 | 0.43 |
| 1:L:361:LEU:HD12 | 1:L:361:LEU:O | 2.18 | 0.43 |
| 1:M:225:ARG:O | 1:M:229:THR:HG23 | 2.18 | 0.43 |
| 1:A:171:ILE:HD11 | 1:B:234:SER:HB3 | 2.01 | 0.43 |
| 1:B:361:LEU:HD12 | 1:B:361:LEU:O | 2.18 | 0.43 |
| 1:B:475:ASN:HA | 1:B:476:GLU:HA | 1.78 | 0.43 |
| 1:C:335:GLN:HB2 | 1:C:417:ASN:HB3 | 2.00 | 0.43 |
| 1:D:221:PRO:HD2 | 1:D:224:ALA:HB2 | 2.00 | 0.43 |
| 1:F:335:GLN:HB2 | 1:F:417:ASN:HB3 | 2.00 | 0.43 |
| 1:J:171:ILE:HD11 | 1:K:234:SER:HB3 | 2.01 | 0.43 |
| 1:N:206:LYS:O | 1:N:218:ILE:HD12 | 2.18 | 0.43 |
| 1:A:234:SER:HB3 | 1:O:171:ILE:HD11 | 2.01 | 0.42 |
| 1:E:221:PRO:HD2 | 1:E:224:ALA:HB2 | 2.00 | 0.42 |
| 1:N:347:ALA:HB2 | 1:N:363:ILE:HG12 | 2.01 | 0.42 |
| 1:O:109:LEU:CD1 | 1:O:162:ASP:HA | 2.50 | 0.42 |
| 1:B:171:ILE:HD11 | 1:C:234:SER:HB3 | 2.01 | 0.42 |
| 1:D:123:GLN:HA | 1:D:126:ASP:HB3 | 2.02 | 0.42 |
| 1:E:124:MET:HB3 | 1:E:154:LEU:HD21 | 2.01 | 0.42 |
| 1:F:124:MET:HB3 | 1:F:154:LEU:HD21 | 2.01 | 0.42 |
| 1:G:335:GLN:HB2 | 1:G:417:ASN:HB3 | 2.00 | 0.42 |
| 1:H:171:ILE:HD11 | 1:I:234:SER:HB3 | 2.01 | 0.42 |
| 1:L:109:LEU:CD1 | 1:L:162:ASP:HA | 2.50 | 0.42 |
| 1:L:124:MET:HB3 | 1:L:154:LEU:HD21 | 2.01 | 0.42 |
| 1:O:475:ASN:HA | 1:O:476:GLU:HA | 1.78 | 0.42 |
| 1:B:117:LEU:HD13 | 1:B:157:VAL:HG12 | 2.01 | 0.42 |
| 1:B:123:GLN:HA | 1:B:126:ASP:HB3 | 2.02 | 0.42 |
| 1:B:206:LYS:O | 1:B:218:ILE:HD12 | 2.18 | 0.42 |
| 1:D:344:VAL:O | 1:D:354:GLN:NE2 | 2.53 | 0.42 |
| 1:E:106:ILE:HG13 | 1:E:106:ILE:O | 2.19 | 0.42 |
| 1:F:109:LEU:CD1 | 1:F:162:ASP:HA | 2.50 | 0.42 |
| 1:F:117:LEU:HD13 | 1:F:157:VAL:HG12 | 2.01 | 0.42 |
| 1:F:210:ASP:OD1 | 1:F:212:ARG:N | 2.51 | 0.42 |
| 1:G:106:ILE:HG13 | 1:G:106:ILE:O | 2.19 | 0.42 |
| 1:K:347:ALA:HB2 | 1:K:363:ILE:HG12 | 2.01 | 0.42 |
| 1:M:124:MET:HB3 | 1:M:154:LEU:HD21 | 2.01 | 0.42 |
| 1:M:206:LYS:O | 1:M:218:ILE:HD12 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:361:LEU:HD12 | 1:O:361:LEU:O | 2.18 | 0.42 |
| 1:A:344:VAL:O | 1:A:354:GLN:NE2 | 2.53 | 0.42 |
| 1:B:344:VAL:O | 1:B:354:GLN:NE2 | 2.53 | 0.42 |
| 1:D:210:ASP:OD1 | 1:D:212:ARG:N | 2.51 | 0.42 |
| 1:F:344:VAL:O | 1:F:354:GLN:NE2 | 2.53 | 0.42 |
| 1:H:106:ILE:O | 1:H:106:ILE:HG13 | 2.19 | 0.42 |
| 1:H:344:VAL:O | 1:H:354:GLN:NE2 | 2.53 | 0.42 |
| 1:J:361:LEU:HD12 | 1:J:361:LEU:O | 2.18 | 0.42 |
| 1:K:117:LEU:HD13 | 1:K:157:VAL:HG12 | 2.01 | 0.42 |
| 1:K:171:ILE:HD11 | 1:L:234:SER:HB3 | 2.01 | 0.42 |
| 1:M:210:ASP:OD1 | 1:M:212:ARG:N | 2.51 | 0.42 |
| 1:O:123:GLN:HA | 1:O:126:ASP:HB3 | 2.02 | 0.42 |
| 1:O:210:ASP:OD1 | 1:O:212:ARG:N | 2.51 | 0.42 |
| 1:A:117:LEU:HD13 | 1:A:157:VAL:HG12 | 2.01 | 0.42 |
| 1:B:335:GLN:HB2 | 1:B:417:ASN:HB3 | 2.00 | 0.42 |
| 1:C:117:LEU:HD13 | 1:C:157:VAL:HG12 | 2.01 | 0.42 |
| 1:C:475:ASN:HA | 1:C:476:GLU:HA | 1.78 | 0.42 |
| 1:E:109:LEU:CD1 | 1:E:162:ASP:HA | 2.50 | 0.42 |
| 1:F:123:GLN:HA | 1:F:126:ASP:HB3 | 2.02 | 0.42 |
| 1:F:262:LEU:HD23 | 1:F:262:LEU:HA | 1.83 | 0.42 |
| 1:G:109:LEU:CD1 | 1:G:162:ASP:HA | 2.50 | 0.42 |
| 1:J:106:ILE:HG13 | 1:J:106:ILE:O | 2.19 | 0.42 |
| 1:B:210:ASP:OD1 | 1:B:212:ARG:N | 2.51 | 0.42 |
| 1:D:109:LEU:CD1 | 1:D:162:ASP:HA | 2.50 | 0.42 |
| 1:D:135:HIS:HE1 | 1:E:120:LEU:HB2 | 1.85 | 0.42 |
| 1:E:344:VAL:O | 1:E:354:GLN:NE2 | 2.53 | 0.42 |
| 1:F:347:ALA:HB2 | 1:F:363:ILE:HG12 | 2.01 | 0.42 |
| 1:G:206:LYS:O | 1:G:218:ILE:HD12 | 2.18 | 0.42 |
| 1:G:344:VAL:O | 1:G:354:GLN:NE2 | 2.53 | 0.42 |
| 1:H:361:LEU:O | 1:H:361:LEU:HD12 | 2.18 | 0.42 |
| 1:M:206:LYS:HZ3 | 1:N:190:ILE:C | 2.23 | 0.42 |
| 1:O:344:VAL:O | 1:O:354:GLN:NE2 | 2.53 | 0.42 |
| 1:B:135:HIS:HE1 | 1:C:120:LEU:HB2 | 1.85 | 0.42 |
| 1:C:171:ILE:HD11 | 1:D:234:SER:HB3 | 2.02 | 0.42 |
| 1:D:347:ALA:HB2 | 1:D:363:ILE:HG12 | 2.01 | 0.42 |
| 1:G:124:MET:HB3 | 1:G:154:LEU:HD21 | 2.01 | 0.42 |
| 1:G:475:ASN:HA | 1:G:476:GLU:HA | 1.78 | 0.42 |
| 1:H:144:LEU:HD11 | 1:H:158:ILE:CD1 | 2.50 | 0.42 |
| 1:J:144:LEU:HD11 | 1:J:158:ILE:CD1 | 2.50 | 0.42 |
| 1:J:344:VAL:O | 1:J:354:GLN:NE2 | 2.53 | 0.42 |
| 1:K:124:MET:HB3 | 1:K:154:LEU:HD21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:221:PRO:HD2 | 1:K:224:ALA:HB2 | 2.00 | 0.42 |
| 1:N:171:ILE:HD11 | 1:O:234:SER:HB3 | 2.01 | 0.42 |
| 1:O:117:LEU:HD13 | 1:O:157:VAL:HG12 | 2.01 | 0.42 |
| 1:O:262:LEU:HD23 | 1:O:262:LEU:HA | 1.83 | 0.42 |
| 1:O:571:ILE:CG2 | 1:O:577:TYR:HB2 | 2.50 | 0.42 |
| 1:A:109:LEU:CD1 | 1:A:162:ASP:HA | 2.50 | 0.42 |
| 1:A:571:ILE:CG2 | 1:A:577:TYR:HB2 | 2.50 | 0.42 |
| 1:C:135:HIS:HE1 | 1:D:120:LEU:HB2 | 1.85 | 0.42 |
| 1:E:135:HIS:HE1 | 1:F:120:LEU:HB2 | 1.85 | 0.42 |
| 1:E:347:ALA:HB2 | 1:E:363:ILE:HG12 | 2.01 | 0.42 |
| 1:G:171:ILE:HD11 | 1:H:234:SER:HB3 | 2.01 | 0.42 |
| 1:H:109:LEU:CD1 | 1:H:162:ASP:HA | 2.50 | 0.42 |
| 1:I:144:LEU:HD11 | 1:I:158:ILE:CD1 | 2.50 | 0.42 |
| 1:I:344:VAL:O | 1:I:354:GLN:NE2 | 2.53 | 0.42 |
| 1:K:109:LEU:CD1 | 1:K:162:ASP:HA | 2.50 | 0.42 |
| 1:K:206:LYS:O | 1:K:218:ILE:HD12 | 2.18 | 0.42 |
| 1:L:144:LEU:HD11 | 1:L:158:ILE:CD1 | 2.50 | 0.42 |
| 1:A:120:LEU:HB2 | 1:O:135:HIS:HE1 | 1.85 | 0.42 |
| 1:C:109:LEU:CD1 | 1:C:162:ASP:HA | 2.50 | 0.42 |
| 1:C:344:VAL:O | 1:C:354:GLN:NE2 | 2.53 | 0.42 |
| 1:D:117:LEU:HD13 | 1:D:157:VAL:HG12 | 2.01 | 0.42 |
| 1:D:184:GLU:O | 1:D:188:GLN:HG2 | 2.20 | 0.42 |
| 1:E:117:LEU:HD13 | 1:E:157:VAL:HG12 | 2.01 | 0.42 |
| 1:E:184:GLU:O | 1:E:188:GLN:HG2 | 2.20 | 0.42 |
| 1:F:221:PRO:HD2 | 1:F:224:ALA:HB2 | 2.00 | 0.42 |
| 1:F:571:ILE:CG2 | 1:F:577:TYR:HB2 | 2.50 | 0.42 |
| 1:I:109:LEU:CD1 | 1:I:162:ASP:HA | 2.50 | 0.42 |
| 1:J:184:GLU:O | 1:J:188:GLN:HG2 | 2.20 | 0.42 |
| 1:L:135:HIS:HE1 | 1:M:120:LEU:HB2 | 1.85 | 0.42 |
| 1:L:344:VAL:O | 1:L:354:GLN:NE2 | 2.53 | 0.42 |
| 1:M:109:LEU:CD1 | 1:M:162:ASP:HA | 2.50 | 0.42 |
| 1:M:184:GLU:O | 1:M:188:GLN:HG2 | 2.20 | 0.42 |
| 1:N:109:LEU:CD1 | 1:N:162:ASP:HA | 2.50 | 0.42 |
| 1:N:184:GLU:O | 1:N:188:GLN:HG2 | 2.20 | 0.42 |
| 1:N:571:ILE:CG2 | 1:N:577:TYR:HB2 | 2.50 | 0.42 |
| 1:O:347:ALA:HB2 | 1:O:363:ILE:HG12 | 2.01 | 0.42 |
| 1:A:436:ASN:HB2 | 1:B:507:THR:HB | 2.02 | 0.42 |
| 1:C:184:GLU:O | 1:C:188:GLN:HG2 | 2.20 | 0.42 |
| 1:C:347:ALA:HB2 | 1:C:363:ILE:HG12 | 2.01 | 0.42 |
| 1:C:571:ILE:CG2 | 1:C:577:TYR:HB2 | 2.50 | 0.42 |
| 1:D:171:ILE:HD11 | 1:E:234:SER:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:206:LYS:HZ3 | 1:F:190:ILE:C | 2.24 | 0.42 |
| 1:H:124:MET:HB3 | 1:H:154:LEU:HD21 | 2.01 | 0.42 |
| 1:I:106:ILE:O | 1:I:106:ILE:HG13 | 2.19 | 0.42 |
| 1:I:124:MET:HB3 | 1:I:154:LEU:HD21 | 2.01 | 0.42 |
| 1:K:144:LEU:HD11 | 1:K:158:ILE:CD1 | 2.50 | 0.42 |
| 1:K:206:LYS:HZ3 | 1:L:190:ILE:C | 2.23 | 0.42 |
| 1:K:344:VAL:O | 1:K:354:GLN:NE2 | 2.53 | 0.42 |
| 1:L:206:LYS:O | 1:L:218:ILE:HD12 | 2.18 | 0.42 |
| 1:M:135:HIS:HE1 | 1:N:120:LEU:HB2 | 1.85 | 0.42 |
| 1:N:475:ASN:HA | 1:N:476:GLU:HA | 1.78 | 0.42 |
| 1:B:118:ALA:HB1 | 1:B:122:ARG:HH21 | 1.85 | 0.41 |
| 1:B:184:GLU:O | 1:B:188:GLN:HG2 | 2.20 | 0.41 |
| 1:D:475:ASN:HA | 1:D:476:GLU:HA | 1.78 | 0.41 |
| 1:D:571:ILE:CG2 | 1:D:577:TYR:HB2 | 2.50 | 0.41 |
| 1:F:106:ILE:O | 1:F:106:ILE:HG13 | 2.19 | 0.41 |
| 1:F:118:ALA:HB1 | 1:F:122:ARG:HH21 | 1.85 | 0.41 |
| 1:F:184:GLU:O | 1:F:188:GLN:HG2 | 2.20 | 0.41 |
| 1:G:123:GLN:HA | 1:G:126:ASP:HB3 | 2.02 | 0.41 |
| 1:G:144:LEU:HD11 | 1:G:158:ILE:CD1 | 2.50 | 0.41 |
| 1:H:232:LEU:HD23 | 1:H:232:LEU:HA | 1.90 | 0.41 |
| 1:J:159:LYS:O | 1:J:162:ASP:HB3 | 2.20 | 0.41 |
| 1:K:118:ALA:HB1 | 1:K:122:ARG:HH21 | 1.85 | 0.41 |
| 1:K:135:HIS:HE1 | 1:L:120:LEU:HB2 | 1.85 | 0.41 |
| 1:M:344:VAL:O | 1:M:354:GLN:NE2 | 2.53 | 0.41 |
| 1:N:144:LEU:HD11 | 1:N:158:ILE:CD1 | 2.50 | 0.41 |
| 1:N:344:VAL:O | 1:N:354:GLN:NE2 | 2.53 | 0.41 |
| 1:A:507:THR:HB | 1:O:436:ASN:HB2 | 2.03 | 0.41 |
| 1:B:175:GLU:HG3 | 1:B:176:TYR:CD2 | 2.56 | 0.41 |
| 1:B:436:ASN:HB2 | 1:C:507:THR:HB | 2.02 | 0.41 |
| 1:D:159:LYS:O | 1:D:162:ASP:HB3 | 2.20 | 0.41 |
| 1:D:175:GLU:HG3 | 1:D:176:TYR:CD2 | 2.55 | 0.41 |
| 1:F:144:LEU:HD11 | 1:F:158:ILE:CD1 | 2.50 | 0.41 |
| 1:F:175:GLU:HG3 | 1:F:176:TYR:CD2 | 2.55 | 0.41 |
| 1:G:175:GLU:HG3 | 1:G:176:TYR:CD2 | 2.56 | 0.41 |
| 1:G:347:ALA:HB2 | 1:G:363:ILE:HG12 | 2.01 | 0.41 |
| 1:H:571:ILE:CG2 | 1:H:577:TYR:HB2 | 2.50 | 0.41 |
| 1:I:123:GLN:HA | 1:I:126:ASP:HB3 | 2.02 | 0.41 |
| 1:I:184:GLU:O | 1:I:188:GLN:HG2 | 2.20 | 0.41 |
| 1:J:118:ALA:HB1 | 1:J:122:ARG:HH21 | 1.85 | 0.41 |
| 1:K:571:ILE:CG2 | 1:K:577:TYR:HB2 | 2.50 | 0.41 |
| 1:L:118:ALA:HB1 | 1:L:122:ARG:HH21 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:123:GLN:HA | 1:L:126:ASP:HB3 | 2.02 | 0.41 |
| 1:L:171:ILE:HD11 | 1:M:234:SER:HB3 | 2.01 | 0.41 |
| 1:L:571:ILE:CG2 | 1:L:577:TYR:HB2 | 2.50 | 0.41 |
| 1:M:144:LEU:HD11 | 1:M:158:ILE:CD1 | 2.50 | 0.41 |
| 1:M:175:GLU:HG3 | 1:M:176:TYR:CD2 | 2.55 | 0.41 |
| 1:M:571:ILE:CG2 | 1:M:577:TYR:HB2 | 2.50 | 0.41 |
| 1:N:117:LEU:HD13 | 1:N:157:VAL:HG12 | 2.01 | 0.41 |
| 1:N:175:GLU:HG3 | 1:N:176:TYR:CD2 | 2.56 | 0.41 |
| 1:A:118:ALA:HB1 | 1:A:122:ARG:HH21 | 1.85 | 0.41 |
| 1:A:184:GLU:O | 1:A:188:GLN:HG2 | 2.20 | 0.41 |
| 1:B:571:ILE:CG2 | 1:B:577:TYR:HB2 | 2.50 | 0.41 |
| 1:E:118:ALA:HB1 | 1:E:122:ARG:HH21 | 1.85 | 0.41 |
| 1:F:135:HIS:HE1 | 1:G:120:LEU:HB2 | 1.85 | 0.41 |
| 1:F:475:ASN:HA | 1:F:476:GLU:HA | 1.78 | 0.41 |
| 1:I:159:LYS:O | 1:I:162:ASP:HB3 | 2.20 | 0.41 |
| 1:J:109:LEU:CD1 | 1:J:162:ASP:HA | 2.50 | 0.41 |
| 1:J:124:MET:HB3 | 1:J:154:LEU:HD21 | 2.01 | 0.41 |
| 1:J:212:ARG:CZ | 1:K:181:ASP:OD2 | 2.69 | 0.41 |
| 1:J:347:ALA:HB2 | 1:J:363:ILE:HG12 | 2.01 | 0.41 |
| 1:L:117:LEU:HD13 | 1:L:157:VAL:HG12 | 2.01 | 0.41 |
| 1:N:123:GLN:HA | 1:N:126:ASP:HB3 | 2.02 | 0.41 |
| 1:O:175:GLU:HG3 | 1:O:176:TYR:CD2 | 2.56 | 0.41 |
| 1:B:109:LEU:CD1 | 1:B:162:ASP:HA | 2.50 | 0.41 |
| 1:E:159:LYS:O | 1:E:162:ASP:HB3 | 2.20 | 0.41 |
| 1:E:571:ILE:CG2 | 1:E:577:TYR:HB2 | 2.50 | 0.41 |
| 1:G:184:GLU:O | 1:G:188:GLN:HG2 | 2.20 | 0.41 |
| 1:H:347:ALA:HB2 | 1:H:363:ILE:HG12 | 2.01 | 0.41 |
| 1:H:436:ASN:HB2 | 1:I:507:THR:HB | 2.02 | 0.41 |
| 1:N:135:HIS:HE1 | 1:O:120:LEU:HB2 | 1.85 | 0.41 |
| 1:N:212:ARG:CZ | 1:O:181:ASP:OD2 | 2.69 | 0.41 |
| 1:O:159:LYS:O | 1:O:162:ASP:HB3 | 2.20 | 0.41 |
| 1:B:159:LYS:O | 1:B:162:ASP:HB3 | 2.20 | 0.41 |
| 1:C:436:ASN:HB2 | 1:D:507:THR:HB | 2.02 | 0.41 |
| 1:E:123:GLN:HA | 1:E:126:ASP:HB3 | 2.02 | 0.41 |
| 1:E:475:ASN:HA | 1:E:476:GLU:HA | 1.78 | 0.41 |
| 1:F:171:ILE:HD11 | 1:G:234:SER:HB3 | 2.01 | 0.41 |
| 1:G:571:ILE:CG2 | 1:G:577:TYR:HB2 | 2.50 | 0.41 |
| 1:I:206:LYS:HZ3 | 1:J:190:ILE:C | 2.24 | 0.41 |
| 1:I:347:ALA:HB2 | 1:I:363:ILE:HG12 | 2.01 | 0.41 |
| 1:O:184:GLU:O | 1:O:188:GLN:HG2 | 2.20 | 0.41 |
| 1:A:123:GLN:HA | 1:A:126:ASP:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:212:ARG:CZ | 1:C:181:ASP:OD2 | 2.69 | 0.41 |
| 1:B:347:ALA:HB2 | 1:B:363:ILE:HG12 | 2.01 | 0.41 |
| 1:C:159:LYS:O | 1:C:162:ASP:HB3 | 2.20 | 0.41 |
| 1:E:171:ILE:HD11 | 1:F:234:SER:HB3 | 2.01 | 0.41 |
| 1:G:149:SER:O | 1:G:152:ASN:HB2 | 2.21 | 0.41 |
| 1:I:548:GLN:HA | 1:I:551:ARG:HG2 | 2.03 | 0.41 |
| 1:J:571:ILE:CG2 | 1:J:577:TYR:HB2 | 2.50 | 0.41 |
| 1:K:159:LYS:O | 1:K:162:ASP:HB3 | 2.20 | 0.41 |
| 1:L:149:SER:O | 1:L:152:ASN:HB2 | 2.21 | 0.41 |
| 1:L:159:LYS:O | 1:L:162:ASP:HB3 | 2.20 | 0.41 |
| 1:M:171:ILE:HD11 | 1:N:234:SER:HB3 | 2.01 | 0.41 |
| 1:N:159:LYS:O | 1:N:162:ASP:HB3 | 2.20 | 0.41 |
| 1:N:436:ASN:HB2 | 1:O:507:THR:HB | 2.02 | 0.41 |
| 1:C:149:SER:O | 1:C:152:ASN:HB2 | 2.21 | 0.41 |
| 1:C:167:GLU:HA | 1:C:221:PRO:CA | 2.50 | 0.41 |
| 1:C:175:GLU:HG3 | 1:C:176:TYR:CD2 | 2.56 | 0.41 |
| 1:D:436:ASN:HB2 | 1:E:507:THR:HB | 2.02 | 0.41 |
| 1:H:159:LYS:O | 1:H:162:ASP:HB3 | 2.20 | 0.41 |
| 1:H:175:GLU:HG3 | 1:H:176:TYR:CD2 | 2.56 | 0.41 |
| 1:I:121:LEU:HD23 | 1:I:121:LEU:HA | 1.86 | 0.41 |
| 1:I:436:ASN:HB2 | 1:J:507:THR:HB | 2.03 | 0.41 |
| 1:J:135:HIS:HE1 | 1:K:120:LEU:HB2 | 1.85 | 0.41 |
| 1:K:184:GLU:O | 1:K:188:GLN:HG2 | 2.20 | 0.41 |
| 1:M:118:ALA:HB1 | 1:M:122:ARG:HH21 | 1.85 | 0.41 |
| 1:M:212:ARG:CZ | 1:N:181:ASP:OD2 | 2.69 | 0.41 |
| 1:A:108:PRO:HB3 | 1:A:141:VAL:HA | 2.03 | 0.41 |
| 1:A:144:LEU:HD11 | 1:A:158:ILE:CD1 | 2.50 | 0.41 |
| 1:A:149:SER:O | 1:A:152:ASN:HB2 | 2.21 | 0.41 |
| 1:B:262:LEU:HD23 | 1:B:262:LEU:HA | 1.83 | 0.41 |
| 1:C:123:GLN:HA | 1:C:126:ASP:HB3 | 2.02 | 0.41 |
| 1:D:167:GLU:HA | 1:D:221:PRO:CA | 2.51 | 0.41 |
| 1:G:436:ASN:HB2 | 1:H:507:THR:HB | 2.02 | 0.41 |
| 1:H:548:GLN:HA | 1:H:551:ARG:HG2 | 2.03 | 0.41 |
| 1:I:118:ALA:HB1 | 1:I:122:ARG:HH21 | 1.85 | 0.41 |
| 1:J:149:SER:O | 1:J:152:ASN:HB2 | 2.21 | 0.41 |
| 1:J:548:GLN:HA | 1:J:551:ARG:HG2 | 2.03 | 0.41 |
| 1:K:108:PRO:HB3 | 1:K:141:VAL:HA | 2.03 | 0.41 |
| 1:L:184:GLU:O | 1:L:188:GLN:HG2 | 2.20 | 0.41 |
| 1:M:117:LEU:HD13 | 1:M:157:VAL:HG12 | 2.01 | 0.41 |
| 1:N:149:SER:O | 1:N:152:ASN:HB2 | 2.21 | 0.41 |
| 1:O:144:LEU:HD11 | 1:O:158:ILE:CD1 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:135:HIS:HE1 | 1:B:120:LEU:HB2 | 1.85 | 0.41 |
| 1:B:144:LEU:HD11 | 1:B:158:ILE:CD1 | 2.50 | 0.41 |
| 1:B:167:GLU:HA | 1:B:221:PRO:CA | 2.50 | 0.41 |
| 1:C:144:LEU:HD11 | 1:C:158:ILE:CD1 | 2.50 | 0.41 |
| 1:D:149:SER:O | 1:D:152:ASN:HB2 | 2.21 | 0.41 |
| 1:D:258:LEU:HD21 | 1:D:318:LEU:CD2 | 2.43 | 0.41 |
| 1:D:536:LYS:HE3 | 1:D:542:ASP:OD1 | 2.21 | 0.41 |
| 1:E:167:GLU:HA | 1:E:221:PRO:CA | 2.51 | 0.41 |
| 1:E:175:GLU:HG3 | 1:E:176:TYR:CD2 | 2.55 | 0.41 |
| 1:E:548:GLN:HA | 1:E:551:ARG:HG2 | 2.03 | 0.41 |
| 1:F:149:SER:O | 1:F:152:ASN:HB2 | 2.21 | 0.41 |
| 1:F:159:LYS:O | 1:F:162:ASP:HB3 | 2.20 | 0.41 |
| 1:I:212:ARG:CZ | 1:J:181:ASP:OD2 | 2.69 | 0.41 |
| 1:J:104:THR:OG1 | 1:J:144:LEU:O | 2.21 | 0.41 |
| 1:J:108:PRO:HB3 | 1:J:141:VAL:HA | 2.03 | 0.41 |
| 1:J:436:ASN:HB2 | 1:K:507:THR:HB | 2.02 | 0.41 |
| 1:K:167:GLU:HA | 1:K:221:PRO:CA | 2.51 | 0.41 |
| 1:L:175:GLU:HG3 | 1:L:176:TYR:CD2 | 2.56 | 0.41 |
| 1:M:108:PRO:HB3 | 1:M:141:VAL:HA | 2.03 | 0.41 |
| 1:M:288:VAL:HG22 | 1:M:303:ALA:HB2 | 2.03 | 0.41 |
| 1:N:121:LEU:HD21 | 1:N:157:VAL:HB | 2.03 | 0.41 |
| 1:O:108:PRO:HB3 | 1:O:141:VAL:HA | 2.03 | 0.41 |
| 1:A:175:GLU:HG3 | 1:A:176:TYR:CD2 | 2.56 | 0.41 |
| 1:A:347:ALA:HB2 | 1:A:363:ILE:HG12 | 2.01 | 0.41 |
| 1:C:258:LEU:HD21 | 1:C:318:LEU:CD2 | 2.43 | 0.41 |
| 1:D:144:LEU:HD11 | 1:D:158:ILE:CD1 | 2.50 | 0.41 |
| 1:D:548:GLN:HA | 1:D:551:ARG:HG2 | 2.03 | 0.41 |
| 1:H:149:SER:O | 1:H:152:ASN:HB2 | 2.21 | 0.41 |
| 1:I:571:ILE:CG2 | 1:I:577:TYR:HB2 | 2.50 | 0.41 |
| 1:K:121:LEU:HD21 | 1:K:157:VAL:HB | 2.03 | 0.41 |
| 1:L:108:PRO:HB3 | 1:L:141:VAL:HA | 2.03 | 0.41 |
| 1:L:121:LEU:HD21 | 1:L:157:VAL:HB | 2.03 | 0.41 |
| 1:M:123:GLN:HA | 1:M:126:ASP:HB3 | 2.02 | 0.41 |
| 1:M:536:LYS:HE3 | 1:M:542:ASP:OD1 | 2.21 | 0.41 |
| 1:O:232:LEU:HD23 | 1:O:232:LEU:HA | 1.90 | 0.41 |
| 1:A:212:ARG:CZ | 1:B:181:ASP:OD2 | 2.69 | 0.40 |
| 1:B:108:PRO:HB3 | 1:B:141:VAL:HA | 2.03 | 0.40 |
| 1:E:536:LYS:HE3 | 1:E:542:ASP:OD1 | 2.21 | 0.40 |
| 1:F:436:ASN:HB2 | 1:G:507:THR:HB | 2.02 | 0.40 |
| 1:H:123:GLN:HA | 1:H:126:ASP:HB3 | 2.02 | 0.40 |
| 1:J:288:VAL:HG22 | 1:J:303:ALA:HB2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:121:LEU:HD21 | 1:M:157:VAL:HB | 2.03 | 0.40 |
| 1:M:232:LEU:HA | 1:M:232:LEU:HD23 | 1.90 | 0.40 |
| 1:N:108:PRO:HB3 | 1:N:141:VAL:HA | 2.03 | 0.40 |
| 1:N:536:LYS:HE3 | 1:N:542:ASP:OD1 | 2.21 | 0.40 |
| 1:O:118:ALA:HB1 | 1:O:122:ARG:HH21 | 1.85 | 0.40 |
| 1:O:536:LYS:HE3 | 1:O:542:ASP:OD1 | 2.21 | 0.40 |
| 1:B:149:SER:O | 1:B:152:ASN:HB2 | 2.21 | 0.40 |
| 1:C:226:GLN:HG3 | 1:C:227:ARG:N | 2.37 | 0.40 |
| 1:E:362:PRO:HD2 | 1:E:388:MET:SD | 2.62 | 0.40 |
| 1:E:436:ASN:HB2 | 1:F:507:THR:HB | 2.02 | 0.40 |
| 1:F:108:PRO:HB3 | 1:F:141:VAL:HA | 2.03 | 0.40 |
| 1:G:108:PRO:HB3 | 1:G:141:VAL:HA | 2.03 | 0.40 |
| 1:G:135:HIS:HE1 | 1:H:120:LEU:HB2 | 1.85 | 0.40 |
| 1:H:226:GLN:HG3 | 1:H:227:ARG:N | 2.37 | 0.40 |
| 1:I:108:PRO:HB3 | 1:I:141:VAL:HA | 2.03 | 0.40 |
| 1:I:175:GLU:HG3 | 1:I:176:TYR:CD2 | 2.56 | 0.40 |
| 1:J:123:GLN:HA | 1:J:126:ASP:HB3 | 2.02 | 0.40 |
| 1:J:226:GLN:HG3 | 1:J:227:ARG:N | 2.37 | 0.40 |
| 1:K:175:GLU:HG3 | 1:K:176:TYR:CD2 | 2.56 | 0.40 |
| 1:K:436:ASN:HB2 | 1:L:507:THR:HB | 2.02 | 0.40 |
| 1:L:536:LYS:HE3 | 1:L:542:ASP:OD1 | 2.21 | 0.40 |
| 1:M:159:LYS:O | 1:M:162:ASP:HB3 | 2.20 | 0.40 |
| 1:M:436:ASN:HB2 | 1:N:507:THR:HB | 2.02 | 0.40 |
| 1:A:121:LEU:HD21 | 1:A:157:VAL:HB | 2.03 | 0.40 |
| 1:A:167:GLU:HA | 1:A:221:PRO:CA | 2.51 | 0.40 |
| 1:A:226:GLN:HG3 | 1:A:227:ARG:N | 2.37 | 0.40 |
| 1:B:226:GLN:HG3 | 1:B:227:ARG:N | 2.37 | 0.40 |
| 1:C:362:PRO:HD2 | 1:C:388:MET:SD | 2.62 | 0.40 |
| 1:C:536:LYS:HE3 | 1:C:542:ASP:OD1 | 2.21 | 0.40 |
| 1:C:548:GLN:HA | 1:C:551:ARG:HG2 | 2.03 | 0.40 |
| 1:D:118:ALA:HB1 | 1:D:122:ARG:HH21 | 1.85 | 0.40 |
| 1:D:121:LEU:HD21 | 1:D:157:VAL:HB | 2.03 | 0.40 |
| 1:E:108:PRO:HB3 | 1:E:141:VAL:HA | 2.03 | 0.40 |
| 1:E:144:LEU:HD11 | 1:E:158:ILE:CD1 | 2.50 | 0.40 |
| 1:F:536:LYS:HE3 | 1:F:542:ASP:OD1 | 2.21 | 0.40 |
| 1:G:159:LYS:O | 1:G:162:ASP:HB3 | 2.20 | 0.40 |
| 1:G:428:LEU:HD11 | 1:H:481:LEU:HD11 | 2.04 | 0.40 |
| 1:H:108:PRO:HB3 | 1:H:141:VAL:HA | 2.03 | 0.40 |
| 1:H:135:HIS:HE1 | 1:I:120:LEU:HB2 | 1.85 | 0.40 |
| 1:H:184:GLU:O | 1:H:188:GLN:HG2 | 2.20 | 0.40 |
| 1:H:428:LEU:HD11 | 1:I:481:LEU:HD11 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:428:LEU:HD11 | 1:J:481:LEU:HD11 | 2.04 | 0.40 |
| 1:J:175:GLU:HG3 | 1:J:176:TYR:CD2 | 2.55 | 0.40 |
| 1:J:262:LEU:HD23 | 1:J:262:LEU:HA | 1.83 | 0.40 |
| 1:J:349:LYS:HE3 | 1:J:349:LYS:HB2 | 1.90 | 0.40 |
| 1:J:536:LYS:HE3 | 1:J:542:ASP:OD1 | 2.21 | 0.40 |
| 1:K:123:GLN:HA | 1:K:126:ASP:HB3 | 2.02 | 0.40 |
| 1:K:548:GLN:HA | 1:K:551:ARG:HG2 | 2.03 | 0.40 |
| 1:O:121:LEU:HD21 | 1:O:157:VAL:HB | 2.03 | 0.40 |
| 1:O:149:SER:O | 1:O:152:ASN:HB2 | 2.21 | 0.40 |
| 1:O:362:PRO:HD2 | 1:O:388:MET:SD | 2.62 | 0.40 |
| 1:O:548:GLN:HA | 1:O:551:ARG:HG2 | 2.03 | 0.40 |
| 1:B:258:LEU:HD21 | 1:B:318:LEU:CD2 | 2.43 | 0.40 |
| 1:D:226:GLN:HG3 | 1:D:227:ARG:N | 2.37 | 0.40 |
| 1:G:226:GLN:HG3 | 1:G:227:ARG:N | 2.37 | 0.40 |
| 1:G:232:LEU:HD23 | 1:G:232:LEU:HA | 1.90 | 0.40 |
| 1:I:135:HIS:HE1 | 1:J:120:LEU:HB2 | 1.85 | 0.40 |
| 1:I:226:GLN:HG3 | 1:I:227:ARG:N | 2.37 | 0.40 |
| 1:I:536:LYS:HE3 | 1:I:542:ASP:OD1 | 2.21 | 0.40 |
| 1:J:167:GLU:HA | 1:J:221:PRO:CA | 2.51 | 0.40 |
| 1:K:536:LYS:HE3 | 1:K:542:ASP:OD1 | 2.21 | 0.40 |
| 1:L:226:GLN:HG3 | 1:L:227:ARG:N | 2.37 | 0.40 |
| 1:M:149:SER:O | 1:M:152:ASN:HB2 | 2.21 | 0.40 |
| 1:M:329:ALA:O | 1:M:422:THR:HA | 2.22 | 0.40 |
| 1:M:475:ASN:HA | 1:M:476:GLU:HA | 1.78 | 0.40 |
| 1:A:362:PRO:HD2 | 1:A:388:MET:SD | 2.62 | 0.40 |
| 1:A:428:LEU:HD11 | 1:B:481:LEU:HD11 | 2.04 | 0.40 |
| 1:C:108:PRO:HB3 | 1:C:141:VAL:HA | 2.03 | 0.40 |
| 1:C:326:LEU:HD21 | 1:C:328:GLU:OE2 | 2.22 | 0.40 |
| 1:D:108:PRO:HB3 | 1:D:141:VAL:HA | 2.03 | 0.40 |
| 1:E:149:SER:O | 1:E:152:ASN:HB2 | 2.21 | 0.40 |
| 1:F:362:PRO:HD2 | 1:F:388:MET:SD | 2.62 | 0.40 |
| 1:G:118:ALA:HB1 | 1:G:122:ARG:HH21 | 1.85 | 0.40 |
| 1:G:329:ALA:O | 1:G:422:THR:HA | 2.22 | 0.40 |
| 1:G:349:LYS:HE3 | 1:G:349:LYS:HB2 | 1.90 | 0.40 |
| 1:G:548:GLN:HA | 1:G:551:ARG:HG2 | 2.03 | 0.40 |
| 1:H:167:GLU:HA | 1:H:221:PRO:CA | 2.50 | 0.40 |
| 1:I:207:ILE:HG23 | 1:I:216:LEU:HD11 | 2.04 | 0.40 |
| 1:J:207:ILE:HG23 | 1:J:216:LEU:HD11 | 2.04 | 0.40 |
| 1:J:428:LEU:HD11 | 1:K:481:LEU:HD11 | 2.04 | 0.40 |
| 1:L:212:ARG:CZ | 1:M:181:ASP:OD2 | 2.69 | 0.40 |
| 1:N:136:TYR:HE1 | 1:N:142:LEU:HG | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:288:VAL:HG22 | 1:N:303:ALA:HB2 | 2.03 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | B | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | C | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | D | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | E | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | F | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | G | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | H | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | I | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | J | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | K | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | L | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | M | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | N | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| 1 | O | 464/627 (74%) | 442 (95%) | 19 (4%) | 3 (1%) | 25 | 60 |
| All | All | 6960/9405 (74%) | 6630 (95%) | 285 (4%) | 45 (1%) | 29 | 60 |

All (45) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 480 | VAL |
| 1 | B | 480 | VAL |
| 1 | C | 480 | VAL |
| 1 | D | 480 | VAL |
| 1 | E | 480 | VAL |
| 1 | F | 480 | VAL |
| 1 | G | 480 | VAL |
| 1 | H | 480 | VAL |
| 1 | I | 480 | VAL |
| 1 | J | 480 | VAL |
| 1 | K | 480 | VAL |
| 1 | L | 480 | VAL |
| 1 | M | 480 | VAL |
| 1 | N | 480 | VAL |
| 1 | O | 480 | VAL |
| 1 | A | 242 | GLU |
| 1 | B | 242 | GLU |
| 1 | C | 242 | GLU |
| 1 | D | 242 | GLU |
| 1 | E | 242 | GLU |
| 1 | F | 242 | GLU |
| 1 | G | 242 | GLU |
| 1 | H | 242 | GLU |
| 1 | I | 242 | GLU |
| 1 | J | 242 | GLU |
| 1 | K | 242 | GLU |
| 1 | L | 242 | GLU |
| 1 | M | 242 | GLU |
| 1 | N | 242 | GLU |
| 1 | O | 242 | GLU |
| 1 | A | 130 | VAL |
| 1 | B | 130 | VAL |
| 1 | C | 130 | VAL |
| 1 | D | 130 | VAL |
| 1 | E | 130 | VAL |
| 1 | F | 130 | VAL |
| 1 | G | 130 | VAL |
| 1 | H | 130 | VAL |
| 1 | I | 130 | VAL |
| 1 | J | 130 | VAL |
| 1 | K | 130 | VAL |
| 1 | L | 130 | VAL |
| 1 | M | 130 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 130 | VAL |
| 1 | O | 130 | VAL |

### 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | B | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | C | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | D | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | E | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | F | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | G | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | H | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | I | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | J | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | K | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | L | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | M | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | N | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| 1 | O | 405/537 (75%) | 404 (100%) | 1 (0%) | 93 | 98 |
| All | All | 6075/8055 (75%) | 6060 (100%) | 15 (0%) | 93 | 98 |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 258 | LEU |
| 1 | B | 258 | LEU |
| 1 | C | 258 | LEU |
| 1 | D | 258 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 258 | LEU |
| 1 | F | 258 | LEU |
| 1 | G | 258 | LEU |
| 1 | H | 258 | LEU |
| 1 | I | 258 | LEU |
| 1 | J | 258 | LEU |
| 1 | K | 258 | LEU |
| 1 | L | 258 | LEU |
| 1 | M | 258 | LEU |
| 1 | N | 258 | LEU |
| 1 | O | 258 | LEU |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 135 | HIS |
| 1 | A | 214 | ASN |
| 1 | A | 257 | ASN |
| 1 | A | 295 | GLN |
| 1 | A | 305 | GLN |
| 1 | A | 308 | GLN |
| 1 | A | 324 | GLN |
| 1 | A | 335 | GLN |
| 1 | A | 368 | GLN |
| 1 | A | 473 | GLN |
| 1 | A | 475 | ASN |
| 1 | B | 135 | HIS |
| 1 | B | 214 | ASN |
| 1 | B | 257 | ASN |
| 1 | B | 295 | GLN |
| 1 | B | 305 | GLN |
| 1 | B | 308 | GLN |
| 1 | B | 324 | GLN |
| 1 | B | 335 | GLN |
| 1 | B | 368 | GLN |
| 1 | B | 473 | GLN |
| 1 | B | 475 | ASN |
| 1 | C | 135 | HIS |
| 1 | C | 214 | ASN |
| 1 | C | 257 | ASN |
| 1 | C | 295 | GLN |
| 1 | C | 305 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 308 | GLN |
| 1 | C | 324 | GLN |
| 1 | C | 335 | GLN |
| 1 | C | 368 | GLN |
| 1 | C | 473 | GLN |
| 1 | C | 475 | ASN |
| 1 | D | 135 | HIS |
| 1 | D | 214 | ASN |
| 1 | D | 257 | ASN |
| 1 | D | 295 | GLN |
| 1 | D | 305 | GLN |
| 1 | D | 308 | GLN |
| 1 | D | 324 | GLN |
| 1 | D | 335 | GLN |
| 1 | D | 368 | GLN |
| 1 | D | 473 | GLN |
| 1 | D | 475 | ASN |
| 1 | E | 135 | HIS |
| 1 | E | 214 | ASN |
| 1 | E | 257 | ASN |
| 1 | E | 295 | GLN |
| 1 | E | 305 | GLN |
| 1 | E | 308 | GLN |
| 1 | E | 324 | GLN |
| 1 | E | 335 | GLN |
| 1 | E | 368 | GLN |
| 1 | E | 473 | GLN |
| 1 | E | 475 | ASN |
| 1 | F | 135 | HIS |
| 1 | F | 214 | ASN |
| 1 | F | 257 | ASN |
| 1 | F | 295 | GLN |
| 1 | F | 305 | GLN |
| 1 | F | 308 | GLN |
| 1 | F | 324 | GLN |
| 1 | F | 335 | GLN |
| 1 | F | 368 | GLN |
| 1 | F | 473 | GLN |
| 1 | F | 475 | ASN |
| 1 | G | 135 | HIS |
| 1 | G | 214 | ASN |
| 1 | G | 257 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 295 | GLN |
| 1 | G | 305 | GLN |
| 1 | G | 308 | GLN |
| 1 | G | 324 | GLN |
| 1 | G | 335 | GLN |
| 1 | G | 368 | GLN |
| 1 | G | 473 | GLN |
| 1 | G | 475 | ASN |
| 1 | H | 135 | HIS |
| 1 | H | 214 | ASN |
| 1 | H | 257 | ASN |
| 1 | H | 295 | GLN |
| 1 | H | 305 | GLN |
| 1 | H | 308 | GLN |
| 1 | H | 324 | GLN |
| 1 | H | 335 | GLN |
| 1 | H | 368 | GLN |
| 1 | H | 473 | GLN |
| 1 | H | 475 | ASN |
| 1 | I | 135 | HIS |
| 1 | I | 214 | ASN |
| 1 | I | 257 | ASN |
| 1 | I | 295 | GLN |
| 1 | I | 305 | GLN |
| 1 | I | 308 | GLN |
| 1 | I | 324 | GLN |
| 1 | I | 335 | GLN |
| 1 | I | 368 | GLN |
| 1 | I | 473 | GLN |
| 1 | I | 475 | ASN |
| 1 | J | 135 | HIS |
| 1 | J | 214 | ASN |
| 1 | J | 257 | ASN |
| 1 | J | 295 | GLN |
| 1 | J | 305 | GLN |
| 1 | J | 308 | GLN |
| 1 | J | 324 | GLN |
| 1 | J | 335 | GLN |
| 1 | J | 368 | GLN |
| 1 | J | 473 | GLN |
| 1 | J | 475 | ASN |
| 1 | K | 135 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 214 | ASN |
| 1 | K | 257 | ASN |
| 1 | K | 295 | GLN |
| 1 | K | 305 | GLN |
| 1 | K | 308 | GLN |
| 1 | K | 324 | GLN |
| 1 | K | 335 | GLN |
| 1 | K | 368 | GLN |
| 1 | K | 473 | GLN |
| 1 | K | 475 | ASN |
| 1 | L | 135 | HIS |
| 1 | L | 214 | ASN |
| 1 | L | 257 | ASN |
| 1 | L | 295 | GLN |
| 1 | L | 305 | GLN |
| 1 | L | 308 | GLN |
| 1 | L | 324 | GLN |
| 1 | L | 335 | GLN |
| 1 | L | 368 | GLN |
| 1 | L | 473 | GLN |
| 1 | L | 475 | ASN |
| 1 | M | 135 | HIS |
| 1 | M | 214 | ASN |
| 1 | M | 257 | ASN |
| 1 | M | 295 | GLN |
| 1 | M | 305 | GLN |
| 1 | M | 308 | GLN |
| 1 | M | 324 | GLN |
| 1 | M | 335 | GLN |
| 1 | M | 368 | GLN |
| 1 | M | 473 | GLN |
| 1 | M | 475 | ASN |
| 1 | N | 135 | HIS |
| 1 | N | 214 | ASN |
| 1 | N | 257 | ASN |
| 1 | N | 295 | GLN |
| 1 | N | 305 | GLN |
| 1 | N | 308 | GLN |
| 1 | N | 324 | GLN |
| 1 | N | 335 | GLN |
| 1 | N | 368 | GLN |
| 1 | N | 473 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 475 | ASN |
| 1 | O | 135 | HIS |
| 1 | O | 214 | ASN |
| 1 | O | 257 | ASN |
| 1 | O | 295 | GLN |
| 1 | O | 305 | GLN |
| 1 | O | 308 | GLN |
| 1 | O | 324 | GLN |
| 1 | O | 335 | GLN |
| 1 | O | 368 | GLN |
| 1 | O | 473 | GLN |
| 1 | O | 475 | ASN |

#### 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 monosaccharides 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.

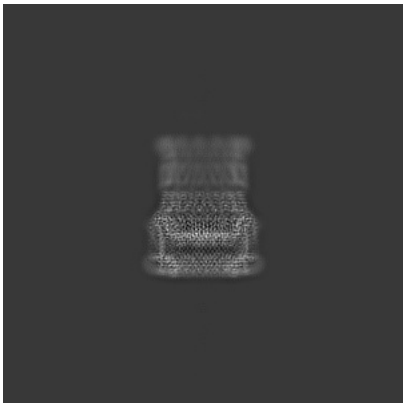
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6675. These allow visual inspection of the internal detail of the map and identification of artifacts.

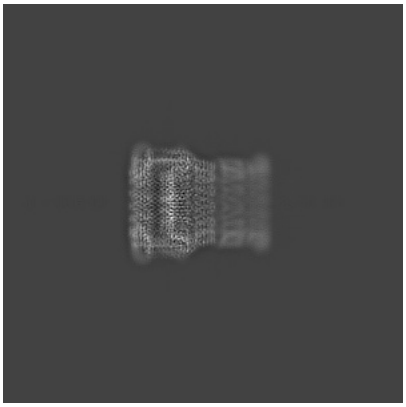
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

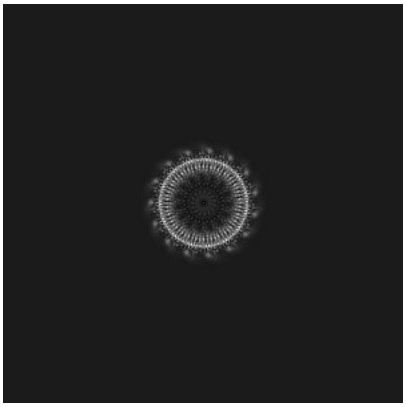
### 6.1.1 Primary map



X



Y

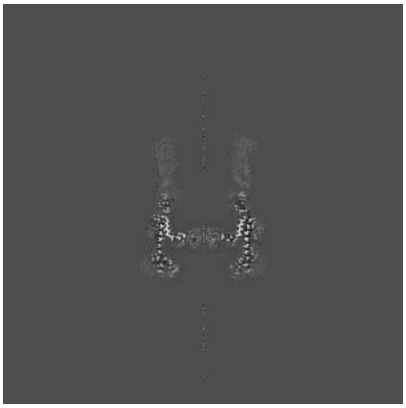


Z

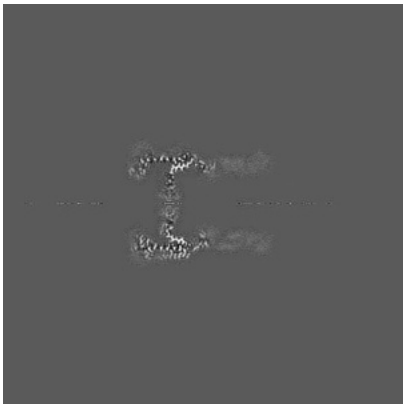
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

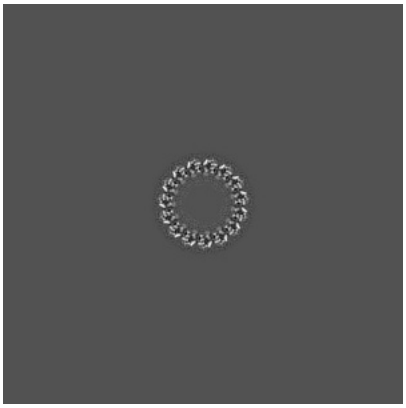
### 6.2.1 Primary map



X Index: 190



Y Index: 190

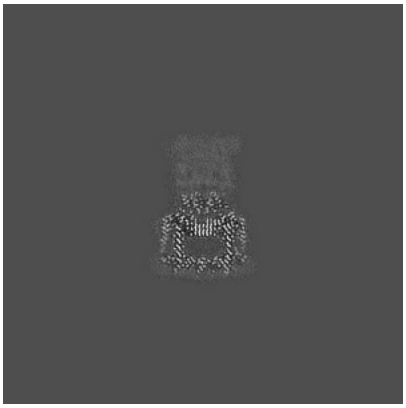


Z Index: 190

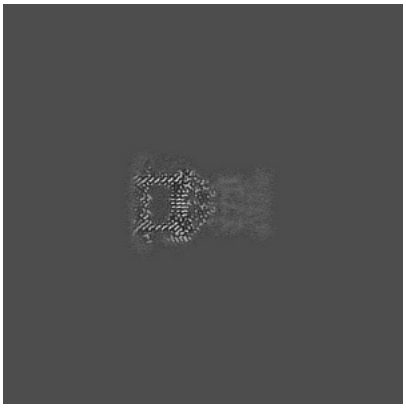
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

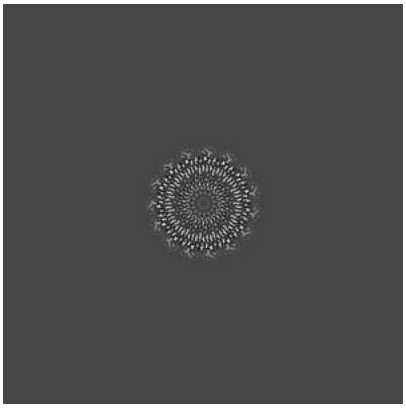
### 6.3.1 Primary map



X Index: 156



Y Index: 155

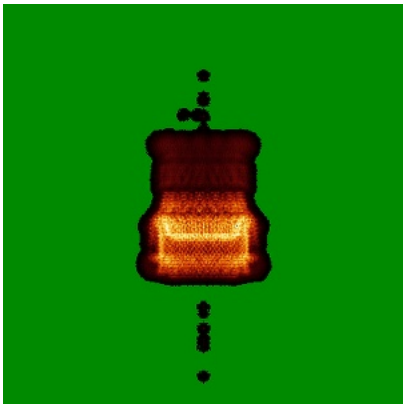


Z Index: 160

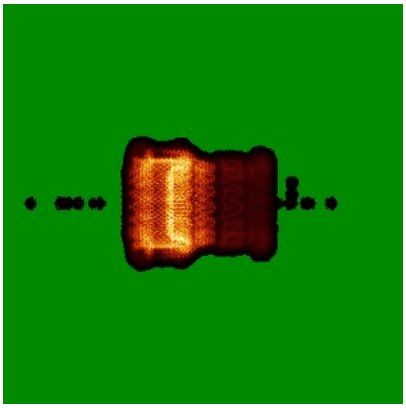
The images above show the largest variance slices of the map in three orthogonal directions.

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

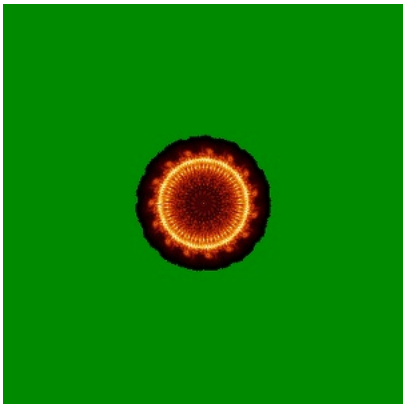
### 6.4.1 Primary map



X



Y

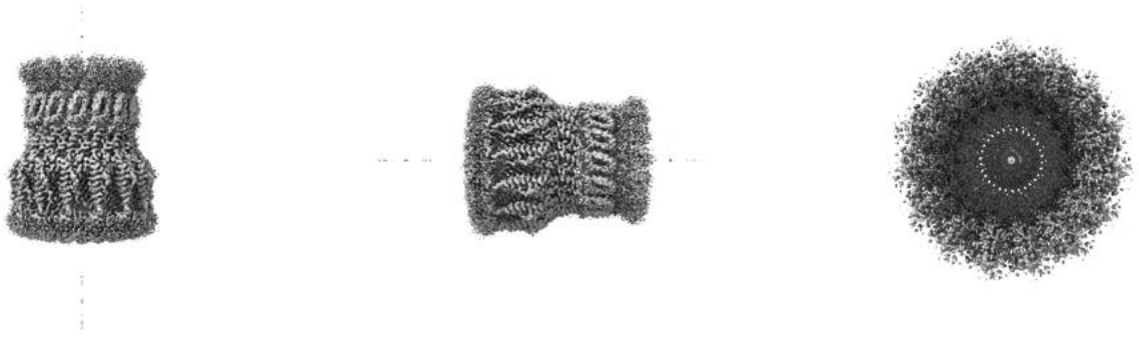


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

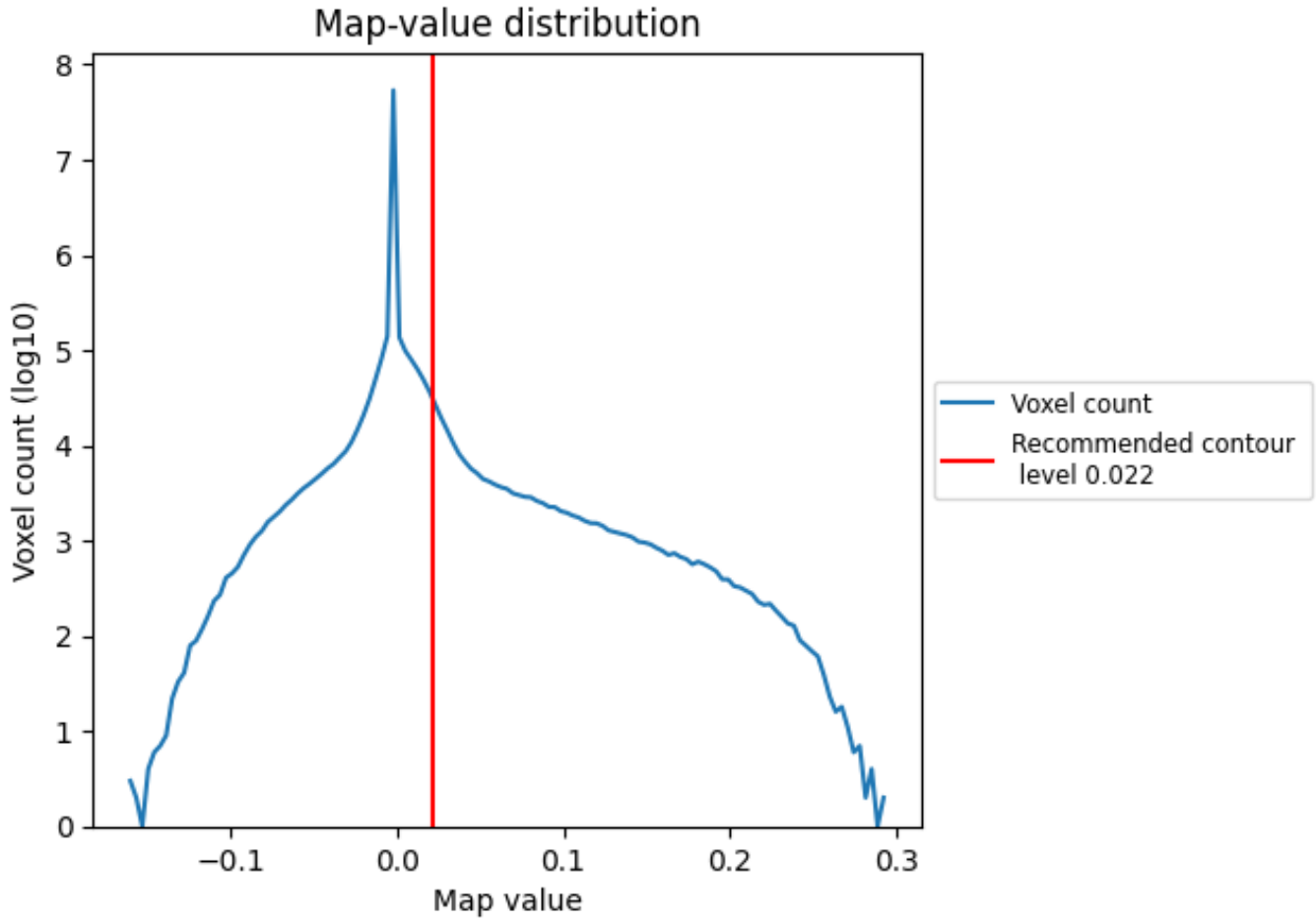
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

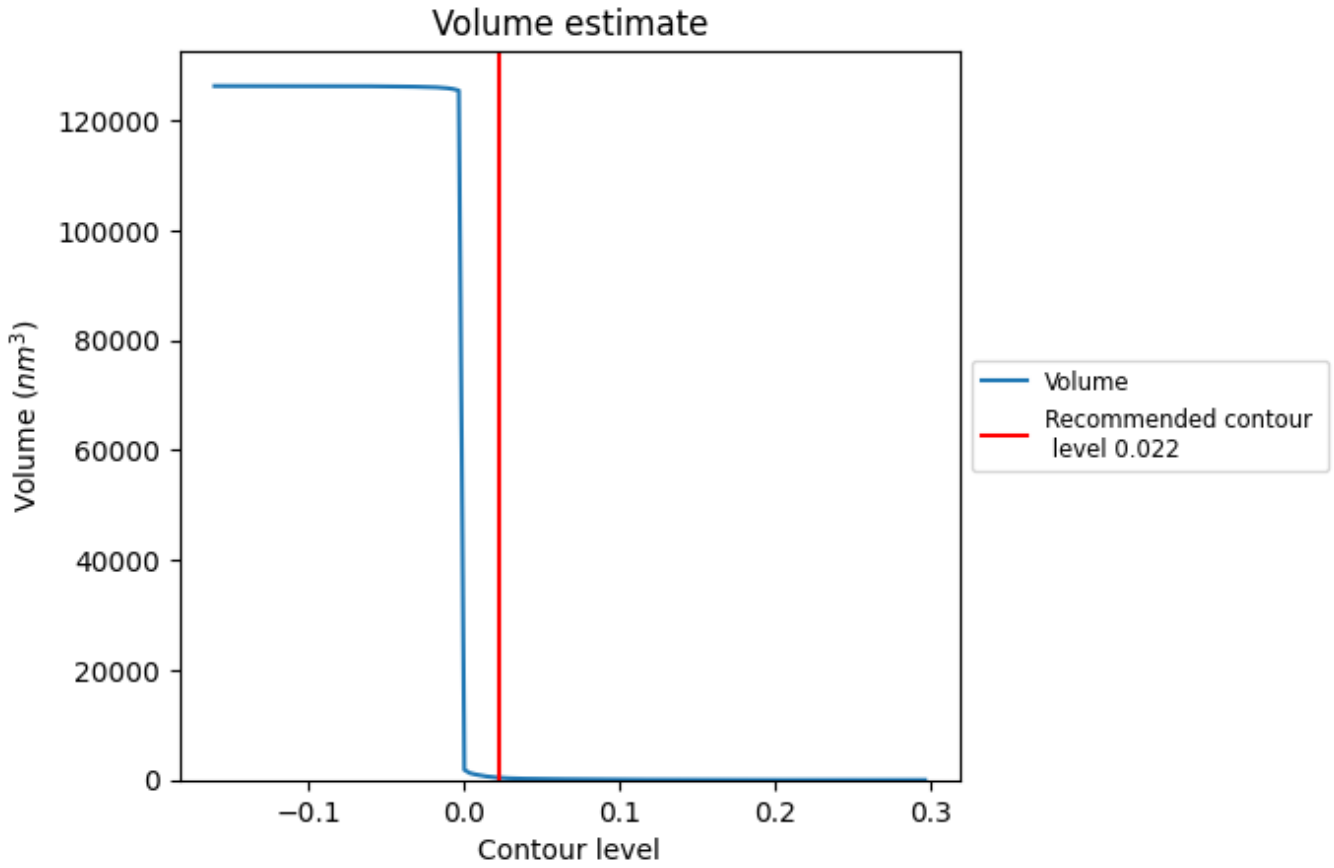
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

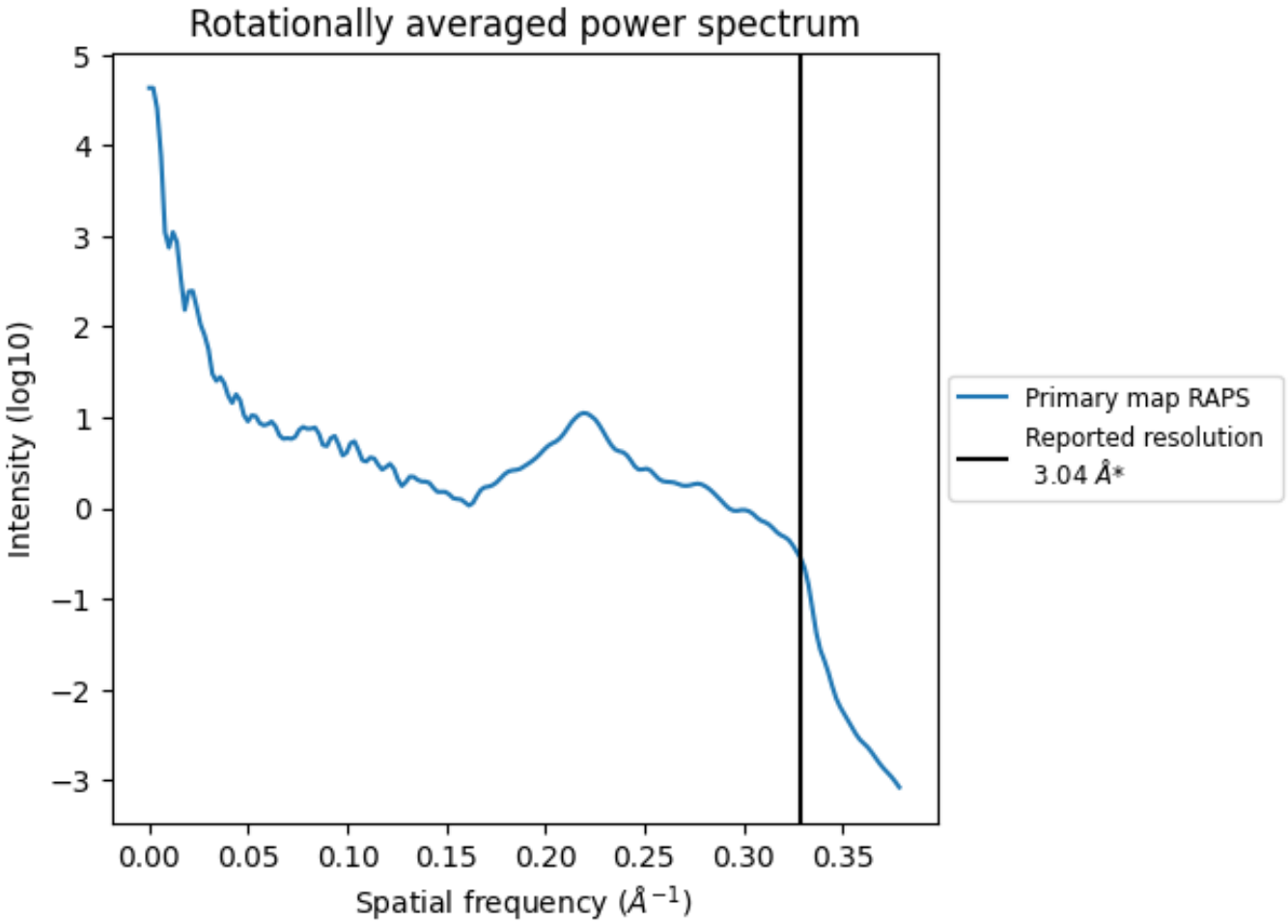
## 7.2 Volume estimate




The volume at the recommended contour level is 416 $nm^3$; this corresponds to an approximate mass of 376 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.329 Å$^{-1}$

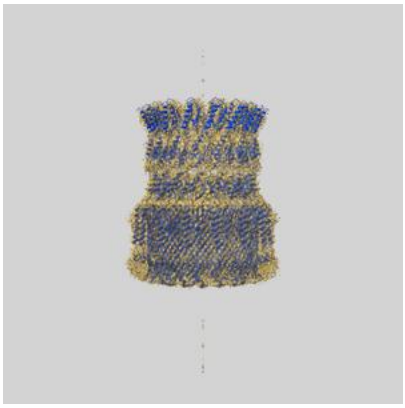
# 8 Fourier-Shell correlation

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

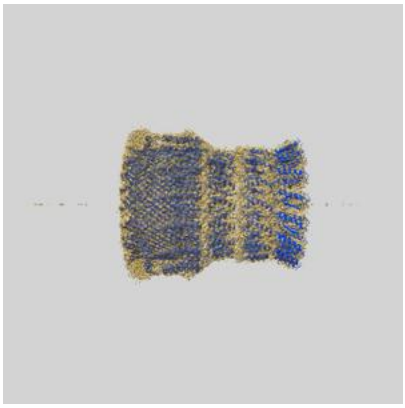
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6675 and PDB model 5WQ7. Per-residue inclusion information can be found in section 3 on page 5.

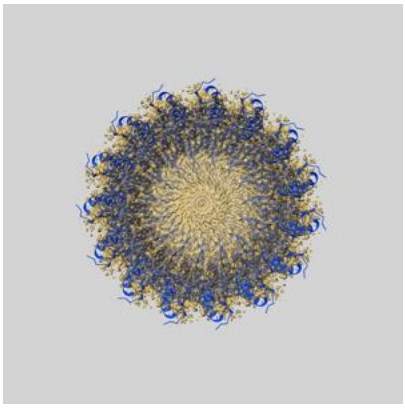
## 9.1 Map-model overlay



X



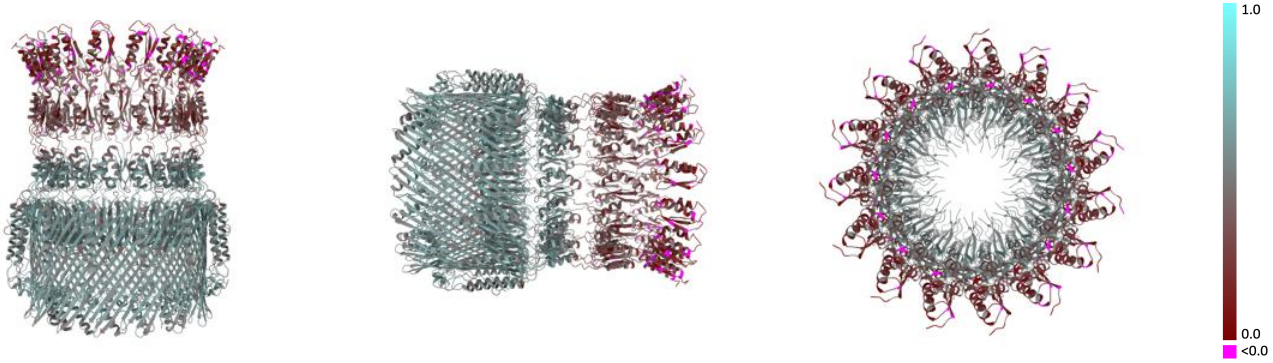
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

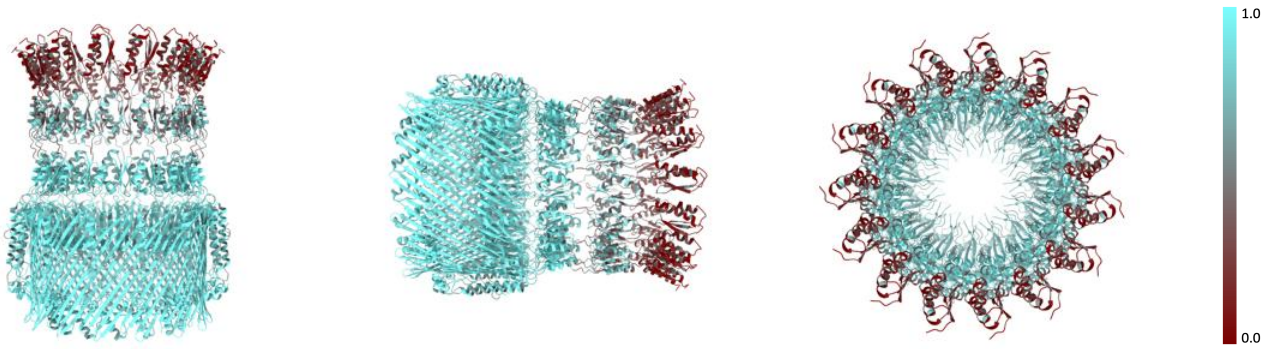
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

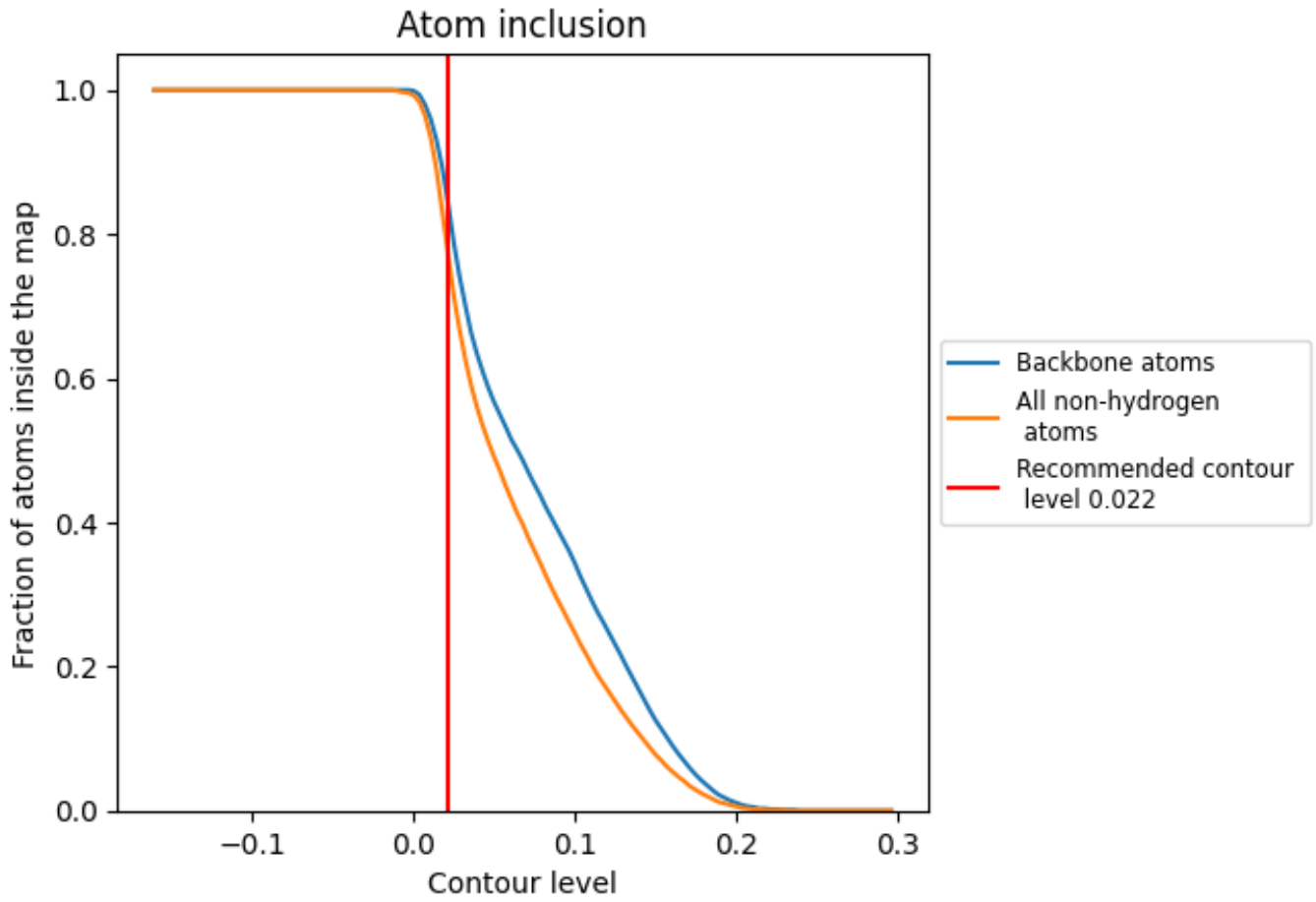
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

## 9.4 Atom inclusion (i)




At the recommended contour level, 84% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7640 | 0.4670 |
| A | 0.7640 | 0.4680 |
| B | 0.7630 | 0.4670 |
| C | 0.7650 | 0.4660 |
| D | 0.7650 | 0.4680 |
| E | 0.7620 | 0.4660 |
| F | 0.7650 | 0.4650 |
| G | 0.7640 | 0.4670 |
| H | 0.7650 | 0.4680 |
| I | 0.7650 | 0.4660 |
| J | 0.7620 | 0.4650 |
| K | 0.7660 | 0.4660 |
| L | 0.7640 | 0.4680 |
| M | 0.7630 | 0.4670 |
| N | 0.7590 | 0.4690 |
| O | 0.7630 | 0.4680 |