# Full wwPDB EM Validation Report

Mar 12, 2026 – 06:19 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 6V1T / pdb_00006v1t |
| EMDB ID | : | EMD-21017 |
| Title | : | Empty AAVrh.39 particle |
| Authors | : | Mietzsch, M.; Agbandje-McKenna, M. |
| Deposited on | : | 2019-11-21 |
| Resolution | : | 3.39 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:

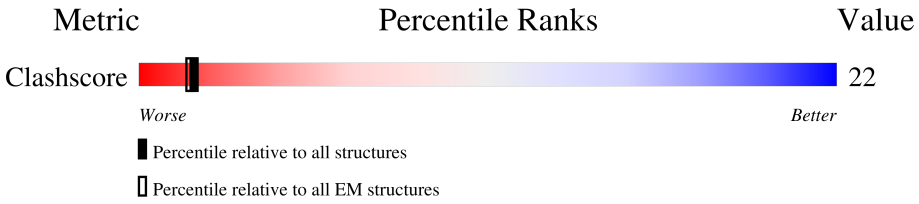
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

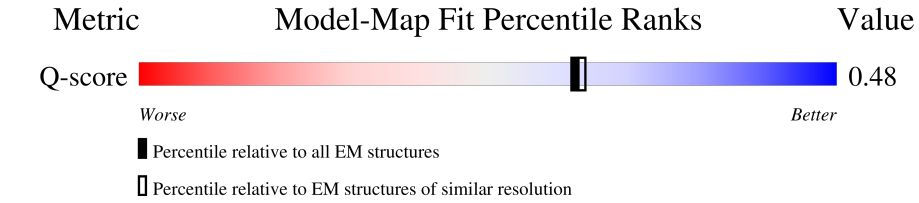
# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.39 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Q-score | - | 25397 | 14220 ( 2.89 - 3.89 ) |

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 | 1 | 521 | 64% 36% |
| 1 | 2 | 521 | 64% 35% |
| 1 | 3 | 521 | 64% 35% |
| 1 | 4 | 521 | 65% 35% |
| 1 | 5 | 521 | 66% 34% |
| 1 | 6 | 521 | 64% 35% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 7 | 521 | 64% 36% |
| 1 | 8 | 521 | 64% 35% |
| 1 | A | 521 | 64% 36% |
| 1 | B | 521 | 65% 35% |
| 1 | C | 521 | 64% 35% |
| 1 | D | 521 | 65% 35% |
| 1 | E | 521 | 64% 36% |
| 1 | F | 521 | 64% 35% |
| 1 | G | 521 | 64% 35% |
| 1 | H | 521 | 64% 35% |
| 1 | I | 521 | 65% 35% |
| 1 | J | 521 | 65% 35% |
| 1 | K | 521 | 65% 35% |
| 1 | L | 521 | 64% 36% |
| 1 | M | 521 | 64% 35% |
| 1 | N | 521 | 65% 35% |
| 1 | O | 521 | 64% 35% |
| 1 | P | 521 | 64% 35% |
| 1 | Q | 521 | 65% 34% |
| 1 | R | 521 | 63% 36% |
| 1 | S | 521 | 63% 36% |
| 1 | T | 521 | 63% 36% |
| 1 | U | 521 | 64% 35% |
| 1 | V | 521 | 64% 35% |
| 1 | W | 521 | 64% 36% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | X | 521 | 64% 35% |
| 1 | Y | 521 | 64% 36% |
| 1 | Z | 521 | 64% 36% |
| 1 | a | 521 | 64% 35% |
| 1 | b | 521 | 65% 35% |
| 1 | c | 521 | 64% 35% |
| 1 | d | 521 | 64% 35% |
| 1 | e | 521 | 65% 35% |
| 1 | f | 521 | 64% 35% |
| 1 | g | 521 | 64% 35% |
| 1 | h | 521 | 64% 36% |
| 1 | i | 521 | 64% 35% |
| 1 | j | 521 | 64% 35% |
| 1 | k | 521 | 64% 36% |
| 1 | l | 521 | 64% 35% |
| 1 | m | 521 | 64% 35% |
| 1 | n | 521 | 65% 35% |
| 1 | o | 521 | 64% 36% |
| 1 | p | 521 | 64% 35% |
| 1 | q | 521 | 64% 36% |
| 1 | r | 521 | 64% 36% |
| 1 | s | 521 | 64% 35% |
| 1 | t | 521 | 64% 35% |
| 1 | u | 521 | 64% 36% |
| 1 | v | 521 | 65% 35% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | w | 521 | |
| 1 | x | 521 | |
| 1 | y | 521 | |
| 1 | z | 521 | |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 248280 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 Capsid protein VP1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | B | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | C | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | D | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | E | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | F | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | G | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | H | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | I | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | J | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | K | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | L | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | M | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | N | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | O | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | P | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | Q | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | R | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | S | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | T | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | U | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | V | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | W | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | X | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | Y | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | Z | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | a | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | b | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | c | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | d | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | e | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | f | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | g | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | h | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | i | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | j | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | k | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | l | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | m | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | n | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | o | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | p | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | q | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | r | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | s | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | t | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | u | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | v | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | w | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | x | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | y | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | z | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | 1 | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | 2 | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | 3 | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | 4 | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | 5 | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | 6 | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |
| 1 | 7 | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 8 | 521 | Total | C | N | O | S | 0 | 0 |
| | | | 4138 | 2612 | 715 | 797 | 14 | | |

There are 120 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 315 | ASN | SER | conflict | UNP B4Y886 |
| A | 417 | GLN | THR | conflict | UNP B4Y886 |
| B | 315 | ASN | SER | conflict | UNP B4Y886 |
| B | 417 | GLN | THR | conflict | UNP B4Y886 |
| C | 315 | ASN | SER | conflict | UNP B4Y886 |
| C | 417 | GLN | THR | conflict | UNP B4Y886 |
| D | 315 | ASN | SER | conflict | UNP B4Y886 |
| D | 417 | GLN | THR | conflict | UNP B4Y886 |
| E | 315 | ASN | SER | conflict | UNP B4Y886 |
| E | 417 | GLN | THR | conflict | UNP B4Y886 |
| F | 315 | ASN | SER | conflict | UNP B4Y886 |
| F | 417 | GLN | THR | conflict | UNP B4Y886 |
| G | 315 | ASN | SER | conflict | UNP B4Y886 |
| G | 417 | GLN | THR | conflict | UNP B4Y886 |
| H | 315 | ASN | SER | conflict | UNP B4Y886 |
| H | 417 | GLN | THR | conflict | UNP B4Y886 |
| I | 315 | ASN | SER | conflict | UNP B4Y886 |
| I | 417 | GLN | THR | conflict | UNP B4Y886 |
| J | 315 | ASN | SER | conflict | UNP B4Y886 |
| J | 417 | GLN | THR | conflict | UNP B4Y886 |
| K | 315 | ASN | SER | conflict | UNP B4Y886 |
| K | 417 | GLN | THR | conflict | UNP B4Y886 |
| L | 315 | ASN | SER | conflict | UNP B4Y886 |
| L | 417 | GLN | THR | conflict | UNP B4Y886 |
| M | 315 | ASN | SER | conflict | UNP B4Y886 |
| M | 417 | GLN | THR | conflict | UNP B4Y886 |
| N | 315 | ASN | SER | conflict | UNP B4Y886 |
| N | 417 | GLN | THR | conflict | UNP B4Y886 |
| O | 315 | ASN | SER | conflict | UNP B4Y886 |
| O | 417 | GLN | THR | conflict | UNP B4Y886 |
| P | 315 | ASN | SER | conflict | UNP B4Y886 |
| P | 417 | GLN | THR | conflict | UNP B4Y886 |
| Q | 315 | ASN | SER | conflict | UNP B4Y886 |
| Q | 417 | GLN | THR | conflict | UNP B4Y886 |
| R | 315 | ASN | SER | conflict | UNP B4Y886 |
| R | 417 | GLN | THR | conflict | UNP B4Y886 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| S | 315 | ASN | SER | conflict | UNP B4Y886 |
| S | 417 | GLN | THR | conflict | UNP B4Y886 |
| T | 315 | ASN | SER | conflict | UNP B4Y886 |
| T | 417 | GLN | THR | conflict | UNP B4Y886 |
| U | 315 | ASN | SER | conflict | UNP B4Y886 |
| U | 417 | GLN | THR | conflict | UNP B4Y886 |
| V | 315 | ASN | SER | conflict | UNP B4Y886 |
| V | 417 | GLN | THR | conflict | UNP B4Y886 |
| W | 315 | ASN | SER | conflict | UNP B4Y886 |
| W | 417 | GLN | THR | conflict | UNP B4Y886 |
| X | 315 | ASN | SER | conflict | UNP B4Y886 |
| X | 417 | GLN | THR | conflict | UNP B4Y886 |
| Y | 315 | ASN | SER | conflict | UNP B4Y886 |
| Y | 417 | GLN | THR | conflict | UNP B4Y886 |
| Z | 315 | ASN | SER | conflict | UNP B4Y886 |
| Z | 417 | GLN | THR | conflict | UNP B4Y886 |
| a | 315 | ASN | SER | conflict | UNP B4Y886 |
| a | 417 | GLN | THR | conflict | UNP B4Y886 |
| b | 315 | ASN | SER | conflict | UNP B4Y886 |
| b | 417 | GLN | THR | conflict | UNP B4Y886 |
| c | 315 | ASN | SER | conflict | UNP B4Y886 |
| c | 417 | GLN | THR | conflict | UNP B4Y886 |
| d | 315 | ASN | SER | conflict | UNP B4Y886 |
| d | 417 | GLN | THR | conflict | UNP B4Y886 |
| e | 315 | ASN | SER | conflict | UNP B4Y886 |
| e | 417 | GLN | THR | conflict | UNP B4Y886 |
| f | 315 | ASN | SER | conflict | UNP B4Y886 |
| f | 417 | GLN | THR | conflict | UNP B4Y886 |
| g | 315 | ASN | SER | conflict | UNP B4Y886 |
| g | 417 | GLN | THR | conflict | UNP B4Y886 |
| h | 315 | ASN | SER | conflict | UNP B4Y886 |
| h | 417 | GLN | THR | conflict | UNP B4Y886 |
| i | 315 | ASN | SER | conflict | UNP B4Y886 |
| i | 417 | GLN | THR | conflict | UNP B4Y886 |
| j | 315 | ASN | SER | conflict | UNP B4Y886 |
| j | 417 | GLN | THR | conflict | UNP B4Y886 |
| k | 315 | ASN | SER | conflict | UNP B4Y886 |
| k | 417 | GLN | THR | conflict | UNP B4Y886 |
| l | 315 | ASN | SER | conflict | UNP B4Y886 |
| l | 417 | GLN | THR | conflict | UNP B4Y886 |
| m | 315 | ASN | SER | conflict | UNP B4Y886 |
| m | 417 | GLN | THR | conflict | UNP B4Y886 |

*Continued on next page...*

*Continued from previous page...*

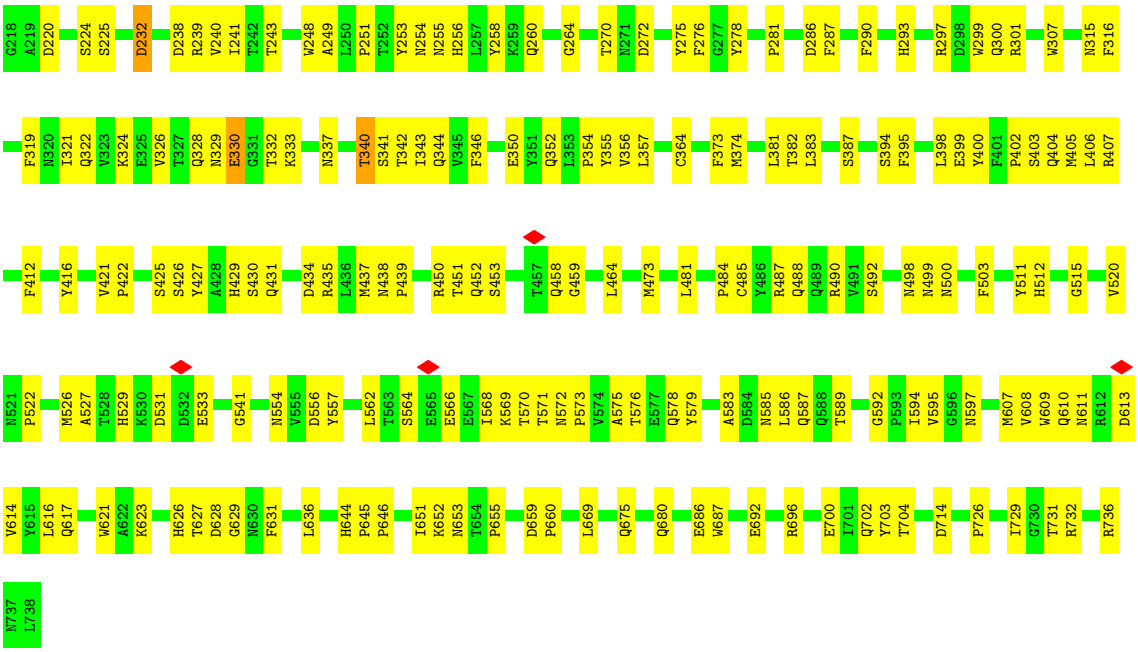
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| n | 315 | ASN | SER | conflict | UNP B4Y886 |
| n | 417 | GLN | THR | conflict | UNP B4Y886 |
| o | 315 | ASN | SER | conflict | UNP B4Y886 |
| o | 417 | GLN | THR | conflict | UNP B4Y886 |
| p | 315 | ASN | SER | conflict | UNP B4Y886 |
| p | 417 | GLN | THR | conflict | UNP B4Y886 |
| q | 315 | ASN | SER | conflict | UNP B4Y886 |
| q | 417 | GLN | THR | conflict | UNP B4Y886 |
| r | 315 | ASN | SER | conflict | UNP B4Y886 |
| r | 417 | GLN | THR | conflict | UNP B4Y886 |
| s | 315 | ASN | SER | conflict | UNP B4Y886 |
| s | 417 | GLN | THR | conflict | UNP B4Y886 |
| t | 315 | ASN | SER | conflict | UNP B4Y886 |
| t | 417 | GLN | THR | conflict | UNP B4Y886 |
| u | 315 | ASN | SER | conflict | UNP B4Y886 |
| u | 417 | GLN | THR | conflict | UNP B4Y886 |
| v | 315 | ASN | SER | conflict | UNP B4Y886 |
| v | 417 | GLN | THR | conflict | UNP B4Y886 |
| w | 315 | ASN | SER | conflict | UNP B4Y886 |
| w | 417 | GLN | THR | conflict | UNP B4Y886 |
| x | 315 | ASN | SER | conflict | UNP B4Y886 |
| x | 417 | GLN | THR | conflict | UNP B4Y886 |
| y | 315 | ASN | SER | conflict | UNP B4Y886 |
| y | 417 | GLN | THR | conflict | UNP B4Y886 |
| z | 315 | ASN | SER | conflict | UNP B4Y886 |
| z | 417 | GLN | THR | conflict | UNP B4Y886 |
| 1 | 315 | ASN | SER | conflict | UNP B4Y886 |
| 1 | 417 | GLN | THR | conflict | UNP B4Y886 |
| 2 | 315 | ASN | SER | conflict | UNP B4Y886 |
| 2 | 417 | GLN | THR | conflict | UNP B4Y886 |
| 3 | 315 | ASN | SER | conflict | UNP B4Y886 |
| 3 | 417 | GLN | THR | conflict | UNP B4Y886 |
| 4 | 315 | ASN | SER | conflict | UNP B4Y886 |
| 4 | 417 | GLN | THR | conflict | UNP B4Y886 |
| 5 | 315 | ASN | SER | conflict | UNP B4Y886 |
| 5 | 417 | GLN | THR | conflict | UNP B4Y886 |
| 6 | 315 | ASN | SER | conflict | UNP B4Y886 |
| 6 | 417 | GLN | THR | conflict | UNP B4Y886 |
| 7 | 315 | ASN | SER | conflict | UNP B4Y886 |
| 7 | 417 | GLN | THR | conflict | UNP B4Y886 |
| 8 | 315 | ASN | SER | conflict | UNP B4Y886 |
| 8 | 417 | GLN | THR | conflict | UNP B4Y886 |

# 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.

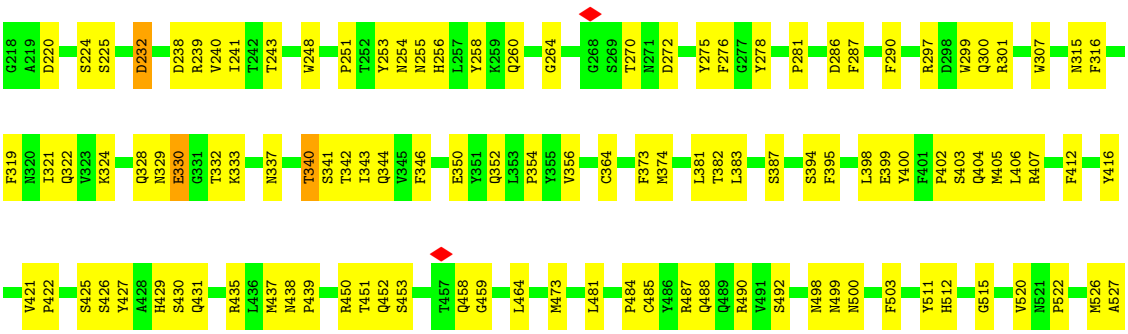
• Molecule 1: Capsid protein VP1

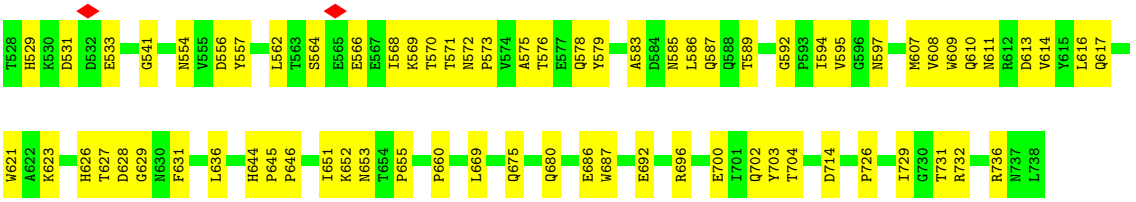
Chain A:




• Molecule 1: Capsid protein VP1

Chain B:

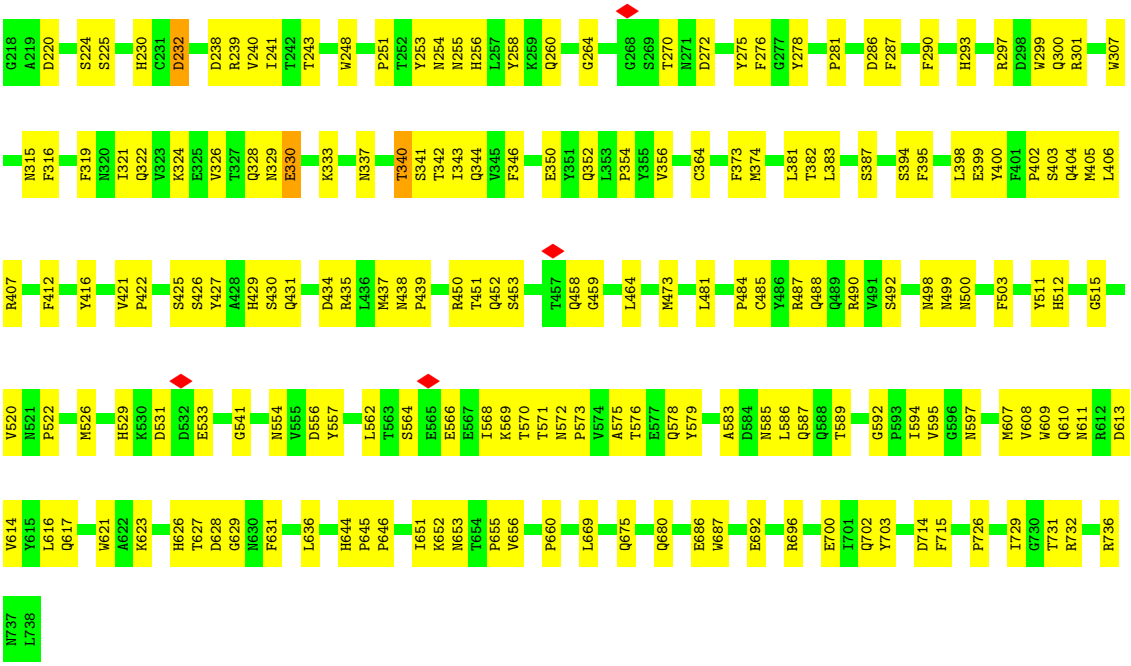






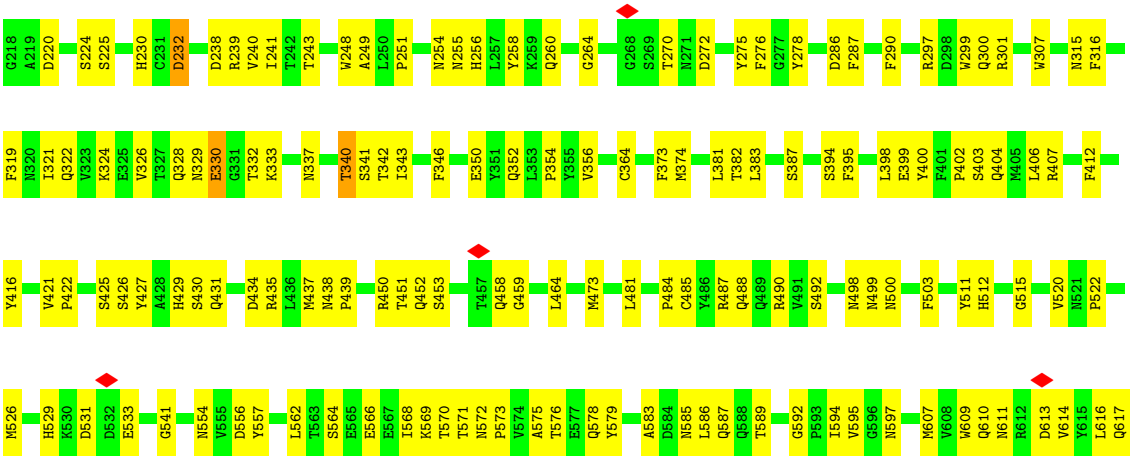
• Molecule 1: Capsid protein VP1

Chain C:



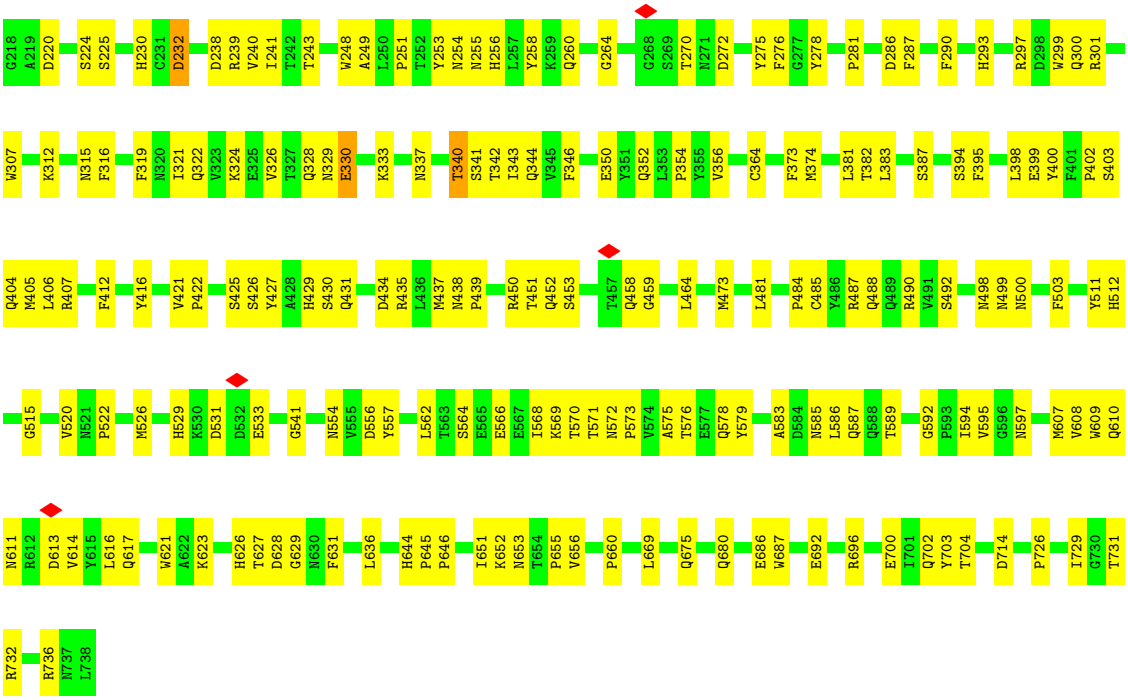
• Molecule 1: Capsid protein VP1

Chain D:



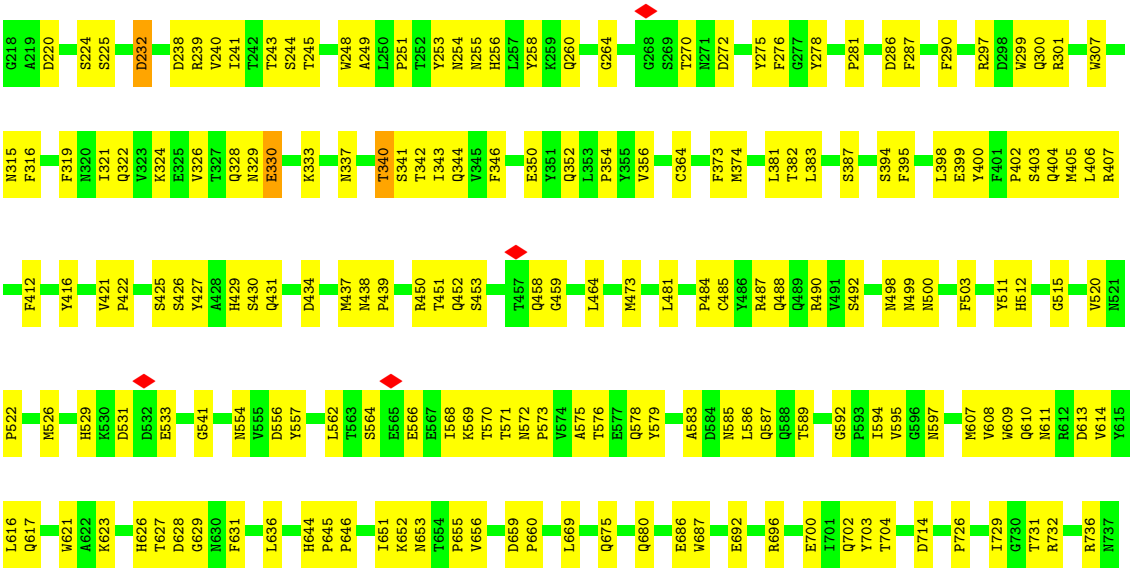
• Molecule 1: Capsid protein VP1

Chain E:



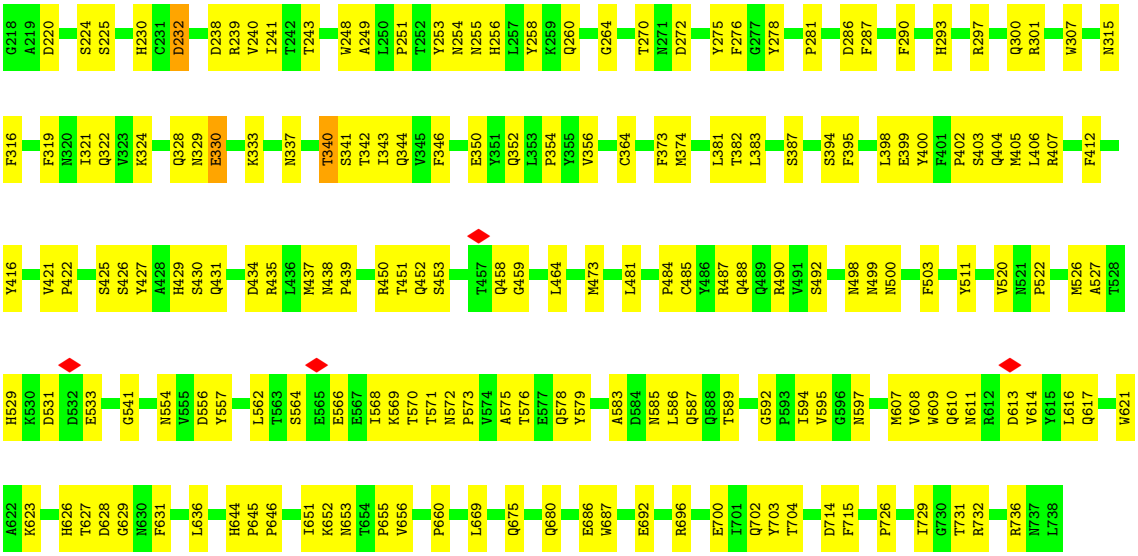

• Molecule 1: Capsid protein VP1

Chain F:



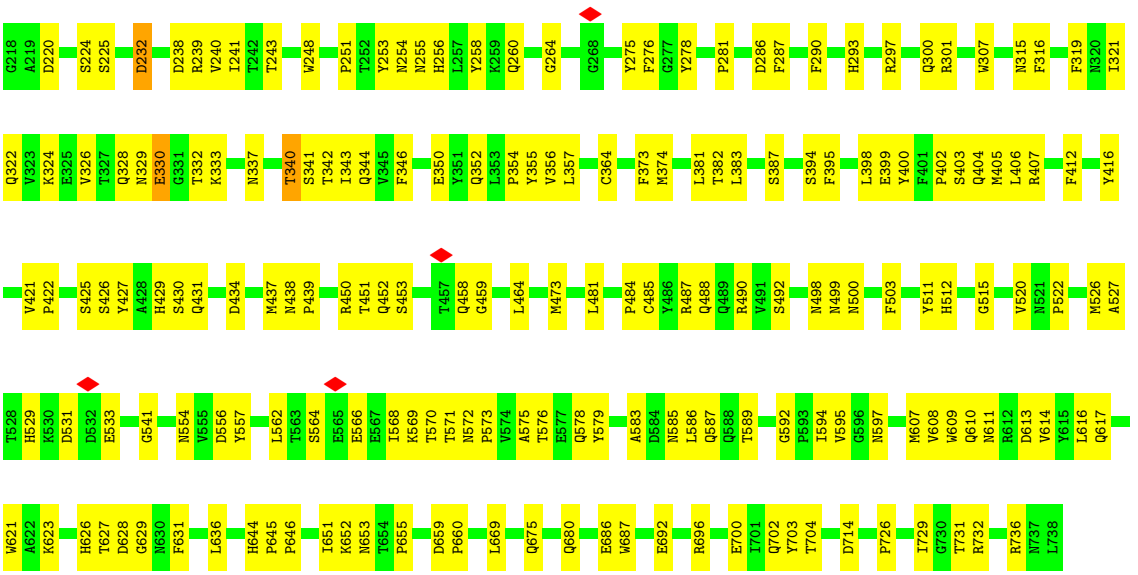
• Molecule 1: Capsid protein VP1

Chain G:



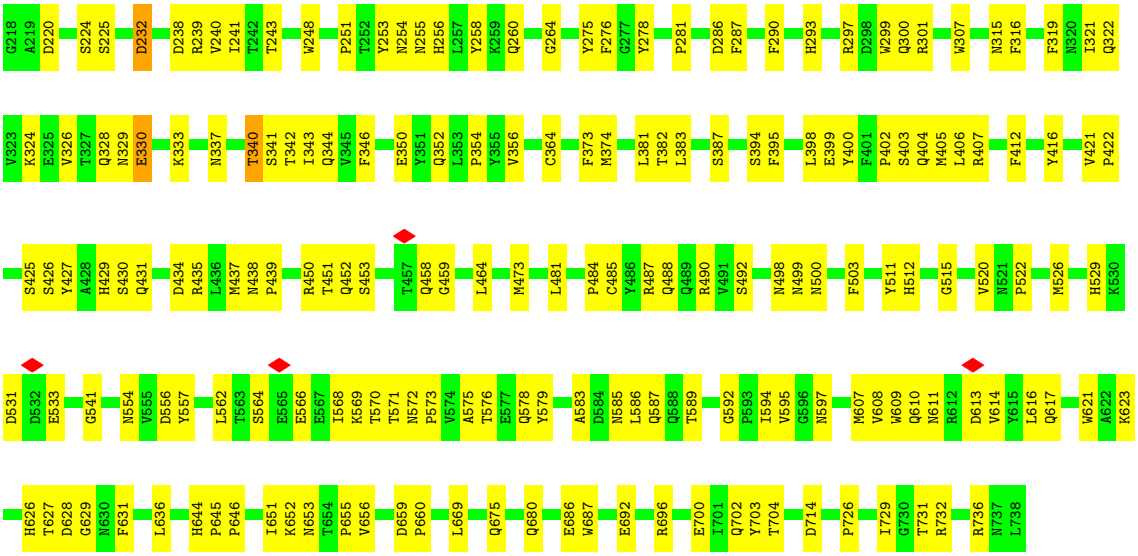

• Molecule 1: Capsid protein VP1

Chain H:



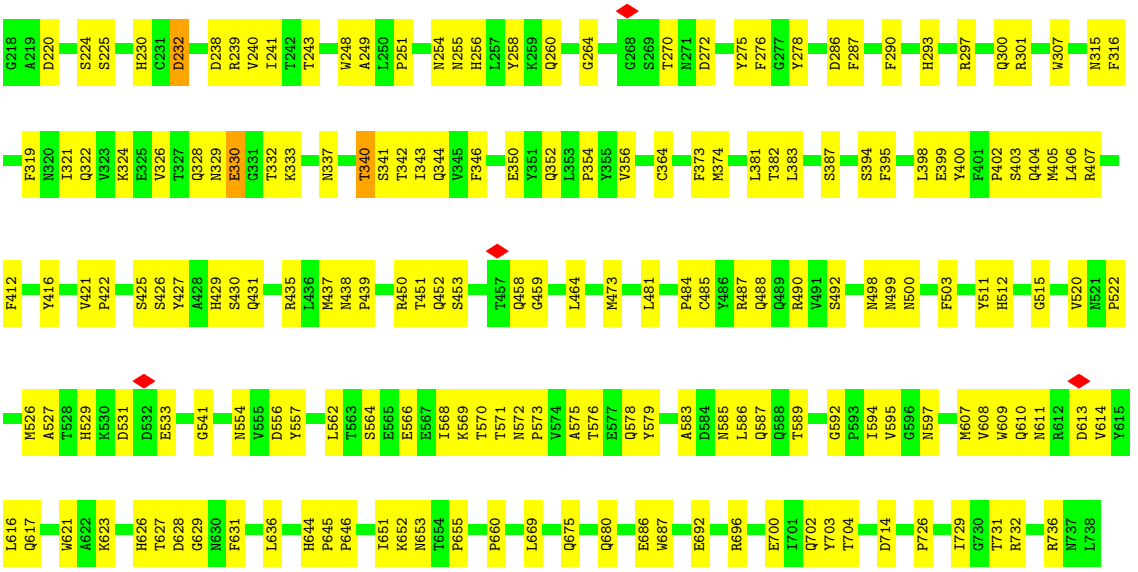

• Molecule 1: Capsid protein VP1

Chain I:



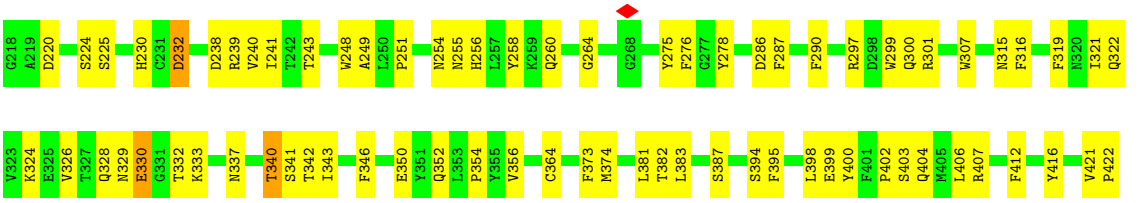
• Molecule 1: Capsid protein VP1

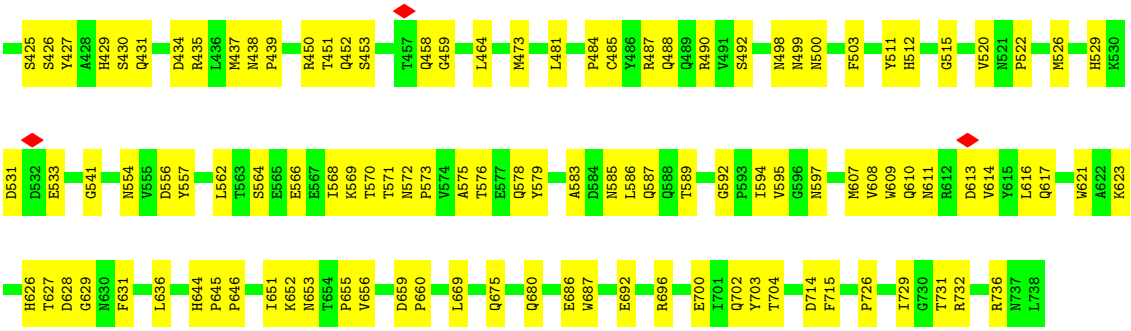
Chain J:



• Molecule 1: Capsid protein VP1

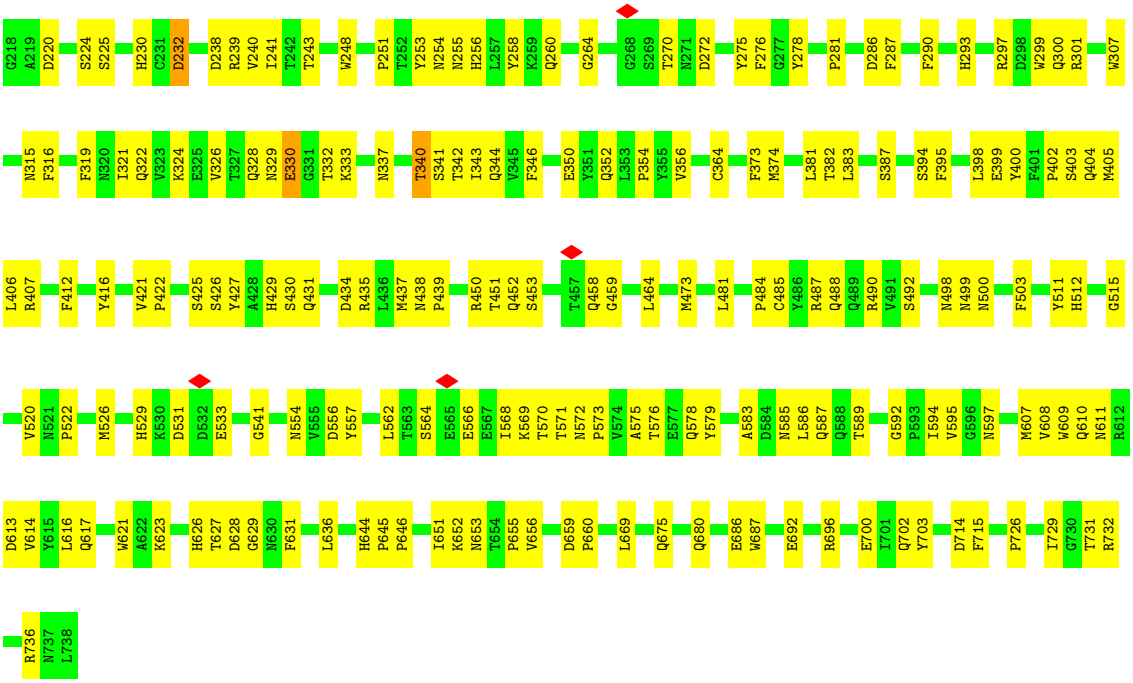
Chain K:





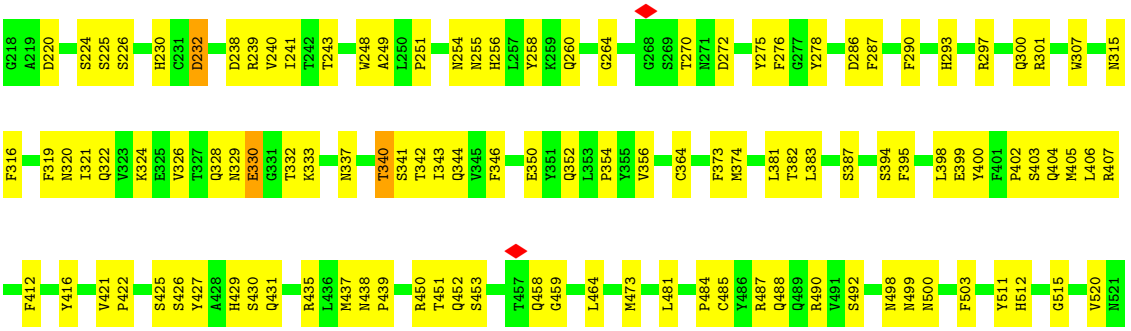

• Molecule 1: Capsid protein VP1

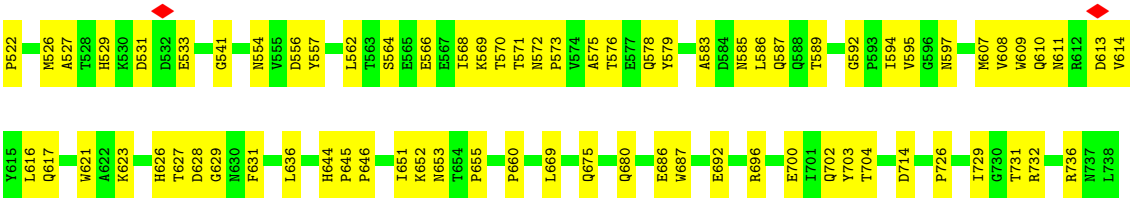
Chain L:




• Molecule 1: Capsid protein VP1

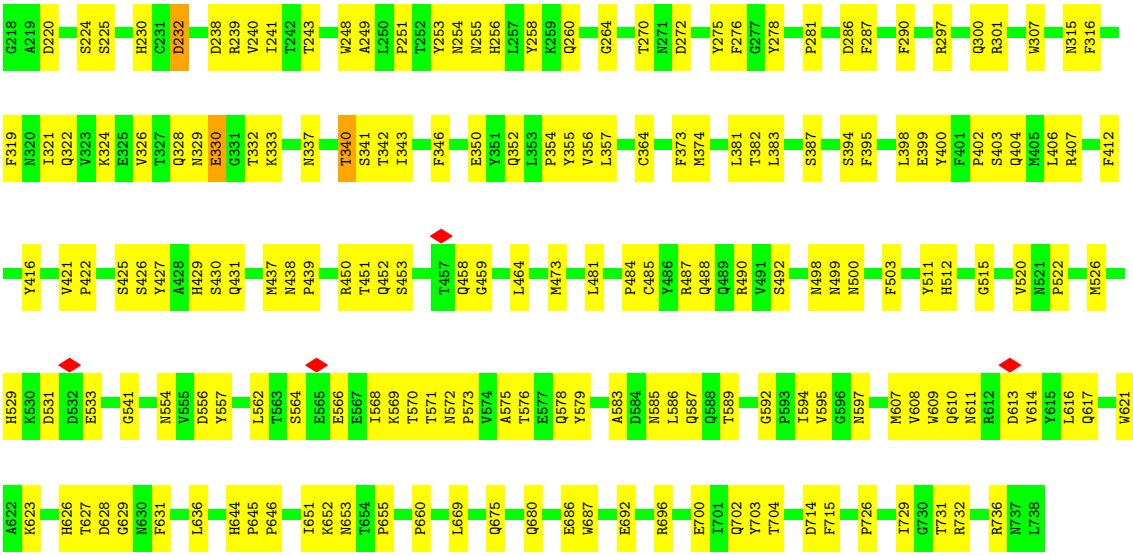
Chain M:





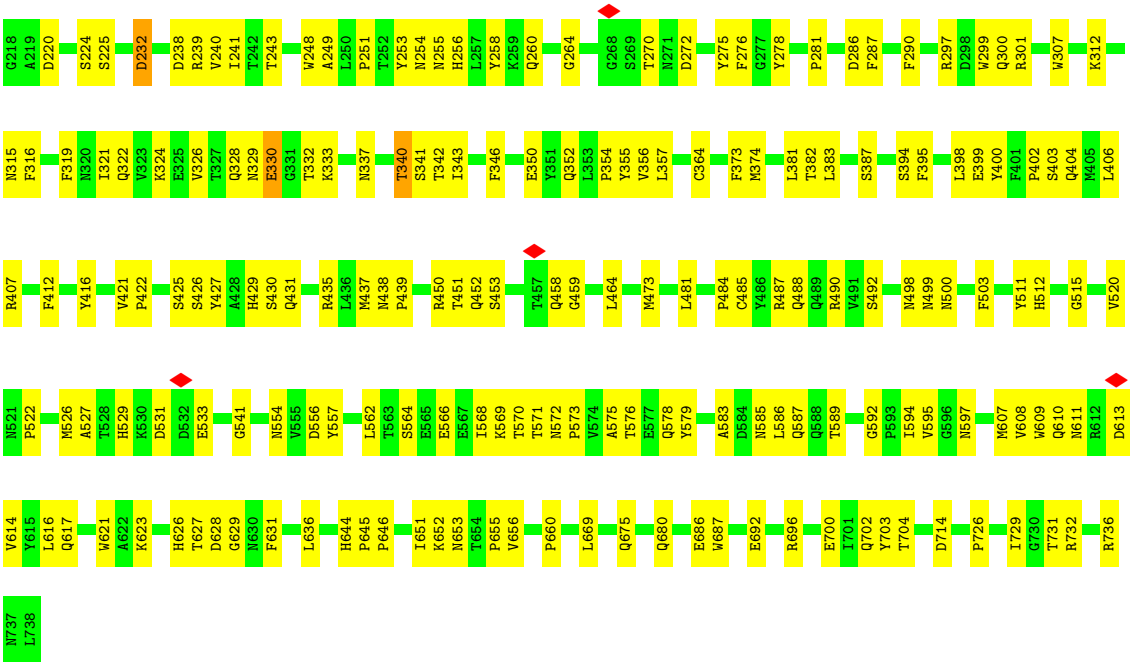
• Molecule 1: Capsid protein VP1

Chain N:



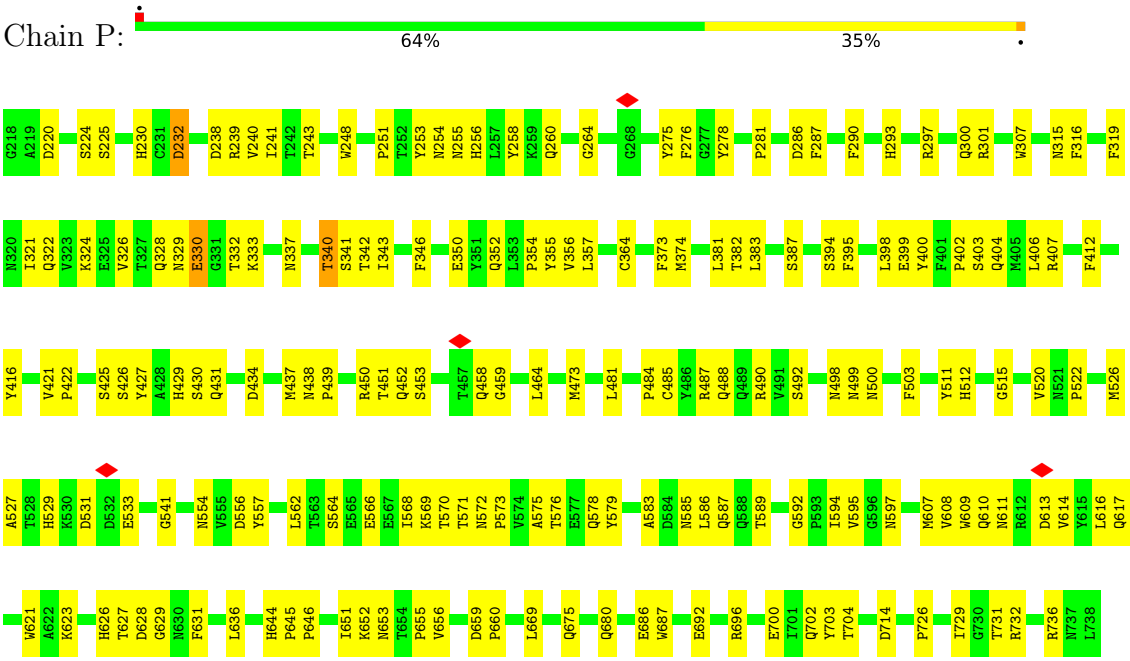
• Molecule 1: Capsid protein VP1

Chain O:



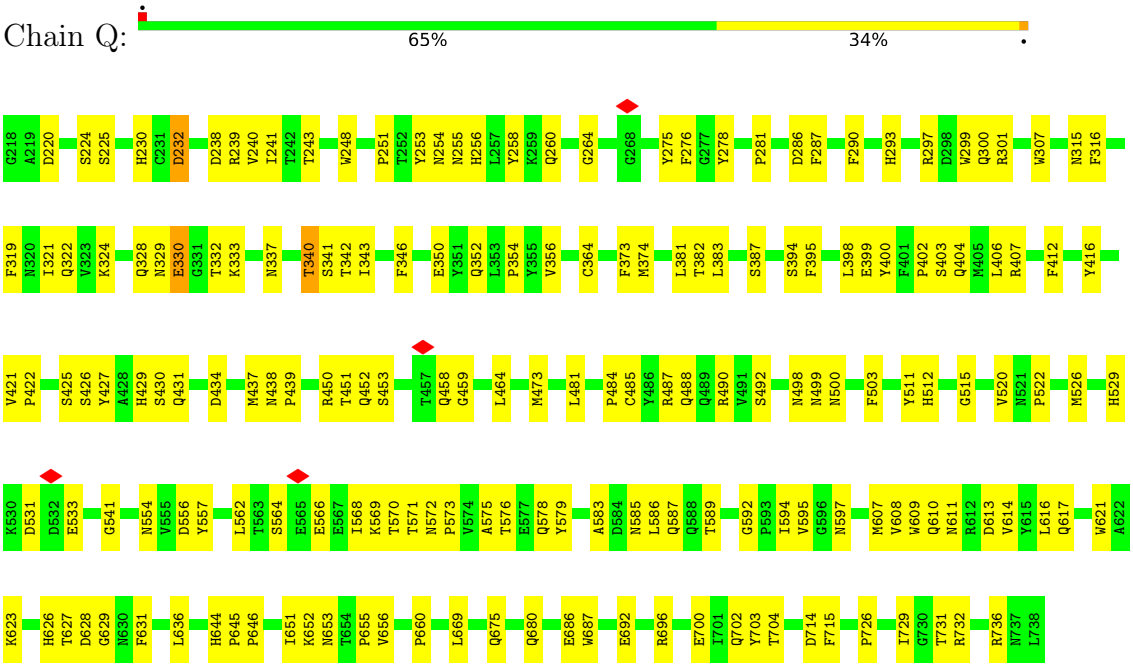
• Molecule 1: Capsid protein VP1

Chain P:



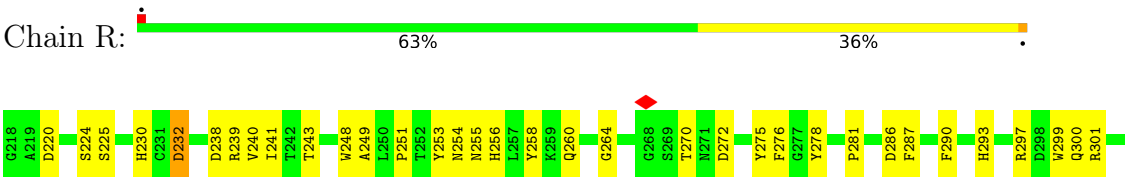

• Molecule 1: Capsid protein VP1

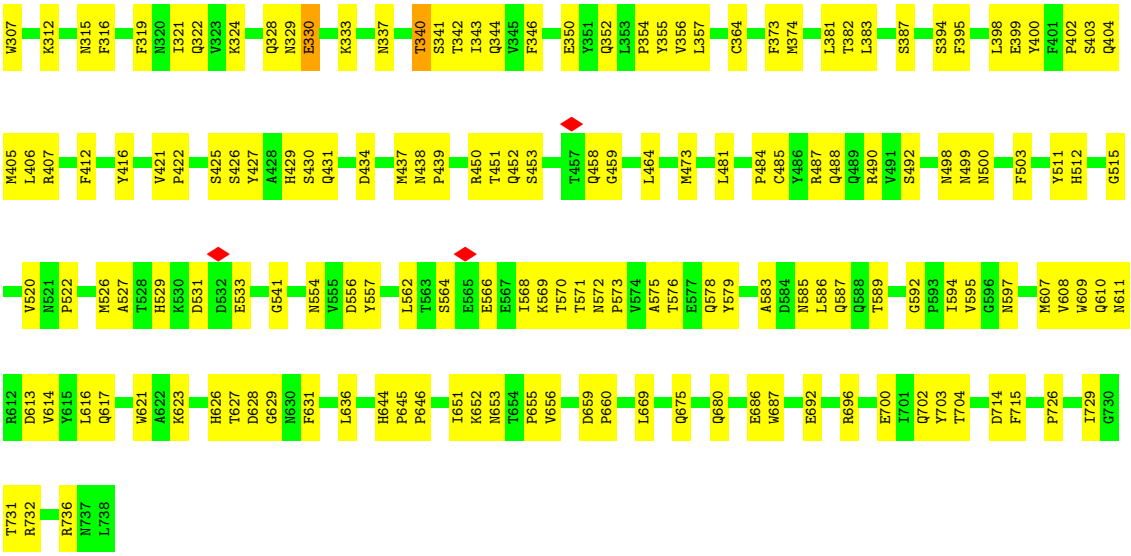
Chain Q:




• Molecule 1: Capsid protein VP1

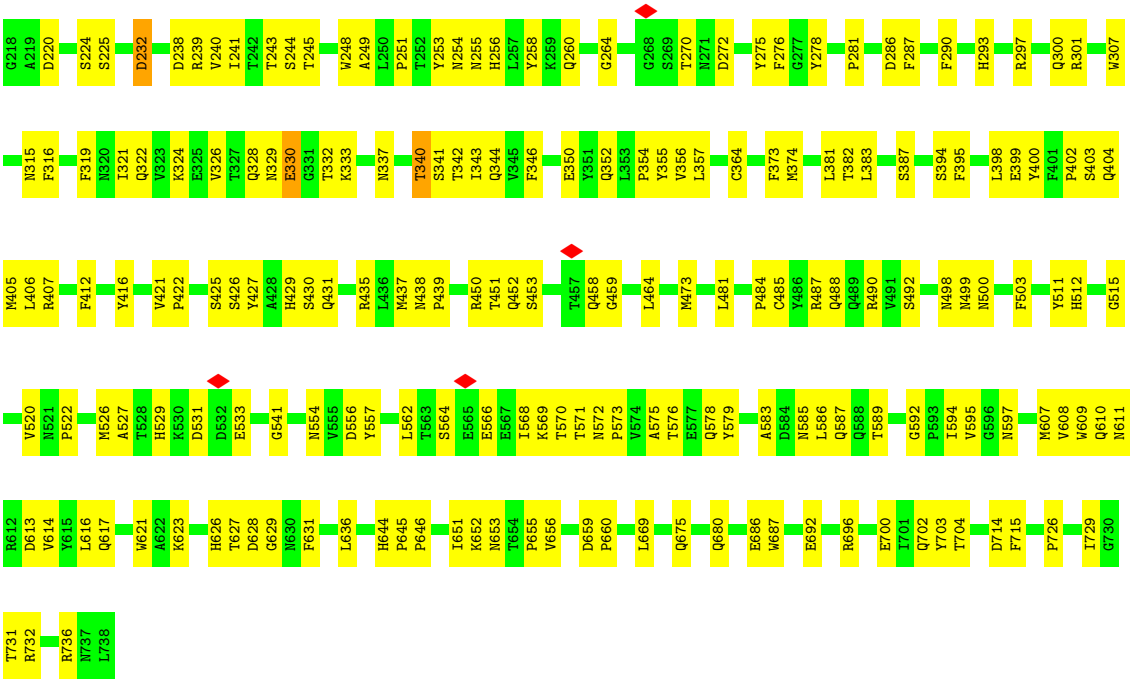
Chain R:





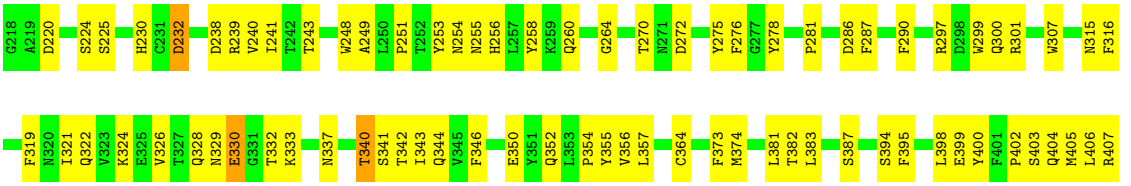

• Molecule 1: Capsid protein VP1

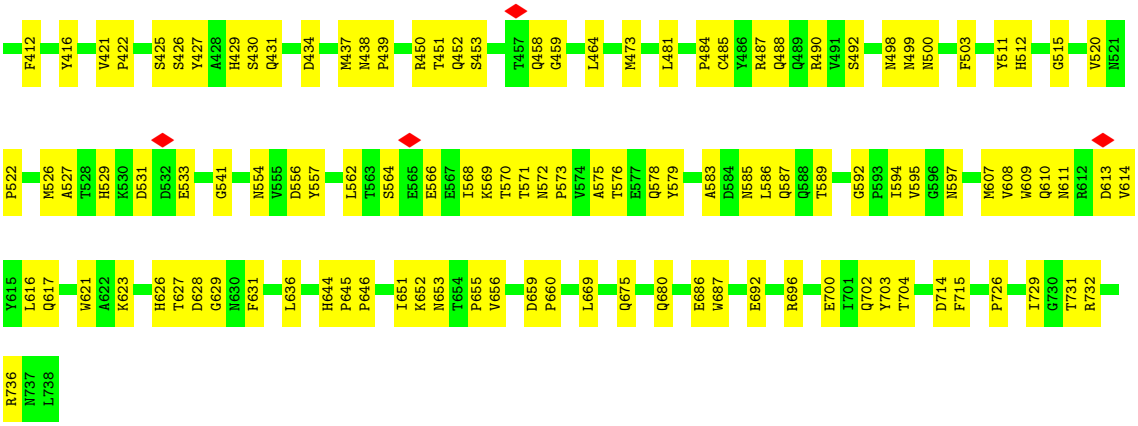
Chain S:




• Molecule 1: Capsid protein VP1

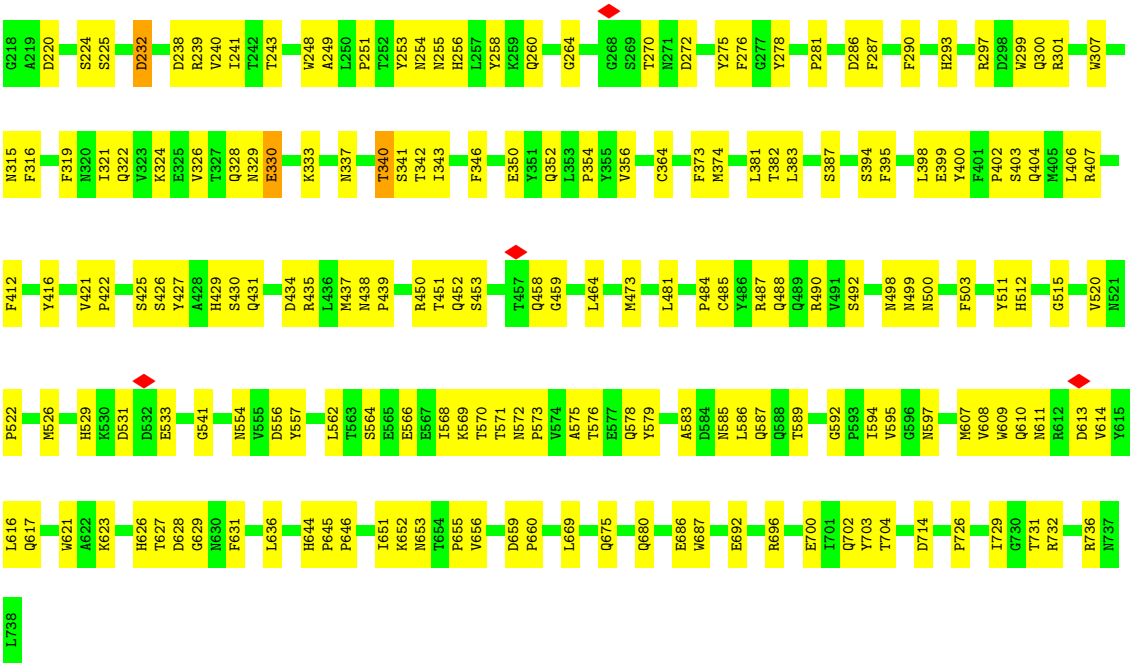
Chain T:





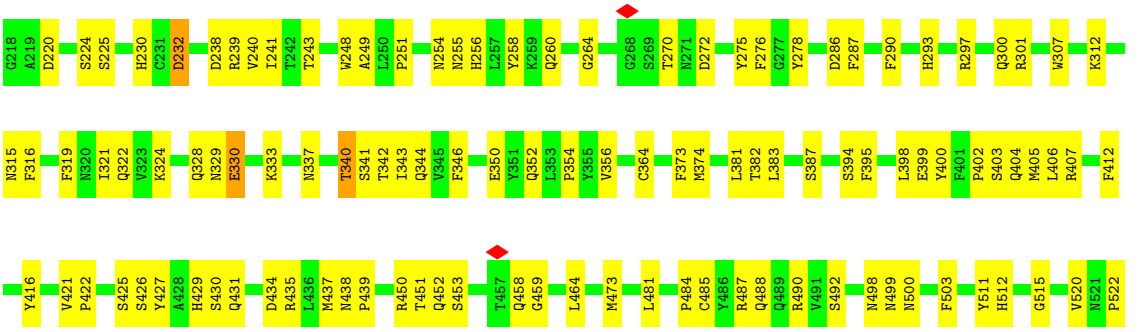

• Molecule 1: Capsid protein VP1

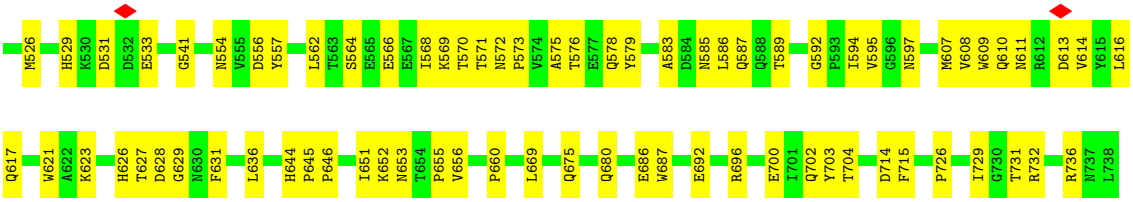
Chain U:




• Molecule 1: Capsid protein VP1

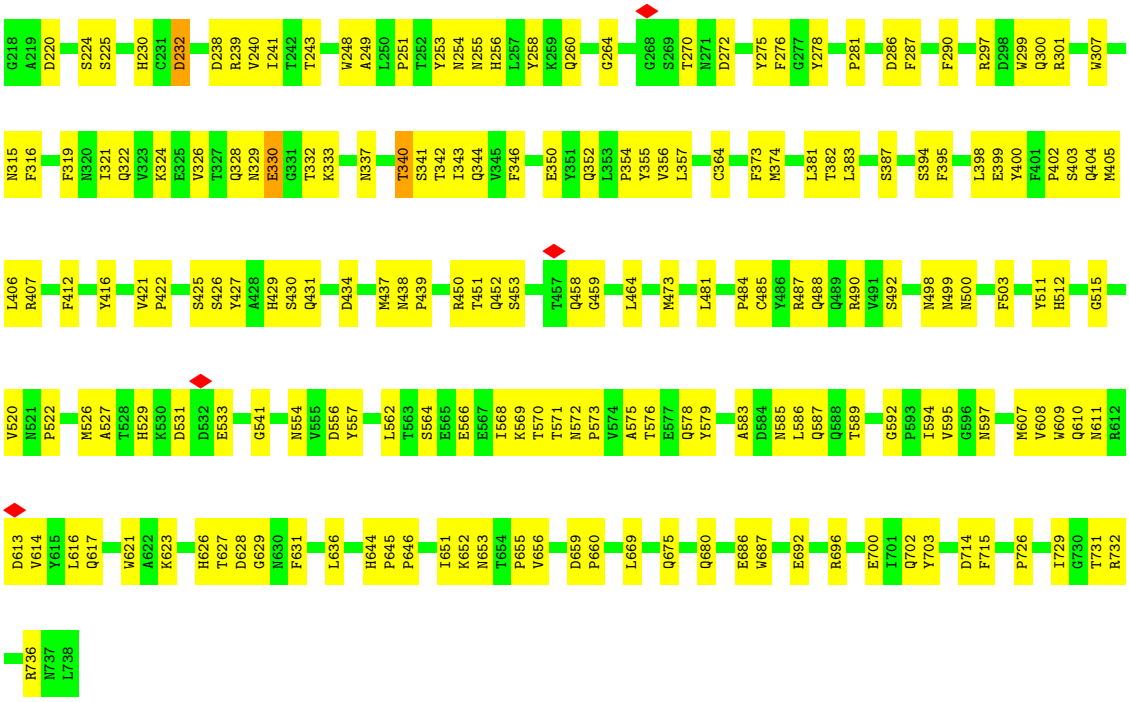
Chain V:





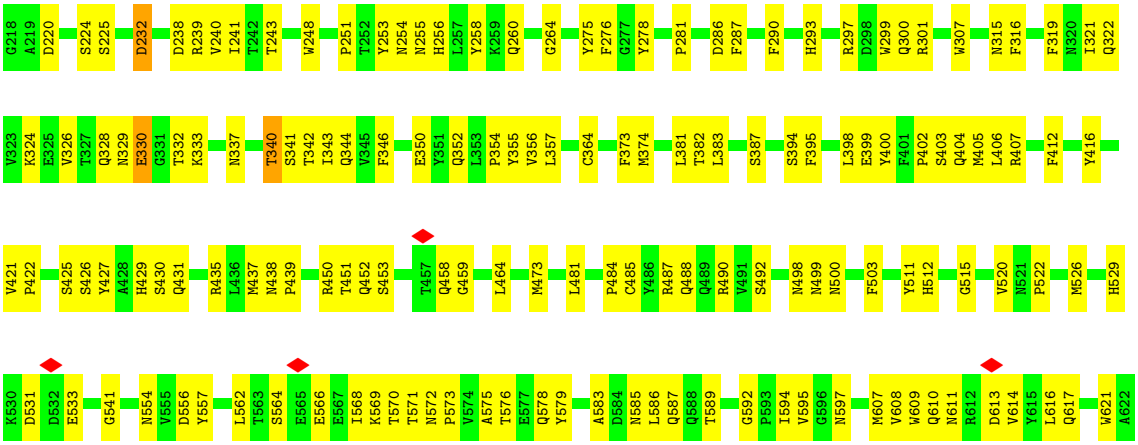
• Molecule 1: Capsid protein VP1

Chain W:



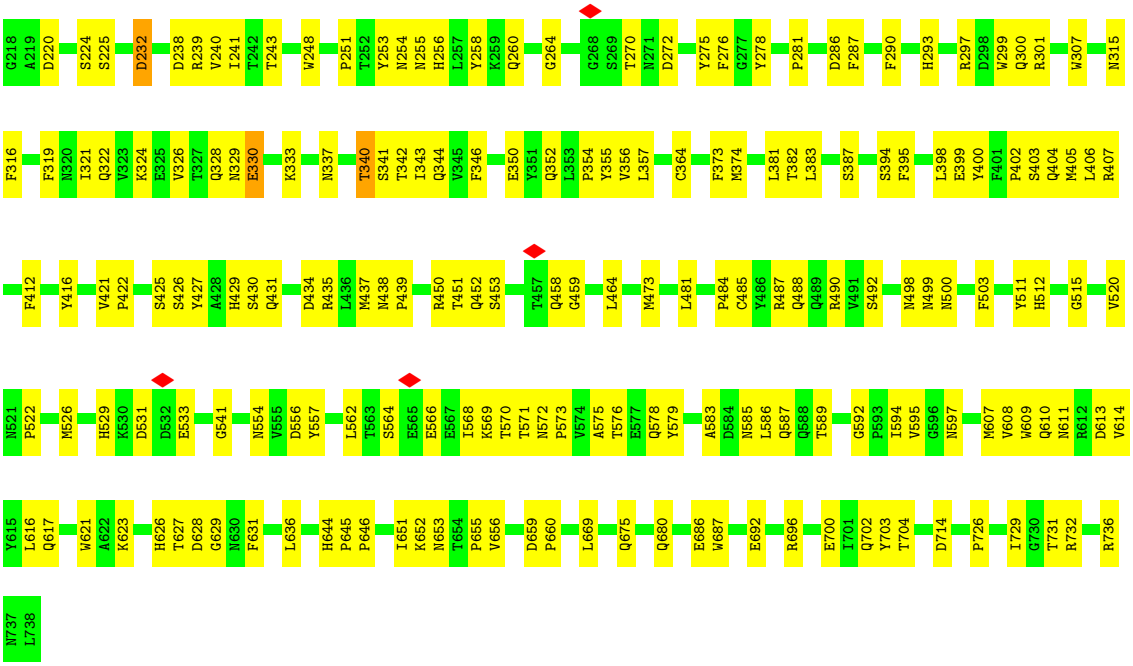
• Molecule 1: Capsid protein VP1

Chain X:



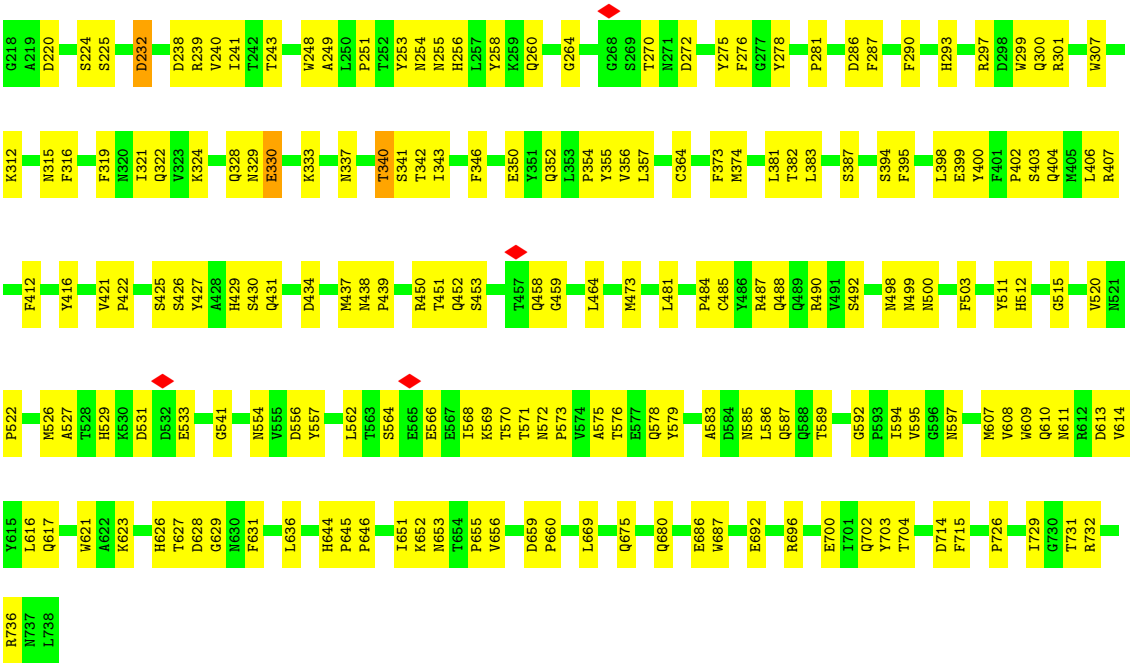
• Molecule 1: Capsid protein VP1

Chain Y:



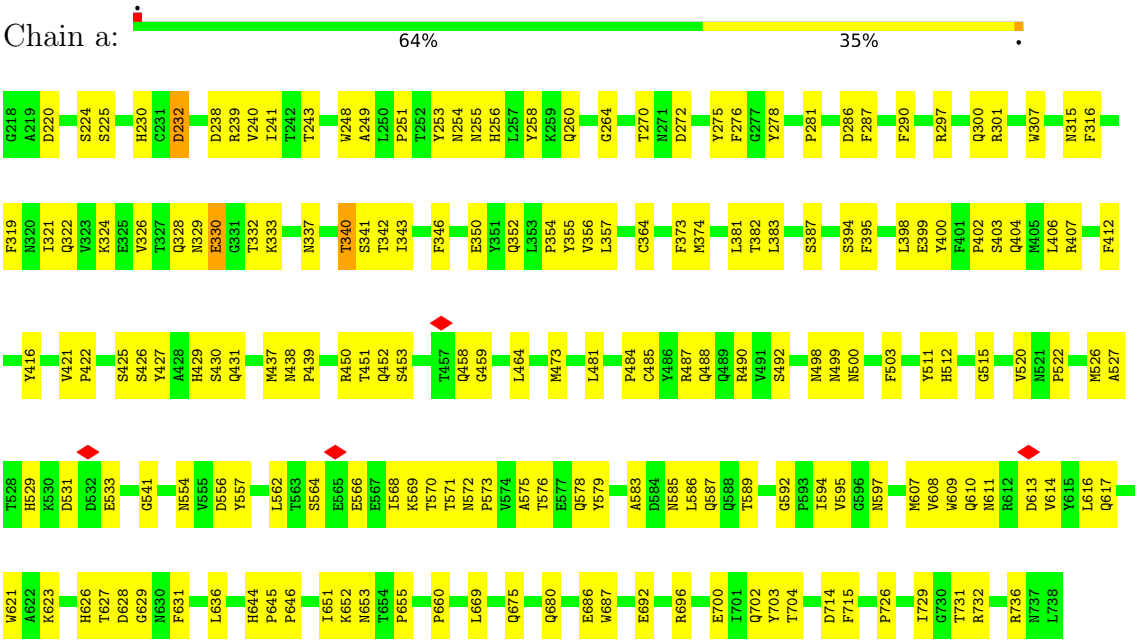

• Molecule 1: Capsid protein VP1

Chain Z:



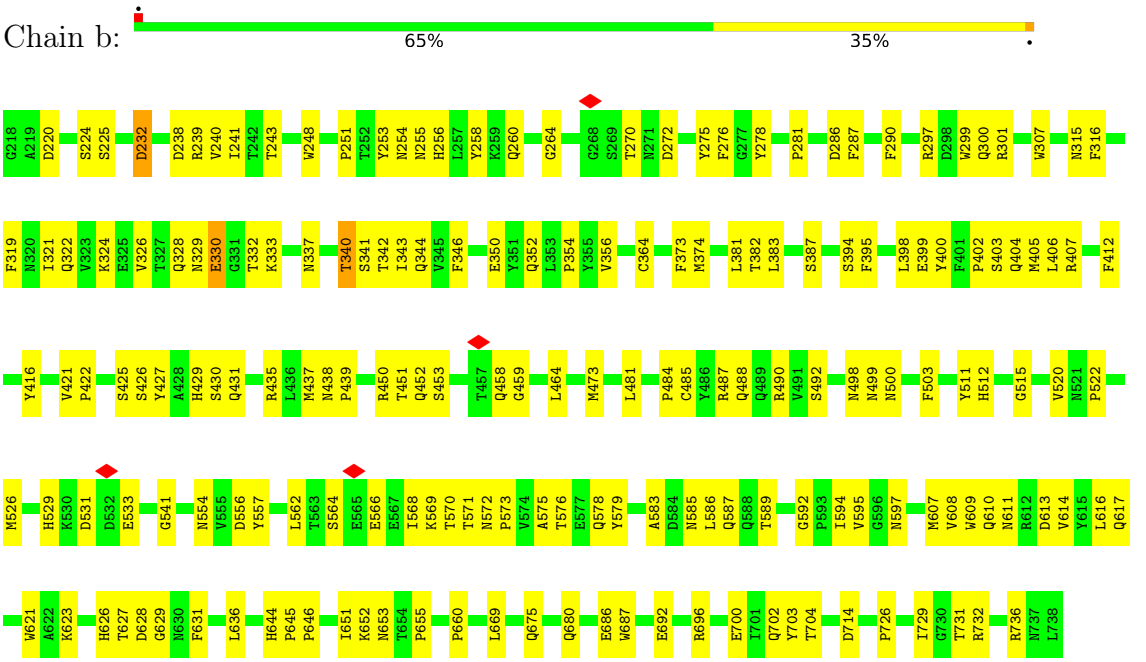
• Molecule 1: Capsid protein VP1

Chain a:



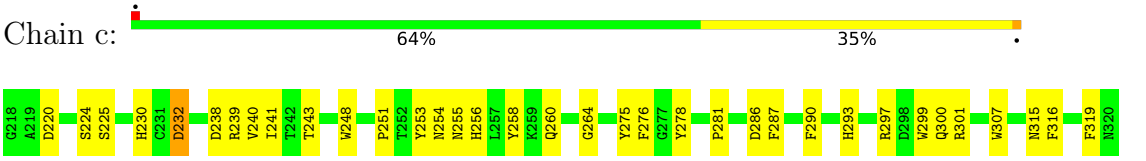

• Molecule 1: Capsid protein VP1

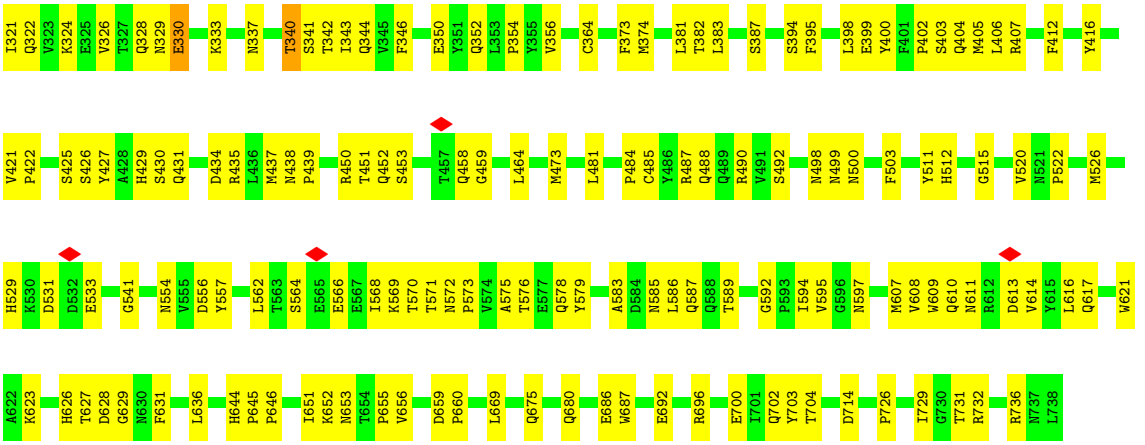
Chain b:




• Molecule 1: Capsid protein VP1

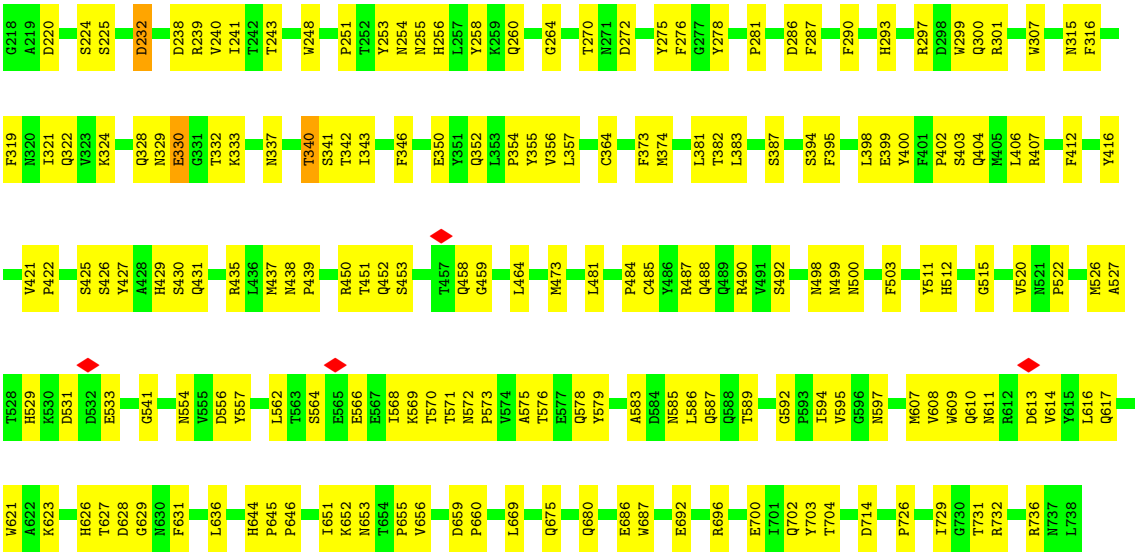
Chain c:





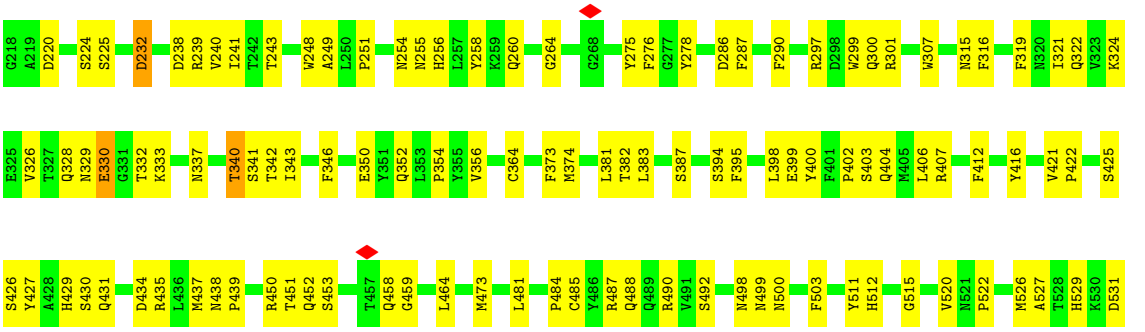
• Molecule 1: Capsid protein VP1

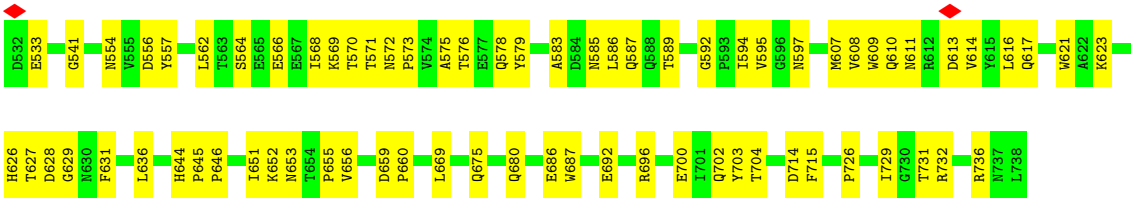
Chain d:



• Molecule 1: Capsid protein VP1

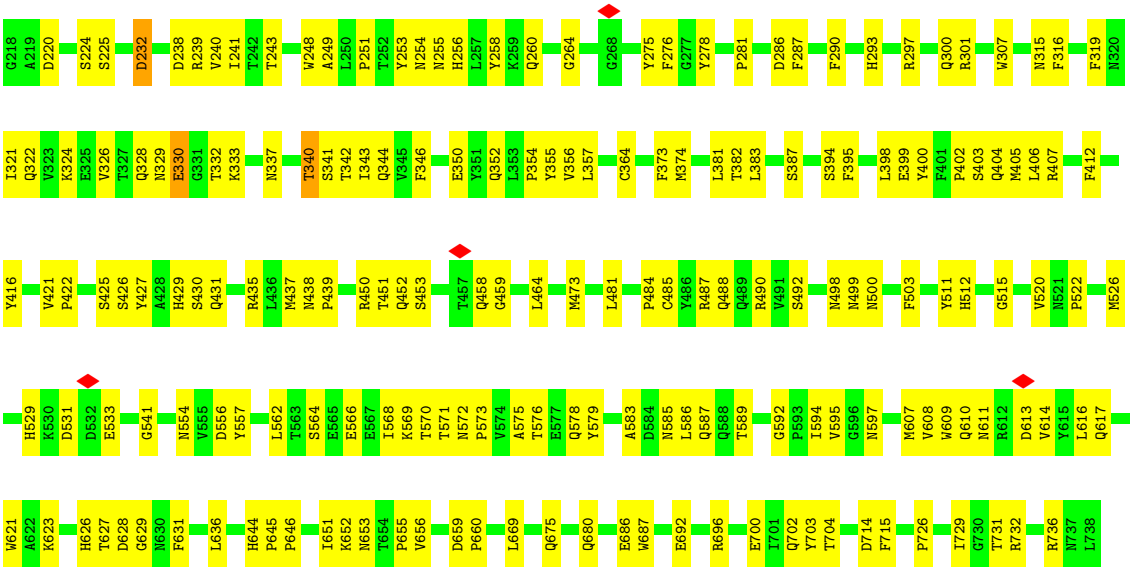
Chain e:





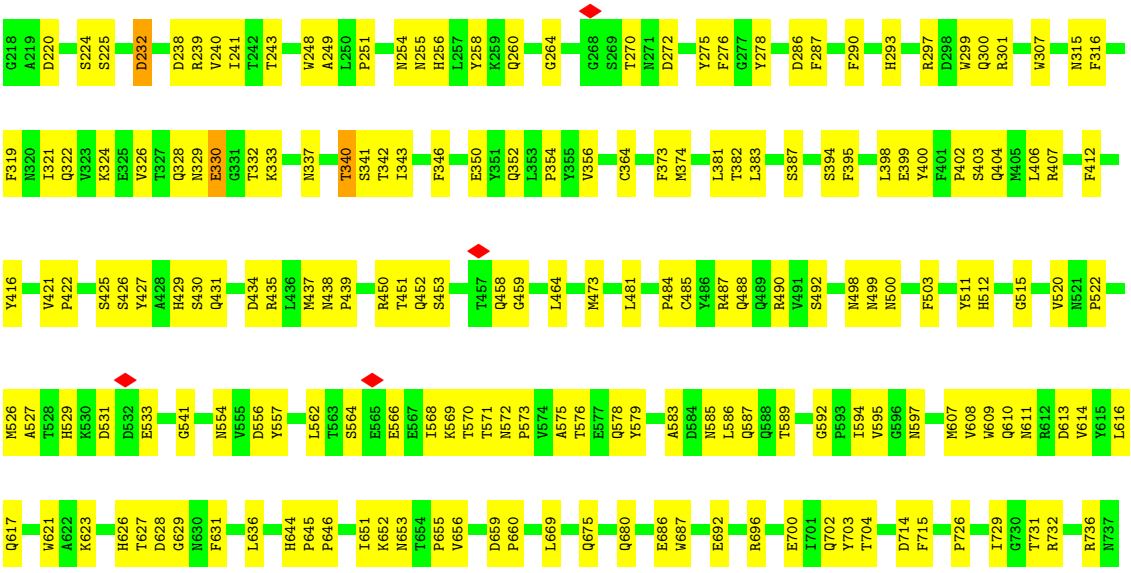

• Molecule 1: Capsid protein VP1

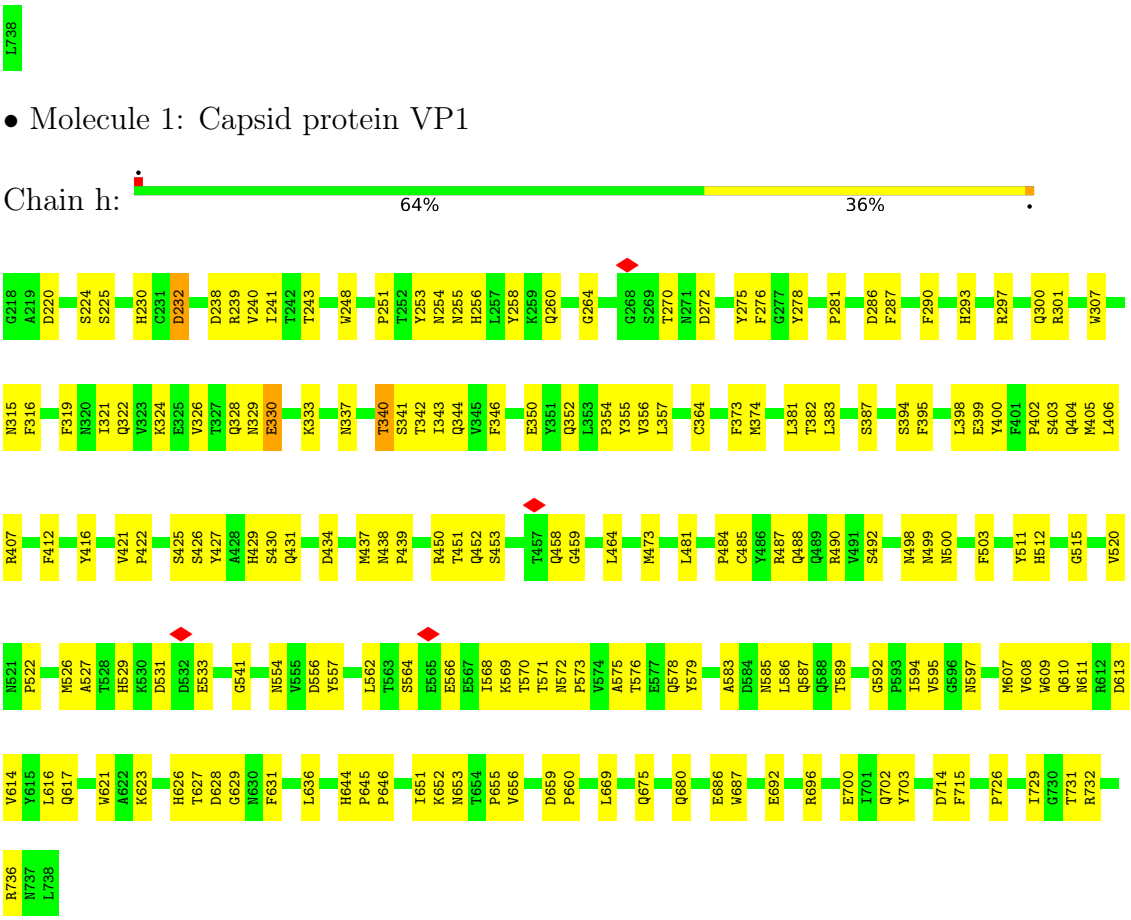
Chain f:




• Molecule 1: Capsid protein VP1

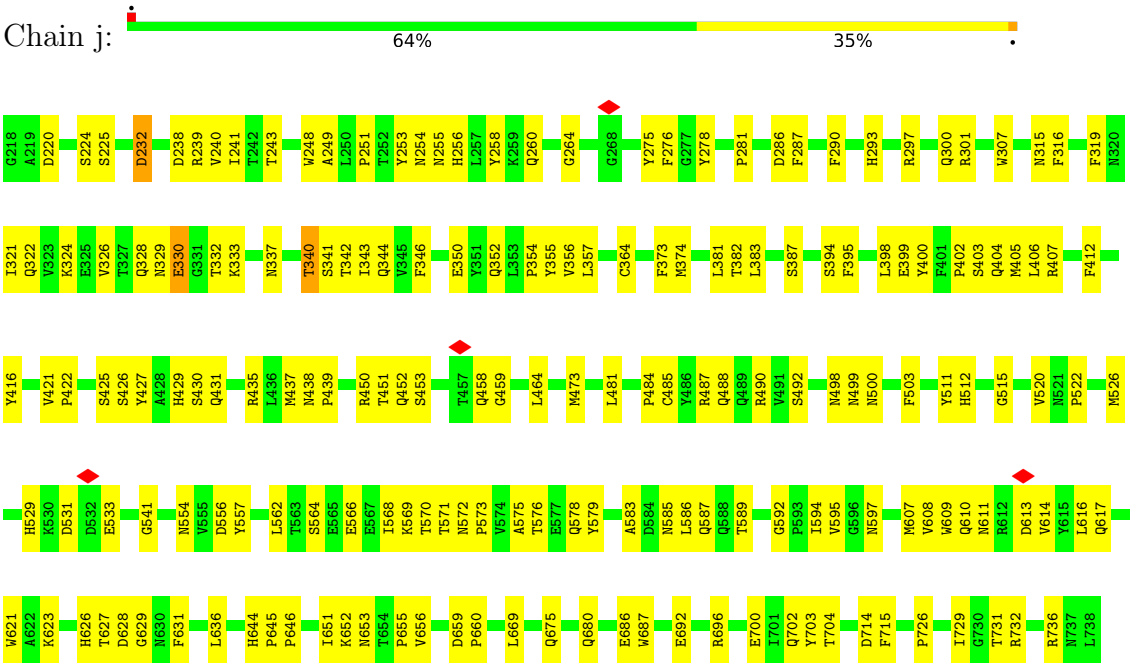
Chain g:




L738
• Molecule 1: Capsid protein VP1
Chain h:
64%
36%
• Molecule 1: Capsid protein VP1
Chain i:
64%
35%

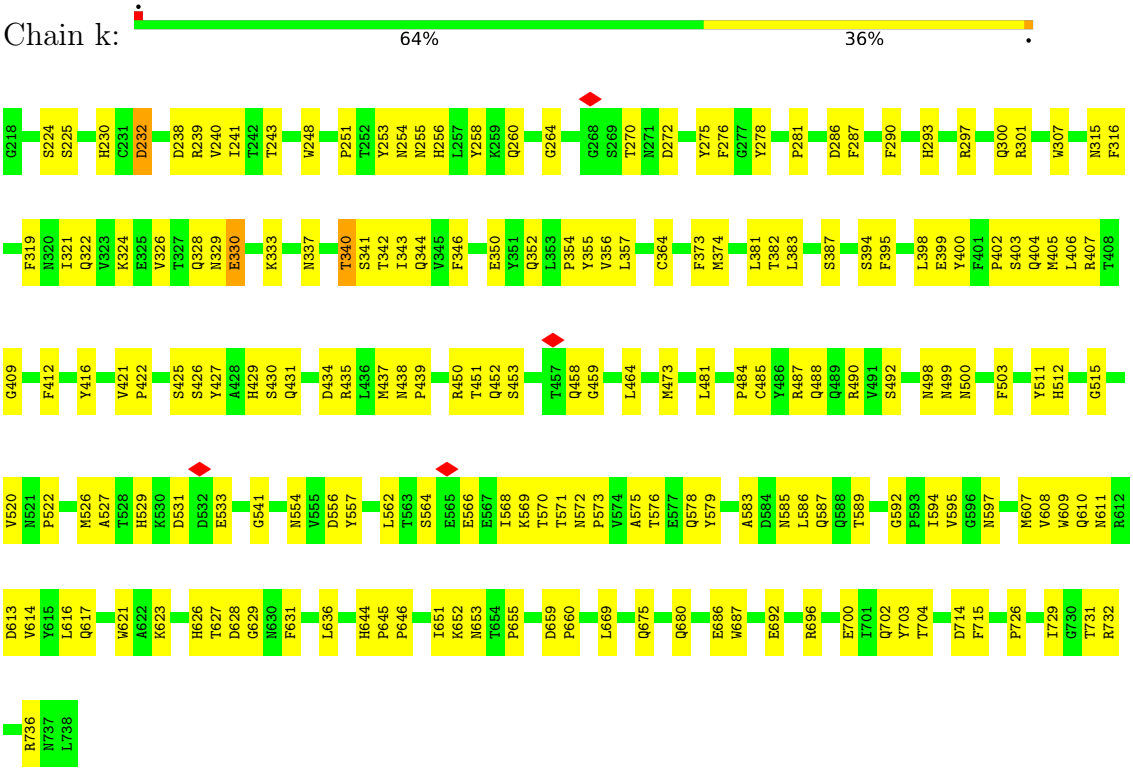
• Molecule 1: Capsid protein VP1

Chain j:



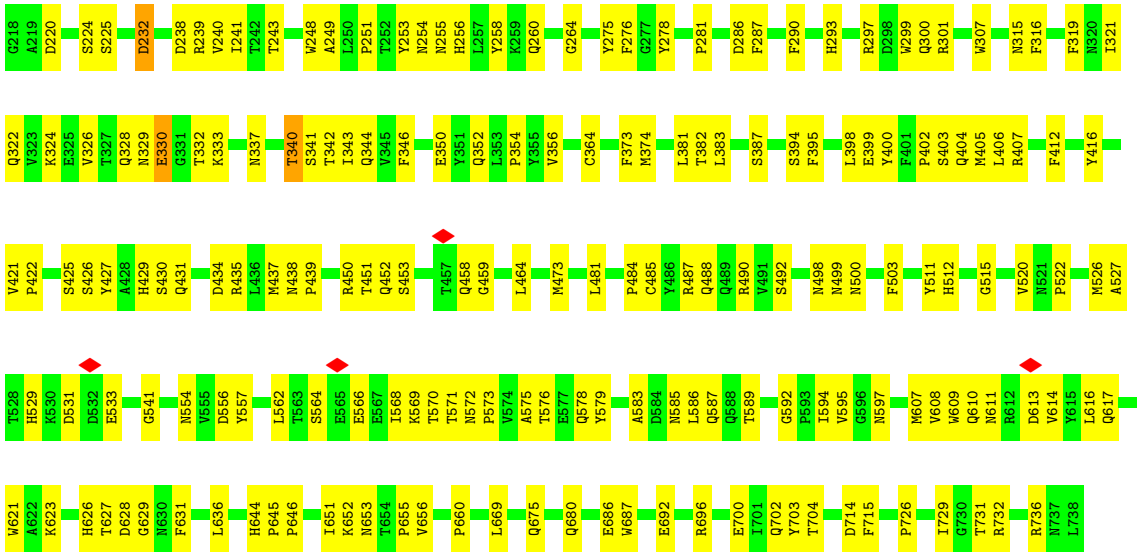

• Molecule 1: Capsid protein VP1

Chain k:



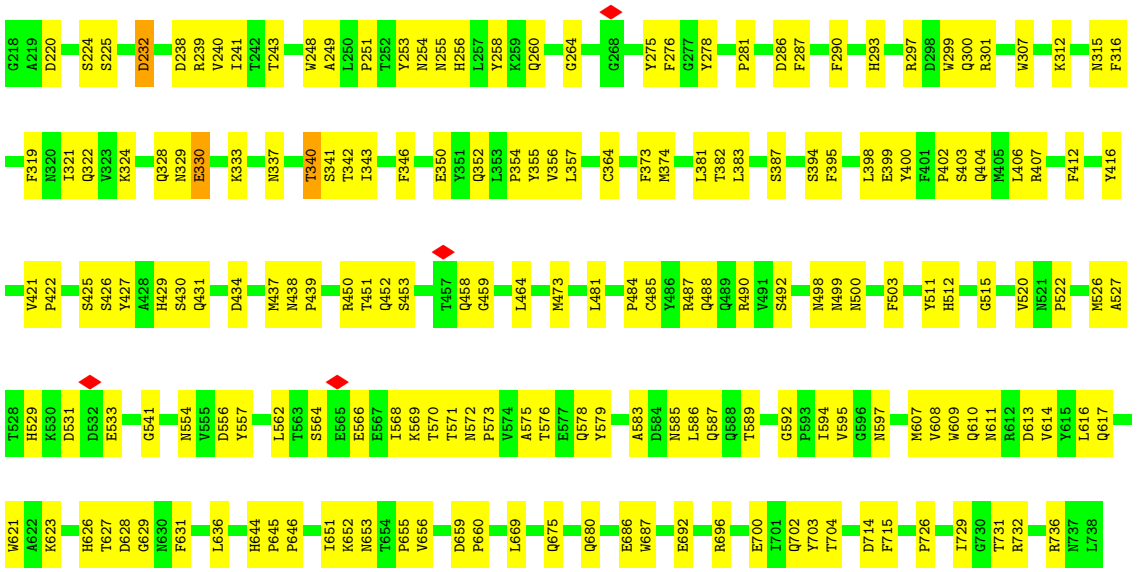

• Molecule 1: Capsid protein VP1

Chain l:



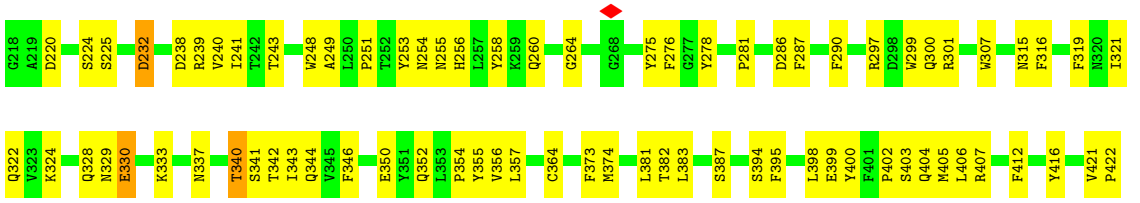

• Molecule 1: Capsid protein VP1

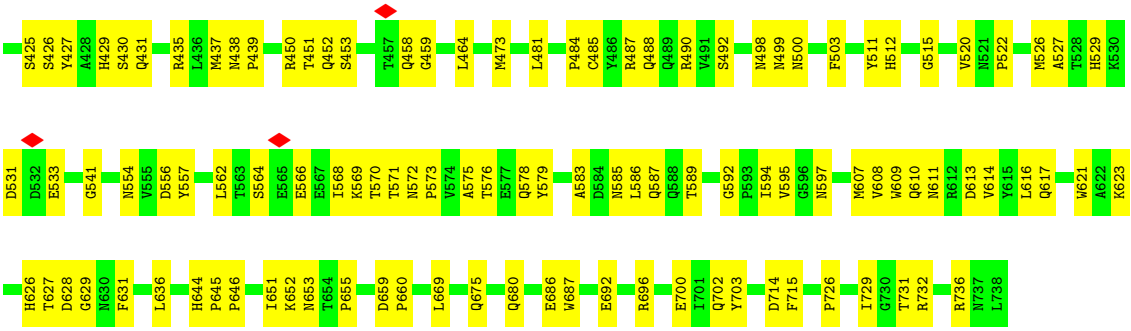
Chain m:




• Molecule 1: Capsid protein VP1

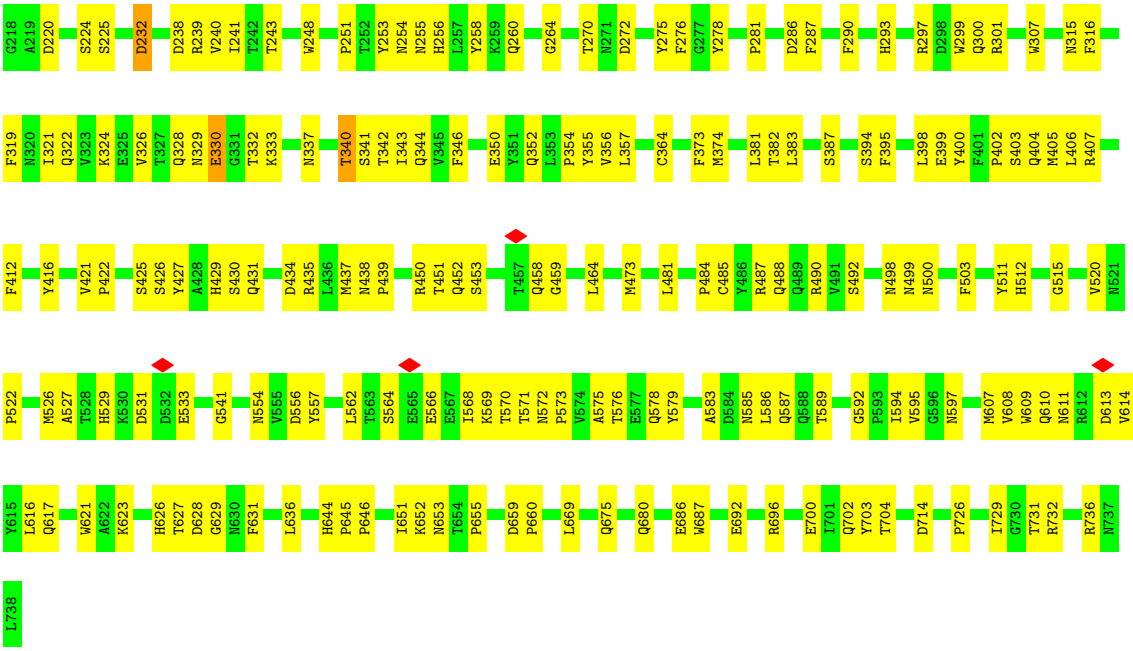
Chain n:





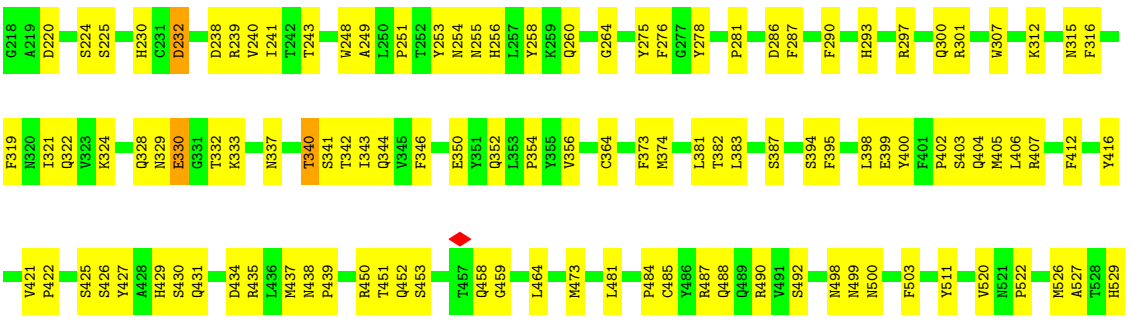

• Molecule 1: Capsid protein VP1

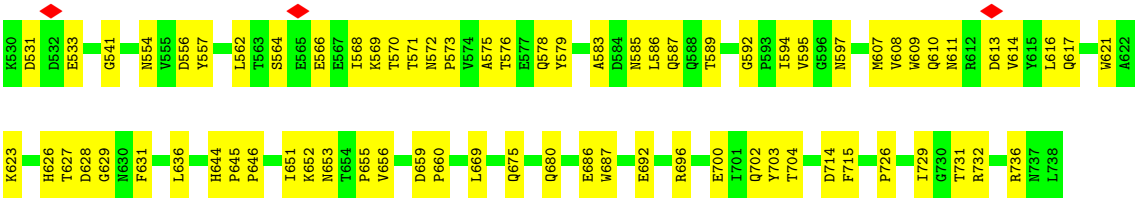
Chain o:




• Molecule 1: Capsid protein VP1

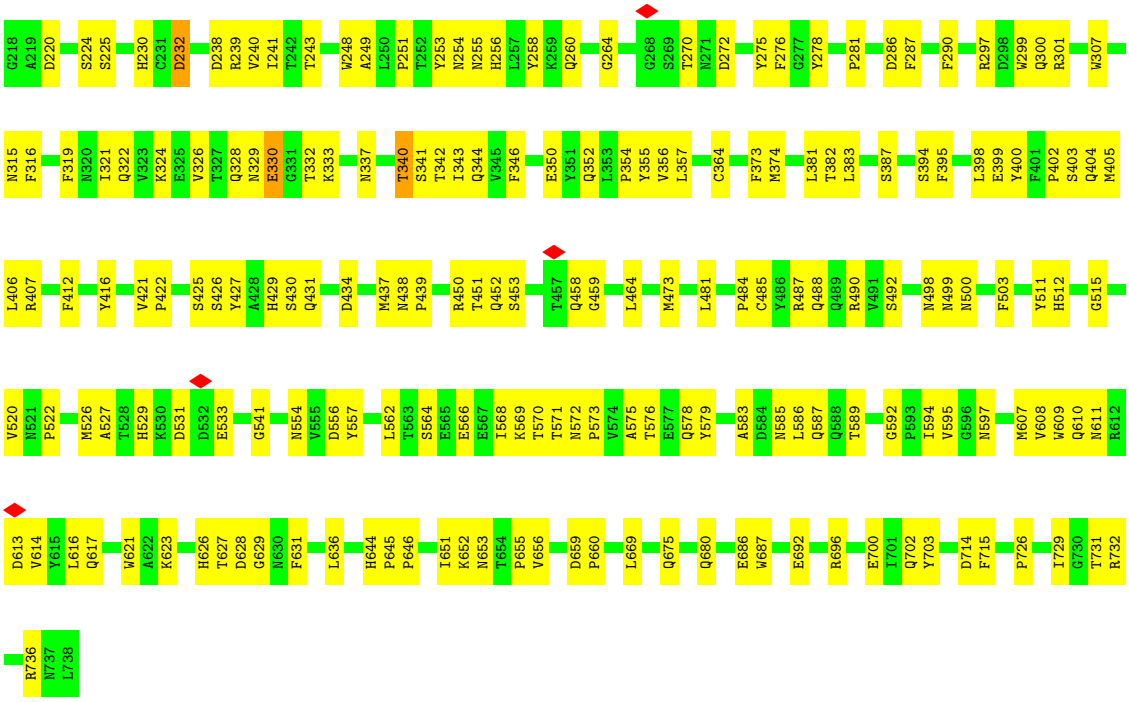
Chain p:





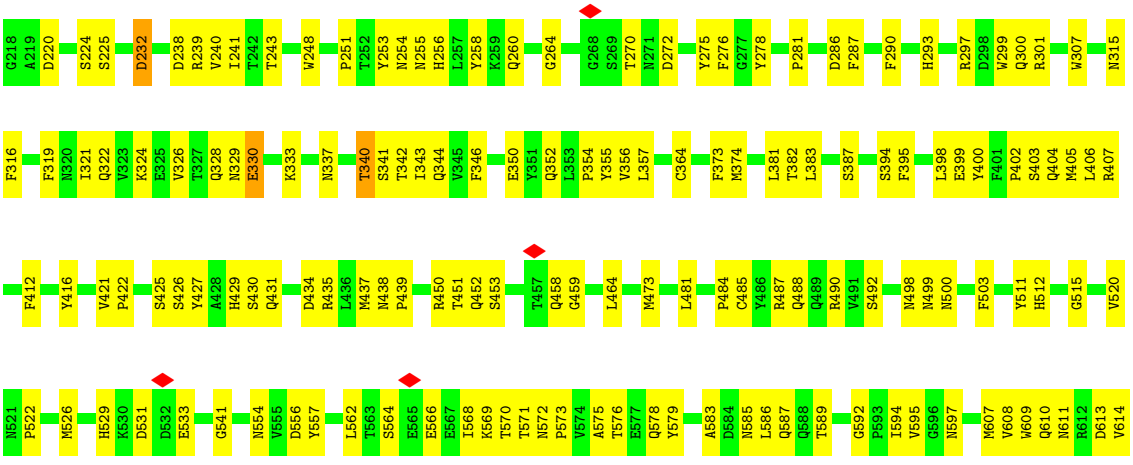

• Molecule 1: Capsid protein VP1

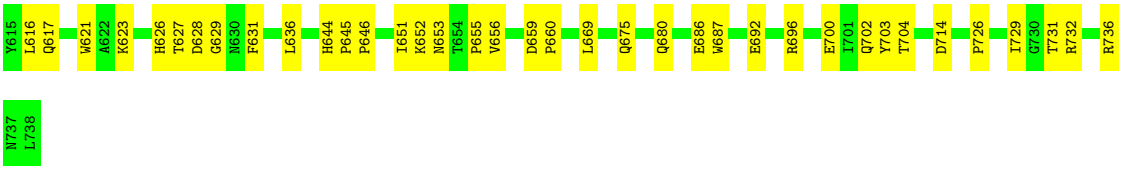
Chain q:




• Molecule 1: Capsid protein VP1

Chain r:

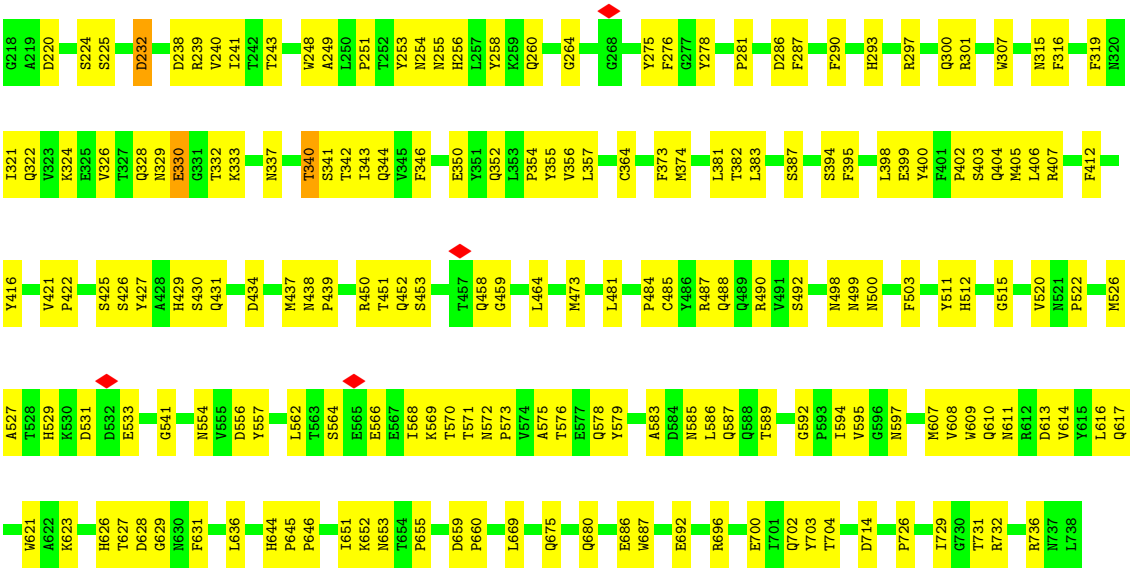






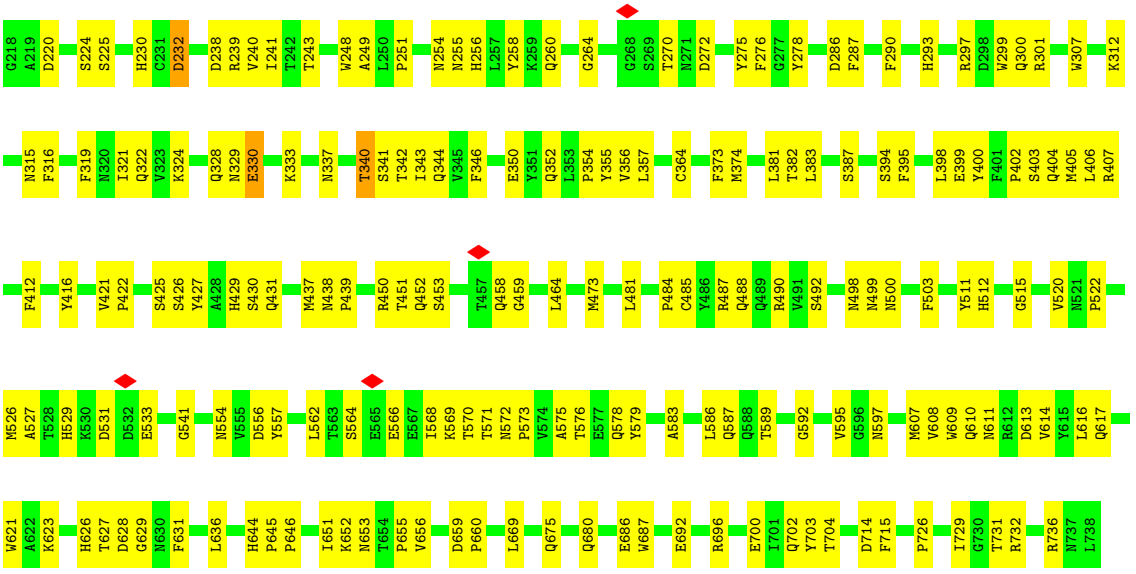
• Molecule 1: Capsid protein VP1

Chain s:



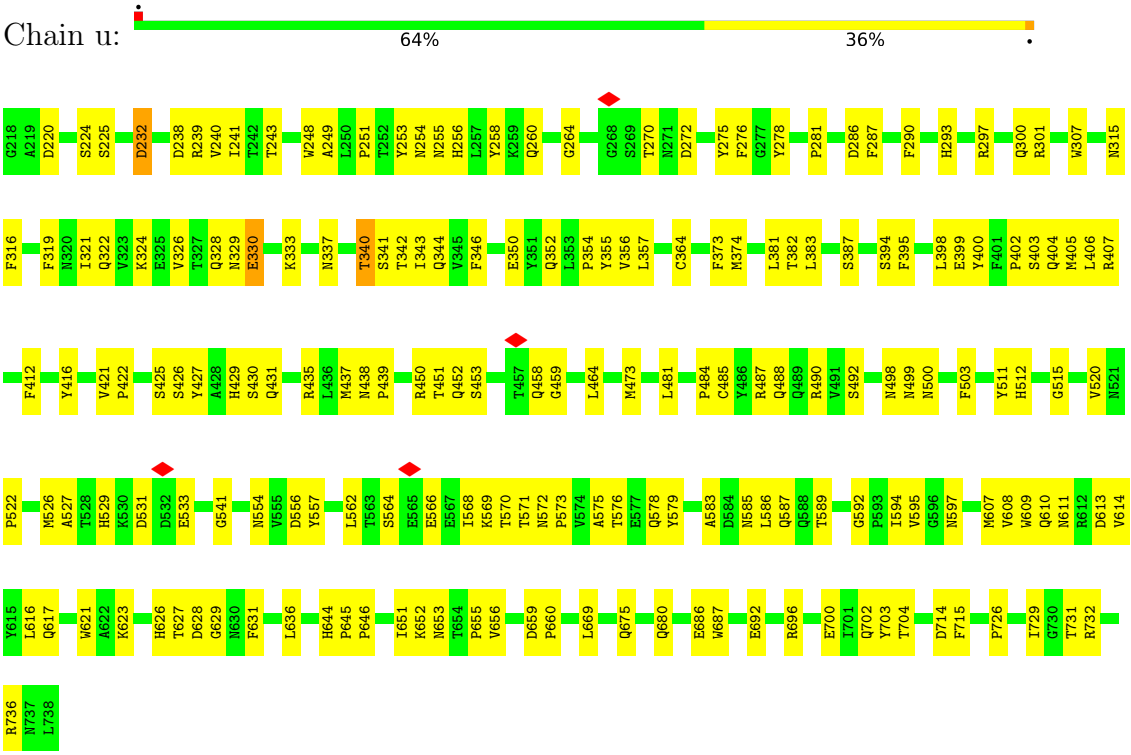
• Molecule 1: Capsid protein VP1

Chain t:



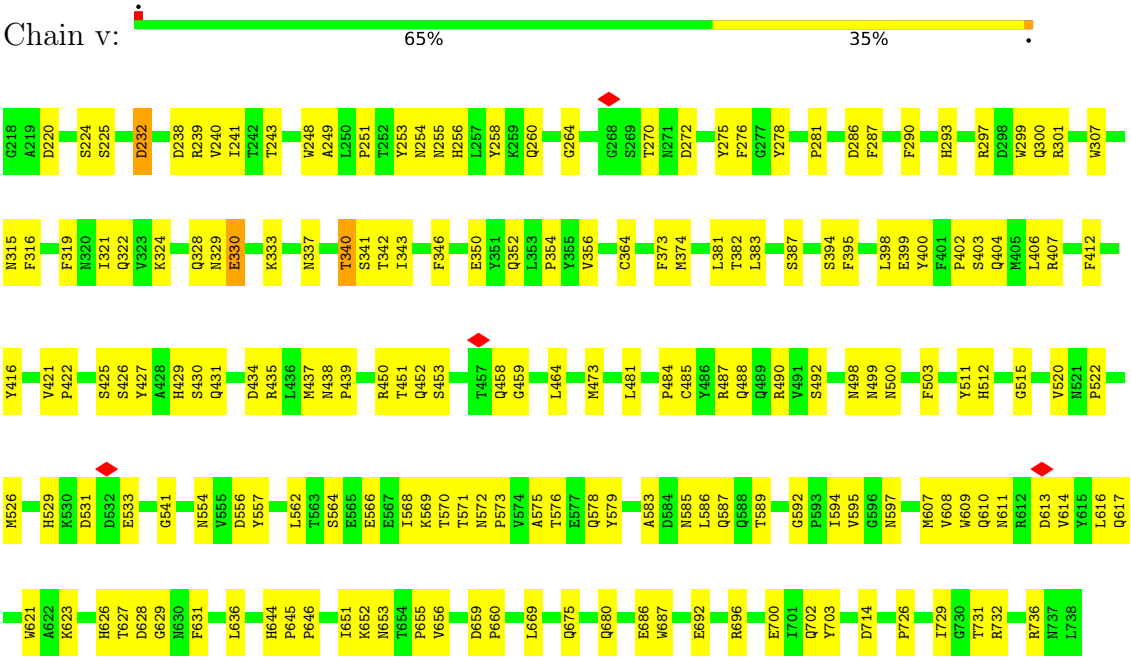
• Molecule 1: Capsid protein VP1

Chain u:



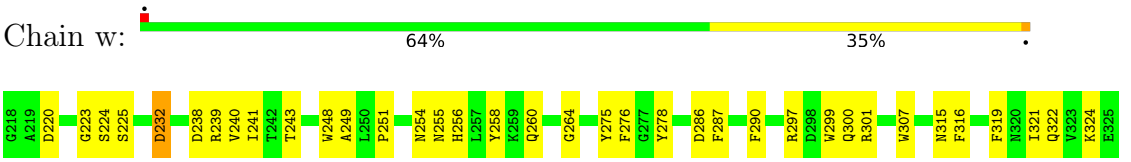

• Molecule 1: Capsid protein VP1

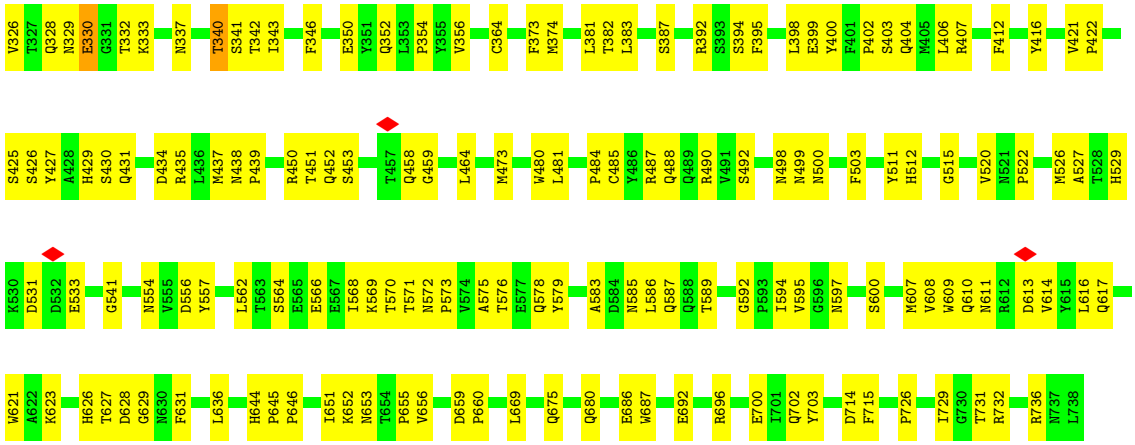
Chain v:




• Molecule 1: Capsid protein VP1

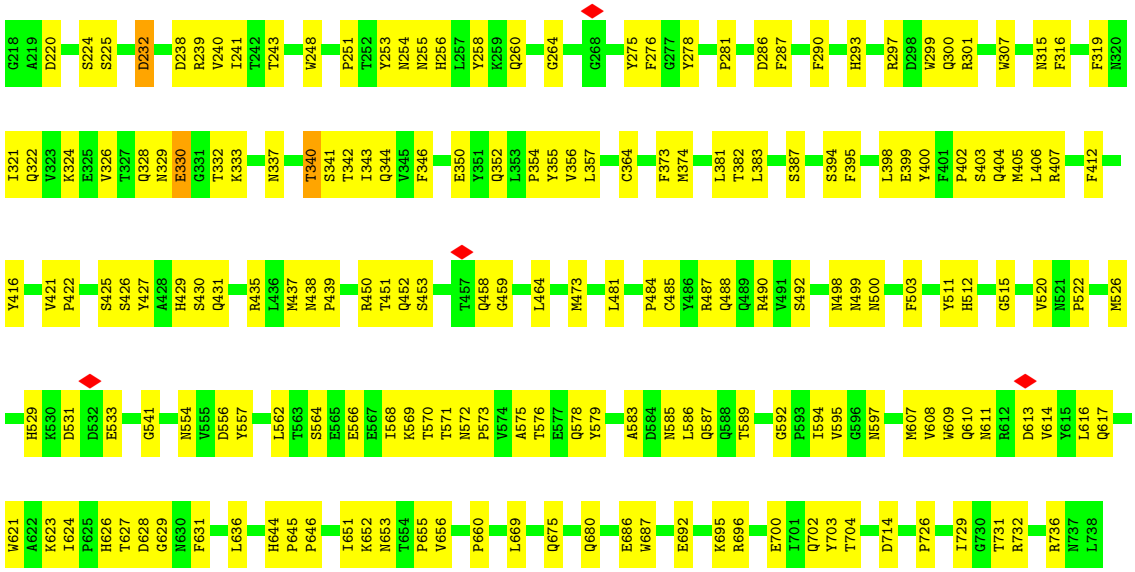
Chain w:





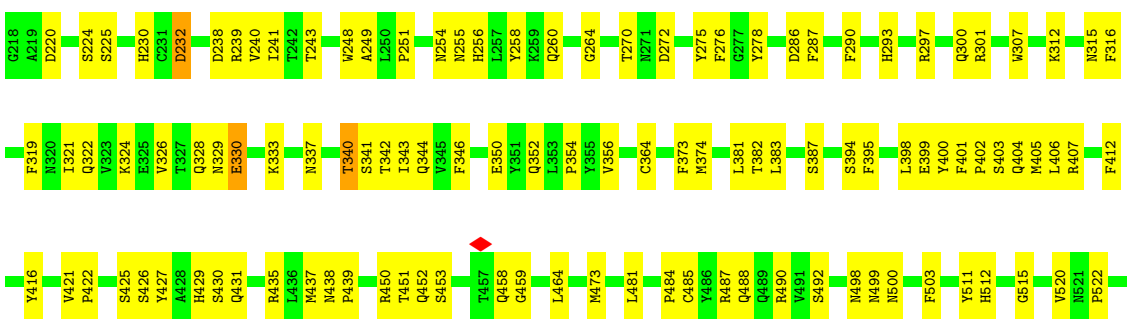
• Molecule 1: Capsid protein VP1

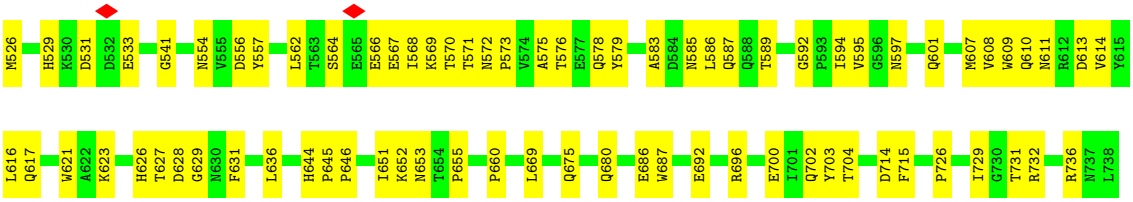
Chain x:



• Molecule 1: Capsid protein VP1

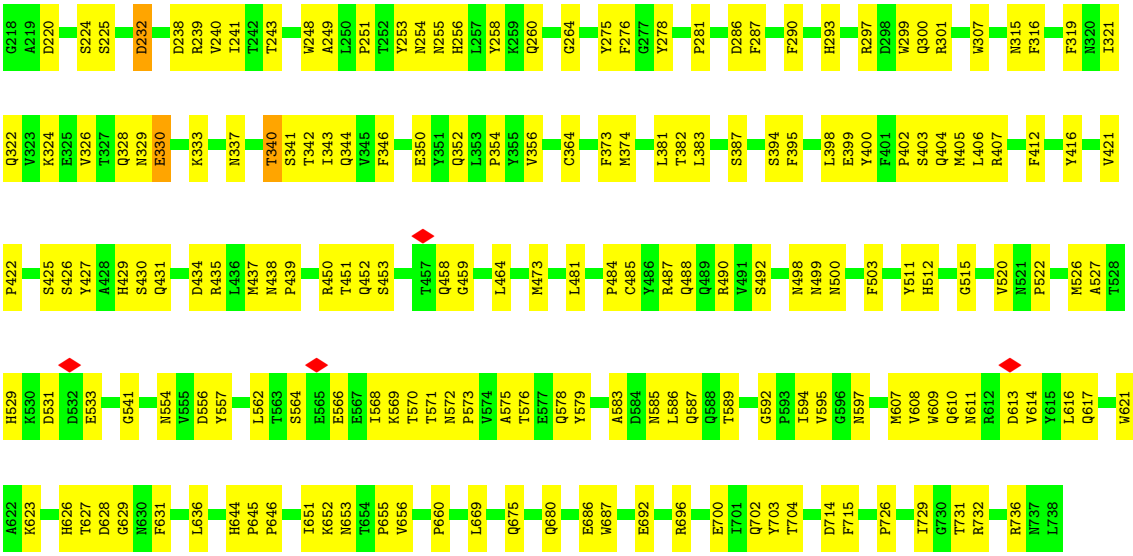
Chain y:





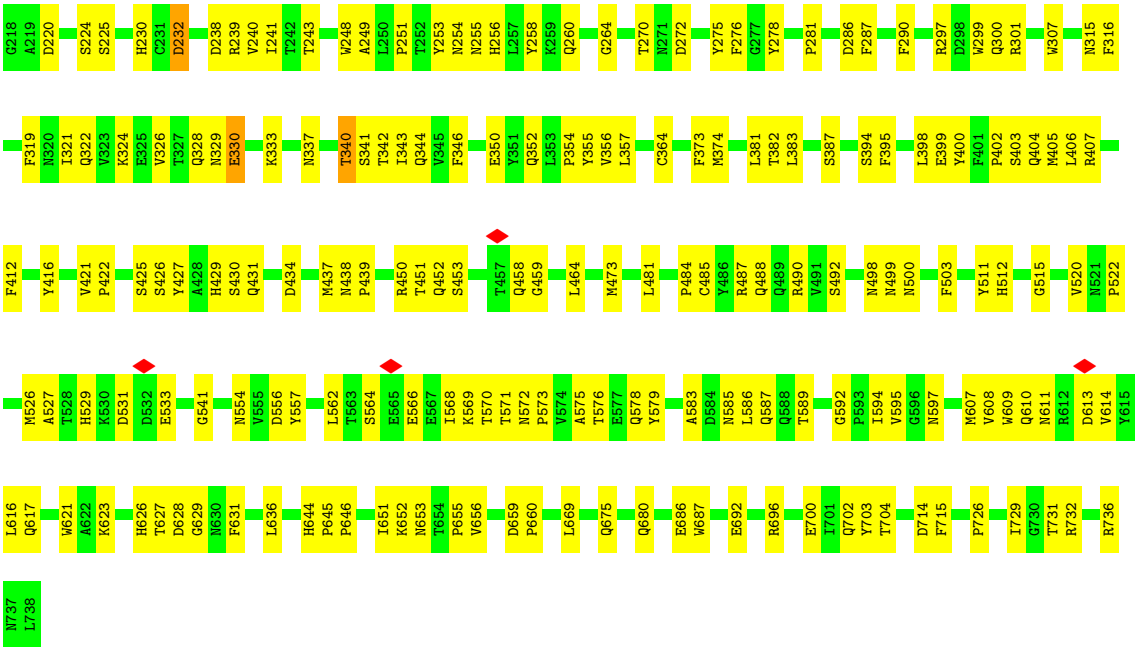

• Molecule 1: Capsid protein VP1

Chain z:



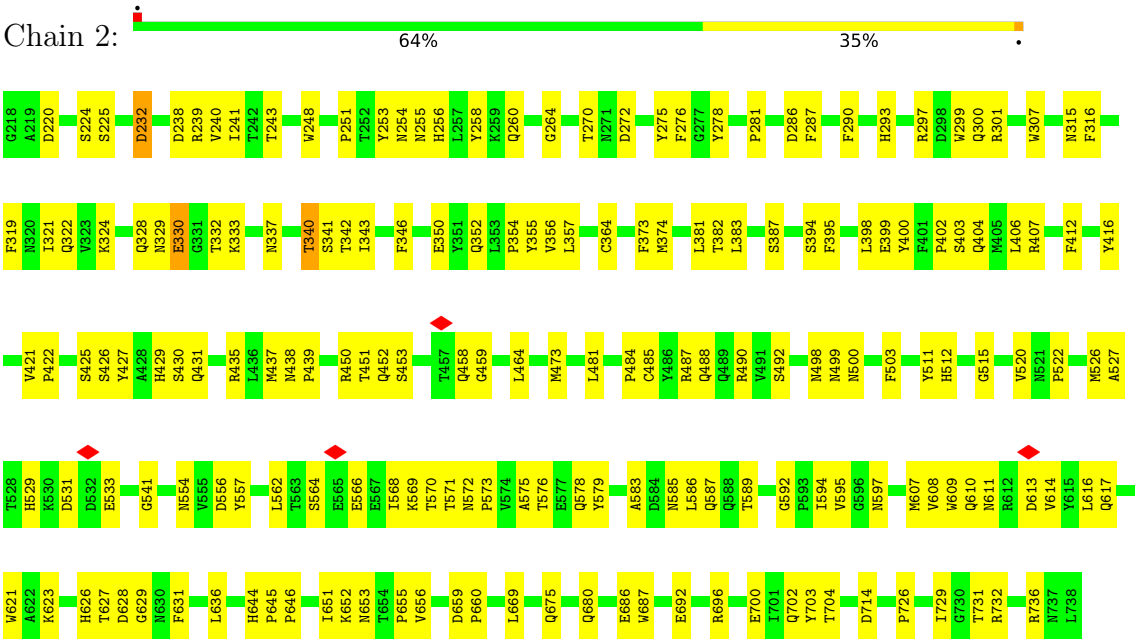

• Molecule 1: Capsid protein VP1

Chain 1:



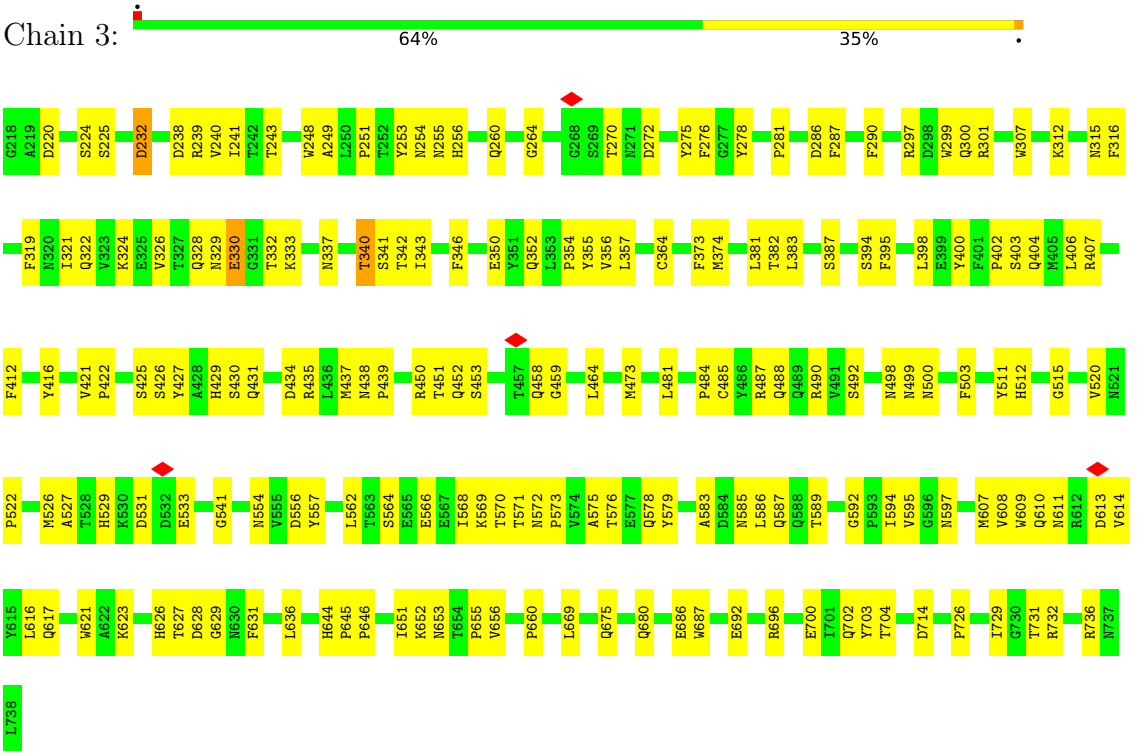
• Molecule 1: Capsid protein VP1

Chain 2:



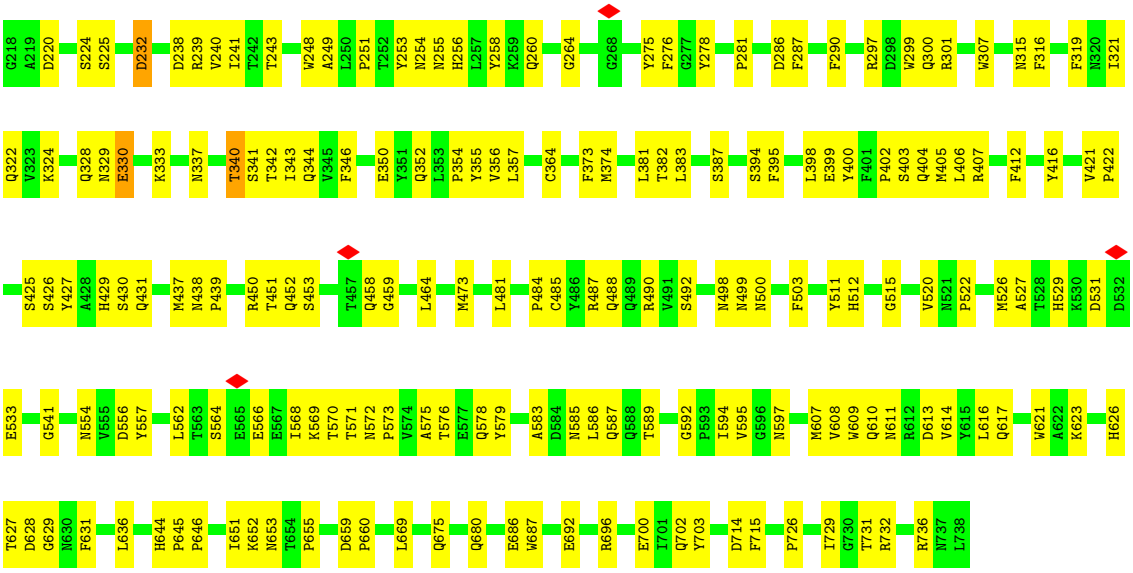

• Molecule 1: Capsid protein VP1

Chain 3:



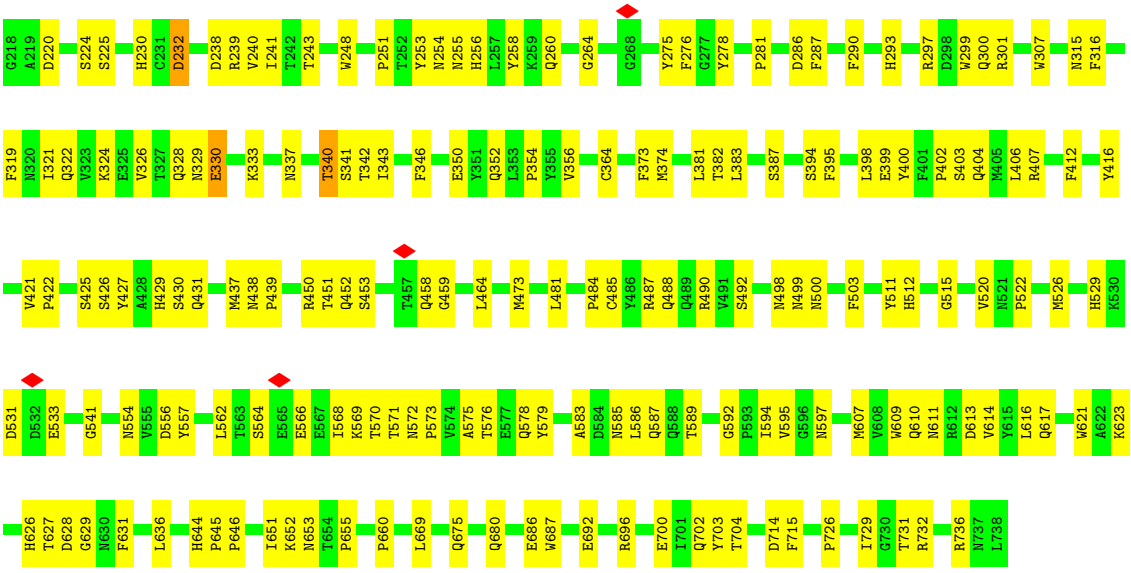

• Molecule 1: Capsid protein VP1

Chain 4:



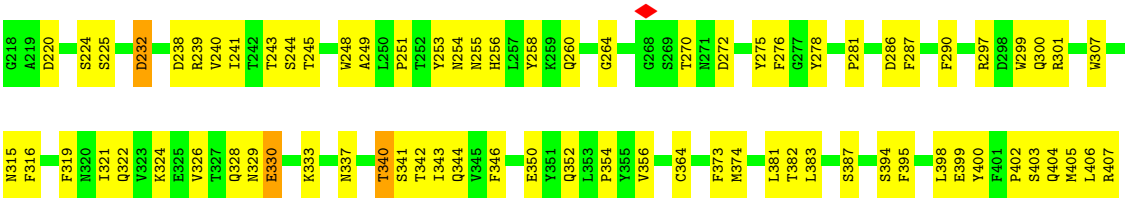
• Molecule 1: Capsid protein VP1

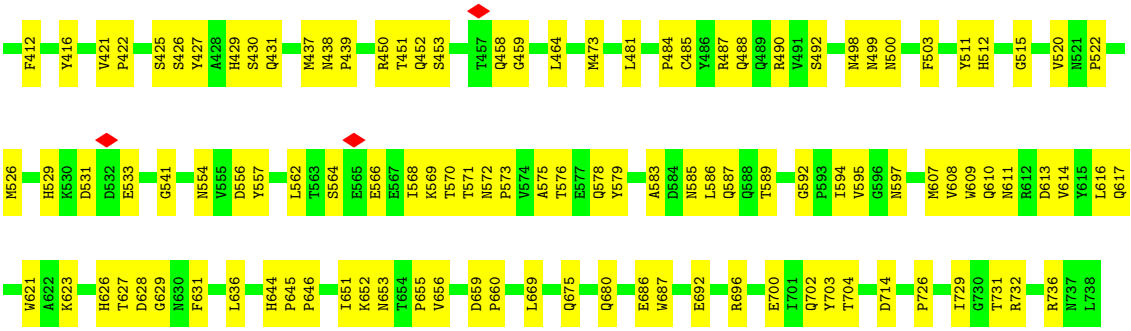
Chain 5:



• Molecule 1: Capsid protein VP1

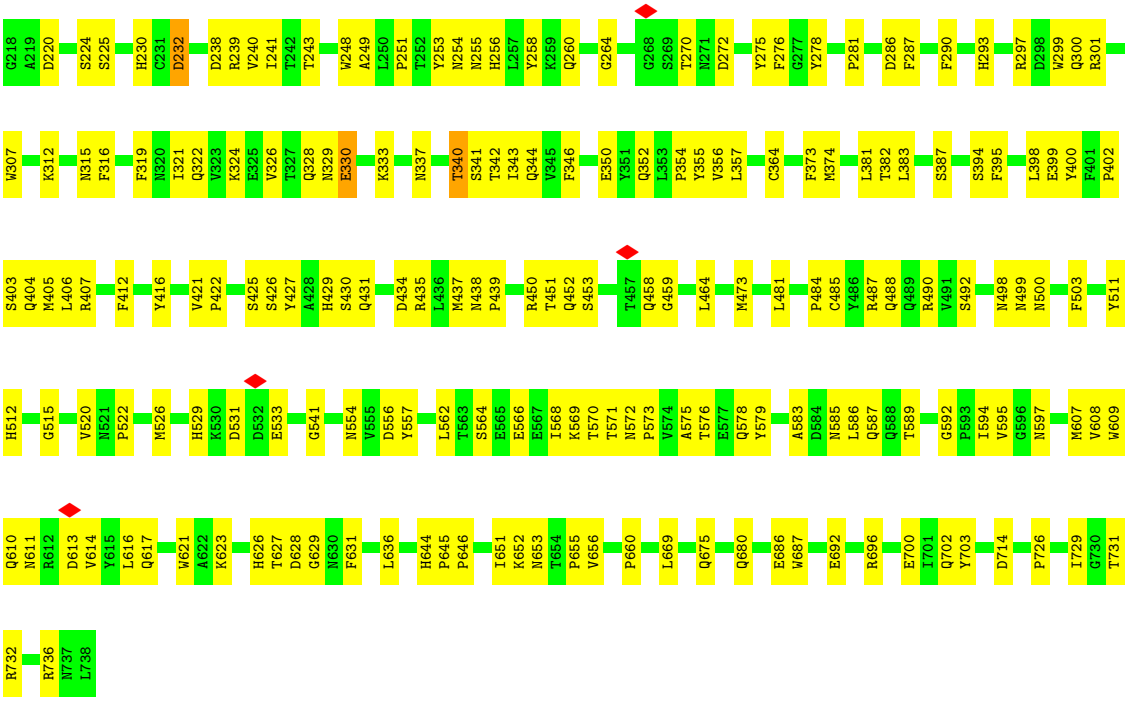
Chain 6:





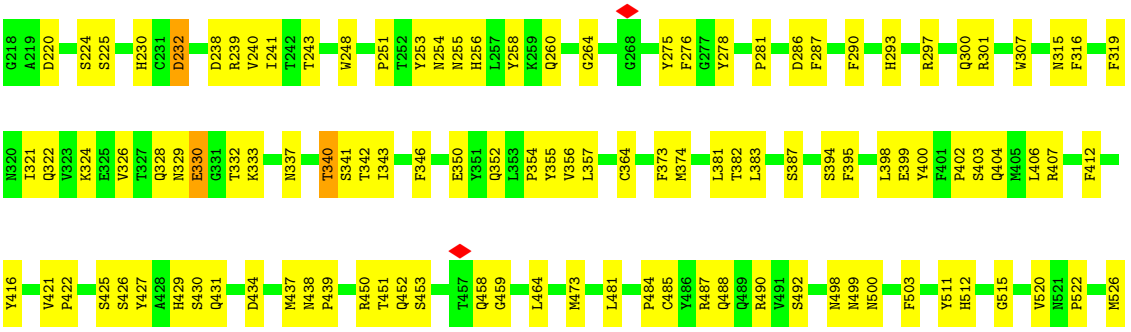
• Molecule 1: Capsid protein VP1

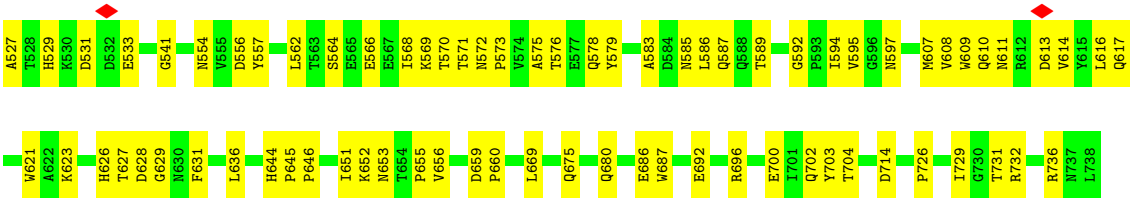
Chain 7:



• Molecule 1: Capsid protein VP1

Chain 8:




A527 T528 H529 K530 D531 D532 E533 G541 N554 V555 D556 Y557 L562 T563 S564 E565 E566 E567 I568 K569 T570 T571 N572 P573 V574 A575 T576 E577 Q578 Y579 A583 D584 N585 L586 Q587 Q588 T589 G592 P593 I594 V595 G596 N597 M607 V608 W609 Q610 N611 R612 D613 V614 Y615 L616 Q617
W621 A622 K623 H626 T627 D628 G629 N630 F631 L636 H644 P645 P646 I651 K652 N653 T654 P655 V656 D659 P660 L669 Q675 Q680 E686 W687 E692 R696 E700 I701 Q702 Y703 T704 D714 P726 I729 G730 T731 R732 R736 N737 L738

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of particles used | 52912 | 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 ($e^-/Å^2$) | 67 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | DIRECT ELECTRON DE-20 (5k x 3k) | Depositor |
| Maximum map value | 18.937 | Depositor |
| Minimum map value | -11.750 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 1 | Depositor |
| Map size (Å) | 384.237, 384.237, 384.237 | wwPDB |
| Map dimensions | 399, 399, 399 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.963, 0.963, 0.963 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 | 1 | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | 2 | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | 3 | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | 4 | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | 5 | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | 6 | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | 7 | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | 8 | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | A | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | B | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | C | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | D | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | E | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | F | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | G | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | H | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | I | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | J | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | K | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | L | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | M | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | N | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | O | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | P | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | Q | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | R | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | S | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | T | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | U | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | V | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | W | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | X | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | Y | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | Z | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | a | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | b | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | c | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | d | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | e | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | f | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | g | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | h | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | i | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | j | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | k | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | l | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | m | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | n | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | o | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | p | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | q | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | r | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | s | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | t | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | u | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | v | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | w | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | x | 0.47 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | y | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| 1 | z | 0.46 | 0/4261 | 0.56 | 3/5810 (0.1%) |
| All | All | 0.47 | 0/255660 | 0.56 | 180/348600 (0.1%) |

There are no bond length outliers.

All (180) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | v | 232 | ASP | N-CA-C | 5.54 | 118.48 | 110.28 |
| 1 | C | 232 | ASP | N-CA-C | 5.54 | 118.47 | 110.28 |
| 1 | L | 232 | ASP | N-CA-C | 5.54 | 118.47 | 110.28 |
| 1 | N | 232 | ASP | N-CA-C | 5.53 | 118.47 | 110.28 |
| 1 | P | 232 | ASP | N-CA-C | 5.53 | 118.47 | 110.28 |
| 1 | k | 232 | ASP | N-CA-C | 5.53 | 118.47 | 110.28 |
| 1 | J | 232 | ASP | N-CA-C | 5.53 | 118.46 | 110.28 |
| 1 | M | 232 | ASP | N-CA-C | 5.53 | 118.46 | 110.28 |
| 1 | W | 232 | ASP | N-CA-C | 5.53 | 118.46 | 110.28 |
| 1 | f | 232 | ASP | N-CA-C | 5.53 | 118.46 | 110.28 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 3 | 232 | ASP | N-CA-C | 5.53 | 118.46 | 110.28 |
| 1 | D | 232 | ASP | N-CA-C | 5.53 | 118.46 | 110.28 |
| 1 | X | 232 | ASP | N-CA-C | 5.53 | 118.46 | 110.28 |
| 1 | a | 232 | ASP | N-CA-C | 5.53 | 118.46 | 110.28 |
| 1 | j | 232 | ASP | N-CA-C | 5.52 | 118.45 | 110.28 |
| 1 | I | 232 | ASP | N-CA-C | 5.52 | 118.45 | 110.28 |
| 1 | c | 232 | ASP | N-CA-C | 5.52 | 118.45 | 110.28 |
| 1 | h | 232 | ASP | N-CA-C | 5.52 | 118.45 | 110.28 |
| 1 | n | 232 | ASP | N-CA-C | 5.52 | 118.45 | 110.28 |
| 1 | s | 232 | ASP | N-CA-C | 5.52 | 118.45 | 110.28 |
| 1 | A | 232 | ASP | N-CA-C | 5.52 | 118.44 | 110.28 |
| 1 | G | 232 | ASP | N-CA-C | 5.52 | 118.44 | 110.28 |
| 1 | d | 232 | ASP | N-CA-C | 5.52 | 118.44 | 110.28 |
| 1 | p | 232 | ASP | N-CA-C | 5.52 | 118.44 | 110.28 |
| 1 | z | 232 | ASP | N-CA-C | 5.52 | 118.44 | 110.28 |
| 1 | 1 | 232 | ASP | N-CA-C | 5.52 | 118.44 | 110.28 |
| 1 | 2 | 232 | ASP | N-CA-C | 5.52 | 118.44 | 110.28 |
| 1 | B | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | Q | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | R | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | b | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | g | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | i | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | m | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | 5 | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | F | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | S | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | Y | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | Z | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | r | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | t | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | 6 | 232 | ASP | N-CA-C | 5.51 | 118.44 | 110.28 |
| 1 | K | 232 | ASP | N-CA-C | 5.51 | 118.43 | 110.28 |
| 1 | T | 232 | ASP | N-CA-C | 5.51 | 118.43 | 110.28 |
| 1 | V | 232 | ASP | N-CA-C | 5.51 | 118.43 | 110.28 |
| 1 | e | 232 | ASP | N-CA-C | 5.51 | 118.43 | 110.28 |
| 1 | l | 232 | ASP | N-CA-C | 5.51 | 118.43 | 110.28 |
| 1 | o | 232 | ASP | N-CA-C | 5.51 | 118.43 | 110.28 |
| 1 | 8 | 232 | ASP | N-CA-C | 5.51 | 118.43 | 110.28 |
| 1 | w | 232 | ASP | N-CA-C | 5.50 | 118.42 | 110.28 |
| 1 | H | 232 | ASP | N-CA-C | 5.50 | 118.42 | 110.28 |
| 1 | x | 232 | ASP | N-CA-C | 5.50 | 118.42 | 110.28 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 4 | 232 | ASP | N-CA-C | 5.50 | 118.42 | 110.28 |
| 1 | U | 232 | ASP | N-CA-C | 5.50 | 118.42 | 110.28 |
| 1 | 7 | 232 | ASP | N-CA-C | 5.50 | 118.42 | 110.28 |
| 1 | u | 232 | ASP | N-CA-C | 5.50 | 118.42 | 110.28 |
| 1 | y | 232 | ASP | N-CA-C | 5.50 | 118.41 | 110.28 |
| 1 | O | 232 | ASP | N-CA-C | 5.49 | 118.41 | 110.28 |
| 1 | q | 232 | ASP | N-CA-C | 5.49 | 118.41 | 110.28 |
| 1 | E | 232 | ASP | N-CA-C | 5.49 | 118.40 | 110.28 |
| 1 | Q | 340 | THR | N-CA-C | 5.40 | 117.17 | 111.28 |
| 1 | R | 340 | THR | N-CA-C | 5.40 | 117.17 | 111.28 |
| 1 | v | 340 | THR | N-CA-C | 5.39 | 117.16 | 111.28 |
| 1 | k | 340 | THR | N-CA-C | 5.39 | 117.15 | 111.28 |
| 1 | O | 340 | THR | N-CA-C | 5.38 | 117.15 | 111.28 |
| 1 | W | 340 | THR | N-CA-C | 5.38 | 117.15 | 111.28 |
| 1 | 3 | 340 | THR | N-CA-C | 5.38 | 117.15 | 111.28 |
| 1 | E | 340 | THR | N-CA-C | 5.38 | 117.15 | 111.28 |
| 1 | F | 340 | THR | N-CA-C | 5.38 | 117.15 | 111.28 |
| 1 | S | 340 | THR | N-CA-C | 5.38 | 117.15 | 111.28 |
| 1 | u | 340 | THR | N-CA-C | 5.38 | 117.15 | 111.28 |
| 1 | 6 | 340 | THR | N-CA-C | 5.38 | 117.15 | 111.28 |
| 1 | D | 340 | THR | N-CA-C | 5.38 | 117.14 | 111.28 |
| 1 | K | 340 | THR | N-CA-C | 5.38 | 117.14 | 111.28 |
| 1 | e | 340 | THR | N-CA-C | 5.38 | 117.14 | 111.28 |
| 1 | l | 340 | THR | N-CA-C | 5.38 | 117.14 | 111.28 |
| 1 | P | 340 | THR | N-CA-C | 5.38 | 117.14 | 111.28 |
| 1 | 5 | 340 | THR | N-CA-C | 5.38 | 117.14 | 111.28 |
| 1 | B | 340 | THR | N-CA-C | 5.37 | 117.13 | 111.28 |
| 1 | H | 340 | THR | N-CA-C | 5.37 | 117.13 | 111.28 |
| 1 | b | 340 | THR | N-CA-C | 5.37 | 117.13 | 111.28 |
| 1 | g | 340 | THR | N-CA-C | 5.37 | 117.13 | 111.28 |
| 1 | i | 340 | THR | N-CA-C | 5.37 | 117.13 | 111.28 |
| 1 | x | 340 | THR | N-CA-C | 5.37 | 117.13 | 111.28 |
| 1 | 4 | 340 | THR | N-CA-C | 5.37 | 117.13 | 111.28 |
| 1 | A | 340 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 1 | j | 340 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 1 | G | 340 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 1 | I | 340 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 1 | c | 340 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 1 | d | 340 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 1 | p | 340 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 1 | 2 | 340 | THR | N-CA-C | 5.36 | 117.12 | 111.28 |
| 1 | n | 340 | THR | N-CA-C | 5.35 | 117.12 | 111.28 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | s | 340 | THR | N-CA-C | 5.35 | 117.12 | 111.28 |
| 1 | U | 340 | THR | N-CA-C | 5.35 | 117.11 | 111.28 |
| 1 | X | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | Y | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | Z | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | a | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | J | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | M | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | f | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | 7 | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | q | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | w | 340 | THR | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | V | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | 8 | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | T | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | o | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | z | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | 1 | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | C | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | L | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | h | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | m | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | r | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | t | 340 | THR | N-CA-C | 5.33 | 117.09 | 111.28 |
| 1 | N | 340 | THR | N-CA-C | 5.33 | 117.08 | 111.28 |
| 1 | y | 340 | THR | N-CA-C | 5.32 | 117.08 | 111.28 |
| 1 | J | 330 | GLU | CB-CA-C | -5.24 | 110.55 | 116.63 |
| 1 | M | 330 | GLU | CB-CA-C | -5.24 | 110.55 | 116.63 |
| 1 | W | 330 | GLU | CB-CA-C | -5.22 | 110.57 | 116.63 |
| 1 | y | 330 | GLU | CB-CA-C | -5.22 | 110.58 | 116.63 |
| 1 | 3 | 330 | GLU | CB-CA-C | -5.22 | 110.58 | 116.63 |
| 1 | K | 330 | GLU | CB-CA-C | -5.22 | 110.58 | 116.63 |
| 1 | e | 330 | GLU | CB-CA-C | -5.22 | 110.58 | 116.63 |
| 1 | E | 330 | GLU | CB-CA-C | -5.21 | 110.58 | 116.63 |
| 1 | U | 330 | GLU | CB-CA-C | -5.21 | 110.58 | 116.63 |
| 1 | 7 | 330 | GLU | CB-CA-C | -5.21 | 110.58 | 116.63 |
| 1 | b | 330 | GLU | CB-CA-C | -5.21 | 110.59 | 116.63 |
| 1 | i | 330 | GLU | CB-CA-C | -5.21 | 110.59 | 116.63 |
| 1 | q | 330 | GLU | CB-CA-C | -5.21 | 110.59 | 116.63 |
| 1 | B | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | F | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | S | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | g | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | u | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | 6 | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | w | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | T | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | 1 | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | D | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | k | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | m | 330 | GLU | CB-CA-C | -5.20 | 110.60 | 116.63 |
| 1 | X | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | a | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | O | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | f | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | j | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | A | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | G | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | I | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | c | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | d | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | o | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | p | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | z | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | 2 | 330 | GLU | CB-CA-C | -5.19 | 110.61 | 116.63 |
| 1 | P | 330 | GLU | CB-CA-C | -5.18 | 110.61 | 116.63 |
| 1 | Q | 330 | GLU | CB-CA-C | -5.18 | 110.62 | 116.63 |
| 1 | R | 330 | GLU | CB-CA-C | -5.18 | 110.62 | 116.63 |
| 1 | t | 330 | GLU | CB-CA-C | -5.18 | 110.62 | 116.63 |
| 1 | 5 | 330 | GLU | CB-CA-C | -5.18 | 110.62 | 116.63 |
| 1 | x | 330 | GLU | CB-CA-C | -5.18 | 110.62 | 116.63 |
| 1 | H | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | N | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | n | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | s | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | 4 | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | L | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | Y | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | Z | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | h | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | r | 330 | GLU | CB-CA-C | -5.17 | 110.63 | 116.63 |
| 1 | l | 330 | GLU | CB-CA-C | -5.16 | 110.64 | 116.63 |
| 1 | v | 330 | GLU | CB-CA-C | -5.16 | 110.64 | 116.63 |
| 1 | C | 330 | GLU | CB-CA-C | -5.16 | 110.65 | 116.63 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | V | 330 | GLU | CB-CA-C | -5.15 | 110.66 | 116.63 |
| 1 | 8 | 330 | GLU | CB-CA-C | -5.15 | 110.66 | 116.63 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | 1 | 4138 | 0 | 3900 | 220 | 0 |
| 1 | 2 | 4138 | 0 | 3900 | 215 | 0 |
| 1 | 3 | 4138 | 0 | 3900 | 220 | 0 |
| 1 | 4 | 4138 | 0 | 3900 | 215 | 0 |
| 1 | 5 | 4138 | 0 | 3900 | 213 | 0 |
| 1 | 6 | 4138 | 0 | 3900 | 214 | 0 |
| 1 | 7 | 4138 | 0 | 3900 | 217 | 0 |
| 1 | 8 | 4138 | 0 | 3900 | 218 | 0 |
| 1 | A | 4138 | 0 | 3900 | 224 | 0 |
| 1 | B | 4138 | 0 | 3900 | 212 | 0 |
| 1 | C | 4138 | 0 | 3900 | 214 | 0 |
| 1 | D | 4138 | 0 | 3900 | 217 | 0 |
| 1 | E | 4138 | 0 | 3900 | 220 | 0 |
| 1 | F | 4138 | 0 | 3900 | 216 | 0 |
| 1 | G | 4138 | 0 | 3900 | 219 | 0 |
| 1 | H | 4138 | 0 | 3900 | 217 | 0 |
| 1 | I | 4138 | 0 | 3900 | 215 | 0 |
| 1 | J | 4138 | 0 | 3900 | 213 | 0 |
| 1 | K | 4138 | 0 | 3900 | 216 | 0 |
| 1 | L | 4138 | 0 | 3900 | 217 | 0 |
| 1 | M | 4138 | 0 | 3900 | 214 | 0 |
| 1 | N | 4138 | 0 | 3900 | 212 | 0 |
| 1 | O | 4138 | 0 | 3900 | 220 | 0 |
| 1 | P | 4138 | 0 | 3900 | 217 | 0 |
| 1 | Q | 4138 | 0 | 3900 | 216 | 0 |
| 1 | R | 4138 | 0 | 3900 | 219 | 0 |
| 1 | S | 4138 | 0 | 3900 | 222 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | T | 4138 | 0 | 3900 | 220 | 0 |
| 1 | U | 4138 | 0 | 3900 | 217 | 0 |
| 1 | V | 4138 | 0 | 3900 | 219 | 0 |
| 1 | W | 4138 | 0 | 3900 | 220 | 0 |
| 1 | X | 4138 | 0 | 3900 | 218 | 0 |
| 1 | Y | 4138 | 0 | 3900 | 217 | 0 |
| 1 | Z | 4138 | 0 | 3900 | 215 | 0 |
| 1 | a | 4138 | 0 | 3900 | 214 | 0 |
| 1 | b | 4138 | 0 | 3900 | 212 | 0 |
| 1 | c | 4138 | 0 | 3900 | 217 | 0 |
| 1 | d | 4138 | 0 | 3900 | 215 | 0 |
| 1 | e | 4138 | 0 | 3900 | 217 | 0 |
| 1 | f | 4138 | 0 | 3900 | 218 | 0 |
| 1 | g | 4138 | 0 | 3900 | 218 | 0 |
| 1 | h | 4138 | 0 | 3900 | 218 | 0 |
| 1 | i | 4138 | 0 | 3900 | 217 | 0 |
| 1 | j | 4138 | 0 | 3900 | 217 | 0 |
| 1 | k | 4138 | 0 | 3900 | 220 | 0 |
| 1 | l | 4138 | 0 | 3900 | 223 | 0 |
| 1 | m | 4138 | 0 | 3900 | 214 | 0 |
| 1 | n | 4138 | 0 | 3900 | 215 | 0 |
| 1 | o | 4138 | 0 | 3900 | 222 | 0 |
| 1 | p | 4138 | 0 | 3900 | 220 | 0 |
| 1 | q | 4138 | 0 | 3900 | 220 | 0 |
| 1 | r | 4138 | 0 | 3900 | 217 | 0 |
| 1 | s | 4138 | 0 | 3900 | 217 | 0 |
| 1 | t | 4138 | 0 | 3900 | 214 | 0 |
| 1 | u | 4138 | 0 | 3900 | 219 | 0 |
| 1 | v | 4138 | 0 | 3900 | 214 | 0 |
| 1 | w | 4138 | 0 | 3900 | 227 | 0 |
| 1 | x | 4138 | 0 | 3900 | 223 | 0 |
| 1 | y | 4138 | 0 | 3900 | 222 | 0 |
| 1 | z | 4138 | 0 | 3900 | 222 | 0 |
| All | All | 248280 | 0 | 234000 | 10820 | 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 22.

All (10820) 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:G:613:ASP:HB3 | 1:G:732:ARG:HD2 | 1.28 | 1.16 |
| 1:p:613:ASP:HB3 | 1:p:732:ARG:HD2 | 1.28 | 1.16 |
| 1:h:613:ASP:HB3 | 1:h:732:ARG:HD2 | 1.28 | 1.16 |
| 1:k:613:ASP:HB3 | 1:k:732:ARG:HD2 | 1.28 | 1.16 |
| 1:I:613:ASP:HB3 | 1:I:732:ARG:HD2 | 1.28 | 1.15 |
| 1:c:613:ASP:HB3 | 1:c:732:ARG:HD2 | 1.28 | 1.15 |
| 1:r:613:ASP:HB3 | 1:r:732:ARG:HD2 | 1.28 | 1.14 |
| 1:w:613:ASP:HB3 | 1:w:732:ARG:HD2 | 1.28 | 1.14 |
| 1:s:613:ASP:HB2 | 1:s:731:THR:HG22 | 1.30 | 1.14 |
| 1:H:613:ASP:HB2 | 1:H:731:THR:HG22 | 1.30 | 1.14 |
| 1:Y:613:ASP:HB3 | 1:Y:732:ARG:HD2 | 1.28 | 1.14 |
| 1:t:613:ASP:HB2 | 1:t:731:THR:HG22 | 1.30 | 1.14 |
| 1:R:613:ASP:HB2 | 1:R:731:THR:HG22 | 1.30 | 1.14 |
| 1:e:613:ASP:HB3 | 1:e:732:ARG:HD2 | 1.28 | 1.14 |
| 1:J:613:ASP:HB2 | 1:J:731:THR:HG22 | 1.30 | 1.14 |
| 1:M:613:ASP:HB2 | 1:M:731:THR:HG22 | 1.30 | 1.14 |
| 1:U:613:ASP:HB3 | 1:U:732:ARG:HD2 | 1.28 | 1.13 |
| 1:o:613:ASP:HB3 | 1:o:732:ARG:HD2 | 1.28 | 1.13 |
| 1:D:613:ASP:HB2 | 1:D:731:THR:HG22 | 1.30 | 1.13 |
| 1:v:613:ASP:HB3 | 1:v:732:ARG:HD2 | 1.28 | 1.13 |
| 1:A:613:ASP:HB3 | 1:A:732:ARG:HD2 | 1.28 | 1.13 |
| 1:E:613:ASP:HB2 | 1:E:731:THR:HG22 | 1.30 | 1.13 |
| 1:Q:613:ASP:HB2 | 1:Q:731:THR:HG22 | 1.30 | 1.13 |
| 1:z:613:ASP:HB2 | 1:z:731:THR:HG22 | 1.30 | 1.13 |
| 1:5:613:ASP:HB2 | 1:5:731:THR:HG22 | 1.30 | 1.13 |
| 1:7:613:ASP:HB2 | 1:7:731:THR:HG22 | 1.30 | 1.13 |
| 1:K:613:ASP:HB2 | 1:K:731:THR:HG22 | 1.30 | 1.13 |
| 1:L:613:ASP:HB2 | 1:L:731:THR:HG22 | 1.30 | 1.13 |
| 1:N:613:ASP:HB3 | 1:N:732:ARG:HD2 | 1.28 | 1.13 |
| 1:R:613:ASP:HB3 | 1:R:732:ARG:HD2 | 1.28 | 1.13 |
| 1:S:613:ASP:HB3 | 1:S:732:ARG:HD2 | 1.28 | 1.13 |
| 1:Z:613:ASP:HB2 | 1:Z:731:THR:HG22 | 1.30 | 1.13 |
| 1:m:613:ASP:HB3 | 1:m:732:ARG:HD2 | 1.28 | 1.13 |
| 1:m:613:ASP:HB2 | 1:m:731:THR:HG22 | 1.30 | 1.13 |
| 1:u:613:ASP:HB3 | 1:u:732:ARG:HD2 | 1.28 | 1.13 |
| 1:2:613:ASP:HB2 | 1:2:731:THR:HG22 | 1.30 | 1.13 |
| 1:C:613:ASP:HB2 | 1:C:731:THR:HG22 | 1.30 | 1.12 |
| 1:w:609:TRP:NE1 | 1:x:629:GLY:HA3 | 1.62 | 1.13 |
| 1:l:613:ASP:HB2 | 1:l:731:THR:HG22 | 1.30 | 1.12 |
| 1:M:613:ASP:HB3 | 1:M:732:ARG:HD2 | 1.28 | 1.12 |
| 1:O:613:ASP:HB3 | 1:O:732:ARG:HD2 | 1.28 | 1.12 |
| 1:Z:613:ASP:HB3 | 1:Z:732:ARG:HD2 | 1.28 | 1.12 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:613:ASP:HB3 | 1:b:732:ARG:HD2 | 1.28 | 1.12 |
| 1:d:613:ASP:HB2 | 1:d:731:THR:HG22 | 1.30 | 1.12 |
| 1:t:613:ASP:HB3 | 1:t:732:ARG:HD2 | 1.28 | 1.12 |
| 1:x:613:ASP:HB2 | 1:x:731:THR:HG22 | 1.30 | 1.12 |
| 1:B:613:ASP:HB3 | 1:B:732:ARG:HD2 | 1.28 | 1.12 |
| 1:J:613:ASP:HB3 | 1:J:732:ARG:HD2 | 1.28 | 1.12 |
| 1:a:613:ASP:HB3 | 1:a:732:ARG:HD2 | 1.28 | 1.12 |
| 1:3:613:ASP:HB3 | 1:3:732:ARG:HD2 | 1.28 | 1.12 |
| 1:U:613:ASP:HB2 | 1:U:731:THR:HG22 | 1.30 | 1.12 |
| 1:k:613:ASP:HB2 | 1:k:731:THR:HG22 | 1.30 | 1.12 |
| 1:u:613:ASP:HB2 | 1:u:731:THR:HG22 | 1.30 | 1.12 |
| 1:v:613:ASP:HB2 | 1:v:731:THR:HG22 | 1.30 | 1.12 |
| 1:N:613:ASP:HB2 | 1:N:731:THR:HG22 | 1.30 | 1.12 |
| 1:S:613:ASP:HB2 | 1:S:731:THR:HG22 | 1.30 | 1.12 |
| 1:X:613:ASP:HB2 | 1:X:731:THR:HG22 | 1.30 | 1.12 |
| 1:x:609:TRP:NE1 | 1:y:629:GLY:HA3 | 1.65 | 1.12 |
| 1:N:609:TRP:NE1 | 1:P:629:GLY:HA3 | 1.66 | 1.11 |
| 1:W:613:ASP:HB2 | 1:W:731:THR:HG22 | 1.30 | 1.11 |
| 1:a:609:TRP:NE1 | 1:8:629:GLY:HA3 | 1.66 | 1.11 |
| 1:h:613:ASP:HB2 | 1:h:731:THR:HG22 | 1.30 | 1.11 |
| 1:q:613:ASP:HB2 | 1:q:731:THR:HG22 | 1.30 | 1.11 |
| 1:a:613:ASP:HB2 | 1:a:731:THR:HG22 | 1.30 | 1.11 |
| 1:A:609:TRP:NE1 | 1:G:629:GLY:HA3 | 1.66 | 1.11 |
| 1:V:629:GLY:HA3 | 1:X:609:TRP:NE1 | 1.66 | 1.11 |
| 1:g:613:ASP:HB2 | 1:g:731:THR:HG22 | 1.30 | 1.11 |
| 1:E:629:GLY:HA3 | 1:F:609:TRP:NE1 | 1.66 | 1.11 |
| 1:H:629:GLY:HA3 | 1:Y:609:TRP:NE1 | 1.66 | 1.11 |
| 1:K:609:TRP:NE1 | 1:a:629:GLY:HA3 | 1.66 | 1.11 |
| 1:V:609:TRP:NE1 | 1:e:629:GLY:HA3 | 1.65 | 1.11 |
| 1:V:613:ASP:HB3 | 1:V:732:ARG:HD2 | 1.28 | 1.11 |
| 1:f:613:ASP:HB3 | 1:f:732:ARG:HD2 | 1.28 | 1.11 |
| 1:r:609:TRP:NE1 | 1:s:629:GLY:HA3 | 1.66 | 1.11 |
| 1:y:613:ASP:HB3 | 1:y:732:ARG:HD2 | 1.28 | 1.11 |
| 1:2:613:ASP:HB3 | 1:2:732:ARG:HD2 | 1.28 | 1.11 |
| 1:6:609:TRP:NE1 | 1:7:629:GLY:HA3 | 1.66 | 1.11 |
| 1:D:609:TRP:NE1 | 1:N:629:GLY:HA3 | 1.66 | 1.11 |
| 1:D:613:ASP:HB3 | 1:D:732:ARG:HD2 | 1.28 | 1.11 |
| 1:c:609:TRP:NE1 | 1:o:629:GLY:HA3 | 1.66 | 1.11 |
| 1:d:613:ASP:HB3 | 1:d:732:ARG:HD2 | 1.28 | 1.11 |
| 1:i:613:ASP:HB2 | 1:i:731:THR:HG22 | 1.30 | 1.11 |
| 1:j:609:TRP:NE1 | 1:k:629:GLY:HA3 | 1.66 | 1.11 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:613:ASP:HB3 | 1:j:732:ARG:HD2 | 1.28 | 1.11 |
| 1:o:609:TRP:NE1 | 1:p:629:GLY:HA3 | 1.66 | 1.11 |
| 1:4:613:ASP:HB2 | 1:4:731:THR:HG22 | 1.30 | 1.11 |
| 1:A:629:GLY:HA3 | 1:I:609:TRP:NE1 | 1.66 | 1.10 |
| 1:C:629:GLY:HA3 | 1:M:609:TRP:NE1 | 1.66 | 1.10 |
| 1:J:609:TRP:NE1 | 1:L:629:GLY:HA3 | 1.66 | 1.10 |
| 1:T:629:GLY:HA3 | 1:l:609:TRP:NE1 | 1.66 | 1.10 |
| 1:f:340:THR:CA | 1:f:407:ARG:HH21 | 1.65 | 1.10 |
| 1:f:609:TRP:NE1 | 1:h:629:GLY:HA3 | 1.66 | 1.10 |
| 1:j:340:THR:CA | 1:j:407:ARG:HH21 | 1.64 | 1.10 |
| 1:l:340:THR:CA | 1:l:407:ARG:HH21 | 1.64 | 1.10 |
| 1:z:340:THR:CA | 1:z:407:ARG:HH21 | 1.64 | 1.10 |
| 1:z:609:TRP:NE1 | 1:1:629:GLY:HA3 | 1.66 | 1.10 |
| 1:B:629:GLY:HA3 | 1:L:609:TRP:NE1 | 1.66 | 1.10 |
| 1:G:609:TRP:NE1 | 1:I:629:GLY:HA3 | 1.66 | 1.10 |
| 1:R:629:GLY:HA3 | 1:U:609:TRP:NE1 | 1.66 | 1.10 |
| 1:W:340:THR:CA | 1:W:407:ARG:HH21 | 1.64 | 1.10 |
| 1:q:340:THR:CA | 1:q:407:ARG:HH21 | 1.64 | 1.10 |
| 1:x:613:ASP:HB3 | 1:x:732:ARG:HD2 | 1.28 | 1.10 |
| 1:1:613:ASP:HB2 | 1:1:731:THR:HG22 | 1.30 | 1.10 |
| 1:C:609:TRP:NE1 | 1:b:629:GLY:HA3 | 1.66 | 1.10 |
| 1:K:613:ASP:HB3 | 1:K:732:ARG:HD2 | 1.28 | 1.10 |
| 1:O:629:GLY:HA3 | 1:n:609:TRP:NE1 | 1.66 | 1.10 |
| 1:T:613:ASP:HB2 | 1:T:731:THR:HG22 | 1.30 | 1.10 |
| 1:c:629:GLY:HA3 | 1:p:609:TRP:NE1 | 1.66 | 1.10 |
| 1:f:613:ASP:HB2 | 1:f:731:THR:HG22 | 1.30 | 1.10 |
| 1:j:613:ASP:HB2 | 1:j:731:THR:HG22 | 1.30 | 1.10 |
| 1:t:629:GLY:HA3 | 1:v:609:TRP:NE1 | 1.66 | 1.10 |
| 1:X:613:ASP:HB3 | 1:X:732:ARG:HD2 | 1.28 | 1.10 |
| 1:l:613:ASP:HB3 | 1:l:732:ARG:HD2 | 1.28 | 1.10 |
| 1:n:613:ASP:HB2 | 1:n:731:THR:HG22 | 1.30 | 1.10 |
| 1:3:629:GLY:HA3 | 1:4:609:TRP:NE1 | 1.66 | 1.10 |
| 1:F:629:GLY:HA3 | 1:Q:609:TRP:NE1 | 1.66 | 1.10 |
| 1:I:340:THR:CA | 1:I:407:ARG:HH21 | 1.65 | 1.10 |
| 1:V:340:THR:CA | 1:V:407:ARG:HH21 | 1.64 | 1.10 |
| 1:W:609:TRP:NE1 | 1:Y:629:GLY:HA3 | 1.66 | 1.10 |
| 1:c:340:THR:CA | 1:c:407:ARG:HH21 | 1.65 | 1.10 |
| 1:e:340:THR:CA | 1:e:407:ARG:HH21 | 1.64 | 1.10 |
| 1:n:613:ASP:HB3 | 1:n:732:ARG:HD2 | 1.28 | 1.10 |
| 1:q:609:TRP:NE1 | 1:r:629:GLY:HA3 | 1.66 | 1.10 |
| 1:z:613:ASP:HB3 | 1:z:732:ARG:HD2 | 1.28 | 1.10 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:340:THR:CA | 1:5:407:ARG:HH21 | 1.65 | 1.10 |
| 1:5:609:TRP:NE1 | 1:6:629:GLY:HA3 | 1.66 | 1.10 |
| 1:Q:340:THR:CA | 1:Q:407:ARG:HH21 | 1.65 | 1.09 |
| 1:X:340:THR:CA | 1:X:407:ARG:HH21 | 1.64 | 1.09 |
| 1:g:613:ASP:HB3 | 1:g:732:ARG:HD2 | 1.28 | 1.09 |
| 1:g:629:GLY:HA3 | 1:h:609:TRP:NE1 | 1.66 | 1.09 |
| 1:i:609:TRP:NE1 | 1:j:629:GLY:HA3 | 1.67 | 1.09 |
| 1:o:613:ASP:HB2 | 1:o:731:THR:HG22 | 1.30 | 1.09 |
| 1:r:340:THR:CA | 1:r:407:ARG:HH21 | 1.64 | 1.09 |
| 1:w:340:THR:CA | 1:w:407:ARG:HH21 | 1.64 | 1.09 |
| 1:x:340:THR:CA | 1:x:407:ARG:HH21 | 1.65 | 1.09 |
| 1:y:340:THR:CA | 1:y:407:ARG:HH21 | 1.64 | 1.09 |
| 1:1:340:THR:CA | 1:1:407:ARG:HH21 | 1.64 | 1.09 |
| 1:4:340:THR:CA | 1:4:407:ARG:HH21 | 1.65 | 1.09 |
| 1:6:613:ASP:HB2 | 1:6:731:THR:HG22 | 1.30 | 1.09 |
| 1:A:613:ASP:HB2 | 1:A:731:THR:HG22 | 1.30 | 1.09 |
| 1:F:613:ASP:HB2 | 1:F:731:THR:HG22 | 1.30 | 1.09 |
| 1:T:340:THR:CA | 1:T:407:ARG:HH21 | 1.64 | 1.09 |
| 1:Y:340:THR:CA | 1:Y:407:ARG:HH21 | 1.64 | 1.09 |
| 1:f:629:GLY:HA3 | 1:g:609:TRP:NE1 | 1.67 | 1.09 |
| 1:i:613:ASP:HB3 | 1:i:732:ARG:HD2 | 1.28 | 1.09 |
| 1:i:629:GLY:HA3 | 1:k:609:TRP:NE1 | 1.66 | 1.09 |
| 1:n:340:THR:CA | 1:n:407:ARG:HH21 | 1.65 | 1.09 |
| 1:u:340:THR:CA | 1:u:407:ARG:HH21 | 1.64 | 1.09 |
| 1:v:340:THR:CA | 1:v:407:ARG:HH21 | 1.64 | 1.09 |
| 1:7:340:THR:CA | 1:7:407:ARG:HH21 | 1.65 | 1.09 |
| 1:C:340:THR:CA | 1:C:407:ARG:HH21 | 1.65 | 1.09 |
| 1:D:340:THR:CA | 1:D:407:ARG:HH21 | 1.64 | 1.09 |
| 1:D:629:GLY:HA3 | 1:P:609:TRP:NE1 | 1.65 | 1.09 |
| 1:E:340:THR:CA | 1:E:407:ARG:HH21 | 1.65 | 1.09 |
| 1:S:340:THR:CA | 1:S:407:ARG:HH21 | 1.64 | 1.09 |
| 1:U:340:THR:CA | 1:U:407:ARG:HH21 | 1.65 | 1.09 |
| 1:W:613:ASP:HB3 | 1:W:732:ARG:HD2 | 1.28 | 1.09 |
| 1:Z:340:THR:CA | 1:Z:407:ARG:HH21 | 1.65 | 1.09 |
| 1:d:609:TRP:NE1 | 1:l:629:GLY:HA3 | 1.65 | 1.09 |
| 1:m:340:THR:CA | 1:m:407:ARG:HH21 | 1.64 | 1.09 |
| 1:q:613:ASP:HB3 | 1:q:732:ARG:HD2 | 1.28 | 1.09 |
| 1:s:613:ASP:HB3 | 1:s:732:ARG:HD2 | 1.28 | 1.09 |
| 1:4:613:ASP:HB3 | 1:4:732:ARG:HD2 | 1.28 | 1.09 |
| 1:E:613:ASP:HB3 | 1:E:732:ARG:HD2 | 1.28 | 1.09 |
| 1:K:340:THR:CA | 1:K:407:ARG:HH21 | 1.64 | 1.09 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:340:THR:CA | 1:L:407:ARG:HH21 | 1.65 | 1.09 |
| 1:M:629:GLY:HA3 | 1:b:609:TRP:NE1 | 1.67 | 1.09 |
| 1:Q:613:ASP:HB3 | 1:Q:732:ARG:HD2 | 1.28 | 1.09 |
| 1:T:613:ASP:HB3 | 1:T:732:ARG:HD2 | 1.28 | 1.09 |
| 1:i:340:THR:CA | 1:i:407:ARG:HH21 | 1.64 | 1.09 |
| 1:z:629:GLY:HA3 | 1:2:609:TRP:NE1 | 1.66 | 1.09 |
| 1:3:613:ASP:HB2 | 1:3:731:THR:HG22 | 1.30 | 1.09 |
| 1:6:340:THR:CA | 1:6:407:ARG:HH21 | 1.64 | 1.09 |
| 1:B:609:TRP:NE1 | 1:J:629:GLY:HA3 | 1.67 | 1.09 |
| 1:F:340:THR:CA | 1:F:407:ARG:HH21 | 1.64 | 1.09 |
| 1:G:613:ASP:HB2 | 1:G:731:THR:HG22 | 1.30 | 1.09 |
| 1:K:629:GLY:HA3 | 1:8:609:TRP:NE1 | 1.65 | 1.09 |
| 1:O:613:ASP:HB2 | 1:O:731:THR:HG22 | 1.30 | 1.09 |
| 1:P:340:THR:CA | 1:P:407:ARG:HH21 | 1.65 | 1.09 |
| 1:a:340:THR:CA | 1:a:407:ARG:HH21 | 1.64 | 1.09 |
| 1:b:340:THR:CA | 1:b:407:ARG:HH21 | 1.64 | 1.09 |
| 1:g:340:THR:CA | 1:g:407:ARG:HH21 | 1.64 | 1.09 |
| 1:t:609:TRP:NE1 | 1:u:629:GLY:HA3 | 1.66 | 1.09 |
| 1:7:613:ASP:HB3 | 1:7:732:ARG:HD2 | 1.28 | 1.09 |
| 1:B:340:THR:CA | 1:B:407:ARG:HH21 | 1.64 | 1.08 |
| 1:H:340:THR:CA | 1:H:407:ARG:HH21 | 1.65 | 1.08 |
| 1:N:340:THR:CA | 1:N:407:ARG:HH21 | 1.65 | 1.08 |
| 1:R:609:TRP:NE1 | 1:S:629:GLY:HA3 | 1.66 | 1.08 |
| 1:m:609:TRP:NE1 | 1:n:629:GLY:HA3 | 1.66 | 1.08 |
| 1:s:340:THR:CA | 1:s:407:ARG:HH21 | 1.64 | 1.08 |
| 1:8:340:THR:CA | 1:8:407:ARG:HH21 | 1.64 | 1.08 |
| 1:B:613:ASP:HB2 | 1:B:731:THR:HG22 | 1.30 | 1.08 |
| 1:E:609:TRP:NE1 | 1:Q:629:GLY:HA3 | 1.66 | 1.08 |
| 1:H:613:ASP:HB3 | 1:H:732:ARG:HD2 | 1.28 | 1.08 |
| 1:M:340:THR:CA | 1:M:407:ARG:HH21 | 1.65 | 1.08 |
| 1:T:609:TRP:NE1 | 1:d:629:GLY:HA3 | 1.66 | 1.08 |
| 1:Z:609:TRP:NE1 | 1:4:629:GLY:HA3 | 1.66 | 1.08 |
| 1:p:613:ASP:HB2 | 1:p:731:THR:HG22 | 1.30 | 1.08 |
| 1:q:629:GLY:HA3 | 1:s:609:TRP:NE1 | 1.66 | 1.08 |
| 1:r:613:ASP:HB2 | 1:r:731:THR:HG22 | 1.30 | 1.08 |
| 1:1:613:ASP:HB3 | 1:1:732:ARG:HD2 | 1.28 | 1.08 |
| 1:3:340:THR:CA | 1:3:407:ARG:HH21 | 1.64 | 1.08 |
| 1:5:613:ASP:HB3 | 1:5:732:ARG:HD2 | 1.28 | 1.08 |
| 1:5:629:GLY:HA3 | 1:7:609:TRP:NE1 | 1.66 | 1.08 |
| 1:A:340:THR:CA | 1:A:407:ARG:HH21 | 1.64 | 1.08 |
| 1:G:340:THR:CA | 1:G:407:ARG:HH21 | 1.65 | 1.08 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:609:TRP:NE1 | 1:W:629:GLY:HA3 | 1.66 | 1.08 |
| 1:J:340:THR:CA | 1:J:407:ARG:HH21 | 1.65 | 1.08 |
| 1:L:613:ASP:HB3 | 1:L:732:ARG:HD2 | 1.28 | 1.08 |
| 1:O:340:THR:CA | 1:O:407:ARG:HH21 | 1.64 | 1.08 |
| 1:X:629:GLY:HA3 | 1:e:609:TRP:NE1 | 1.66 | 1.08 |
| 1:Z:629:GLY:HA3 | 1:3:609:TRP:NE1 | 1.66 | 1.08 |
| 1:b:613:ASP:HB2 | 1:b:731:THR:HG22 | 1.30 | 1.08 |
| 1:d:340:THR:CA | 1:d:407:ARG:HH21 | 1.65 | 1.08 |
| 1:o:340:THR:CA | 1:o:407:ARG:HH21 | 1.64 | 1.08 |
| 1:w:629:GLY:HA3 | 1:y:609:TRP:NE1 | 1.68 | 1.08 |
| 1:1:609:TRP:NE1 | 1:2:629:GLY:HA3 | 1.66 | 1.08 |
| 1:C:613:ASP:HB3 | 1:C:732:ARG:HD2 | 1.28 | 1.08 |
| 1:I:613:ASP:HB2 | 1:I:731:THR:HG22 | 1.30 | 1.08 |
| 1:O:609:TRP:NE1 | 1:m:629:GLY:HA3 | 1.66 | 1.08 |
| 1:R:340:THR:CA | 1:R:407:ARG:HH21 | 1.65 | 1.08 |
| 1:Y:613:ASP:HB2 | 1:Y:731:THR:HG22 | 1.30 | 1.08 |
| 1:p:340:THR:CA | 1:p:407:ARG:HH21 | 1.65 | 1.08 |
| 1:t:340:THR:CA | 1:t:407:ARG:HH21 | 1.64 | 1.08 |
| 1:2:340:THR:CA | 1:2:407:ARG:HH21 | 1.65 | 1.08 |
| 1:h:340:THR:CA | 1:h:407:ARG:HH21 | 1.65 | 1.08 |
| 1:u:609:TRP:NE1 | 1:v:629:GLY:HA3 | 1.66 | 1.08 |
| 1:c:613:ASP:HB2 | 1:c:731:THR:HG22 | 1.30 | 1.07 |
| 1:k:340:THR:CA | 1:k:407:ARG:HH21 | 1.65 | 1.07 |
| 1:P:613:ASP:HB2 | 1:P:731:THR:HG22 | 1.30 | 1.07 |
| 1:P:613:ASP:HB3 | 1:P:732:ARG:HD2 | 1.28 | 1.07 |
| 1:S:609:TRP:NE1 | 1:U:629:GLY:HA3 | 1.66 | 1.07 |
| 1:w:613:ASP:HB2 | 1:w:731:THR:HG22 | 1.30 | 1.07 |
| 1:6:613:ASP:HB3 | 1:6:732:ARG:HD2 | 1.28 | 1.07 |
| 1:e:613:ASP:HB2 | 1:e:731:THR:HG22 | 1.30 | 1.07 |
| 1:F:613:ASP:HB3 | 1:F:732:ARG:HD2 | 1.28 | 1.07 |
| 1:8:613:ASP:HB2 | 1:8:731:THR:HG22 | 1.30 | 1.06 |
| 1:8:613:ASP:HB3 | 1:8:732:ARG:HD2 | 1.28 | 1.06 |
| 1:V:613:ASP:HB2 | 1:V:731:THR:HG22 | 1.30 | 1.06 |
| 1:y:613:ASP:HB2 | 1:y:731:THR:HG22 | 1.30 | 1.06 |
| 1:D:613:ASP:HB3 | 1:D:732:ARG:CD | 1.87 | 1.05 |
| 1:K:613:ASP:HB3 | 1:K:732:ARG:CD | 1.87 | 1.05 |
| 1:A:613:ASP:HB3 | 1:A:732:ARG:CD | 1.87 | 1.05 |
| 1:H:613:ASP:HB3 | 1:H:732:ARG:CD | 1.87 | 1.05 |
| 1:W:613:ASP:HB3 | 1:W:732:ARG:CD | 1.87 | 1.05 |
| 1:o:613:ASP:HB3 | 1:o:732:ARG:CD | 1.87 | 1.05 |
| 1:s:613:ASP:HB3 | 1:s:732:ARG:CD | 1.87 | 1.05 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:613:ASP:HB3 | 1:Y:732:ARG:CD | 1.87 | 1.05 |
| 1:a:613:ASP:HB3 | 1:a:732:ARG:CD | 1.87 | 1.05 |
| 1:q:613:ASP:HB3 | 1:q:732:ARG:CD | 1.87 | 1.05 |
| 1:r:613:ASP:HB3 | 1:r:732:ARG:CD | 1.87 | 1.05 |
| 1:z:613:ASP:HB3 | 1:z:732:ARG:CD | 1.87 | 1.05 |
| 1:8:613:ASP:HB3 | 1:8:732:ARG:CD | 1.87 | 1.05 |
| 1:C:613:ASP:HB3 | 1:C:732:ARG:CD | 1.87 | 1.05 |
| 1:L:613:ASP:HB3 | 1:L:732:ARG:CD | 1.87 | 1.05 |
| 1:N:613:ASP:HB3 | 1:N:732:ARG:CD | 1.87 | 1.05 |
| 1:P:613:ASP:HB3 | 1:P:732:ARG:CD | 1.87 | 1.05 |
| 1:l:613:ASP:HB3 | 1:l:732:ARG:CD | 1.87 | 1.05 |
| 1:t:613:ASP:HB3 | 1:t:732:ARG:CD | 1.87 | 1.05 |
| 1:R:613:ASP:HB3 | 1:R:732:ARG:CD | 1.87 | 1.04 |
| 1:S:613:ASP:HB3 | 1:S:732:ARG:CD | 1.87 | 1.04 |
| 1:X:613:ASP:HB3 | 1:X:732:ARG:CD | 1.87 | 1.04 |
| 1:k:613:ASP:HB3 | 1:k:732:ARG:CD | 1.87 | 1.04 |
| 1:u:613:ASP:HB3 | 1:u:732:ARG:CD | 1.87 | 1.04 |
| 1:x:613:ASP:HB3 | 1:x:732:ARG:CD | 1.87 | 1.04 |
| 1:4:613:ASP:HB3 | 1:4:732:ARG:CD | 1.87 | 1.04 |
| 1:B:613:ASP:HB3 | 1:B:732:ARG:CD | 1.87 | 1.04 |
| 1:b:613:ASP:HB3 | 1:b:732:ARG:CD | 1.87 | 1.04 |
| 1:d:613:ASP:HB3 | 1:d:732:ARG:CD | 1.87 | 1.04 |
| 1:h:613:ASP:HB3 | 1:h:732:ARG:CD | 1.87 | 1.04 |
| 1:n:613:ASP:HB3 | 1:n:732:ARG:CD | 1.87 | 1.04 |
| 1:2:613:ASP:HB3 | 1:2:732:ARG:CD | 1.87 | 1.04 |
| 1:G:613:ASP:HB3 | 1:G:732:ARG:CD | 1.87 | 1.04 |
| 1:J:613:ASP:HB3 | 1:J:732:ARG:CD | 1.87 | 1.04 |
| 1:M:613:ASP:HB3 | 1:M:732:ARG:CD | 1.87 | 1.04 |
| 1:f:613:ASP:HB3 | 1:f:732:ARG:CD | 1.87 | 1.04 |
| 1:m:613:ASP:HB3 | 1:m:732:ARG:CD | 1.87 | 1.04 |
| 1:I:613:ASP:HB3 | 1:I:732:ARG:CD | 1.87 | 1.04 |
| 1:O:613:ASP:HB3 | 1:O:732:ARG:CD | 1.87 | 1.04 |
| 1:Z:613:ASP:HB3 | 1:Z:732:ARG:CD | 1.87 | 1.04 |
| 1:c:613:ASP:HB3 | 1:c:732:ARG:CD | 1.87 | 1.04 |
| 1:p:613:ASP:HB3 | 1:p:732:ARG:CD | 1.87 | 1.04 |
| 1:w:613:ASP:HB3 | 1:w:732:ARG:CD | 1.87 | 1.04 |
| 1:3:613:ASP:HB3 | 1:3:732:ARG:CD | 1.87 | 1.04 |
| 1:E:613:ASP:HB3 | 1:E:732:ARG:CD | 1.87 | 1.04 |
| 1:e:613:ASP:HB3 | 1:e:732:ARG:CD | 1.87 | 1.04 |
| 1:j:613:ASP:HB3 | 1:j:732:ARG:CD | 1.87 | 1.04 |
| 1:v:613:ASP:HB3 | 1:v:732:ARG:CD | 1.86 | 1.04 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:613:ASP:HB3 | 1:U:732:ARG:CD | 1.87 | 1.03 |
| 1:y:613:ASP:HB3 | 1:y:732:ARG:CD | 1.87 | 1.03 |
| 1:7:613:ASP:HB3 | 1:7:732:ARG:CD | 1.87 | 1.03 |
| 1:Q:613:ASP:HB3 | 1:Q:732:ARG:CD | 1.87 | 1.03 |
| 1:g:613:ASP:HB3 | 1:g:732:ARG:CD | 1.87 | 1.03 |
| 1:5:613:ASP:HB3 | 1:5:732:ARG:CD | 1.87 | 1.03 |
| 1:V:613:ASP:HB3 | 1:V:732:ARG:CD | 1.87 | 1.03 |
| 1:i:613:ASP:HB3 | 1:i:732:ARG:CD | 1.87 | 1.03 |
| 1:6:613:ASP:HB3 | 1:6:732:ARG:CD | 1.87 | 1.03 |
| 1:F:613:ASP:HB3 | 1:F:732:ARG:CD | 1.87 | 1.03 |
| 1:T:613:ASP:HB3 | 1:T:732:ARG:CD | 1.87 | 1.03 |
| 1:1:613:ASP:HB3 | 1:1:732:ARG:CD | 1.87 | 1.02 |
| 1:w:609:TRP:CD1 | 1:x:629:GLY:HA3 | 1.94 | 1.01 |
| 1:C:609:TRP:CD1 | 1:b:629:GLY:HA3 | 1.98 | 0.99 |
| 1:B:629:GLY:HA3 | 1:L:609:TRP:CD1 | 1.98 | 0.99 |
| 1:z:629:GLY:HA3 | 1:2:609:TRP:CD1 | 1.97 | 0.99 |
| 1:3:629:GLY:HA3 | 1:4:609:TRP:CD1 | 1.98 | 0.99 |
| 1:E:609:TRP:CD1 | 1:Q:629:GLY:HA3 | 1.98 | 0.99 |
| 1:O:629:GLY:HA3 | 1:n:609:TRP:CD1 | 1.98 | 0.99 |
| 1:V:629:GLY:HA3 | 1:X:609:TRP:CD1 | 1.98 | 0.99 |
| 1:d:609:TRP:CD1 | 1:l:629:GLY:HA3 | 1.97 | 0.99 |
| 1:5:629:GLY:HA3 | 1:7:609:TRP:CD1 | 1.98 | 0.99 |
| 1:K:629:GLY:HA3 | 1:8:609:TRP:CD1 | 1.97 | 0.99 |
| 1:6:609:TRP:CD1 | 1:7:629:GLY:HA3 | 1.98 | 0.99 |
| 1:D:629:GLY:HA3 | 1:P:609:TRP:CD1 | 1.97 | 0.99 |
| 1:E:629:GLY:HA3 | 1:F:609:TRP:CD1 | 1.98 | 0.99 |
| 1:C:629:GLY:HA3 | 1:M:609:TRP:CD1 | 1.98 | 0.99 |
| 1:m:609:TRP:CD1 | 1:n:629:GLY:HA3 | 1.98 | 0.99 |
| 1:V:609:TRP:CD1 | 1:e:629:GLY:HA3 | 1.97 | 0.99 |
| 1:Z:609:TRP:CD1 | 1:4:629:GLY:HA3 | 1.98 | 0.99 |
| 1:g:629:GLY:HA3 | 1:h:609:TRP:CD1 | 1.98 | 0.99 |
| 1:i:629:GLY:HA3 | 1:k:609:TRP:CD1 | 1.97 | 0.99 |
| 1:x:609:TRP:CD1 | 1:y:629:GLY:HA3 | 1.98 | 0.99 |
| 1:J:609:TRP:CD1 | 1:L:629:GLY:HA3 | 1.98 | 0.98 |
| 1:N:609:TRP:CD1 | 1:P:629:GLY:HA3 | 1.98 | 0.98 |
| 1:T:629:GLY:HA3 | 1:l:609:TRP:CD1 | 1.98 | 0.98 |
| 1:Z:629:GLY:HA3 | 1:3:609:TRP:CD1 | 1.98 | 0.98 |
| 1:z:609:TRP:CD1 | 1:1:629:GLY:HA3 | 1.98 | 0.98 |
| 1:O:609:TRP:CD1 | 1:m:629:GLY:HA3 | 1.98 | 0.98 |
| 1:G:609:TRP:CD1 | 1:I:629:GLY:HA3 | 1.97 | 0.98 |
| 1:a:609:TRP:CD1 | 1:8:629:GLY:HA3 | 1.98 | 0.98 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:f:609:TRP:CD1 | 1:h:629:GLY:HA3 | 1.98 | 0.98 |
| 1:1:609:TRP:CD1 | 1:2:629:GLY:HA3 | 1.98 | 0.98 |
| 1:H:609:TRP:CD1 | 1:W:629:GLY:HA3 | 1.98 | 0.98 |
| 1:T:609:TRP:CD1 | 1:d:629:GLY:HA3 | 1.98 | 0.98 |
| 1:W:609:TRP:CD1 | 1:Y:629:GLY:HA3 | 1.98 | 0.98 |
| 1:c:629:GLY:HA3 | 1:p:609:TRP:CD1 | 1.97 | 0.98 |
| 1:q:609:TRP:CD1 | 1:r:629:GLY:HA3 | 1.98 | 0.98 |
| 1:u:609:TRP:CD1 | 1:v:629:GLY:HA3 | 1.97 | 0.98 |
| 1:j:609:TRP:CD1 | 1:k:629:GLY:HA3 | 1.98 | 0.98 |
| 1:D:609:TRP:CD1 | 1:N:629:GLY:HA3 | 1.98 | 0.98 |
| 1:q:629:GLY:HA3 | 1:s:609:TRP:CD1 | 1.98 | 0.98 |
| 1:S:609:TRP:CD1 | 1:U:629:GLY:HA3 | 1.98 | 0.98 |
| 1:c:609:TRP:CD1 | 1:o:629:GLY:HA3 | 1.98 | 0.98 |
| 1:5:609:TRP:CD1 | 1:6:629:GLY:HA3 | 1.98 | 0.98 |
| 1:K:609:TRP:CD1 | 1:a:629:GLY:HA3 | 1.98 | 0.98 |
| 1:X:629:GLY:HA3 | 1:e:609:TRP:CD1 | 1.98 | 0.98 |
| 1:F:629:GLY:HA3 | 1:Q:609:TRP:CD1 | 1.98 | 0.98 |
| 1:t:629:GLY:HA3 | 1:v:609:TRP:CD1 | 1.98 | 0.98 |
| 1:R:629:GLY:HA3 | 1:U:609:TRP:CD1 | 1.98 | 0.97 |
| 1:A:629:GLY:HA3 | 1:I:609:TRP:CD1 | 1.98 | 0.97 |
| 1:R:609:TRP:CD1 | 1:S:629:GLY:HA3 | 1.98 | 0.97 |
| 1:t:609:TRP:CD1 | 1:u:629:GLY:HA3 | 1.98 | 0.97 |
| 1:A:609:TRP:CD1 | 1:G:629:GLY:HA3 | 1.98 | 0.97 |
| 1:M:629:GLY:HA3 | 1:b:609:TRP:CD1 | 1.99 | 0.97 |
| 1:i:609:TRP:CD1 | 1:j:629:GLY:HA3 | 1.98 | 0.97 |
| 1:H:629:GLY:HA3 | 1:Y:609:TRP:CD1 | 1.98 | 0.97 |
| 1:o:609:TRP:CD1 | 1:p:629:GLY:HA3 | 1.98 | 0.97 |
| 1:r:609:TRP:CD1 | 1:s:629:GLY:HA3 | 1.98 | 0.97 |
| 1:B:609:TRP:CD1 | 1:J:629:GLY:HA3 | 1.99 | 0.97 |
| 1:f:629:GLY:HA3 | 1:g:609:TRP:CD1 | 1.99 | 0.97 |
| 1:W:340:THR:HA | 1:W:407:ARG:HH21 | 1.32 | 0.95 |
| 1:z:340:THR:HA | 1:z:407:ARG:HH21 | 1.32 | 0.95 |
| 1:q:340:THR:HA | 1:q:407:ARG:HH21 | 1.32 | 0.95 |
| 1:k:340:THR:HA | 1:k:407:ARG:HH21 | 1.32 | 0.94 |
| 1:l:340:THR:HA | 1:l:407:ARG:HH21 | 1.32 | 0.94 |
| 1:t:340:THR:HA | 1:t:407:ARG:HH21 | 1.32 | 0.94 |
| 1:w:629:GLY:HA3 | 1:y:609:TRP:CD1 | 2.02 | 0.94 |
| 1:g:340:THR:HA | 1:g:407:ARG:HH21 | 1.32 | 0.94 |
| 1:h:340:THR:HA | 1:h:407:ARG:HH21 | 1.32 | 0.94 |
| 1:O:340:THR:HA | 1:O:407:ARG:HH21 | 1.32 | 0.94 |
| 1:i:340:THR:HA | 1:i:407:ARG:HH21 | 1.32 | 0.94 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:6:340:THR:HA | 1:6:407:ARG:HH21 | 1.32 | 0.94 |
| 1:B:340:THR:HA | 1:B:407:ARG:HH21 | 1.32 | 0.94 |
| 1:R:340:THR:HA | 1:R:407:ARG:HH21 | 1.32 | 0.94 |
| 1:1:340:THR:HA | 1:1:407:ARG:HH21 | 1.32 | 0.94 |
| 1:3:340:THR:HA | 1:3:407:ARG:HH21 | 1.32 | 0.94 |
| 1:F:340:THR:HA | 1:F:407:ARG:HH21 | 1.32 | 0.94 |
| 1:T:340:THR:HA | 1:T:407:ARG:HH21 | 1.32 | 0.94 |
| 1:b:340:THR:HA | 1:b:407:ARG:HH21 | 1.32 | 0.94 |
| 1:H:340:THR:HA | 1:H:407:ARG:NH2 | 1.83 | 0.94 |
| 1:T:340:THR:HA | 1:T:407:ARG:NH2 | 1.83 | 0.94 |
| 1:X:340:THR:HA | 1:X:407:ARG:HH21 | 1.32 | 0.94 |
| 1:a:340:THR:HA | 1:a:407:ARG:NH2 | 1.83 | 0.94 |
| 1:e:340:THR:HA | 1:e:407:ARG:NH2 | 1.83 | 0.94 |
| 1:m:340:THR:HA | 1:m:407:ARG:HH21 | 1.32 | 0.94 |
| 1:s:340:THR:HA | 1:s:407:ARG:NH2 | 1.83 | 0.94 |
| 1:E:340:THR:HA | 1:E:407:ARG:NH2 | 1.83 | 0.94 |
| 1:W:340:THR:HA | 1:W:407:ARG:NH2 | 1.83 | 0.94 |
| 1:o:340:THR:HA | 1:o:407:ARG:HH21 | 1.32 | 0.94 |
| 1:w:340:THR:HA | 1:w:407:ARG:NH2 | 1.83 | 0.94 |
| 1:1:340:THR:HA | 1:1:407:ARG:NH2 | 1.83 | 0.94 |
| 1:7:340:THR:HA | 1:7:407:ARG:NH2 | 1.83 | 0.94 |
| 1:A:340:THR:HA | 1:A:407:ARG:HH21 | 1.32 | 0.94 |
| 1:B:340:THR:HA | 1:B:407:ARG:NH2 | 1.83 | 0.94 |
| 1:N:340:THR:HA | 1:N:407:ARG:NH2 | 1.83 | 0.94 |
| 1:V:340:THR:HA | 1:V:407:ARG:NH2 | 1.83 | 0.94 |
| 1:x:340:THR:HA | 1:x:407:ARG:HH21 | 1.32 | 0.94 |
| 1:y:340:THR:HA | 1:y:407:ARG:NH2 | 1.83 | 0.94 |
| 1:Z:340:THR:HA | 1:Z:407:ARG:HH21 | 1.32 | 0.93 |
| 1:b:340:THR:HA | 1:b:407:ARG:NH2 | 1.83 | 0.93 |
| 1:D:340:THR:HA | 1:D:407:ARG:HH21 | 1.32 | 0.93 |
| 1:Y:340:THR:HA | 1:Y:407:ARG:NH2 | 1.83 | 0.93 |
| 1:h:340:THR:HA | 1:h:407:ARG:NH2 | 1.83 | 0.93 |
| 1:l:340:THR:HA | 1:l:407:ARG:NH2 | 1.83 | 0.93 |
| 1:q:340:THR:HA | 1:q:407:ARG:NH2 | 1.83 | 0.93 |
| 1:r:340:THR:HA | 1:r:407:ARG:NH2 | 1.83 | 0.93 |
| 1:z:340:THR:HA | 1:z:407:ARG:NH2 | 1.83 | 0.93 |
| 1:G:340:THR:HA | 1:G:407:ARG:NH2 | 1.83 | 0.93 |
| 1:K:340:THR:HA | 1:K:407:ARG:HH21 | 1.32 | 0.93 |
| 1:k:340:THR:HA | 1:k:407:ARG:NH2 | 1.83 | 0.93 |
| 1:p:340:THR:HA | 1:p:407:ARG:NH2 | 1.83 | 0.93 |
| 1:5:340:THR:HA | 1:5:407:ARG:NH2 | 1.83 | 0.93 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:340:THR:HA | 1:F:407:ARG:NH2 | 1.83 | 0.93 |
| 1:P:340:THR:HA | 1:P:407:ARG:NH2 | 1.83 | 0.93 |
| 1:Q:340:THR:HA | 1:Q:407:ARG:NH2 | 1.83 | 0.93 |
| 1:U:340:THR:HA | 1:U:407:ARG:NH2 | 1.83 | 0.93 |
| 1:d:340:THR:HA | 1:d:407:ARG:NH2 | 1.83 | 0.93 |
| 1:f:340:THR:HA | 1:f:407:ARG:NH2 | 1.83 | 0.93 |
| 1:v:340:THR:HA | 1:v:407:ARG:NH2 | 1.83 | 0.93 |
| 1:8:340:THR:HA | 1:8:407:ARG:NH2 | 1.83 | 0.93 |
| 1:A:340:THR:HA | 1:A:407:ARG:NH2 | 1.83 | 0.93 |
| 1:I:340:THR:HA | 1:I:407:ARG:NH2 | 1.83 | 0.93 |
| 1:J:340:THR:HA | 1:J:407:ARG:NH2 | 1.83 | 0.93 |
| 1:L:340:THR:HA | 1:L:407:ARG:NH2 | 1.83 | 0.93 |
| 1:M:340:THR:HA | 1:M:407:ARG:NH2 | 1.83 | 0.93 |
| 1:O:340:THR:HA | 1:O:407:ARG:NH2 | 1.83 | 0.93 |
| 1:S:340:THR:HA | 1:S:407:ARG:HH21 | 1.32 | 0.93 |
| 1:j:340:THR:HA | 1:j:407:ARG:NH2 | 1.83 | 0.93 |
| 1:2:340:THR:HA | 1:2:407:ARG:NH2 | 1.83 | 0.93 |
| 1:6:340:THR:HA | 1:6:407:ARG:NH2 | 1.83 | 0.93 |
| 1:c:340:THR:HA | 1:c:407:ARG:NH2 | 1.83 | 0.93 |
| 1:o:340:THR:HA | 1:o:407:ARG:NH2 | 1.83 | 0.93 |
| 1:3:340:THR:HA | 1:3:407:ARG:NH2 | 1.83 | 0.93 |
| 1:C:340:THR:HA | 1:C:407:ARG:NH2 | 1.83 | 0.93 |
| 1:u:340:THR:HA | 1:u:407:ARG:HH21 | 1.32 | 0.92 |
| 1:X:340:THR:HA | 1:X:407:ARG:NH2 | 1.83 | 0.92 |
| 1:c:340:THR:HA | 1:c:407:ARG:HH21 | 1.32 | 0.92 |
| 1:n:340:THR:HA | 1:n:407:ARG:NH2 | 1.83 | 0.92 |
| 1:v:340:THR:HA | 1:v:407:ARG:HH21 | 1.32 | 0.92 |
| 1:r:340:THR:HA | 1:r:407:ARG:HH21 | 1.32 | 0.92 |
| 1:U:340:THR:HA | 1:U:407:ARG:HH21 | 1.32 | 0.92 |
| 1:x:340:THR:HA | 1:x:407:ARG:NH2 | 1.83 | 0.92 |
| 1:u:340:THR:HA | 1:u:407:ARG:NH2 | 1.83 | 0.92 |
| 1:4:340:THR:HA | 1:4:407:ARG:NH2 | 1.83 | 0.92 |
| 1:I:340:THR:HA | 1:I:407:ARG:HH21 | 1.32 | 0.92 |
| 1:S:340:THR:HA | 1:S:407:ARG:NH2 | 1.83 | 0.92 |
| 1:Y:340:THR:HA | 1:Y:407:ARG:HH21 | 1.32 | 0.92 |
| 1:i:340:THR:HA | 1:i:407:ARG:NH2 | 1.83 | 0.91 |
| 1:J:340:THR:HA | 1:J:407:ARG:HH21 | 1.32 | 0.91 |
| 1:P:340:THR:HA | 1:P:407:ARG:HH21 | 1.32 | 0.91 |
| 1:C:340:THR:HA | 1:C:407:ARG:HH21 | 1.32 | 0.91 |
| 1:g:340:THR:HA | 1:g:407:ARG:NH2 | 1.83 | 0.91 |
| 1:8:340:THR:HA | 1:8:407:ARG:HH21 | 1.32 | 0.91 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:329:ASN:C | 1:D:330:GLU:OE1 | 2.14 | 0.91 |
| 1:D:340:THR:HA | 1:D:407:ARG:NH2 | 1.83 | 0.91 |
| 1:K:329:ASN:C | 1:K:330:GLU:OE1 | 2.14 | 0.91 |
| 1:N:329:ASN:C | 1:N:330:GLU:OE1 | 2.14 | 0.91 |
| 1:a:329:ASN:C | 1:a:330:GLU:OE1 | 2.14 | 0.91 |
| 1:e:329:ASN:C | 1:e:330:GLU:OE1 | 2.14 | 0.91 |
| 1:h:329:ASN:C | 1:h:330:GLU:OE1 | 2.14 | 0.91 |
| 1:w:329:ASN:C | 1:w:330:GLU:OE1 | 2.14 | 0.91 |
| 1:H:329:ASN:C | 1:H:330:GLU:OE1 | 2.14 | 0.91 |
| 1:R:329:ASN:C | 1:R:330:GLU:OE1 | 2.14 | 0.91 |
| 1:S:329:ASN:C | 1:S:330:GLU:OE1 | 2.14 | 0.91 |
| 1:k:329:ASN:C | 1:k:330:GLU:OE1 | 2.14 | 0.91 |
| 1:s:329:ASN:C | 1:s:330:GLU:OE1 | 2.14 | 0.91 |
| 1:t:340:THR:HA | 1:t:407:ARG:NH2 | 1.83 | 0.91 |
| 1:u:329:ASN:C | 1:u:330:GLU:OE1 | 2.14 | 0.91 |
| 1:E:329:ASN:C | 1:E:330:GLU:OE1 | 2.14 | 0.91 |
| 1:G:329:ASN:C | 1:G:330:GLU:OE1 | 2.14 | 0.91 |
| 1:K:340:THR:HA | 1:K:407:ARG:NH2 | 1.83 | 0.91 |
| 1:O:329:ASN:C | 1:O:330:GLU:OE1 | 2.14 | 0.91 |
| 1:b:329:ASN:C | 1:b:330:GLU:OE1 | 2.14 | 0.91 |
| 1:j:340:THR:HA | 1:j:407:ARG:HH21 | 1.32 | 0.91 |
| 1:p:329:ASN:C | 1:p:330:GLU:OE1 | 2.14 | 0.91 |
| 1:7:329:ASN:C | 1:7:330:GLU:OE1 | 2.14 | 0.91 |
| 1:t:329:ASN:C | 1:t:330:GLU:OE1 | 2.14 | 0.91 |
| 1:3:329:ASN:C | 1:3:330:GLU:OE1 | 2.14 | 0.91 |
| 1:B:329:ASN:C | 1:B:330:GLU:OE1 | 2.14 | 0.91 |
| 1:L:340:THR:HA | 1:L:407:ARG:HH21 | 1.32 | 0.91 |
| 1:R:340:THR:HA | 1:R:407:ARG:NH2 | 1.83 | 0.91 |
| 1:Z:340:THR:HA | 1:Z:407:ARG:NH2 | 1.83 | 0.91 |
| 1:l:329:ASN:C | 1:l:330:GLU:OE1 | 2.14 | 0.91 |
| 1:m:340:THR:HA | 1:m:407:ARG:NH2 | 1.83 | 0.91 |
| 1:g:329:ASN:C | 1:g:330:GLU:OE1 | 2.14 | 0.91 |
| 1:i:329:ASN:C | 1:i:330:GLU:OE1 | 2.14 | 0.91 |
| 1:w:340:THR:HA | 1:w:407:ARG:HH21 | 1.32 | 0.91 |
| 1:J:329:ASN:C | 1:J:330:GLU:OE1 | 2.14 | 0.90 |
| 1:U:329:ASN:C | 1:U:330:GLU:OE1 | 2.14 | 0.90 |
| 1:f:340:THR:HA | 1:f:407:ARG:HH21 | 1.32 | 0.90 |
| 1:z:329:ASN:C | 1:z:330:GLU:OE1 | 2.14 | 0.90 |
| 1:4:340:THR:HA | 1:4:407:ARG:HH21 | 1.32 | 0.90 |
| 1:C:329:ASN:C | 1:C:330:GLU:OE1 | 2.14 | 0.90 |
| 1:F:329:ASN:C | 1:F:330:GLU:OE1 | 2.14 | 0.90 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:329:ASN:C | 1:L:330:GLU:OE1 | 2.14 | 0.90 |
| 1:V:329:ASN:C | 1:V:330:GLU:OE1 | 2.14 | 0.90 |
| 1:X:329:ASN:C | 1:X:330:GLU:OE1 | 2.14 | 0.90 |
| 1:n:340:THR:HA | 1:n:407:ARG:HH21 | 1.32 | 0.90 |
| 1:v:329:ASN:C | 1:v:330:GLU:OE1 | 2.14 | 0.90 |
| 1:2:329:ASN:C | 1:2:330:GLU:OE1 | 2.14 | 0.90 |
| 1:6:329:ASN:C | 1:6:330:GLU:OE1 | 2.14 | 0.90 |
| 1:M:329:ASN:C | 1:M:330:GLU:OE1 | 2.14 | 0.90 |
| 1:Y:329:ASN:C | 1:Y:330:GLU:OE1 | 2.14 | 0.90 |
| 1:e:340:THR:HA | 1:e:407:ARG:HH21 | 1.32 | 0.90 |
| 1:f:329:ASN:C | 1:f:330:GLU:OE1 | 2.14 | 0.90 |
| 1:p:340:THR:HA | 1:p:407:ARG:HH21 | 1.32 | 0.90 |
| 1:A:609:TRP:HH2 | 1:A:631:PHE:CZ | 1.90 | 0.90 |
| 1:N:609:TRP:HH2 | 1:N:631:PHE:CZ | 1.90 | 0.90 |
| 1:a:340:THR:HA | 1:a:407:ARG:HH21 | 1.32 | 0.90 |
| 1:a:609:TRP:HH2 | 1:a:631:PHE:CZ | 1.90 | 0.90 |
| 1:d:329:ASN:C | 1:d:330:GLU:OE1 | 2.14 | 0.90 |
| 1:j:329:ASN:C | 1:j:330:GLU:OE1 | 2.14 | 0.90 |
| 1:x:329:ASN:C | 1:x:330:GLU:OE1 | 2.14 | 0.90 |
| 1:A:329:ASN:C | 1:A:330:GLU:OE1 | 2.14 | 0.90 |
| 1:B:609:TRP:HH2 | 1:B:631:PHE:CZ | 1.90 | 0.90 |
| 1:G:340:THR:HA | 1:G:407:ARG:HH21 | 1.32 | 0.90 |
| 1:P:329:ASN:C | 1:P:330:GLU:OE1 | 2.14 | 0.90 |
| 1:Y:609:TRP:HH2 | 1:Y:631:PHE:CZ | 1.90 | 0.90 |
| 1:Z:329:ASN:C | 1:Z:330:GLU:OE1 | 2.14 | 0.90 |
| 1:b:609:TRP:HH2 | 1:b:631:PHE:CZ | 1.90 | 0.90 |
| 1:o:329:ASN:C | 1:o:330:GLU:OE1 | 2.14 | 0.90 |
| 1:o:609:TRP:HH2 | 1:o:631:PHE:CZ | 1.90 | 0.90 |
| 1:r:329:ASN:C | 1:r:330:GLU:OE1 | 2.14 | 0.90 |
| 1:r:609:TRP:HH2 | 1:r:631:PHE:CZ | 1.90 | 0.90 |
| 1:y:329:ASN:C | 1:y:330:GLU:OE1 | 2.14 | 0.90 |
| 1:Q:329:ASN:C | 1:Q:330:GLU:OE1 | 2.14 | 0.90 |
| 1:m:329:ASN:C | 1:m:330:GLU:OE1 | 2.14 | 0.90 |
| 1:n:329:ASN:C | 1:n:330:GLU:OE1 | 2.14 | 0.90 |
| 1:q:329:ASN:C | 1:q:330:GLU:OE1 | 2.14 | 0.90 |
| 1:5:329:ASN:C | 1:5:330:GLU:OE1 | 2.14 | 0.90 |
| 1:8:329:ASN:C | 1:8:330:GLU:OE1 | 2.14 | 0.90 |
| 1:F:340:THR:C | 1:F:407:ARG:HH21 | 1.80 | 0.90 |
| 1:M:340:THR:HA | 1:M:407:ARG:HH21 | 1.32 | 0.90 |
| 1:Q:340:THR:HA | 1:Q:407:ARG:HH21 | 1.32 | 0.90 |
| 1:T:609:TRP:HH2 | 1:T:631:PHE:CZ | 1.90 | 0.90 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:329:ASN:C | 1:W:330:GLU:OE1 | 2.14 | 0.90 |
| 1:4:329:ASN:C | 1:4:330:GLU:OE1 | 2.14 | 0.90 |
| 1:J:609:TRP:HH2 | 1:J:631:PHE:CZ | 1.90 | 0.90 |
| 1:N:340:THR:HA | 1:N:407:ARG:HH21 | 1.32 | 0.90 |
| 1:S:609:TRP:HH2 | 1:S:631:PHE:CZ | 1.90 | 0.90 |
| 1:1:609:TRP:HH2 | 1:1:631:PHE:CZ | 1.90 | 0.90 |
| 1:6:340:THR:C | 1:6:407:ARG:HH21 | 1.80 | 0.90 |
| 1:O:340:THR:C | 1:O:407:ARG:HH21 | 1.80 | 0.90 |
| 1:R:340:THR:C | 1:R:407:ARG:HH21 | 1.80 | 0.90 |
| 1:U:609:TRP:HH2 | 1:U:631:PHE:CZ | 1.90 | 0.90 |
| 1:X:526:MET:HE2 | 1:X:575:ALA:HA | 1.54 | 0.90 |
| 1:g:340:THR:C | 1:g:407:ARG:HH21 | 1.80 | 0.90 |
| 1:m:609:TRP:HH2 | 1:m:631:PHE:CZ | 1.90 | 0.90 |
| 1:t:340:THR:C | 1:t:407:ARG:HH21 | 1.80 | 0.90 |
| 1:u:609:TRP:HH2 | 1:u:631:PHE:CZ | 1.90 | 0.90 |
| 1:y:609:TRP:HH2 | 1:y:631:PHE:CZ | 1.90 | 0.90 |
| 1:3:340:THR:C | 1:3:407:ARG:HH21 | 1.80 | 0.90 |
| 1:E:526:MET:HE2 | 1:E:575:ALA:HA | 1.54 | 0.90 |
| 1:M:609:TRP:HH2 | 1:M:631:PHE:CZ | 1.90 | 0.90 |
| 1:Z:609:TRP:HH2 | 1:Z:631:PHE:CZ | 1.90 | 0.90 |
| 1:i:340:THR:C | 1:i:407:ARG:HH21 | 1.80 | 0.90 |
| 1:l:526:MET:HE2 | 1:l:575:ALA:HA | 1.54 | 0.90 |
| 1:o:340:THR:C | 1:o:407:ARG:HH21 | 1.80 | 0.90 |
| 1:v:340:THR:C | 1:v:407:ARG:HH21 | 1.80 | 0.90 |
| 1:v:609:TRP:HH2 | 1:v:631:PHE:CZ | 1.90 | 0.90 |
| 1:x:526:MET:HE2 | 1:x:575:ALA:HA | 1.54 | 0.90 |
| 1:7:526:MET:HE2 | 1:7:575:ALA:HA | 1.54 | 0.90 |
| 1:A:340:THR:C | 1:A:407:ARG:HH21 | 1.80 | 0.89 |
| 1:C:526:MET:HE2 | 1:C:575:ALA:HA | 1.54 | 0.89 |
| 1:E:609:TRP:HH2 | 1:E:631:PHE:CZ | 1.90 | 0.89 |
| 1:U:340:THR:C | 1:U:407:ARG:HH21 | 1.80 | 0.89 |
| 1:d:340:THR:C | 1:d:407:ARG:HH21 | 1.80 | 0.89 |
| 1:x:609:TRP:HH2 | 1:x:631:PHE:CZ | 1.90 | 0.89 |
| 1:z:526:MET:HE2 | 1:z:575:ALA:HA | 1.54 | 0.89 |
| 1:7:609:TRP:HH2 | 1:7:631:PHE:CZ | 1.90 | 0.89 |
| 1:I:329:ASN:C | 1:I:330:GLU:OE1 | 2.14 | 0.89 |
| 1:L:526:MET:HE2 | 1:L:575:ALA:HA | 1.54 | 0.89 |
| 1:P:340:THR:C | 1:P:407:ARG:HH21 | 1.80 | 0.89 |
| 1:V:609:TRP:HH2 | 1:V:631:PHE:CZ | 1.90 | 0.89 |
| 1:X:609:TRP:HH2 | 1:X:631:PHE:CZ | 1.90 | 0.89 |
| 1:c:329:ASN:C | 1:c:330:GLU:OE1 | 2.14 | 0.89 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:d:609:TRP:HH2 | 1:d:631:PHE:CZ | 1.90 | 0.89 |
| 1:m:340:THR:C | 1:m:407:ARG:HH21 | 1.80 | 0.89 |
| 1:2:340:THR:C | 1:2:407:ARG:HH21 | 1.80 | 0.89 |
| 1:2:609:TRP:HH2 | 1:2:631:PHE:CZ | 1.90 | 0.89 |
| 1:4:340:THR:C | 1:4:407:ARG:HH21 | 1.80 | 0.89 |
| 1:8:340:THR:C | 1:8:407:ARG:HH21 | 1.80 | 0.89 |
| 1:W:340:THR:C | 1:W:407:ARG:HH21 | 1.80 | 0.89 |
| 1:Y:340:THR:C | 1:Y:407:ARG:HH21 | 1.80 | 0.89 |
| 1:Z:340:THR:C | 1:Z:407:ARG:HH21 | 1.80 | 0.89 |
| 1:f:526:MET:HE2 | 1:f:575:ALA:HA | 1.54 | 0.89 |
| 1:j:526:MET:HE2 | 1:j:575:ALA:HA | 1.54 | 0.89 |
| 1:n:340:THR:C | 1:n:407:ARG:HH21 | 1.80 | 0.89 |
| 1:q:340:THR:C | 1:q:407:ARG:HH21 | 1.80 | 0.89 |
| 1:s:609:TRP:HH2 | 1:s:631:PHE:CZ | 1.90 | 0.89 |
| 1:5:340:THR:HA | 1:5:407:ARG:HH21 | 1.32 | 0.89 |
| 1:C:340:THR:HB | 1:D:322:GLN:HE21 | 1.38 | 0.89 |
| 1:G:340:THR:C | 1:G:407:ARG:HH21 | 1.80 | 0.89 |
| 1:G:526:MET:HE2 | 1:G:575:ALA:HA | 1.54 | 0.89 |
| 1:K:322:GLN:HE21 | 1:L:340:THR:HB | 1.38 | 0.89 |
| 1:c:526:MET:HE2 | 1:c:575:ALA:HA | 1.54 | 0.89 |
| 1:p:340:THR:C | 1:p:407:ARG:HH21 | 1.80 | 0.89 |
| 1:p:526:MET:HE2 | 1:p:575:ALA:HA | 1.54 | 0.89 |
| 1:r:340:THR:C | 1:r:407:ARG:HH21 | 1.80 | 0.89 |
| 1:H:609:TRP:HH2 | 1:H:631:PHE:CZ | 1.90 | 0.89 |
| 1:I:526:MET:HE2 | 1:I:575:ALA:HA | 1.54 | 0.89 |
| 1:e:340:THR:C | 1:e:407:ARG:HH21 | 1.80 | 0.89 |
| 1:w:609:TRP:HH2 | 1:w:631:PHE:CZ | 1.90 | 0.89 |
| 1:F:609:TRP:HH2 | 1:F:631:PHE:CZ | 1.90 | 0.89 |
| 1:P:526:MET:HE2 | 1:P:575:ALA:HA | 1.54 | 0.89 |
| 1:e:609:TRP:HH2 | 1:e:631:PHE:CZ | 1.90 | 0.89 |
| 1:i:609:TRP:HH2 | 1:i:631:PHE:CZ | 1.90 | 0.89 |
| 1:w:340:THR:C | 1:w:407:ARG:HH21 | 1.80 | 0.89 |
| 1:1:329:ASN:C | 1:1:330:GLU:OE1 | 2.14 | 0.89 |
| 1:C:609:TRP:HH2 | 1:C:631:PHE:CZ | 1.90 | 0.89 |
| 1:b:340:THR:C | 1:b:407:ARG:HH21 | 1.80 | 0.89 |
| 1:g:609:TRP:HH2 | 1:g:631:PHE:CZ | 1.90 | 0.89 |
| 1:h:526:MET:HE2 | 1:h:575:ALA:HA | 1.54 | 0.89 |
| 1:r:340:THR:HB | 1:x:322:GLN:HE21 | 1.38 | 0.89 |
| 1:8:526:MET:HE2 | 1:8:575:ALA:HA | 1.54 | 0.89 |
| 1:K:526:MET:HE2 | 1:K:575:ALA:HA | 1.54 | 0.89 |
| 1:S:526:MET:HE2 | 1:S:575:ALA:HA | 1.54 | 0.89 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:329:ASN:C | 1:T:330:GLU:OE1 | 2.14 | 0.89 |
| 1:u:526:MET:HE2 | 1:u:575:ALA:HA | 1.54 | 0.89 |
| 1:6:609:TRP:HH2 | 1:6:631:PHE:CZ | 1.90 | 0.89 |
| 1:8:609:TRP:HH2 | 1:8:631:PHE:CZ | 1.90 | 0.89 |
| 1:B:340:THR:C | 1:B:407:ARG:HH21 | 1.80 | 0.89 |
| 1:D:526:MET:HE2 | 1:D:575:ALA:HA | 1.54 | 0.89 |
| 1:L:609:TRP:HH2 | 1:L:631:PHE:CZ | 1.90 | 0.89 |
| 1:a:340:THR:C | 1:a:407:ARG:HH21 | 1.80 | 0.89 |
| 1:p:609:TRP:HH2 | 1:p:631:PHE:CZ | 1.90 | 0.89 |
| 1:q:322:GLN:HE21 | 1:y:340:THR:HB | 1.36 | 0.89 |
| 1:G:609:TRP:HH2 | 1:G:631:PHE:CZ | 1.90 | 0.89 |
| 1:P:609:TRP:HH2 | 1:P:631:PHE:CZ | 1.90 | 0.89 |
| 1:V:340:THR:C | 1:V:407:ARG:HH21 | 1.80 | 0.89 |
| 1:X:322:GLN:HE21 | 1:Y:340:THR:HB | 1.38 | 0.89 |
| 1:s:340:THR:HA | 1:s:407:ARG:HH21 | 1.32 | 0.89 |
| 1:V:340:THR:HB | 1:W:322:GLN:HE21 | 1.37 | 0.88 |
| 1:k:526:MET:HE2 | 1:k:575:ALA:HA | 1.54 | 0.88 |
| 1:n:526:MET:HE2 | 1:n:575:ALA:HA | 1.54 | 0.88 |
| 1:n:609:TRP:HH2 | 1:n:631:PHE:CZ | 1.90 | 0.88 |
| 1:7:340:THR:HA | 1:7:407:ARG:HH21 | 1.32 | 0.88 |
| 1:E:340:THR:HA | 1:E:407:ARG:HH21 | 1.32 | 0.88 |
| 1:N:340:THR:C | 1:N:407:ARG:HH21 | 1.80 | 0.88 |
| 1:R:526:MET:HE2 | 1:R:575:ALA:HA | 1.54 | 0.88 |
| 1:j:609:TRP:HH2 | 1:j:631:PHE:CZ | 1.90 | 0.88 |
| 1:k:609:TRP:HH2 | 1:k:631:PHE:CZ | 1.90 | 0.88 |
| 1:l:340:THR:C | 1:l:407:ARG:HH21 | 1.80 | 0.88 |
| 1:x:340:THR:C | 1:x:407:ARG:HH21 | 1.80 | 0.88 |
| 1:y:340:THR:C | 1:y:407:ARG:HH21 | 1.80 | 0.88 |
| 1:4:526:MET:HE2 | 1:4:575:ALA:HA | 1.54 | 0.88 |
| 1:I:609:TRP:HH2 | 1:I:631:PHE:CZ | 1.90 | 0.88 |
| 1:J:340:THR:C | 1:J:407:ARG:HH21 | 1.80 | 0.88 |
| 1:X:340:THR:C | 1:X:407:ARG:HH21 | 1.80 | 0.88 |
| 1:c:340:THR:C | 1:c:407:ARG:HH21 | 1.80 | 0.88 |
| 1:f:609:TRP:HH2 | 1:f:631:PHE:CZ | 1.90 | 0.88 |
| 1:h:609:TRP:HH2 | 1:h:631:PHE:CZ | 1.90 | 0.88 |
| 1:l:609:TRP:HH2 | 1:l:631:PHE:CZ | 1.90 | 0.88 |
| 1:q:609:TRP:HH2 | 1:q:631:PHE:CZ | 1.90 | 0.88 |
| 1:u:340:THR:HB | 1:5:322:GLN:HE21 | 1.38 | 0.88 |
| 1:v:322:GLN:HE21 | 1:w:340:THR:HB | 1.38 | 0.88 |
| 1:v:526:MET:HE2 | 1:v:575:ALA:HA | 1.54 | 0.88 |
| 1:z:340:THR:C | 1:z:407:ARG:HH21 | 1.80 | 0.88 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:340:THR:C | 1:D:407:ARG:HH21 | 1.80 | 0.88 |
| 1:I:340:THR:C | 1:I:407:ARG:HH21 | 1.80 | 0.88 |
| 1:L:340:THR:C | 1:L:407:ARG:HH21 | 1.80 | 0.88 |
| 1:M:340:THR:C | 1:M:407:ARG:HH21 | 1.80 | 0.88 |
| 1:U:322:GLN:HE21 | 1:e:340:THR:HB | 1.38 | 0.88 |
| 1:U:526:MET:HE2 | 1:U:575:ALA:HA | 1.54 | 0.88 |
| 1:V:340:THR:HA | 1:V:407:ARG:HH21 | 1.32 | 0.88 |
| 1:W:609:TRP:HH2 | 1:W:631:PHE:CZ | 1.90 | 0.88 |
| 1:e:322:GLN:HE21 | 1:h:340:THR:HB | 1.38 | 0.88 |
| 1:t:526:MET:HE2 | 1:t:575:ALA:HA | 1.54 | 0.88 |
| 1:2:340:THR:HA | 1:2:407:ARG:HH21 | 1.32 | 0.88 |
| 1:3:609:TRP:HH2 | 1:3:631:PHE:CZ | 1.90 | 0.88 |
| 1:4:609:TRP:HH2 | 1:4:631:PHE:CZ | 1.90 | 0.88 |
| 1:B:526:MET:HE2 | 1:B:575:ALA:HA | 1.54 | 0.88 |
| 1:C:340:THR:C | 1:C:407:ARG:HH21 | 1.80 | 0.88 |
| 1:O:609:TRP:HH2 | 1:O:631:PHE:CZ | 1.90 | 0.88 |
| 1:P:322:GLN:HE21 | 1:Q:340:THR:HB | 1.38 | 0.88 |
| 1:Q:340:THR:C | 1:Q:407:ARG:HH21 | 1.80 | 0.88 |
| 1:Q:609:TRP:HH2 | 1:Q:631:PHE:CZ | 1.90 | 0.88 |
| 1:R:609:TRP:HH2 | 1:R:631:PHE:CZ | 1.90 | 0.88 |
| 1:T:340:THR:C | 1:T:407:ARG:HH21 | 1.80 | 0.88 |
| 1:c:609:TRP:HH2 | 1:c:631:PHE:CZ | 1.90 | 0.88 |
| 1:y:340:THR:HA | 1:y:407:ARG:HH21 | 1.32 | 0.88 |
| 1:5:340:THR:C | 1:5:407:ARG:HH21 | 1.80 | 0.88 |
| 1:N:526:MET:HE2 | 1:N:575:ALA:HA | 1.54 | 0.88 |
| 1:Q:322:GLN:HE21 | 1:S:340:THR:HB | 1.38 | 0.88 |
| 1:S:322:GLN:HE21 | 1:d:340:THR:HB | 1.38 | 0.88 |
| 1:b:526:MET:HE2 | 1:b:575:ALA:HA | 1.54 | 0.88 |
| 1:t:609:TRP:HH2 | 1:t:631:PHE:CZ | 1.90 | 0.88 |
| 1:z:609:TRP:HH2 | 1:z:631:PHE:CZ | 1.90 | 0.88 |
| 1:1:340:THR:C | 1:1:407:ARG:HH21 | 1.80 | 0.88 |
| 1:2:322:GLN:HE21 | 1:3:340:THR:HB | 1.39 | 0.88 |
| 1:3:526:MET:HE2 | 1:3:575:ALA:HA | 1.54 | 0.88 |
| 1:5:340:THR:HB | 1:8:322:GLN:HE21 | 1.38 | 0.88 |
| 1:D:609:TRP:HH2 | 1:D:631:PHE:CZ | 1.90 | 0.88 |
| 1:F:526:MET:HE2 | 1:F:575:ALA:HA | 1.54 | 0.88 |
| 1:H:340:THR:HA | 1:H:407:ARG:HH21 | 1.32 | 0.88 |
| 1:K:340:THR:C | 1:K:407:ARG:HH21 | 1.80 | 0.88 |
| 1:e:526:MET:HE2 | 1:e:575:ALA:HA | 1.54 | 0.88 |
| 1:u:322:GLN:HE21 | 1:2:340:THR:HB | 1.38 | 0.88 |
| 1:z:340:THR:HB | 1:4:322:GLN:HE21 | 1.38 | 0.88 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:609:TRP:HH2 | 1:5:631:PHE:CZ | 1.90 | 0.88 |
| 1:K:609:TRP:HH2 | 1:K:631:PHE:CZ | 1.90 | 0.88 |
| 1:O:340:THR:HB | 1:d:322:GLN:HE21 | 1.39 | 0.88 |
| 1:S:340:THR:C | 1:S:407:ARG:HH21 | 1.80 | 0.88 |
| 1:d:340:THR:HA | 1:d:407:ARG:HH21 | 1.32 | 0.88 |
| 1:m:526:MET:HE2 | 1:m:575:ALA:HA | 1.54 | 0.88 |
| 1:w:526:MET:HE2 | 1:w:575:ALA:HA | 1.54 | 0.88 |
| 1:E:340:THR:C | 1:E:407:ARG:HH21 | 1.80 | 0.88 |
| 1:O:526:MET:HE2 | 1:O:575:ALA:HA | 1.54 | 0.88 |
| 1:a:526:MET:HE2 | 1:a:575:ALA:HA | 1.54 | 0.88 |
| 1:l:340:THR:HB | 1:n:322:GLN:HE21 | 1.38 | 0.88 |
| 1:p:340:THR:HB | 1:6:322:GLN:HE21 | 1.38 | 0.88 |
| 1:v:340:THR:HB | 1:1:322:GLN:HE21 | 1.38 | 0.88 |
| 1:1:526:MET:HE2 | 1:1:575:ALA:HA | 1.54 | 0.88 |
| 1:6:526:MET:HE2 | 1:6:575:ALA:HA | 1.54 | 0.88 |
| 1:b:322:GLN:HE21 | 1:o:340:THR:HB | 1.38 | 0.88 |
| 1:h:322:GLN:HE21 | 1:i:340:THR:HB | 1.38 | 0.88 |
| 1:Z:340:THR:HB | 1:a:322:GLN:HE21 | 1.38 | 0.87 |
| 1:Z:526:MET:HE2 | 1:Z:575:ALA:HA | 1.54 | 0.87 |
| 1:g:340:THR:HB | 1:k:322:GLN:HE21 | 1.38 | 0.87 |
| 1:k:340:THR:C | 1:k:407:ARG:HH21 | 1.80 | 0.87 |
| 1:p:322:GLN:HE21 | 1:q:340:THR:HB | 1.39 | 0.87 |
| 1:u:340:THR:C | 1:u:407:ARG:HH21 | 1.80 | 0.87 |
| 1:3:322:GLN:HE21 | 1:8:340:THR:HB | 1.37 | 0.87 |
| 1:7:340:THR:C | 1:7:407:ARG:HH21 | 1.80 | 0.87 |
| 1:F:322:GLN:HE21 | 1:G:340:THR:HB | 1.38 | 0.87 |
| 1:T:322:GLN:HE21 | 1:U:340:THR:HB | 1.38 | 0.87 |
| 1:T:526:MET:HE2 | 1:T:575:ALA:HA | 1.54 | 0.87 |
| 1:f:340:THR:C | 1:f:407:ARG:HH21 | 1.80 | 0.87 |
| 1:G:322:GLN:HE21 | 1:W:340:THR:HB | 1.39 | 0.87 |
| 1:h:340:THR:C | 1:h:407:ARG:HH21 | 1.80 | 0.87 |
| 1:J:613:ASP:CB | 1:J:732:ARG:HD2 | 2.05 | 0.87 |
| 1:j:340:THR:C | 1:j:407:ARG:HH21 | 1.80 | 0.87 |
| 1:s:340:THR:C | 1:s:407:ARG:HH21 | 1.80 | 0.87 |
| 1:y:526:MET:HE2 | 1:y:575:ALA:HA | 1.54 | 0.87 |
| 1:A:340:THR:HB | 1:B:322:GLN:HE21 | 1.38 | 0.87 |
| 1:A:526:MET:HE2 | 1:A:575:ALA:HA | 1.54 | 0.87 |
| 1:B:340:THR:HB | 1:C:322:GLN:HE21 | 1.38 | 0.87 |
| 1:F:613:ASP:CB | 1:F:732:ARG:HD2 | 2.05 | 0.87 |
| 1:G:613:ASP:CB | 1:G:732:ARG:HD2 | 2.05 | 0.87 |
| 1:I:322:GLN:HE21 | 1:J:340:THR:HB | 1.38 | 0.87 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:613:ASP:CB | 1:M:732:ARG:HD2 | 2.05 | 0.87 |
| 1:N:322:GLN:HE21 | 1:m:340:THR:HB | 1.38 | 0.87 |
| 1:X:613:ASP:CB | 1:X:732:ARG:HD2 | 2.05 | 0.87 |
| 1:p:613:ASP:CB | 1:p:732:ARG:HD2 | 2.05 | 0.87 |
| 1:6:613:ASP:CB | 1:6:732:ARG:HD2 | 2.05 | 0.87 |
| 1:H:526:MET:HE2 | 1:H:575:ALA:HA | 1.54 | 0.87 |
| 1:M:340:THR:HB | 1:c:322:GLN:HE21 | 1.38 | 0.87 |
| 1:O:322:GLN:HE21 | 1:P:340:THR:HB | 1.37 | 0.87 |
| 1:V:526:MET:HE2 | 1:V:575:ALA:HA | 1.54 | 0.87 |
| 1:m:613:ASP:CB | 1:m:732:ARG:HD2 | 2.05 | 0.87 |
| 1:x:613:ASP:CB | 1:x:732:ARG:HD2 | 2.05 | 0.87 |
| 1:7:613:ASP:CB | 1:7:732:ARG:HD2 | 2.05 | 0.87 |
| 1:E:613:ASP:CB | 1:E:732:ARG:HD2 | 2.05 | 0.87 |
| 1:H:340:THR:C | 1:H:407:ARG:HH21 | 1.80 | 0.87 |
| 1:Z:613:ASP:CB | 1:Z:732:ARG:HD2 | 2.05 | 0.87 |
| 1:g:613:ASP:CB | 1:g:732:ARG:HD2 | 2.05 | 0.87 |
| 1:i:613:ASP:CB | 1:i:732:ARG:HD2 | 2.05 | 0.87 |
| 1:r:526:MET:HE2 | 1:r:575:ALA:HA | 1.54 | 0.87 |
| 1:s:526:MET:HE2 | 1:s:575:ALA:HA | 1.54 | 0.87 |
| 1:C:613:ASP:CB | 1:C:732:ARG:HD2 | 2.05 | 0.87 |
| 1:L:322:GLN:HE21 | 1:b:340:THR:HB | 1.38 | 0.87 |
| 1:L:613:ASP:CB | 1:L:732:ARG:HD2 | 2.05 | 0.87 |
| 1:X:330:GLU:OE1 | 1:X:330:GLU:N | 2.08 | 0.87 |
| 1:x:330:GLU:OE1 | 1:x:330:GLU:N | 2.08 | 0.87 |
| 1:J:330:GLU:OE1 | 1:J:330:GLU:N | 2.08 | 0.87 |
| 1:M:330:GLU:OE1 | 1:M:330:GLU:N | 2.08 | 0.87 |
| 1:O:330:GLU:OE1 | 1:O:330:GLU:N | 2.08 | 0.87 |
| 1:Y:526:MET:HE2 | 1:Y:575:ALA:HA | 1.54 | 0.87 |
| 1:3:613:ASP:CB | 1:3:732:ARG:HD2 | 2.05 | 0.87 |
| 1:4:613:ASP:CB | 1:4:732:ARG:HD2 | 2.05 | 0.87 |
| 1:5:526:MET:HE2 | 1:5:575:ALA:HA | 1.54 | 0.87 |
| 1:O:613:ASP:CB | 1:O:732:ARG:HD2 | 2.05 | 0.86 |
| 1:Q:330:GLU:OE1 | 1:Q:330:GLU:N | 2.08 | 0.86 |
| 1:Q:526:MET:HE2 | 1:Q:575:ALA:HA | 1.54 | 0.86 |
| 1:W:330:GLU:OE1 | 1:W:330:GLU:N | 2.08 | 0.86 |
| 1:W:526:MET:HE2 | 1:W:575:ALA:HA | 1.54 | 0.86 |
| 1:d:330:GLU:OE1 | 1:d:330:GLU:N | 2.08 | 0.86 |
| 1:n:613:ASP:CB | 1:n:732:ARG:HD2 | 2.05 | 0.86 |
| 1:o:526:MET:HE2 | 1:o:575:ALA:HA | 1.54 | 0.86 |
| 1:q:330:GLU:OE1 | 1:q:330:GLU:N | 2.08 | 0.86 |
| 1:q:613:ASP:CB | 1:q:732:ARG:HD2 | 2.05 | 0.86 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:613:ASP:CB | 1:1:732:ARG:HD2 | 2.05 | 0.86 |
| 1:3:330:GLU:OE1 | 1:3:330:GLU:N | 2.08 | 0.86 |
| 1:J:526:MET:HE2 | 1:J:575:ALA:HA | 1.54 | 0.86 |
| 1:M:322:GLN:HE21 | 1:N:340:THR:HB | 1.39 | 0.86 |
| 1:Q:613:ASP:CB | 1:Q:732:ARG:HD2 | 2.05 | 0.86 |
| 1:S:330:GLU:OE1 | 1:S:330:GLU:N | 2.08 | 0.86 |
| 1:T:613:ASP:CB | 1:T:732:ARG:HD2 | 2.05 | 0.86 |
| 1:j:330:GLU:OE1 | 1:j:330:GLU:N | 2.08 | 0.86 |
| 1:2:330:GLU:OE1 | 1:2:330:GLU:N | 2.08 | 0.86 |
| 1:5:330:GLU:OE1 | 1:5:330:GLU:N | 2.08 | 0.86 |
| 1:5:613:ASP:CB | 1:5:732:ARG:HD2 | 2.05 | 0.86 |
| 1:B:330:GLU:OE1 | 1:B:330:GLU:N | 2.08 | 0.86 |
| 1:F:330:GLU:OE1 | 1:F:330:GLU:N | 2.08 | 0.86 |
| 1:H:330:GLU:OE1 | 1:H:330:GLU:N | 2.08 | 0.86 |
| 1:I:613:ASP:CB | 1:I:732:ARG:HD2 | 2.05 | 0.86 |
| 1:M:526:MET:HE2 | 1:M:575:ALA:HA | 1.54 | 0.86 |
| 1:P:330:GLU:OE1 | 1:P:330:GLU:N | 2.08 | 0.86 |
| 1:W:613:ASP:CB | 1:W:732:ARG:HD2 | 2.05 | 0.86 |
| 1:Y:322:GLN:HE21 | 1:4:340:THR:HB | 1.39 | 0.86 |
| 1:b:330:GLU:OE1 | 1:b:330:GLU:N | 2.08 | 0.86 |
| 1:c:613:ASP:CB | 1:c:732:ARG:HD2 | 2.05 | 0.86 |
| 1:d:613:ASP:CB | 1:d:732:ARG:HD2 | 2.05 | 0.86 |
| 1:h:613:ASP:CB | 1:h:732:ARG:HD2 | 2.05 | 0.86 |
| 1:q:526:MET:HE2 | 1:q:575:ALA:HA | 1.54 | 0.86 |
| 1:s:330:GLU:OE1 | 1:s:330:GLU:N | 2.08 | 0.86 |
| 1:u:330:GLU:OE1 | 1:u:330:GLU:N | 2.08 | 0.86 |
| 1:2:613:ASP:CB | 1:2:732:ARG:HD2 | 2.05 | 0.86 |
| 1:8:330:GLU:OE1 | 1:8:330:GLU:N | 2.08 | 0.86 |
| 1:H:613:ASP:CB | 1:H:732:ARG:HD2 | 2.05 | 0.86 |
| 1:I:330:GLU:OE1 | 1:I:330:GLU:N | 2.08 | 0.86 |
| 1:J:322:GLN:HE21 | 1:a:340:THR:HB | 1.39 | 0.86 |
| 1:Y:330:GLU:OE1 | 1:Y:330:GLU:N | 2.08 | 0.86 |
| 1:c:330:GLU:OE1 | 1:c:330:GLU:N | 2.08 | 0.86 |
| 1:e:330:GLU:OE1 | 1:e:330:GLU:N | 2.08 | 0.86 |
| 1:f:330:GLU:OE1 | 1:f:330:GLU:N | 2.08 | 0.86 |
| 1:k:613:ASP:CB | 1:k:732:ARG:HD2 | 2.05 | 0.86 |
| 1:n:340:THR:CA | 1:n:407:ARG:NH2 | 2.39 | 0.86 |
| 1:n:340:THR:HB | 1:r:322:GLN:HE21 | 1.39 | 0.86 |
| 1:r:330:GLU:OE1 | 1:r:330:GLU:N | 2.08 | 0.86 |
| 1:4:340:THR:CA | 1:4:407:ARG:NH2 | 2.39 | 0.86 |
| 1:6:330:GLU:OE1 | 1:6:330:GLU:N | 2.08 | 0.86 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:340:THR:HB | 1:R:322:GLN:HE21 | 1.38 | 0.86 |
| 1:H:322:GLN:HE21 | 1:I:340:THR:HB | 1.38 | 0.86 |
| 1:Y:613:ASP:CB | 1:Y:732:ARG:HD2 | 2.05 | 0.86 |
| 1:a:613:ASP:CB | 1:a:732:ARG:HD2 | 2.05 | 0.86 |
| 1:e:613:ASP:CB | 1:e:732:ARG:HD2 | 2.05 | 0.86 |
| 1:g:526:MET:HE2 | 1:g:575:ALA:HA | 1.54 | 0.86 |
| 1:k:330:GLU:OE1 | 1:k:330:GLU:N | 2.08 | 0.86 |
| 1:r:613:ASP:CB | 1:r:732:ARG:HD2 | 2.05 | 0.86 |
| 1:w:330:GLU:OE1 | 1:w:330:GLU:N | 2.08 | 0.86 |
| 1:A:330:GLU:OE1 | 1:A:330:GLU:N | 2.08 | 0.86 |
| 1:C:340:THR:CA | 1:C:407:ARG:NH2 | 2.39 | 0.86 |
| 1:D:613:ASP:CB | 1:D:732:ARG:HD2 | 2.05 | 0.86 |
| 1:K:613:ASP:CB | 1:K:732:ARG:HD2 | 2.05 | 0.86 |
| 1:N:613:ASP:CB | 1:N:732:ARG:HD2 | 2.05 | 0.86 |
| 1:b:613:ASP:CB | 1:b:732:ARG:HD2 | 2.05 | 0.86 |
| 1:d:526:MET:HE2 | 1:d:575:ALA:HA | 1.54 | 0.86 |
| 1:g:330:GLU:OE1 | 1:g:330:GLU:N | 2.08 | 0.86 |
| 1:h:330:GLU:OE1 | 1:h:330:GLU:N | 2.08 | 0.86 |
| 1:k:340:THR:HB | 1:w:322:GLN:HE21 | 1.40 | 0.86 |
| 1:o:330:GLU:OE1 | 1:o:330:GLU:N | 2.08 | 0.86 |
| 1:s:613:ASP:CB | 1:s:732:ARG:HD2 | 2.05 | 0.86 |
| 1:B:613:ASP:CB | 1:B:732:ARG:HD2 | 2.05 | 0.86 |
| 1:L:340:THR:CA | 1:L:407:ARG:NH2 | 2.39 | 0.86 |
| 1:a:340:THR:CA | 1:a:407:ARG:NH2 | 2.39 | 0.86 |
| 1:f:613:ASP:CB | 1:f:732:ARG:HD2 | 2.05 | 0.86 |
| 1:i:330:GLU:OE1 | 1:i:330:GLU:N | 2.08 | 0.86 |
| 1:j:613:ASP:CB | 1:j:732:ARG:HD2 | 2.05 | 0.86 |
| 1:2:526:MET:HE2 | 1:2:575:ALA:HA | 1.54 | 0.86 |
| 1:N:340:THR:CA | 1:N:407:ARG:NH2 | 2.39 | 0.86 |
| 1:c:340:THR:HB | 1:s:322:GLN:HE21 | 1.38 | 0.86 |
| 1:i:526:MET:HE2 | 1:i:575:ALA:HA | 1.54 | 0.86 |
| 1:w:613:ASP:CB | 1:w:732:ARG:HD2 | 2.05 | 0.86 |
| 1:t:322:GLN:HE21 | 1:6:340:THR:HB | 1.38 | 0.86 |
| 1:t:613:ASP:CB | 1:t:732:ARG:HD2 | 2.05 | 0.86 |
| 1:y:613:ASP:CB | 1:y:732:ARG:HD2 | 2.05 | 0.86 |
| 1:j:322:GLN:HE21 | 1:x:340:THR:HB | 1.39 | 0.86 |
| 1:l:330:GLU:OE1 | 1:l:330:GLU:N | 2.08 | 0.86 |
| 1:u:406:LEU:HD21 | 1:u:412:PHE:HB2 | 1.58 | 0.86 |
| 1:w:406:LEU:HD21 | 1:w:412:PHE:HB2 | 1.58 | 0.86 |
| 1:z:613:ASP:CB | 1:z:732:ARG:HD2 | 2.05 | 0.86 |
| 1:E:330:GLU:OE1 | 1:E:330:GLU:N | 2.08 | 0.85 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:340:THR:CA | 1:I:407:ARG:NH2 | 2.39 | 0.85 |
| 1:P:613:ASP:CB | 1:P:732:ARG:HD2 | 2.05 | 0.85 |
| 1:R:613:ASP:CB | 1:R:732:ARG:HD2 | 2.05 | 0.85 |
| 1:S:406:LEU:HD21 | 1:S:412:PHE:HB2 | 1.58 | 0.85 |
| 1:V:406:LEU:HD21 | 1:V:412:PHE:HB2 | 1.58 | 0.85 |
| 1:V:613:ASP:CB | 1:V:732:ARG:HD2 | 2.05 | 0.85 |
| 1:X:340:THR:CA | 1:X:407:ARG:NH2 | 2.39 | 0.85 |
| 1:e:406:LEU:HD21 | 1:e:412:PHE:HB2 | 1.58 | 0.85 |
| 1:l:613:ASP:CB | 1:l:732:ARG:HD2 | 2.05 | 0.85 |
| 1:R:330:GLU:OE1 | 1:R:330:GLU:N | 2.08 | 0.85 |
| 1:R:340:THR:HB | 1:V:322:GLN:HE21 | 1.38 | 0.85 |
| 1:U:613:ASP:CB | 1:U:732:ARG:HD2 | 2.05 | 0.85 |
| 1:X:340:THR:HB | 1:f:322:GLN:HE21 | 1.39 | 0.85 |
| 1:c:340:THR:CA | 1:c:407:ARG:NH2 | 2.39 | 0.85 |
| 1:f:340:THR:HB | 1:z:322:GLN:HE21 | 1.38 | 0.85 |
| 1:m:330:GLU:OE1 | 1:m:330:GLU:N | 2.08 | 0.85 |
| 1:v:613:ASP:CB | 1:v:732:ARG:HD2 | 2.05 | 0.85 |
| 1:y:406:LEU:HD21 | 1:y:412:PHE:HB2 | 1.58 | 0.85 |
| 1:z:330:GLU:OE1 | 1:z:330:GLU:N | 2.08 | 0.85 |
| 1:7:330:GLU:OE1 | 1:7:330:GLU:N | 2.08 | 0.85 |
| 1:8:613:ASP:CB | 1:8:732:ARG:HD2 | 2.05 | 0.85 |
| 1:C:330:GLU:OE1 | 1:C:330:GLU:N | 2.08 | 0.85 |
| 1:V:330:GLU:OE1 | 1:V:330:GLU:N | 2.08 | 0.85 |
| 1:m:322:GLN:HE21 | 1:s:340:THR:HB | 1.39 | 0.85 |
| 1:n:406:LEU:HD21 | 1:n:412:PHE:HB2 | 1.58 | 0.85 |
| 1:o:322:GLN:HE21 | 1:7:340:THR:HB | 1.38 | 0.85 |
| 1:o:613:ASP:CB | 1:o:732:ARG:HD2 | 2.05 | 0.85 |
| 1:x:340:THR:CA | 1:x:407:ARG:NH2 | 2.39 | 0.85 |
| 1:z:340:THR:CA | 1:z:407:ARG:NH2 | 2.39 | 0.85 |
| 1:1:330:GLU:OE1 | 1:1:330:GLU:N | 2.08 | 0.85 |
| 1:8:340:THR:CA | 1:8:407:ARG:NH2 | 2.39 | 0.85 |
| 1:D:340:THR:CA | 1:D:407:ARG:NH2 | 2.39 | 0.85 |
| 1:E:340:THR:CA | 1:E:407:ARG:NH2 | 2.39 | 0.85 |
| 1:K:340:THR:CA | 1:K:407:ARG:NH2 | 2.39 | 0.85 |
| 1:L:330:GLU:OE1 | 1:L:330:GLU:N | 2.08 | 0.85 |
| 1:N:330:GLU:OE1 | 1:N:330:GLU:N | 2.08 | 0.85 |
| 1:N:406:LEU:HD21 | 1:N:412:PHE:HB2 | 1.58 | 0.85 |
| 1:O:340:THR:CA | 1:O:407:ARG:NH2 | 2.39 | 0.85 |
| 1:Z:330:GLU:OE1 | 1:Z:330:GLU:N | 2.08 | 0.85 |
| 1:a:406:LEU:HD21 | 1:a:412:PHE:HB2 | 1.58 | 0.85 |
| 1:i:340:THR:CA | 1:i:407:ARG:NH2 | 2.39 | 0.85 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:y:330:GLU:OE1 | 1:y:330:GLU:N | 2.08 | 0.85 |
| 1:3:340:THR:CA | 1:3:407:ARG:NH2 | 2.39 | 0.85 |
| 1:4:406:LEU:HD21 | 1:4:412:PHE:HB2 | 1.58 | 0.85 |
| 1:A:613:ASP:CB | 1:A:732:ARG:HD2 | 2.05 | 0.85 |
| 1:P:340:THR:CA | 1:P:407:ARG:NH2 | 2.39 | 0.85 |
| 1:T:330:GLU:OE1 | 1:T:330:GLU:N | 2.08 | 0.85 |
| 1:b:340:THR:CA | 1:b:407:ARG:NH2 | 2.39 | 0.85 |
| 1:t:330:GLU:OE1 | 1:t:330:GLU:N | 2.08 | 0.85 |
| 1:B:340:THR:CA | 1:B:407:ARG:NH2 | 2.39 | 0.85 |
| 1:H:340:THR:HB | 1:Z:322:GLN:HE21 | 1.39 | 0.85 |
| 1:W:406:LEU:HD21 | 1:W:412:PHE:HB2 | 1.58 | 0.85 |
| 1:a:330:GLU:OE1 | 1:a:330:GLU:N | 2.08 | 0.85 |
| 1:g:340:THR:CA | 1:g:407:ARG:NH2 | 2.39 | 0.85 |
| 1:j:340:THR:HB | 1:l:322:GLN:HE21 | 1.39 | 0.85 |
| 1:l:340:THR:CA | 1:l:407:ARG:NH2 | 2.39 | 0.85 |
| 1:7:340:THR:CA | 1:7:407:ARG:NH2 | 2.39 | 0.85 |
| 1:A:322:GLN:HE21 | 1:E:340:THR:HB | 1.39 | 0.85 |
| 1:H:406:LEU:HD21 | 1:H:412:PHE:HB2 | 1.58 | 0.85 |
| 1:R:340:THR:CA | 1:R:407:ARG:NH2 | 2.39 | 0.85 |
| 1:g:406:LEU:HD21 | 1:g:412:PHE:HB2 | 1.59 | 0.85 |
| 1:h:406:LEU:HD21 | 1:h:412:PHE:HB2 | 1.58 | 0.85 |
| 1:i:406:LEU:HD21 | 1:i:412:PHE:HB2 | 1.59 | 0.85 |
| 1:4:330:GLU:OE1 | 1:4:330:GLU:N | 2.08 | 0.85 |
| 1:D:330:GLU:OE1 | 1:D:330:GLU:N | 2.08 | 0.85 |
| 1:T:340:THR:HB | 1:i:322:GLN:HE21 | 1.38 | 0.85 |
| 1:U:330:GLU:OE1 | 1:U:330:GLU:N | 2.08 | 0.85 |
| 1:n:330:GLU:OE1 | 1:n:330:GLU:N | 2.08 | 0.85 |
| 1:q:406:LEU:HD21 | 1:q:412:PHE:HB2 | 1.58 | 0.85 |
| 1:s:406:LEU:HD21 | 1:s:412:PHE:HB2 | 1.58 | 0.85 |
| 1:t:340:THR:CA | 1:t:407:ARG:NH2 | 2.39 | 0.85 |
| 1:G:340:THR:CA | 1:G:407:ARG:NH2 | 2.39 | 0.85 |
| 1:S:613:ASP:CB | 1:S:732:ARG:HD2 | 2.05 | 0.85 |
| 1:p:340:THR:CA | 1:p:407:ARG:NH2 | 2.39 | 0.85 |
| 1:v:330:GLU:OE1 | 1:v:330:GLU:N | 2.08 | 0.85 |
| 1:K:330:GLU:OE1 | 1:K:330:GLU:N | 2.08 | 0.85 |
| 1:g:322:GLN:HE21 | 1:1:340:THR:HB | 1.38 | 0.85 |
| 1:k:406:LEU:HD21 | 1:k:412:PHE:HB2 | 1.59 | 0.85 |
| 1:q:340:THR:CA | 1:q:407:ARG:NH2 | 2.39 | 0.85 |
| 1:8:406:LEU:HD21 | 1:8:412:PHE:HB2 | 1.58 | 0.85 |
| 1:D:340:THR:HB | 1:E:322:GLN:HE21 | 1.39 | 0.84 |
| 1:D:406:LEU:HD21 | 1:D:412:PHE:HB2 | 1.58 | 0.84 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:406:LEU:HD21 | 1:P:412:PHE:HB2 | 1.59 | 0.84 |
| 1:u:613:ASP:CB | 1:u:732:ARG:HD2 | 2.05 | 0.84 |
| 1:G:330:GLU:OE1 | 1:G:330:GLU:N | 2.08 | 0.84 |
| 1:W:340:THR:CA | 1:W:407:ARG:NH2 | 2.39 | 0.84 |
| 1:G:406:LEU:HD21 | 1:G:412:PHE:HB2 | 1.58 | 0.84 |
| 1:K:406:LEU:HD21 | 1:K:412:PHE:HB2 | 1.59 | 0.84 |
| 1:Q:406:LEU:HD21 | 1:Q:412:PHE:HB2 | 1.58 | 0.84 |
| 1:f:340:THR:CA | 1:f:407:ARG:NH2 | 2.39 | 0.84 |
| 1:j:340:THR:CA | 1:j:407:ARG:NH2 | 2.39 | 0.84 |
| 1:3:406:LEU:HD21 | 1:3:412:PHE:HB2 | 1.58 | 0.84 |
| 1:6:406:LEU:HD21 | 1:6:412:PHE:HB2 | 1.58 | 0.84 |
| 1:F:406:LEU:HD21 | 1:F:412:PHE:HB2 | 1.58 | 0.84 |
| 1:O:406:LEU:HD21 | 1:O:412:PHE:HB2 | 1.58 | 0.84 |
| 1:U:340:THR:CA | 1:U:407:ARG:NH2 | 2.39 | 0.84 |
| 1:p:330:GLU:OE1 | 1:p:330:GLU:N | 2.08 | 0.84 |
| 1:p:406:LEU:HD21 | 1:p:412:PHE:HB2 | 1.58 | 0.84 |
| 1:5:406:LEU:HD21 | 1:5:412:PHE:HB2 | 1.58 | 0.84 |
| 1:K:340:THR:HB | 1:7:322:GLN:HE21 | 1.38 | 0.84 |
| 1:v:340:THR:CA | 1:v:407:ARG:NH2 | 2.39 | 0.84 |
| 1:v:406:LEU:HD21 | 1:v:412:PHE:HB2 | 1.58 | 0.84 |
| 1:U:406:LEU:HD21 | 1:U:412:PHE:HB2 | 1.59 | 0.84 |
| 1:C:406:LEU:HD21 | 1:C:412:PHE:HB2 | 1.58 | 0.84 |
| 1:t:340:THR:HB | 1:y:322:GLN:HE21 | 1.38 | 0.84 |
| 1:u:340:THR:CA | 1:u:407:ARG:NH2 | 2.39 | 0.84 |
| 1:5:340:THR:CA | 1:5:407:ARG:NH2 | 2.39 | 0.84 |
| 1:f:406:LEU:HD21 | 1:f:412:PHE:HB2 | 1.59 | 0.84 |
| 1:2:406:LEU:HD21 | 1:2:412:PHE:HB2 | 1.58 | 0.84 |
| 1:L:406:LEU:HD21 | 1:L:412:PHE:HB2 | 1.58 | 0.84 |
| 1:Q:340:THR:CA | 1:Q:407:ARG:NH2 | 2.39 | 0.84 |
| 1:S:340:THR:CA | 1:S:407:ARG:NH2 | 2.39 | 0.84 |
| 1:d:406:LEU:HD21 | 1:d:412:PHE:HB2 | 1.58 | 0.84 |
| 1:j:406:LEU:HD21 | 1:j:412:PHE:HB2 | 1.58 | 0.84 |
| 1:x:406:LEU:HD21 | 1:x:412:PHE:HB2 | 1.58 | 0.84 |
| 1:Z:406:LEU:HD21 | 1:Z:412:PHE:HB2 | 1.58 | 0.83 |
| 1:m:406:LEU:HD21 | 1:m:412:PHE:HB2 | 1.58 | 0.83 |
| 1:E:406:LEU:HD21 | 1:E:412:PHE:HB2 | 1.59 | 0.83 |
| 1:I:406:LEU:HD21 | 1:I:412:PHE:HB2 | 1.58 | 0.83 |
| 1:X:406:LEU:HD21 | 1:X:412:PHE:HB2 | 1.58 | 0.83 |
| 1:7:406:LEU:HD21 | 1:7:412:PHE:HB2 | 1.59 | 0.83 |
| 1:J:340:THR:CA | 1:J:407:ARG:NH2 | 2.39 | 0.83 |
| 1:T:340:THR:CA | 1:T:407:ARG:NH2 | 2.39 | 0.83 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:c:406:LEU:HD21 | 1:c:412:PHE:HB2 | 1.58 | 0.83 |
| 1:T:406:LEU:HD21 | 1:T:412:PHE:HB2 | 1.58 | 0.83 |
| 1:o:406:LEU:HD21 | 1:o:412:PHE:HB2 | 1.58 | 0.83 |
| 1:r:340:THR:CA | 1:r:407:ARG:NH2 | 2.39 | 0.83 |
| 1:1:406:LEU:HD21 | 1:1:412:PHE:HB2 | 1.58 | 0.83 |
| 1:A:406:LEU:HD21 | 1:A:412:PHE:HB2 | 1.58 | 0.83 |
| 1:M:340:THR:CA | 1:M:407:ARG:NH2 | 2.39 | 0.83 |
| 1:Y:340:THR:CA | 1:Y:407:ARG:NH2 | 2.39 | 0.83 |
| 1:b:406:LEU:HD21 | 1:b:412:PHE:HB2 | 1.59 | 0.83 |
| 1:1:340:THR:CA | 1:1:407:ARG:NH2 | 2.39 | 0.83 |
| 1:B:406:LEU:HD21 | 1:B:412:PHE:HB2 | 1.59 | 0.83 |
| 1:r:406:LEU:HD21 | 1:r:412:PHE:HB2 | 1.58 | 0.83 |
| 1:s:340:THR:CA | 1:s:407:ARG:NH2 | 2.39 | 0.83 |
| 1:H:340:THR:CA | 1:H:407:ARG:NH2 | 2.39 | 0.83 |
| 1:Y:406:LEU:HD21 | 1:Y:412:PHE:HB2 | 1.58 | 0.83 |
| 1:o:340:THR:CA | 1:o:407:ARG:NH2 | 2.39 | 0.83 |
| 1:A:340:THR:CA | 1:A:407:ARG:NH2 | 2.39 | 0.82 |
| 1:V:340:THR:CA | 1:V:407:ARG:NH2 | 2.39 | 0.82 |
| 1:y:340:THR:CA | 1:y:407:ARG:NH2 | 2.39 | 0.82 |
| 1:z:406:LEU:HD21 | 1:z:412:PHE:HB2 | 1.58 | 0.82 |
| 1:F:340:THR:CA | 1:F:407:ARG:NH2 | 2.39 | 0.82 |
| 1:m:340:THR:CA | 1:m:407:ARG:NH2 | 2.39 | 0.82 |
| 1:l:406:LEU:HD21 | 1:l:412:PHE:HB2 | 1.58 | 0.82 |
| 1:t:406:LEU:HD21 | 1:t:412:PHE:HB2 | 1.58 | 0.82 |
| 1:J:406:LEU:HD21 | 1:J:412:PHE:HB2 | 1.59 | 0.82 |
| 1:M:406:LEU:HD21 | 1:M:412:PHE:HB2 | 1.59 | 0.82 |
| 1:Z:340:THR:CA | 1:Z:407:ARG:NH2 | 2.39 | 0.82 |
| 1:6:340:THR:CA | 1:6:407:ARG:NH2 | 2.39 | 0.82 |
| 1:w:340:THR:CA | 1:w:407:ARG:NH2 | 2.39 | 0.81 |
| 1:R:406:LEU:HD21 | 1:R:412:PHE:HB2 | 1.58 | 0.81 |
| 1:O:626:HIS:CD2 | 1:n:736:ARG:HH21 | 1.99 | 0.81 |
| 1:e:340:THR:CA | 1:e:407:ARG:NH2 | 2.39 | 0.81 |
| 1:S:736:ARG:HH21 | 1:U:626:HIS:CD2 | 1.99 | 0.81 |
| 1:i:736:ARG:HH21 | 1:j:626:HIS:CD2 | 1.99 | 0.81 |
| 1:u:736:ARG:HH21 | 1:v:626:HIS:CD2 | 1.99 | 0.81 |
| 1:3:626:HIS:CD2 | 1:4:736:ARG:HH21 | 1.99 | 0.81 |
| 1:f:626:HIS:CD2 | 1:g:736:ARG:HH21 | 1.99 | 0.81 |
| 1:k:340:THR:CA | 1:k:407:ARG:NH2 | 2.39 | 0.81 |
| 1:q:736:ARG:HH21 | 1:r:626:HIS:CD2 | 1.99 | 0.81 |
| 1:B:626:HIS:CD2 | 1:L:736:ARG:HH21 | 1.99 | 0.81 |
| 1:C:736:ARG:HH21 | 1:b:626:HIS:CD2 | 1.99 | 0.81 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:626:HIS:CD2 | 1:Q:736:ARG:HH21 | 1.99 | 0.81 |
| 1:W:736:ARG:HH21 | 1:Y:626:HIS:CD2 | 1.99 | 0.81 |
| 1:o:736:ARG:HH21 | 1:p:626:HIS:CD2 | 1.99 | 0.81 |
| 1:t:626:HIS:CD2 | 1:v:736:ARG:HH21 | 1.99 | 0.81 |
| 1:5:736:ARG:HH21 | 1:6:626:HIS:CD2 | 1.99 | 0.81 |
| 1:B:736:ARG:HH21 | 1:J:626:HIS:CD2 | 1.99 | 0.81 |
| 1:E:626:HIS:CD2 | 1:F:736:ARG:HH21 | 1.99 | 0.81 |
| 1:M:626:HIS:CD2 | 1:b:736:ARG:HH21 | 1.99 | 0.81 |
| 1:C:626:HIS:CD2 | 1:M:736:ARG:HH21 | 1.99 | 0.81 |
| 1:E:736:ARG:HH21 | 1:Q:626:HIS:CD2 | 1.99 | 0.81 |
| 1:J:736:ARG:HH21 | 1:L:626:HIS:CD2 | 1.99 | 0.81 |
| 1:K:626:HIS:CD2 | 1:8:736:ARG:HH21 | 1.99 | 0.81 |
| 1:N:736:ARG:HH21 | 1:P:626:HIS:CD2 | 1.99 | 0.81 |
| 1:a:736:ARG:HH21 | 1:8:626:HIS:CD2 | 1.99 | 0.81 |
| 1:d:340:THR:CA | 1:d:407:ARG:NH2 | 2.39 | 0.81 |
| 1:h:340:THR:CA | 1:h:407:ARG:NH2 | 2.39 | 0.81 |
| 1:i:626:HIS:CD2 | 1:k:736:ARG:HH21 | 1.99 | 0.81 |
| 1:2:340:THR:CA | 1:2:407:ARG:NH2 | 2.39 | 0.81 |
| 1:5:626:HIS:CD2 | 1:7:736:ARG:HH21 | 1.99 | 0.81 |
| 1:6:736:ARG:HH21 | 1:7:626:HIS:CD2 | 1.99 | 0.81 |
| 1:D:626:HIS:CD2 | 1:P:736:ARG:HH21 | 1.99 | 0.81 |
| 1:R:626:HIS:CD2 | 1:U:736:ARG:HH21 | 1.99 | 0.81 |
| 1:c:736:ARG:HH21 | 1:o:626:HIS:CD2 | 1.99 | 0.80 |
| 1:g:626:HIS:CD2 | 1:h:736:ARG:HH21 | 1.99 | 0.80 |
| 1:x:736:ARG:HH21 | 1:y:626:HIS:CD2 | 1.99 | 0.80 |
| 1:O:736:ARG:HH21 | 1:m:626:HIS:CD2 | 1.99 | 0.80 |
| 1:D:736:ARG:HH21 | 1:N:626:HIS:CD2 | 1.99 | 0.80 |
| 1:T:626:HIS:CD2 | 1:l:736:ARG:HH21 | 1.99 | 0.80 |
| 1:Z:626:HIS:CD2 | 1:3:736:ARG:HH21 | 1.99 | 0.80 |
| 1:t:736:ARG:HH21 | 1:u:626:HIS:CD2 | 1.99 | 0.80 |
| 1:A:626:HIS:CD2 | 1:I:736:ARG:HH21 | 1.99 | 0.80 |
| 1:K:736:ARG:HH21 | 1:a:626:HIS:CD2 | 1.99 | 0.80 |
| 1:V:626:HIS:CD2 | 1:X:736:ARG:HH21 | 1.99 | 0.80 |
| 1:z:736:ARG:HH21 | 1:1:626:HIS:CD2 | 1.99 | 0.80 |
| 1:T:736:ARG:HH21 | 1:d:626:HIS:CD2 | 1.99 | 0.80 |
| 1:X:626:HIS:CD2 | 1:e:736:ARG:HH21 | 1.99 | 0.80 |
| 1:A:736:ARG:HH21 | 1:G:626:HIS:CD2 | 2.00 | 0.80 |
| 1:H:736:ARG:HH21 | 1:W:626:HIS:CD2 | 1.99 | 0.80 |
| 1:R:736:ARG:HH21 | 1:S:626:HIS:CD2 | 1.99 | 0.80 |
| 1:1:736:ARG:HH21 | 1:2:626:HIS:CD2 | 1.99 | 0.80 |
| 1:f:736:ARG:HH21 | 1:h:626:HIS:CD2 | 1.99 | 0.80 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:736:ARG:HH21 | 1:k:626:HIS:CD2 | 1.99 | 0.80 |
| 1:d:736:ARG:HH21 | 1:l:626:HIS:CD2 | 1.99 | 0.80 |
| 1:w:626:HIS:CD2 | 1:y:736:ARG:HH21 | 1.99 | 0.80 |
| 1:z:626:HIS:CD2 | 1:2:736:ARG:HH21 | 1.99 | 0.80 |
| 1:q:626:HIS:CD2 | 1:s:736:ARG:HH21 | 1.99 | 0.79 |
| 1:V:736:ARG:HH21 | 1:e:626:HIS:CD2 | 1.99 | 0.79 |
| 1:r:736:ARG:HH21 | 1:s:626:HIS:CD2 | 1.99 | 0.79 |
| 1:H:626:HIS:CD2 | 1:Y:736:ARG:HH21 | 1.99 | 0.79 |
| 1:Z:736:ARG:HH21 | 1:4:626:HIS:CD2 | 1.99 | 0.79 |
| 1:c:626:HIS:CD2 | 1:p:736:ARG:HH21 | 1.99 | 0.79 |
| 1:G:736:ARG:HH21 | 1:I:626:HIS:CD2 | 1.99 | 0.79 |
| 1:m:736:ARG:HH21 | 1:n:626:HIS:CD2 | 1.99 | 0.79 |
| 1:T:429:HIS:CD2 | 1:T:610:GLN:OE1 | 2.36 | 0.79 |
| 1:A:429:HIS:CD2 | 1:A:610:GLN:OE1 | 2.36 | 0.79 |
| 1:S:429:HIS:CD2 | 1:S:610:GLN:OE1 | 2.36 | 0.79 |
| 1:d:429:HIS:CD2 | 1:d:610:GLN:OE1 | 2.36 | 0.79 |
| 1:o:429:HIS:CD2 | 1:o:610:GLN:OE1 | 2.36 | 0.79 |
| 1:u:429:HIS:CD2 | 1:u:610:GLN:OE1 | 2.36 | 0.79 |
| 1:1:429:HIS:CD2 | 1:1:610:GLN:OE1 | 2.36 | 0.79 |
| 1:P:429:HIS:CD2 | 1:P:610:GLN:OE1 | 2.36 | 0.79 |
| 1:l:429:HIS:CD2 | 1:l:610:GLN:OE1 | 2.36 | 0.79 |
| 1:n:429:HIS:CD2 | 1:n:610:GLN:OE1 | 2.36 | 0.79 |
| 1:z:429:HIS:CD2 | 1:z:610:GLN:OE1 | 2.36 | 0.79 |
| 1:4:429:HIS:CD2 | 1:4:610:GLN:OE1 | 2.36 | 0.79 |
| 1:Q:429:HIS:CD2 | 1:Q:610:GLN:OE1 | 2.36 | 0.79 |
| 1:X:429:HIS:CD2 | 1:X:610:GLN:OE1 | 2.36 | 0.79 |
| 1:x:429:HIS:CD2 | 1:x:610:GLN:OE1 | 2.36 | 0.79 |
| 1:2:429:HIS:CD2 | 1:2:610:GLN:OE1 | 2.36 | 0.79 |
| 1:5:429:HIS:CD2 | 1:5:610:GLN:OE1 | 2.36 | 0.79 |
| 1:8:429:HIS:CD2 | 1:8:610:GLN:OE1 | 2.36 | 0.79 |
| 1:K:429:HIS:CD2 | 1:K:610:GLN:OE1 | 2.36 | 0.78 |
| 1:g:429:HIS:CD2 | 1:g:610:GLN:OE1 | 2.36 | 0.78 |
| 1:i:429:HIS:CD2 | 1:i:610:GLN:OE1 | 2.36 | 0.78 |
| 1:j:429:HIS:CD2 | 1:j:610:GLN:OE1 | 2.36 | 0.78 |
| 1:k:429:HIS:CD2 | 1:k:610:GLN:OE1 | 2.36 | 0.78 |
| 1:p:429:HIS:CD2 | 1:p:610:GLN:OE1 | 2.36 | 0.78 |
| 1:D:429:HIS:CD2 | 1:D:610:GLN:OE1 | 2.36 | 0.78 |
| 1:F:429:HIS:CD2 | 1:F:610:GLN:OE1 | 2.36 | 0.78 |
| 1:G:429:HIS:CD2 | 1:G:610:GLN:OE1 | 2.36 | 0.78 |
| 1:Z:429:HIS:CD2 | 1:Z:610:GLN:OE1 | 2.36 | 0.78 |
| 1:e:429:HIS:CD2 | 1:e:610:GLN:OE1 | 2.36 | 0.78 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:f:429:HIS:CD2 | 1:f:610:GLN:OE1 | 2.36 | 0.78 |
| 1:h:429:HIS:CD2 | 1:h:610:GLN:OE1 | 2.36 | 0.78 |
| 1:s:429:HIS:CD2 | 1:s:610:GLN:OE1 | 2.36 | 0.78 |
| 1:H:429:HIS:CD2 | 1:H:610:GLN:OE1 | 2.36 | 0.78 |
| 1:m:429:HIS:CD2 | 1:m:610:GLN:OE1 | 2.36 | 0.78 |
| 1:w:429:HIS:CD2 | 1:w:610:GLN:OE1 | 2.36 | 0.78 |
| 1:6:429:HIS:CD2 | 1:6:610:GLN:OE1 | 2.36 | 0.78 |
| 1:3:429:HIS:CD2 | 1:3:610:GLN:OE1 | 2.36 | 0.78 |
| 1:B:429:HIS:CD2 | 1:B:610:GLN:OE1 | 2.36 | 0.78 |
| 1:E:429:HIS:CD2 | 1:E:610:GLN:OE1 | 2.36 | 0.78 |
| 1:J:429:HIS:CD2 | 1:J:610:GLN:OE1 | 2.36 | 0.78 |
| 1:M:429:HIS:CD2 | 1:M:610:GLN:OE1 | 2.36 | 0.78 |
| 1:7:429:HIS:CD2 | 1:7:610:GLN:OE1 | 2.36 | 0.78 |
| 1:L:429:HIS:CD2 | 1:L:610:GLN:OE1 | 2.36 | 0.78 |
| 1:O:429:HIS:CD2 | 1:O:610:GLN:OE1 | 2.36 | 0.78 |
| 1:a:429:HIS:CD2 | 1:a:610:GLN:OE1 | 2.36 | 0.78 |
| 1:b:429:HIS:CD2 | 1:b:610:GLN:OE1 | 2.36 | 0.78 |
| 1:C:429:HIS:CD2 | 1:C:610:GLN:OE1 | 2.36 | 0.78 |
| 1:N:429:HIS:CD2 | 1:N:610:GLN:OE1 | 2.36 | 0.78 |
| 1:Y:429:HIS:CD2 | 1:Y:610:GLN:OE1 | 2.36 | 0.78 |
| 1:y:429:HIS:CD2 | 1:y:610:GLN:OE1 | 2.36 | 0.78 |
| 1:W:429:HIS:CD2 | 1:W:610:GLN:OE1 | 2.36 | 0.78 |
| 1:q:429:HIS:CD2 | 1:q:610:GLN:OE1 | 2.36 | 0.78 |
| 1:r:429:HIS:CD2 | 1:r:610:GLN:OE1 | 2.36 | 0.78 |
| 1:V:429:HIS:CD2 | 1:V:610:GLN:OE1 | 2.36 | 0.78 |
| 1:v:429:HIS:CD2 | 1:v:610:GLN:OE1 | 2.36 | 0.78 |
| 1:R:429:HIS:CD2 | 1:R:610:GLN:OE1 | 2.36 | 0.77 |
| 1:U:429:HIS:CD2 | 1:U:610:GLN:OE1 | 2.36 | 0.77 |
| 1:S:251:PRO:HG3 | 1:S:374:MET:HE3 | 1.67 | 0.77 |
| 1:u:251:PRO:HG3 | 1:u:374:MET:HE3 | 1.67 | 0.77 |
| 1:t:429:HIS:CD2 | 1:t:610:GLN:OE1 | 2.36 | 0.77 |
| 1:D:251:PRO:HG3 | 1:D:374:MET:HE3 | 1.67 | 0.77 |
| 1:I:429:HIS:CD2 | 1:I:610:GLN:OE1 | 2.36 | 0.77 |
| 1:K:251:PRO:HG3 | 1:K:374:MET:HE3 | 1.67 | 0.77 |
| 1:R:251:PRO:HG3 | 1:R:374:MET:HE3 | 1.67 | 0.77 |
| 1:a:251:PRO:HG3 | 1:a:374:MET:HE3 | 1.67 | 0.77 |
| 1:g:251:PRO:HG3 | 1:g:374:MET:HE3 | 1.67 | 0.77 |
| 1:t:251:PRO:HG3 | 1:t:374:MET:HE3 | 1.67 | 0.77 |
| 1:8:251:PRO:HG3 | 1:8:374:MET:HE3 | 1.67 | 0.77 |
| 1:M:251:PRO:HG3 | 1:M:374:MET:HE3 | 1.67 | 0.77 |
| 1:N:251:PRO:HG3 | 1:N:374:MET:HE3 | 1.67 | 0.77 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:251:PRO:HG3 | 1:P:374:MET:HE3 | 1.67 | 0.77 |
| 1:c:429:HIS:CD2 | 1:c:610:GLN:OE1 | 2.36 | 0.77 |
| 1:i:251:PRO:HG3 | 1:i:374:MET:HE3 | 1.67 | 0.77 |
| 1:f:251:PRO:HG3 | 1:f:374:MET:HE3 | 1.67 | 0.77 |
| 1:A:251:PRO:HG3 | 1:A:374:MET:HE3 | 1.67 | 0.77 |
| 1:E:613:ASP:OD1 | 1:E:732:ARG:HD3 | 1.85 | 0.77 |
| 1:Q:251:PRO:HG3 | 1:Q:374:MET:HE3 | 1.67 | 0.77 |
| 1:U:251:PRO:HG3 | 1:U:374:MET:HE3 | 1.67 | 0.77 |
| 1:Y:251:PRO:HG3 | 1:Y:374:MET:HE3 | 1.67 | 0.77 |
| 1:j:251:PRO:HG3 | 1:j:374:MET:HE3 | 1.67 | 0.77 |
| 1:o:251:PRO:HG3 | 1:o:374:MET:HE3 | 1.67 | 0.77 |
| 1:r:251:PRO:HG3 | 1:r:374:MET:HE3 | 1.67 | 0.77 |
| 1:5:251:PRO:HG3 | 1:5:374:MET:HE3 | 1.67 | 0.77 |
| 1:7:613:ASP:OD1 | 1:7:732:ARG:HD3 | 1.85 | 0.77 |
| 1:J:251:PRO:HG3 | 1:J:374:MET:HE3 | 1.67 | 0.77 |
| 1:v:251:PRO:HG3 | 1:v:374:MET:HE3 | 1.67 | 0.77 |
| 1:w:251:PRO:HG3 | 1:w:374:MET:HE3 | 1.67 | 0.77 |
| 1:J:613:ASP:OD1 | 1:J:732:ARG:HD3 | 1.85 | 0.77 |
| 1:M:613:ASP:OD1 | 1:M:732:ARG:HD3 | 1.85 | 0.77 |
| 1:T:613:ASP:OD1 | 1:T:732:ARG:HD3 | 1.85 | 0.77 |
| 1:d:613:ASP:OD1 | 1:d:732:ARG:HD3 | 1.85 | 0.77 |
| 1:1:613:ASP:OD1 | 1:1:732:ARG:HD3 | 1.85 | 0.77 |
| 1:4:251:PRO:HG3 | 1:4:374:MET:HE3 | 1.67 | 0.77 |
| 1:P:613:ASP:OD1 | 1:P:732:ARG:HD3 | 1.85 | 0.76 |
| 1:n:251:PRO:HG3 | 1:n:374:MET:HE3 | 1.67 | 0.76 |
| 1:2:613:ASP:OD1 | 1:2:732:ARG:HD3 | 1.85 | 0.76 |
| 1:A:613:ASP:OD1 | 1:A:732:ARG:HD3 | 1.85 | 0.76 |
| 1:F:251:PRO:HG3 | 1:F:374:MET:HE3 | 1.67 | 0.76 |
| 1:c:613:ASP:OD1 | 1:c:732:ARG:HD3 | 1.85 | 0.76 |
| 1:e:251:PRO:HG3 | 1:e:374:MET:HE3 | 1.67 | 0.76 |
| 1:8:613:ASP:OD1 | 1:8:732:ARG:HD3 | 1.85 | 0.76 |
| 1:C:613:ASP:OD1 | 1:C:732:ARG:HD3 | 1.85 | 0.76 |
| 1:I:613:ASP:OD1 | 1:I:732:ARG:HD3 | 1.85 | 0.76 |
| 1:O:251:PRO:HG3 | 1:O:374:MET:HE3 | 1.67 | 0.76 |
| 1:X:613:ASP:OD1 | 1:X:732:ARG:HD3 | 1.85 | 0.76 |
| 1:c:251:PRO:HG3 | 1:c:374:MET:HE3 | 1.67 | 0.76 |
| 1:r:613:ASP:OD1 | 1:r:732:ARG:HD3 | 1.85 | 0.76 |
| 1:x:613:ASP:OD1 | 1:x:732:ARG:HD3 | 1.85 | 0.76 |
| 1:5:613:ASP:OD1 | 1:5:732:ARG:HD3 | 1.85 | 0.76 |
| 1:6:251:PRO:HG3 | 1:6:374:MET:HE3 | 1.67 | 0.76 |
| 1:L:613:ASP:OD1 | 1:L:732:ARG:HD3 | 1.85 | 0.76 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:613:ASP:OD1 | 1:Q:732:ARG:HD3 | 1.85 | 0.76 |
| 1:U:613:ASP:OD1 | 1:U:732:ARG:HD3 | 1.85 | 0.76 |
| 1:Y:613:ASP:OD1 | 1:Y:732:ARG:HD3 | 1.85 | 0.76 |
| 1:e:613:ASP:OD1 | 1:e:732:ARG:HD3 | 1.85 | 0.76 |
| 1:o:613:ASP:OD1 | 1:o:732:ARG:HD3 | 1.85 | 0.76 |
| 1:w:613:ASP:OD1 | 1:w:732:ARG:HD3 | 1.85 | 0.76 |
| 1:G:251:PRO:HG3 | 1:G:374:MET:HE3 | 1.67 | 0.76 |
| 1:h:613:ASP:OD1 | 1:h:732:ARG:HD3 | 1.85 | 0.76 |
| 1:t:613:ASP:OD1 | 1:t:732:ARG:HD3 | 1.85 | 0.76 |
| 1:y:613:ASP:OD1 | 1:y:732:ARG:HD3 | 1.85 | 0.76 |
| 1:I:251:PRO:HG3 | 1:I:374:MET:HE3 | 1.67 | 0.76 |
| 1:R:613:ASP:OD1 | 1:R:732:ARG:HD3 | 1.85 | 0.76 |
| 1:V:613:ASP:OD1 | 1:V:732:ARG:HD3 | 1.85 | 0.76 |
| 1:k:613:ASP:OD1 | 1:k:732:ARG:HD3 | 1.85 | 0.76 |
| 1:v:613:ASP:OD1 | 1:v:732:ARG:HD3 | 1.85 | 0.76 |
| 1:1:251:PRO:HG3 | 1:1:374:MET:HE3 | 1.67 | 0.76 |
| 1:3:251:PRO:HG3 | 1:3:374:MET:HE3 | 1.67 | 0.76 |
| 1:4:613:ASP:OD1 | 1:4:732:ARG:HD3 | 1.85 | 0.76 |
| 1:N:613:ASP:OD1 | 1:N:732:ARG:HD3 | 1.85 | 0.76 |
| 1:T:251:PRO:HG3 | 1:T:374:MET:HE3 | 1.67 | 0.76 |
| 1:p:251:PRO:HG3 | 1:p:374:MET:HE3 | 1.67 | 0.76 |
| 1:x:609:TRP:HE1 | 1:y:629:GLY:HA3 | 1.50 | 0.76 |
| 1:F:613:ASP:OD1 | 1:F:732:ARG:HD3 | 1.85 | 0.76 |
| 1:L:251:PRO:HG3 | 1:L:374:MET:HE3 | 1.67 | 0.76 |
| 1:a:613:ASP:OD1 | 1:a:732:ARG:HD3 | 1.85 | 0.76 |
| 1:n:613:ASP:OD1 | 1:n:732:ARG:HD3 | 1.85 | 0.76 |
| 1:6:613:ASP:OD1 | 1:6:732:ARG:HD3 | 1.85 | 0.76 |
| 1:B:613:ASP:OD1 | 1:B:732:ARG:HD3 | 1.85 | 0.76 |
| 1:W:251:PRO:HG3 | 1:W:374:MET:HE3 | 1.67 | 0.76 |
| 1:w:609:TRP:HE1 | 1:x:629:GLY:HA3 | 1.49 | 0.76 |
| 1:C:251:PRO:HG3 | 1:C:374:MET:HE3 | 1.67 | 0.76 |
| 1:V:251:PRO:HG3 | 1:V:374:MET:HE3 | 1.67 | 0.75 |
| 1:b:613:ASP:OD1 | 1:b:732:ARG:HD3 | 1.85 | 0.75 |
| 1:q:251:PRO:HG3 | 1:q:374:MET:HE3 | 1.67 | 0.75 |
| 1:y:251:PRO:HG3 | 1:y:374:MET:HE3 | 1.67 | 0.75 |
| 1:j:613:ASP:OD1 | 1:j:732:ARG:HD3 | 1.85 | 0.75 |
| 1:x:251:PRO:HG3 | 1:x:374:MET:HE3 | 1.67 | 0.75 |
| 1:X:251:PRO:HG3 | 1:X:374:MET:HE3 | 1.67 | 0.75 |
| 1:u:613:ASP:OD1 | 1:u:732:ARG:HD3 | 1.85 | 0.75 |
| 1:2:251:PRO:HG3 | 1:2:374:MET:HE3 | 1.67 | 0.75 |
| 1:O:613:ASP:OD1 | 1:O:732:ARG:HD3 | 1.85 | 0.75 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:d:251:PRO:HG3 | 1:d:374:MET:HE3 | 1.67 | 0.75 |
| 1:f:613:ASP:OD1 | 1:f:732:ARG:HD3 | 1.85 | 0.75 |
| 1:l:251:PRO:HG3 | 1:l:374:MET:HE3 | 1.67 | 0.75 |
| 1:s:251:PRO:HG3 | 1:s:374:MET:HE3 | 1.67 | 0.75 |
| 1:B:251:PRO:HG3 | 1:B:374:MET:HE3 | 1.67 | 0.75 |
| 1:F:613:ASP:CB | 1:F:732:ARG:CD | 2.65 | 0.75 |
| 1:H:251:PRO:HG3 | 1:H:374:MET:HE3 | 1.67 | 0.75 |
| 1:S:613:ASP:OD1 | 1:S:732:ARG:HD3 | 1.85 | 0.75 |
| 1:z:251:PRO:HG3 | 1:z:374:MET:HE3 | 1.67 | 0.75 |
| 1:E:251:PRO:HG3 | 1:E:374:MET:HE3 | 1.67 | 0.75 |
| 1:g:613:ASP:OD1 | 1:g:732:ARG:HD3 | 1.85 | 0.75 |
| 1:6:613:ASP:CB | 1:6:732:ARG:CD | 2.65 | 0.75 |
| 1:m:613:ASP:OD1 | 1:m:732:ARG:HD3 | 1.85 | 0.75 |
| 1:z:613:ASP:OD1 | 1:z:732:ARG:HD3 | 1.85 | 0.75 |
| 1:3:613:ASP:OD1 | 1:3:732:ARG:HD3 | 1.85 | 0.75 |
| 1:b:251:PRO:HG3 | 1:b:374:MET:HE3 | 1.67 | 0.75 |
| 1:h:251:PRO:HG3 | 1:h:374:MET:HE3 | 1.67 | 0.75 |
| 1:i:613:ASP:OD1 | 1:i:732:ARG:HD3 | 1.85 | 0.75 |
| 1:k:251:PRO:HG3 | 1:k:374:MET:HE3 | 1.67 | 0.75 |
| 1:p:613:ASP:OD1 | 1:p:732:ARG:HD3 | 1.85 | 0.75 |
| 1:q:613:ASP:OD1 | 1:q:732:ARG:HD3 | 1.85 | 0.75 |
| 1:7:251:PRO:HG3 | 1:7:374:MET:HE3 | 1.67 | 0.75 |
| 1:A:613:ASP:CB | 1:A:732:ARG:CD | 2.65 | 0.75 |
| 1:G:613:ASP:OD1 | 1:G:732:ARG:HD3 | 1.85 | 0.75 |
| 1:H:613:ASP:OD1 | 1:H:732:ARG:HD3 | 1.85 | 0.75 |
| 1:T:629:GLY:HA3 | 1:l:609:TRP:HE1 | 1.52 | 0.75 |
| 1:Z:613:ASP:OD1 | 1:Z:732:ARG:HD3 | 1.85 | 0.75 |
| 1:e:609:TRP:HH2 | 1:e:631:PHE:HZ | 1.35 | 0.75 |
| 1:f:613:ASP:CB | 1:f:732:ARG:CD | 2.65 | 0.75 |
| 1:j:613:ASP:CB | 1:j:732:ARG:CD | 2.65 | 0.75 |
| 1:o:613:ASP:CB | 1:o:732:ARG:CD | 2.65 | 0.75 |
| 1:w:736:ARG:HH21 | 1:x:626:HIS:CD2 | 2.04 | 0.75 |
| 1:D:613:ASP:OD1 | 1:D:732:ARG:HD3 | 1.85 | 0.74 |
| 1:G:609:TRP:HE1 | 1:I:629:GLY:HA3 | 1.52 | 0.74 |
| 1:l:613:ASP:OD1 | 1:l:732:ARG:HD3 | 1.85 | 0.74 |
| 1:m:251:PRO:HG3 | 1:m:374:MET:HE3 | 1.67 | 0.74 |
| 1:w:609:TRP:HH2 | 1:w:631:PHE:HZ | 1.35 | 0.74 |
| 1:z:609:TRP:HE1 | 1:1:629:GLY:HA3 | 1.52 | 0.74 |
| 1:A:609:TRP:HE1 | 1:G:629:GLY:HA3 | 1.52 | 0.74 |
| 1:E:307:TRP:O | 1:E:426:SER:HB3 | 1.88 | 0.74 |
| 1:F:609:TRP:HH2 | 1:F:631:PHE:HZ | 1.35 | 0.74 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:629:GLY:HA3 | 1:Y:609:TRP:HE1 | 1.52 | 0.74 |
| 1:R:307:TRP:O | 1:R:426:SER:HB3 | 1.88 | 0.74 |
| 1:W:613:ASP:OD1 | 1:W:732:ARG:HD3 | 1.85 | 0.74 |
| 1:c:629:GLY:HA3 | 1:p:609:TRP:HE1 | 1.52 | 0.74 |
| 1:r:609:TRP:HE1 | 1:s:629:GLY:HA3 | 1.52 | 0.74 |
| 1:t:307:TRP:O | 1:t:426:SER:HB3 | 1.88 | 0.74 |
| 1:v:609:TRP:HH2 | 1:v:631:PHE:HZ | 1.35 | 0.74 |
| 1:7:307:TRP:O | 1:7:426:SER:HB3 | 1.88 | 0.74 |
| 1:I:307:TRP:O | 1:I:426:SER:HB3 | 1.87 | 0.74 |
| 1:K:613:ASP:OD1 | 1:K:732:ARG:HD3 | 1.85 | 0.74 |
| 1:U:609:TRP:HH2 | 1:U:631:PHE:HZ | 1.35 | 0.74 |
| 1:W:307:TRP:O | 1:W:426:SER:HB3 | 1.88 | 0.74 |
| 1:X:613:ASP:CB | 1:X:732:ARG:CD | 2.65 | 0.74 |
| 1:Z:251:PRO:HG3 | 1:Z:374:MET:HE3 | 1.67 | 0.74 |
| 1:c:307:TRP:O | 1:c:426:SER:HB3 | 1.87 | 0.74 |
| 1:g:307:TRP:O | 1:g:426:SER:HB3 | 1.88 | 0.74 |
| 1:g:629:GLY:HA3 | 1:h:609:TRP:HE1 | 1.52 | 0.74 |
| 1:i:307:TRP:O | 1:i:426:SER:HB3 | 1.88 | 0.74 |
| 1:m:307:TRP:O | 1:m:426:SER:HB3 | 1.88 | 0.74 |
| 1:n:307:TRP:O | 1:n:426:SER:HB3 | 1.87 | 0.74 |
| 1:o:307:TRP:O | 1:o:426:SER:HB3 | 1.88 | 0.74 |
| 1:s:613:ASP:OD1 | 1:s:732:ARG:HD3 | 1.85 | 0.74 |
| 1:u:307:TRP:O | 1:u:426:SER:HB3 | 1.88 | 0.74 |
| 1:6:609:TRP:HH2 | 1:6:631:PHE:HZ | 1.35 | 0.74 |
| 1:A:307:TRP:O | 1:A:426:SER:HB3 | 1.88 | 0.74 |
| 1:C:609:TRP:HH2 | 1:C:631:PHE:HZ | 1.35 | 0.74 |
| 1:G:307:TRP:O | 1:G:426:SER:HB3 | 1.88 | 0.74 |
| 1:S:307:TRP:O | 1:S:426:SER:HB3 | 1.88 | 0.74 |
| 1:Y:609:TRP:HH2 | 1:Y:631:PHE:HZ | 1.35 | 0.74 |
| 1:i:629:GLY:HA3 | 1:k:609:TRP:HE1 | 1.52 | 0.74 |
| 1:p:307:TRP:O | 1:p:426:SER:HB3 | 1.88 | 0.74 |
| 1:q:307:TRP:O | 1:q:426:SER:HB3 | 1.88 | 0.74 |
| 1:r:609:TRP:HH2 | 1:r:631:PHE:HZ | 1.35 | 0.74 |
| 1:x:613:ASP:CB | 1:x:732:ARG:CD | 2.65 | 0.74 |
| 1:y:609:TRP:HH2 | 1:y:631:PHE:HZ | 1.35 | 0.74 |
| 1:4:307:TRP:O | 1:4:426:SER:HB3 | 1.87 | 0.74 |
| 1:B:609:TRP:HH2 | 1:B:631:PHE:HZ | 1.35 | 0.74 |
| 1:V:609:TRP:HH2 | 1:V:631:PHE:HZ | 1.35 | 0.74 |
| 1:V:613:ASP:CB | 1:V:732:ARG:CD | 2.65 | 0.74 |
| 1:W:609:TRP:HE1 | 1:Y:629:GLY:HA3 | 1.52 | 0.74 |
| 1:Z:307:TRP:O | 1:Z:426:SER:HB3 | 1.88 | 0.74 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:o:609:TRP:HE1 | 1:p:629:GLY:HA3 | 1.52 | 0.74 |
| 1:q:609:TRP:HE1 | 1:r:629:GLY:HA3 | 1.52 | 0.74 |
| 1:u:609:TRP:HE1 | 1:v:629:GLY:HA3 | 1.52 | 0.74 |
| 1:u:613:ASP:CB | 1:u:732:ARG:CD | 2.65 | 0.74 |
| 1:F:307:TRP:O | 1:F:426:SER:HB3 | 1.88 | 0.74 |
| 1:L:609:TRP:HH2 | 1:L:631:PHE:HZ | 1.35 | 0.74 |
| 1:S:613:ASP:CB | 1:S:732:ARG:CD | 2.65 | 0.74 |
| 1:U:613:ASP:CB | 1:U:732:ARG:CD | 2.65 | 0.74 |
| 1:b:609:TRP:HH2 | 1:b:631:PHE:HZ | 1.35 | 0.74 |
| 1:d:613:ASP:CB | 1:d:732:ARG:CD | 2.65 | 0.74 |
| 1:f:609:TRP:HH2 | 1:f:631:PHE:HZ | 1.35 | 0.74 |
| 1:h:609:TRP:HH2 | 1:h:631:PHE:HZ | 1.35 | 0.74 |
| 1:j:609:TRP:HH2 | 1:j:631:PHE:HZ | 1.35 | 0.74 |
| 1:y:307:TRP:O | 1:y:426:SER:HB3 | 1.87 | 0.74 |
| 1:2:613:ASP:CB | 1:2:732:ARG:CD | 2.65 | 0.74 |
| 1:M:307:TRP:O | 1:M:426:SER:HB3 | 1.88 | 0.74 |
| 1:R:629:GLY:HA3 | 1:U:609:TRP:HE1 | 1.53 | 0.74 |
| 1:S:609:TRP:HE1 | 1:U:629:GLY:HA3 | 1.52 | 0.74 |
| 1:T:613:ASP:CB | 1:T:732:ARG:CD | 2.65 | 0.74 |
| 1:k:609:TRP:HH2 | 1:k:631:PHE:HZ | 1.35 | 0.74 |
| 1:v:613:ASP:CB | 1:v:732:ARG:CD | 2.65 | 0.74 |
| 1:1:613:ASP:CB | 1:1:732:ARG:CD | 2.65 | 0.74 |
| 1:6:307:TRP:O | 1:6:426:SER:HB3 | 1.88 | 0.74 |
| 1:D:613:ASP:CB | 1:D:732:ARG:CD | 2.65 | 0.74 |
| 1:J:307:TRP:O | 1:J:426:SER:HB3 | 1.88 | 0.74 |
| 1:K:613:ASP:CB | 1:K:732:ARG:CD | 2.65 | 0.74 |
| 1:M:629:GLY:HA3 | 1:b:609:TRP:HE1 | 1.53 | 0.74 |
| 1:P:613:ASP:CB | 1:P:732:ARG:CD | 2.65 | 0.74 |
| 1:V:307:TRP:O | 1:V:426:SER:HB3 | 1.88 | 0.74 |
| 1:V:629:GLY:HA3 | 1:X:609:TRP:HE1 | 1.52 | 0.74 |
| 1:b:307:TRP:O | 1:b:426:SER:HB3 | 1.88 | 0.74 |
| 1:l:307:TRP:O | 1:l:426:SER:HB3 | 1.87 | 0.74 |
| 1:r:531:ASP:OD1 | 1:r:569:LYS:NZ | 2.21 | 0.74 |
| 1:t:629:GLY:HA3 | 1:v:609:TRP:HE1 | 1.53 | 0.74 |
| 1:z:307:TRP:O | 1:z:426:SER:HB3 | 1.88 | 0.74 |
| 1:B:307:TRP:O | 1:B:426:SER:HB3 | 1.88 | 0.74 |
| 1:B:609:TRP:HE1 | 1:J:629:GLY:HA3 | 1.53 | 0.74 |
| 1:R:531:ASP:OD1 | 1:R:569:LYS:NZ | 2.21 | 0.74 |
| 1:X:609:TRP:HH2 | 1:X:631:PHE:HZ | 1.35 | 0.74 |
| 1:Y:531:ASP:OD1 | 1:Y:569:LYS:NZ | 2.21 | 0.74 |
| 1:5:613:ASP:CB | 1:5:732:ARG:CD | 2.65 | 0.74 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:8:613:ASP:CB | 1:8:732:ARG:CD | 2.65 | 0.74 |
| 1:x:609:TRP:HH2 | 1:x:631:PHE:HZ | 1.35 | 0.74 |
| 1:Q:613:ASP:CB | 1:Q:732:ARG:CD | 2.65 | 0.73 |
| 1:i:613:ASP:CB | 1:i:732:ARG:CD | 2.65 | 0.73 |
| 1:k:307:TRP:O | 1:k:426:SER:HB3 | 1.88 | 0.73 |
| 1:n:531:ASP:OD1 | 1:n:569:LYS:NZ | 2.21 | 0.73 |
| 1:2:307:TRP:O | 1:2:426:SER:HB3 | 1.88 | 0.73 |
| 1:7:531:ASP:OD1 | 1:7:569:LYS:NZ | 2.21 | 0.73 |
| 1:C:307:TRP:O | 1:C:426:SER:HB3 | 1.88 | 0.73 |
| 1:C:629:GLY:HA3 | 1:M:609:TRP:HE1 | 1.52 | 0.73 |
| 1:E:531:ASP:OD1 | 1:E:569:LYS:NZ | 2.21 | 0.73 |
| 1:K:629:GLY:HA3 | 1:8:609:TRP:HE1 | 1.52 | 0.73 |
| 1:L:307:TRP:O | 1:L:426:SER:HB3 | 1.88 | 0.73 |
| 1:Q:307:TRP:O | 1:Q:426:SER:HB3 | 1.88 | 0.73 |
| 1:g:613:ASP:CB | 1:g:732:ARG:CD | 2.65 | 0.73 |
| 1:l:609:TRP:HH2 | 1:l:631:PHE:HZ | 1.35 | 0.73 |
| 1:s:613:ASP:CB | 1:s:732:ARG:CD | 2.65 | 0.73 |
| 1:4:531:ASP:OD1 | 1:4:569:LYS:NZ | 2.21 | 0.73 |
| 1:5:307:TRP:O | 1:5:426:SER:HB3 | 1.88 | 0.73 |
| 1:D:307:TRP:O | 1:D:426:SER:HB3 | 1.87 | 0.73 |
| 1:H:613:ASP:CB | 1:H:732:ARG:CD | 2.65 | 0.73 |
| 1:J:609:TRP:HE1 | 1:L:629:GLY:HA3 | 1.52 | 0.73 |
| 1:S:609:TRP:HH2 | 1:S:631:PHE:HZ | 1.35 | 0.73 |
| 1:d:307:TRP:O | 1:d:426:SER:HB3 | 1.88 | 0.73 |
| 1:h:307:TRP:O | 1:h:426:SER:HB3 | 1.88 | 0.73 |
| 1:j:307:TRP:O | 1:j:426:SER:HB3 | 1.88 | 0.73 |
| 1:8:307:TRP:O | 1:8:426:SER:HB3 | 1.88 | 0.73 |
| 1:D:629:GLY:HA3 | 1:P:609:TRP:HE1 | 1.52 | 0.73 |
| 1:K:307:TRP:O | 1:K:426:SER:HB3 | 1.88 | 0.73 |
| 1:P:307:TRP:O | 1:P:426:SER:HB3 | 1.88 | 0.73 |
| 1:X:629:GLY:HA3 | 1:e:609:TRP:HE1 | 1.52 | 0.73 |
| 1:Y:307:TRP:O | 1:Y:426:SER:HB3 | 1.88 | 0.73 |
| 1:f:609:TRP:HE1 | 1:h:629:GLY:HA3 | 1.52 | 0.73 |
| 1:u:609:TRP:HH2 | 1:u:631:PHE:HZ | 1.35 | 0.73 |
| 1:H:307:TRP:O | 1:H:426:SER:HB3 | 1.87 | 0.73 |
| 1:U:307:TRP:O | 1:U:426:SER:HB3 | 1.88 | 0.73 |
| 1:f:307:TRP:O | 1:f:426:SER:HB3 | 1.88 | 0.73 |
| 1:j:609:TRP:HE1 | 1:k:629:GLY:HA3 | 1.52 | 0.73 |
| 1:r:307:TRP:O | 1:r:426:SER:HB3 | 1.88 | 0.73 |
| 1:s:307:TRP:O | 1:s:426:SER:HB3 | 1.87 | 0.73 |
| 1:z:609:TRP:HH2 | 1:z:631:PHE:HZ | 1.35 | 0.73 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:609:TRP:HH2 | 1:I:631:PHE:HZ | 1.35 | 0.73 |
| 1:7:609:TRP:HH2 | 1:7:631:PHE:HZ | 1.35 | 0.73 |
| 1:i:609:TRP:HE1 | 1:j:629:GLY:HA3 | 1.53 | 0.73 |
| 1:q:531:ASP:OD1 | 1:q:569:LYS:NZ | 2.21 | 0.73 |
| 1:v:307:TRP:O | 1:v:426:SER:HB3 | 1.88 | 0.73 |
| 1:3:531:ASP:OD1 | 1:3:569:LYS:NZ | 2.21 | 0.73 |
| 1:E:609:TRP:HH2 | 1:E:631:PHE:HZ | 1.35 | 0.73 |
| 1:O:531:ASP:OD1 | 1:O:569:LYS:NZ | 2.21 | 0.73 |
| 1:Z:613:ASP:CB | 1:Z:732:ARG:CD | 2.65 | 0.73 |
| 1:c:609:TRP:HE1 | 1:o:629:GLY:HA3 | 1.52 | 0.73 |
| 1:f:629:GLY:HA3 | 1:g:609:TRP:HE1 | 1.53 | 0.73 |
| 1:t:609:TRP:HE1 | 1:u:629:GLY:HA3 | 1.53 | 0.73 |
| 1:R:609:TRP:HE1 | 1:S:629:GLY:HA3 | 1.52 | 0.73 |
| 1:W:531:ASP:OD1 | 1:W:569:LYS:NZ | 2.21 | 0.73 |
| 1:c:609:TRP:HH2 | 1:c:631:PHE:HZ | 1.35 | 0.73 |
| 1:m:613:ASP:CB | 1:m:732:ARG:CD | 2.65 | 0.73 |
| 1:q:629:GLY:HA3 | 1:s:609:TRP:HE1 | 1.53 | 0.73 |
| 1:6:531:ASP:OD1 | 1:6:569:LYS:NZ | 2.21 | 0.73 |
| 1:F:531:ASP:OD1 | 1:F:569:LYS:NZ | 2.21 | 0.73 |
| 1:Z:629:GLY:HA3 | 1:3:609:TRP:HE1 | 1.52 | 0.73 |
| 1:a:307:TRP:O | 1:a:426:SER:HB3 | 1.88 | 0.73 |
| 1:s:609:TRP:HH2 | 1:s:631:PHE:HZ | 1.35 | 0.73 |
| 1:y:531:ASP:OD1 | 1:y:569:LYS:NZ | 2.21 | 0.73 |
| 1:2:609:TRP:HH2 | 1:2:631:PHE:HZ | 1.35 | 0.73 |
| 1:K:531:ASP:OD1 | 1:K:569:LYS:NZ | 2.21 | 0.72 |
| 1:N:307:TRP:O | 1:N:426:SER:HB3 | 1.88 | 0.72 |
| 1:O:307:TRP:O | 1:O:426:SER:HB3 | 1.88 | 0.72 |
| 1:d:609:TRP:HE1 | 1:l:629:GLY:HA3 | 1.52 | 0.72 |
| 1:3:307:TRP:O | 1:3:426:SER:HB3 | 1.88 | 0.72 |
| 1:A:629:GLY:HA3 | 1:I:609:TRP:HE1 | 1.52 | 0.72 |
| 1:V:531:ASP:OD1 | 1:V:569:LYS:NZ | 2.21 | 0.72 |
| 1:d:609:TRP:HH2 | 1:d:631:PHE:HZ | 1.35 | 0.72 |
| 1:m:328:GLN:HE22 | 1:m:333:LYS:HG3 | 1.55 | 0.72 |
| 1:m:531:ASP:OD1 | 1:m:569:LYS:NZ | 2.21 | 0.72 |
| 1:B:328:GLN:HE22 | 1:B:333:LYS:HG3 | 1.55 | 0.72 |
| 1:D:531:ASP:OD1 | 1:D:569:LYS:NZ | 2.21 | 0.72 |
| 1:D:609:TRP:HE1 | 1:N:629:GLY:HA3 | 1.52 | 0.72 |
| 1:E:240:VAL:HG13 | 1:E:687:TRP:HB2 | 1.72 | 0.72 |
| 1:H:609:TRP:HE1 | 1:W:629:GLY:HA3 | 1.53 | 0.72 |
| 1:K:609:TRP:HE1 | 1:a:629:GLY:HA3 | 1.52 | 0.72 |
| 1:O:240:VAL:HG13 | 1:O:687:TRP:HB2 | 1.72 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:609:TRP:HE1 | 1:m:629:GLY:HA3 | 1.52 | 0.72 |
| 1:W:240:VAL:HG13 | 1:W:687:TRP:HB2 | 1.72 | 0.72 |
| 1:Z:328:GLN:HE22 | 1:Z:333:LYS:HG3 | 1.55 | 0.72 |
| 1:a:609:TRP:HH2 | 1:a:631:PHE:HZ | 1.35 | 0.72 |
| 1:b:328:GLN:HE22 | 1:b:333:LYS:HG3 | 1.55 | 0.72 |
| 1:q:240:VAL:HG13 | 1:q:687:TRP:HB2 | 1.72 | 0.72 |
| 1:3:240:VAL:HG13 | 1:3:687:TRP:HB2 | 1.72 | 0.72 |
| 1:7:240:VAL:HG13 | 1:7:687:TRP:HB2 | 1.72 | 0.72 |
| 1:A:609:TRP:HH2 | 1:A:631:PHE:HZ | 1.35 | 0.72 |
| 1:B:629:GLY:HA3 | 1:L:609:TRP:HE1 | 1.52 | 0.72 |
| 1:D:240:VAL:HG13 | 1:D:687:TRP:HB2 | 1.72 | 0.72 |
| 1:I:613:ASP:CB | 1:I:732:ARG:CD | 2.65 | 0.72 |
| 1:K:240:VAL:HG13 | 1:K:687:TRP:HB2 | 1.72 | 0.72 |
| 1:N:240:VAL:HG13 | 1:N:687:TRP:HB2 | 1.71 | 0.72 |
| 1:N:328:GLN:HE22 | 1:N:333:LYS:HG3 | 1.55 | 0.72 |
| 1:O:613:ASP:CB | 1:O:732:ARG:CD | 2.65 | 0.72 |
| 1:P:240:VAL:HG13 | 1:P:687:TRP:HB2 | 1.72 | 0.72 |
| 1:W:609:TRP:HH2 | 1:W:631:PHE:HZ | 1.35 | 0.72 |
| 1:Z:240:VAL:HG13 | 1:Z:687:TRP:HB2 | 1.72 | 0.72 |
| 1:Z:531:ASP:OD1 | 1:Z:569:LYS:NZ | 2.21 | 0.72 |
| 1:a:240:VAL:HG13 | 1:a:687:TRP:HB2 | 1.71 | 0.72 |
| 1:a:328:GLN:HE22 | 1:a:333:LYS:HG3 | 1.55 | 0.72 |
| 1:h:340:THR:O | 1:h:407:ARG:NH2 | 2.23 | 0.72 |
| 1:k:340:THR:O | 1:k:407:ARG:NH2 | 2.23 | 0.72 |
| 1:v:328:GLN:HE22 | 1:v:333:LYS:HG3 | 1.55 | 0.72 |
| 1:1:307:TRP:O | 1:1:426:SER:HB3 | 1.88 | 0.72 |
| 1:C:240:VAL:HG13 | 1:C:687:TRP:HB2 | 1.72 | 0.72 |
| 1:F:340:THR:O | 1:F:407:ARG:NH2 | 2.23 | 0.72 |
| 1:N:609:TRP:HH2 | 1:N:631:PHE:HZ | 1.35 | 0.72 |
| 1:O:340:THR:O | 1:O:407:ARG:NH2 | 2.23 | 0.72 |
| 1:T:307:TRP:O | 1:T:426:SER:HB3 | 1.88 | 0.72 |
| 1:U:328:GLN:HE22 | 1:U:333:LYS:HG3 | 1.55 | 0.72 |
| 1:U:340:THR:O | 1:U:407:ARG:NH2 | 2.23 | 0.72 |
| 1:X:307:TRP:O | 1:X:426:SER:HB3 | 1.88 | 0.72 |
| 1:c:613:ASP:CB | 1:c:732:ARG:CD | 2.65 | 0.72 |
| 1:m:240:VAL:HG13 | 1:m:687:TRP:HB2 | 1.72 | 0.72 |
| 1:q:328:GLN:HE22 | 1:q:333:LYS:HG3 | 1.54 | 0.72 |
| 1:x:307:TRP:O | 1:x:426:SER:HB3 | 1.87 | 0.72 |
| 1:x:431:GLN:HE22 | 1:y:354:PRO:HB3 | 1.55 | 0.72 |
| 1:z:629:GLY:HA3 | 1:2:609:TRP:HE1 | 1.52 | 0.72 |
| 1:3:328:GLN:HE22 | 1:3:333:LYS:HG3 | 1.55 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:8:240:VAL:HG13 | 1:8:687:TRP:HB2 | 1.72 | 0.72 |
| 1:C:328:GLN:HE22 | 1:C:333:LYS:HG3 | 1.55 | 0.72 |
| 1:L:240:VAL:HG13 | 1:L:687:TRP:HB2 | 1.72 | 0.72 |
| 1:L:328:GLN:HE22 | 1:L:333:LYS:HG3 | 1.55 | 0.72 |
| 1:W:328:GLN:HE22 | 1:W:333:LYS:HG3 | 1.55 | 0.72 |
| 1:b:240:VAL:HG13 | 1:b:687:TRP:HB2 | 1.72 | 0.72 |
| 1:d:240:VAL:HG13 | 1:d:687:TRP:HB2 | 1.72 | 0.72 |
| 1:i:613:ASP:CB | 1:i:731:THR:HG22 | 2.17 | 0.72 |
| 1:j:328:GLN:HE22 | 1:j:333:LYS:HG3 | 1.55 | 0.72 |
| 1:o:328:GLN:HE22 | 1:o:333:LYS:HG3 | 1.54 | 0.72 |
| 1:v:340:THR:O | 1:v:407:ARG:NH2 | 2.23 | 0.72 |
| 1:3:340:THR:O | 1:3:407:ARG:NH2 | 2.23 | 0.72 |
| 1:3:613:ASP:CB | 1:3:732:ARG:CD | 2.65 | 0.72 |
| 1:6:340:THR:O | 1:6:407:ARG:NH2 | 2.23 | 0.72 |
| 1:B:240:VAL:HG13 | 1:B:687:TRP:HB2 | 1.72 | 0.72 |
| 1:C:609:TRP:HE1 | 1:b:629:GLY:HA3 | 1.52 | 0.72 |
| 1:G:321:ILE:HD13 | 1:G:343:ILE:HD11 | 1.72 | 0.72 |
| 1:f:531:ASP:OD1 | 1:f:569:LYS:NZ | 2.21 | 0.72 |
| 1:h:240:VAL:HG13 | 1:h:687:TRP:HB2 | 1.72 | 0.72 |
| 1:j:531:ASP:OD1 | 1:j:569:LYS:NZ | 2.21 | 0.72 |
| 1:k:328:GLN:HE22 | 1:k:333:LYS:HG3 | 1.54 | 0.72 |
| 1:p:240:VAL:HG13 | 1:p:687:TRP:HB2 | 1.72 | 0.72 |
| 1:p:321:ILE:HD13 | 1:p:343:ILE:HD11 | 1.72 | 0.72 |
| 1:p:328:GLN:HE22 | 1:p:333:LYS:HG3 | 1.55 | 0.72 |
| 1:p:531:ASP:OD1 | 1:p:569:LYS:NZ | 2.21 | 0.72 |
| 1:q:609:TRP:HH2 | 1:q:631:PHE:HZ | 1.35 | 0.72 |
| 1:x:328:GLN:HE22 | 1:x:333:LYS:HG3 | 1.55 | 0.72 |
| 1:2:240:VAL:HG13 | 1:2:687:TRP:HB2 | 1.72 | 0.72 |
| 1:5:609:TRP:HH2 | 1:5:631:PHE:HZ | 1.35 | 0.72 |
| 1:A:531:ASP:OD1 | 1:A:569:LYS:NZ | 2.21 | 0.72 |
| 1:G:240:VAL:HG13 | 1:G:687:TRP:HB2 | 1.72 | 0.72 |
| 1:G:328:GLN:HE22 | 1:G:333:LYS:HG3 | 1.55 | 0.72 |
| 1:G:531:ASP:OD1 | 1:G:569:LYS:NZ | 2.21 | 0.72 |
| 1:J:340:THR:O | 1:J:407:ARG:NH2 | 2.23 | 0.72 |
| 1:N:531:ASP:OD1 | 1:N:569:LYS:NZ | 2.21 | 0.72 |
| 1:O:328:GLN:HE22 | 1:O:333:LYS:HG3 | 1.55 | 0.72 |
| 1:Q:609:TRP:HH2 | 1:Q:631:PHE:HZ | 1.35 | 0.72 |
| 1:X:240:VAL:HG13 | 1:X:687:TRP:HB2 | 1.71 | 0.72 |
| 1:f:328:GLN:HE22 | 1:f:333:LYS:HG3 | 1.55 | 0.72 |
| 1:g:240:VAL:HG13 | 1:g:687:TRP:HB2 | 1.72 | 0.72 |
| 1:k:240:VAL:HG13 | 1:k:687:TRP:HB2 | 1.72 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:340:THR:O | 1:m:407:ARG:NH2 | 2.23 | 0.72 |
| 1:s:240:VAL:HG13 | 1:s:687:TRP:HB2 | 1.72 | 0.72 |
| 1:w:240:VAL:HG13 | 1:w:687:TRP:HB2 | 1.72 | 0.72 |
| 1:A:328:GLN:HE22 | 1:A:333:LYS:HG3 | 1.55 | 0.72 |
| 1:D:328:GLN:HE22 | 1:D:333:LYS:HG3 | 1.55 | 0.72 |
| 1:H:240:VAL:HG13 | 1:H:687:TRP:HB2 | 1.72 | 0.72 |
| 1:H:321:ILE:HD13 | 1:H:343:ILE:HD11 | 1.72 | 0.72 |
| 1:K:328:GLN:HE22 | 1:K:333:LYS:HG3 | 1.55 | 0.72 |
| 1:K:340:THR:O | 1:K:407:ARG:NH2 | 2.23 | 0.72 |
| 1:L:321:ILE:HD13 | 1:L:343:ILE:HD11 | 1.72 | 0.72 |
| 1:M:340:THR:O | 1:M:407:ARG:NH2 | 2.23 | 0.72 |
| 1:S:328:GLN:HE22 | 1:S:333:LYS:HG3 | 1.55 | 0.72 |
| 1:S:340:THR:O | 1:S:407:ARG:NH2 | 2.23 | 0.72 |
| 1:X:328:GLN:HE22 | 1:X:333:LYS:HG3 | 1.55 | 0.72 |
| 1:Z:340:THR:O | 1:Z:407:ARG:NH2 | 2.23 | 0.72 |
| 1:e:240:VAL:HG13 | 1:e:687:TRP:HB2 | 1.72 | 0.72 |
| 1:i:240:VAL:HG13 | 1:i:687:TRP:HB2 | 1.72 | 0.72 |
| 1:o:609:TRP:HH2 | 1:o:631:PHE:HZ | 1.35 | 0.72 |
| 1:s:321:ILE:HD13 | 1:s:343:ILE:HD11 | 1.72 | 0.72 |
| 1:u:340:THR:O | 1:u:407:ARG:NH2 | 2.23 | 0.72 |
| 1:u:613:ASP:CB | 1:u:731:THR:HG22 | 2.17 | 0.72 |
| 1:C:321:ILE:HD13 | 1:C:343:ILE:HD11 | 1.72 | 0.72 |
| 1:D:340:THR:O | 1:D:407:ARG:NH2 | 2.23 | 0.72 |
| 1:J:613:ASP:CB | 1:J:732:ARG:CD | 2.65 | 0.72 |
| 1:N:321:ILE:HD13 | 1:N:343:ILE:HD11 | 1.72 | 0.72 |
| 1:S:613:ASP:CB | 1:S:731:THR:HG22 | 2.17 | 0.72 |
| 1:U:321:ILE:HD13 | 1:U:343:ILE:HD11 | 1.72 | 0.72 |
| 1:X:340:THR:O | 1:X:407:ARG:NH2 | 2.23 | 0.72 |
| 1:a:321:ILE:HD13 | 1:a:343:ILE:HD11 | 1.72 | 0.72 |
| 1:a:613:ASP:CB | 1:a:732:ARG:CD | 2.65 | 0.72 |
| 1:h:328:GLN:HE22 | 1:h:333:LYS:HG3 | 1.55 | 0.72 |
| 1:n:340:THR:O | 1:n:407:ARG:NH2 | 2.23 | 0.72 |
| 1:o:531:ASP:OD1 | 1:o:569:LYS:NZ | 2.21 | 0.72 |
| 1:u:321:ILE:HD13 | 1:u:343:ILE:HD11 | 1.72 | 0.72 |
| 1:v:321:ILE:HD13 | 1:v:343:ILE:HD11 | 1.72 | 0.72 |
| 1:x:240:VAL:HG13 | 1:x:687:TRP:HB2 | 1.72 | 0.72 |
| 1:x:321:ILE:HD13 | 1:x:343:ILE:HD11 | 1.72 | 0.72 |
| 1:x:340:THR:O | 1:x:407:ARG:NH2 | 2.23 | 0.72 |
| 1:4:340:THR:O | 1:4:407:ARG:NH2 | 2.23 | 0.72 |
| 1:A:340:THR:O | 1:A:407:ARG:NH2 | 2.23 | 0.71 |
| 1:E:328:GLN:HE22 | 1:E:333:LYS:HG3 | 1.55 | 0.71 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:328:GLN:HE22 | 1:F:333:LYS:HG3 | 1.55 | 0.71 |
| 1:M:613:ASP:CB | 1:M:732:ARG:CD | 2.65 | 0.71 |
| 1:S:321:ILE:HD13 | 1:S:343:ILE:HD11 | 1.72 | 0.71 |
| 1:T:340:THR:O | 1:T:407:ARG:NH2 | 2.23 | 0.71 |
| 1:X:321:ILE:HD13 | 1:X:343:ILE:HD11 | 1.72 | 0.71 |
| 1:a:531:ASP:OD1 | 1:a:569:LYS:NZ | 2.21 | 0.71 |
| 1:d:531:ASP:OD1 | 1:d:569:LYS:NZ | 2.21 | 0.71 |
| 1:f:321:ILE:HD13 | 1:f:343:ILE:HD11 | 1.72 | 0.71 |
| 1:o:340:THR:O | 1:o:407:ARG:NH2 | 2.23 | 0.71 |
| 1:u:328:GLN:HE22 | 1:u:333:LYS:HG3 | 1.55 | 0.71 |
| 1:v:240:VAL:HG13 | 1:v:687:TRP:HB2 | 1.72 | 0.71 |
| 1:z:321:ILE:HD13 | 1:z:343:ILE:HD11 | 1.72 | 0.71 |
| 1:1:340:THR:O | 1:1:407:ARG:NH2 | 2.23 | 0.71 |
| 1:2:531:ASP:OD1 | 1:2:569:LYS:NZ | 2.21 | 0.71 |
| 1:4:328:GLN:HE22 | 1:4:333:LYS:HG3 | 1.55 | 0.71 |
| 1:N:340:THR:O | 1:N:407:ARG:NH2 | 2.23 | 0.71 |
| 1:N:613:ASP:CB | 1:N:732:ARG:CD | 2.65 | 0.71 |
| 1:U:240:VAL:HG13 | 1:U:687:TRP:HB2 | 1.72 | 0.71 |
| 1:Y:321:ILE:HD13 | 1:Y:343:ILE:HD11 | 1.72 | 0.71 |
| 1:Y:328:GLN:HE22 | 1:Y:333:LYS:HG3 | 1.55 | 0.71 |
| 1:e:307:TRP:O | 1:e:426:SER:HB3 | 1.88 | 0.71 |
| 1:f:340:THR:O | 1:f:407:ARG:NH2 | 2.23 | 0.71 |
| 1:k:321:ILE:HD13 | 1:k:343:ILE:HD11 | 1.72 | 0.71 |
| 1:l:321:ILE:HD13 | 1:l:343:ILE:HD11 | 1.72 | 0.71 |
| 1:n:328:GLN:HE22 | 1:n:333:LYS:HG3 | 1.54 | 0.71 |
| 1:n:609:TRP:HH2 | 1:n:631:PHE:HZ | 1.35 | 0.71 |
| 1:r:328:GLN:HE22 | 1:r:333:LYS:HG3 | 1.55 | 0.71 |
| 1:y:328:GLN:HE22 | 1:y:333:LYS:HG3 | 1.55 | 0.71 |
| 1:H:328:GLN:HE22 | 1:H:333:LYS:HG3 | 1.55 | 0.71 |
| 1:M:531:ASP:OD1 | 1:M:569:LYS:NZ | 2.21 | 0.71 |
| 1:V:328:GLN:HE22 | 1:V:333:LYS:HG3 | 1.54 | 0.71 |
| 1:Y:240:VAL:HG13 | 1:Y:687:TRP:HB2 | 1.72 | 0.71 |
| 1:Z:609:TRP:HE1 | 1:4:629:GLY:HA3 | 1.52 | 0.71 |
| 1:a:340:THR:O | 1:a:407:ARG:NH2 | 2.23 | 0.71 |
| 1:b:613:ASP:CB | 1:b:732:ARG:CD | 2.65 | 0.71 |
| 1:h:321:ILE:HD13 | 1:h:343:ILE:HD11 | 1.72 | 0.71 |
| 1:i:328:GLN:HE22 | 1:i:333:LYS:HG3 | 1.54 | 0.71 |
| 1:j:340:THR:O | 1:j:407:ARG:NH2 | 2.23 | 0.71 |
| 1:m:609:TRP:HH2 | 1:m:631:PHE:HZ | 1.35 | 0.71 |
| 1:o:321:ILE:HD13 | 1:o:343:ILE:HD11 | 1.72 | 0.71 |
| 1:w:307:TRP:O | 1:w:426:SER:HB3 | 1.88 | 0.71 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:w:340:THR:O | 1:w:407:ARG:NH2 | 2.23 | 0.71 |
| 1:5:340:THR:O | 1:5:407:ARG:NH2 | 2.23 | 0.71 |
| 1:6:328:GLN:HE22 | 1:6:333:LYS:HG3 | 1.55 | 0.71 |
| 1:7:328:GLN:HE22 | 1:7:333:LYS:HG3 | 1.55 | 0.71 |
| 1:B:613:ASP:CB | 1:B:732:ARG:CD | 2.65 | 0.71 |
| 1:F:629:GLY:HA3 | 1:Q:609:TRP:HE1 | 1.52 | 0.71 |
| 1:Q:340:THR:O | 1:Q:407:ARG:NH2 | 2.23 | 0.71 |
| 1:R:328:GLN:HE22 | 1:R:333:LYS:HG3 | 1.55 | 0.71 |
| 1:c:531:ASP:OD1 | 1:c:569:LYS:NZ | 2.21 | 0.71 |
| 1:d:321:ILE:HD13 | 1:d:343:ILE:HD11 | 1.72 | 0.71 |
| 1:e:340:THR:O | 1:e:407:ARG:NH2 | 2.23 | 0.71 |
| 1:j:321:ILE:HD13 | 1:j:343:ILE:HD11 | 1.72 | 0.71 |
| 1:r:240:VAL:HG13 | 1:r:687:TRP:HB2 | 1.72 | 0.71 |
| 1:r:613:ASP:CB | 1:r:732:ARG:CD | 2.65 | 0.71 |
| 1:s:328:GLN:HE22 | 1:s:333:LYS:HG3 | 1.54 | 0.71 |
| 1:2:321:ILE:HD13 | 1:2:343:ILE:HD11 | 1.72 | 0.71 |
| 1:4:609:TRP:HH2 | 1:4:631:PHE:HZ | 1.35 | 0.71 |
| 1:5:240:VAL:HG13 | 1:5:687:TRP:HB2 | 1.72 | 0.71 |
| 1:7:613:ASP:CB | 1:7:732:ARG:CD | 2.65 | 0.71 |
| 1:A:321:ILE:HD13 | 1:A:343:ILE:HD11 | 1.72 | 0.71 |
| 1:B:340:THR:O | 1:B:407:ARG:NH2 | 2.23 | 0.71 |
| 1:E:613:ASP:CB | 1:E:732:ARG:CD | 2.65 | 0.71 |
| 1:I:328:GLN:HE22 | 1:I:333:LYS:HG3 | 1.55 | 0.71 |
| 1:J:531:ASP:OD1 | 1:J:569:LYS:NZ | 2.21 | 0.71 |
| 1:Q:240:VAL:HG13 | 1:Q:687:TRP:HB2 | 1.72 | 0.71 |
| 1:T:328:GLN:HE22 | 1:T:333:LYS:HG3 | 1.54 | 0.71 |
| 1:T:609:TRP:HH2 | 1:T:631:PHE:HZ | 1.35 | 0.71 |
| 1:U:613:ASP:CB | 1:U:731:THR:HG22 | 2.17 | 0.71 |
| 1:V:354:PRO:HB3 | 1:X:431:GLN:HE22 | 1.56 | 0.71 |
| 1:Y:613:ASP:CB | 1:Y:732:ARG:CD | 2.65 | 0.71 |
| 1:Z:609:TRP:HH2 | 1:Z:631:PHE:HZ | 1.35 | 0.71 |
| 1:r:321:ILE:HD13 | 1:r:343:ILE:HD11 | 1.72 | 0.71 |
| 1:t:328:GLN:HE22 | 1:t:333:LYS:HG3 | 1.54 | 0.71 |
| 1:t:340:THR:O | 1:t:407:ARG:NH2 | 2.23 | 0.71 |
| 1:z:340:THR:O | 1:z:407:ARG:NH2 | 2.23 | 0.71 |
| 1:1:240:VAL:HG13 | 1:1:687:TRP:HB2 | 1.72 | 0.71 |
| 1:8:328:GLN:HE22 | 1:8:333:LYS:HG3 | 1.55 | 0.71 |
| 1:C:340:THR:O | 1:C:407:ARG:NH2 | 2.23 | 0.71 |
| 1:I:531:ASP:OD1 | 1:I:569:LYS:NZ | 2.21 | 0.71 |
| 1:L:340:THR:O | 1:L:407:ARG:NH2 | 2.23 | 0.71 |
| 1:R:340:THR:O | 1:R:407:ARG:NH2 | 2.23 | 0.71 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:d:340:THR:O | 1:d:407:ARG:NH2 | 2.23 | 0.71 |
| 1:f:240:VAL:HG13 | 1:f:687:TRP:HB2 | 1.72 | 0.71 |
| 1:g:328:GLN:HE22 | 1:g:333:LYS:HG3 | 1.54 | 0.71 |
| 1:l:340:THR:O | 1:l:407:ARG:NH2 | 2.23 | 0.71 |
| 1:1:328:GLN:HE22 | 1:1:333:LYS:HG3 | 1.54 | 0.71 |
| 1:1:609:TRP:HH2 | 1:1:631:PHE:HZ | 1.35 | 0.71 |
| 1:2:340:THR:O | 1:2:407:ARG:NH2 | 2.23 | 0.71 |
| 1:3:609:TRP:HH2 | 1:3:631:PHE:HZ | 1.35 | 0.71 |
| 1:F:321:ILE:HD13 | 1:F:343:ILE:HD11 | 1.72 | 0.71 |
| 1:G:340:THR:O | 1:G:407:ARG:NH2 | 2.23 | 0.71 |
| 1:N:431:GLN:HE22 | 1:P:354:PRO:HB3 | 1.56 | 0.71 |
| 1:O:609:TRP:HH2 | 1:O:631:PHE:HZ | 1.35 | 0.71 |
| 1:R:240:VAL:HG13 | 1:R:687:TRP:HB2 | 1.72 | 0.71 |
| 1:T:240:VAL:HG13 | 1:T:687:TRP:HB2 | 1.72 | 0.71 |
| 1:V:340:THR:O | 1:V:407:ARG:NH2 | 2.23 | 0.71 |
| 1:b:340:THR:O | 1:b:407:ARG:NH2 | 2.23 | 0.71 |
| 1:i:340:THR:O | 1:i:407:ARG:NH2 | 2.23 | 0.71 |
| 1:j:240:VAL:HG13 | 1:j:687:TRP:HB2 | 1.72 | 0.71 |
| 1:m:609:TRP:HE1 | 1:n:629:GLY:HA3 | 1.52 | 0.71 |
| 1:p:340:THR:O | 1:p:407:ARG:NH2 | 2.23 | 0.71 |
| 1:t:240:VAL:HG13 | 1:t:687:TRP:HB2 | 1.72 | 0.71 |
| 1:5:609:TRP:HE1 | 1:6:629:GLY:HA3 | 1.52 | 0.71 |
| 1:A:240:VAL:HG13 | 1:A:687:TRP:HB2 | 1.72 | 0.71 |
| 1:H:340:THR:O | 1:H:407:ARG:NH2 | 2.23 | 0.71 |
| 1:J:609:TRP:HH2 | 1:J:631:PHE:HZ | 1.35 | 0.71 |
| 1:Z:321:ILE:HD13 | 1:Z:343:ILE:HD11 | 1.72 | 0.71 |
| 1:a:431:GLN:HE22 | 1:8:354:PRO:HB3 | 1.56 | 0.71 |
| 1:c:328:GLN:HE22 | 1:c:333:LYS:HG3 | 1.55 | 0.71 |
| 1:g:340:THR:O | 1:g:407:ARG:NH2 | 2.23 | 0.71 |
| 1:g:609:TRP:HH2 | 1:g:631:PHE:HZ | 1.35 | 0.71 |
| 1:m:321:ILE:HD13 | 1:m:343:ILE:HD11 | 1.72 | 0.71 |
| 1:y:340:THR:O | 1:y:407:ARG:NH2 | 2.23 | 0.71 |
| 1:6:321:ILE:HD13 | 1:6:343:ILE:HD11 | 1.72 | 0.71 |
| 1:G:609:TRP:HH2 | 1:G:631:PHE:HZ | 1.35 | 0.71 |
| 1:P:328:GLN:HE22 | 1:P:333:LYS:HG3 | 1.55 | 0.71 |
| 1:W:340:THR:O | 1:W:407:ARG:NH2 | 2.23 | 0.71 |
| 1:W:613:ASP:CB | 1:W:731:THR:HG22 | 2.17 | 0.71 |
| 1:i:609:TRP:HH2 | 1:i:631:PHE:HZ | 1.35 | 0.71 |
| 1:v:613:ASP:CB | 1:v:731:THR:HG22 | 2.17 | 0.71 |
| 1:2:613:ASP:CB | 1:2:731:THR:HG22 | 2.17 | 0.71 |
| 1:P:321:ILE:HD13 | 1:P:343:ILE:HD11 | 1.72 | 0.71 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:321:ILE:HD13 | 1:R:343:ILE:HD11 | 1.72 | 0.71 |
| 1:R:613:ASP:CB | 1:R:732:ARG:CD | 2.65 | 0.71 |
| 1:l:328:GLN:HE22 | 1:l:333:LYS:HG3 | 1.55 | 0.71 |
| 1:o:240:VAL:HG13 | 1:o:687:TRP:HB2 | 1.72 | 0.71 |
| 1:s:340:THR:O | 1:s:407:ARG:NH2 | 2.23 | 0.71 |
| 1:D:354:PRO:HB3 | 1:P:431:GLN:HE22 | 1.56 | 0.70 |
| 1:F:240:VAL:HG13 | 1:F:687:TRP:HB2 | 1.72 | 0.70 |
| 1:I:240:VAL:HG13 | 1:I:687:TRP:HB2 | 1.72 | 0.70 |
| 1:K:354:PRO:HB3 | 1:8:431:GLN:HE22 | 1.56 | 0.70 |
| 1:L:613:ASP:CB | 1:L:731:THR:HG22 | 2.17 | 0.70 |
| 1:M:609:TRP:HH2 | 1:M:631:PHE:HZ | 1.35 | 0.70 |
| 1:d:613:ASP:CB | 1:d:731:THR:HG22 | 2.17 | 0.70 |
| 1:l:613:ASP:CB | 1:l:731:THR:HG22 | 2.17 | 0.70 |
| 1:n:240:VAL:HG13 | 1:n:687:TRP:HB2 | 1.72 | 0.70 |
| 1:q:340:THR:O | 1:q:407:ARG:NH2 | 2.23 | 0.70 |
| 1:z:613:ASP:CB | 1:z:731:THR:HG22 | 2.17 | 0.70 |
| 1:4:240:VAL:HG13 | 1:4:687:TRP:HB2 | 1.72 | 0.70 |
| 1:4:321:ILE:HD13 | 1:4:343:ILE:HD11 | 1.72 | 0.70 |
| 1:X:531:ASP:OD1 | 1:X:569:LYS:NZ | 2.21 | 0.70 |
| 1:t:613:ASP:CB | 1:t:732:ARG:CD | 2.65 | 0.70 |
| 1:u:531:ASP:OD1 | 1:u:569:LYS:NZ | 2.21 | 0.70 |
| 1:v:531:ASP:OD1 | 1:v:569:LYS:NZ | 2.21 | 0.70 |
| 1:z:328:GLN:HE22 | 1:z:333:LYS:HG3 | 1.55 | 0.70 |
| 1:3:613:ASP:CB | 1:3:731:THR:HG22 | 2.17 | 0.70 |
| 1:8:321:ILE:HD13 | 1:8:343:ILE:HD11 | 1.72 | 0.70 |
| 1:E:340:THR:O | 1:E:407:ARG:NH2 | 2.23 | 0.70 |
| 1:P:340:THR:O | 1:P:407:ARG:NH2 | 2.23 | 0.70 |
| 1:S:531:ASP:OD1 | 1:S:569:LYS:NZ | 2.21 | 0.70 |
| 1:c:240:VAL:HG13 | 1:c:687:TRP:HB2 | 1.72 | 0.70 |
| 1:l:240:VAL:HG13 | 1:l:687:TRP:HB2 | 1.72 | 0.70 |
| 1:p:609:TRP:HH2 | 1:p:631:PHE:HZ | 1.35 | 0.70 |
| 1:q:613:ASP:CB | 1:q:731:THR:HG22 | 2.17 | 0.70 |
| 1:t:321:ILE:HD13 | 1:t:343:ILE:HD11 | 1.72 | 0.70 |
| 1:w:431:GLN:HE22 | 1:x:354:PRO:HB3 | 1.56 | 0.70 |
| 1:z:240:VAL:HG13 | 1:z:687:TRP:HB2 | 1.72 | 0.70 |
| 1:6:240:VAL:HG13 | 1:6:687:TRP:HB2 | 1.72 | 0.70 |
| 1:C:354:PRO:HB3 | 1:M:431:GLN:HE22 | 1.56 | 0.70 |
| 1:J:431:GLN:HE22 | 1:L:354:PRO:HB3 | 1.56 | 0.70 |
| 1:Q:328:GLN:HE22 | 1:Q:333:LYS:HG3 | 1.55 | 0.70 |
| 1:Q:531:ASP:OD1 | 1:Q:569:LYS:NZ | 2.21 | 0.70 |
| 1:U:531:ASP:OD1 | 1:U:569:LYS:NZ | 2.21 | 0.70 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:354:PRO:HB3 | 1:e:431:GLN:HE22 | 1.57 | 0.70 |
| 1:Y:340:THR:O | 1:Y:407:ARG:NH2 | 2.23 | 0.70 |
| 1:c:321:ILE:HD13 | 1:c:343:ILE:HD11 | 1.72 | 0.70 |
| 1:d:328:GLN:HE22 | 1:d:333:LYS:HG3 | 1.55 | 0.70 |
| 1:n:321:ILE:HD13 | 1:n:343:ILE:HD11 | 1.72 | 0.70 |
| 1:q:613:ASP:CB | 1:q:732:ARG:CD | 2.65 | 0.70 |
| 1:1:531:ASP:OD1 | 1:1:569:LYS:NZ | 2.21 | 0.70 |
| 1:3:321:ILE:HD13 | 1:3:343:ILE:HD11 | 1.72 | 0.70 |
| 1:7:340:THR:O | 1:7:407:ARG:NH2 | 2.23 | 0.70 |
| 1:8:340:THR:O | 1:8:407:ARG:NH2 | 2.23 | 0.70 |
| 1:D:321:ILE:HD13 | 1:D:343:ILE:HD11 | 1.72 | 0.70 |
| 1:E:321:ILE:HD13 | 1:E:343:ILE:HD11 | 1.72 | 0.70 |
| 1:I:321:ILE:HD13 | 1:I:343:ILE:HD11 | 1.72 | 0.70 |
| 1:I:340:THR:O | 1:I:407:ARG:NH2 | 2.23 | 0.70 |
| 1:J:321:ILE:HD13 | 1:J:343:ILE:HD11 | 1.72 | 0.70 |
| 1:O:613:ASP:CB | 1:O:731:THR:HG22 | 2.17 | 0.70 |
| 1:V:609:TRP:HE1 | 1:e:629:GLY:HA3 | 1.52 | 0.70 |
| 1:W:613:ASP:CB | 1:W:732:ARG:CD | 2.65 | 0.70 |
| 1:c:354:PRO:HB3 | 1:p:431:GLN:HE22 | 1.56 | 0.70 |
| 1:u:240:VAL:HG13 | 1:u:687:TRP:HB2 | 1.72 | 0.70 |
| 1:2:328:GLN:HE22 | 1:2:333:LYS:HG3 | 1.55 | 0.70 |
| 1:J:240:VAL:HG13 | 1:J:687:TRP:HB2 | 1.72 | 0.70 |
| 1:O:321:ILE:HD13 | 1:O:343:ILE:HD11 | 1.72 | 0.70 |
| 1:S:240:VAL:HG13 | 1:S:687:TRP:HB2 | 1.72 | 0.70 |
| 1:T:354:PRO:HB3 | 1:l:431:GLN:HE22 | 1.56 | 0.70 |
| 1:V:240:VAL:HG13 | 1:V:687:TRP:HB2 | 1.72 | 0.70 |
| 1:V:431:GLN:HE22 | 1:e:354:PRO:HB3 | 1.56 | 0.70 |
| 1:l:613:ASP:CB | 1:l:732:ARG:CD | 2.65 | 0.70 |
| 1:r:340:THR:O | 1:r:407:ARG:NH2 | 2.23 | 0.70 |
| 1:y:240:VAL:HG13 | 1:y:687:TRP:HB2 | 1.72 | 0.70 |
| 1:z:431:GLN:HE22 | 1:1:354:PRO:HB3 | 1.56 | 0.70 |
| 1:7:321:ILE:HD13 | 1:7:343:ILE:HD11 | 1.72 | 0.70 |
| 1:G:431:GLN:HE22 | 1:I:354:PRO:HB3 | 1.56 | 0.70 |
| 1:M:321:ILE:HD13 | 1:M:343:ILE:HD11 | 1.72 | 0.70 |
| 1:T:531:ASP:OD1 | 1:T:569:LYS:NZ | 2.21 | 0.70 |
| 1:c:340:THR:O | 1:c:407:ARG:NH2 | 2.23 | 0.70 |
| 1:e:328:GLN:HE22 | 1:e:333:LYS:HG3 | 1.55 | 0.70 |
| 1:y:613:ASP:CB | 1:y:732:ARG:CD | 2.65 | 0.70 |
| 1:z:613:ASP:CB | 1:z:732:ARG:CD | 2.65 | 0.70 |
| 1:1:609:TRP:HE1 | 1:2:629:GLY:HA3 | 1.52 | 0.70 |
| 1:3:354:PRO:HB3 | 1:4:431:GLN:HE22 | 1.57 | 0.70 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:328:GLN:HE22 | 1:5:333:LYS:HG3 | 1.55 | 0.70 |
| 1:5:531:ASP:OD1 | 1:5:569:LYS:NZ | 2.21 | 0.70 |
| 1:C:431:GLN:HE22 | 1:b:354:PRO:HB3 | 1.57 | 0.70 |
| 1:w:328:GLN:HE22 | 1:w:333:LYS:HG3 | 1.54 | 0.70 |
| 1:w:354:PRO:HB3 | 1:y:431:GLN:HE22 | 1.55 | 0.70 |
| 1:B:354:PRO:HB3 | 1:L:431:GLN:HE22 | 1.57 | 0.70 |
| 1:B:531:ASP:OD1 | 1:B:569:LYS:NZ | 2.21 | 0.70 |
| 1:G:613:ASP:CB | 1:G:732:ARG:CD | 2.65 | 0.70 |
| 1:K:321:ILE:HD13 | 1:K:343:ILE:HD11 | 1.72 | 0.70 |
| 1:M:240:VAL:HG13 | 1:M:687:TRP:HB2 | 1.72 | 0.70 |
| 1:Q:321:ILE:HD13 | 1:Q:343:ILE:HD11 | 1.72 | 0.70 |
| 1:Y:613:ASP:CB | 1:Y:731:THR:HG22 | 2.17 | 0.70 |
| 1:d:431:GLN:HE22 | 1:l:354:PRO:HB3 | 1.56 | 0.70 |
| 1:p:613:ASP:CB | 1:p:732:ARG:CD | 2.65 | 0.70 |
| 1:q:321:ILE:HD13 | 1:q:343:ILE:HD11 | 1.72 | 0.70 |
| 1:5:354:PRO:HB3 | 1:7:431:GLN:HE22 | 1.56 | 0.70 |
| 1:H:354:PRO:HB3 | 1:Y:431:GLN:HE22 | 1.57 | 0.70 |
| 1:O:354:PRO:HB3 | 1:n:431:GLN:HE22 | 1.57 | 0.70 |
| 1:Z:431:GLN:HE22 | 1:4:354:PRO:HB3 | 1.57 | 0.70 |
| 1:h:531:ASP:OD1 | 1:h:569:LYS:NZ | 2.21 | 0.70 |
| 1:m:431:GLN:HE22 | 1:n:354:PRO:HB3 | 1.57 | 0.70 |
| 1:r:613:ASP:CB | 1:r:731:THR:HG22 | 2.17 | 0.70 |
| 1:5:321:ILE:HD13 | 1:5:343:ILE:HD11 | 1.72 | 0.70 |
| 1:E:431:GLN:HE22 | 1:Q:354:PRO:HB3 | 1.56 | 0.69 |
| 1:E:609:TRP:HE1 | 1:Q:629:GLY:HA3 | 1.53 | 0.69 |
| 1:K:609:TRP:HH2 | 1:K:631:PHE:HZ | 1.35 | 0.69 |
| 1:T:321:ILE:HD13 | 1:T:343:ILE:HD11 | 1.72 | 0.69 |
| 1:T:609:TRP:HE1 | 1:d:629:GLY:HA3 | 1.52 | 0.69 |
| 1:b:531:ASP:OD1 | 1:b:569:LYS:NZ | 2.21 | 0.69 |
| 1:k:531:ASP:OD1 | 1:k:569:LYS:NZ | 2.21 | 0.69 |
| 1:x:531:ASP:OD1 | 1:x:569:LYS:NZ | 2.21 | 0.69 |
| 1:1:321:ILE:HD13 | 1:1:343:ILE:HD11 | 1.72 | 0.69 |
| 1:3:629:GLY:HA3 | 1:4:609:TRP:HE1 | 1.53 | 0.69 |
| 1:F:579:TYR:OH | 1:F:607:MET:HE2 | 1.93 | 0.69 |
| 1:P:531:ASP:OD1 | 1:P:569:LYS:NZ | 2.21 | 0.69 |
| 1:i:321:ILE:HD13 | 1:i:343:ILE:HD11 | 1.72 | 0.69 |
| 1:o:431:GLN:HE22 | 1:p:354:PRO:HB3 | 1.57 | 0.69 |
| 1:r:431:GLN:HE22 | 1:s:354:PRO:HB3 | 1.57 | 0.69 |
| 1:z:354:PRO:HB3 | 1:2:431:GLN:HE22 | 1.56 | 0.69 |
| 1:1:431:GLN:HE22 | 1:2:354:PRO:HB3 | 1.57 | 0.69 |
| 1:5:431:GLN:HE22 | 1:6:354:PRO:HB3 | 1.57 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:6:579:TYR:OH | 1:6:607:MET:HE2 | 1.93 | 0.69 |
| 1:C:613:ASP:CB | 1:C:732:ARG:CD | 2.65 | 0.69 |
| 1:F:354:PRO:HB3 | 1:Q:431:GLN:HE22 | 1.57 | 0.69 |
| 1:J:579:TYR:OH | 1:J:607:MET:HE2 | 1.93 | 0.69 |
| 1:M:579:TYR:OH | 1:M:607:MET:HE2 | 1.93 | 0.69 |
| 1:O:431:GLN:HE22 | 1:m:354:PRO:HB3 | 1.56 | 0.69 |
| 1:W:321:ILE:HD13 | 1:W:343:ILE:HD11 | 1.72 | 0.69 |
| 1:W:579:TYR:OH | 1:W:607:MET:HE2 | 1.93 | 0.69 |
| 1:d:579:TYR:OH | 1:d:607:MET:HE2 | 1.93 | 0.69 |
| 1:e:321:ILE:HD13 | 1:e:343:ILE:HD11 | 1.72 | 0.69 |
| 1:f:354:PRO:HB3 | 1:g:431:GLN:HE22 | 1.57 | 0.69 |
| 1:i:431:GLN:HE22 | 1:j:354:PRO:HB3 | 1.57 | 0.69 |
| 1:t:613:ASP:CB | 1:t:731:THR:HG22 | 2.17 | 0.69 |
| 1:w:321:ILE:HD13 | 1:w:343:ILE:HD11 | 1.72 | 0.69 |
| 1:B:431:GLN:HE22 | 1:J:354:PRO:HB3 | 1.57 | 0.69 |
| 1:D:611:ASN:O | 1:D:732:ARG:NH1 | 2.26 | 0.69 |
| 1:H:613:ASP:CB | 1:H:731:THR:HG22 | 2.17 | 0.69 |
| 1:J:328:GLN:HE22 | 1:J:333:LYS:HG3 | 1.55 | 0.69 |
| 1:J:611:ASN:O | 1:J:732:ARG:NH1 | 2.26 | 0.69 |
| 1:J:613:ASP:CB | 1:J:731:THR:HG22 | 2.17 | 0.69 |
| 1:K:611:ASN:O | 1:K:732:ARG:NH1 | 2.26 | 0.69 |
| 1:M:328:GLN:HE22 | 1:M:333:LYS:HG3 | 1.55 | 0.69 |
| 1:M:611:ASN:O | 1:M:732:ARG:NH1 | 2.26 | 0.69 |
| 1:M:613:ASP:CB | 1:M:731:THR:HG22 | 2.17 | 0.69 |
| 1:R:613:ASP:CB | 1:R:731:THR:HG22 | 2.17 | 0.69 |
| 1:S:611:ASN:O | 1:S:732:ARG:NH1 | 2.26 | 0.69 |
| 1:T:431:GLN:HE22 | 1:d:354:PRO:HB3 | 1.57 | 0.69 |
| 1:X:579:TYR:OH | 1:X:607:MET:HE2 | 1.93 | 0.69 |
| 1:Z:354:PRO:HB3 | 1:3:431:GLN:HE22 | 1.56 | 0.69 |
| 1:a:326:VAL:HG21 | 1:a:333:LYS:HZ1 | 1.58 | 0.69 |
| 1:b:579:TYR:OH | 1:b:607:MET:HE2 | 1.93 | 0.69 |
| 1:g:531:ASP:OD1 | 1:g:569:LYS:NZ | 2.21 | 0.69 |
| 1:h:613:ASP:CB | 1:h:732:ARG:CD | 2.65 | 0.69 |
| 1:q:579:TYR:OH | 1:q:607:MET:HE2 | 1.93 | 0.69 |
| 1:q:611:ASN:O | 1:q:732:ARG:NH1 | 2.26 | 0.69 |
| 1:s:531:ASP:OD1 | 1:s:569:LYS:NZ | 2.21 | 0.69 |
| 1:u:611:ASN:O | 1:u:732:ARG:NH1 | 2.26 | 0.69 |
| 1:w:613:ASP:CB | 1:w:732:ARG:CD | 2.65 | 0.69 |
| 1:w:629:GLY:HA3 | 1:y:609:TRP:HE1 | 1.51 | 0.69 |
| 1:x:579:TYR:OH | 1:x:607:MET:HE2 | 1.93 | 0.69 |
| 1:2:579:TYR:OH | 1:2:607:MET:HE2 | 1.93 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:8:531:ASP:OD1 | 1:8:569:LYS:NZ | 2.21 | 0.69 |
| 1:A:431:GLN:HE22 | 1:G:354:PRO:HB3 | 1.57 | 0.69 |
| 1:B:321:ILE:HD13 | 1:B:343:ILE:HD11 | 1.72 | 0.69 |
| 1:B:579:TYR:OH | 1:B:607:MET:HE2 | 1.93 | 0.69 |
| 1:I:611:ASN:O | 1:I:732:ARG:NH1 | 2.26 | 0.69 |
| 1:M:354:PRO:HB3 | 1:b:431:GLN:HE22 | 1.57 | 0.69 |
| 1:O:629:GLY:HA3 | 1:n:609:TRP:HE1 | 1.53 | 0.69 |
| 1:Q:611:ASN:O | 1:Q:732:ARG:NH1 | 2.26 | 0.69 |
| 1:S:579:TYR:OH | 1:S:607:MET:HE2 | 1.93 | 0.69 |
| 1:c:611:ASN:O | 1:c:732:ARG:NH1 | 2.26 | 0.69 |
| 1:e:613:ASP:CB | 1:e:732:ARG:CD | 2.65 | 0.69 |
| 1:g:321:ILE:HD13 | 1:g:343:ILE:HD11 | 1.72 | 0.69 |
| 1:g:354:PRO:HB3 | 1:h:431:GLN:HE22 | 1.57 | 0.69 |
| 1:g:611:ASN:O | 1:g:732:ARG:NH1 | 2.26 | 0.69 |
| 1:i:354:PRO:HB3 | 1:k:431:GLN:HE22 | 1.57 | 0.69 |
| 1:i:611:ASN:O | 1:i:732:ARG:NH1 | 2.26 | 0.69 |
| 1:k:611:ASN:O | 1:k:732:ARG:NH1 | 2.26 | 0.69 |
| 1:l:531:ASP:OD1 | 1:l:569:LYS:NZ | 2.21 | 0.69 |
| 1:n:611:ASN:O | 1:n:732:ARG:NH1 | 2.26 | 0.69 |
| 1:n:613:ASP:CB | 1:n:731:THR:HG22 | 2.17 | 0.69 |
| 1:t:354:PRO:HB3 | 1:v:431:GLN:HE22 | 1.56 | 0.69 |
| 1:u:579:TYR:OH | 1:u:607:MET:HE2 | 1.93 | 0.69 |
| 1:4:611:ASN:O | 1:4:732:ARG:NH1 | 2.26 | 0.69 |
| 1:5:611:ASN:O | 1:5:732:ARG:NH1 | 2.26 | 0.69 |
| 1:D:609:TRP:HH2 | 1:D:631:PHE:HZ | 1.35 | 0.69 |
| 1:L:579:TYR:OH | 1:L:607:MET:HE2 | 1.93 | 0.69 |
| 1:L:613:ASP:CB | 1:L:732:ARG:CD | 2.65 | 0.69 |
| 1:P:613:ASP:CB | 1:P:731:THR:HG22 | 2.17 | 0.69 |
| 1:Q:579:TYR:OH | 1:Q:607:MET:HE2 | 1.93 | 0.69 |
| 1:W:611:ASN:O | 1:W:732:ARG:NH1 | 2.26 | 0.69 |
| 1:h:611:ASN:O | 1:h:732:ARG:NH1 | 2.26 | 0.69 |
| 1:i:531:ASP:OD1 | 1:i:569:LYS:NZ | 2.21 | 0.69 |
| 1:m:611:ASN:O | 1:m:732:ARG:NH1 | 2.26 | 0.69 |
| 1:n:613:ASP:CB | 1:n:732:ARG:CD | 2.65 | 0.69 |
| 1:s:613:ASP:CB | 1:s:731:THR:HG22 | 2.17 | 0.69 |
| 1:4:613:ASP:CB | 1:4:731:THR:HG22 | 2.17 | 0.69 |
| 1:5:579:TYR:OH | 1:5:607:MET:HE2 | 1.93 | 0.69 |
| 1:5:629:GLY:HA3 | 1:7:609:TRP:HE1 | 1.53 | 0.69 |
| 1:E:579:TYR:OH | 1:E:607:MET:HE2 | 1.93 | 0.69 |
| 1:H:531:ASP:OD1 | 1:H:569:LYS:NZ | 2.21 | 0.69 |
| 1:O:579:TYR:OH | 1:O:607:MET:HE2 | 1.93 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:431:GLN:HE22 | 1:Y:354:PRO:HB3 | 1.56 | 0.69 |
| 1:Z:611:ASN:O | 1:Z:732:ARG:NH1 | 2.26 | 0.69 |
| 1:k:579:TYR:OH | 1:k:607:MET:HE2 | 1.93 | 0.69 |
| 1:k:613:ASP:CB | 1:k:731:THR:HG22 | 2.17 | 0.69 |
| 1:q:431:GLN:HE22 | 1:r:354:PRO:HB3 | 1.56 | 0.69 |
| 1:t:609:TRP:HH2 | 1:t:631:PHE:HZ | 1.35 | 0.69 |
| 1:y:321:ILE:HD13 | 1:y:343:ILE:HD11 | 1.72 | 0.69 |
| 1:z:531:ASP:OD1 | 1:z:569:LYS:NZ | 2.21 | 0.69 |
| 1:B:611:ASN:O | 1:B:732:ARG:NH1 | 2.26 | 0.69 |
| 1:C:579:TYR:OH | 1:C:607:MET:HE2 | 1.93 | 0.69 |
| 1:F:611:ASN:O | 1:F:732:ARG:NH1 | 2.26 | 0.69 |
| 1:O:611:ASN:O | 1:O:732:ARG:NH1 | 2.26 | 0.69 |
| 1:P:609:TRP:HH2 | 1:P:631:PHE:HZ | 1.35 | 0.69 |
| 1:R:354:PRO:HB3 | 1:U:431:GLN:HE22 | 1.57 | 0.69 |
| 1:R:431:GLN:HE22 | 1:S:354:PRO:HB3 | 1.57 | 0.69 |
| 1:R:579:TYR:OH | 1:R:607:MET:HE2 | 1.93 | 0.69 |
| 1:R:609:TRP:HH2 | 1:R:631:PHE:HZ | 1.35 | 0.69 |
| 1:V:321:ILE:HD13 | 1:V:343:ILE:HD11 | 1.72 | 0.69 |
| 1:Z:579:TYR:OH | 1:Z:607:MET:HE2 | 1.93 | 0.69 |
| 1:a:579:TYR:OH | 1:a:607:MET:HE2 | 1.93 | 0.69 |
| 1:b:321:ILE:HD13 | 1:b:343:ILE:HD11 | 1.72 | 0.69 |
| 1:f:431:GLN:HE22 | 1:h:354:PRO:HB3 | 1.56 | 0.69 |
| 1:h:579:TYR:OH | 1:h:607:MET:HE2 | 1.93 | 0.69 |
| 1:m:579:TYR:OH | 1:m:607:MET:HE2 | 1.93 | 0.69 |
| 1:t:579:TYR:OH | 1:t:607:MET:HE2 | 1.93 | 0.69 |
| 1:3:579:TYR:OH | 1:3:607:MET:HE2 | 1.93 | 0.69 |
| 1:3:611:ASN:O | 1:3:732:ARG:NH1 | 2.26 | 0.69 |
| 1:4:613:ASP:CB | 1:4:732:ARG:CD | 2.65 | 0.69 |
| 1:6:431:GLN:HE22 | 1:7:354:PRO:HB3 | 1.57 | 0.69 |
| 1:6:611:ASN:O | 1:6:732:ARG:NH1 | 2.26 | 0.69 |
| 1:7:579:TYR:OH | 1:7:607:MET:HE2 | 1.93 | 0.69 |
| 1:7:611:ASN:O | 1:7:732:ARG:NH1 | 2.26 | 0.69 |
| 1:8:613:ASP:CB | 1:8:731:THR:HG22 | 2.17 | 0.69 |
| 1:E:611:ASN:O | 1:E:732:ARG:NH1 | 2.26 | 0.69 |
| 1:G:579:TYR:OH | 1:G:607:MET:HE2 | 1.93 | 0.69 |
| 1:N:579:TYR:OH | 1:N:607:MET:HE2 | 1.93 | 0.69 |
| 1:b:611:ASN:O | 1:b:732:ARG:NH1 | 2.26 | 0.69 |
| 1:1:611:ASN:O | 1:1:732:ARG:NH1 | 2.26 | 0.69 |
| 1:8:609:TRP:HH2 | 1:8:631:PHE:HZ | 1.35 | 0.69 |
| 1:C:611:ASN:O | 1:C:732:ARG:NH1 | 2.26 | 0.69 |
| 1:E:354:PRO:HB3 | 1:F:431:GLN:HE22 | 1.57 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:611:ASN:O | 1:R:732:ARG:NH1 | 2.26 | 0.69 |
| 1:T:611:ASN:O | 1:T:732:ARG:NH1 | 2.26 | 0.69 |
| 1:U:326:VAL:HG21 | 1:U:333:LYS:HZ1 | 1.58 | 0.69 |
| 1:j:431:GLN:HE22 | 1:k:354:PRO:HB3 | 1.57 | 0.69 |
| 1:p:579:TYR:OH | 1:p:607:MET:HE2 | 1.93 | 0.69 |
| 1:s:579:TYR:OH | 1:s:607:MET:HE2 | 1.93 | 0.69 |
| 1:t:611:ASN:O | 1:t:732:ARG:NH1 | 2.26 | 0.69 |
| 1:2:611:ASN:O | 1:2:732:ARG:NH1 | 2.26 | 0.69 |
| 1:4:579:TYR:OH | 1:4:607:MET:HE2 | 1.93 | 0.69 |
| 1:H:579:TYR:OH | 1:H:607:MET:HE2 | 1.93 | 0.68 |
| 1:L:611:ASN:O | 1:L:732:ARG:NH1 | 2.26 | 0.68 |
| 1:T:609:TRP:CH2 | 1:T:631:PHE:CZ | 2.80 | 0.68 |
| 1:d:611:ASN:O | 1:d:732:ARG:NH1 | 2.26 | 0.68 |
| 1:e:611:ASN:O | 1:e:732:ARG:NH1 | 2.26 | 0.68 |
| 1:g:609:TRP:CH2 | 1:g:631:PHE:CZ | 2.80 | 0.68 |
| 1:h:613:ASP:CB | 1:h:731:THR:HG22 | 2.17 | 0.68 |
| 1:n:579:TYR:OH | 1:n:607:MET:HE2 | 1.93 | 0.68 |
| 1:t:431:GLN:HE22 | 1:u:354:PRO:HB3 | 1.57 | 0.68 |
| 1:A:579:TYR:OH | 1:A:607:MET:HE2 | 1.93 | 0.68 |
| 1:B:484:PRO:HD3 | 1:B:609:TRP:HE3 | 1.59 | 0.68 |
| 1:D:579:TYR:OH | 1:D:607:MET:HE2 | 1.93 | 0.68 |
| 1:K:579:TYR:OH | 1:K:607:MET:HE2 | 1.93 | 0.68 |
| 1:P:611:ASN:O | 1:P:732:ARG:NH1 | 2.26 | 0.68 |
| 1:U:484:PRO:HD3 | 1:U:609:TRP:HE3 | 1.59 | 0.68 |
| 1:e:326:VAL:HG21 | 1:e:333:LYS:HZ1 | 1.58 | 0.68 |
| 1:g:579:TYR:OH | 1:g:607:MET:HE2 | 1.93 | 0.68 |
| 1:i:579:TYR:OH | 1:i:607:MET:HE2 | 1.93 | 0.68 |
| 1:l:611:ASN:O | 1:l:732:ARG:NH1 | 2.26 | 0.68 |
| 1:o:579:TYR:OH | 1:o:607:MET:HE2 | 1.93 | 0.68 |
| 1:v:611:ASN:O | 1:v:732:ARG:NH1 | 2.26 | 0.68 |
| 1:w:611:ASN:O | 1:w:732:ARG:NH1 | 2.26 | 0.68 |
| 1:z:611:ASN:O | 1:z:732:ARG:NH1 | 2.26 | 0.68 |
| 1:7:484:PRO:HD3 | 1:7:609:TRP:HE3 | 1.59 | 0.68 |
| 1:8:611:ASN:O | 1:8:732:ARG:NH1 | 2.26 | 0.68 |
| 1:D:484:PRO:HD3 | 1:D:609:TRP:HE3 | 1.59 | 0.68 |
| 1:E:484:PRO:HD3 | 1:E:609:TRP:HE3 | 1.59 | 0.68 |
| 1:K:484:PRO:HD3 | 1:K:609:TRP:HE3 | 1.59 | 0.68 |
| 1:U:611:ASN:O | 1:U:732:ARG:NH1 | 2.26 | 0.68 |
| 1:X:611:ASN:O | 1:X:732:ARG:NH1 | 2.26 | 0.68 |
| 1:b:484:PRO:HD3 | 1:b:609:TRP:HE3 | 1.59 | 0.68 |
| 1:i:609:TRP:CH2 | 1:i:631:PHE:CZ | 2.80 | 0.68 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:q:354:PRO:HB3 | 1:s:431:GLN:HE22 | 1.57 | 0.68 |
| 1:v:484:PRO:HD3 | 1:v:609:TRP:HE3 | 1.59 | 0.68 |
| 1:v:579:TYR:OH | 1:v:607:MET:HE2 | 1.93 | 0.68 |
| 1:x:611:ASN:O | 1:x:732:ARG:NH1 | 2.26 | 0.68 |
| 1:3:484:PRO:HD3 | 1:3:609:TRP:HE3 | 1.59 | 0.68 |
| 1:O:484:PRO:HD3 | 1:O:609:TRP:HE3 | 1.59 | 0.68 |
| 1:T:579:TYR:OH | 1:T:607:MET:HE2 | 1.93 | 0.68 |
| 1:U:579:TYR:OH | 1:U:607:MET:HE2 | 1.93 | 0.68 |
| 1:V:579:TYR:OH | 1:V:607:MET:HE2 | 1.93 | 0.68 |
| 1:e:579:TYR:OH | 1:e:607:MET:HE2 | 1.93 | 0.68 |
| 1:i:613:ASP:HB2 | 1:i:731:THR:CG2 | 2.19 | 0.68 |
| 1:k:402:PRO:HG3 | 1:w:232:ASP:HB3 | 1.76 | 0.68 |
| 1:s:611:ASN:O | 1:s:732:ARG:NH1 | 2.26 | 0.68 |
| 1:8:579:TYR:OH | 1:8:607:MET:HE2 | 1.93 | 0.68 |
| 1:H:431:GLN:HE22 | 1:W:354:PRO:HB3 | 1.57 | 0.68 |
| 1:H:611:ASN:O | 1:H:732:ARG:NH1 | 2.26 | 0.68 |
| 1:N:484:PRO:HD3 | 1:N:609:TRP:HE3 | 1.59 | 0.68 |
| 1:N:609:TRP:HE1 | 1:P:629:GLY:HA3 | 1.52 | 0.68 |
| 1:P:579:TYR:OH | 1:P:607:MET:HE2 | 1.93 | 0.68 |
| 1:e:484:PRO:HD3 | 1:e:609:TRP:HE3 | 1.59 | 0.68 |
| 1:q:322:GLN:NE2 | 1:y:340:THR:CB | 2.57 | 0.68 |
| 1:6:609:TRP:HE1 | 1:7:629:GLY:HA3 | 1.52 | 0.68 |
| 1:8:484:PRO:HD3 | 1:8:609:TRP:HE3 | 1.59 | 0.68 |
| 1:A:611:ASN:O | 1:A:732:ARG:NH1 | 2.26 | 0.68 |
| 1:G:611:ASN:O | 1:G:732:ARG:NH1 | 2.26 | 0.68 |
| 1:H:609:TRP:HH2 | 1:H:631:PHE:HZ | 1.35 | 0.68 |
| 1:H:609:TRP:CH2 | 1:H:631:PHE:CZ | 2.80 | 0.68 |
| 1:I:579:TYR:OH | 1:I:607:MET:HE2 | 1.93 | 0.68 |
| 1:Z:484:PRO:HD3 | 1:Z:609:TRP:HE3 | 1.59 | 0.68 |
| 1:a:484:PRO:HD3 | 1:a:609:TRP:HE3 | 1.59 | 0.68 |
| 1:a:611:ASN:O | 1:a:732:ARG:NH1 | 2.26 | 0.68 |
| 1:a:613:ASP:CB | 1:a:731:THR:HG22 | 2.17 | 0.68 |
| 1:m:484:PRO:HD3 | 1:m:609:TRP:HE3 | 1.59 | 0.68 |
| 1:o:611:ASN:O | 1:o:732:ARG:NH1 | 2.26 | 0.68 |
| 1:w:326:VAL:HG21 | 1:w:333:LYS:HZ1 | 1.58 | 0.68 |
| 1:w:484:PRO:HD3 | 1:w:609:TRP:HE3 | 1.59 | 0.68 |
| 1:w:579:TYR:OH | 1:w:607:MET:HE2 | 1.93 | 0.68 |
| 1:y:579:TYR:OH | 1:y:607:MET:HE2 | 1.93 | 0.68 |
| 1:1:579:TYR:OH | 1:1:607:MET:HE2 | 1.93 | 0.68 |
| 1:C:484:PRO:HD3 | 1:C:609:TRP:HE3 | 1.59 | 0.68 |
| 1:I:484:PRO:HD3 | 1:I:609:TRP:HE3 | 1.59 | 0.68 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:611:ASN:O | 1:N:732:ARG:NH1 | 2.26 | 0.68 |
| 1:V:484:PRO:HD3 | 1:V:609:TRP:HE3 | 1.59 | 0.68 |
| 1:c:579:TYR:OH | 1:c:607:MET:HE2 | 1.93 | 0.68 |
| 1:g:613:ASP:HB2 | 1:g:731:THR:CG2 | 2.19 | 0.68 |
| 1:j:579:TYR:OH | 1:j:607:MET:HE2 | 1.93 | 0.68 |
| 1:r:579:TYR:OH | 1:r:607:MET:HE2 | 1.93 | 0.68 |
| 1:y:611:ASN:O | 1:y:732:ARG:NH1 | 2.26 | 0.68 |
| 1:z:579:TYR:OH | 1:z:607:MET:HE2 | 1.93 | 0.68 |
| 1:2:484:PRO:HD3 | 1:2:609:TRP:HE3 | 1.59 | 0.68 |
| 1:G:609:TRP:CH2 | 1:G:631:PHE:CZ | 2.80 | 0.68 |
| 1:P:484:PRO:HD3 | 1:P:609:TRP:HE3 | 1.59 | 0.68 |
| 1:Y:579:TYR:OH | 1:Y:607:MET:HE2 | 1.93 | 0.68 |
| 1:c:484:PRO:HD3 | 1:c:609:TRP:HE3 | 1.59 | 0.68 |
| 1:f:579:TYR:OH | 1:f:607:MET:HE2 | 1.93 | 0.68 |
| 1:f:613:ASP:HB2 | 1:f:731:THR:CG2 | 2.19 | 0.68 |
| 1:p:611:ASN:O | 1:p:732:ARG:NH1 | 2.26 | 0.68 |
| 1:r:611:ASN:O | 1:r:732:ARG:NH1 | 2.26 | 0.68 |
| 1:s:609:TRP:CH2 | 1:s:631:PHE:CZ | 2.80 | 0.68 |
| 1:t:531:ASP:OD1 | 1:t:569:LYS:NZ | 2.21 | 0.68 |
| 1:u:431:GLN:HE22 | 1:v:354:PRO:HB3 | 1.57 | 0.68 |
| 1:y:484:PRO:HD3 | 1:y:609:TRP:HE3 | 1.59 | 0.68 |
| 1:A:484:PRO:HD3 | 1:A:609:TRP:HE3 | 1.59 | 0.68 |
| 1:E:629:GLY:HA3 | 1:F:609:TRP:HE1 | 1.52 | 0.68 |
| 1:L:484:PRO:HD3 | 1:L:609:TRP:HE3 | 1.59 | 0.68 |
| 1:N:613:ASP:CB | 1:N:731:THR:HG22 | 2.17 | 0.68 |
| 1:S:431:GLN:HE22 | 1:U:354:PRO:HB3 | 1.57 | 0.68 |
| 1:V:611:ASN:O | 1:V:732:ARG:NH1 | 2.26 | 0.68 |
| 1:Y:611:ASN:O | 1:Y:732:ARG:NH1 | 2.26 | 0.68 |
| 1:c:431:GLN:HE22 | 1:o:354:PRO:HB3 | 1.56 | 0.68 |
| 1:d:484:PRO:HD3 | 1:d:609:TRP:HE3 | 1.59 | 0.68 |
| 1:f:611:ASN:O | 1:f:732:ARG:NH1 | 2.26 | 0.68 |
| 1:j:611:ASN:O | 1:j:732:ARG:NH1 | 2.26 | 0.68 |
| 1:l:579:TYR:OH | 1:l:607:MET:HE2 | 1.93 | 0.68 |
| 1:A:354:PRO:HB3 | 1:I:431:GLN:HE22 | 1.57 | 0.68 |
| 1:B:232:ASP:O | 1:B:243:THR:HG22 | 1.94 | 0.68 |
| 1:B:613:ASP:CB | 1:B:731:THR:HG22 | 2.17 | 0.68 |
| 1:D:431:GLN:HE22 | 1:N:354:PRO:HB3 | 1.56 | 0.68 |
| 1:F:232:ASP:O | 1:F:243:THR:HG22 | 1.94 | 0.68 |
| 1:H:232:ASP:O | 1:H:243:THR:HG22 | 1.94 | 0.68 |
| 1:T:326:VAL:HG21 | 1:T:333:LYS:HZ1 | 1.58 | 0.68 |
| 1:W:484:PRO:HD3 | 1:W:609:TRP:HE3 | 1.59 | 0.68 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:613:ASP:CB | 1:X:731:THR:HG22 | 2.17 | 0.68 |
| 1:a:609:TRP:HE1 | 1:8:629:GLY:HA3 | 1.52 | 0.68 |
| 1:g:484:PRO:HD3 | 1:g:609:TRP:HE3 | 1.59 | 0.68 |
| 1:i:484:PRO:HD3 | 1:i:609:TRP:HE3 | 1.59 | 0.68 |
| 1:j:613:ASP:HB2 | 1:j:731:THR:CG2 | 2.19 | 0.68 |
| 1:n:484:PRO:HD3 | 1:n:609:TRP:HE3 | 1.59 | 0.68 |
| 1:o:484:PRO:HD3 | 1:o:609:TRP:HE3 | 1.59 | 0.68 |
| 1:p:609:TRP:CH2 | 1:p:631:PHE:CZ | 2.80 | 0.68 |
| 1:s:232:ASP:O | 1:s:243:THR:HG22 | 1.94 | 0.68 |
| 1:1:326:VAL:HG21 | 1:1:333:LYS:HZ1 | 1.58 | 0.68 |
| 1:6:232:ASP:O | 1:6:243:THR:HG22 | 1.94 | 0.68 |
| 1:A:232:ASP:O | 1:A:243:THR:HG22 | 1.94 | 0.67 |
| 1:C:531:ASP:OD1 | 1:C:569:LYS:NZ | 2.21 | 0.67 |
| 1:G:232:ASP:O | 1:G:243:THR:HG22 | 1.95 | 0.67 |
| 1:N:232:ASP:O | 1:N:243:THR:HG22 | 1.95 | 0.67 |
| 1:S:232:ASP:O | 1:S:243:THR:HG22 | 1.94 | 0.67 |
| 1:a:232:ASP:O | 1:a:243:THR:HG22 | 1.95 | 0.67 |
| 1:b:232:ASP:O | 1:b:243:THR:HG22 | 1.94 | 0.67 |
| 1:d:232:ASP:O | 1:d:243:THR:HG22 | 1.95 | 0.67 |
| 1:f:609:TRP:CH2 | 1:f:631:PHE:CZ | 2.80 | 0.67 |
| 1:o:232:ASP:O | 1:o:243:THR:HG22 | 1.95 | 0.67 |
| 1:p:232:ASP:O | 1:p:243:THR:HG22 | 1.95 | 0.67 |
| 1:u:232:ASP:O | 1:u:243:THR:HG22 | 1.94 | 0.67 |
| 1:x:613:ASP:CB | 1:x:731:THR:HG22 | 2.17 | 0.67 |
| 1:z:484:PRO:HD3 | 1:z:609:TRP:HE3 | 1.59 | 0.67 |
| 1:A:484:PRO:HD3 | 1:A:609:TRP:CE3 | 2.30 | 0.67 |
| 1:G:484:PRO:HD3 | 1:G:609:TRP:CE3 | 2.30 | 0.67 |
| 1:L:531:ASP:OD1 | 1:L:569:LYS:NZ | 2.21 | 0.67 |
| 1:U:484:PRO:HD3 | 1:U:609:TRP:CE3 | 2.30 | 0.67 |
| 1:j:609:TRP:CH2 | 1:j:631:PHE:CZ | 2.80 | 0.67 |
| 1:k:613:ASP:CB | 1:k:732:ARG:CD | 2.65 | 0.67 |
| 1:l:484:PRO:HD3 | 1:l:609:TRP:HE3 | 1.59 | 0.67 |
| 1:p:484:PRO:HD3 | 1:p:609:TRP:CE3 | 2.30 | 0.67 |
| 1:q:484:PRO:HD3 | 1:q:609:TRP:HE3 | 1.59 | 0.67 |
| 1:t:484:PRO:HD3 | 1:t:609:TRP:HE3 | 1.59 | 0.67 |
| 1:2:232:ASP:O | 1:2:243:THR:HG22 | 1.95 | 0.67 |
| 1:3:322:GLN:HE21 | 1:8:340:THR:CB | 2.07 | 0.67 |
| 1:4:484:PRO:HD3 | 1:4:609:TRP:HE3 | 1.59 | 0.67 |
| 1:K:431:GLN:HE22 | 1:a:354:PRO:HB3 | 1.57 | 0.67 |
| 1:Q:232:ASP:O | 1:Q:243:THR:HG22 | 1.95 | 0.67 |
| 1:R:484:PRO:HD3 | 1:R:609:TRP:HE3 | 1.59 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:o:484:PRO:HD3 | 1:o:609:TRP:CE3 | 2.30 | 0.67 |
| 1:v:484:PRO:HD3 | 1:v:609:TRP:CE3 | 2.30 | 0.67 |
| 1:5:232:ASP:O | 1:5:243:THR:HG22 | 1.95 | 0.67 |
| 1:E:232:ASP:O | 1:E:243:THR:HG22 | 1.95 | 0.67 |
| 1:K:232:ASP:O | 1:K:243:THR:HG22 | 1.95 | 0.67 |
| 1:N:484:PRO:HD3 | 1:N:609:TRP:CE3 | 2.30 | 0.67 |
| 1:O:322:GLN:HE21 | 1:P:340:THR:CB | 2.07 | 0.67 |
| 1:P:232:ASP:O | 1:P:243:THR:HG22 | 1.95 | 0.67 |
| 1:R:340:THR:CB | 1:V:322:GLN:HE21 | 2.08 | 0.67 |
| 1:T:613:ASP:CB | 1:T:731:THR:HG22 | 2.17 | 0.67 |
| 1:V:613:ASP:HB2 | 1:V:731:THR:CG2 | 2.19 | 0.67 |
| 1:a:484:PRO:HD3 | 1:a:609:TRP:CE3 | 2.30 | 0.67 |
| 1:b:613:ASP:CB | 1:b:731:THR:HG22 | 2.17 | 0.67 |
| 1:l:484:PRO:HD3 | 1:l:609:TRP:CE3 | 2.30 | 0.67 |
| 1:y:350:GLU:OE1 | 1:y:352:GLN:NE2 | 2.28 | 0.67 |
| 1:1:613:ASP:CB | 1:1:731:THR:HG22 | 2.17 | 0.67 |
| 1:8:232:ASP:O | 1:8:243:THR:HG22 | 1.94 | 0.67 |
| 1:B:340:THR:CB | 1:C:322:GLN:HE21 | 2.08 | 0.67 |
| 1:D:232:ASP:O | 1:D:243:THR:HG22 | 1.95 | 0.67 |
| 1:D:350:GLU:OE1 | 1:D:352:GLN:NE2 | 2.28 | 0.67 |
| 1:D:484:PRO:HD3 | 1:D:609:TRP:CE3 | 2.30 | 0.67 |
| 1:F:350:GLU:OE1 | 1:F:352:GLN:NE2 | 2.28 | 0.67 |
| 1:G:613:ASP:CB | 1:G:731:THR:HG22 | 2.17 | 0.67 |
| 1:H:350:GLU:OE1 | 1:H:352:GLN:NE2 | 2.28 | 0.67 |
| 1:V:350:GLU:OE1 | 1:V:352:GLN:NE2 | 2.28 | 0.67 |
| 1:W:326:VAL:HG21 | 1:W:333:LYS:HZ1 | 1.59 | 0.67 |
| 1:n:484:PRO:HD3 | 1:n:609:TRP:CE3 | 2.30 | 0.67 |
| 1:s:350:GLU:OE1 | 1:s:352:GLN:NE2 | 2.28 | 0.67 |
| 1:t:232:ASP:O | 1:t:243:THR:HG22 | 1.95 | 0.67 |
| 1:v:232:ASP:O | 1:v:243:THR:HG22 | 1.94 | 0.67 |
| 1:w:484:PRO:HD3 | 1:w:609:TRP:CE3 | 2.30 | 0.67 |
| 1:7:232:ASP:O | 1:7:243:THR:HG22 | 1.95 | 0.67 |
| 1:A:613:ASP:CB | 1:A:731:THR:HG22 | 2.17 | 0.67 |
| 1:K:350:GLU:OE1 | 1:K:352:GLN:NE2 | 2.28 | 0.67 |
| 1:K:484:PRO:HD3 | 1:K:609:TRP:CE3 | 2.30 | 0.67 |
| 1:L:322:GLN:HE21 | 1:b:340:THR:CB | 2.08 | 0.67 |
| 1:R:232:ASP:O | 1:R:243:THR:HG22 | 1.95 | 0.67 |
| 1:U:232:ASP:O | 1:U:243:THR:HG22 | 1.95 | 0.67 |
| 1:V:340:THR:CB | 1:W:322:GLN:NE2 | 2.58 | 0.67 |
| 1:X:484:PRO:HD3 | 1:X:609:TRP:HE3 | 1.59 | 0.67 |
| 1:e:484:PRO:HD3 | 1:e:609:TRP:CE3 | 2.30 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:q:322:GLN:HE21 | 1:y:340:THR:CB | 2.05 | 0.67 |
| 1:t:484:PRO:HD3 | 1:t:609:TRP:CE3 | 2.30 | 0.67 |
| 1:x:484:PRO:HD3 | 1:x:609:TRP:HE3 | 1.59 | 0.67 |
| 1:y:613:ASP:HB2 | 1:y:731:THR:CG2 | 2.19 | 0.67 |
| 1:z:484:PRO:HD3 | 1:z:609:TRP:CE3 | 2.30 | 0.67 |
| 1:4:484:PRO:HD3 | 1:4:609:TRP:CE3 | 2.30 | 0.67 |
| 1:6:350:GLU:OE1 | 1:6:352:GLN:NE2 | 2.28 | 0.67 |
| 1:8:350:GLU:OE1 | 1:8:352:GLN:NE2 | 2.28 | 0.67 |
| 1:B:609:TRP:CH2 | 1:B:631:PHE:CZ | 2.80 | 0.67 |
| 1:O:350:GLU:OE1 | 1:O:352:GLN:NE2 | 2.28 | 0.67 |
| 1:P:350:GLU:OE1 | 1:P:352:GLN:NE2 | 2.28 | 0.67 |
| 1:Q:484:PRO:HD3 | 1:Q:609:TRP:HE3 | 1.59 | 0.67 |
| 1:Q:613:ASP:CB | 1:Q:731:THR:HG22 | 2.17 | 0.67 |
| 1:R:484:PRO:HD3 | 1:R:609:TRP:CE3 | 2.30 | 0.67 |
| 1:Y:484:PRO:HD3 | 1:Y:609:TRP:HE3 | 1.59 | 0.67 |
| 1:e:531:ASP:OD1 | 1:e:569:LYS:NZ | 2.21 | 0.67 |
| 1:o:613:ASP:CB | 1:o:731:THR:HG22 | 2.17 | 0.67 |
| 1:r:484:PRO:HD3 | 1:r:609:TRP:HE3 | 1.59 | 0.67 |
| 1:1:484:PRO:HD3 | 1:1:609:TRP:CE3 | 2.30 | 0.67 |
| 1:8:484:PRO:HD3 | 1:8:609:TRP:CE3 | 2.30 | 0.67 |
| 1:I:350:GLU:OE1 | 1:I:352:GLN:NE2 | 2.28 | 0.67 |
| 1:L:484:PRO:HD3 | 1:L:609:TRP:CE3 | 2.30 | 0.67 |
| 1:P:484:PRO:HD3 | 1:P:609:TRP:CE3 | 2.30 | 0.67 |
| 1:Q:350:GLU:OE1 | 1:Q:352:GLN:NE2 | 2.28 | 0.67 |
| 1:T:350:GLU:OE1 | 1:T:352:GLN:NE2 | 2.28 | 0.67 |
| 1:T:484:PRO:HD3 | 1:T:609:TRP:CE3 | 2.30 | 0.67 |
| 1:W:350:GLU:OE1 | 1:W:352:GLN:NE2 | 2.28 | 0.67 |
| 1:b:609:TRP:CH2 | 1:b:631:PHE:CZ | 2.80 | 0.67 |
| 1:c:350:GLU:OE1 | 1:c:352:GLN:NE2 | 2.28 | 0.67 |
| 1:f:613:ASP:CB | 1:f:731:THR:HG22 | 2.17 | 0.67 |
| 1:g:232:ASP:O | 1:g:243:THR:HG22 | 1.94 | 0.67 |
| 1:g:484:PRO:HD3 | 1:g:609:TRP:CE3 | 2.30 | 0.67 |
| 1:j:343:ILE:HD12 | 1:j:651:ILE:HD11 | 1.77 | 0.67 |
| 1:q:350:GLU:OE1 | 1:q:352:GLN:NE2 | 2.28 | 0.67 |
| 1:z:232:ASP:O | 1:z:243:THR:HG22 | 1.95 | 0.67 |
| 1:3:350:GLU:OE1 | 1:3:352:GLN:NE2 | 2.28 | 0.67 |
| 1:A:350:GLU:OE1 | 1:A:352:GLN:NE2 | 2.28 | 0.67 |
| 1:B:484:PRO:HD3 | 1:B:609:TRP:CE3 | 2.30 | 0.67 |
| 1:C:484:PRO:HD3 | 1:C:609:TRP:CE3 | 2.30 | 0.67 |
| 1:I:484:PRO:HD3 | 1:I:609:TRP:CE3 | 2.30 | 0.67 |
| 1:J:484:PRO:HD3 | 1:J:609:TRP:CE3 | 2.30 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:343:ILE:HD12 | 1:Y:651:ILE:HD11 | 1.77 | 0.67 |
| 1:b:322:GLN:HE21 | 1:o:340:THR:CB | 2.08 | 0.67 |
| 1:d:350:GLU:OE1 | 1:d:352:GLN:NE2 | 2.28 | 0.67 |
| 1:f:343:ILE:HD12 | 1:f:651:ILE:HD11 | 1.77 | 0.67 |
| 1:h:484:PRO:HD3 | 1:h:609:TRP:HE3 | 1.59 | 0.67 |
| 1:i:350:GLU:OE1 | 1:i:352:GLN:NE2 | 2.28 | 0.67 |
| 1:i:484:PRO:HD3 | 1:i:609:TRP:CE3 | 2.30 | 0.67 |
| 1:k:484:PRO:HD3 | 1:k:609:TRP:HE3 | 1.59 | 0.67 |
| 1:l:232:ASP:O | 1:l:243:THR:HG22 | 1.95 | 0.67 |
| 1:l:350:GLU:OE1 | 1:l:352:GLN:NE2 | 2.28 | 0.67 |
| 1:m:484:PRO:HD3 | 1:m:609:TRP:CE3 | 2.30 | 0.67 |
| 1:o:350:GLU:OE1 | 1:o:352:GLN:NE2 | 2.28 | 0.67 |
| 1:p:613:ASP:CB | 1:p:731:THR:HG22 | 2.17 | 0.67 |
| 1:r:340:THR:CB | 1:x:322:GLN:HE21 | 2.08 | 0.67 |
| 1:r:343:ILE:HD12 | 1:r:651:ILE:HD11 | 1.77 | 0.67 |
| 1:t:322:GLN:HE21 | 1:6:340:THR:CB | 2.08 | 0.67 |
| 1:u:484:PRO:HD3 | 1:u:609:TRP:CE3 | 2.30 | 0.67 |
| 1:v:340:THR:CB | 1:1:322:GLN:HE21 | 2.08 | 0.67 |
| 1:w:531:ASP:OD1 | 1:w:569:LYS:NZ | 2.21 | 0.67 |
| 1:1:350:GLU:OE1 | 1:1:352:GLN:NE2 | 2.28 | 0.67 |
| 1:2:350:GLU:OE1 | 1:2:352:GLN:NE2 | 2.28 | 0.67 |
| 1:3:484:PRO:HD3 | 1:3:609:TRP:CE3 | 2.30 | 0.67 |
| 1:5:350:GLU:OE1 | 1:5:352:GLN:NE2 | 2.28 | 0.67 |
| 1:5:613:ASP:CB | 1:5:731:THR:HG22 | 2.17 | 0.67 |
| 1:C:232:ASP:O | 1:C:243:THR:HG22 | 1.95 | 0.67 |
| 1:C:326:VAL:HG21 | 1:C:333:LYS:HZ1 | 1.58 | 0.67 |
| 1:K:609:TRP:CH2 | 1:K:631:PHE:CZ | 2.80 | 0.67 |
| 1:L:609:TRP:CH2 | 1:L:631:PHE:CZ | 2.80 | 0.67 |
| 1:S:484:PRO:HD3 | 1:S:609:TRP:CE3 | 2.30 | 0.67 |
| 1:X:350:GLU:OE1 | 1:X:352:GLN:NE2 | 2.28 | 0.67 |
| 1:Z:484:PRO:HD3 | 1:Z:609:TRP:CE3 | 2.30 | 0.67 |
| 1:a:343:ILE:HD12 | 1:a:651:ILE:HD11 | 1.77 | 0.67 |
| 1:c:484:PRO:HD3 | 1:c:609:TRP:CE3 | 2.30 | 0.67 |
| 1:d:343:ILE:HD12 | 1:d:651:ILE:HD11 | 1.77 | 0.67 |
| 1:f:232:ASP:O | 1:f:243:THR:HG22 | 1.94 | 0.67 |
| 1:g:350:GLU:OE1 | 1:g:352:GLN:NE2 | 2.28 | 0.67 |
| 1:h:326:VAL:HG21 | 1:h:333:LYS:HZ1 | 1.60 | 0.67 |
| 1:i:232:ASP:O | 1:i:243:THR:HG22 | 1.95 | 0.67 |
| 1:j:613:ASP:CB | 1:j:731:THR:HG22 | 2.17 | 0.67 |
| 1:k:232:ASP:O | 1:k:243:THR:HG22 | 1.95 | 0.67 |
| 1:r:232:ASP:O | 1:r:243:THR:HG22 | 1.94 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:w:343:ILE:HD12 | 1:w:651:ILE:HD11 | 1.77 | 0.67 |
| 1:x:350:GLU:OE1 | 1:x:352:GLN:NE2 | 2.28 | 0.67 |
| 1:z:350:GLU:OE1 | 1:z:352:GLN:NE2 | 2.28 | 0.67 |
| 1:1:484:PRO:HD3 | 1:1:609:TRP:HE3 | 1.59 | 0.67 |
| 1:2:343:ILE:HD12 | 1:2:651:ILE:HD11 | 1.77 | 0.67 |
| 1:2:484:PRO:HD3 | 1:2:609:TRP:CE3 | 2.30 | 0.67 |
| 1:5:484:PRO:HD3 | 1:5:609:TRP:HE3 | 1.59 | 0.67 |
| 1:A:609:TRP:CH2 | 1:A:631:PHE:CZ | 2.80 | 0.66 |
| 1:C:340:THR:CB | 1:D:322:GLN:NE2 | 2.59 | 0.66 |
| 1:E:350:GLU:OE1 | 1:E:352:GLN:NE2 | 2.28 | 0.66 |
| 1:F:340:THR:CB | 1:R:322:GLN:HE21 | 2.08 | 0.66 |
| 1:K:322:GLN:NE2 | 1:L:340:THR:CB | 2.59 | 0.66 |
| 1:M:232:ASP:O | 1:M:243:THR:HG22 | 1.94 | 0.66 |
| 1:N:343:ILE:HD12 | 1:N:651:ILE:HD11 | 1.77 | 0.66 |
| 1:N:350:GLU:OE1 | 1:N:352:GLN:NE2 | 2.28 | 0.66 |
| 1:O:484:PRO:HD3 | 1:O:609:TRP:CE3 | 2.30 | 0.66 |
| 1:Q:343:ILE:HD12 | 1:Q:651:ILE:HD11 | 1.77 | 0.66 |
| 1:Q:484:PRO:HD3 | 1:Q:609:TRP:CE3 | 2.30 | 0.66 |
| 1:a:350:GLU:OE1 | 1:a:352:GLN:NE2 | 2.28 | 0.66 |
| 1:b:484:PRO:HD3 | 1:b:609:TRP:CE3 | 2.30 | 0.66 |
| 1:d:484:PRO:HD3 | 1:d:609:TRP:CE3 | 2.30 | 0.66 |
| 1:j:322:GLN:HE21 | 1:x:340:THR:CB | 2.08 | 0.66 |
| 1:q:343:ILE:HD12 | 1:q:651:ILE:HD11 | 1.77 | 0.66 |
| 1:v:350:GLU:OE1 | 1:v:352:GLN:NE2 | 2.28 | 0.66 |
| 1:6:343:ILE:HD12 | 1:6:651:ILE:HD11 | 1.77 | 0.66 |
| 1:7:350:GLU:OE1 | 1:7:352:GLN:NE2 | 2.28 | 0.66 |
| 1:C:609:TRP:CH2 | 1:C:631:PHE:CZ | 2.80 | 0.66 |
| 1:F:343:ILE:HD12 | 1:F:651:ILE:HD11 | 1.77 | 0.66 |
| 1:I:609:TRP:CH2 | 1:I:631:PHE:CZ | 2.80 | 0.66 |
| 1:L:232:ASP:O | 1:L:243:THR:HG22 | 1.95 | 0.66 |
| 1:L:350:GLU:OE1 | 1:L:352:GLN:NE2 | 2.28 | 0.66 |
| 1:R:343:ILE:HD12 | 1:R:651:ILE:HD11 | 1.77 | 0.66 |
| 1:W:343:ILE:HD12 | 1:W:651:ILE:HD11 | 1.77 | 0.66 |
| 1:Y:232:ASP:O | 1:Y:243:THR:HG22 | 1.94 | 0.66 |
| 1:c:609:TRP:CH2 | 1:c:631:PHE:CZ | 2.80 | 0.66 |
| 1:h:232:ASP:O | 1:h:243:THR:HG22 | 1.95 | 0.66 |
| 1:i:343:ILE:HD12 | 1:i:651:ILE:HD11 | 1.77 | 0.66 |
| 1:j:232:ASP:O | 1:j:243:THR:HG22 | 1.95 | 0.66 |
| 1:j:484:PRO:HD3 | 1:j:609:TRP:CE3 | 2.30 | 0.66 |
| 1:k:350:GLU:OE1 | 1:k:352:GLN:NE2 | 2.28 | 0.66 |
| 1:p:322:GLN:HE21 | 1:q:340:THR:CB | 2.09 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:z:340:THR:HB | 1:4:322:GLN:NE2 | 2.11 | 0.66 |
| 1:3:343:ILE:HD12 | 1:3:651:ILE:HD11 | 1.77 | 0.66 |
| 1:5:343:ILE:HD12 | 1:5:651:ILE:HD11 | 1.77 | 0.66 |
| 1:B:425:SER:O | 1:B:732:ARG:NH2 | 2.29 | 0.66 |
| 1:C:350:GLU:OE1 | 1:C:352:GLN:NE2 | 2.28 | 0.66 |
| 1:G:322:GLN:HE21 | 1:W:340:THR:CB | 2.09 | 0.66 |
| 1:G:425:SER:O | 1:G:732:ARG:NH2 | 2.29 | 0.66 |
| 1:J:232:ASP:O | 1:J:243:THR:HG22 | 1.94 | 0.66 |
| 1:L:326:VAL:HG21 | 1:L:333:LYS:HZ1 | 1.58 | 0.66 |
| 1:O:343:ILE:HD12 | 1:O:651:ILE:HD11 | 1.77 | 0.66 |
| 1:P:425:SER:O | 1:P:732:ARG:NH2 | 2.29 | 0.66 |
| 1:Q:609:TRP:CH2 | 1:Q:631:PHE:CZ | 2.80 | 0.66 |
| 1:U:350:GLU:OE1 | 1:U:352:GLN:NE2 | 2.28 | 0.66 |
| 1:W:232:ASP:O | 1:W:243:THR:HG22 | 1.94 | 0.66 |
| 1:W:484:PRO:HD3 | 1:W:609:TRP:CE3 | 2.30 | 0.66 |
| 1:Z:343:ILE:HD12 | 1:Z:651:ILE:HD11 | 1.77 | 0.66 |
| 1:b:350:GLU:OE1 | 1:b:352:GLN:NE2 | 2.28 | 0.66 |
| 1:b:425:SER:O | 1:b:732:ARG:NH2 | 2.29 | 0.66 |
| 1:e:343:ILE:HD12 | 1:e:651:ILE:HD11 | 1.77 | 0.66 |
| 1:e:350:GLU:OE1 | 1:e:352:GLN:NE2 | 2.28 | 0.66 |
| 1:f:425:SER:O | 1:f:732:ARG:NH2 | 2.29 | 0.66 |
| 1:g:343:ILE:HD12 | 1:g:651:ILE:HD11 | 1.77 | 0.66 |
| 1:h:350:GLU:OE1 | 1:h:352:GLN:NE2 | 2.28 | 0.66 |
| 1:j:425:SER:O | 1:j:732:ARG:NH2 | 2.29 | 0.66 |
| 1:k:340:THR:CB | 1:w:322:GLN:HE21 | 2.08 | 0.66 |
| 1:l:340:THR:HB | 1:n:322:GLN:NE2 | 2.11 | 0.66 |
| 1:o:609:TRP:CH2 | 1:o:631:PHE:CZ | 2.80 | 0.66 |
| 1:q:232:ASP:O | 1:q:243:THR:HG22 | 1.94 | 0.66 |
| 1:t:343:ILE:HD12 | 1:t:651:ILE:HD11 | 1.77 | 0.66 |
| 1:w:350:GLU:OE1 | 1:w:352:GLN:NE2 | 2.28 | 0.66 |
| 1:1:343:ILE:HD12 | 1:1:651:ILE:HD11 | 1.77 | 0.66 |
| 1:3:322:GLN:NE2 | 1:8:340:THR:CB | 2.58 | 0.66 |
| 1:4:232:ASP:O | 1:4:243:THR:HG22 | 1.94 | 0.66 |
| 1:5:484:PRO:HD3 | 1:5:609:TRP:CE3 | 2.30 | 0.66 |
| 1:5:609:TRP:CH2 | 1:5:631:PHE:CZ | 2.80 | 0.66 |
| 1:7:484:PRO:HD3 | 1:7:609:TRP:CE3 | 2.30 | 0.66 |
| 1:8:425:SER:O | 1:8:732:ARG:NH2 | 2.29 | 0.66 |
| 1:A:340:THR:CB | 1:B:322:GLN:HE21 | 2.09 | 0.66 |
| 1:A:425:SER:O | 1:A:732:ARG:NH2 | 2.29 | 0.66 |
| 1:B:350:GLU:OE1 | 1:B:352:GLN:NE2 | 2.28 | 0.66 |
| 1:D:609:TRP:CH2 | 1:D:631:PHE:CZ | 2.80 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:609:TRP:CH2 | 1:E:631:PHE:CZ | 2.80 | 0.66 |
| 1:H:343:ILE:HD12 | 1:H:651:ILE:HD11 | 1.77 | 0.66 |
| 1:O:232:ASP:O | 1:O:243:THR:HG22 | 1.94 | 0.66 |
| 1:S:343:ILE:HD12 | 1:S:651:ILE:HD11 | 1.77 | 0.66 |
| 1:X:340:THR:CB | 1:f:322:GLN:HE21 | 2.08 | 0.66 |
| 1:Y:484:PRO:HD3 | 1:Y:609:TRP:CE3 | 2.30 | 0.66 |
| 1:c:340:THR:CB | 1:s:322:GLN:HE21 | 2.08 | 0.66 |
| 1:f:484:PRO:HD3 | 1:f:609:TRP:CE3 | 2.30 | 0.66 |
| 1:m:343:ILE:HD12 | 1:m:651:ILE:HD11 | 1.77 | 0.66 |
| 1:o:425:SER:O | 1:o:732:ARG:NH2 | 2.29 | 0.66 |
| 1:p:425:SER:O | 1:p:732:ARG:NH2 | 2.29 | 0.66 |
| 1:q:484:PRO:HD3 | 1:q:609:TRP:CE3 | 2.30 | 0.66 |
| 1:u:343:ILE:HD12 | 1:u:651:ILE:HD11 | 1.77 | 0.66 |
| 1:y:232:ASP:O | 1:y:243:THR:HG22 | 1.94 | 0.66 |
| 1:6:484:PRO:HD3 | 1:6:609:TRP:CE3 | 2.30 | 0.66 |
| 1:D:613:ASP:HB2 | 1:D:731:THR:CG2 | 2.19 | 0.66 |
| 1:E:425:SER:O | 1:E:732:ARG:NH2 | 2.29 | 0.66 |
| 1:E:484:PRO:HD3 | 1:E:609:TRP:CE3 | 2.30 | 0.66 |
| 1:F:425:SER:O | 1:F:732:ARG:NH2 | 2.29 | 0.66 |
| 1:F:484:PRO:HD3 | 1:F:609:TRP:CE3 | 2.30 | 0.66 |
| 1:F:609:TRP:CH2 | 1:F:631:PHE:CZ | 2.80 | 0.66 |
| 1:H:322:GLN:HE21 | 1:I:340:THR:CB | 2.08 | 0.66 |
| 1:I:232:ASP:O | 1:I:243:THR:HG22 | 1.95 | 0.66 |
| 1:M:343:ILE:HD12 | 1:M:651:ILE:HD11 | 1.77 | 0.66 |
| 1:O:322:GLN:NE2 | 1:P:340:THR:CB | 2.58 | 0.66 |
| 1:P:322:GLN:NE2 | 1:Q:340:THR:CB | 2.59 | 0.66 |
| 1:T:343:ILE:HD12 | 1:T:651:ILE:HD11 | 1.77 | 0.66 |
| 1:V:232:ASP:O | 1:V:243:THR:HG22 | 1.94 | 0.66 |
| 1:V:340:THR:HB | 1:W:322:GLN:NE2 | 2.10 | 0.66 |
| 1:X:322:GLN:HE21 | 1:Y:340:THR:CB | 2.08 | 0.66 |
| 1:Z:340:THR:HB | 1:a:322:GLN:NE2 | 2.11 | 0.66 |
| 1:c:232:ASP:O | 1:c:243:THR:HG22 | 1.95 | 0.66 |
| 1:e:322:GLN:HE21 | 1:h:340:THR:CB | 2.08 | 0.66 |
| 1:g:340:THR:CB | 1:k:322:GLN:NE2 | 2.59 | 0.66 |
| 1:h:484:PRO:HD3 | 1:h:609:TRP:CE3 | 2.30 | 0.66 |
| 1:n:232:ASP:O | 1:n:243:THR:HG22 | 1.95 | 0.66 |
| 1:q:232:ASP:HB3 | 1:y:402:PRO:HG3 | 1.76 | 0.66 |
| 1:r:340:THR:CB | 1:x:322:GLN:NE2 | 2.58 | 0.66 |
| 1:r:484:PRO:HD3 | 1:r:609:TRP:CE3 | 2.30 | 0.66 |
| 1:s:343:ILE:HD12 | 1:s:651:ILE:HD11 | 1.77 | 0.66 |
| 1:u:484:PRO:HD3 | 1:u:609:TRP:HE3 | 1.59 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:y:613:ASP:CB | 1:y:731:THR:HG22 | 2.17 | 0.66 |
| 1:3:232:ASP:O | 1:3:243:THR:HG22 | 1.94 | 0.66 |
| 1:4:350:GLU:OE1 | 1:4:352:GLN:NE2 | 2.28 | 0.66 |
| 1:4:425:SER:O | 1:4:732:ARG:NH2 | 2.29 | 0.66 |
| 1:6:609:TRP:CH2 | 1:6:631:PHE:CZ | 2.80 | 0.66 |
| 1:7:425:SER:O | 1:7:732:ARG:NH2 | 2.29 | 0.66 |
| 1:7:609:TRP:CH2 | 1:7:631:PHE:CZ | 2.80 | 0.66 |
| 1:F:322:GLN:NE2 | 1:G:340:THR:CB | 2.59 | 0.66 |
| 1:F:484:PRO:HD3 | 1:F:609:TRP:HE3 | 1.59 | 0.66 |
| 1:G:343:ILE:HD12 | 1:G:651:ILE:HD11 | 1.77 | 0.66 |
| 1:I:343:ILE:HD12 | 1:I:651:ILE:HD11 | 1.77 | 0.66 |
| 1:J:343:ILE:HD12 | 1:J:651:ILE:HD11 | 1.77 | 0.66 |
| 1:R:350:GLU:OE1 | 1:R:352:GLN:NE2 | 2.28 | 0.66 |
| 1:Z:232:ASP:O | 1:Z:243:THR:HG22 | 1.94 | 0.66 |
| 1:a:425:SER:O | 1:a:732:ARG:NH2 | 2.29 | 0.66 |
| 1:f:350:GLU:OE1 | 1:f:352:GLN:NE2 | 2.28 | 0.66 |
| 1:h:322:GLN:NE2 | 1:i:340:THR:CB | 2.59 | 0.66 |
| 1:h:609:TRP:CH2 | 1:h:631:PHE:CZ | 2.80 | 0.66 |
| 1:j:350:GLU:OE1 | 1:j:352:GLN:NE2 | 2.28 | 0.66 |
| 1:k:484:PRO:HD3 | 1:k:609:TRP:CE3 | 2.30 | 0.66 |
| 1:n:350:GLU:OE1 | 1:n:352:GLN:NE2 | 2.28 | 0.66 |
| 1:n:425:SER:O | 1:n:732:ARG:NH2 | 2.29 | 0.66 |
| 1:p:340:THR:CB | 1:6:322:GLN:NE2 | 2.59 | 0.66 |
| 1:p:343:ILE:HD12 | 1:p:651:ILE:HD11 | 1.77 | 0.66 |
| 1:p:350:GLU:OE1 | 1:p:352:GLN:NE2 | 2.28 | 0.66 |
| 1:r:350:GLU:OE1 | 1:r:352:GLN:NE2 | 2.28 | 0.66 |
| 1:v:322:GLN:NE2 | 1:w:340:THR:CB | 2.59 | 0.66 |
| 1:w:232:ASP:O | 1:w:243:THR:HG22 | 1.94 | 0.66 |
| 1:5:340:THR:CB | 1:8:322:GLN:NE2 | 2.59 | 0.66 |
| 1:6:425:SER:O | 1:6:732:ARG:NH2 | 2.29 | 0.66 |
| 1:C:340:THR:CB | 1:D:322:GLN:HE21 | 2.08 | 0.66 |
| 1:G:350:GLU:OE1 | 1:G:352:GLN:NE2 | 2.28 | 0.66 |
| 1:G:484:PRO:HD3 | 1:G:609:TRP:HE3 | 1.59 | 0.66 |
| 1:I:425:SER:O | 1:I:732:ARG:NH2 | 2.29 | 0.66 |
| 1:K:613:ASP:HB2 | 1:K:731:THR:CG2 | 2.18 | 0.66 |
| 1:M:350:GLU:OE1 | 1:M:352:GLN:NE2 | 2.28 | 0.66 |
| 1:N:322:GLN:NE2 | 1:m:340:THR:HB | 2.11 | 0.66 |
| 1:S:484:PRO:HD3 | 1:S:609:TRP:HE3 | 1.59 | 0.66 |
| 1:U:343:ILE:HD12 | 1:U:651:ILE:HD11 | 1.77 | 0.66 |
| 1:V:609:TRP:CH2 | 1:V:631:PHE:CZ | 2.80 | 0.66 |
| 1:V:613:ASP:CB | 1:V:731:THR:HG22 | 2.17 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:350:GLU:OE1 | 1:Y:352:GLN:NE2 | 2.28 | 0.66 |
| 1:Z:350:GLU:OE1 | 1:Z:352:GLN:NE2 | 2.28 | 0.66 |
| 1:c:343:ILE:HD12 | 1:c:651:ILE:HD11 | 1.77 | 0.66 |
| 1:c:425:SER:O | 1:c:732:ARG:NH2 | 2.29 | 0.66 |
| 1:d:425:SER:O | 1:d:732:ARG:NH2 | 2.29 | 0.66 |
| 1:e:425:SER:O | 1:e:732:ARG:NH2 | 2.29 | 0.66 |
| 1:g:326:VAL:HG21 | 1:g:333:LYS:HZ1 | 1.60 | 0.66 |
| 1:g:425:SER:O | 1:g:732:ARG:NH2 | 2.29 | 0.66 |
| 1:k:609:TRP:CH2 | 1:k:631:PHE:CZ | 2.80 | 0.66 |
| 1:l:340:THR:CB | 1:n:322:GLN:HE21 | 2.08 | 0.66 |
| 1:m:350:GLU:OE1 | 1:m:352:GLN:NE2 | 2.28 | 0.66 |
| 1:s:484:PRO:HD3 | 1:s:609:TRP:CE3 | 2.30 | 0.66 |
| 1:t:350:GLU:OE1 | 1:t:352:GLN:NE2 | 2.28 | 0.66 |
| 1:v:343:ILE:HD12 | 1:v:651:ILE:HD11 | 1.77 | 0.66 |
| 1:w:425:SER:O | 1:w:732:ARG:NH2 | 2.29 | 0.66 |
| 1:x:232:ASP:O | 1:x:243:THR:HG22 | 1.95 | 0.66 |
| 1:1:232:ASP:O | 1:1:243:THR:HG22 | 1.95 | 0.66 |
| 1:1:425:SER:O | 1:1:732:ARG:NH2 | 2.29 | 0.66 |
| 1:4:343:ILE:HD12 | 1:4:651:ILE:HD11 | 1.77 | 0.66 |
| 1:D:340:THR:HB | 1:E:322:GLN:NE2 | 2.11 | 0.66 |
| 1:H:484:PRO:HD3 | 1:H:609:TRP:CE3 | 2.30 | 0.66 |
| 1:K:326:VAL:HG21 | 1:K:333:LYS:HZ1 | 1.60 | 0.66 |
| 1:N:425:SER:O | 1:N:732:ARG:NH2 | 2.29 | 0.66 |
| 1:Q:322:GLN:HE21 | 1:S:340:THR:CB | 2.08 | 0.66 |
| 1:S:350:GLU:OE1 | 1:S:352:GLN:NE2 | 2.28 | 0.66 |
| 1:T:232:ASP:O | 1:T:243:THR:HG22 | 1.95 | 0.66 |
| 1:T:425:SER:O | 1:T:732:ARG:NH2 | 2.29 | 0.66 |
| 1:U:609:TRP:CH2 | 1:U:631:PHE:CZ | 2.80 | 0.66 |
| 1:X:232:ASP:O | 1:X:243:THR:HG22 | 1.95 | 0.66 |
| 1:b:343:ILE:HD12 | 1:b:651:ILE:HD11 | 1.77 | 0.66 |
| 1:e:232:ASP:O | 1:e:243:THR:HG22 | 1.95 | 0.66 |
| 1:j:232:ASP:HB3 | 1:x:402:PRO:HG3 | 1.78 | 0.66 |
| 1:m:232:ASP:O | 1:m:243:THR:HG22 | 1.94 | 0.66 |
| 1:n:343:ILE:HD12 | 1:n:651:ILE:HD11 | 1.77 | 0.66 |
| 1:o:322:GLN:NE2 | 1:7:340:THR:HB | 2.11 | 0.66 |
| 1:v:322:GLN:NE2 | 1:w:340:THR:HB | 2.10 | 0.66 |
| 1:v:340:THR:CB | 1:1:322:GLN:NE2 | 2.59 | 0.66 |
| 1:v:609:TRP:CH2 | 1:v:631:PHE:CZ | 2.80 | 0.66 |
| 1:y:425:SER:O | 1:y:732:ARG:NH2 | 2.29 | 0.66 |
| 1:z:613:ASP:HB2 | 1:z:731:THR:CG2 | 2.18 | 0.66 |
| 1:2:425:SER:O | 1:2:732:ARG:NH2 | 2.29 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:343:ILE:HD12 | 1:B:651:ILE:HD11 | 1.77 | 0.66 |
| 1:C:613:ASP:CB | 1:C:731:THR:HG22 | 2.17 | 0.66 |
| 1:D:326:VAL:HG21 | 1:D:333:LYS:HZ1 | 1.61 | 0.66 |
| 1:D:340:THR:CB | 1:E:322:GLN:NE2 | 2.59 | 0.66 |
| 1:D:343:ILE:HD12 | 1:D:651:ILE:HD11 | 1.77 | 0.66 |
| 1:F:613:ASP:CB | 1:F:731:THR:HG22 | 2.17 | 0.66 |
| 1:H:340:THR:CB | 1:Z:322:GLN:NE2 | 2.59 | 0.66 |
| 1:I:322:GLN:NE2 | 1:J:340:THR:CB | 2.59 | 0.66 |
| 1:J:350:GLU:OE1 | 1:J:352:GLN:NE2 | 2.28 | 0.66 |
| 1:K:322:GLN:HE21 | 1:L:340:THR:CB | 2.08 | 0.66 |
| 1:K:340:THR:HB | 1:7:322:GLN:NE2 | 2.11 | 0.66 |
| 1:K:340:THR:CB | 1:7:322:GLN:NE2 | 2.59 | 0.66 |
| 1:M:340:THR:CB | 1:c:322:GLN:NE2 | 2.59 | 0.66 |
| 1:Q:322:GLN:NE2 | 1:S:340:THR:CB | 2.59 | 0.66 |
| 1:U:322:GLN:NE2 | 1:e:340:THR:CB | 2.59 | 0.66 |
| 1:Y:322:GLN:NE2 | 1:4:340:THR:CB | 2.59 | 0.66 |
| 1:h:425:SER:O | 1:h:732:ARG:NH2 | 2.29 | 0.66 |
| 1:i:326:VAL:HG21 | 1:i:333:LYS:HZ1 | 1.60 | 0.66 |
| 1:i:425:SER:O | 1:i:732:ARG:NH2 | 2.29 | 0.66 |
| 1:j:484:PRO:HD3 | 1:j:609:TRP:HE3 | 1.59 | 0.66 |
| 1:k:425:SER:O | 1:k:732:ARG:NH2 | 2.29 | 0.66 |
| 1:l:340:THR:CB | 1:n:322:GLN:NE2 | 2.59 | 0.66 |
| 1:n:340:THR:CB | 1:r:322:GLN:NE2 | 2.59 | 0.66 |
| 1:n:340:THR:CB | 1:r:322:GLN:HE21 | 2.08 | 0.66 |
| 1:p:484:PRO:HD3 | 1:p:609:TRP:HE3 | 1.59 | 0.66 |
| 1:u:340:THR:CB | 1:5:322:GLN:NE2 | 2.59 | 0.66 |
| 1:y:484:PRO:HD3 | 1:y:609:TRP:CE3 | 2.30 | 0.66 |
| 1:y:609:TRP:CH2 | 1:y:631:PHE:CZ | 2.80 | 0.66 |
| 1:z:340:THR:CB | 1:4:322:GLN:HE21 | 2.08 | 0.66 |
| 1:6:484:PRO:HD3 | 1:6:609:TRP:HE3 | 1.59 | 0.66 |
| 1:A:343:ILE:HD12 | 1:A:651:ILE:HD11 | 1.77 | 0.66 |
| 1:J:425:SER:O | 1:J:732:ARG:NH2 | 2.29 | 0.66 |
| 1:K:343:ILE:HD12 | 1:K:651:ILE:HD11 | 1.77 | 0.66 |
| 1:M:425:SER:O | 1:M:732:ARG:NH2 | 2.29 | 0.66 |
| 1:M:484:PRO:HD3 | 1:M:609:TRP:CE3 | 2.30 | 0.66 |
| 1:Q:425:SER:O | 1:Q:732:ARG:NH2 | 2.29 | 0.66 |
| 1:T:340:THR:CB | 1:i:322:GLN:NE2 | 2.59 | 0.66 |
| 1:T:484:PRO:HD3 | 1:T:609:TRP:HE3 | 1.59 | 0.66 |
| 1:V:425:SER:O | 1:V:732:ARG:NH2 | 2.29 | 0.66 |
| 1:V:484:PRO:HD3 | 1:V:609:TRP:CE3 | 2.30 | 0.66 |
| 1:W:425:SER:O | 1:W:732:ARG:NH2 | 2.29 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:322:GLN:NE2 | 1:Y:340:THR:CB | 2.59 | 0.66 |
| 1:Y:322:GLN:HE21 | 1:4:340:THR:CB | 2.08 | 0.66 |
| 1:f:484:PRO:HD3 | 1:f:609:TRP:HE3 | 1.59 | 0.66 |
| 1:g:322:GLN:NE2 | 1:1:340:THR:CB | 2.59 | 0.66 |
| 1:h:343:ILE:HD12 | 1:h:651:ILE:HD11 | 1.77 | 0.66 |
| 1:m:322:GLN:NE2 | 1:s:340:THR:CB | 2.59 | 0.66 |
| 1:o:343:ILE:HD12 | 1:o:651:ILE:HD11 | 1.77 | 0.66 |
| 1:u:340:THR:CB | 1:5:322:GLN:HE21 | 2.08 | 0.66 |
| 1:u:350:GLU:OE1 | 1:u:352:GLN:NE2 | 2.28 | 0.66 |
| 1:2:322:GLN:NE2 | 1:3:340:THR:CB | 2.59 | 0.66 |
| 1:5:425:SER:O | 1:5:732:ARG:NH2 | 2.29 | 0.66 |
| 1:6:613:ASP:CB | 1:6:731:THR:HG22 | 2.17 | 0.66 |
| 1:7:326:VAL:HG21 | 1:7:333:LYS:HZ1 | 1.60 | 0.66 |
| 1:A:322:GLN:NE2 | 1:E:340:THR:HB | 2.11 | 0.65 |
| 1:K:613:ASP:CB | 1:K:731:THR:HG22 | 2.17 | 0.65 |
| 1:O:340:THR:CB | 1:d:322:GLN:NE2 | 2.59 | 0.65 |
| 1:R:340:THR:CB | 1:V:322:GLN:NE2 | 2.59 | 0.65 |
| 1:R:425:SER:O | 1:R:732:ARG:NH2 | 2.29 | 0.65 |
| 1:S:425:SER:O | 1:S:732:ARG:NH2 | 2.29 | 0.65 |
| 1:T:322:GLN:NE2 | 1:U:340:THR:CB | 2.59 | 0.65 |
| 1:U:425:SER:O | 1:U:732:ARG:NH2 | 2.29 | 0.65 |
| 1:e:232:ASP:HB3 | 1:h:402:PRO:HG3 | 1.78 | 0.65 |
| 1:f:340:THR:CB | 1:z:322:GLN:NE2 | 2.59 | 0.65 |
| 1:k:343:ILE:HD12 | 1:k:651:ILE:HD11 | 1.77 | 0.65 |
| 1:l:425:SER:O | 1:l:732:ARG:NH2 | 2.29 | 0.65 |
| 1:q:425:SER:O | 1:q:732:ARG:NH2 | 2.29 | 0.65 |
| 1:r:402:PRO:HG3 | 1:x:232:ASP:HB3 | 1.78 | 0.65 |
| 1:u:425:SER:O | 1:u:732:ARG:NH2 | 2.29 | 0.65 |
| 1:v:425:SER:O | 1:v:732:ARG:NH2 | 2.29 | 0.65 |
| 1:z:343:ILE:HD12 | 1:z:651:ILE:HD11 | 1.77 | 0.65 |
| 1:H:322:GLN:NE2 | 1:I:340:THR:CB | 2.59 | 0.65 |
| 1:H:402:PRO:HG3 | 1:Z:232:ASP:HB3 | 1.79 | 0.65 |
| 1:J:232:ASP:HB3 | 1:a:402:PRO:HG3 | 1.79 | 0.65 |
| 1:J:322:GLN:NE2 | 1:a:340:THR:CB | 2.59 | 0.65 |
| 1:M:232:ASP:HB3 | 1:N:402:PRO:HG3 | 1.79 | 0.65 |
| 1:S:322:GLN:NE2 | 1:d:340:THR:CB | 2.59 | 0.65 |
| 1:X:484:PRO:HD3 | 1:X:609:TRP:CE3 | 2.30 | 0.65 |
| 1:l:343:ILE:HD12 | 1:l:651:ILE:HD11 | 1.77 | 0.65 |
| 1:t:425:SER:O | 1:t:732:ARG:NH2 | 2.29 | 0.65 |
| 1:u:322:GLN:NE2 | 1:2:340:THR:CB | 2.59 | 0.65 |
| 1:z:340:THR:CB | 1:4:322:GLN:NE2 | 2.59 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:z:425:SER:O | 1:z:732:ARG:NH2 | 2.29 | 0.65 |
| 1:D:425:SER:O | 1:D:732:ARG:NH2 | 2.29 | 0.65 |
| 1:J:484:PRO:HD3 | 1:J:609:TRP:HE3 | 1.59 | 0.65 |
| 1:K:425:SER:O | 1:K:732:ARG:NH2 | 2.29 | 0.65 |
| 1:M:322:GLN:HE21 | 1:N:340:THR:CB | 2.08 | 0.65 |
| 1:M:322:GLN:NE2 | 1:N:340:THR:CB | 2.59 | 0.65 |
| 1:M:322:GLN:NE2 | 1:N:340:THR:HB | 2.12 | 0.65 |
| 1:P:322:GLN:HE21 | 1:Q:340:THR:CB | 2.08 | 0.65 |
| 1:V:343:ILE:HD12 | 1:V:651:ILE:HD11 | 1.77 | 0.65 |
| 1:X:402:PRO:HG3 | 1:f:232:ASP:HB3 | 1.79 | 0.65 |
| 1:Y:232:ASP:HB3 | 1:4:402:PRO:HG3 | 1.79 | 0.65 |
| 1:Z:613:ASP:CB | 1:Z:731:THR:HG22 | 2.17 | 0.65 |
| 1:c:340:THR:CB | 1:s:322:GLN:NE2 | 2.59 | 0.65 |
| 1:e:322:GLN:NE2 | 1:h:340:THR:CB | 2.59 | 0.65 |
| 1:j:340:THR:CB | 1:l:322:GLN:NE2 | 2.60 | 0.65 |
| 1:l:613:ASP:HB2 | 1:l:731:THR:CG2 | 2.19 | 0.65 |
| 1:m:232:ASP:HB3 | 1:s:402:PRO:HG3 | 1.79 | 0.65 |
| 1:m:613:ASP:CB | 1:m:731:THR:HG22 | 2.17 | 0.65 |
| 1:n:402:PRO:HG3 | 1:r:232:ASP:HB3 | 1.79 | 0.65 |
| 1:x:484:PRO:HD3 | 1:x:609:TRP:CE3 | 2.30 | 0.65 |
| 1:y:343:ILE:HD12 | 1:y:651:ILE:HD11 | 1.77 | 0.65 |
| 1:2:609:TRP:CH2 | 1:2:631:PHE:CZ | 2.80 | 0.65 |
| 1:F:326:VAL:HG21 | 1:F:333:LYS:HZ1 | 1.61 | 0.65 |
| 1:J:322:GLN:HE21 | 1:a:340:THR:CB | 2.08 | 0.65 |
| 1:S:613:ASP:HB2 | 1:S:731:THR:CG2 | 2.18 | 0.65 |
| 1:W:609:TRP:CH2 | 1:W:631:PHE:CZ | 2.80 | 0.65 |
| 1:b:322:GLN:NE2 | 1:o:340:THR:CB | 2.59 | 0.65 |
| 1:f:340:THR:CB | 1:z:322:GLN:HE21 | 2.09 | 0.65 |
| 1:o:322:GLN:NE2 | 1:7:340:THR:CB | 2.59 | 0.65 |
| 1:p:232:ASP:HB3 | 1:q:402:PRO:HG3 | 1.79 | 0.65 |
| 1:s:425:SER:O | 1:s:732:ARG:NH2 | 2.29 | 0.65 |
| 1:u:613:ASP:HB2 | 1:u:731:THR:CG2 | 2.18 | 0.65 |
| 1:5:402:PRO:HG3 | 1:8:232:ASP:HB3 | 1.78 | 0.65 |
| 1:G:232:ASP:HB3 | 1:W:402:PRO:HG3 | 1.79 | 0.65 |
| 1:H:232:ASP:HB3 | 1:I:402:PRO:HG3 | 1.79 | 0.65 |
| 1:M:484:PRO:HD3 | 1:M:609:TRP:HE3 | 1.59 | 0.65 |
| 1:P:232:ASP:HB3 | 1:Q:402:PRO:HG3 | 1.78 | 0.65 |
| 1:P:343:ILE:HD12 | 1:P:651:ILE:HD11 | 1.77 | 0.65 |
| 1:j:340:THR:CB | 1:l:322:GLN:HE21 | 2.09 | 0.65 |
| 1:r:425:SER:O | 1:r:732:ARG:NH2 | 2.29 | 0.65 |
| 1:s:484:PRO:HD3 | 1:s:609:TRP:HE3 | 1.59 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:u:322:GLN:NE2 | 1:2:340:THR:HB | 2.11 | 0.65 |
| 1:5:340:THR:CB | 1:8:322:GLN:HE21 | 2.08 | 0.65 |
| 1:6:326:VAL:HG21 | 1:6:333:LYS:HZ1 | 1.61 | 0.65 |
| 1:A:340:THR:CB | 1:B:322:GLN:NE2 | 2.59 | 0.65 |
| 1:D:613:ASP:CB | 1:D:731:THR:HG22 | 2.17 | 0.65 |
| 1:E:404:GLN:NE2 | 1:E:406:LEU:HD11 | 2.12 | 0.65 |
| 1:H:425:SER:O | 1:H:732:ARG:NH2 | 2.29 | 0.65 |
| 1:H:484:PRO:HD3 | 1:H:609:TRP:HE3 | 1.59 | 0.65 |
| 1:L:322:GLN:NE2 | 1:b:340:THR:CB | 2.59 | 0.65 |
| 1:O:340:THR:HB | 1:d:322:GLN:NE2 | 2.11 | 0.65 |
| 1:S:232:ASP:HB3 | 1:d:402:PRO:HG3 | 1.79 | 0.65 |
| 1:V:340:THR:CB | 1:W:322:GLN:HE21 | 2.07 | 0.65 |
| 1:c:402:PRO:HG3 | 1:s:232:ASP:HB3 | 1.79 | 0.65 |
| 1:d:609:TRP:CH2 | 1:d:631:PHE:CZ | 2.80 | 0.65 |
| 1:g:340:THR:CB | 1:k:322:GLN:HE21 | 2.08 | 0.65 |
| 1:h:322:GLN:HE21 | 1:i:340:THR:CB | 2.08 | 0.65 |
| 1:8:343:ILE:HD12 | 1:8:651:ILE:HD11 | 1.77 | 0.65 |
| 1:8:609:TRP:CH2 | 1:8:631:PHE:CZ | 2.80 | 0.65 |
| 1:A:232:ASP:HB3 | 1:E:402:PRO:HG3 | 1.79 | 0.65 |
| 1:A:322:GLN:NE2 | 1:E:340:THR:CB | 2.59 | 0.65 |
| 1:C:425:SER:O | 1:C:732:ARG:NH2 | 2.29 | 0.65 |
| 1:F:322:GLN:HE21 | 1:G:340:THR:CB | 2.08 | 0.65 |
| 1:F:340:THR:CB | 1:R:322:GLN:NE2 | 2.59 | 0.65 |
| 1:G:404:GLN:NE2 | 1:G:406:LEU:HD11 | 2.12 | 0.65 |
| 1:H:404:GLN:NE2 | 1:H:406:LEU:HD11 | 2.12 | 0.65 |
| 1:N:322:GLN:NE2 | 1:m:340:THR:CB | 2.59 | 0.65 |
| 1:N:609:TRP:CH2 | 1:N:631:PHE:CZ | 2.80 | 0.65 |
| 1:O:402:PRO:HG3 | 1:d:232:ASP:HB3 | 1.79 | 0.65 |
| 1:R:340:THR:HB | 1:V:322:GLN:NE2 | 2.11 | 0.65 |
| 1:X:232:ASP:HB3 | 1:Y:402:PRO:HG3 | 1.79 | 0.65 |
| 1:Y:425:SER:O | 1:Y:732:ARG:NH2 | 2.29 | 0.65 |
| 1:Z:340:THR:CB | 1:a:322:GLN:NE2 | 2.59 | 0.65 |
| 1:Z:425:SER:O | 1:Z:732:ARG:NH2 | 2.29 | 0.65 |
| 1:h:232:ASP:HB3 | 1:i:402:PRO:HG3 | 1.78 | 0.65 |
| 1:j:322:GLN:NE2 | 1:x:340:THR:CB | 2.59 | 0.65 |
| 1:m:322:GLN:HE21 | 1:s:340:THR:CB | 2.08 | 0.65 |
| 1:p:340:THR:CB | 1:6:322:GLN:HE21 | 2.08 | 0.65 |
| 1:p:404:GLN:NE2 | 1:p:406:LEU:HD11 | 2.12 | 0.65 |
| 1:q:609:TRP:CH2 | 1:q:631:PHE:CZ | 2.80 | 0.65 |
| 1:r:340:THR:HB | 1:x:322:GLN:NE2 | 2.10 | 0.65 |
| 1:s:404:GLN:NE2 | 1:s:406:LEU:HD11 | 2.12 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:t:322:GLN:NE2 | 1:6:340:THR:CB | 2.59 | 0.65 |
| 1:t:340:THR:HB | 1:y:322:GLN:NE2 | 2.10 | 0.65 |
| 1:u:232:ASP:HB3 | 1:2:402:PRO:HG3 | 1.79 | 0.65 |
| 1:3:609:TRP:CH2 | 1:3:631:PHE:CZ | 2.80 | 0.65 |
| 1:7:404:GLN:NE2 | 1:7:406:LEU:HD11 | 2.12 | 0.65 |
| 1:B:340:THR:CB | 1:C:322:GLN:NE2 | 2.59 | 0.65 |
| 1:B:404:GLN:NE2 | 1:B:406:LEU:HD11 | 2.12 | 0.65 |
| 1:C:402:PRO:HG3 | 1:D:232:ASP:HB3 | 1.78 | 0.65 |
| 1:P:609:TRP:CH2 | 1:P:631:PHE:CZ | 2.80 | 0.65 |
| 1:U:322:GLN:NE2 | 1:e:340:THR:HB | 2.11 | 0.65 |
| 1:V:404:GLN:NE2 | 1:V:406:LEU:HD11 | 2.12 | 0.65 |
| 1:X:343:ILE:HD12 | 1:X:651:ILE:HD11 | 1.77 | 0.65 |
| 1:a:609:TRP:CH2 | 1:a:631:PHE:CZ | 2.80 | 0.65 |
| 1:g:402:PRO:HG3 | 1:k:232:ASP:HB3 | 1.78 | 0.65 |
| 1:x:343:ILE:HD12 | 1:x:651:ILE:HD11 | 1.77 | 0.65 |
| 1:x:425:SER:O | 1:x:732:ARG:NH2 | 2.29 | 0.65 |
| 1:y:404:GLN:NE2 | 1:y:406:LEU:HD11 | 2.12 | 0.65 |
| 1:2:232:ASP:HB3 | 1:3:402:PRO:HG3 | 1.79 | 0.65 |
| 1:2:322:GLN:NE2 | 1:3:340:THR:HB | 2.11 | 0.65 |
| 1:C:404:GLN:NE2 | 1:C:406:LEU:HD11 | 2.12 | 0.65 |
| 1:G:322:GLN:NE2 | 1:W:340:THR:CB | 2.59 | 0.65 |
| 1:H:340:THR:CB | 1:Z:322:GLN:HE21 | 2.08 | 0.65 |
| 1:L:404:GLN:NE2 | 1:L:406:LEU:HD11 | 2.12 | 0.65 |
| 1:L:425:SER:O | 1:L:732:ARG:NH2 | 2.29 | 0.65 |
| 1:S:404:GLN:NE2 | 1:S:406:LEU:HD11 | 2.12 | 0.65 |
| 1:S:609:TRP:CH2 | 1:S:631:PHE:CZ | 2.80 | 0.65 |
| 1:X:425:SER:O | 1:X:732:ARG:NH2 | 2.29 | 0.65 |
| 1:a:404:GLN:NE2 | 1:a:406:LEU:HD11 | 2.12 | 0.65 |
| 1:b:404:GLN:NE2 | 1:b:406:LEU:HD11 | 2.12 | 0.65 |
| 1:i:404:GLN:NE2 | 1:i:406:LEU:HD11 | 2.12 | 0.65 |
| 1:j:322:GLN:NE2 | 1:x:340:THR:HB | 2.11 | 0.65 |
| 1:l:404:GLN:NE2 | 1:l:406:LEU:HD11 | 2.12 | 0.65 |
| 1:m:425:SER:O | 1:m:732:ARG:NH2 | 2.29 | 0.65 |
| 1:u:404:GLN:NE2 | 1:u:406:LEU:HD11 | 2.12 | 0.65 |
| 1:u:609:TRP:CH2 | 1:u:631:PHE:CZ | 2.80 | 0.65 |
| 1:1:609:TRP:CH2 | 1:1:631:PHE:CZ | 2.80 | 0.65 |
| 1:E:343:ILE:HD12 | 1:E:651:ILE:HD11 | 1.77 | 0.65 |
| 1:F:340:THR:HB | 1:R:322:GLN:NE2 | 2.11 | 0.65 |
| 1:K:232:ASP:HB3 | 1:L:402:PRO:HG3 | 1.78 | 0.65 |
| 1:N:404:GLN:NE2 | 1:N:406:LEU:HD11 | 2.12 | 0.65 |
| 1:O:609:TRP:CH2 | 1:O:631:PHE:CZ | 2.80 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:404:GLN:NE2 | 1:P:406:LEU:HD11 | 2.12 | 0.65 |
| 1:U:322:GLN:HE21 | 1:e:340:THR:CB | 2.08 | 0.65 |
| 1:X:340:THR:HB | 1:f:322:GLN:NE2 | 2.12 | 0.65 |
| 1:X:340:THR:CB | 1:f:322:GLN:NE2 | 2.59 | 0.65 |
| 1:g:404:GLN:NE2 | 1:g:406:LEU:HD11 | 2.12 | 0.65 |
| 1:p:322:GLN:NE2 | 1:q:340:THR:CB | 2.59 | 0.65 |
| 1:t:340:THR:CB | 1:y:322:GLN:NE2 | 2.59 | 0.65 |
| 1:z:404:GLN:NE2 | 1:z:406:LEU:HD11 | 2.12 | 0.65 |
| 1:4:404:GLN:NE2 | 1:4:406:LEU:HD11 | 2.12 | 0.65 |
| 1:I:613:ASP:HB2 | 1:I:731:THR:CG2 | 2.19 | 0.64 |
| 1:O:232:ASP:HB3 | 1:P:402:PRO:HG3 | 1.78 | 0.64 |
| 1:O:425:SER:O | 1:O:732:ARG:NH2 | 2.29 | 0.64 |
| 1:R:402:PRO:HG3 | 1:V:232:ASP:HB3 | 1.78 | 0.64 |
| 1:T:613:ASP:HB2 | 1:T:731:THR:CG2 | 2.19 | 0.64 |
| 1:X:404:GLN:NE2 | 1:X:406:LEU:HD11 | 2.12 | 0.64 |
| 1:Y:404:GLN:NE2 | 1:Y:406:LEU:HD11 | 2.12 | 0.64 |
| 1:n:404:GLN:NE2 | 1:n:406:LEU:HD11 | 2.12 | 0.64 |
| 1:t:322:GLN:NE2 | 1:6:340:THR:HB | 2.11 | 0.64 |
| 1:x:404:GLN:NE2 | 1:x:406:LEU:HD11 | 2.12 | 0.64 |
| 1:5:613:ASP:HB2 | 1:5:731:THR:CG2 | 2.18 | 0.64 |
| 1:8:404:GLN:NE2 | 1:8:406:LEU:HD11 | 2.12 | 0.64 |
| 1:A:404:GLN:NE2 | 1:A:406:LEU:HD11 | 2.12 | 0.64 |
| 1:D:404:GLN:NE2 | 1:D:406:LEU:HD11 | 2.12 | 0.64 |
| 1:L:322:GLN:NE2 | 1:b:340:THR:HB | 2.11 | 0.64 |
| 1:M:402:PRO:HG3 | 1:c:232:ASP:HB3 | 1.79 | 0.64 |
| 1:X:322:GLN:NE2 | 1:Y:340:THR:HB | 2.11 | 0.64 |
| 1:c:404:GLN:NE2 | 1:c:406:LEU:HD11 | 2.12 | 0.64 |
| 1:g:232:ASP:HB3 | 1:1:402:PRO:HG3 | 1.79 | 0.64 |
| 1:k:404:GLN:NE2 | 1:k:406:LEU:HD11 | 2.12 | 0.64 |
| 1:o:232:ASP:HB3 | 1:7:402:PRO:HG3 | 1.79 | 0.64 |
| 1:r:404:GLN:NE2 | 1:r:406:LEU:HD11 | 2.12 | 0.64 |
| 1:t:232:ASP:HB3 | 1:6:402:PRO:HG3 | 1.79 | 0.64 |
| 1:3:425:SER:O | 1:3:732:ARG:NH2 | 2.29 | 0.64 |
| 1:7:343:ILE:HD12 | 1:7:651:ILE:HD11 | 1.77 | 0.64 |
| 1:B:613:ASP:HB3 | 1:B:732:ARG:NE | 2.13 | 0.64 |
| 1:F:402:PRO:HG3 | 1:R:232:ASP:HB3 | 1.79 | 0.64 |
| 1:I:232:ASP:HB3 | 1:J:402:PRO:HG3 | 1.79 | 0.64 |
| 1:K:404:GLN:NE2 | 1:K:406:LEU:HD11 | 2.12 | 0.64 |
| 1:T:402:PRO:HG3 | 1:i:232:ASP:HB3 | 1.79 | 0.64 |
| 1:T:404:GLN:NE2 | 1:T:406:LEU:HD11 | 2.12 | 0.64 |
| 1:W:613:ASP:HB3 | 1:W:732:ARG:NE | 2.13 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:322:GLN:NE2 | 1:o:340:THR:HB | 2.11 | 0.64 |
| 1:c:340:THR:HB | 1:s:322:GLN:NE2 | 2.11 | 0.64 |
| 1:m:404:GLN:NE2 | 1:m:406:LEU:HD11 | 2.12 | 0.64 |
| 1:o:322:GLN:HE21 | 1:7:340:THR:CB | 2.08 | 0.64 |
| 1:o:404:GLN:NE2 | 1:o:406:LEU:HD11 | 2.12 | 0.64 |
| 1:q:613:ASP:HB3 | 1:q:732:ARG:NE | 2.13 | 0.64 |
| 1:1:404:GLN:NE2 | 1:1:406:LEU:HD11 | 2.12 | 0.64 |
| 1:1:613:ASP:HB2 | 1:1:731:THR:CG2 | 2.19 | 0.64 |
| 1:B:340:THR:HB | 1:C:322:GLN:NE2 | 2.11 | 0.64 |
| 1:I:404:GLN:NE2 | 1:I:406:LEU:HD11 | 2.12 | 0.64 |
| 1:L:343:ILE:HD12 | 1:L:651:ILE:HD11 | 1.77 | 0.64 |
| 1:U:232:ASP:HB3 | 1:e:402:PRO:HG3 | 1.79 | 0.64 |
| 1:Z:613:ASP:HB2 | 1:Z:731:THR:CG2 | 2.19 | 0.64 |
| 1:b:613:ASP:HB3 | 1:b:732:ARG:NE | 2.13 | 0.64 |
| 1:h:404:GLN:NE2 | 1:h:406:LEU:HD11 | 2.12 | 0.64 |
| 1:m:613:ASP:HB2 | 1:m:731:THR:CG2 | 2.19 | 0.64 |
| 1:n:613:ASP:HB3 | 1:n:732:ARG:NE | 2.13 | 0.64 |
| 1:o:613:ASP:HB2 | 1:o:731:THR:CG2 | 2.19 | 0.64 |
| 1:v:340:THR:HB | 1:1:322:GLN:NE2 | 2.11 | 0.64 |
| 1:3:232:ASP:HB3 | 1:8:402:PRO:HG3 | 1.78 | 0.64 |
| 1:4:613:ASP:HB3 | 1:4:732:ARG:NE | 2.13 | 0.64 |
| 1:A:492:SER:O | 1:A:498:ASN:ND2 | 2.31 | 0.64 |
| 1:D:484:PRO:CD | 1:D:609:TRP:HE3 | 2.11 | 0.64 |
| 1:K:484:PRO:CD | 1:K:609:TRP:HE3 | 2.11 | 0.64 |
| 1:Q:404:GLN:NE2 | 1:Q:406:LEU:HD11 | 2.12 | 0.64 |
| 1:Q:613:ASP:HB2 | 1:Q:731:THR:CG2 | 2.18 | 0.64 |
| 1:U:484:PRO:CD | 1:U:609:TRP:HE3 | 2.11 | 0.64 |
| 1:Z:404:GLN:NE2 | 1:Z:406:LEU:HD11 | 2.12 | 0.64 |
| 1:c:613:ASP:HB2 | 1:c:731:THR:CG2 | 2.19 | 0.64 |
| 1:l:613:ASP:HB3 | 1:l:732:ARG:NE | 2.13 | 0.64 |
| 1:o:492:SER:O | 1:o:498:ASN:ND2 | 2.31 | 0.64 |
| 1:p:402:PRO:HG3 | 1:6:232:ASP:HB3 | 1.79 | 0.64 |
| 1:t:492:SER:O | 1:t:498:ASN:ND2 | 2.31 | 0.64 |
| 1:u:326:VAL:HG21 | 1:u:333:LYS:HZ1 | 1.63 | 0.64 |
| 1:v:322:GLN:HE21 | 1:w:340:THR:CB | 2.09 | 0.64 |
| 1:z:613:ASP:HB3 | 1:z:732:ARG:NE | 2.13 | 0.64 |
| 1:5:326:VAL:HG21 | 1:5:333:LYS:HZ1 | 1.63 | 0.64 |
| 1:7:613:ASP:HB3 | 1:7:732:ARG:NE | 2.13 | 0.64 |
| 1:7:613:ASP:CB | 1:7:731:THR:HG22 | 2.17 | 0.64 |
| 1:A:322:GLN:HE21 | 1:E:340:THR:CB | 2.09 | 0.64 |
| 1:A:340:THR:HB | 1:B:322:GLN:NE2 | 2.11 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:484:PRO:CD | 1:A:609:TRP:HE3 | 2.11 | 0.64 |
| 1:B:402:PRO:HG3 | 1:C:232:ASP:HB3 | 1.78 | 0.64 |
| 1:E:613:ASP:HB3 | 1:E:732:ARG:NE | 2.13 | 0.64 |
| 1:K:340:THR:CB | 1:7:322:GLN:HE21 | 2.08 | 0.64 |
| 1:O:484:PRO:CD | 1:O:609:TRP:HE3 | 2.11 | 0.64 |
| 1:P:492:SER:O | 1:P:498:ASN:ND2 | 2.31 | 0.64 |
| 1:S:322:GLN:HE21 | 1:d:340:THR:CB | 2.08 | 0.64 |
| 1:T:492:SER:O | 1:T:498:ASN:ND2 | 2.31 | 0.64 |
| 1:W:382:THR:HG22 | 1:W:383:LEU:H | 1.63 | 0.64 |
| 1:k:340:THR:CB | 1:w:322:GLN:NE2 | 2.60 | 0.64 |
| 1:p:492:SER:O | 1:p:498:ASN:ND2 | 2.31 | 0.64 |
| 1:t:404:GLN:NE2 | 1:t:406:LEU:HD11 | 2.12 | 0.64 |
| 1:u:402:PRO:HG3 | 1:5:232:ASP:HB3 | 1.79 | 0.64 |
| 1:v:484:PRO:CD | 1:v:609:TRP:HE3 | 2.11 | 0.64 |
| 1:w:498:ASN:OD1 | 1:y:587:GLN:NE2 | 2.30 | 0.64 |
| 1:1:492:SER:O | 1:1:498:ASN:ND2 | 2.31 | 0.64 |
| 1:3:484:PRO:CD | 1:3:609:TRP:HE3 | 2.11 | 0.64 |
| 1:5:404:GLN:NE2 | 1:5:406:LEU:HD11 | 2.12 | 0.64 |
| 1:A:613:ASP:HB2 | 1:A:731:THR:CG2 | 2.19 | 0.64 |
| 1:C:613:ASP:HB3 | 1:C:732:ARG:NE | 2.13 | 0.64 |
| 1:D:340:THR:CB | 1:E:322:GLN:HE21 | 2.08 | 0.64 |
| 1:F:232:ASP:HB3 | 1:G:402:PRO:HG3 | 1.79 | 0.64 |
| 1:G:492:SER:O | 1:G:498:ASN:ND2 | 2.31 | 0.64 |
| 1:I:484:PRO:CD | 1:I:609:TRP:HE3 | 2.11 | 0.64 |
| 1:L:613:ASP:HB3 | 1:L:732:ARG:NE | 2.13 | 0.64 |
| 1:P:613:ASP:HB3 | 1:P:732:ARG:NE | 2.13 | 0.64 |
| 1:R:613:ASP:HB3 | 1:R:732:ARG:NE | 2.13 | 0.64 |
| 1:T:322:GLN:NE2 | 1:U:340:THR:HB | 2.11 | 0.64 |
| 1:X:613:ASP:HB2 | 1:X:731:THR:CG2 | 2.18 | 0.64 |
| 1:c:484:PRO:CD | 1:c:609:TRP:HE3 | 2.11 | 0.64 |
| 1:e:492:SER:O | 1:e:498:ASN:ND2 | 2.31 | 0.64 |
| 1:h:613:ASP:HB3 | 1:h:732:ARG:NE | 2.13 | 0.64 |
| 1:j:484:PRO:CD | 1:j:609:TRP:HE3 | 2.11 | 0.64 |
| 1:k:613:ASP:HB3 | 1:k:732:ARG:NE | 2.13 | 0.64 |
| 1:o:484:PRO:CD | 1:o:609:TRP:HE3 | 2.11 | 0.64 |
| 1:q:484:PRO:CD | 1:q:609:TRP:HE3 | 2.11 | 0.64 |
| 1:t:613:ASP:HB3 | 1:t:732:ARG:NE | 2.13 | 0.64 |
| 1:u:322:GLN:HE21 | 1:2:340:THR:CB | 2.08 | 0.64 |
| 1:w:404:GLN:NE2 | 1:w:406:LEU:HD11 | 2.12 | 0.64 |
| 1:w:492:SER:O | 1:w:498:ASN:ND2 | 2.31 | 0.64 |
| 1:y:326:VAL:HG21 | 1:y:333:LYS:HZ1 | 1.61 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:484:PRO:CD | 1:1:609:TRP:HE3 | 2.11 | 0.64 |
| 1:8:613:ASP:HB3 | 1:8:732:ARG:NE | 2.13 | 0.64 |
| 1:C:343:ILE:HD12 | 1:C:651:ILE:HD11 | 1.77 | 0.64 |
| 1:C:484:PRO:CD | 1:C:609:TRP:HE3 | 2.11 | 0.64 |
| 1:F:613:ASP:HB3 | 1:F:732:ARG:NE | 2.13 | 0.64 |
| 1:H:340:THR:HB | 1:Z:322:GLN:NE2 | 2.11 | 0.64 |
| 1:J:404:GLN:NE2 | 1:J:406:LEU:HD11 | 2.12 | 0.64 |
| 1:J:609:TRP:CH2 | 1:J:631:PHE:CZ | 2.80 | 0.64 |
| 1:L:232:ASP:HB3 | 1:b:402:PRO:HG3 | 1.78 | 0.64 |
| 1:M:340:THR:CB | 1:c:322:GLN:HE21 | 2.09 | 0.64 |
| 1:M:404:GLN:NE2 | 1:M:406:LEU:HD11 | 2.12 | 0.64 |
| 1:M:609:TRP:CH2 | 1:M:631:PHE:CZ | 2.80 | 0.64 |
| 1:T:484:PRO:CD | 1:T:609:TRP:HE3 | 2.11 | 0.64 |
| 1:W:484:PRO:CD | 1:W:609:TRP:HE3 | 2.11 | 0.64 |
| 1:Z:609:TRP:CH2 | 1:Z:631:PHE:CZ | 2.80 | 0.64 |
| 1:e:404:GLN:NE2 | 1:e:406:LEU:HD11 | 2.12 | 0.64 |
| 1:g:484:PRO:CD | 1:g:609:TRP:HE3 | 2.11 | 0.64 |
| 1:q:382:THR:HG22 | 1:q:383:LEU:H | 1.63 | 0.64 |
| 1:v:402:PRO:HG3 | 1:1:232:ASP:HB3 | 1.79 | 0.64 |
| 1:w:613:ASP:HB2 | 1:w:731:THR:CG2 | 2.19 | 0.64 |
| 1:2:613:ASP:HB3 | 1:2:732:ARG:NE | 2.13 | 0.64 |
| 1:5:484:PRO:CD | 1:5:609:TRP:HE3 | 2.11 | 0.64 |
| 1:6:484:PRO:CD | 1:6:609:TRP:HE3 | 2.11 | 0.64 |
| 1:B:484:PRO:CD | 1:B:609:TRP:HE3 | 2.11 | 0.64 |
| 1:F:382:THR:HG22 | 1:F:383:LEU:H | 1.63 | 0.64 |
| 1:F:484:PRO:CD | 1:F:609:TRP:HE3 | 2.11 | 0.64 |
| 1:L:484:PRO:CD | 1:L:609:TRP:HE3 | 2.11 | 0.64 |
| 1:N:232:ASP:HB3 | 1:m:402:PRO:HG3 | 1.79 | 0.64 |
| 1:P:484:PRO:CD | 1:P:609:TRP:HE3 | 2.11 | 0.64 |
| 1:Q:232:ASP:HB3 | 1:S:402:PRO:HG3 | 1.79 | 0.64 |
| 1:Q:484:PRO:CD | 1:Q:609:TRP:HE3 | 2.11 | 0.64 |
| 1:R:404:GLN:NE2 | 1:R:406:LEU:HD11 | 2.12 | 0.64 |
| 1:U:382:THR:HG22 | 1:U:383:LEU:H | 1.63 | 0.64 |
| 1:Z:402:PRO:HG3 | 1:a:232:ASP:HB3 | 1.79 | 0.64 |
| 1:b:232:ASP:HB3 | 1:o:402:PRO:HG3 | 1.79 | 0.64 |
| 1:b:484:PRO:CD | 1:b:609:TRP:HE3 | 2.11 | 0.64 |
| 1:d:613:ASP:HB3 | 1:d:732:ARG:NE | 2.13 | 0.64 |
| 1:e:613:ASP:HB2 | 1:e:731:THR:CG2 | 2.18 | 0.64 |
| 1:f:484:PRO:CD | 1:f:609:TRP:HE3 | 2.11 | 0.64 |
| 1:i:382:THR:HG22 | 1:i:383:LEU:H | 1.63 | 0.64 |
| 1:i:484:PRO:CD | 1:i:609:TRP:HE3 | 2.11 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:404:GLN:NE2 | 1:j:406:LEU:HD11 | 2.12 | 0.64 |
| 1:q:322:GLN:NE2 | 1:y:340:THR:OG1 | 2.31 | 0.64 |
| 1:t:609:TRP:CH2 | 1:t:631:PHE:CZ | 2.80 | 0.64 |
| 1:u:484:PRO:CD | 1:u:609:TRP:HE3 | 2.11 | 0.64 |
| 1:v:382:THR:HG22 | 1:v:383:LEU:H | 1.63 | 0.64 |
| 1:3:326:VAL:HG21 | 1:3:333:LYS:HZ1 | 1.63 | 0.64 |
| 1:6:613:ASP:HB3 | 1:6:732:ARG:NE | 2.13 | 0.64 |
| 1:8:484:PRO:CD | 1:8:609:TRP:HE3 | 2.11 | 0.64 |
| 1:D:382:THR:HG22 | 1:D:383:LEU:H | 1.63 | 0.64 |
| 1:E:382:THR:HG22 | 1:E:383:LEU:H | 1.63 | 0.64 |
| 1:E:613:ASP:CB | 1:E:731:THR:HG22 | 2.17 | 0.64 |
| 1:I:322:GLN:HE21 | 1:J:340:THR:CB | 2.09 | 0.64 |
| 1:P:382:THR:HG22 | 1:P:383:LEU:H | 1.63 | 0.64 |
| 1:R:609:TRP:CH2 | 1:R:631:PHE:CZ | 2.80 | 0.64 |
| 1:T:232:ASP:HB3 | 1:U:402:PRO:HG3 | 1.79 | 0.64 |
| 1:T:340:THR:HB | 1:i:322:GLN:NE2 | 2.11 | 0.64 |
| 1:U:613:ASP:HB3 | 1:U:732:ARG:NE | 2.13 | 0.64 |
| 1:f:404:GLN:NE2 | 1:f:406:LEU:HD11 | 2.12 | 0.64 |
| 1:g:382:THR:HG22 | 1:g:383:LEU:H | 1.63 | 0.64 |
| 1:m:322:GLN:NE2 | 1:s:340:THR:HB | 2.11 | 0.64 |
| 1:m:609:TRP:CH2 | 1:m:631:PHE:CZ | 2.80 | 0.64 |
| 1:s:484:PRO:CD | 1:s:609:TRP:HE3 | 2.11 | 0.64 |
| 1:v:404:GLN:NE2 | 1:v:406:LEU:HD11 | 2.12 | 0.64 |
| 1:v:613:ASP:HB3 | 1:v:732:ARG:NE | 2.13 | 0.64 |
| 1:2:484:PRO:CD | 1:2:609:TRP:HE3 | 2.11 | 0.64 |
| 1:6:382:THR:HG22 | 1:6:383:LEU:H | 1.63 | 0.64 |
| 1:7:382:THR:HG22 | 1:7:383:LEU:H | 1.63 | 0.64 |
| 1:A:613:ASP:HB3 | 1:A:732:ARG:NE | 2.13 | 0.63 |
| 1:K:382:THR:HG22 | 1:K:383:LEU:H | 1.63 | 0.63 |
| 1:O:404:GLN:NE2 | 1:O:406:LEU:HD11 | 2.12 | 0.63 |
| 1:O:613:ASP:HB2 | 1:O:731:THR:CG2 | 2.18 | 0.63 |
| 1:R:484:PRO:CD | 1:R:609:TRP:HE3 | 2.11 | 0.63 |
| 1:S:484:PRO:CD | 1:S:609:TRP:HE3 | 2.11 | 0.63 |
| 1:V:402:PRO:HG3 | 1:W:232:ASP:HB3 | 1.78 | 0.63 |
| 1:X:613:ASP:HB3 | 1:X:732:ARG:NE | 2.13 | 0.63 |
| 1:Z:484:PRO:CD | 1:Z:609:TRP:HE3 | 2.11 | 0.63 |
| 1:c:382:THR:HG22 | 1:c:383:LEU:H | 1.63 | 0.63 |
| 1:d:404:GLN:NE2 | 1:d:406:LEU:HD11 | 2.12 | 0.63 |
| 1:d:484:PRO:CD | 1:d:609:TRP:HE3 | 2.11 | 0.63 |
| 1:l:609:TRP:CH2 | 1:l:631:PHE:CZ | 2.80 | 0.63 |
| 1:m:484:PRO:CD | 1:m:609:TRP:HE3 | 2.11 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:o:613:ASP:HB3 | 1:o:732:ARG:NE | 2.13 | 0.63 |
| 1:q:404:GLN:NE2 | 1:q:406:LEU:HD11 | 2.12 | 0.63 |
| 1:t:484:PRO:CD | 1:t:609:TRP:HE3 | 2.11 | 0.63 |
| 1:v:492:SER:O | 1:v:498:ASN:ND2 | 2.31 | 0.63 |
| 1:x:613:ASP:HB2 | 1:x:731:THR:CG2 | 2.18 | 0.63 |
| 1:y:382:THR:HG22 | 1:y:383:LEU:H | 1.63 | 0.63 |
| 1:y:613:ASP:HB3 | 1:y:732:ARG:NE | 2.13 | 0.63 |
| 1:2:404:GLN:NE2 | 1:2:406:LEU:HD11 | 2.12 | 0.63 |
| 1:3:404:GLN:NE2 | 1:3:406:LEU:HD11 | 2.12 | 0.63 |
| 1:6:404:GLN:NE2 | 1:6:406:LEU:HD11 | 2.12 | 0.63 |
| 1:F:404:GLN:NE2 | 1:F:406:LEU:HD11 | 2.12 | 0.63 |
| 1:I:382:THR:HG22 | 1:I:383:LEU:H | 1.63 | 0.63 |
| 1:T:613:ASP:HB3 | 1:T:732:ARG:NE | 2.13 | 0.63 |
| 1:U:404:GLN:NE2 | 1:U:406:LEU:HD11 | 2.12 | 0.63 |
| 1:U:492:SER:O | 1:U:498:ASN:ND2 | 2.31 | 0.63 |
| 1:W:404:GLN:NE2 | 1:W:406:LEU:HD11 | 2.12 | 0.63 |
| 1:Y:484:PRO:CD | 1:Y:609:TRP:HE3 | 2.11 | 0.63 |
| 1:e:484:PRO:CD | 1:e:609:TRP:HE3 | 2.11 | 0.63 |
| 1:g:322:GLN:HE21 | 1:1:340:THR:CB | 2.08 | 0.63 |
| 1:l:402:PRO:HG3 | 1:n:232:ASP:HB3 | 1.79 | 0.63 |
| 1:m:382:THR:HG22 | 1:m:383:LEU:H | 1.63 | 0.63 |
| 1:z:402:PRO:HG3 | 1:4:232:ASP:HB3 | 1.79 | 0.63 |
| 1:z:609:TRP:CH2 | 1:z:631:PHE:CZ | 2.80 | 0.63 |
| 1:3:492:SER:O | 1:3:498:ASN:ND2 | 2.31 | 0.63 |
| 1:7:484:PRO:CD | 1:7:609:TRP:HE3 | 2.11 | 0.63 |
| 1:8:382:THR:HG22 | 1:8:383:LEU:H | 1.63 | 0.63 |
| 1:A:382:THR:HG22 | 1:A:383:LEU:H | 1.63 | 0.63 |
| 1:H:484:PRO:CD | 1:H:609:TRP:HE3 | 2.11 | 0.63 |
| 1:J:613:ASP:HB3 | 1:J:732:ARG:NE | 2.13 | 0.63 |
| 1:N:484:PRO:CD | 1:N:609:TRP:HE3 | 2.11 | 0.63 |
| 1:Q:613:ASP:HB3 | 1:Q:732:ARG:NE | 2.13 | 0.63 |
| 1:V:382:THR:HG22 | 1:V:383:LEU:H | 1.63 | 0.63 |
| 1:V:613:ASP:HB3 | 1:V:732:ARG:NE | 2.13 | 0.63 |
| 1:Z:382:THR:HG22 | 1:Z:383:LEU:H | 1.63 | 0.63 |
| 1:a:484:PRO:CD | 1:a:609:TRP:HE3 | 2.11 | 0.63 |
| 1:e:609:TRP:CH2 | 1:e:631:PHE:CZ | 2.80 | 0.63 |
| 1:f:340:THR:HB | 1:z:322:GLN:NE2 | 2.11 | 0.63 |
| 1:g:322:GLN:NE2 | 1:1:340:THR:HB | 2.11 | 0.63 |
| 1:r:484:PRO:CD | 1:r:609:TRP:HE3 | 2.11 | 0.63 |
| 1:w:484:PRO:CD | 1:w:609:TRP:HE3 | 2.11 | 0.63 |
| 1:w:609:TRP:CH2 | 1:w:631:PHE:CZ | 2.80 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:326:VAL:HG21 | 1:S:333:LYS:HZ1 | 1.64 | 0.63 |
| 1:k:326:VAL:HG21 | 1:k:333:LYS:HZ1 | 1.64 | 0.63 |
| 1:k:484:PRO:CD | 1:k:609:TRP:HE3 | 2.11 | 0.63 |
| 1:o:382:THR:HG22 | 1:o:383:LEU:H | 1.63 | 0.63 |
| 1:x:613:ASP:HB3 | 1:x:732:ARG:NE | 2.13 | 0.63 |
| 1:z:484:PRO:CD | 1:z:609:TRP:HE3 | 2.11 | 0.63 |
| 1:1:613:ASP:HB3 | 1:1:732:ARG:NE | 2.13 | 0.63 |
| 1:3:382:THR:HG22 | 1:3:383:LEU:H | 1.63 | 0.63 |
| 1:3:613:ASP:HB2 | 1:3:731:THR:CG2 | 2.18 | 0.63 |
| 1:4:484:PRO:CD | 1:4:609:TRP:HE3 | 2.11 | 0.63 |
| 1:4:609:TRP:CH2 | 1:4:631:PHE:CZ | 2.80 | 0.63 |
| 1:E:484:PRO:CD | 1:E:609:TRP:HE3 | 2.11 | 0.63 |
| 1:G:613:ASP:HB3 | 1:G:732:ARG:NE | 2.13 | 0.63 |
| 1:M:613:ASP:HB3 | 1:M:732:ARG:NE | 2.13 | 0.63 |
| 1:S:492:SER:O | 1:S:498:ASN:ND2 | 2.31 | 0.63 |
| 1:T:340:THR:CB | 1:i:322:GLN:HE21 | 2.08 | 0.63 |
| 1:Z:613:ASP:HB3 | 1:Z:732:ARG:NE | 2.13 | 0.63 |
| 1:h:484:PRO:CD | 1:h:609:TRP:HE3 | 2.11 | 0.63 |
| 1:l:484:PRO:CD | 1:l:609:TRP:HE3 | 2.11 | 0.63 |
| 1:n:484:PRO:CD | 1:n:609:TRP:HE3 | 2.11 | 0.63 |
| 1:4:382:THR:HG22 | 1:4:383:LEU:H | 1.63 | 0.63 |
| 1:5:613:ASP:HB3 | 1:5:732:ARG:NE | 2.13 | 0.63 |
| 1:A:402:PRO:HG3 | 1:B:232:ASP:HB3 | 1.80 | 0.63 |
| 1:M:484:PRO:CD | 1:M:609:TRP:HE3 | 2.11 | 0.63 |
| 1:O:382:THR:HG22 | 1:O:383:LEU:H | 1.63 | 0.63 |
| 1:X:609:TRP:CH2 | 1:X:631:PHE:CZ | 2.80 | 0.63 |
| 1:Z:340:THR:CB | 1:a:322:GLN:HE21 | 2.08 | 0.63 |
| 1:a:613:ASP:HB3 | 1:a:732:ARG:NE | 2.13 | 0.63 |
| 1:n:382:THR:HG22 | 1:n:383:LEU:H | 1.63 | 0.63 |
| 1:p:613:ASP:HB3 | 1:p:732:ARG:NE | 2.13 | 0.63 |
| 1:u:492:SER:O | 1:u:498:ASN:ND2 | 2.31 | 0.63 |
| 1:3:613:ASP:HB3 | 1:3:732:ARG:NE | 2.13 | 0.63 |
| 1:I:613:ASP:CB | 1:I:731:THR:HG22 | 2.17 | 0.63 |
| 1:N:613:ASP:HB3 | 1:N:732:ARG:NE | 2.13 | 0.63 |
| 1:O:613:ASP:HB3 | 1:O:732:ARG:NE | 2.13 | 0.63 |
| 1:T:382:THR:HG22 | 1:T:383:LEU:H | 1.63 | 0.63 |
| 1:c:613:ASP:CB | 1:c:731:THR:HG22 | 2.17 | 0.63 |
| 1:j:340:THR:HB | 1:l:322:GLN:NE2 | 2.11 | 0.63 |
| 1:j:492:SER:O | 1:j:498:ASN:ND2 | 2.31 | 0.63 |
| 1:m:613:ASP:HB3 | 1:m:732:ARG:NE | 2.13 | 0.63 |
| 1:u:382:THR:HG22 | 1:u:383:LEU:H | 1.63 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:w:613:ASP:HB3 | 1:w:732:ARG:NE | 2.13 | 0.63 |
| 1:J:484:PRO:CD | 1:J:609:TRP:HE3 | 2.11 | 0.63 |
| 1:K:322:GLN:NE2 | 1:L:340:THR:HB | 2.10 | 0.63 |
| 1:S:382:THR:HG22 | 1:S:383:LEU:H | 1.63 | 0.63 |
| 1:e:613:ASP:HB3 | 1:e:732:ARG:NE | 2.13 | 0.63 |
| 1:e:613:ASP:CB | 1:e:731:THR:HG22 | 2.17 | 0.63 |
| 1:f:492:SER:O | 1:f:498:ASN:ND2 | 2.31 | 0.63 |
| 1:m:492:SER:O | 1:m:498:ASN:ND2 | 2.31 | 0.63 |
| 1:n:609:TRP:CH2 | 1:n:631:PHE:CZ | 2.80 | 0.63 |
| 1:q:613:ASP:HB2 | 1:q:731:THR:CG2 | 2.19 | 0.63 |
| 1:t:382:THR:HG22 | 1:t:383:LEU:H | 1.63 | 0.63 |
| 1:u:613:ASP:HB3 | 1:u:732:ARG:NE | 2.13 | 0.63 |
| 1:x:609:TRP:CH2 | 1:x:631:PHE:CZ | 2.80 | 0.63 |
| 1:1:382:THR:HG22 | 1:1:383:LEU:H | 1.63 | 0.63 |
| 1:D:402:PRO:HG3 | 1:E:232:ASP:HB3 | 1.79 | 0.63 |
| 1:a:492:SER:O | 1:a:498:ASN:ND2 | 2.31 | 0.63 |
| 1:x:484:PRO:CD | 1:x:609:TRP:HE3 | 2.11 | 0.63 |
| 1:I:322:GLN:NE2 | 1:J:340:THR:HB | 2.11 | 0.62 |
| 1:M:340:THR:HB | 1:c:322:GLN:NE2 | 2.11 | 0.62 |
| 1:N:492:SER:O | 1:N:498:ASN:ND2 | 2.31 | 0.62 |
| 1:S:613:ASP:HB3 | 1:S:732:ARG:NE | 2.13 | 0.62 |
| 1:X:382:THR:HG22 | 1:X:383:LEU:H | 1.63 | 0.62 |
| 1:X:484:PRO:CD | 1:X:609:TRP:HE3 | 2.11 | 0.62 |
| 1:Z:492:SER:O | 1:Z:498:ASN:ND2 | 2.31 | 0.62 |
| 1:c:613:ASP:HB3 | 1:c:732:ARG:NE | 2.13 | 0.62 |
| 1:f:402:PRO:HG3 | 1:z:232:ASP:HB3 | 1.79 | 0.62 |
| 1:f:613:ASP:HB3 | 1:f:732:ARG:NE | 2.13 | 0.62 |
| 1:h:382:THR:HG22 | 1:h:383:LEU:H | 1.63 | 0.62 |
| 1:w:473:MET:HE1 | 1:x:275:TYR:HB3 | 1.79 | 0.62 |
| 1:x:382:THR:HG22 | 1:x:383:LEU:H | 1.63 | 0.62 |
| 1:C:340:THR:HB | 1:D:322:GLN:NE2 | 2.10 | 0.62 |
| 1:K:402:PRO:HG3 | 1:7:232:ASP:HB3 | 1.79 | 0.62 |
| 1:R:382:THR:HG22 | 1:R:383:LEU:H | 1.63 | 0.62 |
| 1:W:613:ASP:HB2 | 1:W:731:THR:CG2 | 2.18 | 0.62 |
| 1:Y:382:THR:HG22 | 1:Y:383:LEU:H | 1.63 | 0.62 |
| 1:g:613:ASP:HB3 | 1:g:732:ARG:NE | 2.13 | 0.62 |
| 1:i:613:ASP:HB3 | 1:i:732:ARG:NE | 2.13 | 0.62 |
| 1:j:613:ASP:HB3 | 1:j:732:ARG:NE | 2.13 | 0.62 |
| 1:z:382:THR:HG22 | 1:z:383:LEU:H | 1.63 | 0.62 |
| 1:2:382:THR:HG22 | 1:2:383:LEU:H | 1.63 | 0.62 |
| 1:G:484:PRO:CD | 1:G:609:TRP:CE3 | 2.83 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:326:VAL:HG21 | 1:I:333:LYS:HZ1 | 1.65 | 0.62 |
| 1:I:613:ASP:HB3 | 1:I:732:ARG:NE | 2.13 | 0.62 |
| 1:a:382:THR:HG22 | 1:a:383:LEU:H | 1.63 | 0.62 |
| 1:b:382:THR:HG22 | 1:b:383:LEU:H | 1.63 | 0.62 |
| 1:c:326:VAL:HG21 | 1:c:333:LYS:HZ1 | 1.65 | 0.62 |
| 1:d:613:ASP:HB2 | 1:d:731:THR:CG2 | 2.19 | 0.62 |
| 1:g:484:PRO:CD | 1:g:609:TRP:CE3 | 2.83 | 0.62 |
| 1:k:382:THR:HG22 | 1:k:383:LEU:H | 1.63 | 0.62 |
| 1:p:340:THR:HB | 1:6:322:GLN:NE2 | 2.11 | 0.62 |
| 1:p:382:THR:HG22 | 1:p:383:LEU:H | 1.63 | 0.62 |
| 1:p:484:PRO:CD | 1:p:609:TRP:CE3 | 2.83 | 0.62 |
| 1:r:326:VAL:HG21 | 1:r:333:LYS:HZ1 | 1.63 | 0.62 |
| 1:w:499:ASN:HD22 | 1:y:592:GLY:HA2 | 1.64 | 0.62 |
| 1:w:613:ASP:CB | 1:w:731:THR:HG22 | 2.17 | 0.62 |
| 1:y:484:PRO:CD | 1:y:609:TRP:HE3 | 2.11 | 0.62 |
| 1:D:275:TYR:HB3 | 1:P:473:MET:HE1 | 1.81 | 0.62 |
| 1:D:613:ASP:HB3 | 1:D:732:ARG:NE | 2.13 | 0.62 |
| 1:G:484:PRO:CD | 1:G:609:TRP:HE3 | 2.11 | 0.62 |
| 1:H:613:ASP:HB3 | 1:H:732:ARG:NE | 2.13 | 0.62 |
| 1:K:275:TYR:HB3 | 1:8:473:MET:HE1 | 1.81 | 0.62 |
| 1:K:613:ASP:HB3 | 1:K:732:ARG:NE | 2.13 | 0.62 |
| 1:O:484:PRO:CD | 1:O:609:TRP:CE3 | 2.83 | 0.62 |
| 1:U:613:ASP:HB2 | 1:U:731:THR:CG2 | 2.18 | 0.62 |
| 1:h:484:PRO:CD | 1:h:609:TRP:CE3 | 2.83 | 0.62 |
| 1:i:484:PRO:CD | 1:i:609:TRP:CE3 | 2.83 | 0.62 |
| 1:j:402:PRO:HG3 | 1:l:232:ASP:HB3 | 1.79 | 0.62 |
| 1:k:484:PRO:CD | 1:k:609:TRP:CE3 | 2.83 | 0.62 |
| 1:r:382:THR:HG22 | 1:r:383:LEU:H | 1.63 | 0.62 |
| 1:3:484:PRO:CD | 1:3:609:TRP:CE3 | 2.83 | 0.62 |
| 1:5:382:THR:HG22 | 1:5:383:LEU:H | 1.63 | 0.62 |
| 1:8:613:ASP:HB2 | 1:8:731:THR:CG2 | 2.19 | 0.62 |
| 1:B:382:THR:HG22 | 1:B:383:LEU:H | 1.63 | 0.62 |
| 1:N:382:THR:HG22 | 1:N:383:LEU:H | 1.63 | 0.62 |
| 1:Q:382:THR:HG22 | 1:Q:383:LEU:H | 1.63 | 0.62 |
| 1:R:613:ASP:HB2 | 1:R:731:THR:CG2 | 2.18 | 0.62 |
| 1:T:275:TYR:HB3 | 1:l:473:MET:HE1 | 1.82 | 0.62 |
| 1:U:484:PRO:CD | 1:U:609:TRP:CE3 | 2.83 | 0.62 |
| 1:V:484:PRO:CD | 1:V:609:TRP:HE3 | 2.11 | 0.62 |
| 1:d:382:THR:HG22 | 1:d:383:LEU:H | 1.63 | 0.62 |
| 1:f:473:MET:HE1 | 1:h:275:TYR:HB3 | 1.82 | 0.62 |
| 1:j:484:PRO:CD | 1:j:609:TRP:CE3 | 2.83 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:l:382:THR:HG22 | 1:l:383:LEU:H | 1.63 | 0.62 |
| 1:l:484:PRO:CD | 1:l:609:TRP:CE3 | 2.83 | 0.62 |
| 1:p:613:ASP:HB2 | 1:p:731:THR:CG2 | 2.19 | 0.62 |
| 1:y:484:PRO:CD | 1:y:609:TRP:CE3 | 2.83 | 0.62 |
| 1:B:484:PRO:CD | 1:B:609:TRP:CE3 | 2.83 | 0.62 |
| 1:F:322:GLN:NE2 | 1:G:340:THR:HB | 2.11 | 0.62 |
| 1:G:382:THR:HG22 | 1:G:383:LEU:H | 1.63 | 0.62 |
| 1:G:613:ASP:HB2 | 1:G:731:THR:CG2 | 2.19 | 0.62 |
| 1:H:613:ASP:HB2 | 1:H:731:THR:CG2 | 2.18 | 0.62 |
| 1:P:613:ASP:HB2 | 1:P:731:THR:CG2 | 2.19 | 0.62 |
| 1:R:484:PRO:CD | 1:R:609:TRP:CE3 | 2.83 | 0.62 |
| 1:V:275:TYR:HB3 | 1:X:473:MET:HE1 | 1.81 | 0.62 |
| 1:V:484:PRO:CD | 1:V:609:TRP:CE3 | 2.83 | 0.62 |
| 1:Y:326:VAL:HG21 | 1:Y:333:LYS:HZ1 | 1.63 | 0.62 |
| 1:Y:613:ASP:HB3 | 1:Y:732:ARG:NE | 2.13 | 0.62 |
| 1:b:613:ASP:HB2 | 1:b:731:THR:CG2 | 2.19 | 0.62 |
| 1:f:484:PRO:CD | 1:f:609:TRP:CE3 | 2.83 | 0.62 |
| 1:p:484:PRO:CD | 1:p:609:TRP:HE3 | 2.11 | 0.62 |
| 1:s:613:ASP:HB3 | 1:s:732:ARG:NE | 2.13 | 0.62 |
| 1:t:484:PRO:CD | 1:t:609:TRP:CE3 | 2.83 | 0.62 |
| 1:v:484:PRO:CD | 1:v:609:TRP:CE3 | 2.83 | 0.62 |
| 1:x:473:MET:HE1 | 1:y:275:TYR:HB3 | 1.81 | 0.62 |
| 1:z:484:PRO:CD | 1:z:609:TRP:CE3 | 2.83 | 0.62 |
| 1:2:613:ASP:HB2 | 1:2:731:THR:CG2 | 2.19 | 0.62 |
| 1:I:484:PRO:CD | 1:I:609:TRP:CE3 | 2.83 | 0.62 |
| 1:N:484:PRO:CD | 1:N:609:TRP:CE3 | 2.83 | 0.62 |
| 1:a:484:PRO:CD | 1:a:609:TRP:CE3 | 2.83 | 0.62 |
| 1:b:484:PRO:CD | 1:b:609:TRP:CE3 | 2.83 | 0.62 |
| 1:j:473:MET:HE1 | 1:k:275:TYR:HB3 | 1.82 | 0.62 |
| 1:B:473:MET:HE1 | 1:J:275:TYR:HB3 | 1.82 | 0.62 |
| 1:E:484:PRO:CD | 1:E:609:TRP:CE3 | 2.83 | 0.62 |
| 1:K:473:MET:HE1 | 1:a:275:TYR:HB3 | 1.82 | 0.62 |
| 1:c:484:PRO:CD | 1:c:609:TRP:CE3 | 2.83 | 0.62 |
| 1:e:484:PRO:CD | 1:e:609:TRP:CE3 | 2.83 | 0.62 |
| 1:f:382:THR:HG22 | 1:f:383:LEU:H | 1.63 | 0.62 |
| 1:k:340:THR:OG1 | 1:w:322:GLN:NE2 | 2.33 | 0.62 |
| 1:n:340:THR:HB | 1:r:322:GLN:NE2 | 2.11 | 0.62 |
| 1:r:613:ASP:HB3 | 1:r:732:ARG:NE | 2.13 | 0.62 |
| 1:t:613:ASP:HB2 | 1:t:731:THR:CG2 | 2.18 | 0.62 |
| 1:u:473:MET:HE1 | 1:v:275:TYR:HB3 | 1.82 | 0.62 |
| 1:z:473:MET:HE1 | 1:1:275:TYR:HB3 | 1.82 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:7:484:PRO:CD | 1:7:609:TRP:CE3 | 2.83 | 0.62 |
| 1:B:613:ASP:HB2 | 1:B:731:THR:CG2 | 2.19 | 0.62 |
| 1:F:484:PRO:CD | 1:F:609:TRP:CE3 | 2.83 | 0.62 |
| 1:K:484:PRO:CD | 1:K:609:TRP:CE3 | 2.83 | 0.62 |
| 1:L:492:SER:O | 1:L:498:ASN:ND2 | 2.31 | 0.62 |
| 1:M:275:TYR:HB3 | 1:b:473:MET:HE1 | 1.82 | 0.62 |
| 1:Q:484:PRO:CD | 1:Q:609:TRP:CE3 | 2.83 | 0.62 |
| 1:T:484:PRO:CD | 1:T:609:TRP:CE3 | 2.83 | 0.62 |
| 1:W:484:PRO:CD | 1:W:609:TRP:CE3 | 2.83 | 0.62 |
| 1:Z:484:PRO:CD | 1:Z:609:TRP:CE3 | 2.83 | 0.62 |
| 1:j:382:THR:HG22 | 1:j:383:LEU:H | 1.63 | 0.62 |
| 1:m:484:PRO:CD | 1:m:609:TRP:CE3 | 2.83 | 0.62 |
| 1:q:484:PRO:CD | 1:q:609:TRP:CE3 | 2.83 | 0.62 |
| 1:s:382:THR:HG22 | 1:s:383:LEU:H | 1.63 | 0.62 |
| 1:s:613:ASP:HB2 | 1:s:731:THR:CG2 | 2.18 | 0.62 |
| 1:t:402:PRO:HG3 | 1:y:232:ASP:HB3 | 1.80 | 0.62 |
| 1:w:484:PRO:CD | 1:w:609:TRP:CE3 | 2.83 | 0.62 |
| 1:1:484:PRO:CD | 1:1:609:TRP:CE3 | 2.83 | 0.62 |
| 1:5:484:PRO:CD | 1:5:609:TRP:CE3 | 2.83 | 0.62 |
| 1:6:484:PRO:CD | 1:6:609:TRP:CE3 | 2.83 | 0.62 |
| 1:D:473:MET:HE1 | 1:N:275:TYR:HB3 | 1.82 | 0.62 |
| 1:D:484:PRO:CD | 1:D:609:TRP:CE3 | 2.83 | 0.62 |
| 1:E:473:MET:HE1 | 1:Q:275:TYR:HB3 | 1.82 | 0.62 |
| 1:G:473:MET:HE1 | 1:I:275:TYR:HB3 | 1.82 | 0.62 |
| 1:H:484:PRO:CD | 1:H:609:TRP:CE3 | 2.83 | 0.62 |
| 1:H:492:SER:O | 1:H:498:ASN:ND2 | 2.31 | 0.62 |
| 1:J:322:GLN:NE2 | 1:a:340:THR:HB | 2.12 | 0.62 |
| 1:J:382:THR:HG22 | 1:J:383:LEU:H | 1.63 | 0.62 |
| 1:M:382:THR:HG22 | 1:M:383:LEU:H | 1.63 | 0.62 |
| 1:M:484:PRO:CD | 1:M:609:TRP:CE3 | 2.83 | 0.62 |
| 1:S:473:MET:HE1 | 1:U:275:TYR:HB3 | 1.82 | 0.62 |
| 1:S:484:PRO:CD | 1:S:609:TRP:CE3 | 2.83 | 0.62 |
| 1:Z:473:MET:HE1 | 1:4:275:TYR:HB3 | 1.82 | 0.62 |
| 1:m:473:MET:HE1 | 1:n:275:TYR:HB3 | 1.82 | 0.62 |
| 1:5:275:TYR:HB3 | 1:7:473:MET:HE1 | 1.82 | 0.62 |
| 1:A:484:PRO:CD | 1:A:609:TRP:CE3 | 2.83 | 0.61 |
| 1:C:492:SER:O | 1:C:498:ASN:ND2 | 2.31 | 0.61 |
| 1:H:275:TYR:HB3 | 1:Y:473:MET:HE1 | 1.82 | 0.61 |
| 1:H:382:THR:HG22 | 1:H:383:LEU:H | 1.63 | 0.61 |
| 1:J:484:PRO:CD | 1:J:609:TRP:CE3 | 2.83 | 0.61 |
| 1:V:473:MET:HE1 | 1:e:275:TYR:HB3 | 1.81 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:322:GLN:NE2 | 1:4:340:THR:HB | 2.11 | 0.61 |
| 1:Y:609:TRP:CH2 | 1:Y:631:PHE:CZ | 2.80 | 0.61 |
| 1:c:275:TYR:HB3 | 1:p:473:MET:HE1 | 1.82 | 0.61 |
| 1:l:492:SER:O | 1:l:498:ASN:ND2 | 2.31 | 0.61 |
| 1:n:484:PRO:CD | 1:n:609:TRP:CE3 | 2.83 | 0.61 |
| 1:r:473:MET:HE1 | 1:s:275:TYR:HB3 | 1.82 | 0.61 |
| 1:r:484:PRO:CD | 1:r:609:TRP:CE3 | 2.83 | 0.61 |
| 1:s:484:PRO:CD | 1:s:609:TRP:CE3 | 2.83 | 0.61 |
| 1:u:484:PRO:CD | 1:u:609:TRP:CE3 | 2.83 | 0.61 |
| 1:w:382:THR:HG22 | 1:w:383:LEU:H | 1.63 | 0.61 |
| 1:x:492:SER:O | 1:x:498:ASN:ND2 | 2.31 | 0.61 |
| 1:4:484:PRO:CD | 1:4:609:TRP:CE3 | 2.83 | 0.61 |
| 1:C:275:TYR:HB3 | 1:M:473:MET:HE1 | 1.82 | 0.61 |
| 1:X:492:SER:O | 1:X:498:ASN:ND2 | 2.31 | 0.61 |
| 1:Y:484:PRO:CD | 1:Y:609:TRP:CE3 | 2.83 | 0.61 |
| 1:d:492:SER:O | 1:d:498:ASN:ND2 | 2.31 | 0.61 |
| 1:o:484:PRO:CD | 1:o:609:TRP:CE3 | 2.83 | 0.61 |
| 1:z:492:SER:O | 1:z:498:ASN:ND2 | 2.31 | 0.61 |
| 1:2:492:SER:O | 1:2:498:ASN:ND2 | 2.31 | 0.61 |
| 1:E:275:TYR:HB3 | 1:F:473:MET:HE1 | 1.82 | 0.61 |
| 1:J:473:MET:HE1 | 1:L:275:TYR:HB3 | 1.82 | 0.61 |
| 1:s:492:SER:O | 1:s:498:ASN:ND2 | 2.31 | 0.61 |
| 1:O:473:MET:HE1 | 1:m:275:TYR:HB3 | 1.82 | 0.61 |
| 1:Z:275:TYR:HB3 | 1:3:473:MET:HE1 | 1.82 | 0.61 |
| 1:e:382:THR:HG22 | 1:e:383:LEU:H | 1.63 | 0.61 |
| 1:6:473:MET:HE1 | 1:7:275:TYR:HB3 | 1.82 | 0.61 |
| 1:C:484:PRO:CD | 1:C:609:TRP:CE3 | 2.83 | 0.61 |
| 1:R:275:TYR:HB3 | 1:U:473:MET:HE1 | 1.82 | 0.61 |
| 1:X:484:PRO:CD | 1:X:609:TRP:CE3 | 2.83 | 0.61 |
| 1:d:484:PRO:CD | 1:d:609:TRP:CE3 | 2.83 | 0.61 |
| 1:r:492:SER:O | 1:r:498:ASN:ND2 | 2.31 | 0.61 |
| 1:r:609:TRP:CH2 | 1:r:631:PHE:CZ | 2.80 | 0.61 |
| 1:s:326:VAL:HG21 | 1:s:333:LYS:HZ1 | 1.64 | 0.61 |
| 1:t:275:TYR:HB3 | 1:v:473:MET:HE1 | 1.82 | 0.61 |
| 1:x:484:PRO:CD | 1:x:609:TRP:CE3 | 2.83 | 0.61 |
| 1:L:484:PRO:CD | 1:L:609:TRP:CE3 | 2.83 | 0.61 |
| 1:O:275:TYR:HB3 | 1:n:473:MET:HE1 | 1.82 | 0.61 |
| 1:2:484:PRO:CD | 1:2:609:TRP:CE3 | 2.83 | 0.61 |
| 1:3:275:TYR:HB3 | 1:4:473:MET:HE1 | 1.82 | 0.61 |
| 1:H:326:VAL:HG21 | 1:H:333:LYS:HZ1 | 1.65 | 0.61 |
| 1:Y:492:SER:O | 1:Y:498:ASN:ND2 | 2.31 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:f:275:TYR:HB3 | 1:g:473:MET:HE1 | 1.82 | 0.61 |
| 1:A:473:MET:HE1 | 1:G:275:TYR:HB3 | 1.81 | 0.61 |
| 1:C:382:THR:HG22 | 1:C:383:LEU:H | 1.63 | 0.61 |
| 1:F:492:SER:O | 1:F:498:ASN:ND2 | 2.31 | 0.61 |
| 1:P:322:GLN:NE2 | 1:Q:340:THR:HB | 2.11 | 0.61 |
| 1:V:340:THR:OG1 | 1:W:322:GLN:NE2 | 2.34 | 0.61 |
| 1:e:322:GLN:NE2 | 1:h:340:THR:HB | 2.10 | 0.61 |
| 1:i:473:MET:HE1 | 1:j:275:TYR:HB3 | 1.82 | 0.61 |
| 1:q:492:SER:O | 1:q:498:ASN:ND2 | 2.31 | 0.61 |
| 1:v:613:ASP:HB2 | 1:v:731:THR:CG2 | 2.19 | 0.61 |
| 1:6:492:SER:O | 1:6:498:ASN:ND2 | 2.31 | 0.61 |
| 1:D:578:GLN:OE1 | 1:D:597:ASN:ND2 | 2.34 | 0.61 |
| 1:F:578:GLN:OE1 | 1:F:597:ASN:ND2 | 2.34 | 0.61 |
| 1:I:342:THR:HG22 | 1:I:407:ARG:HG3 | 1.83 | 0.61 |
| 1:K:578:GLN:OE1 | 1:K:597:ASN:ND2 | 2.34 | 0.61 |
| 1:T:473:MET:HE1 | 1:d:275:TYR:HB3 | 1.82 | 0.61 |
| 1:c:342:THR:HG22 | 1:c:407:ARG:HG3 | 1.83 | 0.61 |
| 1:h:492:SER:O | 1:h:498:ASN:ND2 | 2.31 | 0.61 |
| 1:l:578:GLN:OE1 | 1:l:597:ASN:ND2 | 2.34 | 0.61 |
| 1:r:342:THR:HG22 | 1:r:407:ARG:HG3 | 1.83 | 0.61 |
| 1:z:578:GLN:OE1 | 1:z:597:ASN:ND2 | 2.34 | 0.61 |
| 1:1:473:MET:HE1 | 1:2:275:TYR:HB3 | 1.82 | 0.61 |
| 1:5:340:THR:HB | 1:8:322:GLN:NE2 | 2.11 | 0.61 |
| 1:6:578:GLN:OE1 | 1:6:597:ASN:ND2 | 2.34 | 0.61 |
| 1:I:437:MET:HE1 | 1:I:473:MET:HB3 | 1.83 | 0.61 |
| 1:J:613:ASP:HB2 | 1:J:731:THR:CG2 | 2.19 | 0.61 |
| 1:N:473:MET:HE1 | 1:P:275:TYR:HB3 | 1.81 | 0.61 |
| 1:N:578:GLN:OE1 | 1:N:597:ASN:ND2 | 2.34 | 0.61 |
| 1:P:484:PRO:CD | 1:P:609:TRP:CE3 | 2.83 | 0.61 |
| 1:V:578:GLN:OE1 | 1:V:597:ASN:ND2 | 2.34 | 0.61 |
| 1:W:492:SER:O | 1:W:498:ASN:ND2 | 2.31 | 0.61 |
| 1:Y:342:THR:HG22 | 1:Y:407:ARG:HG3 | 1.83 | 0.61 |
| 1:Y:437:MET:HE1 | 1:Y:473:MET:HB3 | 1.83 | 0.61 |
| 1:a:473:MET:HE1 | 1:8:275:TYR:HB3 | 1.81 | 0.61 |
| 1:a:578:GLN:OE1 | 1:a:597:ASN:ND2 | 2.34 | 0.61 |
| 1:e:578:GLN:OE1 | 1:e:597:ASN:ND2 | 2.34 | 0.61 |
| 1:k:578:GLN:OE1 | 1:k:597:ASN:ND2 | 2.34 | 0.61 |
| 1:v:578:GLN:OE1 | 1:v:597:ASN:ND2 | 2.34 | 0.61 |
| 1:w:578:GLN:OE1 | 1:w:597:ASN:ND2 | 2.34 | 0.61 |
| 1:y:578:GLN:OE1 | 1:y:597:ASN:ND2 | 2.34 | 0.61 |
| 1:3:578:GLN:OE1 | 1:3:597:ASN:ND2 | 2.34 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:8:484:PRO:CD | 1:8:609:TRP:CE3 | 2.83 | 0.61 |
| 1:A:437:MET:HE1 | 1:A:473:MET:HB3 | 1.83 | 0.60 |
| 1:A:578:GLN:OE1 | 1:A:597:ASN:ND2 | 2.34 | 0.60 |
| 1:C:404:GLN:HE21 | 1:C:406:LEU:CD1 | 2.14 | 0.60 |
| 1:F:275:TYR:HB3 | 1:Q:473:MET:HE1 | 1.82 | 0.60 |
| 1:H:342:THR:HG22 | 1:H:407:ARG:HG3 | 1.83 | 0.60 |
| 1:J:578:GLN:OE1 | 1:J:597:ASN:ND2 | 2.34 | 0.60 |
| 1:L:382:THR:HG22 | 1:L:383:LEU:H | 1.63 | 0.60 |
| 1:M:578:GLN:OE1 | 1:M:597:ASN:ND2 | 2.34 | 0.60 |
| 1:O:322:GLN:NE2 | 1:P:340:THR:OG1 | 2.34 | 0.60 |
| 1:O:578:GLN:OE1 | 1:O:597:ASN:ND2 | 2.34 | 0.60 |
| 1:R:340:THR:OG1 | 1:V:322:GLN:NE2 | 2.34 | 0.60 |
| 1:U:578:GLN:OE1 | 1:U:597:ASN:ND2 | 2.34 | 0.60 |
| 1:V:492:SER:O | 1:V:498:ASN:ND2 | 2.31 | 0.60 |
| 1:c:437:MET:HE1 | 1:c:473:MET:HB3 | 1.83 | 0.60 |
| 1:h:578:GLN:OE1 | 1:h:597:ASN:ND2 | 2.34 | 0.60 |
| 1:n:437:MET:HE1 | 1:n:473:MET:HB3 | 1.83 | 0.60 |
| 1:o:437:MET:HE1 | 1:o:473:MET:HB3 | 1.83 | 0.60 |
| 1:r:437:MET:HE1 | 1:r:473:MET:HB3 | 1.83 | 0.60 |
| 1:s:342:THR:HG22 | 1:s:407:ARG:HG3 | 1.83 | 0.60 |
| 1:3:322:GLN:NE2 | 1:8:340:THR:OG1 | 2.34 | 0.60 |
| 1:5:473:MET:HE1 | 1:6:275:TYR:HB3 | 1.82 | 0.60 |
| 1:B:275:TYR:HB3 | 1:L:473:MET:HE1 | 1.82 | 0.60 |
| 1:E:404:GLN:HE21 | 1:E:406:LEU:CD1 | 2.14 | 0.60 |
| 1:E:578:GLN:OE1 | 1:E:597:ASN:ND2 | 2.34 | 0.60 |
| 1:E:613:ASP:HB2 | 1:E:731:THR:CG2 | 2.18 | 0.60 |
| 1:J:404:GLN:HE21 | 1:J:406:LEU:CD1 | 2.14 | 0.60 |
| 1:L:404:GLN:HE21 | 1:L:406:LEU:CD1 | 2.14 | 0.60 |
| 1:M:404:GLN:HE21 | 1:M:406:LEU:CD1 | 2.15 | 0.60 |
| 1:O:342:THR:HG22 | 1:O:407:ARG:HG3 | 1.83 | 0.60 |
| 1:O:437:MET:HE1 | 1:O:473:MET:HB3 | 1.83 | 0.60 |
| 1:T:578:GLN:OE1 | 1:T:597:ASN:ND2 | 2.34 | 0.60 |
| 1:U:437:MET:HE1 | 1:U:473:MET:HB3 | 1.83 | 0.60 |
| 1:W:342:THR:HG22 | 1:W:407:ARG:HG3 | 1.83 | 0.60 |
| 1:W:437:MET:HE1 | 1:W:473:MET:HB3 | 1.83 | 0.60 |
| 1:b:404:GLN:HE21 | 1:b:406:LEU:CD1 | 2.15 | 0.60 |
| 1:f:404:GLN:HE21 | 1:f:406:LEU:CD1 | 2.14 | 0.60 |
| 1:i:275:TYR:HB3 | 1:k:473:MET:HE1 | 1.81 | 0.60 |
| 1:k:492:SER:O | 1:k:498:ASN:ND2 | 2.31 | 0.60 |
| 1:n:342:THR:HG22 | 1:n:407:ARG:HG3 | 1.83 | 0.60 |
| 1:o:578:GLN:OE1 | 1:o:597:ASN:ND2 | 2.34 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:q:342:THR:HG22 | 1:q:407:ARG:HG3 | 1.83 | 0.60 |
| 1:r:340:THR:OG1 | 1:x:322:GLN:NE2 | 2.34 | 0.60 |
| 1:r:578:GLN:OE1 | 1:r:597:ASN:ND2 | 2.34 | 0.60 |
| 1:t:404:GLN:HE21 | 1:t:406:LEU:CD1 | 2.14 | 0.60 |
| 1:v:232:ASP:HB3 | 1:w:402:PRO:HG3 | 1.82 | 0.60 |
| 1:v:437:MET:HE1 | 1:v:473:MET:HB3 | 1.83 | 0.60 |
| 1:y:437:MET:HE1 | 1:y:473:MET:HB3 | 1.83 | 0.60 |
| 1:z:275:TYR:HB3 | 1:2:473:MET:HE1 | 1.82 | 0.60 |
| 1:1:578:GLN:OE1 | 1:1:597:ASN:ND2 | 2.34 | 0.60 |
| 1:3:342:THR:HG22 | 1:3:407:ARG:HG3 | 1.83 | 0.60 |
| 1:4:342:THR:HG22 | 1:4:407:ARG:HG3 | 1.83 | 0.60 |
| 1:4:437:MET:HE1 | 1:4:473:MET:HB3 | 1.83 | 0.60 |
| 1:7:578:GLN:OE1 | 1:7:597:ASN:ND2 | 2.34 | 0.60 |
| 1:B:404:GLN:HE21 | 1:B:406:LEU:CD1 | 2.15 | 0.60 |
| 1:C:473:MET:HE1 | 1:b:275:TYR:HB3 | 1.82 | 0.60 |
| 1:J:326:VAL:HG21 | 1:J:333:LYS:HZ1 | 1.65 | 0.60 |
| 1:P:578:GLN:OE1 | 1:P:597:ASN:ND2 | 2.34 | 0.60 |
| 1:R:404:GLN:HE21 | 1:R:406:LEU:CD1 | 2.15 | 0.60 |
| 1:R:473:MET:HE1 | 1:S:275:TYR:HB3 | 1.82 | 0.60 |
| 1:S:342:THR:HG22 | 1:S:407:ARG:HG3 | 1.83 | 0.60 |
| 1:T:404:GLN:HE21 | 1:T:406:LEU:CD1 | 2.15 | 0.60 |
| 1:Y:578:GLN:OE1 | 1:Y:597:ASN:ND2 | 2.34 | 0.60 |
| 1:j:404:GLN:HE21 | 1:j:406:LEU:CD1 | 2.14 | 0.60 |
| 1:q:437:MET:HE1 | 1:q:473:MET:HB3 | 1.83 | 0.60 |
| 1:w:404:GLN:HE21 | 1:w:406:LEU:HD11 | 1.67 | 0.60 |
| 1:x:578:GLN:OE1 | 1:x:597:ASN:ND2 | 2.34 | 0.60 |
| 1:y:342:THR:HG22 | 1:y:407:ARG:HG3 | 1.83 | 0.60 |
| 1:y:404:GLN:HE21 | 1:y:406:LEU:CD1 | 2.14 | 0.60 |
| 1:y:404:GLN:HE21 | 1:y:406:LEU:HD11 | 1.67 | 0.60 |
| 1:1:404:GLN:HE21 | 1:1:406:LEU:CD1 | 2.15 | 0.60 |
| 1:3:404:GLN:HE21 | 1:3:406:LEU:HD11 | 1.67 | 0.60 |
| 1:3:437:MET:HE1 | 1:3:473:MET:HB3 | 1.83 | 0.60 |
| 1:4:578:GLN:OE1 | 1:4:597:ASN:ND2 | 2.34 | 0.60 |
| 1:7:404:GLN:HE21 | 1:7:406:LEU:CD1 | 2.15 | 0.60 |
| 1:8:578:GLN:OE1 | 1:8:597:ASN:ND2 | 2.34 | 0.60 |
| 1:A:404:GLN:HE21 | 1:A:406:LEU:HD11 | 1.67 | 0.60 |
| 1:B:340:THR:OG1 | 1:C:322:GLN:NE2 | 2.34 | 0.60 |
| 1:D:492:SER:O | 1:D:498:ASN:ND2 | 2.31 | 0.60 |
| 1:E:404:GLN:HE21 | 1:E:406:LEU:HD11 | 1.67 | 0.60 |
| 1:E:492:SER:O | 1:E:498:ASN:ND2 | 2.31 | 0.60 |
| 1:M:613:ASP:HB2 | 1:M:731:THR:CG2 | 2.18 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:437:MET:HE1 | 1:N:473:MET:HB3 | 1.84 | 0.60 |
| 1:S:404:GLN:HE21 | 1:S:406:LEU:CD1 | 2.14 | 0.60 |
| 1:V:342:THR:HG22 | 1:V:407:ARG:HG3 | 1.83 | 0.60 |
| 1:V:404:GLN:HE21 | 1:V:406:LEU:CD1 | 2.15 | 0.60 |
| 1:V:437:MET:HE1 | 1:V:473:MET:HB3 | 1.84 | 0.60 |
| 1:Z:437:MET:HE1 | 1:Z:473:MET:HB3 | 1.83 | 0.60 |
| 1:b:322:GLN:NE2 | 1:o:340:THR:OG1 | 2.35 | 0.60 |
| 1:d:473:MET:HE1 | 1:l:275:TYR:HB3 | 1.82 | 0.60 |
| 1:f:326:VAL:HG21 | 1:f:333:LYS:HZ1 | 1.64 | 0.60 |
| 1:g:275:TYR:HB3 | 1:h:473:MET:HE1 | 1.82 | 0.60 |
| 1:j:322:GLN:NE2 | 1:x:340:THR:OG1 | 2.35 | 0.60 |
| 1:o:404:GLN:HE21 | 1:o:406:LEU:HD11 | 1.67 | 0.60 |
| 1:t:473:MET:HE1 | 1:u:275:TYR:HB3 | 1.82 | 0.60 |
| 1:u:404:GLN:HE21 | 1:u:406:LEU:CD1 | 2.14 | 0.60 |
| 1:w:587:GLN:NE2 | 1:x:498:ASN:OD1 | 2.34 | 0.60 |
| 1:7:404:GLN:HE21 | 1:7:406:LEU:HD11 | 1.67 | 0.60 |
| 1:8:342:THR:HG22 | 1:8:407:ARG:HG3 | 1.83 | 0.60 |
| 1:A:275:TYR:HB3 | 1:I:473:MET:HE1 | 1.82 | 0.60 |
| 1:C:578:GLN:OE1 | 1:C:597:ASN:ND2 | 2.34 | 0.60 |
| 1:L:322:GLN:NE2 | 1:b:340:THR:OG1 | 2.34 | 0.60 |
| 1:L:578:GLN:OE1 | 1:L:597:ASN:ND2 | 2.34 | 0.60 |
| 1:M:492:SER:O | 1:M:498:ASN:ND2 | 2.31 | 0.60 |
| 1:O:404:GLN:HE21 | 1:O:406:LEU:HD11 | 1.67 | 0.60 |
| 1:P:342:THR:HG22 | 1:P:407:ARG:HG3 | 1.83 | 0.60 |
| 1:S:578:GLN:OE1 | 1:S:597:ASN:ND2 | 2.34 | 0.60 |
| 1:T:342:THR:HG22 | 1:T:407:ARG:HG3 | 1.83 | 0.60 |
| 1:X:437:MET:HE1 | 1:X:473:MET:HB3 | 1.84 | 0.60 |
| 1:X:578:GLN:OE1 | 1:X:597:ASN:ND2 | 2.34 | 0.60 |
| 1:a:437:MET:HE1 | 1:a:473:MET:HB3 | 1.84 | 0.60 |
| 1:d:578:GLN:OE1 | 1:d:597:ASN:ND2 | 2.34 | 0.60 |
| 1:e:404:GLN:HE21 | 1:e:406:LEU:HD11 | 1.67 | 0.60 |
| 1:i:404:GLN:HE21 | 1:i:406:LEU:HD11 | 1.67 | 0.60 |
| 1:l:404:GLN:HE21 | 1:l:406:LEU:HD11 | 1.67 | 0.60 |
| 1:m:437:MET:HE1 | 1:m:473:MET:HB3 | 1.83 | 0.60 |
| 1:n:578:GLN:OE1 | 1:n:597:ASN:ND2 | 2.34 | 0.60 |
| 1:p:404:GLN:HE21 | 1:p:406:LEU:CD1 | 2.14 | 0.60 |
| 1:u:342:THR:HG22 | 1:u:407:ARG:HG3 | 1.83 | 0.60 |
| 1:u:578:GLN:OE1 | 1:u:597:ASN:ND2 | 2.34 | 0.60 |
| 1:x:437:MET:HE1 | 1:x:473:MET:HB3 | 1.83 | 0.60 |
| 1:y:492:SER:O | 1:y:498:ASN:ND2 | 2.31 | 0.60 |
| 1:1:342:THR:HG22 | 1:1:407:ARG:HG3 | 1.83 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2:404:GLN:HE21 | 1:2:406:LEU:CD1 | 2.14 | 0.60 |
| 1:5:437:MET:HE1 | 1:5:473:MET:HB3 | 1.83 | 0.60 |
| 1:G:404:GLN:HE21 | 1:G:406:LEU:CD1 | 2.14 | 0.60 |
| 1:J:492:SER:O | 1:J:498:ASN:ND2 | 2.31 | 0.60 |
| 1:K:322:GLN:NE2 | 1:L:340:THR:OG1 | 2.34 | 0.60 |
| 1:Q:437:MET:HE1 | 1:Q:473:MET:HB3 | 1.83 | 0.60 |
| 1:U:322:GLN:NE2 | 1:e:340:THR:OG1 | 2.35 | 0.60 |
| 1:V:404:GLN:HE21 | 1:V:406:LEU:HD11 | 1.67 | 0.60 |
| 1:W:578:GLN:OE1 | 1:W:597:ASN:ND2 | 2.34 | 0.60 |
| 1:X:322:GLN:NE2 | 1:Y:340:THR:OG1 | 2.35 | 0.60 |
| 1:X:340:THR:OG1 | 1:f:322:GLN:NE2 | 2.35 | 0.60 |
| 1:c:473:MET:HE1 | 1:o:275:TYR:HB3 | 1.82 | 0.60 |
| 1:d:342:THR:HG22 | 1:d:407:ARG:HG3 | 1.83 | 0.60 |
| 1:d:404:GLN:HE21 | 1:d:406:LEU:CD1 | 2.14 | 0.60 |
| 1:e:322:GLN:NE2 | 1:h:340:THR:OG1 | 2.34 | 0.60 |
| 1:e:404:GLN:HE21 | 1:e:406:LEU:CD1 | 2.15 | 0.60 |
| 1:h:404:GLN:HE21 | 1:h:406:LEU:HD11 | 1.67 | 0.60 |
| 1:i:342:THR:HG22 | 1:i:407:ARG:HG3 | 1.83 | 0.60 |
| 1:l:404:GLN:HE21 | 1:l:406:LEU:CD1 | 2.14 | 0.60 |
| 1:p:342:THR:HG22 | 1:p:407:ARG:HG3 | 1.83 | 0.60 |
| 1:t:404:GLN:HE21 | 1:t:406:LEU:HD11 | 1.67 | 0.60 |
| 1:w:404:GLN:HE21 | 1:w:406:LEU:CD1 | 2.14 | 0.60 |
| 1:z:404:GLN:HE21 | 1:z:406:LEU:CD1 | 2.15 | 0.60 |
| 1:2:342:THR:HG22 | 1:2:407:ARG:HG3 | 1.83 | 0.60 |
| 1:2:578:GLN:OE1 | 1:2:597:ASN:ND2 | 2.34 | 0.60 |
| 1:7:613:ASP:HB2 | 1:7:731:THR:CG2 | 2.18 | 0.60 |
| 1:C:340:THR:OG1 | 1:D:322:GLN:NE2 | 2.34 | 0.60 |
| 1:C:342:THR:HG22 | 1:C:407:ARG:HG3 | 1.83 | 0.60 |
| 1:D:404:GLN:HE21 | 1:D:406:LEU:CD1 | 2.15 | 0.60 |
| 1:G:342:THR:HG22 | 1:G:407:ARG:HG3 | 1.83 | 0.60 |
| 1:I:578:GLN:OE1 | 1:I:597:ASN:ND2 | 2.34 | 0.60 |
| 1:K:404:GLN:HE21 | 1:K:406:LEU:CD1 | 2.15 | 0.60 |
| 1:K:492:SER:O | 1:K:498:ASN:ND2 | 2.31 | 0.60 |
| 1:L:342:THR:HG22 | 1:L:407:ARG:HG3 | 1.83 | 0.60 |
| 1:L:404:GLN:HE21 | 1:L:406:LEU:HD11 | 1.67 | 0.60 |
| 1:O:492:SER:O | 1:O:498:ASN:ND2 | 2.31 | 0.60 |
| 1:R:342:THR:HG22 | 1:R:407:ARG:HG3 | 1.83 | 0.60 |
| 1:R:404:GLN:HE21 | 1:R:406:LEU:HD11 | 1.67 | 0.60 |
| 1:X:275:TYR:HB3 | 1:e:473:MET:HE1 | 1.82 | 0.60 |
| 1:c:404:GLN:HE21 | 1:c:406:LEU:CD1 | 2.14 | 0.60 |
| 1:c:578:GLN:OE1 | 1:c:597:ASN:ND2 | 2.34 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:e:342:THR:HG22 | 1:e:407:ARG:HG3 | 1.83 | 0.60 |
| 1:g:404:GLN:HE21 | 1:g:406:LEU:CD1 | 2.15 | 0.60 |
| 1:g:404:GLN:HE21 | 1:g:406:LEU:HD11 | 1.67 | 0.60 |
| 1:g:578:GLN:OE1 | 1:g:597:ASN:ND2 | 2.34 | 0.60 |
| 1:h:342:THR:HG22 | 1:h:407:ARG:HG3 | 1.83 | 0.60 |
| 1:i:578:GLN:OE1 | 1:i:597:ASN:ND2 | 2.34 | 0.60 |
| 1:j:437:MET:HE1 | 1:j:473:MET:HB3 | 1.83 | 0.60 |
| 1:l:437:MET:HE1 | 1:l:473:MET:HB3 | 1.83 | 0.60 |
| 1:o:404:GLN:HE21 | 1:o:406:LEU:CD1 | 2.15 | 0.60 |
| 1:o:473:MET:HE1 | 1:p:275:TYR:HB3 | 1.82 | 0.60 |
| 1:q:578:GLN:OE1 | 1:q:597:ASN:ND2 | 2.34 | 0.60 |
| 1:z:404:GLN:HE21 | 1:z:406:LEU:HD11 | 1.67 | 0.60 |
| 1:z:437:MET:HE1 | 1:z:473:MET:HB3 | 1.83 | 0.60 |
| 1:5:340:THR:OG1 | 1:8:322:GLN:NE2 | 2.34 | 0.60 |
| 1:5:342:THR:HG22 | 1:5:407:ARG:HG3 | 1.83 | 0.60 |
| 1:7:492:SER:O | 1:7:498:ASN:ND2 | 2.31 | 0.60 |
| 1:A:342:THR:HG22 | 1:A:407:ARG:HG3 | 1.83 | 0.60 |
| 1:A:404:GLN:HE21 | 1:A:406:LEU:CD1 | 2.14 | 0.60 |
| 1:C:404:GLN:HE21 | 1:C:406:LEU:HD11 | 1.67 | 0.60 |
| 1:C:437:MET:HE1 | 1:C:473:MET:HB3 | 1.83 | 0.60 |
| 1:F:340:THR:OG1 | 1:R:322:GLN:NE2 | 2.35 | 0.60 |
| 1:I:404:GLN:HE21 | 1:I:406:LEU:CD1 | 2.14 | 0.60 |
| 1:K:340:THR:OG1 | 1:7:322:GLN:NE2 | 2.35 | 0.60 |
| 1:O:326:VAL:HG21 | 1:O:333:LYS:HZ1 | 1.66 | 0.60 |
| 1:P:322:GLN:NE2 | 1:Q:340:THR:OG1 | 2.34 | 0.60 |
| 1:Q:342:THR:HG22 | 1:Q:407:ARG:HG3 | 1.83 | 0.60 |
| 1:Z:404:GLN:HE21 | 1:Z:406:LEU:CD1 | 2.14 | 0.60 |
| 1:f:437:MET:HE1 | 1:f:473:MET:HB3 | 1.83 | 0.60 |
| 1:g:340:THR:OG1 | 1:k:322:GLN:NE2 | 2.34 | 0.60 |
| 1:g:342:THR:HG22 | 1:g:407:ARG:HG3 | 1.83 | 0.60 |
| 1:h:322:GLN:NE2 | 1:i:340:THR:OG1 | 2.34 | 0.60 |
| 1:i:404:GLN:HE21 | 1:i:406:LEU:CD1 | 2.14 | 0.60 |
| 1:k:342:THR:HG22 | 1:k:407:ARG:HG3 | 1.83 | 0.60 |
| 1:k:404:GLN:HE21 | 1:k:406:LEU:HD11 | 1.67 | 0.60 |
| 1:l:326:VAL:HG21 | 1:l:333:LYS:HZ1 | 1.66 | 0.60 |
| 1:m:404:GLN:HE21 | 1:m:406:LEU:CD1 | 2.14 | 0.60 |
| 1:s:404:GLN:HE21 | 1:s:406:LEU:CD1 | 2.15 | 0.60 |
| 1:w:342:THR:HG22 | 1:w:407:ARG:HG3 | 1.83 | 0.60 |
| 1:D:340:THR:OG1 | 1:E:322:GLN:NE2 | 2.35 | 0.60 |
| 1:G:578:GLN:OE1 | 1:G:597:ASN:ND2 | 2.34 | 0.60 |
| 1:H:404:GLN:HE21 | 1:H:406:LEU:CD1 | 2.15 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:578:GLN:OE1 | 1:H:597:ASN:ND2 | 2.34 | 0.60 |
| 1:J:322:GLN:NE2 | 1:a:340:THR:OG1 | 2.35 | 0.60 |
| 1:L:437:MET:HE1 | 1:L:473:MET:HB3 | 1.83 | 0.60 |
| 1:T:437:MET:HE1 | 1:T:473:MET:HB3 | 1.83 | 0.60 |
| 1:Z:404:GLN:HE21 | 1:Z:406:LEU:HD11 | 1.67 | 0.60 |
| 1:b:578:GLN:OE1 | 1:b:597:ASN:ND2 | 2.34 | 0.60 |
| 1:d:437:MET:HE1 | 1:d:473:MET:HB3 | 1.83 | 0.60 |
| 1:g:613:ASP:CB | 1:g:731:THR:HG22 | 2.17 | 0.60 |
| 1:k:407:ARG:HD3 | 1:w:224:SER:O | 2.01 | 0.60 |
| 1:m:404:GLN:HE21 | 1:m:406:LEU:HD11 | 1.67 | 0.60 |
| 1:s:578:GLN:OE1 | 1:s:597:ASN:ND2 | 2.34 | 0.60 |
| 1:t:322:GLN:NE2 | 1:6:340:THR:OG1 | 2.35 | 0.60 |
| 1:x:342:THR:HG22 | 1:x:407:ARG:HG3 | 1.83 | 0.60 |
| 1:1:437:MET:HE1 | 1:1:473:MET:HB3 | 1.83 | 0.60 |
| 1:2:437:MET:HE1 | 1:2:473:MET:HB3 | 1.83 | 0.60 |
| 1:7:342:THR:HG22 | 1:7:407:ARG:HG3 | 1.83 | 0.60 |
| 1:A:322:GLN:NE2 | 1:E:340:THR:OG1 | 2.35 | 0.60 |
| 1:A:340:THR:OG1 | 1:B:322:GLN:NE2 | 2.35 | 0.60 |
| 1:I:322:GLN:NE2 | 1:J:340:THR:OG1 | 2.35 | 0.60 |
| 1:M:340:THR:OG1 | 1:c:322:GLN:NE2 | 2.35 | 0.60 |
| 1:Q:404:GLN:HE21 | 1:Q:406:LEU:CD1 | 2.15 | 0.60 |
| 1:X:342:THR:HG22 | 1:X:407:ARG:HG3 | 1.83 | 0.60 |
| 1:Z:340:THR:OG1 | 1:a:322:GLN:NE2 | 2.35 | 0.60 |
| 1:b:342:THR:HG22 | 1:b:407:ARG:HG3 | 1.83 | 0.60 |
| 1:h:404:GLN:HE21 | 1:h:406:LEU:CD1 | 2.14 | 0.60 |
| 1:l:340:THR:OG1 | 1:n:322:GLN:NE2 | 2.35 | 0.60 |
| 1:o:342:THR:HG22 | 1:o:407:ARG:HG3 | 1.83 | 0.60 |
| 1:p:322:GLN:NE2 | 1:q:340:THR:OG1 | 2.35 | 0.60 |
| 1:p:340:THR:OG1 | 1:6:322:GLN:NE2 | 2.35 | 0.60 |
| 1:p:578:GLN:OE1 | 1:p:597:ASN:ND2 | 2.34 | 0.60 |
| 1:s:404:GLN:HE21 | 1:s:406:LEU:HD11 | 1.67 | 0.60 |
| 1:t:342:THR:HG22 | 1:t:407:ARG:HG3 | 1.83 | 0.60 |
| 1:v:374:MET:HB2 | 1:w:669:LEU:HD11 | 1.84 | 0.60 |
| 1:z:326:VAL:HG21 | 1:z:333:LYS:HZ1 | 1.66 | 0.60 |
| 1:2:404:GLN:HE21 | 1:2:406:LEU:HD11 | 1.67 | 0.60 |
| 1:4:613:ASP:HB2 | 1:4:731:THR:CG2 | 2.18 | 0.60 |
| 1:5:404:GLN:HE21 | 1:5:406:LEU:CD1 | 2.15 | 0.60 |
| 1:8:404:GLN:HE21 | 1:8:406:LEU:CD1 | 2.15 | 0.60 |
| 1:B:342:THR:HG22 | 1:B:407:ARG:HG3 | 1.83 | 0.59 |
| 1:B:437:MET:HE1 | 1:B:473:MET:HB3 | 1.83 | 0.59 |
| 1:B:578:GLN:OE1 | 1:B:597:ASN:ND2 | 2.34 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:342:THR:HG22 | 1:E:407:ARG:HG3 | 1.83 | 0.59 |
| 1:F:322:GLN:NE2 | 1:G:340:THR:OG1 | 2.35 | 0.59 |
| 1:F:613:ASP:HB2 | 1:F:731:THR:CG2 | 2.18 | 0.59 |
| 1:G:322:GLN:NE2 | 1:W:340:THR:OG1 | 2.35 | 0.59 |
| 1:J:342:THR:HG22 | 1:J:407:ARG:HG3 | 1.83 | 0.59 |
| 1:M:322:GLN:NE2 | 1:N:340:THR:OG1 | 2.35 | 0.59 |
| 1:M:342:THR:HG22 | 1:M:407:ARG:HG3 | 1.83 | 0.59 |
| 1:N:322:GLN:NE2 | 1:m:340:THR:OG1 | 2.35 | 0.59 |
| 1:O:404:GLN:HE21 | 1:O:406:LEU:CD1 | 2.15 | 0.59 |
| 1:P:404:GLN:HE21 | 1:P:406:LEU:CD1 | 2.14 | 0.59 |
| 1:P:437:MET:HE1 | 1:P:473:MET:HB3 | 1.83 | 0.59 |
| 1:W:473:MET:HE1 | 1:Y:275:TYR:HB3 | 1.82 | 0.59 |
| 1:b:437:MET:HE1 | 1:b:473:MET:HB3 | 1.83 | 0.59 |
| 1:d:404:GLN:HE21 | 1:d:406:LEU:HD11 | 1.67 | 0.59 |
| 1:k:404:GLN:HE21 | 1:k:406:LEU:CD1 | 2.15 | 0.59 |
| 1:q:275:TYR:HB3 | 1:s:473:MET:HE1 | 1.82 | 0.59 |
| 1:w:589:THR:HA | 1:x:499:ASN:HA | 1.84 | 0.59 |
| 1:x:404:GLN:HE21 | 1:x:406:LEU:CD1 | 2.14 | 0.59 |
| 1:3:404:GLN:HE21 | 1:3:406:LEU:CD1 | 2.14 | 0.59 |
| 1:4:404:GLN:HE21 | 1:4:406:LEU:CD1 | 2.15 | 0.59 |
| 1:5:492:SER:O | 1:5:498:ASN:ND2 | 2.31 | 0.59 |
| 1:H:404:GLN:HE21 | 1:H:406:LEU:HD11 | 1.67 | 0.59 |
| 1:Q:322:GLN:NE2 | 1:S:340:THR:OG1 | 2.35 | 0.59 |
| 1:c:340:THR:OG1 | 1:s:322:GLN:NE2 | 2.35 | 0.59 |
| 1:f:578:GLN:OE1 | 1:f:597:ASN:ND2 | 2.34 | 0.59 |
| 1:g:696:ARG:HD3 | 1:g:700:GLU:OE2 | 2.03 | 0.59 |
| 1:i:696:ARG:HD3 | 1:i:700:GLU:OE2 | 2.03 | 0.59 |
| 1:j:578:GLN:OE1 | 1:j:597:ASN:ND2 | 2.34 | 0.59 |
| 1:n:404:GLN:HE21 | 1:n:406:LEU:CD1 | 2.15 | 0.59 |
| 1:n:492:SER:O | 1:n:498:ASN:ND2 | 2.31 | 0.59 |
| 1:q:473:MET:HE1 | 1:r:275:TYR:HB3 | 1.82 | 0.59 |
| 1:s:437:MET:HE1 | 1:s:473:MET:HB3 | 1.83 | 0.59 |
| 1:u:340:THR:OG1 | 1:5:322:GLN:NE2 | 2.35 | 0.59 |
| 1:x:404:GLN:HE21 | 1:x:406:LEU:HD11 | 1.67 | 0.59 |
| 1:4:404:GLN:HE21 | 1:4:406:LEU:HD11 | 1.67 | 0.59 |
| 1:8:437:MET:HE1 | 1:8:473:MET:HB3 | 1.84 | 0.59 |
| 1:B:404:GLN:HE21 | 1:B:406:LEU:HD11 | 1.67 | 0.59 |
| 1:G:437:MET:HE1 | 1:G:473:MET:HB3 | 1.83 | 0.59 |
| 1:H:322:GLN:NE2 | 1:I:340:THR:OG1 | 2.35 | 0.59 |
| 1:H:473:MET:HE1 | 1:W:275:TYR:HB3 | 1.82 | 0.59 |
| 1:Q:492:SER:O | 1:Q:498:ASN:ND2 | 2.31 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:322:GLN:NE2 | 1:d:340:THR:OG1 | 2.35 | 0.59 |
| 1:S:696:ARG:HD3 | 1:S:700:GLU:OE2 | 2.03 | 0.59 |
| 1:T:340:THR:OG1 | 1:i:322:GLN:NE2 | 2.35 | 0.59 |
| 1:W:404:GLN:HE21 | 1:W:406:LEU:HD11 | 1.67 | 0.59 |
| 1:Y:404:GLN:HE21 | 1:Y:406:LEU:HD11 | 1.67 | 0.59 |
| 1:f:340:THR:OG1 | 1:z:322:GLN:NE2 | 2.35 | 0.59 |
| 1:n:404:GLN:HE21 | 1:n:406:LEU:HD11 | 1.67 | 0.59 |
| 1:n:613:ASP:HB2 | 1:n:731:THR:CG2 | 2.18 | 0.59 |
| 1:p:437:MET:HE1 | 1:p:473:MET:HB3 | 1.83 | 0.59 |
| 1:r:404:GLN:HE21 | 1:r:406:LEU:HD11 | 1.67 | 0.59 |
| 1:u:322:GLN:NE2 | 1:2:340:THR:OG1 | 2.35 | 0.59 |
| 1:u:340:THR:HB | 1:5:322:GLN:NE2 | 2.11 | 0.59 |
| 1:u:696:ARG:HD3 | 1:u:700:GLU:OE2 | 2.03 | 0.59 |
| 1:z:340:THR:OG1 | 1:4:322:GLN:NE2 | 2.35 | 0.59 |
| 1:5:578:GLN:OE1 | 1:5:597:ASN:ND2 | 2.34 | 0.59 |
| 1:6:437:MET:HE1 | 1:6:473:MET:HB3 | 1.84 | 0.59 |
| 1:F:437:MET:HE1 | 1:F:473:MET:HB3 | 1.84 | 0.59 |
| 1:H:437:MET:HE1 | 1:H:473:MET:HB3 | 1.83 | 0.59 |
| 1:N:374:MET:HB2 | 1:m:669:LEU:HD11 | 1.85 | 0.59 |
| 1:N:696:ARG:HD3 | 1:N:700:GLU:OE2 | 2.03 | 0.59 |
| 1:P:696:ARG:HD3 | 1:P:700:GLU:OE2 | 2.03 | 0.59 |
| 1:Q:578:GLN:OE1 | 1:Q:597:ASN:ND2 | 2.34 | 0.59 |
| 1:T:404:GLN:HE21 | 1:T:406:LEU:HD11 | 1.67 | 0.59 |
| 1:W:404:GLN:HE21 | 1:W:406:LEU:CD1 | 2.14 | 0.59 |
| 1:X:404:GLN:HE21 | 1:X:406:LEU:CD1 | 2.15 | 0.59 |
| 1:X:404:GLN:HE21 | 1:X:406:LEU:HD11 | 1.67 | 0.59 |
| 1:Z:578:GLN:OE1 | 1:Z:597:ASN:ND2 | 2.34 | 0.59 |
| 1:a:342:THR:HG22 | 1:a:407:ARG:HG3 | 1.83 | 0.59 |
| 1:f:342:THR:HG22 | 1:f:407:ARG:HG3 | 1.83 | 0.59 |
| 1:i:437:MET:HE1 | 1:i:473:MET:HB3 | 1.83 | 0.59 |
| 1:j:340:THR:OG1 | 1:l:322:GLN:NE2 | 2.35 | 0.59 |
| 1:j:342:THR:HG22 | 1:j:407:ARG:HG3 | 1.83 | 0.59 |
| 1:n:340:THR:OG1 | 1:r:322:GLN:NE2 | 2.35 | 0.59 |
| 1:o:322:GLN:NE2 | 1:7:340:THR:OG1 | 2.35 | 0.59 |
| 1:q:404:GLN:HE21 | 1:q:406:LEU:HD11 | 1.67 | 0.59 |
| 1:y:696:ARG:HD3 | 1:y:700:GLU:OE2 | 2.03 | 0.59 |
| 1:1:404:GLN:HE21 | 1:1:406:LEU:HD11 | 1.67 | 0.59 |
| 1:8:696:ARG:HD3 | 1:8:700:GLU:OE2 | 2.03 | 0.59 |
| 1:B:696:ARG:HD3 | 1:B:700:GLU:OE2 | 2.03 | 0.59 |
| 1:E:696:ARG:HD3 | 1:E:700:GLU:OE2 | 2.03 | 0.59 |
| 1:F:404:GLN:HE21 | 1:F:406:LEU:CD1 | 2.14 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:499:ASN:OD1 | 1:I:500:ASN:N | 2.36 | 0.59 |
| 1:N:342:THR:HG22 | 1:N:407:ARG:HG3 | 1.83 | 0.59 |
| 1:T:322:GLN:HE21 | 1:U:340:THR:CB | 2.08 | 0.59 |
| 1:V:499:ASN:OD1 | 1:V:500:ASN:N | 2.36 | 0.59 |
| 1:V:696:ARG:HD3 | 1:V:700:GLU:OE2 | 2.03 | 0.59 |
| 1:Y:322:GLN:NE2 | 1:4:340:THR:OG1 | 2.35 | 0.59 |
| 1:a:696:ARG:HD3 | 1:a:700:GLU:OE2 | 2.03 | 0.59 |
| 1:c:499:ASN:OD1 | 1:c:500:ASN:N | 2.36 | 0.59 |
| 1:d:696:ARG:HD3 | 1:d:700:GLU:OE2 | 2.03 | 0.59 |
| 1:g:322:GLN:NE2 | 1:1:340:THR:OG1 | 2.35 | 0.59 |
| 1:g:437:MET:HE1 | 1:g:473:MET:HB3 | 1.83 | 0.59 |
| 1:m:578:GLN:OE1 | 1:m:597:ASN:ND2 | 2.34 | 0.59 |
| 1:o:696:ARG:HD3 | 1:o:700:GLU:OE2 | 2.03 | 0.59 |
| 1:r:404:GLN:HE21 | 1:r:406:LEU:CD1 | 2.14 | 0.59 |
| 1:y:499:ASN:OD1 | 1:y:500:ASN:N | 2.36 | 0.59 |
| 1:4:492:SER:O | 1:4:498:ASN:ND2 | 2.31 | 0.59 |
| 1:7:696:ARG:HD3 | 1:7:700:GLU:OE2 | 2.03 | 0.59 |
| 1:E:324:LYS:NZ | 1:E:337:ASN:OD1 | 2.35 | 0.59 |
| 1:F:342:THR:HG22 | 1:F:407:ARG:HG3 | 1.83 | 0.59 |
| 1:J:437:MET:HE1 | 1:J:473:MET:HB3 | 1.83 | 0.59 |
| 1:M:437:MET:HE1 | 1:M:473:MET:HB3 | 1.83 | 0.59 |
| 1:N:404:GLN:HE21 | 1:N:406:LEU:HD11 | 1.67 | 0.59 |
| 1:T:696:ARG:HD3 | 1:T:700:GLU:OE2 | 2.03 | 0.59 |
| 1:Y:404:GLN:HE21 | 1:Y:406:LEU:CD1 | 2.14 | 0.59 |
| 1:Z:669:LEU:HD11 | 1:a:374:MET:HB2 | 1.85 | 0.59 |
| 1:b:696:ARG:HD3 | 1:b:700:GLU:OE2 | 2.03 | 0.59 |
| 1:f:696:ARG:HD3 | 1:f:700:GLU:OE2 | 2.03 | 0.59 |
| 1:j:696:ARG:HD3 | 1:j:700:GLU:OE2 | 2.03 | 0.59 |
| 1:q:404:GLN:HE21 | 1:q:406:LEU:CD1 | 2.14 | 0.59 |
| 1:t:499:ASN:OD1 | 1:t:500:ASN:N | 2.36 | 0.59 |
| 1:t:578:GLN:OE1 | 1:t:597:ASN:ND2 | 2.34 | 0.59 |
| 1:v:404:GLN:HE21 | 1:v:406:LEU:CD1 | 2.14 | 0.59 |
| 1:w:499:ASN:OD1 | 1:w:500:ASN:N | 2.36 | 0.59 |
| 1:2:696:ARG:HD3 | 1:2:700:GLU:OE2 | 2.03 | 0.59 |
| 1:3:696:ARG:HD3 | 1:3:700:GLU:OE2 | 2.03 | 0.59 |
| 1:6:342:THR:HG22 | 1:6:407:ARG:HG3 | 1.83 | 0.59 |
| 1:6:613:ASP:HB2 | 1:6:731:THR:CG2 | 2.18 | 0.59 |
| 1:A:696:ARG:HD3 | 1:A:700:GLU:OE2 | 2.03 | 0.59 |
| 1:D:404:GLN:HE21 | 1:D:406:LEU:HD11 | 1.67 | 0.59 |
| 1:D:696:ARG:HD3 | 1:D:700:GLU:OE2 | 2.03 | 0.59 |
| 1:F:404:GLN:HE21 | 1:F:406:LEU:HD11 | 1.67 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:696:ARG:HD3 | 1:K:700:GLU:OE2 | 2.03 | 0.59 |
| 1:N:404:GLN:HE21 | 1:N:406:LEU:CD1 | 2.14 | 0.59 |
| 1:O:696:ARG:HD3 | 1:O:700:GLU:OE2 | 2.03 | 0.59 |
| 1:Q:322:GLN:NE2 | 1:S:340:THR:HB | 2.11 | 0.59 |
| 1:R:499:ASN:OD1 | 1:R:500:ASN:N | 2.36 | 0.59 |
| 1:R:578:GLN:OE1 | 1:R:597:ASN:ND2 | 2.34 | 0.59 |
| 1:U:374:MET:HB2 | 1:e:669:LEU:HD11 | 1.85 | 0.59 |
| 1:e:499:ASN:OD1 | 1:e:500:ASN:N | 2.36 | 0.59 |
| 1:f:499:ASN:OD1 | 1:f:500:ASN:N | 2.36 | 0.59 |
| 1:h:499:ASN:OD1 | 1:h:500:ASN:N | 2.36 | 0.59 |
| 1:j:499:ASN:OD1 | 1:j:500:ASN:N | 2.36 | 0.59 |
| 1:k:499:ASN:OD1 | 1:k:500:ASN:N | 2.36 | 0.59 |
| 1:v:404:GLN:HE21 | 1:v:406:LEU:HD11 | 1.67 | 0.59 |
| 1:w:275:TYR:HB3 | 1:y:473:MET:HE1 | 1.84 | 0.59 |
| 1:z:342:THR:HG22 | 1:z:407:ARG:HG3 | 1.83 | 0.59 |
| 1:1:696:ARG:HD3 | 1:1:700:GLU:OE2 | 2.03 | 0.59 |
| 1:4:696:ARG:HD3 | 1:4:700:GLU:OE2 | 2.03 | 0.59 |
| 1:6:404:GLN:HE21 | 1:6:406:LEU:CD1 | 2.14 | 0.59 |
| 1:7:324:LYS:NZ | 1:7:337:ASN:OD1 | 2.35 | 0.59 |
| 1:C:324:LYS:NZ | 1:C:337:ASN:OD1 | 2.35 | 0.59 |
| 1:G:499:ASN:OD1 | 1:G:500:ASN:N | 2.36 | 0.59 |
| 1:H:340:THR:OG1 | 1:Z:322:GLN:NE2 | 2.35 | 0.59 |
| 1:L:324:LYS:NZ | 1:L:337:ASN:OD1 | 2.35 | 0.59 |
| 1:O:499:ASN:OD1 | 1:O:500:ASN:N | 2.36 | 0.59 |
| 1:P:404:GLN:HE21 | 1:P:406:LEU:HD11 | 1.67 | 0.59 |
| 1:T:499:ASN:OD1 | 1:T:500:ASN:N | 2.36 | 0.59 |
| 1:U:404:GLN:HE21 | 1:U:406:LEU:CD1 | 2.15 | 0.59 |
| 1:U:404:GLN:HE21 | 1:U:406:LEU:HD11 | 1.67 | 0.59 |
| 1:U:499:ASN:OD1 | 1:U:500:ASN:N | 2.36 | 0.59 |
| 1:Z:499:ASN:OD1 | 1:Z:500:ASN:N | 2.36 | 0.59 |
| 1:a:404:GLN:HE21 | 1:a:406:LEU:HD11 | 1.67 | 0.59 |
| 1:d:499:ASN:OD1 | 1:d:500:ASN:N | 2.36 | 0.59 |
| 1:m:322:GLN:NE2 | 1:s:340:THR:OG1 | 2.35 | 0.59 |
| 1:m:499:ASN:OD1 | 1:m:500:ASN:N | 2.36 | 0.59 |
| 1:n:696:ARG:HD3 | 1:n:700:GLU:OE2 | 2.03 | 0.59 |
| 1:p:499:ASN:OD1 | 1:p:500:ASN:N | 2.36 | 0.59 |
| 1:q:499:ASN:OD1 | 1:q:500:ASN:N | 2.36 | 0.59 |
| 1:v:340:THR:OG1 | 1:1:322:GLN:NE2 | 2.35 | 0.59 |
| 1:v:499:ASN:OD1 | 1:v:500:ASN:N | 2.36 | 0.59 |
| 1:w:437:MET:HE1 | 1:w:473:MET:HB3 | 1.83 | 0.59 |
| 1:2:322:GLN:NE2 | 1:3:340:THR:OG1 | 2.35 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:499:ASN:OD1 | 1:3:500:ASN:N | 2.36 | 0.59 |
| 1:4:324:LYS:NZ | 1:4:337:ASN:OD1 | 2.35 | 0.59 |
| 1:A:374:MET:HB2 | 1:E:669:LEU:HD11 | 1.85 | 0.59 |
| 1:B:499:ASN:OD1 | 1:B:500:ASN:N | 2.36 | 0.59 |
| 1:E:499:ASN:OD1 | 1:E:500:ASN:N | 2.36 | 0.59 |
| 1:K:404:GLN:HE21 | 1:K:406:LEU:HD11 | 1.67 | 0.59 |
| 1:K:437:MET:HE1 | 1:K:473:MET:HB3 | 1.84 | 0.59 |
| 1:L:696:ARG:HD3 | 1:L:700:GLU:OE2 | 2.03 | 0.59 |
| 1:O:340:THR:OG1 | 1:d:322:GLN:NE2 | 2.35 | 0.59 |
| 1:W:499:ASN:OD1 | 1:W:500:ASN:N | 2.36 | 0.59 |
| 1:W:696:ARG:HD3 | 1:W:700:GLU:OE2 | 2.03 | 0.59 |
| 1:Z:342:THR:HG22 | 1:Z:407:ARG:HG3 | 1.83 | 0.59 |
| 1:b:499:ASN:OD1 | 1:b:500:ASN:N | 2.36 | 0.59 |
| 1:e:374:MET:HB2 | 1:h:669:LEU:HD11 | 1.85 | 0.59 |
| 1:h:696:ARG:HD3 | 1:h:700:GLU:OE2 | 2.03 | 0.59 |
| 1:k:696:ARG:HD3 | 1:k:700:GLU:OE2 | 2.03 | 0.59 |
| 1:l:342:THR:HG22 | 1:l:407:ARG:HG3 | 1.83 | 0.59 |
| 1:m:342:THR:HG22 | 1:m:407:ARG:HG3 | 1.83 | 0.59 |
| 1:n:324:LYS:NZ | 1:n:337:ASN:OD1 | 2.35 | 0.59 |
| 1:q:696:ARG:HD3 | 1:q:700:GLU:OE2 | 2.03 | 0.59 |
| 1:v:342:THR:HG22 | 1:v:407:ARG:HG3 | 1.83 | 0.59 |
| 1:1:499:ASN:OD1 | 1:1:500:ASN:N | 2.36 | 0.59 |
| 1:2:499:ASN:OD1 | 1:2:500:ASN:N | 2.36 | 0.59 |
| 1:5:499:ASN:OD1 | 1:5:500:ASN:N | 2.36 | 0.59 |
| 1:7:499:ASN:OD1 | 1:7:500:ASN:N | 2.36 | 0.59 |
| 1:C:696:ARG:HD3 | 1:C:700:GLU:OE2 | 2.03 | 0.59 |
| 1:D:437:MET:HE1 | 1:D:473:MET:HB3 | 1.84 | 0.59 |
| 1:F:696:ARG:HD3 | 1:F:700:GLU:OE2 | 2.03 | 0.59 |
| 1:Q:499:ASN:OD1 | 1:Q:500:ASN:N | 2.36 | 0.59 |
| 1:R:696:ARG:HD3 | 1:R:700:GLU:OE2 | 2.03 | 0.59 |
| 1:T:322:GLN:NE2 | 1:U:340:THR:OG1 | 2.35 | 0.59 |
| 1:Y:613:ASP:HB2 | 1:Y:731:THR:CG2 | 2.19 | 0.59 |
| 1:e:437:MET:HE1 | 1:e:473:MET:HB3 | 1.84 | 0.59 |
| 1:v:322:GLN:NE2 | 1:w:340:THR:OG1 | 2.36 | 0.59 |
| 1:8:404:GLN:HE21 | 1:8:406:LEU:HD11 | 1.67 | 0.59 |
| 1:R:669:LEU:HD11 | 1:V:374:MET:HB2 | 1.85 | 0.58 |
| 1:X:669:LEU:HD11 | 1:f:374:MET:HB2 | 1.85 | 0.58 |
| 1:a:404:GLN:HE21 | 1:a:406:LEU:CD1 | 2.15 | 0.58 |
| 1:p:404:GLN:HE21 | 1:p:406:LEU:HD11 | 1.67 | 0.58 |
| 1:t:696:ARG:HD3 | 1:t:700:GLU:OE2 | 2.03 | 0.58 |
| 1:A:669:LEU:HD11 | 1:B:374:MET:HB2 | 1.85 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:374:MET:HB2 | 1:G:669:LEU:HD11 | 1.85 | 0.58 |
| 1:G:404:GLN:HE21 | 1:G:406:LEU:HD11 | 1.67 | 0.58 |
| 1:R:437:MET:HE1 | 1:R:473:MET:HB3 | 1.83 | 0.58 |
| 1:S:404:GLN:HE21 | 1:S:406:LEU:HD11 | 1.67 | 0.58 |
| 1:S:437:MET:HE1 | 1:S:473:MET:HB3 | 1.84 | 0.58 |
| 1:U:342:THR:HG22 | 1:U:407:ARG:HG3 | 1.83 | 0.58 |
| 1:X:499:ASN:OD1 | 1:X:500:ASN:N | 2.36 | 0.58 |
| 1:b:374:MET:HB2 | 1:o:669:LEU:HD11 | 1.85 | 0.58 |
| 1:j:669:LEU:HD11 | 1:l:374:MET:HB2 | 1.85 | 0.58 |
| 1:k:437:MET:HE1 | 1:k:473:MET:HB3 | 1.83 | 0.58 |
| 1:p:669:LEU:HD11 | 1:6:374:MET:HB2 | 1.85 | 0.58 |
| 1:u:404:GLN:HE21 | 1:u:406:LEU:HD11 | 1.67 | 0.58 |
| 1:w:341:SER:HB3 | 1:w:675:GLN:HE22 | 1.69 | 0.58 |
| 1:5:696:ARG:HD3 | 1:5:700:GLU:OE2 | 2.03 | 0.58 |
| 1:6:696:ARG:HD3 | 1:6:700:GLU:OE2 | 2.03 | 0.58 |
| 1:7:437:MET:HE1 | 1:7:473:MET:HB3 | 1.83 | 0.58 |
| 1:C:669:LEU:HD11 | 1:D:374:MET:HB2 | 1.85 | 0.58 |
| 1:D:342:THR:HG22 | 1:D:407:ARG:HG3 | 1.83 | 0.58 |
| 1:E:437:MET:HE1 | 1:E:473:MET:HB3 | 1.83 | 0.58 |
| 1:F:669:LEU:HD11 | 1:R:374:MET:HB2 | 1.85 | 0.58 |
| 1:G:696:ARG:HD3 | 1:G:700:GLU:OE2 | 2.03 | 0.58 |
| 1:K:374:MET:HB2 | 1:L:669:LEU:HD11 | 1.85 | 0.58 |
| 1:U:341:SER:HB3 | 1:U:675:GLN:HE22 | 1.69 | 0.58 |
| 1:a:341:SER:HB3 | 1:a:675:GLN:HE22 | 1.69 | 0.58 |
| 1:b:404:GLN:HE21 | 1:b:406:LEU:HD11 | 1.67 | 0.58 |
| 1:c:669:LEU:HD11 | 1:s:374:MET:HB2 | 1.85 | 0.58 |
| 1:e:341:SER:HB3 | 1:e:675:GLN:HE22 | 1.69 | 0.58 |
| 1:f:669:LEU:HD11 | 1:z:374:MET:HB2 | 1.85 | 0.58 |
| 1:h:437:MET:HE1 | 1:h:473:MET:HB3 | 1.83 | 0.58 |
| 1:o:374:MET:HB2 | 1:7:669:LEU:HD11 | 1.86 | 0.58 |
| 1:p:696:ARG:HD3 | 1:p:700:GLU:OE2 | 2.03 | 0.58 |
| 1:r:613:ASP:HB2 | 1:r:731:THR:CG2 | 2.19 | 0.58 |
| 1:r:669:LEU:HD11 | 1:x:374:MET:HB2 | 1.85 | 0.58 |
| 1:t:374:MET:HB2 | 1:6:669:LEU:HD11 | 1.85 | 0.58 |
| 1:u:437:MET:HE1 | 1:u:473:MET:HB3 | 1.84 | 0.58 |
| 1:v:341:SER:HB3 | 1:v:675:GLN:HE22 | 1.69 | 0.58 |
| 1:8:492:SER:O | 1:8:498:ASN:ND2 | 2.31 | 0.58 |
| 1:D:499:ASN:OD1 | 1:D:500:ASN:N | 2.36 | 0.58 |
| 1:H:374:MET:HB2 | 1:I:669:LEU:HD11 | 1.85 | 0.58 |
| 1:K:499:ASN:OD1 | 1:K:500:ASN:N | 2.36 | 0.58 |
| 1:N:499:ASN:OD1 | 1:N:500:ASN:N | 2.36 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:499:ASN:OD1 | 1:P:500:ASN:N | 2.36 | 0.58 |
| 1:Q:696:ARG:HD3 | 1:Q:700:GLU:OE2 | 2.03 | 0.58 |
| 1:Z:341:SER:HB3 | 1:Z:675:GLN:HE22 | 1.69 | 0.58 |
| 1:a:324:LYS:NZ | 1:a:337:ASN:OD1 | 2.35 | 0.58 |
| 1:j:374:MET:HB2 | 1:x:669:LEU:HD11 | 1.85 | 0.58 |
| 1:l:696:ARG:HD3 | 1:l:700:GLU:OE2 | 2.03 | 0.58 |
| 1:m:341:SER:HB3 | 1:m:675:GLN:HE22 | 1.69 | 0.58 |
| 1:t:437:MET:HE1 | 1:t:473:MET:HB3 | 1.83 | 0.58 |
| 1:w:696:ARG:HD3 | 1:w:700:GLU:OE2 | 2.03 | 0.58 |
| 1:x:499:ASN:OD1 | 1:x:500:ASN:N | 2.36 | 0.58 |
| 1:x:696:ARG:HD3 | 1:x:700:GLU:OE2 | 2.03 | 0.58 |
| 1:z:696:ARG:HD3 | 1:z:700:GLU:OE2 | 2.03 | 0.58 |
| 1:8:499:ASN:OD1 | 1:8:500:ASN:N | 2.36 | 0.58 |
| 1:G:341:SER:HB3 | 1:G:675:GLN:HE22 | 1.69 | 0.58 |
| 1:J:499:ASN:OD1 | 1:J:500:ASN:N | 2.36 | 0.58 |
| 1:K:342:THR:HG22 | 1:K:407:ARG:HG3 | 1.83 | 0.58 |
| 1:M:499:ASN:OD1 | 1:M:500:ASN:N | 2.36 | 0.58 |
| 1:N:324:LYS:NZ | 1:N:337:ASN:OD1 | 2.35 | 0.58 |
| 1:N:341:SER:HB3 | 1:N:675:GLN:HE22 | 1.69 | 0.58 |
| 1:X:696:ARG:HD3 | 1:X:700:GLU:OE2 | 2.03 | 0.58 |
| 1:Y:341:SER:HB3 | 1:Y:675:GLN:HE22 | 1.69 | 0.58 |
| 1:Y:696:ARG:HD3 | 1:Y:700:GLU:OE2 | 2.03 | 0.58 |
| 1:e:254:ASN:O | 1:e:255:ASN:C | 2.47 | 0.58 |
| 1:e:696:ARG:HD3 | 1:e:700:GLU:OE2 | 2.03 | 0.58 |
| 1:k:613:ASP:HB2 | 1:k:731:THR:CG2 | 2.18 | 0.58 |
| 1:l:341:SER:HB3 | 1:l:675:GLN:HE22 | 1.69 | 0.58 |
| 1:n:613:ASP:OD1 | 1:n:732:ARG:CD | 2.52 | 0.58 |
| 1:p:341:SER:HB3 | 1:p:675:GLN:HE22 | 1.69 | 0.58 |
| 1:r:341:SER:HB3 | 1:r:675:GLN:HE22 | 1.69 | 0.58 |
| 1:z:341:SER:HB3 | 1:z:675:GLN:HE22 | 1.69 | 0.58 |
| 1:3:341:SER:HB3 | 1:3:675:GLN:HE22 | 1.69 | 0.58 |
| 1:4:613:ASP:OD1 | 1:4:732:ARG:CD | 2.52 | 0.58 |
| 1:C:232:ASP:OD1 | 1:C:232:ASP:N | 2.37 | 0.58 |
| 1:I:324:LYS:NZ | 1:I:337:ASN:OD1 | 2.35 | 0.58 |
| 1:J:613:ASP:OD1 | 1:J:732:ARG:CD | 2.52 | 0.58 |
| 1:K:669:LEU:HD11 | 1:7:374:MET:HB2 | 1.85 | 0.58 |
| 1:L:232:ASP:OD1 | 1:L:232:ASP:N | 2.37 | 0.58 |
| 1:M:613:ASP:OD1 | 1:M:732:ARG:CD | 2.52 | 0.58 |
| 1:O:341:SER:HB3 | 1:O:675:GLN:HE22 | 1.69 | 0.58 |
| 1:P:613:ASP:OD1 | 1:P:732:ARG:CD | 2.52 | 0.58 |
| 1:Q:254:ASN:O | 1:Q:255:ASN:C | 2.47 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:499:ASN:OD1 | 1:S:500:ASN:N | 2.36 | 0.58 |
| 1:V:232:ASP:OD1 | 1:V:232:ASP:N | 2.37 | 0.58 |
| 1:X:374:MET:HB2 | 1:Y:669:LEU:HD11 | 1.85 | 0.58 |
| 1:Z:254:ASN:O | 1:Z:255:ASN:C | 2.47 | 0.58 |
| 1:a:499:ASN:OD1 | 1:a:500:ASN:N | 2.36 | 0.58 |
| 1:c:696:ARG:HD3 | 1:c:700:GLU:OE2 | 2.03 | 0.58 |
| 1:h:232:ASP:OD1 | 1:h:232:ASP:N | 2.37 | 0.58 |
| 1:h:613:ASP:HB2 | 1:h:731:THR:CG2 | 2.19 | 0.58 |
| 1:l:669:LEU:HD11 | 1:n:374:MET:HB2 | 1.85 | 0.58 |
| 1:m:254:ASN:O | 1:m:255:ASN:C | 2.47 | 0.58 |
| 1:m:696:ARG:HD3 | 1:m:700:GLU:OE2 | 2.03 | 0.58 |
| 1:t:340:THR:OG1 | 1:y:322:GLN:NE2 | 2.37 | 0.58 |
| 1:w:254:ASN:O | 1:w:255:ASN:C | 2.47 | 0.58 |
| 1:4:499:ASN:OD1 | 1:4:500:ASN:N | 2.36 | 0.58 |
| 1:5:254:ASN:O | 1:5:255:ASN:C | 2.47 | 0.58 |
| 1:5:404:GLN:HE21 | 1:5:406:LEU:HD11 | 1.67 | 0.58 |
| 1:5:613:ASP:OD1 | 1:5:732:ARG:CD | 2.52 | 0.58 |
| 1:J:696:ARG:HD3 | 1:J:700:GLU:OE2 | 2.03 | 0.58 |
| 1:M:696:ARG:HD3 | 1:M:700:GLU:OE2 | 2.03 | 0.58 |
| 1:Q:404:GLN:HE21 | 1:Q:406:LEU:HD11 | 1.67 | 0.58 |
| 1:Q:613:ASP:OD1 | 1:Q:732:ARG:CD | 2.52 | 0.58 |
| 1:S:341:SER:HB3 | 1:S:675:GLN:HE22 | 1.69 | 0.58 |
| 1:Y:499:ASN:OD1 | 1:Y:500:ASN:N | 2.36 | 0.58 |
| 1:Z:696:ARG:HD3 | 1:Z:700:GLU:OE2 | 2.03 | 0.58 |
| 1:b:492:SER:O | 1:b:498:ASN:ND2 | 2.31 | 0.58 |
| 1:c:324:LYS:NZ | 1:c:337:ASN:OD1 | 2.35 | 0.58 |
| 1:g:499:ASN:OD1 | 1:g:500:ASN:N | 2.36 | 0.58 |
| 1:k:232:ASP:OD1 | 1:k:232:ASP:N | 2.37 | 0.58 |
| 1:n:499:ASN:OD1 | 1:n:500:ASN:N | 2.36 | 0.58 |
| 1:q:374:MET:HB2 | 1:y:669:LEU:HD11 | 1.84 | 0.58 |
| 1:r:499:ASN:OD1 | 1:r:500:ASN:N | 2.36 | 0.58 |
| 1:r:696:ARG:HD3 | 1:r:700:GLU:OE2 | 2.03 | 0.58 |
| 1:u:341:SER:HB3 | 1:u:675:GLN:HE22 | 1.69 | 0.58 |
| 1:u:499:ASN:OD1 | 1:u:500:ASN:N | 2.36 | 0.58 |
| 1:v:696:ARG:HD3 | 1:v:700:GLU:OE2 | 2.03 | 0.58 |
| 1:y:232:ASP:OD1 | 1:y:232:ASP:N | 2.37 | 0.58 |
| 1:6:499:ASN:OD1 | 1:6:500:ASN:N | 2.36 | 0.58 |
| 1:8:613:ASP:OD1 | 1:8:732:ARG:CD | 2.52 | 0.58 |
| 1:F:499:ASN:OD1 | 1:F:500:ASN:N | 2.36 | 0.58 |
| 1:G:613:ASP:OD1 | 1:G:732:ARG:CD | 2.52 | 0.58 |
| 1:I:232:ASP:OD1 | 1:I:232:ASP:N | 2.37 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:492:SER:O | 1:I:498:ASN:ND2 | 2.31 | 0.58 |
| 1:I:613:ASP:OD1 | 1:I:732:ARG:CD | 2.52 | 0.58 |
| 1:I:696:ARG:HD3 | 1:I:700:GLU:OE2 | 2.03 | 0.58 |
| 1:U:696:ARG:HD3 | 1:U:700:GLU:OE2 | 2.03 | 0.58 |
| 1:c:232:ASP:OD1 | 1:c:232:ASP:N | 2.37 | 0.58 |
| 1:c:613:ASP:OD1 | 1:c:732:ARG:CD | 2.52 | 0.58 |
| 1:l:613:ASP:OD1 | 1:l:732:ARG:CD | 2.52 | 0.58 |
| 1:p:613:ASP:OD1 | 1:p:732:ARG:CD | 2.52 | 0.58 |
| 1:t:340:THR:CB | 1:y:322:GLN:HE21 | 2.10 | 0.58 |
| 1:z:499:ASN:OD1 | 1:z:500:ASN:N | 2.36 | 0.58 |
| 1:D:669:LEU:HD11 | 1:E:374:MET:HB2 | 1.85 | 0.58 |
| 1:I:404:GLN:HE21 | 1:I:406:LEU:HD11 | 1.67 | 0.58 |
| 1:L:341:SER:HB3 | 1:L:675:GLN:HE22 | 1.69 | 0.58 |
| 1:L:499:ASN:OD1 | 1:L:500:ASN:N | 2.36 | 0.58 |
| 1:L:613:ASP:OD1 | 1:L:732:ARG:CD | 2.52 | 0.58 |
| 1:Q:374:MET:HB2 | 1:S:669:LEU:HD11 | 1.85 | 0.58 |
| 1:W:613:ASP:OD1 | 1:W:732:ARG:CD | 2.52 | 0.58 |
| 1:c:492:SER:O | 1:c:498:ASN:ND2 | 2.31 | 0.58 |
| 1:i:499:ASN:OD1 | 1:i:500:ASN:N | 2.36 | 0.58 |
| 1:i:613:ASP:OD1 | 1:i:732:ARG:CD | 2.52 | 0.58 |
| 1:j:404:GLN:HE21 | 1:j:406:LEU:HD11 | 1.67 | 0.58 |
| 1:l:499:ASN:OD1 | 1:l:500:ASN:N | 2.36 | 0.58 |
| 1:n:254:ASN:O | 1:n:255:ASN:C | 2.47 | 0.58 |
| 1:n:341:SER:HB3 | 1:n:675:GLN:HE22 | 1.69 | 0.58 |
| 1:q:613:ASP:OD1 | 1:q:732:ARG:CD | 2.52 | 0.58 |
| 1:r:232:ASP:OD1 | 1:r:232:ASP:N | 2.37 | 0.58 |
| 1:s:696:ARG:HD3 | 1:s:700:GLU:OE2 | 2.03 | 0.58 |
| 1:z:613:ASP:OD1 | 1:z:732:ARG:CD | 2.52 | 0.58 |
| 1:z:669:LEU:HD11 | 1:4:374:MET:HB2 | 1.85 | 0.58 |
| 1:4:254:ASN:O | 1:4:255:ASN:C | 2.47 | 0.58 |
| 1:A:341:SER:HB3 | 1:A:675:GLN:HE22 | 1.69 | 0.58 |
| 1:C:341:SER:HB3 | 1:C:675:GLN:HE22 | 1.69 | 0.58 |
| 1:C:499:ASN:OD1 | 1:C:500:ASN:N | 2.36 | 0.58 |
| 1:C:613:ASP:OD1 | 1:C:732:ARG:CD | 2.52 | 0.58 |
| 1:D:498:ASN:OD1 | 1:P:587:GLN:NE2 | 2.37 | 0.58 |
| 1:J:404:GLN:HE21 | 1:J:406:LEU:HD11 | 1.67 | 0.58 |
| 1:K:498:ASN:OD1 | 1:8:587:GLN:NE2 | 2.37 | 0.58 |
| 1:N:613:ASP:HB2 | 1:N:731:THR:CG2 | 2.18 | 0.58 |
| 1:P:341:SER:HB3 | 1:P:675:GLN:HE22 | 1.69 | 0.58 |
| 1:Y:232:ASP:OD1 | 1:Y:232:ASP:N | 2.37 | 0.58 |
| 1:a:613:ASP:HB2 | 1:a:731:THR:CG2 | 2.18 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:c:404:GLN:HE21 | 1:c:406:LEU:HD11 | 1.67 | 0.58 |
| 1:f:404:GLN:HE21 | 1:f:406:LEU:HD11 | 1.67 | 0.58 |
| 1:g:613:ASP:OD1 | 1:g:732:ARG:CD | 2.52 | 0.58 |
| 1:g:669:LEU:HD11 | 1:k:374:MET:HB2 | 1.85 | 0.58 |
| 1:o:341:SER:HB3 | 1:o:675:GLN:HE22 | 1.69 | 0.58 |
| 1:o:499:ASN:OD1 | 1:o:500:ASN:N | 2.36 | 0.58 |
| 1:u:669:LEU:HD11 | 1:5:374:MET:HB2 | 1.85 | 0.58 |
| 1:y:254:ASN:O | 1:y:255:ASN:C | 2.47 | 0.58 |
| 1:4:341:SER:HB3 | 1:4:675:GLN:HE22 | 1.69 | 0.58 |
| 1:7:341:SER:HB3 | 1:7:675:GLN:HE22 | 1.69 | 0.58 |
| 1:A:499:ASN:OD1 | 1:A:500:ASN:N | 2.36 | 0.57 |
| 1:B:492:SER:O | 1:B:498:ASN:ND2 | 2.31 | 0.57 |
| 1:E:341:SER:HB3 | 1:E:675:GLN:HE22 | 1.69 | 0.57 |
| 1:F:232:ASP:OD1 | 1:F:232:ASP:N | 2.37 | 0.57 |
| 1:G:374:MET:HB2 | 1:W:669:LEU:HD11 | 1.86 | 0.57 |
| 1:H:696:ARG:HD3 | 1:H:700:GLU:OE2 | 2.03 | 0.57 |
| 1:T:254:ASN:O | 1:T:255:ASN:C | 2.47 | 0.57 |
| 1:V:254:ASN:O | 1:V:255:ASN:C | 2.47 | 0.57 |
| 1:c:341:SER:HB3 | 1:c:675:GLN:HE22 | 1.69 | 0.57 |
| 1:k:613:ASP:OD1 | 1:k:732:ARG:CD | 2.52 | 0.57 |
| 1:o:613:ASP:OD1 | 1:o:732:ARG:CD | 2.52 | 0.57 |
| 1:q:224:SER:O | 1:y:407:ARG:HD3 | 2.04 | 0.57 |
| 1:w:609:TRP:NE1 | 1:x:629:GLY:CA | 2.54 | 0.57 |
| 1:1:254:ASN:O | 1:1:255:ASN:C | 2.47 | 0.57 |
| 1:6:341:SER:HB3 | 1:6:675:GLN:HE22 | 1.69 | 0.57 |
| 1:A:613:ASP:OD1 | 1:A:732:ARG:CD | 2.52 | 0.57 |
| 1:D:341:SER:HB3 | 1:D:675:GLN:HE22 | 1.69 | 0.57 |
| 1:W:617:GLN:OE1 | 1:W:617:GLN:N | 2.38 | 0.57 |
| 1:h:374:MET:HB2 | 1:i:669:LEU:HD11 | 1.85 | 0.57 |
| 1:h:613:ASP:OD1 | 1:h:732:ARG:CD | 2.52 | 0.57 |
| 1:k:669:LEU:HD11 | 1:w:374:MET:HB2 | 1.86 | 0.57 |
| 1:n:232:ASP:OD1 | 1:n:232:ASP:N | 2.37 | 0.57 |
| 1:q:617:GLN:N | 1:q:617:GLN:OE1 | 2.38 | 0.57 |
| 1:t:232:ASP:OD1 | 1:t:232:ASP:N | 2.37 | 0.57 |
| 1:2:341:SER:HB3 | 1:2:675:GLN:HE22 | 1.69 | 0.57 |
| 1:6:324:LYS:NZ | 1:6:337:ASN:OD1 | 2.35 | 0.57 |
| 1:A:617:GLN:OE1 | 1:A:617:GLN:N | 2.38 | 0.57 |
| 1:F:341:SER:HB3 | 1:F:675:GLN:HE22 | 1.69 | 0.57 |
| 1:H:669:LEU:HD11 | 1:Z:374:MET:HB2 | 1.85 | 0.57 |
| 1:I:341:SER:HB3 | 1:I:675:GLN:HE22 | 1.69 | 0.57 |
| 1:K:341:SER:HB3 | 1:K:675:GLN:HE22 | 1.69 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:404:GLN:HE21 | 1:M:406:LEU:HD11 | 1.67 | 0.57 |
| 1:R:232:ASP:OD1 | 1:R:232:ASP:N | 2.37 | 0.57 |
| 1:S:232:ASP:OD1 | 1:S:232:ASP:N | 2.37 | 0.57 |
| 1:U:613:ASP:OD1 | 1:U:732:ARG:CD | 2.52 | 0.57 |
| 1:f:341:SER:HB3 | 1:f:675:GLN:HE22 | 1.69 | 0.57 |
| 1:f:613:ASP:OD1 | 1:f:732:ARG:CD | 2.52 | 0.57 |
| 1:j:613:ASP:OD1 | 1:j:732:ARG:CD | 2.52 | 0.57 |
| 1:o:617:GLN:OE1 | 1:o:617:GLN:N | 2.38 | 0.57 |
| 1:p:374:MET:HB2 | 1:q:669:LEU:HD11 | 1.86 | 0.57 |
| 1:p:617:GLN:OE1 | 1:p:617:GLN:N | 2.38 | 0.57 |
| 1:v:613:ASP:OD1 | 1:v:732:ARG:CD | 2.52 | 0.57 |
| 1:4:232:ASP:OD1 | 1:4:232:ASP:N | 2.37 | 0.57 |
| 1:8:341:SER:HB3 | 1:8:675:GLN:HE22 | 1.69 | 0.57 |
| 1:F:617:GLN:N | 1:F:617:GLN:OE1 | 2.38 | 0.57 |
| 1:G:617:GLN:OE1 | 1:G:617:GLN:N | 2.38 | 0.57 |
| 1:J:374:MET:HB2 | 1:a:669:LEU:HD11 | 1.85 | 0.57 |
| 1:O:254:ASN:O | 1:O:255:ASN:C | 2.47 | 0.57 |
| 1:b:613:ASP:OD1 | 1:b:732:ARG:CD | 2.52 | 0.57 |
| 1:d:341:SER:HB3 | 1:d:675:GLN:HE22 | 1.69 | 0.57 |
| 1:u:232:ASP:OD1 | 1:u:232:ASP:N | 2.37 | 0.57 |
| 1:w:232:ASP:N | 1:w:232:ASP:OD1 | 2.37 | 0.57 |
| 1:x:587:GLN:NE2 | 1:y:498:ASN:OD1 | 2.37 | 0.57 |
| 1:1:341:SER:HB3 | 1:1:675:GLN:HE22 | 1.69 | 0.57 |
| 1:3:232:ASP:OD1 | 1:3:232:ASP:N | 2.37 | 0.57 |
| 1:5:617:GLN:OE1 | 1:5:617:GLN:N | 2.38 | 0.57 |
| 1:6:617:GLN:N | 1:6:617:GLN:OE1 | 2.38 | 0.57 |
| 1:D:613:ASP:OD1 | 1:D:732:ARG:CD | 2.52 | 0.57 |
| 1:F:613:ASP:OD1 | 1:F:732:ARG:CD | 2.52 | 0.57 |
| 1:K:324:LYS:NZ | 1:K:337:ASN:OD1 | 2.35 | 0.57 |
| 1:M:374:MET:HB2 | 1:N:669:LEU:HD11 | 1.85 | 0.57 |
| 1:O:232:ASP:OD1 | 1:O:232:ASP:N | 2.37 | 0.57 |
| 1:O:617:GLN:OE1 | 1:O:617:GLN:N | 2.38 | 0.57 |
| 1:Q:341:SER:HB3 | 1:Q:675:GLN:HE22 | 1.69 | 0.57 |
| 1:Q:617:GLN:OE1 | 1:Q:617:GLN:N | 2.38 | 0.57 |
| 1:R:492:SER:O | 1:R:498:ASN:ND2 | 2.31 | 0.57 |
| 1:S:374:MET:HB2 | 1:d:669:LEU:HD11 | 1.85 | 0.57 |
| 1:V:669:LEU:HD11 | 1:W:374:MET:HB2 | 1.86 | 0.57 |
| 1:Z:617:GLN:OE1 | 1:Z:617:GLN:N | 2.38 | 0.57 |
| 1:a:254:ASN:O | 1:a:255:ASN:C | 2.47 | 0.57 |
| 1:b:341:SER:HB3 | 1:b:675:GLN:HE22 | 1.69 | 0.57 |
| 1:d:613:ASP:OD1 | 1:d:732:ARG:CD | 2.52 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:f:258:TYR:OH | 1:f:399:GLU:OE1 | 2.22 | 0.57 |
| 1:i:492:SER:O | 1:i:498:ASN:ND2 | 2.31 | 0.57 |
| 1:k:652:LYS:HG2 | 1:k:653:ASN:O | 2.05 | 0.57 |
| 1:m:374:MET:HB2 | 1:s:669:LEU:HD11 | 1.85 | 0.57 |
| 1:m:617:GLN:OE1 | 1:m:617:GLN:N | 2.38 | 0.57 |
| 1:2:374:MET:HB2 | 1:3:669:LEU:HD11 | 1.86 | 0.57 |
| 1:2:613:ASP:OD1 | 1:2:732:ARG:CD | 2.52 | 0.57 |
| 1:3:254:ASN:O | 1:3:255:ASN:C | 2.47 | 0.57 |
| 1:4:617:GLN:OE1 | 1:4:617:GLN:N | 2.38 | 0.57 |
| 1:6:254:ASN:O | 1:6:255:ASN:C | 2.47 | 0.57 |
| 1:8:557:TYR:HE1 | 1:8:562:LEU:HD11 | 1.70 | 0.57 |
| 1:B:613:ASP:OD1 | 1:B:732:ARG:CD | 2.52 | 0.57 |
| 1:D:324:LYS:NZ | 1:D:337:ASN:OD1 | 2.35 | 0.57 |
| 1:F:254:ASN:O | 1:F:255:ASN:C | 2.47 | 0.57 |
| 1:G:557:TYR:HE1 | 1:G:562:LEU:HD11 | 1.70 | 0.57 |
| 1:H:499:ASN:OD1 | 1:H:500:ASN:N | 2.36 | 0.57 |
| 1:P:557:TYR:HE1 | 1:P:562:LEU:HD11 | 1.70 | 0.57 |
| 1:R:557:TYR:HE1 | 1:R:562:LEU:HD11 | 1.70 | 0.57 |
| 1:R:652:LYS:HG2 | 1:R:653:ASN:O | 2.05 | 0.57 |
| 1:T:341:SER:HB3 | 1:T:675:GLN:HE22 | 1.69 | 0.57 |
| 1:W:557:TYR:HE1 | 1:W:562:LEU:HD11 | 1.70 | 0.57 |
| 1:g:374:MET:HB2 | 1:1:669:LEU:HD11 | 1.85 | 0.57 |
| 1:j:341:SER:HB3 | 1:j:675:GLN:HE22 | 1.69 | 0.57 |
| 1:n:557:TYR:HE1 | 1:n:562:LEU:HD11 | 1.70 | 0.57 |
| 1:n:617:GLN:N | 1:n:617:GLN:OE1 | 2.38 | 0.57 |
| 1:p:557:TYR:HE1 | 1:p:562:LEU:HD11 | 1.70 | 0.57 |
| 1:s:499:ASN:OD1 | 1:s:500:ASN:N | 2.36 | 0.57 |
| 1:t:557:TYR:HE1 | 1:t:562:LEU:HD11 | 1.70 | 0.57 |
| 1:t:652:LYS:HG2 | 1:t:653:ASN:O | 2.05 | 0.57 |
| 1:3:617:GLN:N | 1:3:617:GLN:OE1 | 2.38 | 0.57 |
| 1:5:341:SER:HB3 | 1:5:675:GLN:HE22 | 1.69 | 0.57 |
| 1:B:341:SER:HB3 | 1:B:675:GLN:HE22 | 1.69 | 0.57 |
| 1:I:254:ASN:O | 1:I:255:ASN:C | 2.47 | 0.57 |
| 1:K:254:ASN:O | 1:K:255:ASN:C | 2.47 | 0.57 |
| 1:K:613:ASP:OD1 | 1:K:732:ARG:CD | 2.52 | 0.57 |
| 1:N:254:ASN:O | 1:N:255:ASN:C | 2.47 | 0.57 |
| 1:N:652:LYS:HG2 | 1:N:653:ASN:O | 2.05 | 0.57 |
| 1:O:557:TYR:HE1 | 1:O:562:LEU:HD11 | 1.70 | 0.57 |
| 1:P:382:THR:HG21 | 1:P:394:SER:H | 1.70 | 0.57 |
| 1:S:241:ILE:HG12 | 1:S:686:GLU:HG3 | 1.87 | 0.57 |
| 1:T:669:LEU:HD11 | 1:i:374:MET:HB2 | 1.85 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:a:652:LYS:HG2 | 1:a:653:ASN:O | 2.05 | 0.57 |
| 1:d:652:LYS:HG2 | 1:d:653:ASN:O | 2.05 | 0.57 |
| 1:h:254:ASN:O | 1:h:255:ASN:C | 2.47 | 0.57 |
| 1:h:652:LYS:HG2 | 1:h:653:ASN:O | 2.05 | 0.57 |
| 1:j:382:THR:HG21 | 1:j:394:SER:H | 1.70 | 0.57 |
| 1:l:652:LYS:HG2 | 1:l:653:ASN:O | 2.05 | 0.57 |
| 1:o:557:TYR:HE1 | 1:o:562:LEU:HD11 | 1.70 | 0.57 |
| 1:r:254:ASN:O | 1:r:255:ASN:C | 2.47 | 0.57 |
| 1:u:241:ILE:HG12 | 1:u:686:GLU:HG3 | 1.87 | 0.57 |
| 1:u:374:MET:HB2 | 1:2:669:LEU:HD11 | 1.85 | 0.57 |
| 1:u:652:LYS:HG2 | 1:u:653:ASN:O | 2.05 | 0.57 |
| 1:y:341:SER:HB3 | 1:y:675:GLN:HE22 | 1.69 | 0.57 |
| 1:2:652:LYS:HG2 | 1:2:653:ASN:O | 2.05 | 0.57 |
| 1:3:557:TYR:HE1 | 1:3:562:LEU:HD11 | 1.70 | 0.57 |
| 1:4:557:TYR:HE1 | 1:4:562:LEU:HD11 | 1.70 | 0.57 |
| 1:6:613:ASP:OD1 | 1:6:732:ARG:CD | 2.52 | 0.57 |
| 1:8:382:THR:HG21 | 1:8:394:SER:H | 1.70 | 0.57 |
| 1:A:557:TYR:HE1 | 1:A:562:LEU:HD11 | 1.70 | 0.57 |
| 1:C:241:ILE:HG12 | 1:C:686:GLU:HG3 | 1.87 | 0.57 |
| 1:C:617:GLN:N | 1:C:617:GLN:OE1 | 2.38 | 0.57 |
| 1:D:254:ASN:O | 1:D:255:ASN:C | 2.47 | 0.57 |
| 1:D:382:THR:HG21 | 1:D:394:SER:H | 1.70 | 0.57 |
| 1:G:232:ASP:OD1 | 1:G:232:ASP:N | 2.37 | 0.57 |
| 1:H:241:ILE:HG12 | 1:H:686:GLU:HG3 | 1.87 | 0.57 |
| 1:H:258:TYR:OH | 1:H:399:GLU:OE1 | 2.22 | 0.57 |
| 1:H:617:GLN:OE1 | 1:H:617:GLN:N | 2.38 | 0.57 |
| 1:I:260:GLN:NE2 | 1:I:276:PHE:HE1 | 2.03 | 0.57 |
| 1:I:374:MET:HB2 | 1:J:669:LEU:HD11 | 1.85 | 0.57 |
| 1:L:617:GLN:OE1 | 1:L:617:GLN:N | 2.38 | 0.57 |
| 1:M:669:LEU:HD11 | 1:c:374:MET:HB2 | 1.85 | 0.57 |
| 1:O:382:THR:HG21 | 1:O:394:SER:H | 1.70 | 0.57 |
| 1:O:669:LEU:HD11 | 1:d:374:MET:HB2 | 1.86 | 0.57 |
| 1:S:382:THR:HG21 | 1:S:394:SER:H | 1.70 | 0.57 |
| 1:S:652:LYS:HG2 | 1:S:653:ASN:O | 2.05 | 0.57 |
| 1:T:613:ASP:OD1 | 1:T:732:ARG:CD | 2.52 | 0.57 |
| 1:T:617:GLN:OE1 | 1:T:617:GLN:N | 2.38 | 0.57 |
| 1:V:341:SER:HB3 | 1:V:675:GLN:HE22 | 1.69 | 0.57 |
| 1:V:617:GLN:N | 1:V:617:GLN:OE1 | 2.38 | 0.57 |
| 1:W:241:ILE:HG12 | 1:W:686:GLU:HG3 | 1.87 | 0.57 |
| 1:W:652:LYS:HG2 | 1:W:653:ASN:O | 2.05 | 0.57 |
| 1:Z:613:ASP:OD1 | 1:Z:732:ARG:CD | 2.52 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:c:254:ASN:O | 1:c:255:ASN:C | 2.47 | 0.57 |
| 1:c:260:GLN:NE2 | 1:c:276:PHE:HE1 | 2.03 | 0.57 |
| 1:d:382:THR:HG21 | 1:d:394:SER:H | 1.70 | 0.57 |
| 1:f:382:THR:HG21 | 1:f:394:SER:H | 1.70 | 0.57 |
| 1:g:492:SER:O | 1:g:498:ASN:ND2 | 2.31 | 0.57 |
| 1:j:258:TYR:OH | 1:j:399:GLU:OE1 | 2.22 | 0.57 |
| 1:k:254:ASN:O | 1:k:255:ASN:C | 2.47 | 0.57 |
| 1:m:613:ASP:OD1 | 1:m:732:ARG:CD | 2.52 | 0.57 |
| 1:q:241:ILE:HG12 | 1:q:686:GLU:HG3 | 1.87 | 0.57 |
| 1:q:557:TYR:HE1 | 1:q:562:LEU:HD11 | 1.70 | 0.57 |
| 1:q:652:LYS:HG2 | 1:q:653:ASN:O | 2.05 | 0.57 |
| 1:s:241:ILE:HG12 | 1:s:686:GLU:HG3 | 1.87 | 0.57 |
| 1:s:617:GLN:OE1 | 1:s:617:GLN:N | 2.38 | 0.57 |
| 1:t:613:ASP:OD1 | 1:t:732:ARG:CD | 2.52 | 0.57 |
| 1:w:617:GLN:OE1 | 1:w:617:GLN:N | 2.38 | 0.57 |
| 1:y:617:GLN:N | 1:y:617:GLN:OE1 | 2.38 | 0.57 |
| 1:y:652:LYS:HG2 | 1:y:653:ASN:O | 2.05 | 0.57 |
| 1:z:652:LYS:HG2 | 1:z:653:ASN:O | 2.05 | 0.57 |
| 1:1:617:GLN:OE1 | 1:1:617:GLN:N | 2.38 | 0.57 |
| 1:2:382:THR:HG21 | 1:2:394:SER:H | 1.70 | 0.57 |
| 1:B:652:LYS:HG2 | 1:B:653:ASN:O | 2.05 | 0.57 |
| 1:B:669:LEU:HD11 | 1:C:374:MET:HB2 | 1.85 | 0.57 |
| 1:C:260:GLN:NE2 | 1:C:276:PHE:HE1 | 2.03 | 0.57 |
| 1:E:617:GLN:OE1 | 1:E:617:GLN:N | 2.38 | 0.57 |
| 1:K:382:THR:HG21 | 1:K:394:SER:H | 1.70 | 0.57 |
| 1:L:241:ILE:HG12 | 1:L:686:GLU:HG3 | 1.87 | 0.57 |
| 1:L:260:GLN:NE2 | 1:L:276:PHE:HE1 | 2.03 | 0.57 |
| 1:P:232:ASP:OD1 | 1:P:232:ASP:N | 2.37 | 0.57 |
| 1:P:374:MET:HB2 | 1:Q:669:LEU:HD11 | 1.85 | 0.57 |
| 1:Q:260:GLN:NE2 | 1:Q:276:PHE:HE1 | 2.03 | 0.57 |
| 1:Q:290:PHE:CE2 | 1:Q:614:VAL:HB | 2.40 | 0.57 |
| 1:U:290:PHE:CE2 | 1:U:614:VAL:HB | 2.40 | 0.57 |
| 1:U:617:GLN:OE1 | 1:U:617:GLN:N | 2.38 | 0.57 |
| 1:V:260:GLN:NE2 | 1:V:276:PHE:HE1 | 2.03 | 0.57 |
| 1:V:652:LYS:HG2 | 1:V:653:ASN:O | 2.05 | 0.57 |
| 1:X:382:THR:HG21 | 1:X:394:SER:H | 1.70 | 0.57 |
| 1:Y:254:ASN:O | 1:Y:255:ASN:C | 2.47 | 0.57 |
| 1:Z:241:ILE:HG12 | 1:Z:686:GLU:HG3 | 1.87 | 0.57 |
| 1:Z:404:GLN:HG2 | 1:Z:406:LEU:CD1 | 2.35 | 0.57 |
| 1:b:652:LYS:HG2 | 1:b:653:ASN:O | 2.05 | 0.57 |
| 1:c:617:GLN:OE1 | 1:c:617:GLN:N | 2.38 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:e:617:GLN:OE1 | 1:e:617:GLN:N | 2.38 | 0.57 |
| 1:f:260:GLN:NE2 | 1:f:276:PHE:HE1 | 2.03 | 0.57 |
| 1:g:341:SER:HB3 | 1:g:675:GLN:HE22 | 1.69 | 0.57 |
| 1:h:290:PHE:CE2 | 1:h:614:VAL:HB | 2.40 | 0.57 |
| 1:i:260:GLN:NE2 | 1:i:276:PHE:HE1 | 2.03 | 0.57 |
| 1:j:260:GLN:NE2 | 1:j:276:PHE:HE1 | 2.03 | 0.57 |
| 1:j:557:TYR:HE1 | 1:j:562:LEU:HD11 | 1.70 | 0.57 |
| 1:k:290:PHE:CE2 | 1:k:614:VAL:HB | 2.40 | 0.57 |
| 1:m:241:ILE:HG12 | 1:m:686:GLU:HG3 | 1.87 | 0.57 |
| 1:m:404:GLN:HG2 | 1:m:406:LEU:CD1 | 2.35 | 0.57 |
| 1:m:557:TYR:HE1 | 1:m:562:LEU:HD11 | 1.70 | 0.57 |
| 1:n:241:ILE:HG12 | 1:n:686:GLU:HG3 | 1.87 | 0.57 |
| 1:o:241:ILE:HG12 | 1:o:686:GLU:HG3 | 1.87 | 0.57 |
| 1:p:652:LYS:HG2 | 1:p:653:ASN:O | 2.05 | 0.57 |
| 1:u:382:THR:HG21 | 1:u:394:SER:H | 1.70 | 0.57 |
| 1:v:617:GLN:N | 1:v:617:GLN:OE1 | 2.38 | 0.57 |
| 1:x:232:ASP:OD1 | 1:x:232:ASP:N | 2.37 | 0.57 |
| 1:x:613:ASP:OD1 | 1:x:732:ARG:CD | 2.52 | 0.57 |
| 1:1:613:ASP:OD1 | 1:1:732:ARG:CD | 2.52 | 0.57 |
| 1:3:382:THR:HG21 | 1:3:394:SER:H | 1.70 | 0.57 |
| 1:4:241:ILE:HG12 | 1:4:686:GLU:HG3 | 1.87 | 0.57 |
| 1:5:260:GLN:NE2 | 1:5:276:PHE:HE1 | 2.03 | 0.57 |
| 1:5:669:LEU:HD11 | 1:8:374:MET:HB2 | 1.85 | 0.57 |
| 1:G:652:LYS:HG2 | 1:G:653:ASN:O | 2.05 | 0.57 |
| 1:K:623:LYS:HB2 | 1:K:645:PRO:HG3 | 1.87 | 0.57 |
| 1:L:374:MET:HB2 | 1:b:669:LEU:HD11 | 1.85 | 0.57 |
| 1:P:617:GLN:OE1 | 1:P:617:GLN:N | 2.38 | 0.57 |
| 1:Q:556:ASP:OD1 | 1:Q:557:TYR:N | 2.38 | 0.57 |
| 1:R:382:THR:HG21 | 1:R:394:SER:H | 1.70 | 0.57 |
| 1:R:613:ASP:OD1 | 1:R:732:ARG:CD | 2.52 | 0.57 |
| 1:U:241:ILE:HG12 | 1:U:686:GLU:HG3 | 1.87 | 0.57 |
| 1:U:260:GLN:NE2 | 1:U:276:PHE:HE1 | 2.03 | 0.57 |
| 1:V:404:GLN:HG2 | 1:V:406:LEU:CD1 | 2.35 | 0.57 |
| 1:V:587:GLN:NE2 | 1:e:498:ASN:OD1 | 2.37 | 0.57 |
| 1:X:341:SER:HB3 | 1:X:675:GLN:HE22 | 1.69 | 0.57 |
| 1:X:613:ASP:OD1 | 1:X:732:ARG:CD | 2.52 | 0.57 |
| 1:Y:382:THR:HG21 | 1:Y:394:SER:H | 1.70 | 0.57 |
| 1:Z:557:TYR:HE1 | 1:Z:562:LEU:HD11 | 1.70 | 0.57 |
| 1:e:290:PHE:CE2 | 1:e:614:VAL:HB | 2.40 | 0.57 |
| 1:f:557:TYR:HE1 | 1:f:562:LEU:HD11 | 1.70 | 0.57 |
| 1:f:617:GLN:N | 1:f:617:GLN:OE1 | 2.38 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:g:241:ILE:HG12 | 1:g:686:GLU:HG3 | 1.87 | 0.57 |
| 1:g:260:GLN:NE2 | 1:g:276:PHE:HE1 | 2.03 | 0.57 |
| 1:g:652:LYS:HG2 | 1:g:653:ASN:O | 2.05 | 0.57 |
| 1:h:341:SER:HB3 | 1:h:675:GLN:HE22 | 1.69 | 0.57 |
| 1:i:241:ILE:HG12 | 1:i:686:GLU:HG3 | 1.87 | 0.57 |
| 1:k:341:SER:HB3 | 1:k:675:GLN:HE22 | 1.69 | 0.57 |
| 1:n:260:GLN:NE2 | 1:n:276:PHE:HE1 | 2.03 | 0.57 |
| 1:p:232:ASP:OD1 | 1:p:232:ASP:N | 2.37 | 0.57 |
| 1:r:382:THR:HG21 | 1:r:394:SER:H | 1.70 | 0.57 |
| 1:s:258:TYR:OH | 1:s:399:GLU:OE1 | 2.22 | 0.57 |
| 1:t:341:SER:HB3 | 1:t:675:GLN:HE22 | 1.69 | 0.57 |
| 1:t:382:THR:HG21 | 1:t:394:SER:H | 1.70 | 0.57 |
| 1:u:617:GLN:OE1 | 1:u:617:GLN:N | 2.38 | 0.57 |
| 1:v:241:ILE:HG12 | 1:v:686:GLU:HG3 | 1.87 | 0.57 |
| 1:v:260:GLN:NE2 | 1:v:276:PHE:HE1 | 2.03 | 0.57 |
| 1:v:290:PHE:CE2 | 1:v:614:VAL:HB | 2.40 | 0.57 |
| 1:x:341:SER:HB3 | 1:x:675:GLN:HE22 | 1.69 | 0.57 |
| 1:x:382:THR:HG21 | 1:x:394:SER:H | 1.70 | 0.57 |
| 1:y:260:GLN:NE2 | 1:y:276:PHE:HE1 | 2.03 | 0.57 |
| 1:1:557:TYR:HE1 | 1:1:562:LEU:HD11 | 1.70 | 0.57 |
| 1:4:260:GLN:NE2 | 1:4:276:PHE:HE1 | 2.03 | 0.57 |
| 1:5:290:PHE:CE2 | 1:5:614:VAL:HB | 2.40 | 0.57 |
| 1:5:556:ASP:OD1 | 1:5:557:TYR:N | 2.38 | 0.57 |
| 1:7:617:GLN:OE1 | 1:7:617:GLN:N | 2.38 | 0.57 |
| 1:B:241:ILE:HG12 | 1:B:686:GLU:HG3 | 1.87 | 0.56 |
| 1:D:404:GLN:HG2 | 1:D:406:LEU:CD1 | 2.35 | 0.56 |
| 1:D:623:LYS:HB2 | 1:D:645:PRO:HG3 | 1.87 | 0.56 |
| 1:E:623:LYS:HB2 | 1:E:645:PRO:HG3 | 1.87 | 0.56 |
| 1:E:652:LYS:HG2 | 1:E:653:ASN:O | 2.05 | 0.56 |
| 1:F:260:GLN:NE2 | 1:F:276:PHE:HE1 | 2.03 | 0.56 |
| 1:H:382:THR:HG21 | 1:H:394:SER:H | 1.70 | 0.56 |
| 1:I:290:PHE:CE2 | 1:I:614:VAL:HB | 2.40 | 0.56 |
| 1:I:617:GLN:OE1 | 1:I:617:GLN:N | 2.38 | 0.56 |
| 1:J:341:SER:HB3 | 1:J:675:GLN:HE22 | 1.69 | 0.56 |
| 1:J:404:GLN:HG2 | 1:J:406:LEU:CD1 | 2.35 | 0.56 |
| 1:M:404:GLN:HG2 | 1:M:406:LEU:CD1 | 2.35 | 0.56 |
| 1:M:652:LYS:HG2 | 1:M:653:ASN:O | 2.05 | 0.56 |
| 1:P:652:LYS:HG2 | 1:P:653:ASN:O | 2.05 | 0.56 |
| 1:Q:241:ILE:HG12 | 1:Q:686:GLU:HG3 | 1.87 | 0.56 |
| 1:Q:404:GLN:HG2 | 1:Q:406:LEU:CD1 | 2.35 | 0.56 |
| 1:R:341:SER:HB3 | 1:R:675:GLN:HE22 | 1.69 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:382:THR:HG21 | 1:T:394:SER:H | 1.70 | 0.56 |
| 1:T:557:TYR:HE1 | 1:T:562:LEU:HD11 | 1.70 | 0.56 |
| 1:X:232:ASP:OD1 | 1:X:232:ASP:N | 2.37 | 0.56 |
| 1:Y:329:ASN:CG | 1:Y:330:GLU:OE1 | 2.48 | 0.56 |
| 1:Z:260:GLN:NE2 | 1:Z:276:PHE:HE1 | 2.03 | 0.56 |
| 1:b:241:ILE:HG12 | 1:b:686:GLU:HG3 | 1.87 | 0.56 |
| 1:c:290:PHE:CE2 | 1:c:614:VAL:HB | 2.40 | 0.56 |
| 1:f:329:ASN:CG | 1:f:330:GLU:OE1 | 2.49 | 0.56 |
| 1:g:290:PHE:CE2 | 1:g:614:VAL:HB | 2.40 | 0.56 |
| 1:i:652:LYS:HG2 | 1:i:653:ASN:O | 2.05 | 0.56 |
| 1:j:232:ASP:OD1 | 1:j:232:ASP:N | 2.37 | 0.56 |
| 1:j:290:PHE:CE2 | 1:j:614:VAL:HB | 2.40 | 0.56 |
| 1:j:617:GLN:OE1 | 1:j:617:GLN:N | 2.38 | 0.56 |
| 1:k:557:TYR:HE1 | 1:k:562:LEU:HD11 | 1.70 | 0.56 |
| 1:l:617:GLN:OE1 | 1:l:617:GLN:N | 2.38 | 0.56 |
| 1:m:260:GLN:NE2 | 1:m:276:PHE:HE1 | 2.03 | 0.56 |
| 1:m:382:THR:HG21 | 1:m:394:SER:H | 1.70 | 0.56 |
| 1:n:556:ASP:OD1 | 1:n:557:TYR:N | 2.38 | 0.56 |
| 1:r:329:ASN:CG | 1:r:330:GLU:OE1 | 2.48 | 0.56 |
| 1:s:613:ASP:OD1 | 1:s:732:ARG:CD | 2.52 | 0.56 |
| 1:v:404:GLN:HG2 | 1:v:406:LEU:CD1 | 2.35 | 0.56 |
| 1:w:382:THR:HG21 | 1:w:394:SER:H | 1.70 | 0.56 |
| 1:2:557:TYR:HE1 | 1:2:562:LEU:HD11 | 1.70 | 0.56 |
| 1:4:652:LYS:HG2 | 1:4:653:ASN:O | 2.05 | 0.56 |
| 1:5:241:ILE:HG12 | 1:5:686:GLU:HG3 | 1.87 | 0.56 |
| 1:5:404:GLN:HG2 | 1:5:406:LEU:CD1 | 2.35 | 0.56 |
| 1:7:232:ASP:OD1 | 1:7:232:ASP:N | 2.37 | 0.56 |
| 1:7:652:LYS:HG2 | 1:7:653:ASN:O | 2.05 | 0.56 |
| 1:A:241:ILE:HG12 | 1:A:686:GLU:HG3 | 1.87 | 0.56 |
| 1:A:587:GLN:NE2 | 1:G:498:ASN:OD1 | 2.38 | 0.56 |
| 1:B:623:LYS:HB2 | 1:B:645:PRO:HG3 | 1.88 | 0.56 |
| 1:C:404:GLN:HG2 | 1:C:406:LEU:CD1 | 2.35 | 0.56 |
| 1:C:652:LYS:HG2 | 1:C:653:ASN:O | 2.05 | 0.56 |
| 1:E:232:ASP:OD1 | 1:E:232:ASP:N | 2.37 | 0.56 |
| 1:E:404:GLN:HG2 | 1:E:406:LEU:CD1 | 2.35 | 0.56 |
| 1:G:324:LYS:NZ | 1:G:337:ASN:OD1 | 2.35 | 0.56 |
| 1:G:404:GLN:HG2 | 1:G:406:LEU:CD1 | 2.35 | 0.56 |
| 1:H:329:ASN:CG | 1:H:330:GLU:OE1 | 2.49 | 0.56 |
| 1:H:623:LYS:HB2 | 1:H:645:PRO:HG3 | 1.88 | 0.56 |
| 1:J:652:LYS:HG2 | 1:J:653:ASN:O | 2.05 | 0.56 |
| 1:K:404:GLN:HG2 | 1:K:406:LEU:CD1 | 2.35 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:652:LYS:HG2 | 1:L:653:ASN:O | 2.05 | 0.56 |
| 1:M:260:GLN:NE2 | 1:M:276:PHE:HE1 | 2.03 | 0.56 |
| 1:P:241:ILE:HG12 | 1:P:686:GLU:HG3 | 1.87 | 0.56 |
| 1:Q:557:TYR:HE1 | 1:Q:562:LEU:HD11 | 1.70 | 0.56 |
| 1:R:241:ILE:HG12 | 1:R:686:GLU:HG3 | 1.87 | 0.56 |
| 1:S:260:GLN:NE2 | 1:S:276:PHE:HE1 | 2.03 | 0.56 |
| 1:S:617:GLN:N | 1:S:617:GLN:OE1 | 2.38 | 0.56 |
| 1:T:290:PHE:CE2 | 1:T:614:VAL:HB | 2.40 | 0.56 |
| 1:U:404:GLN:HG2 | 1:U:406:LEU:CD1 | 2.35 | 0.56 |
| 1:V:623:LYS:HB2 | 1:V:645:PRO:HG3 | 1.87 | 0.56 |
| 1:W:329:ASN:CG | 1:W:330:GLU:OE1 | 2.49 | 0.56 |
| 1:X:557:TYR:HE1 | 1:X:562:LEU:HD11 | 1.70 | 0.56 |
| 1:Y:258:TYR:OH | 1:Y:399:GLU:OE1 | 2.22 | 0.56 |
| 1:Y:374:MET:HB2 | 1:4:669:LEU:HD11 | 1.85 | 0.56 |
| 1:Y:623:LYS:HB2 | 1:Y:645:PRO:HG3 | 1.87 | 0.56 |
| 1:Z:382:THR:HG21 | 1:Z:394:SER:H | 1.70 | 0.56 |
| 1:b:326:VAL:HG21 | 1:b:333:LYS:HZ1 | 1.69 | 0.56 |
| 1:b:623:LYS:HB2 | 1:b:645:PRO:HG3 | 1.88 | 0.56 |
| 1:c:404:GLN:HG2 | 1:c:406:LEU:CD1 | 2.35 | 0.56 |
| 1:d:254:ASN:O | 1:d:255:ASN:C | 2.47 | 0.56 |
| 1:d:329:ASN:CG | 1:d:330:GLU:OE1 | 2.49 | 0.56 |
| 1:d:557:TYR:HE1 | 1:d:562:LEU:HD11 | 1.70 | 0.56 |
| 1:f:232:ASP:OD1 | 1:f:232:ASP:N | 2.37 | 0.56 |
| 1:f:556:ASP:OD1 | 1:f:557:TYR:N | 2.38 | 0.56 |
| 1:i:341:SER:HB3 | 1:i:675:GLN:HE22 | 1.69 | 0.56 |
| 1:j:329:ASN:CG | 1:j:330:GLU:OE1 | 2.49 | 0.56 |
| 1:l:556:ASP:OD1 | 1:l:557:TYR:N | 2.38 | 0.56 |
| 1:n:652:LYS:HG2 | 1:n:653:ASN:O | 2.05 | 0.56 |
| 1:q:251:PRO:HB3 | 1:y:660:PRO:HG2 | 1.88 | 0.56 |
| 1:q:329:ASN:CG | 1:q:330:GLU:OE1 | 2.49 | 0.56 |
| 1:r:557:TYR:HE1 | 1:r:562:LEU:HD11 | 1.70 | 0.56 |
| 1:r:623:LYS:HB2 | 1:r:645:PRO:HG3 | 1.87 | 0.56 |
| 1:s:329:ASN:CG | 1:s:330:GLU:OE1 | 2.48 | 0.56 |
| 1:s:382:THR:HG21 | 1:s:394:SER:H | 1.70 | 0.56 |
| 1:s:623:LYS:HB2 | 1:s:645:PRO:HG3 | 1.88 | 0.56 |
| 1:w:290:PHE:CE2 | 1:w:614:VAL:HB | 2.40 | 0.56 |
| 1:w:652:LYS:HG2 | 1:w:653:ASN:O | 2.05 | 0.56 |
| 1:x:557:TYR:HE1 | 1:x:562:LEU:HD11 | 1.70 | 0.56 |
| 1:y:404:GLN:HG2 | 1:y:406:LEU:CD1 | 2.35 | 0.56 |
| 1:z:556:ASP:OD1 | 1:z:557:TYR:N | 2.38 | 0.56 |
| 1:1:382:THR:HG21 | 1:1:394:SER:H | 1.70 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:623:LYS:HB2 | 1:1:645:PRO:HG3 | 1.87 | 0.56 |
| 1:2:324:LYS:NZ | 1:2:337:ASN:OD1 | 2.35 | 0.56 |
| 1:2:329:ASN:CG | 1:2:330:GLU:OE1 | 2.49 | 0.56 |
| 1:3:652:LYS:HG2 | 1:3:653:ASN:O | 2.05 | 0.56 |
| 1:4:290:PHE:CE2 | 1:4:614:VAL:HB | 2.40 | 0.56 |
| 1:4:556:ASP:OD1 | 1:4:557:TYR:N | 2.38 | 0.56 |
| 1:5:557:TYR:HE1 | 1:5:562:LEU:HD11 | 1.70 | 0.56 |
| 1:6:260:GLN:NE2 | 1:6:276:PHE:HE1 | 2.03 | 0.56 |
| 1:7:382:THR:HG21 | 1:7:394:SER:H | 1.70 | 0.56 |
| 1:7:404:GLN:HG2 | 1:7:406:LEU:CD1 | 2.35 | 0.56 |
| 1:8:617:GLN:N | 1:8:617:GLN:OE1 | 2.38 | 0.56 |
| 1:8:652:LYS:HG2 | 1:8:653:ASN:O | 2.05 | 0.56 |
| 1:A:260:GLN:NE2 | 1:A:276:PHE:HE1 | 2.03 | 0.56 |
| 1:A:290:PHE:CE2 | 1:A:614:VAL:HB | 2.40 | 0.56 |
| 1:A:329:ASN:CG | 1:A:330:GLU:OE1 | 2.49 | 0.56 |
| 1:A:556:ASP:OD1 | 1:A:557:TYR:N | 2.38 | 0.56 |
| 1:B:404:GLN:HG2 | 1:B:406:LEU:CD1 | 2.35 | 0.56 |
| 1:C:613:ASP:HB2 | 1:C:731:THR:CG2 | 2.18 | 0.56 |
| 1:E:382:THR:HG21 | 1:E:394:SER:H | 1.70 | 0.56 |
| 1:F:557:TYR:HE1 | 1:F:562:LEU:HD11 | 1.70 | 0.56 |
| 1:G:241:ILE:HG12 | 1:G:686:GLU:HG3 | 1.87 | 0.56 |
| 1:G:382:THR:HG21 | 1:G:394:SER:H | 1.70 | 0.56 |
| 1:H:557:TYR:HE1 | 1:H:562:LEU:HD11 | 1.70 | 0.56 |
| 1:H:613:ASP:OD1 | 1:H:732:ARG:CD | 2.52 | 0.56 |
| 1:I:404:GLN:HG2 | 1:I:406:LEU:CD1 | 2.35 | 0.56 |
| 1:I:557:TYR:HE1 | 1:I:562:LEU:HD11 | 1.70 | 0.56 |
| 1:J:260:GLN:NE2 | 1:J:276:PHE:HE1 | 2.03 | 0.56 |
| 1:J:329:ASN:CG | 1:J:330:GLU:OE1 | 2.49 | 0.56 |
| 1:J:557:TYR:HE1 | 1:J:562:LEU:HD11 | 1.70 | 0.56 |
| 1:L:404:GLN:HG2 | 1:L:406:LEU:CD1 | 2.35 | 0.56 |
| 1:L:613:ASP:HB2 | 1:L:731:THR:CG2 | 2.18 | 0.56 |
| 1:M:241:ILE:HG12 | 1:M:686:GLU:HG3 | 1.87 | 0.56 |
| 1:M:290:PHE:CE2 | 1:M:614:VAL:HB | 2.40 | 0.56 |
| 1:M:341:SER:HB3 | 1:M:675:GLN:HE22 | 1.69 | 0.56 |
| 1:M:382:THR:HG21 | 1:M:394:SER:H | 1.70 | 0.56 |
| 1:M:623:LYS:HB2 | 1:M:645:PRO:HG3 | 1.87 | 0.56 |
| 1:N:241:ILE:HG12 | 1:N:686:GLU:HG3 | 1.87 | 0.56 |
| 1:O:290:PHE:CE2 | 1:O:614:VAL:HB | 2.40 | 0.56 |
| 1:O:556:ASP:OD1 | 1:O:557:TYR:N | 2.38 | 0.56 |
| 1:O:623:LYS:HB2 | 1:O:645:PRO:HG3 | 1.87 | 0.56 |
| 1:O:652:LYS:HG2 | 1:O:653:ASN:O | 2.05 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:290:PHE:CE2 | 1:P:614:VAL:HB | 2.40 | 0.56 |
| 1:P:623:LYS:HB2 | 1:P:645:PRO:HG3 | 1.88 | 0.56 |
| 1:R:260:GLN:NE2 | 1:R:276:PHE:HE1 | 2.03 | 0.56 |
| 1:R:290:PHE:CE2 | 1:R:614:VAL:HB | 2.40 | 0.56 |
| 1:R:623:LYS:HB2 | 1:R:645:PRO:HG3 | 1.87 | 0.56 |
| 1:S:556:ASP:OD1 | 1:S:557:TYR:N | 2.38 | 0.56 |
| 1:T:241:ILE:HG12 | 1:T:686:GLU:HG3 | 1.87 | 0.56 |
| 1:T:587:GLN:NE2 | 1:d:498:ASN:OD1 | 2.39 | 0.56 |
| 1:T:623:LYS:HB2 | 1:T:645:PRO:HG3 | 1.87 | 0.56 |
| 1:V:290:PHE:CE2 | 1:V:614:VAL:HB | 2.40 | 0.56 |
| 1:W:260:GLN:NE2 | 1:W:276:PHE:HE1 | 2.03 | 0.56 |
| 1:X:617:GLN:OE1 | 1:X:617:GLN:N | 2.38 | 0.56 |
| 1:Y:557:TYR:HE1 | 1:Y:562:LEU:HD11 | 1.70 | 0.56 |
| 1:a:241:ILE:HG12 | 1:a:686:GLU:HG3 | 1.87 | 0.56 |
| 1:b:404:GLN:HG2 | 1:b:406:LEU:CD1 | 2.35 | 0.56 |
| 1:c:241:ILE:HG12 | 1:c:686:GLU:HG3 | 1.87 | 0.56 |
| 1:d:241:ILE:HG12 | 1:d:686:GLU:HG3 | 1.87 | 0.56 |
| 1:d:324:LYS:NZ | 1:d:337:ASN:OD1 | 2.35 | 0.56 |
| 1:d:404:GLN:HG2 | 1:d:406:LEU:CD1 | 2.35 | 0.56 |
| 1:d:587:GLN:NE2 | 1:l:498:ASN:OD1 | 2.39 | 0.56 |
| 1:e:382:THR:HG21 | 1:e:394:SER:H | 1.70 | 0.56 |
| 1:e:557:TYR:HE1 | 1:e:562:LEU:HD11 | 1.70 | 0.56 |
| 1:e:652:LYS:HG2 | 1:e:653:ASN:O | 2.05 | 0.56 |
| 1:f:290:PHE:CE2 | 1:f:614:VAL:HB | 2.40 | 0.56 |
| 1:f:404:GLN:HG2 | 1:f:406:LEU:CD1 | 2.35 | 0.56 |
| 1:g:404:GLN:HG2 | 1:g:406:LEU:CD1 | 2.35 | 0.56 |
| 1:g:617:GLN:OE1 | 1:g:617:GLN:N | 2.38 | 0.56 |
| 1:h:404:GLN:HG2 | 1:h:406:LEU:CD1 | 2.35 | 0.56 |
| 1:h:557:TYR:HE1 | 1:h:562:LEU:HD11 | 1.70 | 0.56 |
| 1:h:623:LYS:HB2 | 1:h:645:PRO:HG3 | 1.87 | 0.56 |
| 1:i:290:PHE:CE2 | 1:i:614:VAL:HB | 2.40 | 0.56 |
| 1:i:324:LYS:NZ | 1:i:337:ASN:OD1 | 2.35 | 0.56 |
| 1:i:404:GLN:HG2 | 1:i:406:LEU:CD1 | 2.35 | 0.56 |
| 1:i:617:GLN:N | 1:i:617:GLN:OE1 | 2.38 | 0.56 |
| 1:j:404:GLN:HG2 | 1:j:406:LEU:CD1 | 2.35 | 0.56 |
| 1:j:556:ASP:OD1 | 1:j:557:TYR:N | 2.38 | 0.56 |
| 1:k:404:GLN:HG2 | 1:k:406:LEU:CD1 | 2.35 | 0.56 |
| 1:l:557:TYR:HE1 | 1:l:562:LEU:HD11 | 1.70 | 0.56 |
| 1:n:290:PHE:CE2 | 1:n:614:VAL:HB | 2.40 | 0.56 |
| 1:n:404:GLN:HG2 | 1:n:406:LEU:CD1 | 2.35 | 0.56 |
| 1:n:669:LEU:HD11 | 1:r:374:MET:HB2 | 1.85 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:o:260:GLN:NE2 | 1:o:276:PHE:HE1 | 2.03 | 0.56 |
| 1:o:290:PHE:CE2 | 1:o:614:VAL:HB | 2.40 | 0.56 |
| 1:o:324:LYS:NZ | 1:o:337:ASN:OD1 | 2.35 | 0.56 |
| 1:o:329:ASN:CG | 1:o:330:GLU:OE1 | 2.49 | 0.56 |
| 1:o:556:ASP:OD1 | 1:o:557:TYR:N | 2.38 | 0.56 |
| 1:p:241:ILE:HG12 | 1:p:686:GLU:HG3 | 1.87 | 0.56 |
| 1:p:382:THR:HG21 | 1:p:394:SER:H | 1.70 | 0.56 |
| 1:p:404:GLN:HG2 | 1:p:406:LEU:CD1 | 2.35 | 0.56 |
| 1:p:623:LYS:HB2 | 1:p:645:PRO:HG3 | 1.87 | 0.56 |
| 1:r:258:TYR:OH | 1:r:399:GLU:OE1 | 2.22 | 0.56 |
| 1:r:290:PHE:CE2 | 1:r:614:VAL:HB | 2.40 | 0.56 |
| 1:s:341:SER:HB3 | 1:s:675:GLN:HE22 | 1.69 | 0.56 |
| 1:t:241:ILE:HG12 | 1:t:686:GLU:HG3 | 1.87 | 0.56 |
| 1:u:260:GLN:NE2 | 1:u:276:PHE:HE1 | 2.03 | 0.56 |
| 1:w:557:TYR:HE1 | 1:w:562:LEU:HD11 | 1.70 | 0.56 |
| 1:x:617:GLN:OE1 | 1:x:617:GLN:N | 2.38 | 0.56 |
| 1:y:290:PHE:CE2 | 1:y:614:VAL:HB | 2.40 | 0.56 |
| 1:y:623:LYS:HB2 | 1:y:645:PRO:HG3 | 1.87 | 0.56 |
| 1:z:498:ASN:OD1 | 1:2:587:GLN:NE2 | 2.39 | 0.56 |
| 1:z:617:GLN:OE1 | 1:z:617:GLN:N | 2.38 | 0.56 |
| 1:1:241:ILE:HG12 | 1:1:686:GLU:HG3 | 1.87 | 0.56 |
| 1:1:290:PHE:CE2 | 1:1:614:VAL:HB | 2.40 | 0.56 |
| 1:1:587:GLN:NE2 | 1:2:498:ASN:OD1 | 2.39 | 0.56 |
| 1:2:254:ASN:O | 1:2:255:ASN:C | 2.47 | 0.56 |
| 1:2:404:GLN:HG2 | 1:2:406:LEU:CD1 | 2.35 | 0.56 |
| 1:3:290:PHE:CE2 | 1:3:614:VAL:HB | 2.40 | 0.56 |
| 1:3:556:ASP:OD1 | 1:3:557:TYR:N | 2.38 | 0.56 |
| 1:3:623:LYS:HB2 | 1:3:645:PRO:HG3 | 1.87 | 0.56 |
| 1:6:557:TYR:HE1 | 1:6:562:LEU:HD11 | 1.70 | 0.56 |
| 1:7:623:LYS:HB2 | 1:7:645:PRO:HG3 | 1.87 | 0.56 |
| 1:8:241:ILE:HG12 | 1:8:686:GLU:HG3 | 1.87 | 0.56 |
| 1:8:290:PHE:CE2 | 1:8:614:VAL:HB | 2.40 | 0.56 |
| 1:8:623:LYS:HB2 | 1:8:645:PRO:HG3 | 1.87 | 0.56 |
| 1:A:324:LYS:NZ | 1:A:337:ASN:OD1 | 2.35 | 0.56 |
| 1:C:290:PHE:CE2 | 1:C:614:VAL:HB | 2.40 | 0.56 |
| 1:D:587:GLN:NE2 | 1:N:498:ASN:OD1 | 2.39 | 0.56 |
| 1:G:623:LYS:HB2 | 1:G:645:PRO:HG3 | 1.87 | 0.56 |
| 1:H:324:LYS:NZ | 1:H:337:ASN:OD1 | 2.35 | 0.56 |
| 1:I:241:ILE:HG12 | 1:I:686:GLU:HG3 | 1.87 | 0.56 |
| 1:J:241:ILE:HG12 | 1:J:686:GLU:HG3 | 1.87 | 0.56 |
| 1:J:251:PRO:HB3 | 1:a:660:PRO:HG2 | 1.88 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:382:THR:HG21 | 1:J:394:SER:H | 1.70 | 0.56 |
| 1:J:617:GLN:OE1 | 1:J:617:GLN:N | 2.38 | 0.56 |
| 1:J:623:LYS:HB2 | 1:J:645:PRO:HG3 | 1.87 | 0.56 |
| 1:K:587:GLN:NE2 | 1:a:498:ASN:OD1 | 2.39 | 0.56 |
| 1:L:382:THR:HG21 | 1:L:394:SER:H | 1.70 | 0.56 |
| 1:M:329:ASN:CG | 1:M:330:GLU:OE1 | 2.49 | 0.56 |
| 1:M:617:GLN:OE1 | 1:M:617:GLN:N | 2.38 | 0.56 |
| 1:N:617:GLN:N | 1:N:617:GLN:OE1 | 2.38 | 0.56 |
| 1:S:290:PHE:CE2 | 1:S:614:VAL:HB | 2.40 | 0.56 |
| 1:T:374:MET:HB2 | 1:U:669:LEU:HD11 | 1.86 | 0.56 |
| 1:T:404:GLN:HG2 | 1:T:406:LEU:CD1 | 2.35 | 0.56 |
| 1:W:341:SER:HB3 | 1:W:675:GLN:HE22 | 1.69 | 0.56 |
| 1:Y:290:PHE:CE2 | 1:Y:614:VAL:HB | 2.40 | 0.56 |
| 1:Z:258:TYR:OH | 1:Z:399:GLU:OE1 | 2.22 | 0.56 |
| 1:c:557:TYR:HE1 | 1:c:562:LEU:HD11 | 1.70 | 0.56 |
| 1:e:251:PRO:HB3 | 1:h:660:PRO:HG2 | 1.87 | 0.56 |
| 1:e:329:ASN:CG | 1:e:330:GLU:OE1 | 2.49 | 0.56 |
| 1:f:652:LYS:HG2 | 1:f:653:ASN:O | 2.05 | 0.56 |
| 1:j:652:LYS:HG2 | 1:j:653:ASN:O | 2.05 | 0.56 |
| 1:k:556:ASP:OD1 | 1:k:557:TYR:N | 2.38 | 0.56 |
| 1:k:623:LYS:HB2 | 1:k:645:PRO:HG3 | 1.87 | 0.56 |
| 1:n:382:THR:HG21 | 1:n:394:SER:H | 1.70 | 0.56 |
| 1:p:260:GLN:NE2 | 1:p:276:PHE:HE1 | 2.03 | 0.56 |
| 1:p:324:LYS:NZ | 1:p:337:ASN:OD1 | 2.35 | 0.56 |
| 1:q:232:ASP:OD1 | 1:q:232:ASP:N | 2.37 | 0.56 |
| 1:q:260:GLN:NE2 | 1:q:276:PHE:HE1 | 2.03 | 0.56 |
| 1:t:260:GLN:NE2 | 1:t:276:PHE:HE1 | 2.03 | 0.56 |
| 1:t:290:PHE:CE2 | 1:t:614:VAL:HB | 2.40 | 0.56 |
| 1:t:329:ASN:CG | 1:t:330:GLU:OE1 | 2.48 | 0.56 |
| 1:t:498:ASN:OD1 | 1:v:587:GLN:NE2 | 2.39 | 0.56 |
| 1:t:617:GLN:OE1 | 1:t:617:GLN:N | 2.38 | 0.56 |
| 1:t:623:LYS:HB2 | 1:t:645:PRO:HG3 | 1.87 | 0.56 |
| 1:u:329:ASN:CG | 1:u:330:GLU:OE1 | 2.49 | 0.56 |
| 1:u:556:ASP:OD1 | 1:u:557:TYR:N | 2.38 | 0.56 |
| 1:w:329:ASN:CG | 1:w:330:GLU:OE1 | 2.49 | 0.56 |
| 1:2:617:GLN:OE1 | 1:2:617:GLN:N | 2.38 | 0.56 |
| 1:4:382:THR:HG21 | 1:4:394:SER:H | 1.70 | 0.56 |
| 1:4:404:GLN:HG2 | 1:4:406:LEU:CD1 | 2.35 | 0.56 |
| 1:B:260:GLN:NE2 | 1:B:276:PHE:HE1 | 2.03 | 0.56 |
| 1:B:556:ASP:OD1 | 1:B:557:TYR:N | 2.38 | 0.56 |
| 1:B:587:GLN:NE2 | 1:J:498:ASN:OD1 | 2.39 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:254:ASN:O | 1:C:255:ASN:C | 2.47 | 0.56 |
| 1:C:329:ASN:CG | 1:C:330:GLU:OE1 | 2.48 | 0.56 |
| 1:C:382:THR:HG21 | 1:C:394:SER:H | 1.70 | 0.56 |
| 1:E:254:ASN:O | 1:E:255:ASN:C | 2.47 | 0.56 |
| 1:E:329:ASN:CG | 1:E:330:GLU:OE1 | 2.49 | 0.56 |
| 1:F:251:PRO:HB3 | 1:G:660:PRO:HG2 | 1.88 | 0.56 |
| 1:F:382:THR:HG21 | 1:F:394:SER:H | 1.70 | 0.56 |
| 1:G:254:ASN:O | 1:G:255:ASN:C | 2.47 | 0.56 |
| 1:G:260:GLN:NE2 | 1:G:276:PHE:HE1 | 2.03 | 0.56 |
| 1:I:329:ASN:CG | 1:I:330:GLU:OE1 | 2.49 | 0.56 |
| 1:I:623:LYS:HB2 | 1:I:645:PRO:HG3 | 1.87 | 0.56 |
| 1:J:290:PHE:CE2 | 1:J:614:VAL:HB | 2.40 | 0.56 |
| 1:K:557:TYR:HE1 | 1:K:562:LEU:HD11 | 1.70 | 0.56 |
| 1:L:290:PHE:CE2 | 1:L:614:VAL:HB | 2.40 | 0.56 |
| 1:L:329:ASN:CG | 1:L:330:GLU:OE1 | 2.48 | 0.56 |
| 1:M:251:PRO:HB3 | 1:N:660:PRO:HG2 | 1.88 | 0.56 |
| 1:M:556:ASP:OD1 | 1:M:557:TYR:N | 2.38 | 0.56 |
| 1:M:557:TYR:HE1 | 1:M:562:LEU:HD11 | 1.70 | 0.56 |
| 1:N:613:ASP:OD1 | 1:N:732:ARG:CD | 2.52 | 0.56 |
| 1:O:260:GLN:NE2 | 1:O:276:PHE:HE1 | 2.03 | 0.56 |
| 1:O:374:MET:HB2 | 1:P:669:LEU:HD11 | 1.86 | 0.56 |
| 1:O:587:GLN:NE2 | 1:m:498:ASN:OD1 | 2.39 | 0.56 |
| 1:R:329:ASN:CG | 1:R:330:GLU:OE1 | 2.48 | 0.56 |
| 1:S:329:ASN:CG | 1:S:330:GLU:OE1 | 2.49 | 0.56 |
| 1:T:498:ASN:OD1 | 1:l:587:GLN:NE2 | 2.39 | 0.56 |
| 1:U:329:ASN:CG | 1:U:330:GLU:OE1 | 2.49 | 0.56 |
| 1:V:557:TYR:HE1 | 1:V:562:LEU:HD11 | 1.70 | 0.56 |
| 1:W:232:ASP:OD1 | 1:W:232:ASP:N | 2.37 | 0.56 |
| 1:W:404:GLN:HG2 | 1:W:406:LEU:CD1 | 2.35 | 0.56 |
| 1:X:329:ASN:CG | 1:X:330:GLU:OE1 | 2.49 | 0.56 |
| 1:Y:241:ILE:HG12 | 1:Y:686:GLU:HG3 | 1.87 | 0.56 |
| 1:Z:498:ASN:OD1 | 1:3:587:GLN:NE2 | 2.39 | 0.56 |
| 1:a:260:GLN:NE2 | 1:a:276:PHE:HE1 | 2.03 | 0.56 |
| 1:b:290:PHE:CE2 | 1:b:614:VAL:HB | 2.40 | 0.56 |
| 1:b:556:ASP:OD1 | 1:b:557:TYR:N | 2.38 | 0.56 |
| 1:c:329:ASN:CG | 1:c:330:GLU:OE1 | 2.49 | 0.56 |
| 1:d:260:GLN:NE2 | 1:d:276:PHE:HE1 | 2.03 | 0.56 |
| 1:d:617:GLN:OE1 | 1:d:617:GLN:N | 2.38 | 0.56 |
| 1:f:623:LYS:HB2 | 1:f:645:PRO:HG3 | 1.87 | 0.56 |
| 1:g:557:TYR:HE1 | 1:g:562:LEU:HD11 | 1.70 | 0.56 |
| 1:g:623:LYS:HB2 | 1:g:645:PRO:HG3 | 1.87 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:h:556:ASP:OD1 | 1:h:557:TYR:N | 2.38 | 0.56 |
| 1:j:623:LYS:HB2 | 1:j:645:PRO:HG3 | 1.87 | 0.56 |
| 1:k:324:LYS:NZ | 1:k:337:ASN:OD1 | 2.35 | 0.56 |
| 1:p:660:PRO:HG2 | 1:6:251:PRO:HB3 | 1.88 | 0.56 |
| 1:q:404:GLN:HG2 | 1:q:406:LEU:CD1 | 2.35 | 0.56 |
| 1:r:241:ILE:HG12 | 1:r:686:GLU:HG3 | 1.87 | 0.56 |
| 1:r:260:GLN:NE2 | 1:r:276:PHE:HE1 | 2.03 | 0.56 |
| 1:s:324:LYS:NZ | 1:s:337:ASN:OD1 | 2.35 | 0.56 |
| 1:s:557:TYR:HE1 | 1:s:562:LEU:HD11 | 1.70 | 0.56 |
| 1:v:329:ASN:CG | 1:v:330:GLU:OE1 | 2.49 | 0.56 |
| 1:v:669:LEU:HD11 | 1:1:374:MET:HB2 | 1.86 | 0.56 |
| 1:w:499:ASN:HA | 1:y:589:THR:HA | 1.87 | 0.56 |
| 1:x:260:GLN:NE2 | 1:x:276:PHE:HE1 | 2.03 | 0.56 |
| 1:x:329:ASN:CG | 1:x:330:GLU:OE1 | 2.49 | 0.56 |
| 1:y:557:TYR:HE1 | 1:y:562:LEU:HD11 | 1.70 | 0.56 |
| 1:z:258:TYR:OH | 1:z:399:GLU:OE1 | 2.22 | 0.56 |
| 1:z:557:TYR:HE1 | 1:z:562:LEU:HD11 | 1.70 | 0.56 |
| 1:1:404:GLN:HG2 | 1:1:406:LEU:CD1 | 2.35 | 0.56 |
| 1:2:241:ILE:HG12 | 1:2:686:GLU:HG3 | 1.87 | 0.56 |
| 1:3:374:MET:HB2 | 1:8:669:LEU:HD11 | 1.86 | 0.56 |
| 1:6:241:ILE:HG12 | 1:6:686:GLU:HG3 | 1.87 | 0.56 |
| 1:B:290:PHE:CE2 | 1:B:614:VAL:HB | 2.40 | 0.56 |
| 1:D:557:TYR:HE1 | 1:D:562:LEU:HD11 | 1.70 | 0.56 |
| 1:E:260:GLN:NE2 | 1:E:276:PHE:HE1 | 2.03 | 0.56 |
| 1:F:241:ILE:HG12 | 1:F:686:GLU:HG3 | 1.87 | 0.56 |
| 1:F:329:ASN:CG | 1:F:330:GLU:OE1 | 2.49 | 0.56 |
| 1:G:251:PRO:HB3 | 1:W:660:PRO:HG2 | 1.88 | 0.56 |
| 1:G:290:PHE:CE2 | 1:G:614:VAL:HB | 2.40 | 0.56 |
| 1:H:290:PHE:CE2 | 1:H:614:VAL:HB | 2.40 | 0.56 |
| 1:H:341:SER:HB3 | 1:H:675:GLN:HE22 | 1.69 | 0.56 |
| 1:H:498:ASN:OD1 | 1:Y:587:GLN:NE2 | 2.39 | 0.56 |
| 1:J:556:ASP:OD1 | 1:J:557:TYR:N | 2.38 | 0.56 |
| 1:L:254:ASN:O | 1:L:255:ASN:C | 2.47 | 0.56 |
| 1:L:556:ASP:OD1 | 1:L:557:TYR:N | 2.38 | 0.56 |
| 1:M:498:ASN:OD1 | 1:b:587:GLN:NE2 | 2.39 | 0.56 |
| 1:N:260:GLN:NE2 | 1:N:276:PHE:HE1 | 2.03 | 0.56 |
| 1:O:241:ILE:HG12 | 1:O:686:GLU:HG3 | 1.87 | 0.56 |
| 1:O:322:GLN:NE2 | 1:P:340:THR:HB | 2.10 | 0.56 |
| 1:O:613:ASP:OD1 | 1:O:732:ARG:CD | 2.52 | 0.56 |
| 1:R:498:ASN:OD1 | 1:U:587:GLN:NE2 | 2.39 | 0.56 |
| 1:R:617:GLN:OE1 | 1:R:617:GLN:N | 2.38 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:322:GLN:NE2 | 1:d:340:THR:HB | 2.11 | 0.56 |
| 1:T:251:PRO:HB3 | 1:U:660:PRO:HG2 | 1.88 | 0.56 |
| 1:T:260:GLN:NE2 | 1:T:276:PHE:HE1 | 2.03 | 0.56 |
| 1:V:660:PRO:HG2 | 1:W:251:PRO:HB3 | 1.88 | 0.56 |
| 1:X:290:PHE:CE2 | 1:X:614:VAL:HB | 2.40 | 0.56 |
| 1:Y:251:PRO:HB3 | 1:4:660:PRO:HG2 | 1.88 | 0.56 |
| 1:Y:260:GLN:NE2 | 1:Y:276:PHE:HE1 | 2.03 | 0.56 |
| 1:a:613:ASP:OD1 | 1:a:732:ARG:CD | 2.52 | 0.56 |
| 1:a:617:GLN:N | 1:a:617:GLN:OE1 | 2.38 | 0.56 |
| 1:b:260:GLN:NE2 | 1:b:276:PHE:HE1 | 2.03 | 0.56 |
| 1:c:623:LYS:HB2 | 1:c:645:PRO:HG3 | 1.87 | 0.56 |
| 1:d:589:THR:HA | 1:l:499:ASN:HA | 1.88 | 0.56 |
| 1:d:623:LYS:HB2 | 1:d:645:PRO:HG3 | 1.87 | 0.56 |
| 1:e:232:ASP:OD1 | 1:e:232:ASP:N | 2.37 | 0.56 |
| 1:e:260:GLN:NE2 | 1:e:276:PHE:HE1 | 2.03 | 0.56 |
| 1:g:324:LYS:NZ | 1:g:337:ASN:OD1 | 2.35 | 0.56 |
| 1:g:498:ASN:OD1 | 1:h:587:GLN:NE2 | 2.39 | 0.56 |
| 1:h:324:LYS:NZ | 1:h:337:ASN:OD1 | 2.35 | 0.56 |
| 1:i:254:ASN:O | 1:i:255:ASN:C | 2.47 | 0.56 |
| 1:i:498:ASN:OD1 | 1:k:587:GLN:NE2 | 2.39 | 0.56 |
| 1:i:623:LYS:HB2 | 1:i:645:PRO:HG3 | 1.88 | 0.56 |
| 1:k:382:THR:HG21 | 1:k:394:SER:H | 1.70 | 0.56 |
| 1:l:260:GLN:NE2 | 1:l:276:PHE:HE1 | 2.03 | 0.56 |
| 1:l:329:ASN:CG | 1:l:330:GLU:OE1 | 2.48 | 0.56 |
| 1:m:556:ASP:OD1 | 1:m:557:TYR:N | 2.38 | 0.56 |
| 1:n:660:PRO:HG2 | 1:r:251:PRO:HB3 | 1.88 | 0.56 |
| 1:o:652:LYS:HG2 | 1:o:653:ASN:O | 2.05 | 0.56 |
| 1:p:254:ASN:O | 1:p:255:ASN:C | 2.47 | 0.56 |
| 1:p:290:PHE:CE2 | 1:p:614:VAL:HB | 2.40 | 0.56 |
| 1:q:341:SER:HB3 | 1:q:675:GLN:HE22 | 1.69 | 0.56 |
| 1:u:290:PHE:CE2 | 1:u:614:VAL:HB | 2.40 | 0.56 |
| 1:v:660:PRO:HG2 | 1:1:251:PRO:HB3 | 1.88 | 0.56 |
| 1:w:260:GLN:NE2 | 1:w:276:PHE:HE1 | 2.03 | 0.56 |
| 1:w:613:ASP:OD1 | 1:w:732:ARG:CD | 2.52 | 0.56 |
| 1:z:260:GLN:NE2 | 1:z:276:PHE:HE1 | 2.03 | 0.56 |
| 1:z:499:ASN:HA | 1:2:589:THR:HA | 1.88 | 0.56 |
| 1:z:587:GLN:NE2 | 1:1:498:ASN:OD1 | 2.39 | 0.56 |
| 1:1:260:GLN:NE2 | 1:1:276:PHE:HE1 | 2.03 | 0.56 |
| 1:2:260:GLN:NE2 | 1:2:276:PHE:HE1 | 2.03 | 0.56 |
| 1:2:623:LYS:HB2 | 1:2:645:PRO:HG3 | 1.87 | 0.56 |
| 1:6:382:THR:HG21 | 1:6:394:SER:H | 1.70 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:7:260:GLN:NE2 | 1:7:276:PHE:HE1 | 2.03 | 0.56 |
| 1:7:329:ASN:CG | 1:7:330:GLU:OE1 | 2.49 | 0.56 |
| 1:A:652:LYS:HG2 | 1:A:653:ASN:O | 2.05 | 0.56 |
| 1:B:329:ASN:CG | 1:B:330:GLU:OE1 | 2.49 | 0.56 |
| 1:E:498:ASN:OD1 | 1:F:587:GLN:NE2 | 2.39 | 0.56 |
| 1:I:251:PRO:HB3 | 1:J:660:PRO:HG2 | 1.88 | 0.56 |
| 1:K:290:PHE:CE2 | 1:K:614:VAL:HB | 2.40 | 0.56 |
| 1:L:258:TYR:OH | 1:L:399:GLU:OE1 | 2.22 | 0.56 |
| 1:N:290:PHE:CE2 | 1:N:614:VAL:HB | 2.40 | 0.56 |
| 1:N:382:THR:HG21 | 1:N:394:SER:H | 1.70 | 0.56 |
| 1:O:340:THR:CB | 1:d:322:GLN:HE21 | 2.09 | 0.56 |
| 1:P:329:ASN:CG | 1:P:330:GLU:OE1 | 2.49 | 0.56 |
| 1:Q:652:LYS:HG2 | 1:Q:653:ASN:O | 2.05 | 0.56 |
| 1:T:556:ASP:OD1 | 1:T:557:TYR:N | 2.38 | 0.56 |
| 1:T:652:LYS:HG2 | 1:T:653:ASN:O | 2.05 | 0.56 |
| 1:W:556:ASP:OD1 | 1:W:557:TYR:N | 2.38 | 0.56 |
| 1:X:260:GLN:NE2 | 1:X:276:PHE:HE1 | 2.03 | 0.56 |
| 1:Z:556:ASP:OD1 | 1:Z:557:TYR:N | 2.38 | 0.56 |
| 1:d:232:ASP:OD1 | 1:d:232:ASP:N | 2.37 | 0.56 |
| 1:e:613:ASP:OD1 | 1:e:732:ARG:CD | 2.52 | 0.56 |
| 1:f:254:ASN:O | 1:f:255:ASN:C | 2.47 | 0.56 |
| 1:f:498:ASN:OD1 | 1:g:587:GLN:NE2 | 2.39 | 0.56 |
| 1:h:258:TYR:OH | 1:h:399:GLU:OE1 | 2.22 | 0.56 |
| 1:h:382:THR:HG21 | 1:h:394:SER:H | 1.70 | 0.56 |
| 1:i:587:GLN:NE2 | 1:j:498:ASN:OD1 | 2.39 | 0.56 |
| 1:j:254:ASN:O | 1:j:255:ASN:C | 2.47 | 0.56 |
| 1:l:258:TYR:OH | 1:l:399:GLU:OE1 | 2.22 | 0.56 |
| 1:l:404:GLN:HG2 | 1:l:406:LEU:CD1 | 2.35 | 0.56 |
| 1:m:329:ASN:CG | 1:m:330:GLU:OE1 | 2.48 | 0.56 |
| 1:o:587:GLN:NE2 | 1:p:498:ASN:OD1 | 2.39 | 0.56 |
| 1:p:251:PRO:HB3 | 1:q:660:PRO:HG2 | 1.88 | 0.56 |
| 1:q:290:PHE:CE2 | 1:q:614:VAL:HB | 2.40 | 0.56 |
| 1:r:587:GLN:NE2 | 1:s:498:ASN:OD1 | 2.39 | 0.56 |
| 1:s:290:PHE:CE2 | 1:s:614:VAL:HB | 2.40 | 0.56 |
| 1:x:290:PHE:CE2 | 1:x:614:VAL:HB | 2.40 | 0.56 |
| 1:3:241:ILE:HG12 | 1:3:686:GLU:HG3 | 1.87 | 0.56 |
| 1:3:260:GLN:NE2 | 1:3:276:PHE:HE1 | 2.03 | 0.56 |
| 1:3:322:GLN:NE2 | 1:8:340:THR:HB | 2.10 | 0.56 |
| 1:6:329:ASN:CG | 1:6:330:GLU:OE1 | 2.49 | 0.56 |
| 1:6:587:GLN:NE2 | 1:7:498:ASN:OD1 | 2.39 | 0.56 |
| 1:7:254:ASN:O | 1:7:255:ASN:C | 2.47 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:8:329:ASN:CG | 1:8:330:GLU:OE1 | 2.48 | 0.56 |
| 1:8:556:ASP:OD1 | 1:8:557:TYR:N | 2.38 | 0.56 |
| 1:A:382:THR:HG21 | 1:A:394:SER:H | 1.70 | 0.56 |
| 1:A:404:GLN:HG2 | 1:A:406:LEU:CD1 | 2.35 | 0.56 |
| 1:B:382:THR:HG21 | 1:B:394:SER:H | 1.70 | 0.56 |
| 1:B:660:PRO:HG2 | 1:C:251:PRO:HB3 | 1.88 | 0.56 |
| 1:C:258:TYR:OH | 1:C:399:GLU:OE1 | 2.22 | 0.56 |
| 1:C:499:ASN:HA | 1:M:589:THR:HA | 1.88 | 0.56 |
| 1:D:290:PHE:CE2 | 1:D:614:VAL:HB | 2.40 | 0.56 |
| 1:G:587:GLN:NE2 | 1:I:498:ASN:OD1 | 2.39 | 0.56 |
| 1:J:589:THR:HA | 1:L:499:ASN:HA | 1.88 | 0.56 |
| 1:M:660:PRO:HG2 | 1:c:251:PRO:HB3 | 1.88 | 0.56 |
| 1:N:329:ASN:CG | 1:N:330:GLU:OE1 | 2.48 | 0.56 |
| 1:P:556:ASP:OD1 | 1:P:557:TYR:N | 2.38 | 0.56 |
| 1:R:404:GLN:HG2 | 1:R:406:LEU:CD1 | 2.35 | 0.56 |
| 1:V:329:ASN:CG | 1:V:330:GLU:OE1 | 2.48 | 0.56 |
| 1:W:290:PHE:CE2 | 1:W:614:VAL:HB | 2.40 | 0.56 |
| 1:Z:329:ASN:CG | 1:Z:330:GLU:OE1 | 2.48 | 0.56 |
| 1:Z:587:GLN:NE2 | 1:4:498:ASN:OD1 | 2.39 | 0.56 |
| 1:a:290:PHE:CE2 | 1:a:614:VAL:HB | 2.40 | 0.56 |
| 1:a:382:THR:HG21 | 1:a:394:SER:H | 1.70 | 0.56 |
| 1:b:329:ASN:CG | 1:b:330:GLU:OE1 | 2.49 | 0.56 |
| 1:c:498:ASN:OD1 | 1:p:587:GLN:NE2 | 2.39 | 0.56 |
| 1:g:254:ASN:O | 1:g:255:ASN:C | 2.47 | 0.56 |
| 1:i:557:TYR:HE1 | 1:i:562:LEU:HD11 | 1.70 | 0.56 |
| 1:j:251:PRO:HB3 | 1:x:660:PRO:HG2 | 1.87 | 0.56 |
| 1:m:652:LYS:HG2 | 1:m:653:ASN:O | 2.05 | 0.56 |
| 1:r:652:LYS:HG2 | 1:r:653:ASN:O | 2.05 | 0.56 |
| 1:s:652:LYS:HG2 | 1:s:653:ASN:O | 2.05 | 0.56 |
| 1:t:669:LEU:HD11 | 1:y:374:MET:HB2 | 1.88 | 0.56 |
| 1:v:251:PRO:HB3 | 1:w:660:PRO:HG2 | 1.87 | 0.56 |
| 1:v:652:LYS:HG2 | 1:v:653:ASN:O | 2.05 | 0.56 |
| 1:w:623:LYS:HB2 | 1:w:645:PRO:HG3 | 1.87 | 0.56 |
| 1:y:329:ASN:CG | 1:y:330:GLU:OE1 | 2.49 | 0.56 |
| 1:y:613:ASP:OD1 | 1:y:732:ARG:CD | 2.52 | 0.56 |
| 1:z:329:ASN:CG | 1:z:330:GLU:OE1 | 2.49 | 0.56 |
| 1:z:404:GLN:HG2 | 1:z:406:LEU:CD1 | 2.35 | 0.56 |
| 1:1:556:ASP:OD1 | 1:1:557:TYR:N | 2.38 | 0.56 |
| 1:1:652:LYS:HG2 | 1:1:653:ASN:O | 2.05 | 0.56 |
| 1:2:232:ASP:OD1 | 1:2:232:ASP:N | 2.37 | 0.56 |
| 1:2:290:PHE:CE2 | 1:2:614:VAL:HB | 2.40 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:613:ASP:OD1 | 1:3:732:ARG:CD | 2.52 | 0.56 |
| 1:C:623:LYS:HB2 | 1:C:645:PRO:HG3 | 1.87 | 0.56 |
| 1:D:652:LYS:HG2 | 1:D:653:ASN:O | 2.05 | 0.56 |
| 1:H:652:LYS:HG2 | 1:H:653:ASN:O | 2.05 | 0.56 |
| 1:I:258:TYR:OH | 1:I:399:GLU:OE1 | 2.22 | 0.56 |
| 1:J:254:ASN:O | 1:J:255:ASN:C | 2.47 | 0.56 |
| 1:J:587:GLN:NE2 | 1:L:498:ASN:OD1 | 2.39 | 0.56 |
| 1:K:556:ASP:OD1 | 1:K:557:TYR:N | 2.38 | 0.56 |
| 1:K:652:LYS:HG2 | 1:K:653:ASN:O | 2.05 | 0.56 |
| 1:L:251:PRO:HB3 | 1:b:660:PRO:HG2 | 1.88 | 0.56 |
| 1:L:557:TYR:HE1 | 1:L:562:LEU:HD11 | 1.70 | 0.56 |
| 1:L:623:LYS:HB2 | 1:L:645:PRO:HG3 | 1.87 | 0.56 |
| 1:P:404:GLN:HG2 | 1:P:406:LEU:CD1 | 2.35 | 0.56 |
| 1:S:404:GLN:HG2 | 1:S:406:LEU:CD1 | 2.35 | 0.56 |
| 1:U:652:LYS:HG2 | 1:U:653:ASN:O | 2.05 | 0.56 |
| 1:X:404:GLN:HG2 | 1:X:406:LEU:CD1 | 2.35 | 0.56 |
| 1:X:556:ASP:OD1 | 1:X:557:TYR:N | 2.38 | 0.56 |
| 1:Y:556:ASP:OD1 | 1:Y:557:TYR:N | 2.38 | 0.56 |
| 1:Z:652:LYS:HG2 | 1:Z:653:ASN:O | 2.05 | 0.56 |
| 1:a:329:ASN:CG | 1:a:330:GLU:OE1 | 2.49 | 0.56 |
| 1:c:556:ASP:OD1 | 1:c:557:TYR:N | 2.38 | 0.56 |
| 1:d:290:PHE:CE2 | 1:d:614:VAL:HB | 2.40 | 0.56 |
| 1:e:404:GLN:HG2 | 1:e:406:LEU:CD1 | 2.35 | 0.56 |
| 1:e:623:LYS:HB2 | 1:e:645:PRO:HG3 | 1.87 | 0.56 |
| 1:h:329:ASN:CG | 1:h:330:GLU:OE1 | 2.48 | 0.56 |
| 1:k:241:ILE:HG12 | 1:k:686:GLU:HG3 | 1.87 | 0.56 |
| 1:m:290:PHE:CE2 | 1:m:614:VAL:HB | 2.40 | 0.56 |
| 1:m:587:GLN:NE2 | 1:n:498:ASN:OD1 | 2.39 | 0.56 |
| 1:o:382:THR:HG21 | 1:o:394:SER:H | 1.70 | 0.56 |
| 1:o:404:GLN:HG2 | 1:o:406:LEU:CD1 | 2.35 | 0.56 |
| 1:q:556:ASP:OD1 | 1:q:557:TYR:N | 2.38 | 0.56 |
| 1:r:556:ASP:OD1 | 1:r:557:TYR:N | 2.38 | 0.56 |
| 1:r:617:GLN:OE1 | 1:r:617:GLN:N | 2.38 | 0.56 |
| 1:t:404:GLN:HG2 | 1:t:406:LEU:CD1 | 2.35 | 0.56 |
| 1:u:404:GLN:HG2 | 1:u:406:LEU:CD1 | 2.35 | 0.56 |
| 1:w:241:ILE:HG12 | 1:w:686:GLU:HG3 | 1.87 | 0.56 |
| 1:w:404:GLN:HG2 | 1:w:406:LEU:CD1 | 2.35 | 0.56 |
| 1:2:251:PRO:HB3 | 1:3:660:PRO:HG2 | 1.88 | 0.56 |
| 1:6:290:PHE:CE2 | 1:6:614:VAL:HB | 2.40 | 0.56 |
| 1:6:652:LYS:HG2 | 1:6:653:ASN:O | 2.05 | 0.56 |
| 1:7:290:PHE:CE2 | 1:7:614:VAL:HB | 2.40 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:8:254:ASN:O | 1:8:255:ASN:C | 2.47 | 0.56 |
| 1:8:404:GLN:HG2 | 1:8:406:LEU:CD1 | 2.35 | 0.56 |
| 1:B:617:GLN:OE1 | 1:B:617:GLN:N | 2.38 | 0.56 |
| 1:C:498:ASN:OD1 | 1:M:587:GLN:NE2 | 2.39 | 0.56 |
| 1:C:557:TYR:HE1 | 1:C:562:LEU:HD11 | 1.70 | 0.56 |
| 1:D:241:ILE:HG12 | 1:D:686:GLU:HG3 | 1.87 | 0.56 |
| 1:D:556:ASP:OD1 | 1:D:557:TYR:N | 2.38 | 0.56 |
| 1:E:290:PHE:CE2 | 1:E:614:VAL:HB | 2.40 | 0.56 |
| 1:E:557:TYR:HE1 | 1:E:562:LEU:HD11 | 1.70 | 0.56 |
| 1:F:290:PHE:CE2 | 1:F:614:VAL:HB | 2.40 | 0.56 |
| 1:F:556:ASP:OD1 | 1:F:557:TYR:N | 2.38 | 0.56 |
| 1:G:556:ASP:OD1 | 1:G:557:TYR:N | 2.38 | 0.56 |
| 1:I:556:ASP:OD1 | 1:I:557:TYR:N | 2.38 | 0.56 |
| 1:M:254:ASN:O | 1:M:255:ASN:C | 2.47 | 0.56 |
| 1:O:498:ASN:OD1 | 1:n:587:GLN:NE2 | 2.39 | 0.56 |
| 1:O:660:PRO:HG2 | 1:d:251:PRO:HB3 | 1.88 | 0.56 |
| 1:P:254:ASN:O | 1:P:255:ASN:C | 2.47 | 0.56 |
| 1:Q:329:ASN:CG | 1:Q:330:GLU:OE1 | 2.48 | 0.56 |
| 1:S:557:TYR:HE1 | 1:S:562:LEU:HD11 | 1.70 | 0.56 |
| 1:U:254:ASN:O | 1:U:255:ASN:C | 2.47 | 0.56 |
| 1:U:258:TYR:OH | 1:U:399:GLU:OE1 | 2.22 | 0.56 |
| 1:V:589:THR:HA | 1:e:499:ASN:HA | 1.87 | 0.56 |
| 1:V:613:ASP:OD1 | 1:V:732:ARG:CD | 2.52 | 0.56 |
| 1:X:407:ARG:HD3 | 1:f:224:SER:O | 2.06 | 0.56 |
| 1:Y:652:LYS:HG2 | 1:Y:653:ASN:O | 2.05 | 0.56 |
| 1:b:382:THR:HG21 | 1:b:394:SER:H | 1.70 | 0.56 |
| 1:h:241:ILE:HG12 | 1:h:686:GLU:HG3 | 1.87 | 0.56 |
| 1:j:224:SER:O | 1:x:407:ARG:HD3 | 2.06 | 0.56 |
| 1:k:617:GLN:OE1 | 1:k:617:GLN:N | 2.38 | 0.56 |
| 1:l:660:PRO:HG2 | 1:n:251:PRO:HB3 | 1.88 | 0.56 |
| 1:n:623:LYS:HB2 | 1:n:645:PRO:HG3 | 1.88 | 0.56 |
| 1:v:324:LYS:NZ | 1:v:337:ASN:OD1 | 2.35 | 0.56 |
| 1:x:404:GLN:HG2 | 1:x:406:LEU:CD1 | 2.35 | 0.56 |
| 1:x:556:ASP:OD1 | 1:x:557:TYR:N | 2.38 | 0.56 |
| 1:z:254:ASN:O | 1:z:255:ASN:C | 2.47 | 0.56 |
| 1:z:290:PHE:CE2 | 1:z:614:VAL:HB | 2.40 | 0.56 |
| 1:3:404:GLN:HG2 | 1:3:406:LEU:CD1 | 2.35 | 0.56 |
| 1:3:498:ASN:OD1 | 1:4:587:GLN:NE2 | 2.39 | 0.56 |
| 1:4:329:ASN:CG | 1:4:330:GLU:OE1 | 2.49 | 0.56 |
| 1:4:623:LYS:HB2 | 1:4:645:PRO:HG3 | 1.88 | 0.56 |
| 1:5:258:TYR:OH | 1:5:399:GLU:OE1 | 2.22 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:623:LYS:HB2 | 1:5:645:PRO:HG3 | 1.87 | 0.56 |
| 1:5:652:LYS:HG2 | 1:5:653:ASN:O | 2.05 | 0.56 |
| 1:C:660:PRO:HG2 | 1:D:251:PRO:HB3 | 1.87 | 0.55 |
| 1:D:329:ASN:CG | 1:D:330:GLU:OE1 | 2.49 | 0.55 |
| 1:D:660:PRO:HG2 | 1:E:251:PRO:HB3 | 1.88 | 0.55 |
| 1:E:241:ILE:HG12 | 1:E:686:GLU:HG3 | 1.87 | 0.55 |
| 1:E:587:GLN:NE2 | 1:Q:498:ASN:OD1 | 2.39 | 0.55 |
| 1:F:652:LYS:HG2 | 1:F:653:ASN:O | 2.05 | 0.55 |
| 1:F:660:PRO:HG2 | 1:R:251:PRO:HB3 | 1.88 | 0.55 |
| 1:K:329:ASN:CG | 1:K:330:GLU:OE1 | 2.49 | 0.55 |
| 1:N:557:TYR:HE1 | 1:N:562:LEU:HD11 | 1.70 | 0.55 |
| 1:N:587:GLN:NE2 | 1:P:498:ASN:OD1 | 2.39 | 0.55 |
| 1:O:251:PRO:HB3 | 1:P:660:PRO:HG2 | 1.88 | 0.55 |
| 1:O:404:GLN:HG2 | 1:O:406:LEU:CD1 | 2.35 | 0.55 |
| 1:Q:623:LYS:HB2 | 1:Q:645:PRO:HG3 | 1.87 | 0.55 |
| 1:R:324:LYS:NZ | 1:R:337:ASN:OD1 | 2.35 | 0.55 |
| 1:U:324:LYS:NZ | 1:U:337:ASN:OD1 | 2.35 | 0.55 |
| 1:X:499:ASN:HA | 1:e:589:THR:HA | 1.88 | 0.55 |
| 1:Z:290:PHE:CE2 | 1:Z:614:VAL:HB | 2.40 | 0.55 |
| 1:a:587:GLN:NE2 | 1:8:498:ASN:OD1 | 2.39 | 0.55 |
| 1:c:258:TYR:OH | 1:c:399:GLU:OE1 | 2.22 | 0.55 |
| 1:e:241:ILE:HG12 | 1:e:686:GLU:HG3 | 1.87 | 0.55 |
| 1:h:260:GLN:NE2 | 1:h:276:PHE:HE1 | 2.03 | 0.55 |
| 1:h:617:GLN:OE1 | 1:h:617:GLN:N | 2.38 | 0.55 |
| 1:k:329:ASN:CG | 1:k:330:GLU:OE1 | 2.49 | 0.55 |
| 1:l:290:PHE:CE2 | 1:l:614:VAL:HB | 2.40 | 0.55 |
| 1:l:382:THR:HG21 | 1:l:394:SER:H | 1.70 | 0.55 |
| 1:l:623:LYS:HB2 | 1:l:645:PRO:HG3 | 1.87 | 0.55 |
| 1:m:232:ASP:OD1 | 1:m:232:ASP:N | 2.37 | 0.55 |
| 1:n:329:ASN:CG | 1:n:330:GLU:OE1 | 2.48 | 0.55 |
| 1:p:556:ASP:OD1 | 1:p:557:TYR:N | 2.38 | 0.55 |
| 1:q:324:LYS:NZ | 1:q:337:ASN:OD1 | 2.35 | 0.55 |
| 1:s:556:ASP:OD1 | 1:s:557:TYR:N | 2.38 | 0.55 |
| 1:t:251:PRO:HB3 | 1:6:660:PRO:HG2 | 1.88 | 0.55 |
| 1:u:613:ASP:OD1 | 1:u:732:ARG:CD | 2.52 | 0.55 |
| 1:v:258:TYR:OH | 1:v:399:GLU:OE1 | 2.22 | 0.55 |
| 1:v:557:TYR:HE1 | 1:v:562:LEU:HD11 | 1.70 | 0.55 |
| 1:z:382:THR:HG21 | 1:z:394:SER:H | 1.70 | 0.55 |
| 1:z:623:LYS:HB2 | 1:z:645:PRO:HG3 | 1.87 | 0.55 |
| 1:z:660:PRO:HG2 | 1:4:251:PRO:HB3 | 1.88 | 0.55 |
| 1:2:322:GLN:HE21 | 1:3:340:THR:CB | 2.09 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:251:PRO:HB3 | 1:8:660:PRO:HG2 | 1.88 | 0.55 |
| 1:5:329:ASN:CG | 1:5:330:GLU:OE1 | 2.48 | 0.55 |
| 1:6:404:GLN:HE21 | 1:6:406:LEU:HD11 | 1.67 | 0.55 |
| 1:6:556:ASP:OD1 | 1:6:557:TYR:N | 2.38 | 0.55 |
| 1:7:556:ASP:OD1 | 1:7:557:TYR:N | 2.38 | 0.55 |
| 1:7:557:TYR:HE1 | 1:7:562:LEU:HD11 | 1.70 | 0.55 |
| 1:D:499:ASN:HA | 1:P:589:THR:HA | 1.87 | 0.55 |
| 1:D:589:THR:HA | 1:N:499:ASN:HA | 1.88 | 0.55 |
| 1:D:617:GLN:OE1 | 1:D:617:GLN:N | 2.38 | 0.55 |
| 1:E:499:ASN:HA | 1:F:589:THR:HA | 1.88 | 0.55 |
| 1:E:556:ASP:OD1 | 1:E:557:TYR:N | 2.38 | 0.55 |
| 1:E:589:THR:HA | 1:Q:499:ASN:HA | 1.89 | 0.55 |
| 1:H:254:ASN:O | 1:H:255:ASN:C | 2.47 | 0.55 |
| 1:H:556:ASP:OD1 | 1:H:557:TYR:N | 2.38 | 0.55 |
| 1:K:251:PRO:HB3 | 1:L:660:PRO:HG2 | 1.87 | 0.55 |
| 1:K:499:ASN:HA | 1:8:589:THR:HA | 1.87 | 0.55 |
| 1:K:589:THR:HA | 1:a:499:ASN:HA | 1.88 | 0.55 |
| 1:K:660:PRO:HG2 | 1:7:251:PRO:HB3 | 1.88 | 0.55 |
| 1:N:556:ASP:OD1 | 1:N:557:TYR:N | 2.38 | 0.55 |
| 1:P:260:GLN:NE2 | 1:P:276:PHE:HE1 | 2.03 | 0.55 |
| 1:Q:251:PRO:HB3 | 1:S:660:PRO:HG2 | 1.88 | 0.55 |
| 1:Q:258:TYR:OH | 1:Q:399:GLU:OE1 | 2.22 | 0.55 |
| 1:S:613:ASP:OD1 | 1:S:732:ARG:CD | 2.52 | 0.55 |
| 1:T:660:PRO:HG2 | 1:i:251:PRO:HB3 | 1.88 | 0.55 |
| 1:V:498:ASN:OD1 | 1:X:587:GLN:NE2 | 2.39 | 0.55 |
| 1:a:556:ASP:OD1 | 1:a:557:TYR:N | 2.38 | 0.55 |
| 1:b:617:GLN:OE1 | 1:b:617:GLN:N | 2.38 | 0.55 |
| 1:g:251:PRO:HB3 | 1:1:660:PRO:HG2 | 1.88 | 0.55 |
| 1:g:382:THR:HG21 | 1:g:394:SER:H | 1.70 | 0.55 |
| 1:l:241:ILE:HG12 | 1:l:686:GLU:HG3 | 1.87 | 0.55 |
| 1:l:254:ASN:O | 1:l:255:ASN:C | 2.47 | 0.55 |
| 1:u:557:TYR:HE1 | 1:u:562:LEU:HD11 | 1.70 | 0.55 |
| 1:v:254:ASN:O | 1:v:255:ASN:C | 2.47 | 0.55 |
| 1:z:241:ILE:HG12 | 1:z:686:GLU:HG3 | 1.87 | 0.55 |
| 1:5:498:ASN:OD1 | 1:7:587:GLN:NE2 | 2.39 | 0.55 |
| 1:5:499:ASN:HA | 1:7:589:THR:HA | 1.89 | 0.55 |
| 1:6:589:THR:HA | 1:7:499:ASN:HA | 1.89 | 0.55 |
| 1:7:241:ILE:HG12 | 1:7:686:GLU:HG3 | 1.87 | 0.55 |
| 1:A:499:ASN:HA | 1:I:589:THR:HA | 1.88 | 0.55 |
| 1:A:660:PRO:HG2 | 1:B:251:PRO:HB3 | 1.88 | 0.55 |
| 1:F:404:GLN:HG2 | 1:F:406:LEU:CD1 | 2.35 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:241:ILE:HG12 | 1:K:686:GLU:HG3 | 1.87 | 0.55 |
| 1:K:617:GLN:N | 1:K:617:GLN:OE1 | 2.38 | 0.55 |
| 1:N:404:GLN:HG2 | 1:N:406:LEU:CD1 | 2.35 | 0.55 |
| 1:R:254:ASN:O | 1:R:255:ASN:C | 2.47 | 0.55 |
| 1:R:587:GLN:NE2 | 1:S:498:ASN:OD1 | 2.39 | 0.55 |
| 1:U:556:ASP:OD1 | 1:U:557:TYR:N | 2.38 | 0.55 |
| 1:X:652:LYS:HG2 | 1:X:653:ASN:O | 2.05 | 0.55 |
| 1:X:660:PRO:HG2 | 1:f:251:PRO:HB3 | 1.88 | 0.55 |
| 1:Y:617:GLN:N | 1:Y:617:GLN:OE1 | 2.38 | 0.55 |
| 1:a:404:GLN:HG2 | 1:a:406:LEU:CD1 | 2.35 | 0.55 |
| 1:a:557:TYR:HE1 | 1:a:562:LEU:HD11 | 1.70 | 0.55 |
| 1:c:589:THR:HA | 1:o:499:ASN:HA | 1.88 | 0.55 |
| 1:c:652:LYS:HG2 | 1:c:653:ASN:O | 2.05 | 0.55 |
| 1:f:587:GLN:NE2 | 1:h:498:ASN:OD1 | 2.39 | 0.55 |
| 1:f:589:THR:HA | 1:h:499:ASN:HA | 1.88 | 0.55 |
| 1:k:260:GLN:NE2 | 1:k:276:PHE:HE1 | 2.03 | 0.55 |
| 1:p:329:ASN:CG | 1:p:330:GLU:OE1 | 2.49 | 0.55 |
| 1:r:660:PRO:HG2 | 1:x:251:PRO:HB3 | 1.87 | 0.55 |
| 1:u:660:PRO:HG2 | 1:5:251:PRO:HB3 | 1.88 | 0.55 |
| 1:w:556:ASP:OD1 | 1:w:557:TYR:N | 2.38 | 0.55 |
| 1:z:589:THR:HA | 1:1:499:ASN:HA | 1.88 | 0.55 |
| 1:5:587:GLN:NE2 | 1:6:498:ASN:OD1 | 2.39 | 0.55 |
| 1:D:260:GLN:NE2 | 1:D:276:PHE:HE1 | 2.03 | 0.55 |
| 1:G:258:TYR:OH | 1:G:399:GLU:OE1 | 2.22 | 0.55 |
| 1:S:254:ASN:O | 1:S:255:ASN:C | 2.47 | 0.55 |
| 1:T:499:ASN:HA | 1:l:589:THR:HA | 1.88 | 0.55 |
| 1:U:251:PRO:HB3 | 1:e:660:PRO:HG2 | 1.88 | 0.55 |
| 1:U:557:TYR:HE1 | 1:U:562:LEU:HD11 | 1.70 | 0.55 |
| 1:U:623:LYS:HB2 | 1:U:645:PRO:HG3 | 1.87 | 0.55 |
| 1:V:556:ASP:OD1 | 1:V:557:TYR:N | 2.38 | 0.55 |
| 1:W:324:LYS:NZ | 1:W:337:ASN:OD1 | 2.35 | 0.55 |
| 1:X:251:PRO:HB3 | 1:Y:660:PRO:HG2 | 1.87 | 0.55 |
| 1:X:623:LYS:HB2 | 1:X:645:PRO:HG3 | 1.87 | 0.55 |
| 1:Z:232:ASP:OD1 | 1:Z:232:ASP:N | 2.37 | 0.55 |
| 1:b:251:PRO:HB3 | 1:o:660:PRO:HG2 | 1.88 | 0.55 |
| 1:e:556:ASP:OD1 | 1:e:557:TYR:N | 2.38 | 0.55 |
| 1:h:224:SER:O | 1:i:407:ARG:HD3 | 2.07 | 0.55 |
| 1:i:382:THR:HG21 | 1:i:394:SER:H | 1.70 | 0.55 |
| 1:j:241:ILE:HG12 | 1:j:686:GLU:HG3 | 1.87 | 0.55 |
| 1:m:589:THR:HA | 1:n:499:ASN:HA | 1.88 | 0.55 |
| 1:s:254:ASN:O | 1:s:255:ASN:C | 2.47 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:s:404:GLN:HG2 | 1:s:406:LEU:CD1 | 2.35 | 0.55 |
| 1:t:587:GLN:NE2 | 1:u:498:ASN:OD1 | 2.39 | 0.55 |
| 1:v:623:LYS:HB2 | 1:v:645:PRO:HG3 | 1.87 | 0.55 |
| 1:x:589:THR:HA | 1:y:499:ASN:HA | 1.88 | 0.55 |
| 1:x:652:LYS:HG2 | 1:x:653:ASN:O | 2.05 | 0.55 |
| 1:y:556:ASP:OD1 | 1:y:557:TYR:N | 2.38 | 0.55 |
| 1:6:404:GLN:HG2 | 1:6:406:LEU:CD1 | 2.35 | 0.55 |
| 1:6:623:LYS:HB2 | 1:6:645:PRO:HG3 | 1.87 | 0.55 |
| 1:7:613:ASP:OD1 | 1:7:732:ARG:CD | 2.52 | 0.55 |
| 1:8:260:GLN:NE2 | 1:8:276:PHE:HE1 | 2.03 | 0.55 |
| 1:E:613:ASP:OD1 | 1:E:732:ARG:CD | 2.52 | 0.55 |
| 1:F:498:ASN:OD1 | 1:Q:587:GLN:NE2 | 2.39 | 0.55 |
| 1:G:329:ASN:CG | 1:G:330:GLU:OE1 | 2.49 | 0.55 |
| 1:H:404:GLN:HG2 | 1:H:406:LEU:CD1 | 2.35 | 0.55 |
| 1:I:652:LYS:HG2 | 1:I:653:ASN:O | 2.05 | 0.55 |
| 1:K:260:GLN:NE2 | 1:K:276:PHE:HE1 | 2.03 | 0.55 |
| 1:N:322:GLN:HE21 | 1:m:340:THR:CB | 2.08 | 0.55 |
| 1:Q:382:THR:HG21 | 1:Q:394:SER:H | 1.70 | 0.55 |
| 1:R:407:ARG:HD3 | 1:V:224:SER:O | 2.06 | 0.55 |
| 1:S:251:PRO:HB3 | 1:d:660:PRO:HG2 | 1.88 | 0.55 |
| 1:U:382:THR:HG21 | 1:U:394:SER:H | 1.70 | 0.55 |
| 1:V:499:ASN:HA | 1:X:589:THR:HA | 1.88 | 0.55 |
| 1:W:587:GLN:NE2 | 1:Y:498:ASN:OD1 | 2.39 | 0.55 |
| 1:Y:224:SER:O | 1:4:407:ARG:HD3 | 2.07 | 0.55 |
| 1:Z:589:THR:HA | 1:4:499:ASN:HA | 1.88 | 0.55 |
| 1:c:499:ASN:HA | 1:p:589:THR:HA | 1.88 | 0.55 |
| 1:g:407:ARG:HD3 | 1:k:224:SER:O | 2.07 | 0.55 |
| 1:g:556:ASP:OD1 | 1:g:557:TYR:N | 2.38 | 0.55 |
| 1:j:587:GLN:NE2 | 1:k:498:ASN:OD1 | 2.39 | 0.55 |
| 1:n:407:ARG:HD3 | 1:r:224:SER:O | 2.07 | 0.55 |
| 1:q:587:GLN:NE2 | 1:r:498:ASN:OD1 | 2.39 | 0.55 |
| 1:r:613:ASP:OD1 | 1:r:732:ARG:CD | 2.52 | 0.55 |
| 1:t:254:ASN:O | 1:t:255:ASN:C | 2.47 | 0.55 |
| 1:t:324:LYS:NZ | 1:t:337:ASN:OD1 | 2.35 | 0.55 |
| 1:u:251:PRO:HB3 | 1:2:660:PRO:HG2 | 1.88 | 0.55 |
| 1:u:254:ASN:O | 1:u:255:ASN:C | 2.47 | 0.55 |
| 1:1:232:ASP:OD1 | 1:1:232:ASP:N | 2.37 | 0.55 |
| 1:5:329:ASN:OD1 | 1:5:330:GLU:OE1 | 2.25 | 0.55 |
| 1:5:382:THR:HG21 | 1:5:394:SER:H | 1.70 | 0.55 |
| 1:B:329:ASN:OD1 | 1:B:330:GLU:OE1 | 2.25 | 0.55 |
| 1:B:557:TYR:HE1 | 1:B:562:LEU:HD11 | 1.70 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:589:THR:HA | 1:I:499:ASN:HA | 1.88 | 0.55 |
| 1:H:251:PRO:HB3 | 1:I:660:PRO:HG2 | 1.88 | 0.55 |
| 1:O:329:ASN:CG | 1:O:330:GLU:OE1 | 2.49 | 0.55 |
| 1:O:329:ASN:OD1 | 1:O:330:GLU:OE1 | 2.25 | 0.55 |
| 1:Q:329:ASN:OD1 | 1:Q:330:GLU:OE1 | 2.25 | 0.55 |
| 1:T:232:ASP:OD1 | 1:T:232:ASP:N | 2.37 | 0.55 |
| 1:U:329:ASN:OD1 | 1:U:330:GLU:OE1 | 2.25 | 0.55 |
| 1:X:241:ILE:HG12 | 1:X:686:GLU:HG3 | 1.87 | 0.55 |
| 1:X:498:ASN:OD1 | 1:e:587:GLN:NE2 | 2.39 | 0.55 |
| 1:b:329:ASN:OD1 | 1:b:330:GLU:OE1 | 2.25 | 0.55 |
| 1:c:660:PRO:HG2 | 1:s:251:PRO:HB3 | 1.88 | 0.55 |
| 1:o:254:ASN:O | 1:o:255:ASN:C | 2.47 | 0.55 |
| 1:p:258:TYR:OH | 1:p:399:GLU:OE1 | 2.22 | 0.55 |
| 1:q:589:THR:HA | 1:r:499:ASN:HA | 1.88 | 0.55 |
| 1:s:329:ASN:OD1 | 1:s:330:GLU:OE1 | 2.25 | 0.55 |
| 1:t:499:ASN:HA | 1:v:589:THR:HA | 1.88 | 0.55 |
| 1:v:329:ASN:OD1 | 1:v:330:GLU:OE1 | 2.25 | 0.55 |
| 1:v:556:ASP:OD1 | 1:v:557:TYR:N | 2.38 | 0.55 |
| 1:3:329:ASN:CG | 1:3:330:GLU:OE1 | 2.49 | 0.55 |
| 1:3:329:ASN:OD1 | 1:3:330:GLU:OE1 | 2.25 | 0.55 |
| 1:A:224:SER:O | 1:E:407:ARG:HD3 | 2.07 | 0.55 |
| 1:A:254:ASN:O | 1:A:255:ASN:C | 2.47 | 0.55 |
| 1:C:587:GLN:NE2 | 1:b:498:ASN:OD1 | 2.39 | 0.55 |
| 1:D:407:ARG:HD3 | 1:E:224:SER:O | 2.07 | 0.55 |
| 1:F:623:LYS:HB2 | 1:F:645:PRO:HG3 | 1.87 | 0.55 |
| 1:H:329:ASN:OD1 | 1:H:330:GLU:OE1 | 2.25 | 0.55 |
| 1:N:251:PRO:HB3 | 1:m:660:PRO:HG2 | 1.87 | 0.55 |
| 1:P:329:ASN:OD1 | 1:P:330:GLU:OE1 | 2.25 | 0.55 |
| 1:R:499:ASN:HA | 1:U:589:THR:HA | 1.89 | 0.55 |
| 1:T:329:ASN:OD1 | 1:T:330:GLU:OE1 | 2.25 | 0.55 |
| 1:U:224:SER:O | 1:e:407:ARG:HD3 | 2.07 | 0.55 |
| 1:V:329:ASN:OD1 | 1:V:330:GLU:OE1 | 2.25 | 0.55 |
| 1:W:382:THR:HG21 | 1:W:394:SER:H | 1.70 | 0.55 |
| 1:f:241:ILE:HG12 | 1:f:686:GLU:HG3 | 1.87 | 0.55 |
| 1:f:660:PRO:HG2 | 1:z:251:PRO:HB3 | 1.88 | 0.55 |
| 1:g:660:PRO:HG2 | 1:k:251:PRO:HB3 | 1.88 | 0.55 |
| 1:h:251:PRO:HB3 | 1:i:660:PRO:HG2 | 1.88 | 0.55 |
| 1:i:556:ASP:OD1 | 1:i:557:TYR:N | 2.38 | 0.55 |
| 1:j:589:THR:HA | 1:k:499:ASN:HA | 1.89 | 0.55 |
| 1:p:322:GLN:NE2 | 1:q:340:THR:HB | 2.11 | 0.55 |
| 1:q:623:LYS:HB2 | 1:q:645:PRO:HG3 | 1.87 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:r:329:ASN:OD1 | 1:r:330:GLU:OE1 | 2.25 | 0.55 |
| 1:r:404:GLN:HG2 | 1:r:406:LEU:CD1 | 2.35 | 0.55 |
| 1:y:329:ASN:OD1 | 1:y:330:GLU:OE1 | 2.25 | 0.55 |
| 1:1:329:ASN:OD1 | 1:1:330:GLU:OE1 | 2.25 | 0.55 |
| 1:8:258:TYR:OH | 1:8:399:GLU:OE1 | 2.22 | 0.55 |
| 1:8:329:ASN:OD1 | 1:8:330:GLU:OE1 | 2.25 | 0.55 |
| 1:B:498:ASN:OD1 | 1:L:587:GLN:NE2 | 2.39 | 0.55 |
| 1:F:499:ASN:HA | 1:Q:589:THR:HA | 1.88 | 0.55 |
| 1:H:660:PRO:HG2 | 1:Z:251:PRO:HB3 | 1.88 | 0.55 |
| 1:J:324:LYS:NZ | 1:J:337:ASN:OD1 | 2.35 | 0.55 |
| 1:K:407:ARG:HD3 | 1:7:224:SER:O | 2.07 | 0.55 |
| 1:Q:224:SER:O | 1:S:407:ARG:HD3 | 2.07 | 0.55 |
| 1:T:329:ASN:CG | 1:T:330:GLU:OE1 | 2.49 | 0.55 |
| 1:V:258:TYR:OH | 1:V:399:GLU:OE1 | 2.22 | 0.55 |
| 1:W:589:THR:HA | 1:Y:499:ASN:HA | 1.88 | 0.55 |
| 1:Y:329:ASN:OD1 | 1:Y:330:GLU:OE1 | 2.25 | 0.55 |
| 1:Y:404:GLN:HG2 | 1:Y:406:LEU:CD1 | 2.35 | 0.55 |
| 1:Y:613:ASP:OD1 | 1:Y:732:ARG:CD | 2.52 | 0.55 |
| 1:Z:660:PRO:HG2 | 1:a:251:PRO:HB3 | 1.87 | 0.55 |
| 1:b:557:TYR:HE1 | 1:b:562:LEU:HD11 | 1.70 | 0.55 |
| 1:j:660:PRO:HG2 | 1:l:251:PRO:HB3 | 1.88 | 0.55 |
| 1:m:251:PRO:HB3 | 1:s:660:PRO:HG2 | 1.88 | 0.55 |
| 1:o:623:LYS:HB2 | 1:o:645:PRO:HG3 | 1.87 | 0.55 |
| 1:p:224:SER:O | 1:q:407:ARG:HD3 | 2.07 | 0.55 |
| 1:u:407:ARG:HD3 | 1:5:224:SER:O | 2.07 | 0.55 |
| 1:v:382:THR:HG21 | 1:v:394:SER:H | 1.70 | 0.55 |
| 1:w:329:ASN:OD1 | 1:w:330:GLU:OE1 | 2.25 | 0.55 |
| 1:x:241:ILE:HG12 | 1:x:686:GLU:HG3 | 1.87 | 0.55 |
| 1:x:623:LYS:HB2 | 1:x:645:PRO:HG3 | 1.87 | 0.55 |
| 1:y:241:ILE:HG12 | 1:y:686:GLU:HG3 | 1.87 | 0.55 |
| 1:y:258:TYR:OH | 1:y:399:GLU:OE1 | 2.22 | 0.55 |
| 1:1:329:ASN:CG | 1:1:330:GLU:OE1 | 2.49 | 0.55 |
| 1:2:556:ASP:OD1 | 1:2:557:TYR:N | 2.38 | 0.55 |
| 1:5:589:THR:HA | 1:6:499:ASN:HA | 1.88 | 0.55 |
| 1:C:329:ASN:OD1 | 1:C:330:GLU:OE1 | 2.25 | 0.55 |
| 1:G:224:SER:O | 1:W:407:ARG:HD3 | 2.07 | 0.55 |
| 1:H:260:GLN:NE2 | 1:H:276:PHE:HE1 | 2.03 | 0.55 |
| 1:H:587:GLN:NE2 | 1:W:498:ASN:OD1 | 2.39 | 0.55 |
| 1:K:329:ASN:OD1 | 1:K:330:GLU:OE1 | 2.25 | 0.55 |
| 1:N:224:SER:O | 1:m:407:ARG:HD3 | 2.07 | 0.55 |
| 1:V:241:ILE:HG12 | 1:V:686:GLU:HG3 | 1.87 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:258:TYR:OH | 1:W:399:GLU:OE1 | 2.22 | 0.55 |
| 1:W:623:LYS:HB2 | 1:W:645:PRO:HG3 | 1.87 | 0.55 |
| 1:Z:407:ARG:HD3 | 1:a:224:SER:O | 2.07 | 0.55 |
| 1:Z:623:LYS:HB2 | 1:Z:645:PRO:HG3 | 1.87 | 0.55 |
| 1:a:623:LYS:HB2 | 1:a:645:PRO:HG3 | 1.87 | 0.55 |
| 1:c:587:GLN:NE2 | 1:o:498:ASN:OD1 | 2.39 | 0.55 |
| 1:d:258:TYR:OH | 1:d:399:GLU:OE1 | 2.22 | 0.55 |
| 1:i:329:ASN:CG | 1:i:330:GLU:OE1 | 2.49 | 0.55 |
| 1:q:382:THR:HG21 | 1:q:394:SER:H | 1.70 | 0.55 |
| 1:q:498:ASN:OD1 | 1:s:587:GLN:NE2 | 2.40 | 0.55 |
| 1:5:407:ARG:HD3 | 1:8:224:SER:O | 2.06 | 0.55 |
| 1:A:498:ASN:OD1 | 1:I:587:GLN:NE2 | 2.39 | 0.55 |
| 1:A:623:LYS:HB2 | 1:A:645:PRO:HG3 | 1.87 | 0.55 |
| 1:B:499:ASN:HA | 1:L:589:THR:HA | 1.88 | 0.55 |
| 1:D:329:ASN:OD1 | 1:D:330:GLU:OE1 | 2.25 | 0.55 |
| 1:I:340:THR:CB | 1:I:407:ARG:HH21 | 2.20 | 0.55 |
| 1:J:224:SER:O | 1:a:407:ARG:HD3 | 2.06 | 0.55 |
| 1:L:329:ASN:OD1 | 1:L:330:GLU:OE1 | 2.25 | 0.55 |
| 1:N:589:THR:HA | 1:P:499:ASN:HA | 1.88 | 0.55 |
| 1:N:623:LYS:HB2 | 1:N:645:PRO:HG3 | 1.87 | 0.55 |
| 1:P:224:SER:O | 1:Q:407:ARG:HD3 | 2.06 | 0.55 |
| 1:P:258:TYR:OH | 1:P:399:GLU:OE1 | 2.22 | 0.55 |
| 1:S:587:GLN:NE2 | 1:U:498:ASN:OD1 | 2.39 | 0.55 |
| 1:T:589:THR:HA | 1:d:499:ASN:HA | 1.88 | 0.55 |
| 1:a:589:THR:HA | 1:8:499:ASN:HA | 1.88 | 0.55 |
| 1:b:324:LYS:NZ | 1:b:337:ASN:OD1 | 2.35 | 0.55 |
| 1:c:340:THR:CB | 1:c:407:ARG:HH21 | 2.20 | 0.55 |
| 1:d:556:ASP:OD1 | 1:d:557:TYR:N | 2.38 | 0.55 |
| 1:e:329:ASN:OD1 | 1:e:330:GLU:OE1 | 2.25 | 0.55 |
| 1:f:499:ASN:HA | 1:g:589:THR:HA | 1.89 | 0.55 |
| 1:g:329:ASN:CG | 1:g:330:GLU:OE1 | 2.49 | 0.55 |
| 1:g:329:ASN:OD1 | 1:g:330:GLU:OE1 | 2.25 | 0.55 |
| 1:g:499:ASN:HA | 1:h:589:THR:HA | 1.88 | 0.55 |
| 1:i:499:ASN:HA | 1:k:589:THR:HA | 1.88 | 0.55 |
| 1:m:623:LYS:HB2 | 1:m:645:PRO:HG3 | 1.87 | 0.55 |
| 1:s:260:GLN:NE2 | 1:s:276:PHE:HE1 | 2.03 | 0.55 |
| 1:w:324:LYS:NZ | 1:w:337:ASN:OD1 | 2.35 | 0.55 |
| 1:1:589:THR:HA | 1:2:499:ASN:HA | 1.88 | 0.55 |
| 1:6:329:ASN:OD1 | 1:6:330:GLU:OE1 | 2.25 | 0.55 |
| 1:C:589:THR:HA | 1:b:499:ASN:HA | 1.88 | 0.54 |
| 1:F:329:ASN:OD1 | 1:F:330:GLU:OE1 | 2.25 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:322:GLN:NE2 | 1:W:340:THR:HB | 2.11 | 0.54 |
| 1:J:258:TYR:OH | 1:J:399:GLU:OE1 | 2.22 | 0.54 |
| 1:M:224:SER:O | 1:N:407:ARG:HD3 | 2.06 | 0.54 |
| 1:M:329:ASN:OD1 | 1:M:330:GLU:OE1 | 2.25 | 0.54 |
| 1:P:251:PRO:HB3 | 1:Q:660:PRO:HG2 | 1.88 | 0.54 |
| 1:Q:714:ASP:HB3 | 1:Q:726:PRO:HG3 | 1.90 | 0.54 |
| 1:R:556:ASP:OD1 | 1:R:557:TYR:N | 2.38 | 0.54 |
| 1:V:407:ARG:HD3 | 1:W:224:SER:O | 2.08 | 0.54 |
| 1:X:254:ASN:O | 1:X:255:ASN:C | 2.47 | 0.54 |
| 1:a:329:ASN:OD1 | 1:a:330:GLU:OE1 | 2.25 | 0.54 |
| 1:i:329:ASN:OD1 | 1:i:330:GLU:OE1 | 2.25 | 0.54 |
| 1:i:589:THR:HA | 1:j:499:ASN:HA | 1.89 | 0.54 |
| 1:q:258:TYR:OH | 1:q:399:GLU:OE1 | 2.22 | 0.54 |
| 1:s:714:ASP:HB3 | 1:s:726:PRO:HG3 | 1.90 | 0.54 |
| 1:u:324:LYS:NZ | 1:u:337:ASN:OD1 | 2.35 | 0.54 |
| 1:u:587:GLN:NE2 | 1:v:498:ASN:OD1 | 2.39 | 0.54 |
| 1:w:592:GLY:HA2 | 1:x:499:ASN:HD22 | 1.72 | 0.54 |
| 1:2:258:TYR:OH | 1:2:399:GLU:OE1 | 2.22 | 0.54 |
| 1:5:714:ASP:HB3 | 1:5:726:PRO:HG3 | 1.90 | 0.54 |
| 1:B:324:LYS:NZ | 1:B:337:ASN:OD1 | 2.35 | 0.54 |
| 1:C:340:THR:CB | 1:C:407:ARG:HH21 | 2.20 | 0.54 |
| 1:C:407:ARG:HD3 | 1:D:224:SER:O | 2.07 | 0.54 |
| 1:J:329:ASN:OD1 | 1:J:330:GLU:OE1 | 2.25 | 0.54 |
| 1:K:224:SER:O | 1:L:407:ARG:HD3 | 2.07 | 0.54 |
| 1:L:340:THR:CB | 1:L:407:ARG:HH21 | 2.20 | 0.54 |
| 1:N:329:ASN:OD1 | 1:N:330:GLU:OE1 | 2.25 | 0.54 |
| 1:X:714:ASP:HB3 | 1:X:726:PRO:HG3 | 1.90 | 0.54 |
| 1:c:714:ASP:HB3 | 1:c:726:PRO:HG3 | 1.90 | 0.54 |
| 1:e:324:LYS:NZ | 1:e:337:ASN:OD1 | 2.35 | 0.54 |
| 1:o:714:ASP:HB3 | 1:o:726:PRO:HG3 | 1.90 | 0.54 |
| 1:t:556:ASP:OD1 | 1:t:557:TYR:N | 2.38 | 0.54 |
| 1:u:623:LYS:HB2 | 1:u:645:PRO:HG3 | 1.87 | 0.54 |
| 1:x:254:ASN:O | 1:x:255:ASN:C | 2.47 | 0.54 |
| 1:x:714:ASP:HB3 | 1:x:726:PRO:HG3 | 1.90 | 0.54 |
| 1:y:382:THR:HG21 | 1:y:394:SER:H | 1.70 | 0.54 |
| 1:3:499:ASN:HA | 1:4:589:THR:HA | 1.89 | 0.54 |
| 1:A:589:THR:HA | 1:G:499:ASN:HA | 1.88 | 0.54 |
| 1:A:714:ASP:HB3 | 1:A:726:PRO:HG3 | 1.90 | 0.54 |
| 1:B:714:ASP:HB3 | 1:B:726:PRO:HG3 | 1.90 | 0.54 |
| 1:E:340:THR:CB | 1:E:407:ARG:HH21 | 2.21 | 0.54 |
| 1:H:714:ASP:HB3 | 1:H:726:PRO:HG3 | 1.90 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:714:ASP:HB3 | 1:I:726:PRO:HG3 | 1.90 | 0.54 |
| 1:O:499:ASN:HA | 1:n:589:THR:HA | 1.89 | 0.54 |
| 1:R:660:PRO:HG2 | 1:V:251:PRO:HB3 | 1.88 | 0.54 |
| 1:S:623:LYS:HB2 | 1:S:645:PRO:HG3 | 1.87 | 0.54 |
| 1:T:714:ASP:HB3 | 1:T:726:PRO:HG3 | 1.90 | 0.54 |
| 1:V:382:THR:HG21 | 1:V:394:SER:H | 1.70 | 0.54 |
| 1:t:714:ASP:HB3 | 1:t:726:PRO:HG3 | 1.89 | 0.54 |
| 1:z:324:LYS:NZ | 1:z:337:ASN:OD1 | 2.35 | 0.54 |
| 1:1:714:ASP:HB3 | 1:1:726:PRO:HG3 | 1.90 | 0.54 |
| 1:5:660:PRO:HG2 | 1:8:251:PRO:HB3 | 1.88 | 0.54 |
| 1:7:340:THR:CB | 1:7:407:ARG:HH21 | 2.20 | 0.54 |
| 1:C:714:ASP:HB3 | 1:C:726:PRO:HG3 | 1.90 | 0.54 |
| 1:L:224:SER:O | 1:b:407:ARG:HD3 | 2.07 | 0.54 |
| 1:M:258:TYR:OH | 1:M:399:GLU:OE1 | 2.22 | 0.54 |
| 1:R:714:ASP:HB3 | 1:R:726:PRO:HG3 | 1.90 | 0.54 |
| 1:W:254:ASN:O | 1:W:255:ASN:C | 2.47 | 0.54 |
| 1:Z:714:ASP:HB3 | 1:Z:726:PRO:HG3 | 1.89 | 0.54 |
| 1:b:714:ASP:HB3 | 1:b:726:PRO:HG3 | 1.90 | 0.54 |
| 1:k:329:ASN:OD1 | 1:k:330:GLU:OE1 | 2.25 | 0.54 |
| 1:l:340:THR:CB | 1:l:407:ARG:HH21 | 2.20 | 0.54 |
| 1:m:224:SER:O | 1:s:407:ARG:HD3 | 2.07 | 0.54 |
| 1:w:340:THR:CB | 1:w:407:ARG:HH21 | 2.20 | 0.54 |
| 1:B:407:ARG:HD3 | 1:C:224:SER:O | 2.07 | 0.54 |
| 1:D:714:ASP:HB3 | 1:D:726:PRO:HG3 | 1.90 | 0.54 |
| 1:H:224:SER:O | 1:I:407:ARG:HD3 | 2.08 | 0.54 |
| 1:L:714:ASP:HB3 | 1:L:726:PRO:HG3 | 1.90 | 0.54 |
| 1:N:714:ASP:HB3 | 1:N:726:PRO:HG3 | 1.90 | 0.54 |
| 1:O:407:ARG:HD3 | 1:d:224:SER:O | 2.07 | 0.54 |
| 1:S:324:LYS:NZ | 1:S:337:ASN:OD1 | 2.35 | 0.54 |
| 1:S:714:ASP:HB3 | 1:S:726:PRO:HG3 | 1.90 | 0.54 |
| 1:T:340:THR:CB | 1:T:407:ARG:HH21 | 2.20 | 0.54 |
| 1:a:714:ASP:HB3 | 1:a:726:PRO:HG3 | 1.90 | 0.54 |
| 1:c:407:ARG:HD3 | 1:s:224:SER:O | 2.08 | 0.54 |
| 1:d:714:ASP:HB3 | 1:d:726:PRO:HG3 | 1.90 | 0.54 |
| 1:h:329:ASN:OD1 | 1:h:330:GLU:OE1 | 2.25 | 0.54 |
| 1:k:660:PRO:HG2 | 1:w:251:PRO:HB3 | 1.89 | 0.54 |
| 1:l:329:ASN:OD1 | 1:l:330:GLU:OE1 | 2.25 | 0.54 |
| 1:n:714:ASP:HB3 | 1:n:726:PRO:HG3 | 1.90 | 0.54 |
| 1:1:340:THR:CB | 1:1:407:ARG:HH21 | 2.20 | 0.54 |
| 1:2:714:ASP:HB3 | 1:2:726:PRO:HG3 | 1.90 | 0.54 |
| 1:4:714:ASP:HB3 | 1:4:726:PRO:HG3 | 1.90 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:407:ARG:HD3 | 1:Z:224:SER:O | 2.07 | 0.54 |
| 1:H:499:ASN:HA | 1:Y:589:THR:HA | 1.88 | 0.54 |
| 1:V:714:ASP:HB3 | 1:V:726:PRO:HG3 | 1.90 | 0.54 |
| 1:X:329:ASN:OD1 | 1:X:330:GLU:OE1 | 2.25 | 0.54 |
| 1:e:340:THR:CB | 1:e:407:ARG:HH21 | 2.21 | 0.54 |
| 1:l:324:LYS:NZ | 1:l:337:ASN:OD1 | 2.35 | 0.54 |
| 1:l:407:ARG:HD3 | 1:n:224:SER:O | 2.08 | 0.54 |
| 1:q:329:ASN:OD1 | 1:q:330:GLU:OE1 | 2.25 | 0.54 |
| 1:u:714:ASP:HB3 | 1:u:726:PRO:HG3 | 1.90 | 0.54 |
| 1:x:340:THR:CB | 1:x:407:ARG:HH21 | 2.21 | 0.54 |
| 1:z:329:ASN:OD1 | 1:z:330:GLU:OE1 | 2.25 | 0.54 |
| 1:z:340:THR:CB | 1:z:407:ARG:HH21 | 2.21 | 0.54 |
| 1:z:407:ARG:HD3 | 1:4:224:SER:O | 2.08 | 0.54 |
| 1:3:340:THR:CB | 1:3:407:ARG:HH21 | 2.20 | 0.54 |
| 1:5:340:THR:CB | 1:5:407:ARG:HH21 | 2.21 | 0.54 |
| 1:8:324:LYS:NZ | 1:8:337:ASN:OD1 | 2.35 | 0.54 |
| 1:A:258:TYR:OH | 1:A:399:GLU:OE1 | 2.22 | 0.54 |
| 1:G:340:THR:CB | 1:G:407:ARG:HH21 | 2.20 | 0.54 |
| 1:O:340:THR:CB | 1:O:407:ARG:HH21 | 2.20 | 0.54 |
| 1:P:324:LYS:NZ | 1:P:337:ASN:OD1 | 2.35 | 0.54 |
| 1:Q:340:THR:CB | 1:Q:407:ARG:HH21 | 2.21 | 0.54 |
| 1:W:329:ASN:OD1 | 1:W:330:GLU:OE1 | 2.25 | 0.54 |
| 1:X:340:THR:CB | 1:X:407:ARG:HH21 | 2.20 | 0.54 |
| 1:m:714:ASP:HB3 | 1:m:726:PRO:HG3 | 1.90 | 0.54 |
| 1:q:254:ASN:O | 1:q:255:ASN:C | 2.47 | 0.54 |
| 1:x:329:ASN:OD1 | 1:x:330:GLU:OE1 | 2.25 | 0.54 |
| 1:2:224:SER:O | 1:3:407:ARG:HD3 | 2.07 | 0.54 |
| 1:A:251:PRO:HB3 | 1:E:660:PRO:HG2 | 1.88 | 0.54 |
| 1:A:329:ASN:OD1 | 1:A:330:GLU:OE1 | 2.25 | 0.54 |
| 1:A:340:THR:CB | 1:A:407:ARG:HH21 | 2.20 | 0.54 |
| 1:B:232:ASP:N | 1:B:232:ASP:OD1 | 2.37 | 0.54 |
| 1:K:714:ASP:HB3 | 1:K:726:PRO:HG3 | 1.90 | 0.54 |
| 1:R:329:ASN:OD1 | 1:R:330:GLU:OE1 | 2.25 | 0.54 |
| 1:f:329:ASN:OD1 | 1:f:330:GLU:OE1 | 2.25 | 0.54 |
| 1:o:224:SER:O | 1:7:407:ARG:HD3 | 2.08 | 0.54 |
| 1:o:329:ASN:OD1 | 1:o:330:GLU:OE1 | 2.25 | 0.54 |
| 1:o:340:THR:CB | 1:o:407:ARG:HH21 | 2.20 | 0.54 |
| 1:p:340:THR:CB | 1:p:407:ARG:HH21 | 2.20 | 0.54 |
| 1:r:589:THR:HA | 1:s:499:ASN:HA | 1.89 | 0.54 |
| 1:t:329:ASN:OD1 | 1:t:330:GLU:OE1 | 2.25 | 0.54 |
| 1:u:589:THR:HA | 1:v:499:ASN:HA | 1.88 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:y:714:ASP:HB3 | 1:y:726:PRO:HG3 | 1.90 | 0.54 |
| 1:1:324:LYS:NZ | 1:1:337:ASN:OD1 | 2.35 | 0.54 |
| 1:G:714:ASP:HB3 | 1:G:726:PRO:HG3 | 1.90 | 0.54 |
| 1:M:324:LYS:NZ | 1:M:337:ASN:OD1 | 2.35 | 0.54 |
| 1:R:589:THR:HA | 1:S:499:ASN:HA | 1.88 | 0.54 |
| 1:S:589:THR:HA | 1:U:499:ASN:HA | 1.89 | 0.54 |
| 1:T:324:LYS:NZ | 1:T:337:ASN:OD1 | 2.35 | 0.54 |
| 1:W:714:ASP:HB3 | 1:W:726:PRO:HG3 | 1.90 | 0.54 |
| 1:X:324:LYS:NZ | 1:X:337:ASN:OD1 | 2.35 | 0.54 |
| 1:b:254:ASN:O | 1:b:255:ASN:C | 2.47 | 0.54 |
| 1:j:407:ARG:HD3 | 1:l:224:SER:O | 2.08 | 0.54 |
| 1:m:329:ASN:OD1 | 1:m:330:GLU:OE1 | 2.25 | 0.54 |
| 1:o:251:PRO:HB3 | 1:7:660:PRO:HG2 | 1.88 | 0.54 |
| 1:G:329:ASN:OD1 | 1:G:330:GLU:OE1 | 2.25 | 0.54 |
| 1:J:340:THR:CB | 1:J:407:ARG:HH21 | 2.21 | 0.54 |
| 1:M:340:THR:CB | 1:M:407:ARG:HH21 | 2.21 | 0.54 |
| 1:X:224:SER:O | 1:Y:407:ARG:HD3 | 2.07 | 0.54 |
| 1:c:382:THR:HG21 | 1:c:394:SER:H | 1.70 | 0.54 |
| 1:d:329:ASN:OD1 | 1:d:330:GLU:OE1 | 2.25 | 0.54 |
| 1:g:714:ASP:HB3 | 1:g:726:PRO:HG3 | 1.90 | 0.54 |
| 1:j:329:ASN:OD1 | 1:j:330:GLU:OE1 | 2.25 | 0.54 |
| 1:p:714:ASP:HB3 | 1:p:726:PRO:HG3 | 1.90 | 0.54 |
| 1:q:714:ASP:HB3 | 1:q:726:PRO:HG3 | 1.90 | 0.54 |
| 1:2:329:ASN:OD1 | 1:2:330:GLU:OE1 | 2.25 | 0.54 |
| 1:B:589:THR:HA | 1:J:499:ASN:HA | 1.89 | 0.53 |
| 1:I:382:THR:HG21 | 1:I:394:SER:H | 1.70 | 0.53 |
| 1:M:232:ASP:OD1 | 1:M:232:ASP:N | 2.37 | 0.53 |
| 1:O:224:SER:O | 1:P:407:ARG:HD3 | 2.08 | 0.53 |
| 1:R:434:ASP:OD1 | 1:R:434:ASP:N | 2.41 | 0.53 |
| 1:T:224:SER:O | 1:U:407:ARG:HD3 | 2.08 | 0.53 |
| 1:T:340:THR:CB | 1:T:407:ARG:NH2 | 2.72 | 0.53 |
| 1:Z:329:ASN:OD1 | 1:Z:330:GLU:OE1 | 2.25 | 0.53 |
| 1:b:232:ASP:N | 1:b:232:ASP:OD1 | 2.37 | 0.53 |
| 1:i:714:ASP:HB3 | 1:i:726:PRO:HG3 | 1.90 | 0.53 |
| 1:t:589:THR:HA | 1:u:499:ASN:HA | 1.89 | 0.53 |
| 1:u:224:SER:O | 1:2:407:ARG:HD3 | 2.08 | 0.53 |
| 1:u:329:ASN:OD1 | 1:u:330:GLU:OE1 | 2.25 | 0.53 |
| 1:1:340:THR:CB | 1:1:407:ARG:NH2 | 2.72 | 0.53 |
| 1:8:340:THR:CB | 1:8:407:ARG:NH2 | 2.72 | 0.53 |
| 1:B:254:ASN:O | 1:B:255:ASN:C | 2.47 | 0.53 |
| 1:E:329:ASN:OD1 | 1:E:330:GLU:OE1 | 2.25 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:322:GLN:NE2 | 1:I:340:THR:HB | 2.11 | 0.53 |
| 1:M:499:ASN:HA | 1:b:589:THR:HA | 1.89 | 0.53 |
| 1:M:714:ASP:HB3 | 1:M:726:PRO:HG3 | 1.90 | 0.53 |
| 1:N:340:THR:CB | 1:N:407:ARG:NH2 | 2.72 | 0.53 |
| 1:O:714:ASP:HB3 | 1:O:726:PRO:HG3 | 1.90 | 0.53 |
| 1:P:340:THR:CB | 1:P:407:ARG:NH2 | 2.72 | 0.53 |
| 1:Q:340:THR:CB | 1:Q:407:ARG:NH2 | 2.72 | 0.53 |
| 1:S:224:SER:O | 1:d:407:ARG:HD3 | 2.08 | 0.53 |
| 1:S:329:ASN:OD1 | 1:S:330:GLU:OE1 | 2.25 | 0.53 |
| 1:Y:324:LYS:NZ | 1:Y:337:ASN:OD1 | 2.35 | 0.53 |
| 1:a:340:THR:CB | 1:a:407:ARG:NH2 | 2.72 | 0.53 |
| 1:a:340:THR:CB | 1:a:407:ARG:HH21 | 2.20 | 0.53 |
| 1:h:340:THR:CB | 1:h:407:ARG:NH2 | 2.71 | 0.53 |
| 1:n:329:ASN:OD1 | 1:n:330:GLU:OE1 | 2.25 | 0.53 |
| 1:o:589:THR:HA | 1:p:499:ASN:HA | 1.88 | 0.53 |
| 1:p:329:ASN:OD1 | 1:p:330:GLU:OE1 | 2.25 | 0.53 |
| 1:r:407:ARG:HD3 | 1:x:224:SER:O | 2.08 | 0.53 |
| 1:s:232:ASP:OD1 | 1:s:232:ASP:N | 2.37 | 0.53 |
| 1:v:407:ARG:HD3 | 1:1:224:SER:O | 2.08 | 0.53 |
| 1:w:258:TYR:OH | 1:w:399:GLU:OE1 | 2.22 | 0.53 |
| 1:x:324:LYS:NZ | 1:x:337:ASN:OD1 | 2.35 | 0.53 |
| 1:3:224:SER:O | 1:8:407:ARG:HD3 | 2.08 | 0.53 |
| 1:3:714:ASP:HB3 | 1:3:726:PRO:HG3 | 1.90 | 0.53 |
| 1:4:329:ASN:OD1 | 1:4:330:GLU:OE1 | 2.25 | 0.53 |
| 1:5:340:THR:CB | 1:5:407:ARG:NH2 | 2.72 | 0.53 |
| 1:7:329:ASN:OD1 | 1:7:330:GLU:OE1 | 2.25 | 0.53 |
| 1:C:556:ASP:OD1 | 1:C:557:TYR:N | 2.38 | 0.53 |
| 1:J:232:ASP:OD1 | 1:J:232:ASP:N | 2.37 | 0.53 |
| 1:J:714:ASP:HB3 | 1:J:726:PRO:HG3 | 1.90 | 0.53 |
| 1:N:340:THR:CB | 1:N:407:ARG:HH21 | 2.21 | 0.53 |
| 1:U:340:THR:CB | 1:U:407:ARG:NH2 | 2.72 | 0.53 |
| 1:Z:629:GLY:CA | 1:3:609:TRP:CD1 | 2.85 | 0.53 |
| 1:d:340:THR:CB | 1:d:407:ARG:NH2 | 2.72 | 0.53 |
| 1:e:258:TYR:OH | 1:e:399:GLU:OE1 | 2.22 | 0.53 |
| 1:f:407:ARG:HD3 | 1:z:224:SER:O | 2.08 | 0.53 |
| 1:k:340:THR:CB | 1:k:407:ARG:NH2 | 2.72 | 0.53 |
| 1:q:499:ASN:HA | 1:s:589:THR:HA | 1.89 | 0.53 |
| 1:v:340:THR:CB | 1:v:407:ARG:NH2 | 2.72 | 0.53 |
| 1:w:340:THR:CB | 1:w:407:ARG:NH2 | 2.71 | 0.53 |
| 1:2:340:THR:CB | 1:2:407:ARG:NH2 | 2.72 | 0.53 |
| 1:8:232:ASP:OD1 | 1:8:232:ASP:N | 2.37 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:232:ASP:OD1 | 1:H:232:ASP:N | 2.37 | 0.53 |
| 1:H:589:THR:HA | 1:W:499:ASN:HA | 1.89 | 0.53 |
| 1:O:589:THR:HA | 1:m:499:ASN:HA | 1.88 | 0.53 |
| 1:T:407:ARG:HD3 | 1:i:224:SER:O | 2.08 | 0.53 |
| 1:Z:499:ASN:HA | 1:3:589:THR:HA | 1.88 | 0.53 |
| 1:b:224:SER:O | 1:o:407:ARG:HD3 | 2.08 | 0.53 |
| 1:d:328:GLN:NE2 | 1:d:333:LYS:HG3 | 2.24 | 0.53 |
| 1:e:224:SER:O | 1:h:407:ARG:HD3 | 2.07 | 0.53 |
| 1:e:340:THR:CB | 1:e:407:ARG:NH2 | 2.72 | 0.53 |
| 1:t:224:SER:O | 1:6:407:ARG:HD3 | 2.07 | 0.53 |
| 1:A:232:ASP:OD1 | 1:A:232:ASP:N | 2.37 | 0.53 |
| 1:C:328:GLN:NE2 | 1:C:333:LYS:HG3 | 2.24 | 0.53 |
| 1:H:425:SER:HB3 | 1:W:628:ASP:OD1 | 2.09 | 0.53 |
| 1:O:609:TRP:CD1 | 1:m:629:GLY:CA | 2.85 | 0.53 |
| 1:U:714:ASP:HB3 | 1:U:726:PRO:HG3 | 1.90 | 0.53 |
| 1:V:592:GLY:HA2 | 1:e:499:ASN:HD22 | 1.74 | 0.53 |
| 1:Z:324:LYS:NZ | 1:Z:337:ASN:OD1 | 2.35 | 0.53 |
| 1:g:340:THR:CB | 1:g:407:ARG:NH2 | 2.72 | 0.53 |
| 1:g:340:THR:CB | 1:g:407:ARG:HH21 | 2.20 | 0.53 |
| 1:j:340:THR:CB | 1:j:407:ARG:NH2 | 2.72 | 0.53 |
| 1:k:258:TYR:OH | 1:k:399:GLU:OE1 | 2.22 | 0.53 |
| 1:m:324:LYS:NZ | 1:m:337:ASN:OD1 | 2.35 | 0.53 |
| 1:n:340:THR:CB | 1:n:407:ARG:NH2 | 2.72 | 0.53 |
| 1:o:232:ASP:OD1 | 1:o:232:ASP:N | 2.37 | 0.53 |
| 1:q:628:ASP:OD1 | 1:s:425:SER:HB3 | 2.09 | 0.53 |
| 1:r:324:LYS:NZ | 1:r:337:ASN:OD1 | 2.35 | 0.53 |
| 1:F:407:ARG:HD3 | 1:R:224:SER:O | 2.07 | 0.53 |
| 1:H:529:HIS:ND1 | 1:H:533:GLU:O | 2.42 | 0.53 |
| 1:I:329:ASN:OD1 | 1:I:330:GLU:OE1 | 2.25 | 0.53 |
| 1:O:324:LYS:NZ | 1:O:337:ASN:OD1 | 2.35 | 0.53 |
| 1:b:529:HIS:ND1 | 1:b:533:GLU:O | 2.42 | 0.53 |
| 1:c:329:ASN:OD1 | 1:c:330:GLU:OE1 | 2.25 | 0.53 |
| 1:e:434:ASP:OD1 | 1:e:434:ASP:N | 2.41 | 0.53 |
| 1:f:340:THR:CB | 1:f:407:ARG:NH2 | 2.72 | 0.53 |
| 1:f:714:ASP:HB3 | 1:f:726:PRO:HG3 | 1.90 | 0.53 |
| 1:g:224:SER:O | 1:1:407:ARG:HD3 | 2.08 | 0.53 |
| 1:i:258:TYR:OH | 1:i:399:GLU:OE1 | 2.22 | 0.53 |
| 1:i:340:THR:CB | 1:i:407:ARG:NH2 | 2.72 | 0.53 |
| 1:i:340:THR:CB | 1:i:407:ARG:HH21 | 2.20 | 0.53 |
| 1:p:407:ARG:HD3 | 1:6:224:SER:O | 2.08 | 0.53 |
| 1:s:529:HIS:ND1 | 1:s:533:GLU:O | 2.42 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:w:586:LEU:HD21 | 1:x:490:ARG:NH1 | 2.24 | 0.53 |
| 1:y:529:HIS:ND1 | 1:y:533:GLU:O | 2.42 | 0.53 |
| 1:4:340:THR:CB | 1:4:407:ARG:NH2 | 2.72 | 0.53 |
| 1:A:340:THR:CB | 1:A:407:ARG:NH2 | 2.72 | 0.53 |
| 1:B:529:HIS:ND1 | 1:B:533:GLU:O | 2.42 | 0.53 |
| 1:D:340:THR:CB | 1:D:407:ARG:NH2 | 2.72 | 0.53 |
| 1:D:529:HIS:ND1 | 1:D:533:GLU:O | 2.42 | 0.53 |
| 1:E:434:ASP:OD1 | 1:E:434:ASP:N | 2.41 | 0.53 |
| 1:F:224:SER:O | 1:G:407:ARG:HD3 | 2.08 | 0.53 |
| 1:F:529:HIS:ND1 | 1:F:533:GLU:O | 2.42 | 0.53 |
| 1:F:714:ASP:HB3 | 1:F:726:PRO:HG3 | 1.90 | 0.53 |
| 1:H:340:THR:CB | 1:H:407:ARG:HH21 | 2.21 | 0.53 |
| 1:K:340:THR:CB | 1:K:407:ARG:HH21 | 2.21 | 0.53 |
| 1:S:340:THR:CB | 1:S:407:ARG:NH2 | 2.72 | 0.53 |
| 1:V:529:HIS:ND1 | 1:V:533:GLU:O | 2.42 | 0.53 |
| 1:e:529:HIS:ND1 | 1:e:533:GLU:O | 2.42 | 0.53 |
| 1:o:340:THR:CB | 1:o:407:ARG:NH2 | 2.72 | 0.53 |
| 1:s:340:THR:CB | 1:s:407:ARG:HH21 | 2.20 | 0.53 |
| 1:w:434:ASP:OD1 | 1:w:434:ASP:N | 2.41 | 0.53 |
| 1:3:324:LYS:NZ | 1:3:337:ASN:OD1 | 2.35 | 0.53 |
| 1:6:529:HIS:ND1 | 1:6:533:GLU:O | 2.42 | 0.53 |
| 1:6:714:ASP:HB3 | 1:6:726:PRO:HG3 | 1.90 | 0.53 |
| 1:7:434:ASP:OD1 | 1:7:434:ASP:N | 2.41 | 0.53 |
| 1:B:328:GLN:NE2 | 1:B:333:LYS:HG3 | 2.24 | 0.53 |
| 1:D:340:THR:CB | 1:D:407:ARG:HH21 | 2.20 | 0.53 |
| 1:G:340:THR:CB | 1:G:407:ARG:NH2 | 2.72 | 0.53 |
| 1:I:529:HIS:ND1 | 1:I:533:GLU:O | 2.42 | 0.53 |
| 1:J:340:THR:CB | 1:J:407:ARG:NH2 | 2.72 | 0.53 |
| 1:K:340:THR:CB | 1:K:407:ARG:NH2 | 2.72 | 0.53 |
| 1:K:529:HIS:ND1 | 1:K:533:GLU:O | 2.42 | 0.53 |
| 1:M:340:THR:CB | 1:M:407:ARG:NH2 | 2.72 | 0.53 |
| 1:O:628:ASP:OD1 | 1:n:425:SER:HB3 | 2.09 | 0.53 |
| 1:R:529:HIS:ND1 | 1:R:533:GLU:O | 2.42 | 0.53 |
| 1:W:340:THR:CB | 1:W:407:ARG:NH2 | 2.72 | 0.53 |
| 1:Y:714:ASP:HB3 | 1:Y:726:PRO:HG3 | 1.89 | 0.53 |
| 1:c:529:HIS:ND1 | 1:c:533:GLU:O | 2.42 | 0.53 |
| 1:f:324:LYS:NZ | 1:f:337:ASN:OD1 | 2.35 | 0.53 |
| 1:j:328:GLN:NE2 | 1:j:333:LYS:HG3 | 2.24 | 0.53 |
| 1:j:714:ASP:HB3 | 1:j:726:PRO:HG3 | 1.90 | 0.53 |
| 1:q:340:THR:CB | 1:q:407:ARG:NH2 | 2.71 | 0.53 |
| 1:t:529:HIS:ND1 | 1:t:533:GLU:O | 2.42 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:u:340:THR:CB | 1:u:407:ARG:NH2 | 2.72 | 0.53 |
| 1:u:416:TYR:OH | 1:u:644:HIS:O | 2.27 | 0.53 |
| 1:v:714:ASP:HB3 | 1:v:726:PRO:HG3 | 1.90 | 0.53 |
| 1:w:529:HIS:ND1 | 1:w:533:GLU:O | 2.42 | 0.53 |
| 1:1:328:GLN:NE2 | 1:1:333:LYS:HG3 | 2.24 | 0.53 |
| 1:3:328:GLN:NE2 | 1:3:333:LYS:HG3 | 2.24 | 0.53 |
| 1:3:628:ASP:OD1 | 1:4:425:SER:HB3 | 2.09 | 0.53 |
| 1:7:340:THR:CB | 1:7:407:ARG:NH2 | 2.72 | 0.53 |
| 1:A:407:ARG:HD3 | 1:B:224:SER:O | 2.08 | 0.53 |
| 1:A:529:HIS:ND1 | 1:A:533:GLU:O | 2.42 | 0.53 |
| 1:B:340:THR:CB | 1:B:407:ARG:NH2 | 2.72 | 0.53 |
| 1:J:529:HIS:ND1 | 1:J:533:GLU:O | 2.42 | 0.53 |
| 1:O:328:GLN:NE2 | 1:O:333:LYS:HG3 | 2.24 | 0.53 |
| 1:P:714:ASP:HB3 | 1:P:726:PRO:HG3 | 1.90 | 0.53 |
| 1:Q:232:ASP:OD1 | 1:Q:232:ASP:N | 2.37 | 0.53 |
| 1:T:328:GLN:NE2 | 1:T:333:LYS:HG3 | 2.24 | 0.53 |
| 1:V:340:THR:CB | 1:V:407:ARG:NH2 | 2.72 | 0.53 |
| 1:b:328:GLN:NE2 | 1:b:333:LYS:HG3 | 2.24 | 0.53 |
| 1:b:340:THR:CB | 1:b:407:ARG:NH2 | 2.72 | 0.53 |
| 1:l:529:HIS:ND1 | 1:l:533:GLU:O | 2.42 | 0.53 |
| 1:p:340:THR:CB | 1:p:407:ARG:NH2 | 2.72 | 0.53 |
| 1:v:529:HIS:ND1 | 1:v:533:GLU:O | 2.42 | 0.53 |
| 1:y:340:THR:CB | 1:y:407:ARG:NH2 | 2.72 | 0.53 |
| 1:z:529:HIS:ND1 | 1:z:533:GLU:O | 2.42 | 0.53 |
| 1:C:340:THR:CB | 1:C:407:ARG:NH2 | 2.71 | 0.53 |
| 1:D:499:ASN:HD22 | 1:P:592:GLY:HA2 | 1.74 | 0.53 |
| 1:F:340:THR:CB | 1:F:407:ARG:NH2 | 2.72 | 0.53 |
| 1:M:529:HIS:ND1 | 1:M:533:GLU:O | 2.42 | 0.53 |
| 1:O:583:ALA:HA | 1:O:595:VAL:HG12 | 1.91 | 0.53 |
| 1:S:340:THR:CB | 1:S:407:ARG:HH21 | 2.20 | 0.53 |
| 1:U:529:HIS:ND1 | 1:U:533:GLU:O | 2.42 | 0.53 |
| 1:Z:628:ASP:OD1 | 1:3:425:SER:HB3 | 2.09 | 0.53 |
| 1:f:328:GLN:NE2 | 1:f:333:LYS:HG3 | 2.24 | 0.53 |
| 1:g:258:TYR:OH | 1:g:399:GLU:OE1 | 2.22 | 0.53 |
| 1:h:714:ASP:HB3 | 1:h:726:PRO:HG3 | 1.90 | 0.53 |
| 1:l:714:ASP:HB3 | 1:l:726:PRO:HG3 | 1.90 | 0.53 |
| 1:o:529:HIS:ND1 | 1:o:533:GLU:O | 2.42 | 0.53 |
| 1:q:529:HIS:ND1 | 1:q:533:GLU:O | 2.42 | 0.53 |
| 1:t:660:PRO:HG2 | 1:y:251:PRO:HB3 | 1.90 | 0.53 |
| 1:z:340:THR:CB | 1:z:407:ARG:NH2 | 2.72 | 0.53 |
| 1:z:714:ASP:HB3 | 1:z:726:PRO:HG3 | 1.90 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:4:529:HIS:ND1 | 1:4:533:GLU:O | 2.42 | 0.53 |
| 1:D:425:SER:HB3 | 1:N:628:ASP:OD1 | 2.10 | 0.52 |
| 1:E:340:THR:CB | 1:E:407:ARG:NH2 | 2.72 | 0.52 |
| 1:K:425:SER:HB3 | 1:a:628:ASP:OD1 | 2.10 | 0.52 |
| 1:L:340:THR:CB | 1:L:407:ARG:NH2 | 2.71 | 0.52 |
| 1:M:407:ARG:HD3 | 1:c:224:SER:O | 2.08 | 0.52 |
| 1:M:628:ASP:OD1 | 1:b:425:SER:HB3 | 2.09 | 0.52 |
| 1:N:232:ASP:OD1 | 1:N:232:ASP:N | 2.37 | 0.52 |
| 1:O:425:SER:HB3 | 1:m:628:ASP:OD1 | 2.09 | 0.52 |
| 1:R:258:TYR:OH | 1:R:399:GLU:OE1 | 2.22 | 0.52 |
| 1:S:328:GLN:NE2 | 1:S:333:LYS:HG3 | 2.24 | 0.52 |
| 1:T:254:ASN:O | 1:T:256:HIS:N | 2.43 | 0.52 |
| 1:X:529:HIS:ND1 | 1:X:533:GLU:O | 2.42 | 0.52 |
| 1:l:340:THR:CB | 1:l:407:ARG:NH2 | 2.72 | 0.52 |
| 1:n:416:TYR:OH | 1:n:644:HIS:O | 2.27 | 0.52 |
| 1:n:529:HIS:ND1 | 1:n:533:GLU:O | 2.42 | 0.52 |
| 1:r:254:ASN:O | 1:r:256:HIS:N | 2.43 | 0.52 |
| 1:s:340:THR:CB | 1:s:407:ARG:NH2 | 2.72 | 0.52 |
| 1:x:592:GLY:HA2 | 1:y:499:ASN:HD22 | 1.73 | 0.52 |
| 1:z:425:SER:HB3 | 1:1:628:ASP:OD1 | 2.09 | 0.52 |
| 1:3:583:ALA:HA | 1:3:595:VAL:HG12 | 1.91 | 0.52 |
| 1:5:583:ALA:HA | 1:5:595:VAL:HG12 | 1.92 | 0.52 |
| 1:C:628:ASP:OD1 | 1:M:425:SER:HB3 | 2.10 | 0.52 |
| 1:E:529:HIS:ND1 | 1:E:533:GLU:O | 2.42 | 0.52 |
| 1:G:254:ASN:O | 1:G:256:HIS:N | 2.43 | 0.52 |
| 1:I:224:SER:O | 1:J:407:ARG:HD3 | 2.08 | 0.52 |
| 1:J:425:SER:HB3 | 1:L:628:ASP:OD1 | 2.10 | 0.52 |
| 1:K:499:ASN:HD22 | 1:8:592:GLY:HA2 | 1.74 | 0.52 |
| 1:P:340:THR:CB | 1:P:407:ARG:HH21 | 2.21 | 0.52 |
| 1:Q:583:ALA:HA | 1:Q:595:VAL:HG12 | 1.92 | 0.52 |
| 1:S:254:ASN:O | 1:S:256:HIS:N | 2.43 | 0.52 |
| 1:S:583:ALA:HA | 1:S:595:VAL:HG12 | 1.92 | 0.52 |
| 1:U:232:ASP:OD1 | 1:U:232:ASP:N | 2.37 | 0.52 |
| 1:W:529:HIS:ND1 | 1:W:533:GLU:O | 2.42 | 0.52 |
| 1:W:583:ALA:HA | 1:W:595:VAL:HG12 | 1.91 | 0.52 |
| 1:X:340:THR:CB | 1:X:407:ARG:NH2 | 2.72 | 0.52 |
| 1:X:416:TYR:OH | 1:X:644:HIS:O | 2.27 | 0.52 |
| 1:Y:254:ASN:O | 1:Y:256:HIS:N | 2.43 | 0.52 |
| 1:g:416:TYR:OH | 1:g:644:HIS:O | 2.27 | 0.52 |
| 1:g:529:HIS:ND1 | 1:g:533:GLU:O | 2.42 | 0.52 |
| 1:h:322:GLN:NE2 | 1:i:340:THR:HB | 2.11 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:i:416:TYR:OH | 1:i:644:HIS:O | 2.27 | 0.52 |
| 1:j:324:LYS:NZ | 1:j:337:ASN:OD1 | 2.35 | 0.52 |
| 1:m:340:THR:CB | 1:m:407:ARG:NH2 | 2.71 | 0.52 |
| 1:p:254:ASN:O | 1:p:256:HIS:N | 2.43 | 0.52 |
| 1:q:583:ALA:HA | 1:q:595:VAL:HG12 | 1.91 | 0.52 |
| 1:r:529:HIS:ND1 | 1:r:533:GLU:O | 2.42 | 0.52 |
| 1:r:714:ASP:HB3 | 1:r:726:PRO:HG3 | 1.90 | 0.52 |
| 1:t:425:SER:HB3 | 1:u:628:ASP:OD1 | 2.09 | 0.52 |
| 1:u:254:ASN:O | 1:u:256:HIS:N | 2.43 | 0.52 |
| 1:u:529:HIS:ND1 | 1:u:533:GLU:O | 2.42 | 0.52 |
| 1:u:583:ALA:HA | 1:u:595:VAL:HG12 | 1.92 | 0.52 |
| 1:x:416:TYR:OH | 1:x:644:HIS:O | 2.27 | 0.52 |
| 1:x:529:HIS:ND1 | 1:x:533:GLU:O | 2.42 | 0.52 |
| 1:1:254:ASN:O | 1:1:256:HIS:N | 2.43 | 0.52 |
| 1:4:416:TYR:OH | 1:4:644:HIS:O | 2.27 | 0.52 |
| 1:5:232:ASP:OD1 | 1:5:232:ASP:N | 2.37 | 0.52 |
| 1:6:340:THR:CB | 1:6:407:ARG:NH2 | 2.72 | 0.52 |
| 1:6:425:SER:HB3 | 1:7:628:ASP:OD1 | 2.09 | 0.52 |
| 1:7:529:HIS:ND1 | 1:7:533:GLU:O | 2.42 | 0.52 |
| 1:8:340:THR:CB | 1:8:407:ARG:HH21 | 2.20 | 0.52 |
| 1:8:714:ASP:HB3 | 1:8:726:PRO:HG3 | 1.90 | 0.52 |
| 1:B:425:SER:HB3 | 1:J:628:ASP:OD1 | 2.09 | 0.52 |
| 1:C:254:ASN:O | 1:C:256:HIS:N | 2.43 | 0.52 |
| 1:C:425:SER:HB3 | 1:b:628:ASP:OD1 | 2.10 | 0.52 |
| 1:E:628:ASP:OD1 | 1:F:425:SER:HB3 | 2.09 | 0.52 |
| 1:F:583:ALA:HA | 1:F:595:VAL:HG12 | 1.92 | 0.52 |
| 1:H:340:THR:CB | 1:H:407:ARG:NH2 | 2.72 | 0.52 |
| 1:I:254:ASN:O | 1:I:256:HIS:N | 2.43 | 0.52 |
| 1:L:254:ASN:O | 1:L:256:HIS:N | 2.43 | 0.52 |
| 1:L:529:HIS:ND1 | 1:L:533:GLU:O | 2.42 | 0.52 |
| 1:R:340:THR:CB | 1:R:407:ARG:HH21 | 2.21 | 0.52 |
| 1:S:529:HIS:ND1 | 1:S:533:GLU:O | 2.42 | 0.52 |
| 1:T:628:ASP:OD1 | 1:l:425:SER:HB3 | 2.09 | 0.52 |
| 1:Y:529:HIS:ND1 | 1:Y:533:GLU:O | 2.42 | 0.52 |
| 1:Z:340:THR:CB | 1:Z:407:ARG:HH21 | 2.20 | 0.52 |
| 1:c:254:ASN:O | 1:c:256:HIS:N | 2.43 | 0.52 |
| 1:f:628:ASP:OD1 | 1:g:425:SER:HB3 | 2.09 | 0.52 |
| 1:h:340:THR:CB | 1:h:407:ARG:HH21 | 2.20 | 0.52 |
| 1:i:425:SER:HB3 | 1:j:628:ASP:OD1 | 2.09 | 0.52 |
| 1:k:714:ASP:HB3 | 1:k:726:PRO:HG3 | 1.90 | 0.52 |
| 1:m:254:ASN:O | 1:m:256:HIS:N | 2.43 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:340:THR:CB | 1:m:407:ARG:HH21 | 2.20 | 0.52 |
| 1:o:425:SER:HB3 | 1:p:628:ASP:OD1 | 2.09 | 0.52 |
| 1:t:340:THR:CB | 1:t:407:ARG:HH21 | 2.20 | 0.52 |
| 1:u:328:GLN:NE2 | 1:u:333:LYS:HG3 | 2.24 | 0.52 |
| 1:u:340:THR:CB | 1:u:407:ARG:HH21 | 2.21 | 0.52 |
| 1:6:583:ALA:HA | 1:6:595:VAL:HG12 | 1.92 | 0.52 |
| 1:7:328:GLN:NE2 | 1:7:333:LYS:HG3 | 2.24 | 0.52 |
| 1:A:609:TRP:CD1 | 1:G:629:GLY:CA | 2.85 | 0.52 |
| 1:B:628:ASP:OD1 | 1:L:425:SER:HB3 | 2.10 | 0.52 |
| 1:C:529:HIS:ND1 | 1:C:533:GLU:O | 2.42 | 0.52 |
| 1:E:254:ASN:O | 1:E:256:HIS:N | 2.43 | 0.52 |
| 1:F:254:ASN:O | 1:F:256:HIS:N | 2.43 | 0.52 |
| 1:K:232:ASP:OD1 | 1:K:232:ASP:N | 2.37 | 0.52 |
| 1:R:425:SER:HB3 | 1:S:628:ASP:OD1 | 2.09 | 0.52 |
| 1:R:583:ALA:HA | 1:R:595:VAL:HG12 | 1.92 | 0.52 |
| 1:S:425:SER:HB3 | 1:U:628:ASP:OD1 | 2.09 | 0.52 |
| 1:U:570:THR:OG1 | 1:U:571:THR:N | 2.43 | 0.52 |
| 1:V:254:ASN:O | 1:V:256:HIS:N | 2.43 | 0.52 |
| 1:X:583:ALA:HA | 1:X:595:VAL:HG12 | 1.92 | 0.52 |
| 1:Z:340:THR:CB | 1:Z:407:ARG:NH2 | 2.71 | 0.52 |
| 1:a:232:ASP:OD1 | 1:a:232:ASP:N | 2.37 | 0.52 |
| 1:h:254:ASN:O | 1:h:256:HIS:N | 2.43 | 0.52 |
| 1:i:529:HIS:ND1 | 1:i:533:GLU:O | 2.42 | 0.52 |
| 1:i:592:GLY:HA2 | 1:j:499:ASN:HD22 | 1.75 | 0.52 |
| 1:k:254:ASN:O | 1:k:256:HIS:N | 2.43 | 0.52 |
| 1:o:416:TYR:OH | 1:o:644:HIS:O | 2.27 | 0.52 |
| 1:o:583:ALA:HA | 1:o:595:VAL:HG12 | 1.91 | 0.52 |
| 1:q:425:SER:HB3 | 1:r:628:ASP:OD1 | 2.09 | 0.52 |
| 1:r:340:THR:CB | 1:r:407:ARG:NH2 | 2.71 | 0.52 |
| 1:t:258:TYR:OH | 1:t:399:GLU:OE1 | 2.22 | 0.52 |
| 1:v:232:ASP:OD1 | 1:v:232:ASP:N | 2.37 | 0.52 |
| 1:x:340:THR:CB | 1:x:407:ARG:NH2 | 2.72 | 0.52 |
| 1:x:583:ALA:HA | 1:x:595:VAL:HG12 | 1.92 | 0.52 |
| 1:y:254:ASN:O | 1:y:256:HIS:N | 2.43 | 0.52 |
| 1:1:592:GLY:HA2 | 1:2:499:ASN:HD22 | 1.75 | 0.52 |
| 1:6:254:ASN:O | 1:6:256:HIS:N | 2.43 | 0.52 |
| 1:7:254:ASN:O | 1:7:256:HIS:N | 2.43 | 0.52 |
| 1:A:416:TYR:OH | 1:A:644:HIS:O | 2.27 | 0.52 |
| 1:A:583:ALA:HA | 1:A:595:VAL:HG12 | 1.92 | 0.52 |
| 1:E:328:GLN:NE2 | 1:E:333:LYS:HG3 | 2.24 | 0.52 |
| 1:H:254:ASN:O | 1:H:256:HIS:N | 2.43 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:628:ASP:OD1 | 1:Y:425:SER:HB3 | 2.09 | 0.52 |
| 1:K:583:ALA:HA | 1:K:595:VAL:HG12 | 1.92 | 0.52 |
| 1:M:254:ASN:O | 1:M:256:HIS:N | 2.43 | 0.52 |
| 1:P:254:ASN:O | 1:P:256:HIS:N | 2.43 | 0.52 |
| 1:Q:254:ASN:O | 1:Q:256:HIS:N | 2.43 | 0.52 |
| 1:T:529:HIS:ND1 | 1:T:533:GLU:O | 2.42 | 0.52 |
| 1:T:592:GLY:HA2 | 1:d:499:ASN:HD22 | 1.75 | 0.52 |
| 1:W:328:GLN:NE2 | 1:W:333:LYS:HG3 | 2.24 | 0.52 |
| 1:W:425:SER:HB3 | 1:Y:628:ASP:OD1 | 2.09 | 0.52 |
| 1:Y:340:THR:CB | 1:Y:407:ARG:NH2 | 2.71 | 0.52 |
| 1:Z:254:ASN:O | 1:Z:256:HIS:N | 2.43 | 0.52 |
| 1:a:258:TYR:OH | 1:a:399:GLU:OE1 | 2.22 | 0.52 |
| 1:c:628:ASP:OD1 | 1:p:425:SER:HB3 | 2.10 | 0.52 |
| 1:d:570:THR:OG1 | 1:d:571:THR:N | 2.43 | 0.52 |
| 1:e:328:GLN:NE2 | 1:e:333:LYS:HG3 | 2.24 | 0.52 |
| 1:f:529:HIS:ND1 | 1:f:533:GLU:O | 2.42 | 0.52 |
| 1:h:529:HIS:ND1 | 1:h:533:GLU:O | 2.42 | 0.52 |
| 1:j:340:THR:CB | 1:j:407:ARG:HH21 | 2.20 | 0.52 |
| 1:j:529:HIS:ND1 | 1:j:533:GLU:O | 2.42 | 0.52 |
| 1:q:328:GLN:NE2 | 1:q:333:LYS:HG3 | 2.24 | 0.52 |
| 1:v:340:THR:CB | 1:v:407:ARG:HH21 | 2.20 | 0.52 |
| 1:v:570:THR:OG1 | 1:v:571:THR:N | 2.43 | 0.52 |
| 1:w:628:ASP:OD1 | 1:y:425:SER:HB3 | 2.09 | 0.52 |
| 1:z:583:ALA:HA | 1:z:595:VAL:HG12 | 1.91 | 0.52 |
| 1:1:529:HIS:ND1 | 1:1:533:GLU:O | 2.42 | 0.52 |
| 1:2:529:HIS:ND1 | 1:2:533:GLU:O | 2.42 | 0.52 |
| 1:2:570:THR:OG1 | 1:2:571:THR:N | 2.43 | 0.52 |
| 1:5:254:ASN:O | 1:5:256:HIS:N | 2.43 | 0.52 |
| 1:7:416:TYR:OH | 1:7:644:HIS:O | 2.27 | 0.52 |
| 1:8:254:ASN:O | 1:8:256:HIS:N | 2.43 | 0.52 |
| 1:A:254:ASN:O | 1:A:256:HIS:N | 2.43 | 0.52 |
| 1:C:583:ALA:HA | 1:C:595:VAL:HG12 | 1.92 | 0.52 |
| 1:D:232:ASP:N | 1:D:232:ASP:OD1 | 2.37 | 0.52 |
| 1:E:416:TYR:OH | 1:E:644:HIS:O | 2.27 | 0.52 |
| 1:G:425:SER:HB3 | 1:I:628:ASP:OD1 | 2.10 | 0.52 |
| 1:J:254:ASN:O | 1:J:256:HIS:N | 2.43 | 0.52 |
| 1:P:570:THR:OG1 | 1:P:571:THR:N | 2.43 | 0.52 |
| 1:V:324:LYS:NZ | 1:V:337:ASN:OD1 | 2.35 | 0.52 |
| 1:W:254:ASN:O | 1:W:256:HIS:N | 2.43 | 0.52 |
| 1:c:570:THR:OG1 | 1:c:571:THR:N | 2.43 | 0.52 |
| 1:d:254:ASN:O | 1:d:256:HIS:N | 2.43 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:d:529:HIS:ND1 | 1:d:533:GLU:O | 2.42 | 0.52 |
| 1:e:254:ASN:O | 1:e:256:HIS:N | 2.43 | 0.52 |
| 1:g:340:THR:HB | 1:k:322:GLN:NE2 | 2.11 | 0.52 |
| 1:k:340:THR:CB | 1:k:407:ARG:HH21 | 2.21 | 0.52 |
| 1:q:254:ASN:O | 1:q:256:HIS:N | 2.43 | 0.52 |
| 1:r:425:SER:HB3 | 1:s:628:ASP:OD1 | 2.09 | 0.52 |
| 1:s:254:ASN:O | 1:s:256:HIS:N | 2.43 | 0.52 |
| 1:t:583:ALA:HA | 1:t:595:VAL:HG12 | 1.92 | 0.52 |
| 1:w:254:ASN:O | 1:w:256:HIS:N | 2.43 | 0.52 |
| 1:w:328:GLN:NE2 | 1:w:333:LYS:HG3 | 2.24 | 0.52 |
| 1:w:570:THR:OG1 | 1:w:571:THR:N | 2.43 | 0.52 |
| 1:1:425:SER:HB3 | 1:2:628:ASP:OD1 | 2.09 | 0.52 |
| 1:2:254:ASN:O | 1:2:256:HIS:N | 2.43 | 0.52 |
| 1:3:340:THR:CB | 1:3:407:ARG:NH2 | 2.72 | 0.52 |
| 1:5:628:ASP:OD1 | 1:7:425:SER:HB3 | 2.09 | 0.52 |
| 1:8:570:THR:OG1 | 1:8:571:THR:N | 2.43 | 0.52 |
| 1:C:499:ASN:HD22 | 1:M:592:GLY:HA2 | 1.75 | 0.52 |
| 1:E:425:SER:HB3 | 1:Q:628:ASP:OD1 | 2.09 | 0.52 |
| 1:I:340:THR:CB | 1:I:407:ARG:NH2 | 2.72 | 0.52 |
| 1:I:609:TRP:CH2 | 1:I:631:PHE:CE2 | 2.98 | 0.52 |
| 1:L:583:ALA:HA | 1:L:595:VAL:HG12 | 1.92 | 0.52 |
| 1:M:583:ALA:HA | 1:M:595:VAL:HG12 | 1.92 | 0.52 |
| 1:O:340:THR:CB | 1:O:407:ARG:NH2 | 2.72 | 0.52 |
| 1:S:609:TRP:CH2 | 1:S:631:PHE:CE2 | 2.98 | 0.52 |
| 1:T:425:SER:HB3 | 1:d:628:ASP:OD1 | 2.09 | 0.52 |
| 1:X:570:THR:OG1 | 1:X:571:THR:N | 2.43 | 0.52 |
| 1:Y:570:THR:OG1 | 1:Y:571:THR:N | 2.43 | 0.52 |
| 1:b:583:ALA:HA | 1:b:595:VAL:HG12 | 1.92 | 0.52 |
| 1:c:340:THR:CB | 1:c:407:ARG:NH2 | 2.72 | 0.52 |
| 1:c:609:TRP:CH2 | 1:c:631:PHE:CE2 | 2.98 | 0.52 |
| 1:f:499:ASN:HD22 | 1:g:592:GLY:HA2 | 1.75 | 0.52 |
| 1:k:529:HIS:ND1 | 1:k:533:GLU:O | 2.42 | 0.52 |
| 1:l:416:TYR:OH | 1:l:644:HIS:O | 2.27 | 0.52 |
| 1:m:570:THR:OG1 | 1:m:571:THR:N | 2.43 | 0.52 |
| 1:o:254:ASN:O | 1:o:256:HIS:N | 2.43 | 0.52 |
| 1:q:322:GLN:NE2 | 1:y:340:THR:HB | 2.10 | 0.52 |
| 1:r:570:THR:OG1 | 1:r:571:THR:N | 2.43 | 0.52 |
| 1:t:340:THR:CB | 1:t:407:ARG:NH2 | 2.71 | 0.52 |
| 1:u:425:SER:HB3 | 1:v:628:ASP:OD1 | 2.09 | 0.52 |
| 1:u:609:TRP:CH2 | 1:u:631:PHE:CE2 | 2.98 | 0.52 |
| 1:w:714:ASP:HB3 | 1:w:726:PRO:HG3 | 1.90 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:629:GLY:CA | 1:4:609:TRP:CD1 | 2.85 | 0.52 |
| 1:6:232:ASP:OD1 | 1:6:232:ASP:N | 2.37 | 0.52 |
| 1:A:425:SER:HB3 | 1:G:628:ASP:OD1 | 2.10 | 0.52 |
| 1:A:609:TRP:CH2 | 1:A:631:PHE:CE2 | 2.98 | 0.52 |
| 1:B:583:ALA:HA | 1:B:595:VAL:HG12 | 1.92 | 0.52 |
| 1:B:609:TRP:CH2 | 1:B:631:PHE:CE2 | 2.98 | 0.52 |
| 1:D:570:THR:OG1 | 1:D:571:THR:N | 2.43 | 0.52 |
| 1:D:583:ALA:HA | 1:D:595:VAL:HG12 | 1.92 | 0.52 |
| 1:G:583:ALA:HA | 1:G:595:VAL:HG12 | 1.92 | 0.52 |
| 1:J:583:ALA:HA | 1:J:595:VAL:HG12 | 1.92 | 0.52 |
| 1:J:592:GLY:HA2 | 1:L:499:ASN:HD22 | 1.75 | 0.52 |
| 1:L:609:TRP:CH2 | 1:L:631:PHE:CE2 | 2.98 | 0.52 |
| 1:N:258:TYR:OH | 1:N:399:GLU:OE1 | 2.22 | 0.52 |
| 1:O:503:PHE:CE2 | 1:n:451:THR:HG21 | 2.45 | 0.52 |
| 1:O:609:TRP:CH2 | 1:O:631:PHE:CE2 | 2.98 | 0.52 |
| 1:S:439:PRO:HB3 | 1:U:381:LEU:HD21 | 1.92 | 0.52 |
| 1:U:340:THR:CB | 1:U:407:ARG:HH21 | 2.20 | 0.52 |
| 1:Z:570:THR:OG1 | 1:Z:571:THR:N | 2.43 | 0.52 |
| 1:a:609:TRP:CH2 | 1:a:631:PHE:CE2 | 2.98 | 0.52 |
| 1:b:609:TRP:CH2 | 1:b:631:PHE:CE2 | 2.98 | 0.52 |
| 1:d:609:TRP:CH2 | 1:d:631:PHE:CE2 | 2.98 | 0.52 |
| 1:e:570:THR:OG1 | 1:e:571:THR:N | 2.43 | 0.52 |
| 1:e:714:ASP:HB3 | 1:e:726:PRO:HG3 | 1.90 | 0.52 |
| 1:f:340:THR:CB | 1:f:407:ARG:HH21 | 2.21 | 0.52 |
| 1:g:629:GLY:CA | 1:h:609:TRP:CD1 | 2.85 | 0.52 |
| 1:j:254:ASN:O | 1:j:256:HIS:N | 2.43 | 0.52 |
| 1:j:416:TYR:OH | 1:j:644:HIS:O | 2.27 | 0.52 |
| 1:l:570:THR:OG1 | 1:l:571:THR:N | 2.43 | 0.52 |
| 1:l:583:ALA:HA | 1:l:595:VAL:HG12 | 1.92 | 0.52 |
| 1:o:609:TRP:CD1 | 1:p:629:GLY:CA | 2.85 | 0.52 |
| 1:o:609:TRP:CH2 | 1:o:631:PHE:CE2 | 2.98 | 0.52 |
| 1:p:583:ALA:HA | 1:p:595:VAL:HG12 | 1.92 | 0.52 |
| 1:t:499:ASN:HD22 | 1:v:592:GLY:HA2 | 1.75 | 0.52 |
| 1:v:609:TRP:CH2 | 1:v:631:PHE:CE2 | 2.98 | 0.52 |
| 1:x:570:THR:OG1 | 1:x:571:THR:N | 2.43 | 0.52 |
| 1:y:609:TRP:CH2 | 1:y:631:PHE:CE2 | 2.98 | 0.52 |
| 1:z:416:TYR:OH | 1:z:644:HIS:O | 2.27 | 0.52 |
| 1:z:570:THR:OG1 | 1:z:571:THR:N | 2.43 | 0.52 |
| 1:1:570:THR:OG1 | 1:1:571:THR:N | 2.43 | 0.52 |
| 1:2:609:TRP:CH2 | 1:2:631:PHE:CE2 | 2.98 | 0.52 |
| 1:3:503:PHE:CE2 | 1:4:451:THR:HG21 | 2.45 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:609:TRP:CH2 | 1:3:631:PHE:CE2 | 2.98 | 0.52 |
| 1:6:570:THR:OG1 | 1:6:571:THR:N | 2.43 | 0.52 |
| 1:7:714:ASP:HB3 | 1:7:726:PRO:HG3 | 1.90 | 0.52 |
| 1:A:499:ASN:HD22 | 1:I:592:GLY:HA2 | 1.75 | 0.52 |
| 1:A:592:GLY:HA2 | 1:G:499:ASN:HD22 | 1.75 | 0.52 |
| 1:A:628:ASP:OD1 | 1:I:425:SER:HB3 | 2.09 | 0.52 |
| 1:C:609:TRP:CH2 | 1:C:631:PHE:CE2 | 2.98 | 0.52 |
| 1:E:583:ALA:HA | 1:E:595:VAL:HG12 | 1.91 | 0.52 |
| 1:E:714:ASP:HB3 | 1:E:726:PRO:HG3 | 1.90 | 0.52 |
| 1:F:570:THR:OG1 | 1:F:571:THR:N | 2.43 | 0.52 |
| 1:G:416:TYR:OH | 1:G:644:HIS:O | 2.27 | 0.52 |
| 1:K:570:THR:OG1 | 1:K:571:THR:N | 2.43 | 0.52 |
| 1:L:416:TYR:OH | 1:L:644:HIS:O | 2.27 | 0.52 |
| 1:N:609:TRP:CH2 | 1:N:631:PHE:CE2 | 2.98 | 0.52 |
| 1:O:258:TYR:OH | 1:O:399:GLU:OE1 | 2.22 | 0.52 |
| 1:R:340:THR:CB | 1:R:407:ARG:NH2 | 2.72 | 0.52 |
| 1:R:499:ASN:HD22 | 1:U:592:GLY:HA2 | 1.75 | 0.52 |
| 1:R:592:GLY:HA2 | 1:S:499:ASN:HD22 | 1.75 | 0.52 |
| 1:T:570:THR:OG1 | 1:T:571:THR:N | 2.43 | 0.52 |
| 1:U:609:TRP:CH2 | 1:U:631:PHE:CE2 | 2.98 | 0.52 |
| 1:V:609:TRP:CH2 | 1:V:631:PHE:CE2 | 2.98 | 0.52 |
| 1:W:609:TRP:CH2 | 1:W:631:PHE:CE2 | 2.98 | 0.52 |
| 1:c:425:SER:HB3 | 1:o:628:ASP:OD1 | 2.09 | 0.52 |
| 1:c:592:GLY:HA2 | 1:o:499:ASN:HD22 | 1.75 | 0.52 |
| 1:f:254:ASN:O | 1:f:256:HIS:N | 2.43 | 0.52 |
| 1:f:416:TYR:OH | 1:f:644:HIS:O | 2.27 | 0.52 |
| 1:i:629:GLY:CA | 1:k:609:TRP:CD1 | 2.85 | 0.52 |
| 1:l:609:TRP:CH2 | 1:l:631:PHE:CE2 | 2.98 | 0.52 |
| 1:m:425:SER:HB3 | 1:n:628:ASP:OD1 | 2.09 | 0.52 |
| 1:n:583:ALA:HA | 1:n:595:VAL:HG12 | 1.92 | 0.52 |
| 1:q:609:TRP:CH2 | 1:q:631:PHE:CE2 | 2.98 | 0.52 |
| 1:t:629:GLY:CA | 1:v:609:TRP:CD1 | 2.85 | 0.52 |
| 1:w:609:TRP:CD1 | 1:x:629:GLY:CA | 2.82 | 0.52 |
| 1:z:609:TRP:CH2 | 1:z:631:PHE:CE2 | 2.98 | 0.52 |
| 1:4:258:TYR:OH | 1:4:399:GLU:OE1 | 2.22 | 0.52 |
| 1:4:583:ALA:HA | 1:4:595:VAL:HG12 | 1.92 | 0.52 |
| 1:7:583:ALA:HA | 1:7:595:VAL:HG12 | 1.91 | 0.52 |
| 1:A:381:LEU:HD21 | 1:I:439:PRO:HB3 | 1.92 | 0.52 |
| 1:O:529:HIS:ND1 | 1:O:533:GLU:O | 2.42 | 0.52 |
| 1:P:529:HIS:ND1 | 1:P:533:GLU:O | 2.42 | 0.52 |
| 1:X:499:ASN:HD22 | 1:e:592:GLY:HA2 | 1.75 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z:425:SER:HB3 | 1:4:628:ASP:OD1 | 2.09 | 0.52 |
| 1:Z:609:TRP:CD1 | 1:4:629:GLY:CA | 2.85 | 0.52 |
| 1:d:583:ALA:HA | 1:d:595:VAL:HG12 | 1.92 | 0.52 |
| 1:j:451:THR:HG21 | 1:k:503:PHE:CE2 | 2.45 | 0.52 |
| 1:l:254:ASN:O | 1:l:256:HIS:N | 2.43 | 0.52 |
| 1:p:529:HIS:ND1 | 1:p:533:GLU:O | 2.42 | 0.52 |
| 1:t:628:ASP:OD1 | 1:v:425:SER:HB3 | 2.09 | 0.52 |
| 1:u:439:PRO:HB3 | 1:v:381:LEU:HD21 | 1.92 | 0.52 |
| 1:w:439:PRO:HB3 | 1:x:381:LEU:HD21 | 1.91 | 0.52 |
| 1:x:254:ASN:O | 1:x:256:HIS:N | 2.43 | 0.52 |
| 1:y:324:LYS:NZ | 1:y:337:ASN:OD1 | 2.35 | 0.52 |
| 1:z:628:ASP:OD1 | 1:2:425:SER:HB3 | 2.10 | 0.52 |
| 1:2:583:ALA:HA | 1:2:595:VAL:HG12 | 1.92 | 0.52 |
| 1:8:529:HIS:ND1 | 1:8:533:GLU:O | 2.42 | 0.52 |
| 1:A:328:GLN:NE2 | 1:A:333:LYS:HG3 | 2.24 | 0.51 |
| 1:B:592:GLY:HA2 | 1:J:499:ASN:HD22 | 1.75 | 0.51 |
| 1:C:416:TYR:OH | 1:C:644:HIS:O | 2.27 | 0.51 |
| 1:C:439:PRO:HB3 | 1:b:381:LEU:HD21 | 1.92 | 0.51 |
| 1:D:254:ASN:O | 1:D:256:HIS:N | 2.43 | 0.51 |
| 1:F:628:ASP:OD1 | 1:Q:425:SER:HB3 | 2.09 | 0.51 |
| 1:G:529:HIS:ND1 | 1:G:533:GLU:O | 2.42 | 0.51 |
| 1:H:609:TRP:CH2 | 1:H:631:PHE:CE2 | 2.98 | 0.51 |
| 1:M:499:ASN:HD22 | 1:b:592:GLY:HA2 | 1.75 | 0.51 |
| 1:N:254:ASN:O | 1:N:256:HIS:N | 2.43 | 0.51 |
| 1:N:425:SER:HB3 | 1:P:628:ASP:OD1 | 2.10 | 0.51 |
| 1:O:629:GLY:CA | 1:n:609:TRP:CD1 | 2.85 | 0.51 |
| 1:Q:529:HIS:ND1 | 1:Q:533:GLU:O | 2.42 | 0.51 |
| 1:R:629:GLY:CA | 1:U:609:TRP:CD1 | 2.85 | 0.51 |
| 1:V:583:ALA:HA | 1:V:595:VAL:HG12 | 1.92 | 0.51 |
| 1:Y:340:THR:CB | 1:Y:407:ARG:HH21 | 2.20 | 0.51 |
| 1:Z:451:THR:HG21 | 1:4:503:PHE:CE2 | 2.45 | 0.51 |
| 1:a:529:HIS:ND1 | 1:a:533:GLU:O | 2.42 | 0.51 |
| 1:g:381:LEU:HD21 | 1:h:439:PRO:HB3 | 1.92 | 0.51 |
| 1:m:451:THR:HG21 | 1:n:503:PHE:CE2 | 2.45 | 0.51 |
| 1:m:609:TRP:CD1 | 1:n:629:GLY:CA | 2.85 | 0.51 |
| 1:m:609:TRP:CH2 | 1:m:631:PHE:CE2 | 2.98 | 0.51 |
| 1:p:416:TYR:OH | 1:p:644:HIS:O | 2.27 | 0.51 |
| 1:r:340:THR:CB | 1:r:407:ARG:HH21 | 2.20 | 0.51 |
| 1:r:583:ALA:HA | 1:r:595:VAL:HG12 | 1.92 | 0.51 |
| 1:s:609:TRP:CH2 | 1:s:631:PHE:CE2 | 2.98 | 0.51 |
| 1:t:328:GLN:NE2 | 1:t:333:LYS:HG3 | 2.24 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:t:592:GLY:HA2 | 1:u:499:ASN:HD22 | 1.75 | 0.51 |
| 1:t:609:TRP:CH2 | 1:t:631:PHE:CE2 | 2.98 | 0.51 |
| 1:v:583:ALA:HA | 1:v:595:VAL:HG12 | 1.92 | 0.51 |
| 1:x:609:TRP:CH2 | 1:x:631:PHE:CE2 | 2.98 | 0.51 |
| 1:y:583:ALA:HA | 1:y:595:VAL:HG12 | 1.92 | 0.51 |
| 1:z:254:ASN:O | 1:z:256:HIS:N | 2.43 | 0.51 |
| 1:3:529:HIS:ND1 | 1:3:533:GLU:O | 2.42 | 0.51 |
| 1:B:254:ASN:O | 1:B:256:HIS:N | 2.43 | 0.51 |
| 1:B:381:LEU:HD21 | 1:L:439:PRO:HB3 | 1.92 | 0.51 |
| 1:B:499:ASN:HD22 | 1:L:592:GLY:HA2 | 1.75 | 0.51 |
| 1:D:628:ASP:OD1 | 1:P:425:SER:HB3 | 2.10 | 0.51 |
| 1:E:451:THR:HG21 | 1:Q:503:PHE:CE2 | 2.46 | 0.51 |
| 1:F:609:TRP:CH2 | 1:F:631:PHE:CE2 | 2.98 | 0.51 |
| 1:I:570:THR:OG1 | 1:I:571:THR:N | 2.43 | 0.51 |
| 1:I:583:ALA:HA | 1:I:595:VAL:HG12 | 1.92 | 0.51 |
| 1:K:254:ASN:O | 1:K:256:HIS:N | 2.43 | 0.51 |
| 1:K:628:ASP:OD1 | 1:8:425:SER:HB3 | 2.10 | 0.51 |
| 1:N:529:HIS:ND1 | 1:N:533:GLU:O | 2.42 | 0.51 |
| 1:O:254:ASN:O | 1:O:256:HIS:N | 2.43 | 0.51 |
| 1:R:609:TRP:CH2 | 1:R:631:PHE:CE2 | 2.98 | 0.51 |
| 1:R:628:ASP:OD1 | 1:U:425:SER:HB3 | 2.09 | 0.51 |
| 1:X:254:ASN:O | 1:X:256:HIS:N | 2.43 | 0.51 |
| 1:X:609:TRP:CH2 | 1:X:631:PHE:CE2 | 2.98 | 0.51 |
| 1:Y:583:ALA:HA | 1:Y:595:VAL:HG12 | 1.92 | 0.51 |
| 1:Z:609:TRP:CH2 | 1:Z:631:PHE:CE2 | 2.98 | 0.51 |
| 1:a:254:ASN:O | 1:a:256:HIS:N | 2.43 | 0.51 |
| 1:a:570:THR:OG1 | 1:a:571:THR:N | 2.43 | 0.51 |
| 1:b:254:ASN:O | 1:b:256:HIS:N | 2.43 | 0.51 |
| 1:d:425:SER:HB3 | 1:l:628:ASP:OD1 | 2.10 | 0.51 |
| 1:i:381:LEU:HD21 | 1:k:439:PRO:HB3 | 1.92 | 0.51 |
| 1:m:529:HIS:ND1 | 1:m:533:GLU:O | 2.42 | 0.51 |
| 1:n:609:TRP:CH2 | 1:n:631:PHE:CE2 | 2.98 | 0.51 |
| 1:o:328:GLN:NE2 | 1:o:333:LYS:HG3 | 2.24 | 0.51 |
| 1:o:592:GLY:HA2 | 1:p:499:ASN:HD22 | 1.75 | 0.51 |
| 1:t:254:ASN:O | 1:t:256:HIS:N | 2.43 | 0.51 |
| 1:1:258:TYR:OH | 1:1:399:GLU:OE1 | 2.22 | 0.51 |
| 1:4:609:TRP:CH2 | 1:4:631:PHE:CE2 | 2.98 | 0.51 |
| 1:5:324:LYS:NZ | 1:5:337:ASN:OD1 | 2.35 | 0.51 |
| 1:5:425:SER:HB3 | 1:6:628:ASP:OD1 | 2.09 | 0.51 |
| 1:6:609:TRP:CH2 | 1:6:631:PHE:CE2 | 2.98 | 0.51 |
| 1:C:592:GLY:HA2 | 1:b:499:ASN:HD22 | 1.75 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:592:GLY:HA2 | 1:I:499:ASN:HD22 | 1.75 | 0.51 |
| 1:J:609:TRP:CH2 | 1:J:631:PHE:CE2 | 2.98 | 0.51 |
| 1:M:609:TRP:CH2 | 1:M:631:PHE:CE2 | 2.98 | 0.51 |
| 1:N:570:THR:OG1 | 1:N:571:THR:N | 2.43 | 0.51 |
| 1:R:254:ASN:O | 1:R:256:HIS:N | 2.43 | 0.51 |
| 1:R:328:GLN:NE2 | 1:R:333:LYS:HG3 | 2.24 | 0.51 |
| 1:T:583:ALA:HA | 1:T:595:VAL:HG12 | 1.91 | 0.51 |
| 1:U:583:ALA:HA | 1:U:595:VAL:HG12 | 1.92 | 0.51 |
| 1:V:425:SER:HB3 | 1:e:628:ASP:OD1 | 2.10 | 0.51 |
| 1:W:592:GLY:HA2 | 1:Y:499:ASN:HD22 | 1.75 | 0.51 |
| 1:a:425:SER:HB3 | 1:8:628:ASP:OD1 | 2.10 | 0.51 |
| 1:c:439:PRO:HB3 | 1:o:381:LEU:HD21 | 1.92 | 0.51 |
| 1:c:583:ALA:HA | 1:c:595:VAL:HG12 | 1.92 | 0.51 |
| 1:f:451:THR:HG21 | 1:h:503:PHE:CE2 | 2.46 | 0.51 |
| 1:g:232:ASP:N | 1:g:232:ASP:OD1 | 2.37 | 0.51 |
| 1:i:628:ASP:OD1 | 1:k:425:SER:HB3 | 2.10 | 0.51 |
| 1:l:232:ASP:OD1 | 1:l:232:ASP:N | 2.37 | 0.51 |
| 1:n:258:TYR:OH | 1:n:399:GLU:OE1 | 2.22 | 0.51 |
| 1:n:570:THR:OG1 | 1:n:571:THR:N | 2.43 | 0.51 |
| 1:u:609:TRP:NE1 | 1:v:629:GLY:CA | 2.58 | 0.51 |
| 1:v:254:ASN:O | 1:v:256:HIS:N | 2.43 | 0.51 |
| 1:4:254:ASN:O | 1:4:256:HIS:N | 2.43 | 0.51 |
| 1:4:570:THR:OG1 | 1:4:571:THR:N | 2.43 | 0.51 |
| 1:5:503:PHE:CE2 | 1:7:451:THR:HG21 | 2.46 | 0.51 |
| 1:5:529:HIS:ND1 | 1:5:533:GLU:O | 2.42 | 0.51 |
| 1:F:340:THR:CB | 1:F:407:ARG:HH21 | 2.20 | 0.51 |
| 1:N:592:GLY:HA2 | 1:P:499:ASN:HD22 | 1.75 | 0.51 |
| 1:U:254:ASN:O | 1:U:256:HIS:N | 2.43 | 0.51 |
| 1:X:503:PHE:CE2 | 1:e:451:THR:HG21 | 2.46 | 0.51 |
| 1:Z:529:HIS:ND1 | 1:Z:533:GLU:O | 2.42 | 0.51 |
| 1:g:254:ASN:O | 1:g:256:HIS:N | 2.43 | 0.51 |
| 1:g:328:GLN:NE2 | 1:g:333:LYS:HG3 | 2.24 | 0.51 |
| 1:q:592:GLY:HA2 | 1:r:499:ASN:HD22 | 1.75 | 0.51 |
| 1:r:609:TRP:CH2 | 1:r:631:PHE:CE2 | 2.98 | 0.51 |
| 1:w:583:ALA:O | 1:x:487:ARG:HD2 | 2.11 | 0.51 |
| 1:3:254:ASN:O | 1:3:256:HIS:N | 2.43 | 0.51 |
| 1:3:499:ASN:HD22 | 1:4:592:GLY:HA2 | 1.76 | 0.51 |
| 1:6:439:PRO:HB3 | 1:7:381:LEU:HD21 | 1.92 | 0.51 |
| 1:D:609:TRP:CH2 | 1:D:631:PHE:CE2 | 2.98 | 0.51 |
| 1:E:381:LEU:HD21 | 1:F:439:PRO:HB3 | 1.92 | 0.51 |
| 1:E:439:PRO:HB3 | 1:Q:381:LEU:HD21 | 1.93 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:503:PHE:CE2 | 1:F:451:THR:HG21 | 2.45 | 0.51 |
| 1:G:570:THR:OG1 | 1:G:571:THR:N | 2.43 | 0.51 |
| 1:I:286:ASP:O | 1:I:364:CYS:HA | 2.11 | 0.51 |
| 1:L:570:THR:OG1 | 1:L:571:THR:N | 2.43 | 0.51 |
| 1:N:583:ALA:HA | 1:N:595:VAL:HG12 | 1.92 | 0.51 |
| 1:O:439:PRO:HB3 | 1:m:381:LEU:HD21 | 1.93 | 0.51 |
| 1:O:499:ASN:HD22 | 1:n:592:GLY:HA2 | 1.76 | 0.51 |
| 1:Q:286:ASP:O | 1:Q:364:CYS:HA | 2.11 | 0.51 |
| 1:V:328:GLN:NE2 | 1:V:333:LYS:HG3 | 2.24 | 0.51 |
| 1:V:570:THR:OG1 | 1:V:571:THR:N | 2.43 | 0.51 |
| 1:W:451:THR:HG21 | 1:Y:503:PHE:CE2 | 2.46 | 0.51 |
| 1:Y:609:TRP:CH2 | 1:Y:631:PHE:CE2 | 2.98 | 0.51 |
| 1:Z:381:LEU:HD21 | 1:3:439:PRO:HB3 | 1.93 | 0.51 |
| 1:b:570:THR:OG1 | 1:b:571:THR:N | 2.43 | 0.51 |
| 1:c:286:ASP:O | 1:c:364:CYS:HA | 2.11 | 0.51 |
| 1:c:499:ASN:HD22 | 1:p:592:GLY:HA2 | 1.75 | 0.51 |
| 1:d:416:TYR:OH | 1:d:644:HIS:O | 2.27 | 0.51 |
| 1:g:434:ASP:OD1 | 1:g:434:ASP:N | 2.41 | 0.51 |
| 1:i:328:GLN:NE2 | 1:i:333:LYS:HG3 | 2.24 | 0.51 |
| 1:n:254:ASN:O | 1:n:256:HIS:N | 2.43 | 0.51 |
| 1:o:429:HIS:NE2 | 1:p:627:THR:HG22 | 2.26 | 0.51 |
| 1:o:570:THR:OG1 | 1:o:571:THR:N | 2.43 | 0.51 |
| 1:q:451:THR:HG21 | 1:r:503:PHE:CE2 | 2.46 | 0.51 |
| 1:s:583:ALA:HA | 1:s:595:VAL:HG12 | 1.92 | 0.51 |
| 1:t:407:ARG:HD3 | 1:y:224:SER:O | 2.10 | 0.51 |
| 1:t:451:THR:HG21 | 1:u:503:PHE:CE2 | 2.45 | 0.51 |
| 1:2:416:TYR:OH | 1:2:644:HIS:O | 2.27 | 0.51 |
| 1:5:381:LEU:HD21 | 1:7:439:PRO:HB3 | 1.93 | 0.51 |
| 1:6:340:THR:CB | 1:6:407:ARG:HH21 | 2.21 | 0.51 |
| 1:7:609:TRP:CH2 | 1:7:631:PHE:CE2 | 2.98 | 0.51 |
| 1:A:286:ASP:O | 1:A:364:CYS:HA | 2.11 | 0.51 |
| 1:A:570:THR:OG1 | 1:A:571:THR:N | 2.43 | 0.51 |
| 1:B:570:THR:OG1 | 1:B:571:THR:N | 2.43 | 0.51 |
| 1:C:570:THR:OG1 | 1:C:571:THR:N | 2.43 | 0.51 |
| 1:E:592:GLY:HA2 | 1:Q:499:ASN:HD22 | 1.75 | 0.51 |
| 1:E:609:TRP:CH2 | 1:E:631:PHE:CE2 | 2.98 | 0.51 |
| 1:F:499:ASN:HD22 | 1:Q:592:GLY:HA2 | 1.75 | 0.51 |
| 1:K:609:TRP:CH2 | 1:K:631:PHE:CE2 | 2.98 | 0.51 |
| 1:M:381:LEU:HD21 | 1:b:439:PRO:HB3 | 1.92 | 0.51 |
| 1:M:627:THR:HG22 | 1:b:429:HIS:NE2 | 2.26 | 0.51 |
| 1:Q:324:LYS:NZ | 1:Q:337:ASN:OD1 | 2.35 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:609:TRP:CH2 | 1:Q:631:PHE:CE2 | 2.98 | 0.51 |
| 1:R:381:LEU:HD21 | 1:U:439:PRO:HB3 | 1.93 | 0.51 |
| 1:S:286:ASP:O | 1:S:364:CYS:HA | 2.11 | 0.51 |
| 1:S:429:HIS:NE2 | 1:U:627:THR:HG22 | 2.26 | 0.51 |
| 1:T:258:TYR:OH | 1:T:399:GLU:OE1 | 2.22 | 0.51 |
| 1:T:609:TRP:CH2 | 1:T:631:PHE:CE2 | 2.98 | 0.51 |
| 1:V:627:THR:HG22 | 1:X:429:HIS:NE2 | 2.26 | 0.51 |
| 1:a:583:ALA:HA | 1:a:595:VAL:HG12 | 1.92 | 0.51 |
| 1:a:592:GLY:HA2 | 1:8:499:ASN:HD22 | 1.75 | 0.51 |
| 1:g:628:ASP:OD1 | 1:h:425:SER:HB3 | 2.10 | 0.51 |
| 1:h:583:ALA:HA | 1:h:595:VAL:HG12 | 1.92 | 0.51 |
| 1:i:254:ASN:O | 1:i:256:HIS:N | 2.43 | 0.51 |
| 1:o:286:ASP:O | 1:o:364:CYS:HA | 2.11 | 0.51 |
| 1:p:570:THR:OG1 | 1:p:571:THR:N | 2.43 | 0.51 |
| 1:u:429:HIS:NE2 | 1:v:627:THR:HG22 | 2.26 | 0.51 |
| 1:y:570:THR:OG1 | 1:y:571:THR:N | 2.43 | 0.51 |
| 1:z:232:ASP:OD1 | 1:z:232:ASP:N | 2.37 | 0.51 |
| 1:z:451:THR:HG21 | 1:1:503:PHE:CE2 | 2.46 | 0.51 |
| 1:1:583:ALA:HA | 1:1:595:VAL:HG12 | 1.92 | 0.51 |
| 1:1:609:TRP:CH2 | 1:1:631:PHE:CE2 | 2.98 | 0.51 |
| 1:4:286:ASP:O | 1:4:364:CYS:HA | 2.11 | 0.51 |
| 1:5:286:ASP:O | 1:5:364:CYS:HA | 2.11 | 0.51 |
| 1:5:609:TRP:CH2 | 1:5:631:PHE:CE2 | 2.98 | 0.51 |
| 1:6:286:ASP:O | 1:6:364:CYS:HA | 2.11 | 0.51 |
| 1:A:503:PHE:CE2 | 1:I:451:THR:HG21 | 2.46 | 0.51 |
| 1:B:286:ASP:O | 1:B:364:CYS:HA | 2.11 | 0.51 |
| 1:B:429:HIS:NE2 | 1:J:627:THR:HG22 | 2.26 | 0.51 |
| 1:B:439:PRO:HB3 | 1:J:381:LEU:HD21 | 1.92 | 0.51 |
| 1:D:381:LEU:HD21 | 1:P:439:PRO:HB3 | 1.93 | 0.51 |
| 1:F:286:ASP:O | 1:F:364:CYS:HA | 2.11 | 0.51 |
| 1:O:451:THR:HG21 | 1:m:503:PHE:CE2 | 2.46 | 0.51 |
| 1:T:381:LEU:HD21 | 1:l:439:PRO:HB3 | 1.92 | 0.51 |
| 1:U:286:ASP:O | 1:U:364:CYS:HA | 2.11 | 0.51 |
| 1:V:628:ASP:OD1 | 1:X:425:SER:HB3 | 2.10 | 0.51 |
| 1:Z:503:PHE:CE2 | 1:3:451:THR:HG21 | 2.46 | 0.51 |
| 1:c:451:THR:HG21 | 1:o:503:PHE:CE2 | 2.46 | 0.51 |
| 1:e:583:ALA:HA | 1:e:595:VAL:HG12 | 1.92 | 0.51 |
| 1:g:583:ALA:HA | 1:g:595:VAL:HG12 | 1.91 | 0.51 |
| 1:g:609:TRP:CH2 | 1:g:631:PHE:CE2 | 2.98 | 0.51 |
| 1:i:232:ASP:OD1 | 1:i:232:ASP:N | 2.37 | 0.51 |
| 1:i:583:ALA:HA | 1:i:595:VAL:HG12 | 1.92 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:609:TRP:CH2 | 1:j:631:PHE:CE2 | 2.98 | 0.51 |
| 1:n:286:ASP:O | 1:n:364:CYS:HA | 2.11 | 0.51 |
| 1:p:609:TRP:CH2 | 1:p:631:PHE:CE2 | 2.98 | 0.51 |
| 1:q:429:HIS:NE2 | 1:r:627:THR:HG22 | 2.26 | 0.51 |
| 1:t:381:LEU:HD21 | 1:v:439:PRO:HB3 | 1.93 | 0.51 |
| 1:t:503:PHE:CE2 | 1:v:451:THR:HG21 | 2.46 | 0.51 |
| 1:u:286:ASP:O | 1:u:364:CYS:HA | 2.11 | 0.51 |
| 1:v:224:SER:O | 1:w:407:ARG:HD3 | 2.11 | 0.51 |
| 1:v:286:ASP:O | 1:v:364:CYS:HA | 2.11 | 0.51 |
| 1:w:583:ALA:HA | 1:w:595:VAL:HG12 | 1.91 | 0.51 |
| 1:y:328:GLN:NE2 | 1:y:333:LYS:HG3 | 2.24 | 0.51 |
| 1:z:286:ASP:O | 1:z:364:CYS:HA | 2.11 | 0.51 |
| 1:z:439:PRO:HB3 | 1:1:381:LEU:HD21 | 1.93 | 0.51 |
| 1:z:503:PHE:CE2 | 1:2:451:THR:HG21 | 2.46 | 0.51 |
| 1:5:499:ASN:HD22 | 1:7:592:GLY:HA2 | 1.75 | 0.51 |
| 1:5:592:GLY:HA2 | 1:6:499:ASN:HD22 | 1.75 | 0.51 |
| 1:6:451:THR:HG21 | 1:7:503:PHE:CE2 | 2.45 | 0.51 |
| 1:8:609:TRP:CH2 | 1:8:631:PHE:CE2 | 2.98 | 0.51 |
| 1:B:503:PHE:CE2 | 1:L:451:THR:HG21 | 2.46 | 0.51 |
| 1:C:627:THR:HG22 | 1:M:429:HIS:NE2 | 2.26 | 0.51 |
| 1:E:499:ASN:HD22 | 1:F:592:GLY:HA2 | 1.75 | 0.51 |
| 1:F:627:THR:HG22 | 1:Q:429:HIS:NE2 | 2.26 | 0.51 |
| 1:G:609:TRP:CH2 | 1:G:631:PHE:CE2 | 2.98 | 0.51 |
| 1:H:286:ASP:O | 1:H:364:CYS:HA | 2.11 | 0.51 |
| 1:H:583:ALA:HA | 1:H:595:VAL:HG12 | 1.92 | 0.51 |
| 1:J:429:HIS:NE2 | 1:L:627:THR:HG22 | 2.26 | 0.51 |
| 1:K:381:LEU:HD21 | 1:8:439:PRO:HB3 | 1.93 | 0.51 |
| 1:P:609:TRP:CH2 | 1:P:631:PHE:CE2 | 2.98 | 0.51 |
| 1:R:451:THR:HG21 | 1:S:503:PHE:CE2 | 2.46 | 0.51 |
| 1:R:503:PHE:CE2 | 1:U:451:THR:HG21 | 2.46 | 0.51 |
| 1:S:592:GLY:HA2 | 1:U:499:ASN:HD22 | 1.75 | 0.51 |
| 1:T:503:PHE:CE2 | 1:l:451:THR:HG21 | 2.46 | 0.51 |
| 1:V:439:PRO:HB3 | 1:e:381:LEU:HD21 | 1.93 | 0.51 |
| 1:W:429:HIS:NE2 | 1:Y:627:THR:HG22 | 2.26 | 0.51 |
| 1:W:609:TRP:CD1 | 1:Y:629:GLY:CA | 2.85 | 0.51 |
| 1:Z:499:ASN:HD22 | 1:3:592:GLY:HA2 | 1.75 | 0.51 |
| 1:Z:627:THR:HG22 | 1:3:429:HIS:NE2 | 2.26 | 0.51 |
| 1:b:286:ASP:O | 1:b:364:CYS:HA | 2.11 | 0.51 |
| 1:d:451:THR:HG21 | 1:l:503:PHE:CE2 | 2.46 | 0.51 |
| 1:f:609:TRP:CH2 | 1:f:631:PHE:CE2 | 2.98 | 0.51 |
| 1:h:286:ASP:O | 1:h:364:CYS:HA | 2.11 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:583:ALA:HA | 1:j:595:VAL:HG12 | 1.92 | 0.51 |
| 1:k:286:ASP:O | 1:k:364:CYS:HA | 2.11 | 0.51 |
| 1:k:570:THR:OG1 | 1:k:571:THR:N | 2.43 | 0.51 |
| 1:k:583:ALA:HA | 1:k:595:VAL:HG12 | 1.92 | 0.51 |
| 1:l:286:ASP:O | 1:l:364:CYS:HA | 2.11 | 0.51 |
| 1:r:429:HIS:NE2 | 1:s:627:THR:HG22 | 2.26 | 0.51 |
| 1:s:286:ASP:O | 1:s:364:CYS:HA | 2.11 | 0.51 |
| 1:t:439:PRO:HB3 | 1:u:381:LEU:HD21 | 1.92 | 0.51 |
| 1:u:592:GLY:HA2 | 1:v:499:ASN:HD22 | 1.76 | 0.51 |
| 1:z:429:HIS:NE2 | 1:1:627:THR:HG22 | 2.26 | 0.51 |
| 1:3:286:ASP:O | 1:3:364:CYS:HA | 2.11 | 0.51 |
| 1:3:627:THR:HG22 | 1:4:429:HIS:NE2 | 2.26 | 0.51 |
| 1:4:490:ARG:HB2 | 1:4:576:THR:HB | 1.93 | 0.51 |
| 1:6:592:GLY:HA2 | 1:7:499:ASN:HD22 | 1.75 | 0.51 |
| 1:C:451:THR:HG21 | 1:b:503:PHE:CE2 | 2.46 | 0.51 |
| 1:G:439:PRO:HB3 | 1:I:381:LEU:HD21 | 1.93 | 0.51 |
| 1:G:451:THR:HG21 | 1:I:503:PHE:CE2 | 2.46 | 0.51 |
| 1:H:439:PRO:HB3 | 1:W:381:LEU:HD21 | 1.92 | 0.51 |
| 1:H:627:THR:HG22 | 1:Y:429:HIS:NE2 | 2.26 | 0.51 |
| 1:J:570:THR:OG1 | 1:J:571:THR:N | 2.43 | 0.51 |
| 1:K:451:THR:HG21 | 1:a:503:PHE:CE2 | 2.46 | 0.51 |
| 1:O:286:ASP:O | 1:O:364:CYS:HA | 2.11 | 0.51 |
| 1:O:429:HIS:NE2 | 1:m:627:THR:HG22 | 2.26 | 0.51 |
| 1:O:592:GLY:HA2 | 1:m:499:ASN:HD22 | 1.75 | 0.51 |
| 1:O:627:THR:HG22 | 1:n:429:HIS:NE2 | 2.26 | 0.51 |
| 1:P:286:ASP:O | 1:P:364:CYS:HA | 2.11 | 0.51 |
| 1:Q:328:GLN:NE2 | 1:Q:333:LYS:HG3 | 2.24 | 0.51 |
| 1:R:439:PRO:HB3 | 1:S:381:LEU:HD21 | 1.92 | 0.51 |
| 1:T:627:THR:HG22 | 1:l:429:HIS:NE2 | 2.26 | 0.51 |
| 1:c:328:GLN:NE2 | 1:c:333:LYS:HG3 | 2.24 | 0.51 |
| 1:c:503:PHE:CE2 | 1:p:451:THR:HG21 | 2.46 | 0.51 |
| 1:f:583:ALA:HA | 1:f:595:VAL:HG12 | 1.92 | 0.51 |
| 1:f:592:GLY:HA2 | 1:h:499:ASN:HD22 | 1.75 | 0.51 |
| 1:g:286:ASP:O | 1:g:364:CYS:HA | 2.11 | 0.51 |
| 1:g:503:PHE:CE2 | 1:h:451:THR:HG21 | 2.46 | 0.51 |
| 1:g:570:THR:OG1 | 1:g:571:THR:N | 2.43 | 0.51 |
| 1:h:490:ARG:HB2 | 1:h:576:THR:HB | 1.93 | 0.51 |
| 1:i:439:PRO:HB3 | 1:j:381:LEU:HD21 | 1.92 | 0.51 |
| 1:i:503:PHE:CE2 | 1:k:451:THR:HG21 | 2.46 | 0.51 |
| 1:i:609:TRP:CH2 | 1:i:631:PHE:CE2 | 2.98 | 0.51 |
| 1:i:627:THR:HG22 | 1:k:429:HIS:NE2 | 2.26 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:429:HIS:NE2 | 1:k:627:THR:HG22 | 2.26 | 0.51 |
| 1:j:609:TRP:CD1 | 1:k:629:GLY:CA | 2.85 | 0.51 |
| 1:k:609:TRP:CH2 | 1:k:631:PHE:CE2 | 2.98 | 0.51 |
| 1:l:490:ARG:HB2 | 1:l:576:THR:HB | 1.93 | 0.51 |
| 1:n:490:ARG:HB2 | 1:n:576:THR:HB | 1.93 | 0.51 |
| 1:p:286:ASP:O | 1:p:364:CYS:HA | 2.11 | 0.51 |
| 1:q:503:PHE:CE2 | 1:s:451:THR:HG21 | 2.45 | 0.51 |
| 1:u:451:THR:HG21 | 1:v:503:PHE:CE2 | 2.46 | 0.51 |
| 1:x:429:HIS:NE2 | 1:y:627:THR:HG22 | 2.26 | 0.51 |
| 1:z:490:ARG:HB2 | 1:z:576:THR:HB | 1.93 | 0.51 |
| 1:5:328:GLN:NE2 | 1:5:333:LYS:HG3 | 2.24 | 0.51 |
| 1:5:429:HIS:NE2 | 1:6:627:THR:HG22 | 2.26 | 0.51 |
| 1:C:307:TRP:O | 1:C:426:SER:CB | 2.59 | 0.51 |
| 1:D:258:TYR:OH | 1:D:399:GLU:OE1 | 2.22 | 0.51 |
| 1:D:451:THR:HG21 | 1:N:503:PHE:CE2 | 2.46 | 0.51 |
| 1:F:503:PHE:CE2 | 1:Q:451:THR:HG21 | 2.46 | 0.51 |
| 1:G:286:ASP:O | 1:G:364:CYS:HA | 2.11 | 0.51 |
| 1:I:328:GLN:NE2 | 1:I:333:LYS:HG3 | 2.24 | 0.51 |
| 1:J:286:ASP:O | 1:J:364:CYS:HA | 2.11 | 0.51 |
| 1:J:328:GLN:NE2 | 1:J:333:LYS:HG3 | 2.24 | 0.51 |
| 1:J:439:PRO:HB3 | 1:L:381:LEU:HD21 | 1.93 | 0.51 |
| 1:J:451:THR:HG21 | 1:L:503:PHE:CE2 | 2.46 | 0.51 |
| 1:L:307:TRP:O | 1:L:426:SER:CB | 2.59 | 0.51 |
| 1:M:328:GLN:NE2 | 1:M:333:LYS:HG3 | 2.24 | 0.51 |
| 1:M:570:THR:OG1 | 1:M:571:THR:N | 2.43 | 0.51 |
| 1:N:609:TRP:NE1 | 1:P:629:GLY:CA | 2.58 | 0.51 |
| 1:O:416:TYR:OH | 1:O:644:HIS:O | 2.27 | 0.51 |
| 1:P:490:ARG:HB2 | 1:P:576:THR:HB | 1.93 | 0.51 |
| 1:Q:346:PHE:HB3 | 1:Q:403:SER:HA | 1.93 | 0.51 |
| 1:Q:570:THR:OG1 | 1:Q:571:THR:N | 2.43 | 0.51 |
| 1:U:328:GLN:NE2 | 1:U:333:LYS:HG3 | 2.24 | 0.51 |
| 1:V:503:PHE:CE2 | 1:X:451:THR:HG21 | 2.46 | 0.51 |
| 1:W:439:PRO:HB3 | 1:Y:381:LEU:HD21 | 1.93 | 0.51 |
| 1:c:381:LEU:HD21 | 1:p:439:PRO:HB3 | 1.93 | 0.51 |
| 1:e:609:TRP:CH2 | 1:e:631:PHE:CE2 | 2.98 | 0.51 |
| 1:f:381:LEU:HD21 | 1:g:439:PRO:HB3 | 1.92 | 0.51 |
| 1:f:429:HIS:NE2 | 1:h:627:THR:HG22 | 2.26 | 0.51 |
| 1:g:627:THR:HG22 | 1:h:429:HIS:NE2 | 2.26 | 0.51 |
| 1:h:570:THR:OG1 | 1:h:571:THR:N | 2.43 | 0.51 |
| 1:i:286:ASP:O | 1:i:364:CYS:HA | 2.11 | 0.51 |
| 1:j:592:GLY:HA2 | 1:k:499:ASN:HD22 | 1.75 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:k:490:ARG:HB2 | 1:k:576:THR:HB | 1.93 | 0.51 |
| 1:q:381:LEU:HD21 | 1:s:439:PRO:HB3 | 1.92 | 0.51 |
| 1:q:439:PRO:HB3 | 1:r:381:LEU:HD21 | 1.93 | 0.51 |
| 1:s:346:PHE:HB3 | 1:s:403:SER:HA | 1.93 | 0.51 |
| 1:t:490:ARG:HB2 | 1:t:576:THR:HB | 1.93 | 0.51 |
| 1:3:629:GLY:CA | 1:4:609:TRP:NE1 | 2.58 | 0.51 |
| 1:7:490:ARG:HB2 | 1:7:576:THR:HB | 1.93 | 0.51 |
| 1:8:286:ASP:O | 1:8:364:CYS:HA | 2.11 | 0.51 |
| 1:A:346:PHE:HB3 | 1:A:403:SER:HA | 1.93 | 0.50 |
| 1:C:381:LEU:HD21 | 1:M:439:PRO:HB3 | 1.93 | 0.50 |
| 1:C:503:PHE:CE2 | 1:M:451:THR:HG21 | 2.46 | 0.50 |
| 1:E:609:TRP:CD1 | 1:Q:629:GLY:CA | 2.85 | 0.50 |
| 1:H:451:THR:HG21 | 1:W:503:PHE:CE2 | 2.45 | 0.50 |
| 1:H:503:PHE:CE2 | 1:Y:451:THR:HG21 | 2.45 | 0.50 |
| 1:M:286:ASP:O | 1:M:364:CYS:HA | 2.11 | 0.50 |
| 1:N:439:PRO:HB3 | 1:P:381:LEU:HD21 | 1.93 | 0.50 |
| 1:R:286:ASP:O | 1:R:364:CYS:HA | 2.11 | 0.50 |
| 1:S:258:TYR:OH | 1:S:399:GLU:OE1 | 2.22 | 0.50 |
| 1:S:451:THR:HG21 | 1:U:503:PHE:CE2 | 2.45 | 0.50 |
| 1:Y:286:ASP:O | 1:Y:364:CYS:HA | 2.11 | 0.50 |
| 1:a:439:PRO:HB3 | 1:8:381:LEU:HD21 | 1.93 | 0.50 |
| 1:a:609:TRP:NE1 | 1:8:629:GLY:CA | 2.58 | 0.50 |
| 1:c:490:ARG:HB2 | 1:c:576:THR:HB | 1.93 | 0.50 |
| 1:d:307:TRP:O | 1:d:426:SER:CB | 2.59 | 0.50 |
| 1:f:286:ASP:O | 1:f:364:CYS:HA | 2.11 | 0.50 |
| 1:i:570:THR:OG1 | 1:i:571:THR:N | 2.43 | 0.50 |
| 1:j:286:ASP:O | 1:j:364:CYS:HA | 2.11 | 0.50 |
| 1:m:439:PRO:HB3 | 1:n:381:LEU:HD21 | 1.92 | 0.50 |
| 1:m:583:ALA:HA | 1:m:595:VAL:HG12 | 1.92 | 0.50 |
| 1:t:286:ASP:O | 1:t:364:CYS:HA | 2.11 | 0.50 |
| 1:w:609:TRP:CH2 | 1:w:631:PHE:CE2 | 2.98 | 0.50 |
| 1:2:307:TRP:O | 1:2:426:SER:CB | 2.59 | 0.50 |
| 1:3:490:ARG:HB2 | 1:3:576:THR:HB | 1.93 | 0.50 |
| 1:5:346:PHE:HB3 | 1:5:403:SER:HA | 1.93 | 0.50 |
| 1:5:451:THR:HG21 | 1:6:503:PHE:CE2 | 2.46 | 0.50 |
| 1:8:490:ARG:HB2 | 1:8:576:THR:HB | 1.93 | 0.50 |
| 1:B:451:THR:HG21 | 1:J:503:PHE:CE2 | 2.46 | 0.50 |
| 1:C:490:ARG:HB2 | 1:C:576:THR:HB | 1.93 | 0.50 |
| 1:E:490:ARG:HB2 | 1:E:576:THR:HB | 1.93 | 0.50 |
| 1:G:490:ARG:HB2 | 1:G:576:THR:HB | 1.93 | 0.50 |
| 1:H:346:PHE:HB3 | 1:H:403:SER:HA | 1.93 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:490:ARG:HB2 | 1:H:576:THR:HB | 1.93 | 0.50 |
| 1:I:490:ARG:HB2 | 1:I:576:THR:HB | 1.93 | 0.50 |
| 1:K:258:TYR:OH | 1:K:399:GLU:OE1 | 2.22 | 0.50 |
| 1:K:592:GLY:HA2 | 1:a:499:ASN:HD22 | 1.75 | 0.50 |
| 1:L:490:ARG:HB2 | 1:L:576:THR:HB | 1.93 | 0.50 |
| 1:M:503:PHE:CE2 | 1:b:451:THR:HG21 | 2.46 | 0.50 |
| 1:P:583:ALA:HA | 1:P:595:VAL:HG12 | 1.92 | 0.50 |
| 1:T:429:HIS:NE2 | 1:d:627:THR:HG22 | 2.26 | 0.50 |
| 1:T:451:THR:HG21 | 1:d:503:PHE:CE2 | 2.46 | 0.50 |
| 1:b:416:TYR:OH | 1:b:644:HIS:O | 2.27 | 0.50 |
| 1:c:429:HIS:NE2 | 1:o:627:THR:HG22 | 2.26 | 0.50 |
| 1:c:609:TRP:CD1 | 1:o:629:GLY:CA | 2.85 | 0.50 |
| 1:d:346:PHE:HB3 | 1:d:403:SER:HA | 1.93 | 0.50 |
| 1:d:429:HIS:NE2 | 1:l:627:THR:HG22 | 2.26 | 0.50 |
| 1:f:503:PHE:CE2 | 1:g:451:THR:HG21 | 2.46 | 0.50 |
| 1:f:609:TRP:CD1 | 1:h:629:GLY:CA | 2.85 | 0.50 |
| 1:h:609:TRP:CH2 | 1:h:631:PHE:CE2 | 2.98 | 0.50 |
| 1:i:451:THR:HG21 | 1:j:503:PHE:CE2 | 2.46 | 0.50 |
| 1:k:346:PHE:HB3 | 1:k:403:SER:HA | 1.93 | 0.50 |
| 1:p:490:ARG:HB2 | 1:p:576:THR:HB | 1.93 | 0.50 |
| 1:s:490:ARG:HB2 | 1:s:576:THR:HB | 1.93 | 0.50 |
| 1:u:258:TYR:OH | 1:u:399:GLU:OE1 | 2.22 | 0.50 |
| 1:v:328:GLN:NE2 | 1:v:333:LYS:HG3 | 2.24 | 0.50 |
| 1:x:346:PHE:HB3 | 1:x:403:SER:HA | 1.93 | 0.50 |
| 1:z:592:GLY:HA2 | 1:1:499:ASN:HD22 | 1.75 | 0.50 |
| 1:z:627:THR:HG22 | 1:2:429:HIS:NE2 | 2.26 | 0.50 |
| 1:2:346:PHE:HB3 | 1:2:403:SER:HA | 1.93 | 0.50 |
| 1:5:570:THR:OG1 | 1:5:571:THR:N | 2.43 | 0.50 |
| 1:5:629:GLY:CA | 1:7:609:TRP:CD1 | 2.85 | 0.50 |
| 1:B:416:TYR:OH | 1:B:644:HIS:O | 2.27 | 0.50 |
| 1:F:324:LYS:NZ | 1:F:337:ASN:OD1 | 2.35 | 0.50 |
| 1:G:328:GLN:NE2 | 1:G:333:LYS:HG3 | 2.24 | 0.50 |
| 1:H:340:THR:HB | 1:H:407:ARG:NH2 | 2.27 | 0.50 |
| 1:O:490:ARG:HB2 | 1:O:576:THR:HB | 1.94 | 0.50 |
| 1:P:346:PHE:HB3 | 1:P:403:SER:HA | 1.93 | 0.50 |
| 1:R:490:ARG:HB2 | 1:R:576:THR:HB | 1.94 | 0.50 |
| 1:T:340:THR:HB | 1:T:407:ARG:NH2 | 2.27 | 0.50 |
| 1:T:439:PRO:HB3 | 1:d:381:LEU:HD21 | 1.93 | 0.50 |
| 1:T:499:ASN:HD22 | 1:l:592:GLY:HA2 | 1.75 | 0.50 |
| 1:X:346:PHE:HB3 | 1:X:403:SER:HA | 1.94 | 0.50 |
| 1:X:381:LEU:HD21 | 1:e:439:PRO:HB3 | 1.93 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z:439:PRO:HB3 | 1:4:381:LEU:HD21 | 1.92 | 0.50 |
| 1:Z:583:ALA:HA | 1:Z:595:VAL:HG12 | 1.92 | 0.50 |
| 1:i:499:ASN:HD22 | 1:k:592:GLY:HA2 | 1.75 | 0.50 |
| 1:o:346:PHE:HB3 | 1:o:403:SER:HA | 1.93 | 0.50 |
| 1:o:490:ARG:HB2 | 1:o:576:THR:HB | 1.93 | 0.50 |
| 1:p:328:GLN:NE2 | 1:p:333:LYS:HG3 | 2.24 | 0.50 |
| 1:q:609:TRP:CD1 | 1:r:629:GLY:CA | 2.85 | 0.50 |
| 1:r:286:ASP:O | 1:r:364:CYS:HA | 2.11 | 0.50 |
| 1:r:451:THR:HG21 | 1:s:503:PHE:CE2 | 2.45 | 0.50 |
| 1:s:340:THR:HB | 1:s:407:ARG:NH2 | 2.27 | 0.50 |
| 1:w:286:ASP:O | 1:w:364:CYS:HA | 2.11 | 0.50 |
| 1:w:490:ARG:NH1 | 1:y:586:LEU:HD21 | 2.26 | 0.50 |
| 1:1:340:THR:HB | 1:1:407:ARG:NH2 | 2.27 | 0.50 |
| 1:1:429:HIS:NE2 | 1:2:627:THR:HG22 | 2.26 | 0.50 |
| 1:1:439:PRO:HB3 | 1:2:381:LEU:HD21 | 1.93 | 0.50 |
| 1:1:451:THR:HG21 | 1:2:503:PHE:CE2 | 2.46 | 0.50 |
| 1:3:416:TYR:OH | 1:3:644:HIS:O | 2.27 | 0.50 |
| 1:4:340:THR:CB | 1:4:407:ARG:HH21 | 2.21 | 0.50 |
| 1:7:340:THR:HB | 1:7:407:ARG:NH2 | 2.27 | 0.50 |
| 1:8:346:PHE:HB3 | 1:8:403:SER:HA | 1.93 | 0.50 |
| 1:8:583:ALA:HA | 1:8:595:VAL:HG12 | 1.92 | 0.50 |
| 1:A:429:HIS:NE2 | 1:G:627:THR:HG22 | 2.27 | 0.50 |
| 1:A:490:ARG:HB2 | 1:A:576:THR:HB | 1.93 | 0.50 |
| 1:B:346:PHE:HB3 | 1:B:403:SER:HA | 1.93 | 0.50 |
| 1:D:592:GLY:HA2 | 1:N:499:ASN:HD22 | 1.75 | 0.50 |
| 1:E:340:THR:HB | 1:E:407:ARG:NH2 | 2.27 | 0.50 |
| 1:E:627:THR:HG22 | 1:F:429:HIS:NE2 | 2.26 | 0.50 |
| 1:X:490:ARG:HB2 | 1:X:576:THR:HB | 1.93 | 0.50 |
| 1:a:340:THR:HB | 1:a:407:ARG:NH2 | 2.27 | 0.50 |
| 1:f:425:SER:HB3 | 1:h:628:ASP:OD1 | 2.10 | 0.50 |
| 1:g:490:ARG:HB2 | 1:g:576:THR:HB | 1.93 | 0.50 |
| 1:g:499:ASN:HD22 | 1:h:592:GLY:HA2 | 1.75 | 0.50 |
| 1:h:328:GLN:NE2 | 1:h:333:LYS:HG3 | 2.24 | 0.50 |
| 1:h:346:PHE:HB3 | 1:h:403:SER:HA | 1.93 | 0.50 |
| 1:i:429:HIS:NE2 | 1:j:627:THR:HG22 | 2.26 | 0.50 |
| 1:i:490:ARG:HB2 | 1:i:576:THR:HB | 1.93 | 0.50 |
| 1:j:425:SER:HB3 | 1:k:628:ASP:OD1 | 2.10 | 0.50 |
| 1:r:416:TYR:OH | 1:r:644:HIS:O | 2.27 | 0.50 |
| 1:w:636:LEU:HD11 | 1:y:481:LEU:CD1 | 2.41 | 0.50 |
| 1:x:490:ARG:HB2 | 1:x:576:THR:HB | 1.94 | 0.50 |
| 1:4:340:THR:HB | 1:4:407:ARG:NH2 | 2.27 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:7:346:PHE:HB3 | 1:7:403:SER:HA | 1.93 | 0.50 |
| 1:A:439:PRO:HB3 | 1:G:381:LEU:HD21 | 1.92 | 0.50 |
| 1:E:346:PHE:HB3 | 1:E:403:SER:HA | 1.93 | 0.50 |
| 1:H:592:GLY:HA2 | 1:W:499:ASN:HD22 | 1.76 | 0.50 |
| 1:N:340:THR:HB | 1:N:407:ARG:NH2 | 2.27 | 0.50 |
| 1:N:429:HIS:NE2 | 1:P:627:THR:HG22 | 2.26 | 0.50 |
| 1:O:381:LEU:HD21 | 1:n:439:PRO:HB3 | 1.92 | 0.50 |
| 1:P:328:GLN:NE2 | 1:P:333:LYS:HG3 | 2.24 | 0.50 |
| 1:S:570:THR:OG1 | 1:S:571:THR:N | 2.43 | 0.50 |
| 1:U:346:PHE:HB3 | 1:U:403:SER:HA | 1.93 | 0.50 |
| 1:U:490:ARG:HB2 | 1:U:576:THR:HB | 1.93 | 0.50 |
| 1:W:490:ARG:HB2 | 1:W:576:THR:HB | 1.93 | 0.50 |
| 1:X:627:THR:HG22 | 1:e:429:HIS:NE2 | 2.26 | 0.50 |
| 1:Y:328:GLN:NE2 | 1:Y:333:LYS:HG3 | 2.24 | 0.50 |
| 1:Z:429:HIS:NE2 | 1:4:627:THR:HG22 | 2.26 | 0.50 |
| 1:a:451:THR:HG21 | 1:8:503:PHE:CE2 | 2.46 | 0.50 |
| 1:b:346:PHE:HB3 | 1:b:403:SER:HA | 1.93 | 0.50 |
| 1:d:592:GLY:HA2 | 1:l:499:ASN:HD22 | 1.75 | 0.50 |
| 1:e:286:ASP:O | 1:e:364:CYS:HA | 2.11 | 0.50 |
| 1:f:627:THR:HG22 | 1:g:429:HIS:NE2 | 2.26 | 0.50 |
| 1:j:340:THR:HB | 1:j:407:ARG:NH2 | 2.27 | 0.50 |
| 1:k:328:GLN:NE2 | 1:k:333:LYS:HG3 | 2.24 | 0.50 |
| 1:m:592:GLY:HA2 | 1:n:499:ASN:HD22 | 1.75 | 0.50 |
| 1:n:328:GLN:NE2 | 1:n:333:LYS:HG3 | 2.24 | 0.50 |
| 1:n:340:THR:HB | 1:n:407:ARG:NH2 | 2.27 | 0.50 |
| 1:q:490:ARG:HB2 | 1:q:576:THR:HB | 1.93 | 0.50 |
| 1:u:570:THR:OG1 | 1:u:571:THR:N | 2.43 | 0.50 |
| 1:z:381:LEU:HD21 | 1:2:439:PRO:HB3 | 1.93 | 0.50 |
| 1:2:286:ASP:O | 1:2:364:CYS:HA | 2.11 | 0.50 |
| 1:2:340:THR:CB | 1:2:407:ARG:HH21 | 2.20 | 0.50 |
| 1:6:429:HIS:NE2 | 1:7:627:THR:HG22 | 2.26 | 0.50 |
| 1:8:340:THR:HB | 1:8:407:ARG:NH2 | 2.27 | 0.50 |
| 1:C:429:HIS:NE2 | 1:b:627:THR:HG22 | 2.26 | 0.50 |
| 1:G:346:PHE:HB3 | 1:G:403:SER:HA | 1.93 | 0.50 |
| 1:N:451:THR:HG21 | 1:P:503:PHE:CE2 | 2.46 | 0.50 |
| 1:P:340:THR:HB | 1:P:407:ARG:NH2 | 2.27 | 0.50 |
| 1:S:340:THR:HB | 1:S:407:ARG:NH2 | 2.27 | 0.50 |
| 1:V:429:HIS:NE2 | 1:e:627:THR:HG22 | 2.26 | 0.50 |
| 1:V:499:ASN:HD22 | 1:X:592:GLY:HA2 | 1.75 | 0.50 |
| 1:X:315:ASN:OD1 | 1:X:316:PHE:N | 2.45 | 0.50 |
| 1:e:416:TYR:OH | 1:e:644:HIS:O | 2.27 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:f:439:PRO:HB3 | 1:h:381:LEU:HD21 | 1.93 | 0.50 |
| 1:h:340:THR:HB | 1:h:407:ARG:NH2 | 2.27 | 0.50 |
| 1:j:439:PRO:HB3 | 1:k:381:LEU:HD21 | 1.93 | 0.50 |
| 1:j:570:THR:OG1 | 1:j:571:THR:N | 2.43 | 0.50 |
| 1:k:340:THR:HB | 1:k:407:ARG:NH2 | 2.27 | 0.50 |
| 1:m:429:HIS:NE2 | 1:n:627:THR:HG22 | 2.26 | 0.50 |
| 1:n:340:THR:CB | 1:n:407:ARG:HH21 | 2.21 | 0.50 |
| 1:p:346:PHE:HB3 | 1:p:403:SER:HA | 1.93 | 0.50 |
| 1:r:328:GLN:NE2 | 1:r:333:LYS:HG3 | 2.24 | 0.50 |
| 1:t:346:PHE:HB3 | 1:t:403:SER:HA | 1.93 | 0.50 |
| 1:v:490:ARG:HB2 | 1:v:576:THR:HB | 1.93 | 0.50 |
| 1:x:315:ASN:OD1 | 1:x:316:PHE:N | 2.45 | 0.50 |
| 1:x:425:SER:HB3 | 1:y:628:ASP:OD1 | 2.11 | 0.50 |
| 1:3:381:LEU:HD21 | 1:4:439:PRO:HB3 | 1.92 | 0.50 |
| 1:5:429:HIS:NE2 | 1:5:610:GLN:OE1 | 2.45 | 0.50 |
| 1:6:416:TYR:OH | 1:6:644:HIS:O | 2.27 | 0.50 |
| 1:7:286:ASP:O | 1:7:364:CYS:HA | 2.11 | 0.50 |
| 1:8:328:GLN:NE2 | 1:8:333:LYS:HG3 | 2.24 | 0.50 |
| 1:D:429:HIS:NE2 | 1:N:627:THR:HG22 | 2.26 | 0.50 |
| 1:E:286:ASP:O | 1:E:364:CYS:HA | 2.11 | 0.50 |
| 1:E:315:ASN:OD1 | 1:E:316:PHE:N | 2.45 | 0.50 |
| 1:F:346:PHE:HB3 | 1:F:403:SER:HA | 1.93 | 0.50 |
| 1:G:429:HIS:NE2 | 1:I:627:THR:HG22 | 2.26 | 0.50 |
| 1:H:499:ASN:HD22 | 1:Y:592:GLY:HA2 | 1.75 | 0.50 |
| 1:M:315:ASN:OD1 | 1:M:316:PHE:N | 2.45 | 0.50 |
| 1:N:346:PHE:HB3 | 1:N:403:SER:HA | 1.93 | 0.50 |
| 1:Q:340:THR:HB | 1:Q:407:ARG:NH2 | 2.27 | 0.50 |
| 1:Q:429:HIS:NE2 | 1:Q:610:GLN:OE1 | 2.45 | 0.50 |
| 1:R:346:PHE:HB3 | 1:R:403:SER:HA | 1.93 | 0.50 |
| 1:V:315:ASN:OD1 | 1:V:316:PHE:N | 2.45 | 0.50 |
| 1:X:340:THR:HB | 1:X:407:ARG:NH2 | 2.27 | 0.50 |
| 1:Y:416:TYR:OH | 1:Y:644:HIS:O | 2.27 | 0.50 |
| 1:Z:286:ASP:O | 1:Z:364:CYS:HA | 2.11 | 0.50 |
| 1:Z:490:ARG:HB2 | 1:Z:576:THR:HB | 1.93 | 0.50 |
| 1:Z:592:GLY:HA2 | 1:4:499:ASN:HD22 | 1.75 | 0.50 |
| 1:a:429:HIS:NE2 | 1:8:627:THR:HG22 | 2.26 | 0.50 |
| 1:d:286:ASP:O | 1:d:364:CYS:HA | 2.11 | 0.50 |
| 1:d:340:THR:CB | 1:d:407:ARG:HH21 | 2.20 | 0.50 |
| 1:d:439:PRO:HB3 | 1:l:381:LEU:HD21 | 1.93 | 0.50 |
| 1:f:315:ASN:OD1 | 1:f:316:PHE:N | 2.45 | 0.50 |
| 1:g:346:PHE:HB3 | 1:g:403:SER:HA | 1.93 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:h:315:ASN:OD1 | 1:h:316:PHE:N | 2.45 | 0.50 |
| 1:i:346:PHE:HB3 | 1:i:403:SER:HA | 1.93 | 0.50 |
| 1:k:315:ASN:OD1 | 1:k:316:PHE:N | 2.45 | 0.50 |
| 1:m:286:ASP:O | 1:m:364:CYS:HA | 2.11 | 0.50 |
| 1:r:592:GLY:HA2 | 1:s:499:ASN:HD22 | 1.75 | 0.50 |
| 1:t:570:THR:OG1 | 1:t:571:THR:N | 2.43 | 0.50 |
| 1:u:340:THR:HB | 1:u:407:ARG:NH2 | 2.27 | 0.50 |
| 1:v:346:PHE:HB3 | 1:v:403:SER:HA | 1.93 | 0.50 |
| 1:y:315:ASN:OD1 | 1:y:316:PHE:N | 2.45 | 0.50 |
| 1:z:499:ASN:HD22 | 1:2:592:GLY:HA2 | 1.75 | 0.50 |
| 1:5:300:GLN:NE2 | 1:5:703:TYR:O | 2.45 | 0.50 |
| 1:5:416:TYR:OH | 1:5:644:HIS:O | 2.27 | 0.50 |
| 1:7:315:ASN:OD1 | 1:7:316:PHE:N | 2.45 | 0.50 |
| 1:B:340:THR:HB | 1:B:407:ARG:NH2 | 2.27 | 0.50 |
| 1:B:627:THR:HG22 | 1:L:429:HIS:NE2 | 2.26 | 0.50 |
| 1:E:258:TYR:OH | 1:E:399:GLU:OE1 | 2.22 | 0.50 |
| 1:F:381:LEU:HD21 | 1:Q:439:PRO:HB3 | 1.92 | 0.50 |
| 1:F:416:TYR:OH | 1:F:644:HIS:O | 2.27 | 0.50 |
| 1:F:490:ARG:HB2 | 1:F:576:THR:HB | 1.94 | 0.50 |
| 1:J:315:ASN:OD1 | 1:J:316:PHE:N | 2.45 | 0.50 |
| 1:K:429:HIS:NE2 | 1:a:627:THR:HG22 | 2.26 | 0.50 |
| 1:K:627:THR:HG22 | 1:8:429:HIS:NE2 | 2.26 | 0.50 |
| 1:N:328:GLN:NE2 | 1:N:333:LYS:HG3 | 2.24 | 0.50 |
| 1:Q:416:TYR:OH | 1:Q:644:HIS:O | 2.27 | 0.50 |
| 1:R:429:HIS:NE2 | 1:S:627:THR:HG22 | 2.26 | 0.50 |
| 1:R:570:THR:OG1 | 1:R:571:THR:N | 2.43 | 0.50 |
| 1:S:315:ASN:OD1 | 1:S:316:PHE:N | 2.45 | 0.50 |
| 1:S:609:TRP:CD1 | 1:U:629:GLY:CA | 2.85 | 0.50 |
| 1:T:490:ARG:HB2 | 1:T:576:THR:HB | 1.93 | 0.50 |
| 1:U:340:THR:HB | 1:U:407:ARG:NH2 | 2.27 | 0.50 |
| 1:V:381:LEU:HD21 | 1:X:439:PRO:HB3 | 1.93 | 0.50 |
| 1:W:286:ASP:O | 1:W:364:CYS:HA | 2.11 | 0.50 |
| 1:X:628:ASP:OD1 | 1:e:425:SER:HB3 | 2.10 | 0.50 |
| 1:Z:429:HIS:NE2 | 1:Z:610:GLN:OE1 | 2.45 | 0.50 |
| 1:a:328:GLN:NE2 | 1:a:333:LYS:HG3 | 2.24 | 0.50 |
| 1:a:346:PHE:HB3 | 1:a:403:SER:HA | 1.94 | 0.50 |
| 1:b:340:THR:HB | 1:b:407:ARG:NH2 | 2.27 | 0.50 |
| 1:c:627:THR:HG22 | 1:p:429:HIS:NE2 | 2.26 | 0.50 |
| 1:e:315:ASN:OD1 | 1:e:316:PHE:N | 2.45 | 0.50 |
| 1:e:490:ARG:HB2 | 1:e:576:THR:HB | 1.93 | 0.50 |
| 1:f:340:THR:HB | 1:f:407:ARG:NH2 | 2.27 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:315:ASN:OD1 | 1:j:316:PHE:N | 2.45 | 0.50 |
| 1:m:490:ARG:HB2 | 1:m:576:THR:HB | 1.93 | 0.50 |
| 1:q:340:THR:HB | 1:q:407:ARG:NH2 | 2.27 | 0.50 |
| 1:q:499:ASN:HD22 | 1:s:592:GLY:HA2 | 1.76 | 0.50 |
| 1:u:315:ASN:OD1 | 1:u:316:PHE:N | 2.45 | 0.50 |
| 1:w:315:ASN:OD1 | 1:w:316:PHE:N | 2.45 | 0.50 |
| 1:w:416:TYR:OH | 1:w:644:HIS:O | 2.27 | 0.50 |
| 1:x:340:THR:HB | 1:x:407:ARG:NH2 | 2.27 | 0.50 |
| 1:z:346:PHE:HB3 | 1:z:403:SER:HA | 1.93 | 0.50 |
| 1:4:328:GLN:NE2 | 1:4:333:LYS:HG3 | 2.24 | 0.50 |
| 1:5:340:THR:HB | 1:5:407:ARG:NH2 | 2.27 | 0.50 |
| 1:6:346:PHE:HB3 | 1:6:403:SER:HA | 1.93 | 0.50 |
| 1:A:627:THR:HG22 | 1:I:429:HIS:NE2 | 2.27 | 0.50 |
| 1:B:429:HIS:NE2 | 1:B:610:GLN:OE1 | 2.45 | 0.50 |
| 1:D:627:THR:HG22 | 1:P:429:HIS:NE2 | 2.26 | 0.50 |
| 1:E:429:HIS:NE2 | 1:E:610:GLN:OE1 | 2.45 | 0.50 |
| 1:L:315:ASN:OD1 | 1:L:316:PHE:N | 2.45 | 0.50 |
| 1:Q:490:ARG:HB2 | 1:Q:576:THR:HB | 1.94 | 0.50 |
| 1:T:315:ASN:OD1 | 1:T:316:PHE:N | 2.45 | 0.50 |
| 1:V:340:THR:HB | 1:V:407:ARG:NH2 | 2.27 | 0.50 |
| 1:V:629:GLY:CA | 1:X:609:TRP:CD1 | 2.85 | 0.50 |
| 1:X:629:GLY:CA | 1:e:609:TRP:NE1 | 2.58 | 0.50 |
| 1:Z:328:GLN:NE2 | 1:Z:333:LYS:HG3 | 2.24 | 0.50 |
| 1:a:490:ARG:HB2 | 1:a:576:THR:HB | 1.93 | 0.50 |
| 1:c:340:THR:HB | 1:c:407:ARG:NH2 | 2.27 | 0.50 |
| 1:f:570:THR:OG1 | 1:f:571:THR:N | 2.43 | 0.50 |
| 1:h:307:TRP:O | 1:h:426:SER:CB | 2.59 | 0.50 |
| 1:m:429:HIS:NE2 | 1:m:610:GLN:OE1 | 2.45 | 0.50 |
| 1:o:451:THR:HG21 | 1:p:503:PHE:CE2 | 2.46 | 0.50 |
| 1:q:300:GLN:NE2 | 1:q:703:TYR:O | 2.45 | 0.50 |
| 1:t:315:ASN:OD1 | 1:t:316:PHE:N | 2.45 | 0.50 |
| 1:t:627:THR:HG22 | 1:v:429:HIS:NE2 | 2.26 | 0.50 |
| 1:v:340:THR:HB | 1:v:407:ARG:NH2 | 2.27 | 0.50 |
| 1:w:490:ARG:HB2 | 1:w:576:THR:HB | 1.94 | 0.50 |
| 1:1:315:ASN:OD1 | 1:1:316:PHE:N | 2.45 | 0.50 |
| 1:1:490:ARG:HB2 | 1:1:576:THR:HB | 1.93 | 0.50 |
| 1:6:490:ARG:HB2 | 1:6:576:THR:HB | 1.94 | 0.50 |
| 1:7:258:TYR:OH | 1:7:399:GLU:OE1 | 2.22 | 0.50 |
| 1:7:429:HIS:NE2 | 1:7:610:GLN:OE1 | 2.45 | 0.50 |
| 1:7:570:THR:OG1 | 1:7:571:THR:N | 2.43 | 0.50 |
| 1:A:340:THR:HB | 1:A:407:ARG:NH2 | 2.27 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:315:ASN:OD1 | 1:C:316:PHE:N | 2.45 | 0.49 |
| 1:E:570:THR:OG1 | 1:E:571:THR:N | 2.43 | 0.49 |
| 1:G:315:ASN:OD1 | 1:G:316:PHE:N | 2.45 | 0.49 |
| 1:H:307:TRP:O | 1:H:426:SER:CB | 2.59 | 0.49 |
| 1:I:315:ASN:OD1 | 1:I:316:PHE:N | 2.45 | 0.49 |
| 1:K:328:GLN:NE2 | 1:K:333:LYS:HG3 | 2.24 | 0.49 |
| 1:N:490:ARG:HB2 | 1:N:576:THR:HB | 1.93 | 0.49 |
| 1:O:340:THR:HB | 1:O:407:ARG:NH2 | 2.27 | 0.49 |
| 1:P:315:ASN:OD1 | 1:P:316:PHE:N | 2.45 | 0.49 |
| 1:R:315:ASN:OD1 | 1:R:316:PHE:N | 2.45 | 0.49 |
| 1:V:300:GLN:NE2 | 1:V:703:TYR:O | 2.45 | 0.49 |
| 1:W:300:GLN:NE2 | 1:W:703:TYR:O | 2.45 | 0.49 |
| 1:W:307:TRP:O | 1:W:426:SER:CB | 2.59 | 0.49 |
| 1:Z:346:PHE:HB3 | 1:Z:403:SER:HA | 1.93 | 0.49 |
| 1:b:300:GLN:NE2 | 1:b:703:TYR:O | 2.45 | 0.49 |
| 1:h:429:HIS:NE2 | 1:h:610:GLN:OE1 | 2.45 | 0.49 |
| 1:k:307:TRP:O | 1:k:426:SER:CB | 2.59 | 0.49 |
| 1:k:429:HIS:NE2 | 1:k:610:GLN:OE1 | 2.45 | 0.49 |
| 1:l:346:PHE:HB3 | 1:l:403:SER:HA | 1.93 | 0.49 |
| 1:m:346:PHE:HB3 | 1:m:403:SER:HA | 1.93 | 0.49 |
| 1:o:439:PRO:HB3 | 1:p:381:LEU:HD21 | 1.93 | 0.49 |
| 1:p:315:ASN:OD1 | 1:p:316:PHE:N | 2.45 | 0.49 |
| 1:r:346:PHE:HB3 | 1:r:403:SER:HA | 1.93 | 0.49 |
| 1:t:429:HIS:NE2 | 1:u:627:THR:HG22 | 2.26 | 0.49 |
| 1:u:609:TRP:CD1 | 1:v:629:GLY:CA | 2.85 | 0.49 |
| 1:w:340:THR:HB | 1:w:407:ARG:NH2 | 2.27 | 0.49 |
| 1:y:340:THR:HB | 1:y:407:ARG:NH2 | 2.27 | 0.49 |
| 1:3:570:THR:OG1 | 1:3:571:THR:N | 2.43 | 0.49 |
| 1:5:439:PRO:HB3 | 1:6:381:LEU:HD21 | 1.92 | 0.49 |
| 1:5:490:ARG:HB2 | 1:5:576:THR:HB | 1.94 | 0.49 |
| 1:C:286:ASP:O | 1:C:364:CYS:HA | 2.11 | 0.49 |
| 1:E:429:HIS:NE2 | 1:Q:627:THR:HG22 | 2.26 | 0.49 |
| 1:F:629:GLY:CA | 1:Q:609:TRP:CD1 | 2.85 | 0.49 |
| 1:H:434:ASP:OD1 | 1:H:434:ASP:N | 2.41 | 0.49 |
| 1:I:340:THR:HB | 1:I:407:ARG:NH2 | 2.27 | 0.49 |
| 1:J:329:ASN:O | 1:J:332:THR:OG1 | 2.30 | 0.49 |
| 1:J:340:THR:HB | 1:J:407:ARG:NH2 | 2.27 | 0.49 |
| 1:O:570:THR:OG1 | 1:O:571:THR:N | 2.43 | 0.49 |
| 1:R:627:THR:HG22 | 1:U:429:HIS:NE2 | 2.26 | 0.49 |
| 1:S:307:TRP:O | 1:S:426:SER:CB | 2.59 | 0.49 |
| 1:V:340:THR:CB | 1:V:407:ARG:HH21 | 2.20 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:340:THR:HB | 1:W:407:ARG:NH2 | 2.27 | 0.49 |
| 1:W:570:THR:OG1 | 1:W:571:THR:N | 2.43 | 0.49 |
| 1:X:487:ARG:HG2 | 1:X:488:GLN:N | 2.28 | 0.49 |
| 1:Y:346:PHE:HB3 | 1:Y:403:SER:HA | 1.93 | 0.49 |
| 1:b:429:HIS:NE2 | 1:b:610:GLN:OE1 | 2.45 | 0.49 |
| 1:c:315:ASN:OD1 | 1:c:316:PHE:N | 2.45 | 0.49 |
| 1:g:429:HIS:NE2 | 1:g:610:GLN:OE1 | 2.45 | 0.49 |
| 1:j:346:PHE:HB3 | 1:j:403:SER:HA | 1.93 | 0.49 |
| 1:m:340:THR:HB | 1:m:407:ARG:NH2 | 2.27 | 0.49 |
| 1:q:286:ASP:O | 1:q:364:CYS:HA | 2.11 | 0.49 |
| 1:q:570:THR:OG1 | 1:q:571:THR:N | 2.43 | 0.49 |
| 1:s:434:ASP:OD1 | 1:s:434:ASP:N | 2.41 | 0.49 |
| 1:u:307:TRP:O | 1:u:426:SER:CB | 2.59 | 0.49 |
| 1:x:487:ARG:HG2 | 1:x:488:GLN:N | 2.28 | 0.49 |
| 1:y:300:GLN:NE2 | 1:y:703:TYR:O | 2.45 | 0.49 |
| 1:y:429:HIS:NE2 | 1:y:610:GLN:OE1 | 2.45 | 0.49 |
| 1:3:340:THR:HB | 1:3:407:ARG:NH2 | 2.27 | 0.49 |
| 1:5:609:TRP:CD1 | 1:6:629:GLY:CA | 2.85 | 0.49 |
| 1:6:429:HIS:NE2 | 1:6:610:GLN:OE1 | 2.45 | 0.49 |
| 1:8:315:ASN:OD1 | 1:8:316:PHE:N | 2.45 | 0.49 |
| 1:A:451:THR:HG21 | 1:G:503:PHE:CE2 | 2.47 | 0.49 |
| 1:C:340:THR:HB | 1:C:407:ARG:NH2 | 2.27 | 0.49 |
| 1:C:429:HIS:NE2 | 1:C:610:GLN:OE1 | 2.45 | 0.49 |
| 1:C:609:TRP:NE1 | 1:b:629:GLY:CA | 2.58 | 0.49 |
| 1:D:286:ASP:O | 1:D:364:CYS:HA | 2.11 | 0.49 |
| 1:D:328:GLN:NE2 | 1:D:333:LYS:HG3 | 2.24 | 0.49 |
| 1:D:346:PHE:HB3 | 1:D:403:SER:HA | 1.93 | 0.49 |
| 1:F:340:THR:HB | 1:F:407:ARG:NH2 | 2.27 | 0.49 |
| 1:F:429:HIS:NE2 | 1:F:610:GLN:OE1 | 2.45 | 0.49 |
| 1:G:429:HIS:NE2 | 1:G:610:GLN:OE1 | 2.45 | 0.49 |
| 1:H:429:HIS:NE2 | 1:H:610:GLN:OE1 | 2.45 | 0.49 |
| 1:K:346:PHE:HB3 | 1:K:403:SER:HA | 1.93 | 0.49 |
| 1:L:286:ASP:O | 1:L:364:CYS:HA | 2.11 | 0.49 |
| 1:L:429:HIS:NE2 | 1:L:610:GLN:OE1 | 2.45 | 0.49 |
| 1:M:340:THR:HB | 1:M:407:ARG:NH2 | 2.27 | 0.49 |
| 1:T:286:ASP:O | 1:T:364:CYS:HA | 2.11 | 0.49 |
| 1:T:429:HIS:NE2 | 1:T:610:GLN:OE1 | 2.45 | 0.49 |
| 1:T:487:ARG:HG2 | 1:T:488:GLN:N | 2.28 | 0.49 |
| 1:V:429:HIS:NE2 | 1:V:610:GLN:OE1 | 2.45 | 0.49 |
| 1:W:315:ASN:OD1 | 1:W:316:PHE:N | 2.45 | 0.49 |
| 1:W:340:THR:CB | 1:W:407:ARG:HH21 | 2.20 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:d:340:THR:HB | 1:d:407:ARG:NH2 | 2.27 | 0.49 |
| 1:d:490:ARG:HB2 | 1:d:576:THR:HB | 1.93 | 0.49 |
| 1:e:340:THR:HB | 1:e:407:ARG:NH2 | 2.27 | 0.49 |
| 1:e:346:PHE:HB3 | 1:e:403:SER:HA | 1.93 | 0.49 |
| 1:f:346:PHE:HB3 | 1:f:403:SER:HA | 1.94 | 0.49 |
| 1:g:315:ASN:OD1 | 1:g:316:PHE:N | 2.45 | 0.49 |
| 1:i:429:HIS:NE2 | 1:i:610:GLN:OE1 | 2.45 | 0.49 |
| 1:k:487:ARG:HG2 | 1:k:488:GLN:N | 2.28 | 0.49 |
| 1:o:340:THR:HB | 1:o:407:ARG:NH2 | 2.27 | 0.49 |
| 1:q:307:TRP:O | 1:q:426:SER:CB | 2.59 | 0.49 |
| 1:q:315:ASN:OD1 | 1:q:316:PHE:N | 2.45 | 0.49 |
| 1:q:429:HIS:NE2 | 1:q:610:GLN:OE1 | 2.45 | 0.49 |
| 1:s:307:TRP:O | 1:s:426:SER:CB | 2.59 | 0.49 |
| 1:s:429:HIS:NE2 | 1:s:610:GLN:OE1 | 2.45 | 0.49 |
| 1:t:426:SER:OG | 1:t:731:THR:O | 2.31 | 0.49 |
| 1:x:609:TRP:CD1 | 1:y:629:GLY:CA | 2.85 | 0.49 |
| 1:z:629:GLY:CA | 1:2:609:TRP:CD1 | 2.85 | 0.49 |
| 1:1:286:ASP:O | 1:1:364:CYS:HA | 2.11 | 0.49 |
| 1:1:487:ARG:HG2 | 1:1:488:GLN:N | 2.28 | 0.49 |
| 1:4:429:HIS:NE2 | 1:4:610:GLN:OE1 | 2.45 | 0.49 |
| 1:5:627:THR:HG22 | 1:7:429:HIS:NE2 | 2.26 | 0.49 |
| 1:6:307:TRP:O | 1:6:426:SER:CB | 2.59 | 0.49 |
| 1:A:629:GLY:CA | 1:I:609:TRP:CD1 | 2.86 | 0.49 |
| 1:B:487:ARG:HG2 | 1:B:488:GLN:N | 2.27 | 0.49 |
| 1:B:629:GLY:CA | 1:L:609:TRP:NE1 | 2.58 | 0.49 |
| 1:D:315:ASN:OD1 | 1:D:316:PHE:N | 2.45 | 0.49 |
| 1:D:503:PHE:CE2 | 1:P:451:THR:HG21 | 2.47 | 0.49 |
| 1:G:340:THR:HB | 1:G:407:ARG:NH2 | 2.27 | 0.49 |
| 1:H:381:LEU:HD21 | 1:Y:439:PRO:HB3 | 1.92 | 0.49 |
| 1:J:346:PHE:HB3 | 1:J:403:SER:HA | 1.94 | 0.49 |
| 1:J:490:ARG:HB2 | 1:J:576:THR:HB | 1.93 | 0.49 |
| 1:K:286:ASP:O | 1:K:364:CYS:HA | 2.11 | 0.49 |
| 1:K:503:PHE:CE2 | 1:8:451:THR:HG21 | 2.47 | 0.49 |
| 1:L:340:THR:HB | 1:L:407:ARG:NH2 | 2.27 | 0.49 |
| 1:N:315:ASN:OD1 | 1:N:316:PHE:N | 2.45 | 0.49 |
| 1:N:429:HIS:NE2 | 1:N:610:GLN:OE1 | 2.45 | 0.49 |
| 1:P:429:HIS:NE2 | 1:P:610:GLN:OE1 | 2.45 | 0.49 |
| 1:W:429:HIS:NE2 | 1:W:610:GLN:OE1 | 2.45 | 0.49 |
| 1:X:300:GLN:NE2 | 1:X:703:TYR:O | 2.45 | 0.49 |
| 1:Y:490:ARG:HB2 | 1:Y:576:THR:HB | 1.93 | 0.49 |
| 1:Z:340:THR:HB | 1:Z:407:ARG:NH2 | 2.27 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:a:315:ASN:OD1 | 1:a:316:PHE:N | 2.45 | 0.49 |
| 1:d:315:ASN:OD1 | 1:d:316:PHE:N | 2.45 | 0.49 |
| 1:d:609:TRP:CD1 | 1:l:629:GLY:CA | 2.85 | 0.49 |
| 1:e:426:SER:OG | 1:e:731:THR:O | 2.31 | 0.49 |
| 1:h:416:TYR:OH | 1:h:644:HIS:O | 2.27 | 0.49 |
| 1:h:487:ARG:HG2 | 1:h:488:GLN:N | 2.28 | 0.49 |
| 1:i:315:ASN:OD1 | 1:i:316:PHE:N | 2.45 | 0.49 |
| 1:k:416:TYR:OH | 1:k:644:HIS:O | 2.27 | 0.49 |
| 1:l:429:HIS:NE2 | 1:l:610:GLN:OE1 | 2.45 | 0.49 |
| 1:m:328:GLN:NE2 | 1:m:333:LYS:HG3 | 2.24 | 0.49 |
| 1:n:429:HIS:NE2 | 1:n:610:GLN:OE1 | 2.45 | 0.49 |
| 1:r:439:PRO:HB3 | 1:s:381:LEU:HD21 | 1.92 | 0.49 |
| 1:r:490:ARG:HB2 | 1:r:576:THR:HB | 1.93 | 0.49 |
| 1:u:490:ARG:HB2 | 1:u:576:THR:HB | 1.94 | 0.49 |
| 1:w:481:LEU:CD1 | 1:x:636:LEU:HD11 | 2.43 | 0.49 |
| 1:y:340:THR:CB | 1:y:407:ARG:HH21 | 2.20 | 0.49 |
| 1:z:429:HIS:NE2 | 1:z:610:GLN:OE1 | 2.45 | 0.49 |
| 1:1:429:HIS:NE2 | 1:1:610:GLN:OE1 | 2.45 | 0.49 |
| 1:2:315:ASN:OD1 | 1:2:316:PHE:N | 2.45 | 0.49 |
| 1:2:340:THR:HB | 1:2:407:ARG:NH2 | 2.27 | 0.49 |
| 1:2:490:ARG:HB2 | 1:2:576:THR:HB | 1.93 | 0.49 |
| 1:6:340:THR:HB | 1:6:407:ARG:NH2 | 2.27 | 0.49 |
| 1:7:307:TRP:O | 1:7:426:SER:CB | 2.59 | 0.49 |
| 1:8:416:TYR:OH | 1:8:644:HIS:O | 2.27 | 0.49 |
| 1:8:429:HIS:NE2 | 1:8:610:GLN:OE1 | 2.45 | 0.49 |
| 1:B:315:ASN:OD1 | 1:B:316:PHE:N | 2.45 | 0.49 |
| 1:E:426:SER:OG | 1:E:731:THR:O | 2.31 | 0.49 |
| 1:F:307:TRP:O | 1:F:426:SER:CB | 2.59 | 0.49 |
| 1:I:429:HIS:NE2 | 1:I:610:GLN:OE1 | 2.45 | 0.49 |
| 1:K:429:HIS:NE2 | 1:K:610:GLN:OE1 | 2.45 | 0.49 |
| 1:L:426:SER:OG | 1:L:731:THR:O | 2.31 | 0.49 |
| 1:M:346:PHE:HB3 | 1:M:403:SER:HA | 1.94 | 0.49 |
| 1:M:490:ARG:HB2 | 1:M:576:THR:HB | 1.93 | 0.49 |
| 1:R:416:TYR:OH | 1:R:644:HIS:O | 2.27 | 0.49 |
| 1:a:429:HIS:NE2 | 1:a:610:GLN:OE1 | 2.45 | 0.49 |
| 1:b:487:ARG:HG2 | 1:b:488:GLN:N | 2.27 | 0.49 |
| 1:l:340:THR:HB | 1:l:407:ARG:NH2 | 2.27 | 0.49 |
| 1:p:340:THR:HB | 1:p:407:ARG:NH2 | 2.27 | 0.49 |
| 1:p:429:HIS:NE2 | 1:p:610:GLN:OE1 | 2.45 | 0.49 |
| 1:q:340:THR:CB | 1:q:407:ARG:HH21 | 2.20 | 0.49 |
| 1:q:627:THR:HG22 | 1:s:429:HIS:NE2 | 2.26 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:t:416:TYR:OH | 1:t:644:HIS:O | 2.27 | 0.49 |
| 1:w:346:PHE:HB3 | 1:w:403:SER:HA | 1.93 | 0.49 |
| 1:w:627:THR:HG22 | 1:y:429:HIS:NE2 | 2.26 | 0.49 |
| 1:x:300:GLN:NE2 | 1:x:703:TYR:O | 2.45 | 0.49 |
| 1:y:286:ASP:O | 1:y:364:CYS:HA | 2.11 | 0.49 |
| 1:y:429:HIS:HD2 | 1:y:610:GLN:OE1 | 1.94 | 0.49 |
| 1:z:328:GLN:NE2 | 1:z:333:LYS:HG3 | 2.24 | 0.49 |
| 1:1:307:TRP:O | 1:1:426:SER:CB | 2.59 | 0.49 |
| 1:4:315:ASN:OD1 | 1:4:316:PHE:N | 2.45 | 0.49 |
| 1:C:346:PHE:HB3 | 1:C:403:SER:HA | 1.93 | 0.49 |
| 1:C:426:SER:OG | 1:C:731:THR:O | 2.31 | 0.49 |
| 1:D:340:THR:HB | 1:D:407:ARG:NH2 | 2.27 | 0.49 |
| 1:E:307:TRP:O | 1:E:426:SER:CB | 2.59 | 0.49 |
| 1:E:487:ARG:HG2 | 1:E:488:GLN:N | 2.27 | 0.49 |
| 1:H:429:HIS:NE2 | 1:W:627:THR:HG22 | 2.26 | 0.49 |
| 1:K:315:ASN:OD1 | 1:K:316:PHE:N | 2.45 | 0.49 |
| 1:K:340:THR:HB | 1:K:407:ARG:NH2 | 2.27 | 0.49 |
| 1:L:346:PHE:HB3 | 1:L:403:SER:HA | 1.93 | 0.49 |
| 1:R:300:GLN:NE2 | 1:R:703:TYR:O | 2.45 | 0.49 |
| 1:S:487:ARG:HG2 | 1:S:488:GLN:N | 2.28 | 0.49 |
| 1:S:490:ARG:HB2 | 1:S:576:THR:HB | 1.94 | 0.49 |
| 1:V:346:PHE:HB3 | 1:V:403:SER:HA | 1.93 | 0.49 |
| 1:V:429:HIS:HD2 | 1:V:610:GLN:OE1 | 1.94 | 0.49 |
| 1:X:286:ASP:O | 1:X:364:CYS:HA | 2.11 | 0.49 |
| 1:Y:429:HIS:NE2 | 1:Y:610:GLN:OE1 | 2.45 | 0.49 |
| 1:Z:487:ARG:HG2 | 1:Z:488:GLN:N | 2.28 | 0.49 |
| 1:b:315:ASN:OD1 | 1:b:316:PHE:N | 2.45 | 0.49 |
| 1:b:490:ARG:HB2 | 1:b:576:THR:HB | 1.93 | 0.49 |
| 1:c:429:HIS:NE2 | 1:c:610:GLN:OE1 | 2.45 | 0.49 |
| 1:e:429:HIS:NE2 | 1:e:610:GLN:OE1 | 2.45 | 0.49 |
| 1:g:426:SER:OG | 1:g:731:THR:O | 2.31 | 0.49 |
| 1:j:429:HIS:NE2 | 1:j:610:GLN:OE1 | 2.45 | 0.49 |
| 1:l:328:GLN:NE2 | 1:l:333:LYS:HG3 | 2.24 | 0.49 |
| 1:m:315:ASN:OD1 | 1:m:316:PHE:N | 2.45 | 0.49 |
| 1:n:346:PHE:HB3 | 1:n:403:SER:HA | 1.93 | 0.49 |
| 1:s:487:ARG:HG2 | 1:s:488:GLN:N | 2.28 | 0.49 |
| 1:u:487:ARG:HG2 | 1:u:488:GLN:N | 2.28 | 0.49 |
| 1:x:286:ASP:O | 1:x:364:CYS:HA | 2.11 | 0.49 |
| 1:x:328:GLN:NE2 | 1:x:333:LYS:HG3 | 2.24 | 0.49 |
| 1:y:346:PHE:HB3 | 1:y:403:SER:HA | 1.93 | 0.49 |
| 1:z:340:THR:HB | 1:z:407:ARG:NH2 | 2.27 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:487:ARG:HG2 | 1:5:488:GLN:N | 2.28 | 0.49 |
| 1:7:300:GLN:NE2 | 1:7:703:TYR:O | 2.45 | 0.49 |
| 1:A:307:TRP:O | 1:A:426:SER:CB | 2.59 | 0.49 |
| 1:B:490:ARG:HB2 | 1:B:576:THR:HB | 1.93 | 0.49 |
| 1:D:429:HIS:NE2 | 1:D:610:GLN:OE1 | 2.45 | 0.49 |
| 1:H:487:ARG:HG2 | 1:H:488:GLN:N | 2.27 | 0.49 |
| 1:N:286:ASP:O | 1:N:364:CYS:HA | 2.11 | 0.49 |
| 1:Q:487:ARG:HG2 | 1:Q:488:GLN:N | 2.27 | 0.49 |
| 1:T:307:TRP:O | 1:T:426:SER:CB | 2.59 | 0.49 |
| 1:V:286:ASP:O | 1:V:364:CYS:HA | 2.11 | 0.49 |
| 1:X:328:GLN:NE2 | 1:X:333:LYS:HG3 | 2.24 | 0.49 |
| 1:Y:315:ASN:OD1 | 1:Y:316:PHE:N | 2.45 | 0.49 |
| 1:i:340:THR:HB | 1:i:407:ARG:NH2 | 2.27 | 0.49 |
| 1:i:426:SER:OG | 1:i:731:THR:O | 2.31 | 0.49 |
| 1:j:300:GLN:NE2 | 1:j:703:TYR:O | 2.45 | 0.49 |
| 1:m:487:ARG:HG2 | 1:m:488:GLN:N | 2.28 | 0.49 |
| 1:n:315:ASN:OD1 | 1:n:316:PHE:N | 2.45 | 0.49 |
| 1:o:429:HIS:NE2 | 1:o:610:GLN:OE1 | 2.45 | 0.49 |
| 1:w:429:HIS:NE2 | 1:w:610:GLN:OE1 | 2.45 | 0.49 |
| 1:x:429:HIS:HD2 | 1:x:610:GLN:OE1 | 1.94 | 0.49 |
| 1:3:429:HIS:NE2 | 1:3:610:GLN:OE1 | 2.45 | 0.49 |
| 1:4:346:PHE:HB3 | 1:4:403:SER:HA | 1.93 | 0.49 |
| 1:5:609:TRP:NE1 | 1:6:629:GLY:CA | 2.58 | 0.49 |
| 1:6:609:TRP:CD1 | 1:7:629:GLY:CA | 2.85 | 0.49 |
| 1:A:315:ASN:OD1 | 1:A:316:PHE:N | 2.45 | 0.49 |
| 1:A:429:HIS:NE2 | 1:A:610:GLN:OE1 | 2.45 | 0.49 |
| 1:C:487:ARG:HG2 | 1:C:488:GLN:N | 2.28 | 0.49 |
| 1:D:439:PRO:HB3 | 1:N:381:LEU:HD21 | 1.93 | 0.49 |
| 1:E:300:GLN:NE2 | 1:E:703:TYR:O | 2.45 | 0.49 |
| 1:F:487:ARG:HG2 | 1:F:488:GLN:N | 2.28 | 0.49 |
| 1:I:346:PHE:HB3 | 1:I:403:SER:HA | 1.93 | 0.49 |
| 1:K:439:PRO:HB3 | 1:a:381:LEU:HD21 | 1.93 | 0.49 |
| 1:L:487:ARG:HG2 | 1:L:488:GLN:N | 2.28 | 0.49 |
| 1:V:451:THR:HG21 | 1:e:503:PHE:CE2 | 2.47 | 0.49 |
| 1:V:487:ARG:HG2 | 1:V:488:GLN:N | 2.27 | 0.49 |
| 1:V:490:ARG:HB2 | 1:V:576:THR:HB | 1.93 | 0.49 |
| 1:W:487:ARG:HG2 | 1:W:488:GLN:N | 2.28 | 0.49 |
| 1:Z:315:ASN:OD1 | 1:Z:316:PHE:N | 2.45 | 0.49 |
| 1:a:286:ASP:O | 1:a:364:CYS:HA | 2.11 | 0.49 |
| 1:f:300:GLN:NE2 | 1:f:703:TYR:O | 2.45 | 0.49 |
| 1:f:429:HIS:NE2 | 1:f:610:GLN:OE1 | 2.45 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:g:300:GLN:NE2 | 1:g:703:TYR:O | 2.45 | 0.49 |
| 1:l:487:ARG:HG2 | 1:l:488:GLN:N | 2.28 | 0.49 |
| 1:o:315:ASN:OD1 | 1:o:316:PHE:N | 2.45 | 0.49 |
| 1:r:340:THR:HB | 1:r:407:ARG:NH2 | 2.27 | 0.49 |
| 1:r:429:HIS:NE2 | 1:r:610:GLN:OE1 | 2.45 | 0.49 |
| 1:t:340:THR:HB | 1:t:407:ARG:NH2 | 2.27 | 0.49 |
| 1:u:300:GLN:NE2 | 1:u:703:TYR:O | 2.45 | 0.49 |
| 1:v:315:ASN:OD1 | 1:v:316:PHE:N | 2.45 | 0.49 |
| 1:v:429:HIS:NE2 | 1:v:610:GLN:OE1 | 2.45 | 0.49 |
| 1:z:487:ARG:HG2 | 1:z:488:GLN:N | 2.28 | 0.49 |
| 1:1:346:PHE:HB3 | 1:1:403:SER:HA | 1.93 | 0.49 |
| 1:1:434:ASP:OD1 | 1:1:434:ASP:N | 2.41 | 0.49 |
| 1:6:487:ARG:HG2 | 1:6:488:GLN:N | 2.28 | 0.49 |
| 1:7:487:ARG:HG2 | 1:7:488:GLN:N | 2.28 | 0.49 |
| 1:I:416:TYR:OH | 1:I:644:HIS:O | 2.27 | 0.49 |
| 1:O:429:HIS:NE2 | 1:O:610:GLN:OE1 | 2.45 | 0.49 |
| 1:P:416:TYR:OH | 1:P:644:HIS:O | 2.27 | 0.49 |
| 1:Q:315:ASN:OD1 | 1:Q:316:PHE:N | 2.45 | 0.49 |
| 1:S:300:GLN:NE2 | 1:S:703:TYR:O | 2.45 | 0.49 |
| 1:S:429:HIS:NE2 | 1:S:610:GLN:OE1 | 2.45 | 0.49 |
| 1:T:346:PHE:HB3 | 1:T:403:SER:HA | 1.93 | 0.49 |
| 1:U:315:ASN:OD1 | 1:U:316:PHE:N | 2.45 | 0.49 |
| 1:U:487:ARG:HG2 | 1:U:488:GLN:N | 2.28 | 0.49 |
| 1:W:346:PHE:HB3 | 1:W:403:SER:HA | 1.93 | 0.49 |
| 1:X:429:HIS:HD2 | 1:X:610:GLN:OE1 | 1.94 | 0.49 |
| 1:c:346:PHE:HB3 | 1:c:403:SER:HA | 1.93 | 0.49 |
| 1:d:429:HIS:NE2 | 1:d:610:GLN:OE1 | 2.45 | 0.49 |
| 1:f:490:ARG:HB2 | 1:f:576:THR:HB | 1.93 | 0.49 |
| 1:g:340:THR:HB | 1:g:407:ARG:NH2 | 2.27 | 0.49 |
| 1:i:300:GLN:NE2 | 1:i:703:TYR:O | 2.45 | 0.49 |
| 1:n:254:ASN:C | 1:n:256:HIS:N | 2.71 | 0.49 |
| 1:o:307:TRP:O | 1:o:426:SER:CB | 2.59 | 0.49 |
| 1:q:346:PHE:HB3 | 1:q:403:SER:HA | 1.93 | 0.49 |
| 1:q:487:ARG:HG2 | 1:q:488:GLN:N | 2.28 | 0.49 |
| 1:r:315:ASN:OD1 | 1:r:316:PHE:N | 2.45 | 0.49 |
| 1:r:487:ARG:HG2 | 1:r:488:GLN:N | 2.27 | 0.49 |
| 1:s:570:THR:OG1 | 1:s:571:THR:N | 2.43 | 0.49 |
| 1:u:346:PHE:HB3 | 1:u:403:SER:HA | 1.93 | 0.49 |
| 1:u:429:HIS:NE2 | 1:u:610:GLN:OE1 | 2.45 | 0.49 |
| 1:x:429:HIS:NE2 | 1:x:610:GLN:OE1 | 2.45 | 0.49 |
| 1:y:254:ASN:C | 1:y:256:HIS:N | 2.71 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:y:487:ARG:HG2 | 1:y:488:GLN:N | 2.27 | 0.49 |
| 1:y:490:ARG:HB2 | 1:y:576:THR:HB | 1.93 | 0.49 |
| 1:2:429:HIS:NE2 | 1:2:610:GLN:OE1 | 2.45 | 0.49 |
| 1:3:346:PHE:HB3 | 1:3:403:SER:HA | 1.93 | 0.49 |
| 1:4:254:ASN:C | 1:4:256:HIS:N | 2.71 | 0.49 |
| 1:4:307:TRP:O | 1:4:426:SER:CB | 2.59 | 0.49 |
| 1:5:315:ASN:OD1 | 1:5:316:PHE:N | 2.45 | 0.49 |
| 1:D:490:ARG:HB2 | 1:D:576:THR:HB | 1.93 | 0.49 |
| 1:H:300:GLN:NE2 | 1:H:703:TYR:O | 2.45 | 0.49 |
| 1:J:300:GLN:NE2 | 1:J:703:TYR:O | 2.45 | 0.49 |
| 1:N:609:TRP:CD1 | 1:P:629:GLY:CA | 2.85 | 0.49 |
| 1:P:300:GLN:NE2 | 1:P:703:TYR:O | 2.45 | 0.49 |
| 1:S:346:PHE:HB3 | 1:S:403:SER:HA | 1.93 | 0.49 |
| 1:U:429:HIS:NE2 | 1:U:610:GLN:OE1 | 2.45 | 0.49 |
| 1:V:254:ASN:C | 1:V:256:HIS:N | 2.71 | 0.49 |
| 1:X:429:HIS:NE2 | 1:X:610:GLN:OE1 | 2.45 | 0.49 |
| 1:Y:254:ASN:C | 1:Y:256:HIS:N | 2.71 | 0.49 |
| 1:Y:340:THR:HB | 1:Y:407:ARG:NH2 | 2.27 | 0.49 |
| 1:Y:487:ARG:HG2 | 1:Y:488:GLN:N | 2.28 | 0.49 |
| 1:r:254:ASN:C | 1:r:256:HIS:N | 2.71 | 0.49 |
| 1:s:300:GLN:NE2 | 1:s:703:TYR:O | 2.45 | 0.49 |
| 1:t:429:HIS:NE2 | 1:t:610:GLN:OE1 | 2.45 | 0.49 |
| 1:w:464:LEU:HD23 | 1:x:554:ASN:HB3 | 1.95 | 0.49 |
| 1:8:429:HIS:HD2 | 1:8:610:GLN:OE1 | 1.94 | 0.49 |
| 1:E:629:GLY:CA | 1:F:609:TRP:CD1 | 2.85 | 0.48 |
| 1:F:585:ASN:OD1 | 1:F:594:ILE:N | 2.45 | 0.48 |
| 1:H:570:THR:OG1 | 1:H:571:THR:N | 2.43 | 0.48 |
| 1:I:487:ARG:HG2 | 1:I:488:GLN:N | 2.28 | 0.48 |
| 1:J:487:ARG:HG2 | 1:J:488:GLN:N | 2.28 | 0.48 |
| 1:K:490:ARG:HB2 | 1:K:576:THR:HB | 1.93 | 0.48 |
| 1:M:300:GLN:NE2 | 1:M:703:TYR:O | 2.45 | 0.48 |
| 1:M:429:HIS:NE2 | 1:M:610:GLN:OE1 | 2.45 | 0.48 |
| 1:O:254:ASN:C | 1:O:256:HIS:N | 2.71 | 0.48 |
| 1:O:346:PHE:HB3 | 1:O:403:SER:HA | 1.93 | 0.48 |
| 1:Q:307:TRP:O | 1:Q:426:SER:CB | 2.59 | 0.48 |
| 1:R:340:THR:HB | 1:R:407:ARG:NH2 | 2.27 | 0.48 |
| 1:R:429:HIS:NE2 | 1:R:610:GLN:OE1 | 2.45 | 0.48 |
| 1:T:434:ASP:OD1 | 1:T:434:ASP:N | 2.41 | 0.48 |
| 1:W:434:ASP:OD1 | 1:W:434:ASP:N | 2.41 | 0.48 |
| 1:Y:307:TRP:O | 1:Y:426:SER:CB | 2.59 | 0.48 |
| 1:g:329:ASN:O | 1:g:332:THR:OG1 | 2.31 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:490:ARG:HB2 | 1:j:576:THR:HB | 1.94 | 0.48 |
| 1:l:426:SER:OG | 1:l:731:THR:O | 2.31 | 0.48 |
| 1:m:416:TYR:OH | 1:m:644:HIS:O | 2.27 | 0.48 |
| 1:n:307:TRP:O | 1:n:426:SER:CB | 2.59 | 0.48 |
| 1:p:254:ASN:C | 1:p:256:HIS:N | 2.71 | 0.48 |
| 1:t:487:ARG:HG2 | 1:t:488:GLN:N | 2.28 | 0.48 |
| 1:v:487:ARG:HG2 | 1:v:488:GLN:N | 2.28 | 0.48 |
| 1:x:481:LEU:CD1 | 1:y:636:LEU:HD11 | 2.43 | 0.48 |
| 1:z:315:ASN:OD1 | 1:z:316:PHE:N | 2.45 | 0.48 |
| 1:z:426:SER:OG | 1:z:731:THR:O | 2.30 | 0.48 |
| 1:8:300:GLN:NE2 | 1:8:703:TYR:O | 2.45 | 0.48 |
| 1:D:487:ARG:HG2 | 1:D:488:GLN:N | 2.28 | 0.48 |
| 1:J:429:HIS:NE2 | 1:J:610:GLN:OE1 | 2.45 | 0.48 |
| 1:K:629:GLY:CA | 1:8:609:TRP:CD1 | 2.84 | 0.48 |
| 1:M:307:TRP:O | 1:M:426:SER:CB | 2.59 | 0.48 |
| 1:M:487:ARG:HG2 | 1:M:488:GLN:N | 2.28 | 0.48 |
| 1:N:487:ARG:HG2 | 1:N:488:GLN:N | 2.27 | 0.48 |
| 1:P:429:HIS:HD2 | 1:P:610:GLN:OE1 | 1.94 | 0.48 |
| 1:P:487:ARG:HG2 | 1:P:488:GLN:N | 2.28 | 0.48 |
| 1:Q:254:ASN:C | 1:Q:256:HIS:N | 2.71 | 0.48 |
| 1:R:487:ARG:HG2 | 1:R:488:GLN:N | 2.28 | 0.48 |
| 1:U:416:TYR:OH | 1:U:644:HIS:O | 2.27 | 0.48 |
| 1:c:307:TRP:O | 1:c:426:SER:CB | 2.59 | 0.48 |
| 1:c:487:ARG:HG2 | 1:c:488:GLN:N | 2.28 | 0.48 |
| 1:h:426:SER:OG | 1:h:731:THR:O | 2.31 | 0.48 |
| 1:k:426:SER:OG | 1:k:731:THR:O | 2.31 | 0.48 |
| 1:l:315:ASN:OD1 | 1:l:316:PHE:N | 2.45 | 0.48 |
| 1:n:487:ARG:HG2 | 1:n:488:GLN:N | 2.28 | 0.48 |
| 1:q:416:TYR:OH | 1:q:644:HIS:O | 2.27 | 0.48 |
| 1:2:254:ASN:C | 1:2:256:HIS:N | 2.71 | 0.48 |
| 1:3:254:ASN:C | 1:3:256:HIS:N | 2.71 | 0.48 |
| 1:4:487:ARG:HG2 | 1:4:488:GLN:N | 2.27 | 0.48 |
| 1:F:629:GLY:CA | 1:Q:609:TRP:NE1 | 2.58 | 0.48 |
| 1:J:307:TRP:O | 1:J:426:SER:CB | 2.59 | 0.48 |
| 1:K:487:ARG:HG2 | 1:K:488:GLN:N | 2.28 | 0.48 |
| 1:S:254:ASN:C | 1:S:256:HIS:N | 2.71 | 0.48 |
| 1:a:426:SER:OG | 1:a:731:THR:O | 2.31 | 0.48 |
| 1:d:254:ASN:C | 1:d:256:HIS:N | 2.71 | 0.48 |
| 1:d:609:TRP:NE1 | 1:l:629:GLY:CA | 2.58 | 0.48 |
| 1:j:585:ASN:OD1 | 1:j:594:ILE:N | 2.45 | 0.48 |
| 1:r:307:TRP:O | 1:r:426:SER:CB | 2.59 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:t:254:ASN:C | 1:t:256:HIS:N | 2.71 | 0.48 |
| 1:w:487:ARG:HG2 | 1:w:488:GLN:N | 2.27 | 0.48 |
| 1:y:382:THR:HG22 | 1:y:383:LEU:N | 2.29 | 0.48 |
| 1:3:382:THR:HG22 | 1:3:383:LEU:N | 2.29 | 0.48 |
| 1:3:487:ARG:HG2 | 1:3:488:GLN:N | 2.28 | 0.48 |
| 1:5:254:ASN:C | 1:5:256:HIS:N | 2.71 | 0.48 |
| 1:5:307:TRP:O | 1:5:426:SER:CB | 2.59 | 0.48 |
| 1:6:315:ASN:OD1 | 1:6:316:PHE:N | 2.45 | 0.48 |
| 1:I:307:TRP:O | 1:I:426:SER:CB | 2.59 | 0.48 |
| 1:K:434:ASP:OD1 | 1:K:434:ASP:N | 2.41 | 0.48 |
| 1:O:315:ASN:OD1 | 1:O:316:PHE:N | 2.45 | 0.48 |
| 1:O:382:THR:HG22 | 1:O:383:LEU:N | 2.29 | 0.48 |
| 1:O:487:ARG:HG2 | 1:O:488:GLN:N | 2.28 | 0.48 |
| 1:R:254:ASN:C | 1:R:256:HIS:N | 2.71 | 0.48 |
| 1:X:629:GLY:CA | 1:e:609:TRP:CD1 | 2.85 | 0.48 |
| 1:Z:416:TYR:OH | 1:Z:644:HIS:O | 2.27 | 0.48 |
| 1:a:609:TRP:CD1 | 1:8:629:GLY:CA | 2.85 | 0.48 |
| 1:b:307:TRP:O | 1:b:426:SER:CB | 2.59 | 0.48 |
| 1:f:585:ASN:OD1 | 1:f:594:ILE:N | 2.45 | 0.48 |
| 1:v:416:TYR:OH | 1:v:644:HIS:O | 2.27 | 0.48 |
| 1:3:315:ASN:OD1 | 1:3:316:PHE:N | 2.45 | 0.48 |
| 1:8:329:ASN:O | 1:8:332:THR:OG1 | 2.31 | 0.48 |
| 1:8:487:ARG:HG2 | 1:8:488:GLN:N | 2.27 | 0.48 |
| 1:A:254:ASN:C | 1:A:256:HIS:N | 2.71 | 0.48 |
| 1:B:307:TRP:O | 1:B:426:SER:CB | 2.59 | 0.48 |
| 1:B:382:THR:HG22 | 1:B:383:LEU:N | 2.29 | 0.48 |
| 1:F:300:GLN:NE2 | 1:F:703:TYR:O | 2.45 | 0.48 |
| 1:F:315:ASN:OD1 | 1:F:316:PHE:N | 2.45 | 0.48 |
| 1:G:426:SER:OG | 1:G:731:THR:O | 2.31 | 0.48 |
| 1:H:315:ASN:OD1 | 1:H:316:PHE:N | 2.45 | 0.48 |
| 1:H:328:GLN:NE2 | 1:H:333:LYS:HG3 | 2.24 | 0.48 |
| 1:V:382:THR:HG22 | 1:V:383:LEU:N | 2.29 | 0.48 |
| 1:V:609:TRP:CD1 | 1:e:629:GLY:CA | 2.84 | 0.48 |
| 1:W:416:TYR:OH | 1:W:644:HIS:O | 2.27 | 0.48 |
| 1:Y:429:HIS:HD2 | 1:Y:610:GLN:OE1 | 1.94 | 0.48 |
| 1:b:382:THR:HG22 | 1:b:383:LEU:N | 2.29 | 0.48 |
| 1:c:434:ASP:OD1 | 1:c:434:ASP:N | 2.41 | 0.48 |
| 1:o:254:ASN:C | 1:o:256:HIS:N | 2.71 | 0.48 |
| 1:r:429:HIS:HD2 | 1:r:610:GLN:OE1 | 1.94 | 0.48 |
| 1:s:315:ASN:OD1 | 1:s:316:PHE:N | 2.45 | 0.48 |
| 1:u:254:ASN:C | 1:u:256:HIS:N | 2.71 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:w:554:ASN:HB3 | 1:y:464:LEU:HD23 | 1.95 | 0.48 |
| 1:x:451:THR:HG21 | 1:y:503:PHE:CE2 | 2.48 | 0.48 |
| 1:y:307:TRP:O | 1:y:426:SER:CB | 2.59 | 0.48 |
| 1:z:307:TRP:O | 1:z:426:SER:CB | 2.59 | 0.48 |
| 1:C:300:GLN:NE2 | 1:C:703:TYR:O | 2.45 | 0.48 |
| 1:D:629:GLY:CA | 1:P:609:TRP:CD1 | 2.84 | 0.48 |
| 1:E:382:THR:HG22 | 1:E:383:LEU:N | 2.29 | 0.48 |
| 1:E:585:ASN:OD1 | 1:E:594:ILE:N | 2.45 | 0.48 |
| 1:a:487:ARG:HG2 | 1:a:488:GLN:N | 2.28 | 0.48 |
| 1:e:487:ARG:HG2 | 1:e:488:GLN:N | 2.28 | 0.48 |
| 1:f:329:ASN:O | 1:f:332:THR:OG1 | 2.30 | 0.48 |
| 1:j:487:ARG:HG2 | 1:j:488:GLN:N | 2.28 | 0.48 |
| 1:l:307:TRP:O | 1:l:426:SER:CB | 2.59 | 0.48 |
| 1:p:426:SER:OG | 1:p:731:THR:O | 2.31 | 0.48 |
| 1:q:434:ASP:OD1 | 1:q:434:ASP:N | 2.41 | 0.48 |
| 1:w:490:ARG:CZ | 1:y:586:LEU:HD21 | 2.43 | 0.48 |
| 1:7:585:ASN:OD1 | 1:7:594:ILE:N | 2.45 | 0.48 |
| 1:8:254:ASN:C | 1:8:256:HIS:N | 2.71 | 0.48 |
| 1:A:429:HIS:HD2 | 1:A:610:GLN:OE1 | 1.94 | 0.48 |
| 1:D:434:ASP:OD1 | 1:D:434:ASP:N | 2.41 | 0.48 |
| 1:I:382:THR:HG22 | 1:I:383:LEU:N | 2.29 | 0.48 |
| 1:I:434:ASP:OD1 | 1:I:434:ASP:N | 2.41 | 0.48 |
| 1:L:300:GLN:NE2 | 1:L:703:TYR:O | 2.45 | 0.48 |
| 1:U:300:GLN:NE2 | 1:U:703:TYR:O | 2.45 | 0.48 |
| 1:V:307:TRP:O | 1:V:426:SER:CB | 2.59 | 0.48 |
| 1:V:585:ASN:OD1 | 1:V:594:ILE:N | 2.45 | 0.48 |
| 1:Y:585:ASN:OD1 | 1:Y:594:ILE:N | 2.45 | 0.48 |
| 1:c:300:GLN:NE2 | 1:c:703:TYR:O | 2.45 | 0.48 |
| 1:c:382:THR:HG22 | 1:c:383:LEU:N | 2.29 | 0.48 |
| 1:c:426:SER:OG | 1:c:731:THR:O | 2.31 | 0.48 |
| 1:d:382:THR:HG22 | 1:d:383:LEU:N | 2.29 | 0.48 |
| 1:g:307:TRP:O | 1:g:426:SER:CB | 2.59 | 0.48 |
| 1:r:585:ASN:OD1 | 1:r:594:ILE:N | 2.45 | 0.48 |
| 1:s:328:GLN:NE2 | 1:s:333:LYS:HG3 | 2.24 | 0.48 |
| 1:x:382:THR:HG22 | 1:x:383:LEU:N | 2.29 | 0.48 |
| 1:1:426:SER:OG | 1:1:731:THR:O | 2.31 | 0.48 |
| 1:6:300:GLN:NE2 | 1:6:703:TYR:O | 2.45 | 0.48 |
| 1:7:382:THR:HG22 | 1:7:383:LEU:N | 2.29 | 0.48 |
| 1:G:487:ARG:HG2 | 1:G:488:GLN:N | 2.28 | 0.48 |
| 1:I:426:SER:OG | 1:I:731:THR:O | 2.31 | 0.48 |
| 1:M:226:SER:HG | 1:M:320:ASN:H | 1.60 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:287:PHE:CE1 | 1:N:621:TRP:HH2 | 2.32 | 0.48 |
| 1:T:426:SER:OG | 1:T:731:THR:O | 2.31 | 0.48 |
| 1:U:254:ASN:C | 1:U:256:HIS:N | 2.71 | 0.48 |
| 1:W:287:PHE:CE1 | 1:W:621:TRP:HH2 | 2.32 | 0.48 |
| 1:X:382:THR:HG22 | 1:X:383:LEU:N | 2.29 | 0.48 |
| 1:f:487:ARG:HG2 | 1:f:488:GLN:N | 2.28 | 0.48 |
| 1:g:487:ARG:HG2 | 1:g:488:GLN:N | 2.27 | 0.48 |
| 1:j:329:ASN:O | 1:j:332:THR:OG1 | 2.31 | 0.48 |
| 1:k:300:GLN:NE2 | 1:k:703:TYR:O | 2.45 | 0.48 |
| 1:p:487:ARG:HG2 | 1:p:488:GLN:N | 2.28 | 0.48 |
| 1:q:287:PHE:CE1 | 1:q:621:TRP:HH2 | 2.32 | 0.48 |
| 1:v:254:ASN:C | 1:v:256:HIS:N | 2.71 | 0.48 |
| 1:y:585:ASN:OD1 | 1:y:594:ILE:N | 2.45 | 0.48 |
| 1:2:382:THR:HG22 | 1:2:383:LEU:N | 2.29 | 0.48 |
| 1:3:329:ASN:O | 1:3:332:THR:OG1 | 2.31 | 0.48 |
| 1:5:429:HIS:HD2 | 1:5:610:GLN:OE1 | 1.94 | 0.48 |
| 1:6:328:GLN:NE2 | 1:6:333:LYS:HG3 | 2.24 | 0.48 |
| 1:F:328:GLN:NE2 | 1:F:333:LYS:HG3 | 2.24 | 0.48 |
| 1:I:300:GLN:NE2 | 1:I:703:TYR:O | 2.45 | 0.48 |
| 1:J:382:THR:HG22 | 1:J:383:LEU:N | 2.29 | 0.48 |
| 1:K:287:PHE:CE1 | 1:K:621:TRP:HH2 | 2.32 | 0.48 |
| 1:L:328:GLN:NE2 | 1:L:333:LYS:HG3 | 2.24 | 0.48 |
| 1:M:382:THR:HG22 | 1:M:383:LEU:N | 2.29 | 0.48 |
| 1:Q:429:HIS:HD2 | 1:Q:610:GLN:OE1 | 1.94 | 0.48 |
| 1:a:287:PHE:CE1 | 1:a:621:TRP:HH2 | 2.32 | 0.48 |
| 1:d:487:ARG:HG2 | 1:d:488:GLN:N | 2.28 | 0.48 |
| 1:m:254:ASN:C | 1:m:256:HIS:N | 2.71 | 0.48 |
| 1:o:429:HIS:HD2 | 1:o:610:GLN:OE1 | 1.94 | 0.48 |
| 1:o:487:ARG:HG2 | 1:o:488:GLN:N | 2.28 | 0.48 |
| 1:t:629:GLY:CA | 1:v:609:TRP:NE1 | 2.58 | 0.48 |
| 1:w:429:HIS:NE2 | 1:x:627:THR:HG22 | 2.28 | 0.48 |
| 1:z:629:GLY:CA | 1:2:609:TRP:NE1 | 2.58 | 0.48 |
| 1:1:287:PHE:CE1 | 1:1:621:TRP:HH2 | 2.32 | 0.48 |
| 1:2:487:ARG:HG2 | 1:2:488:GLN:N | 2.28 | 0.48 |
| 1:A:487:ARG:HG2 | 1:A:488:GLN:N | 2.28 | 0.48 |
| 1:D:287:PHE:CE1 | 1:D:621:TRP:HH2 | 2.32 | 0.48 |
| 1:L:382:THR:HG22 | 1:L:383:LEU:N | 2.29 | 0.48 |
| 1:O:329:ASN:O | 1:O:332:THR:OG1 | 2.31 | 0.48 |
| 1:T:287:PHE:CE1 | 1:T:621:TRP:HH2 | 2.32 | 0.48 |
| 1:U:585:ASN:OD1 | 1:U:594:ILE:N | 2.45 | 0.48 |
| 1:W:585:ASN:OD1 | 1:W:594:ILE:N | 2.45 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z:254:ASN:C | 1:Z:256:HIS:N | 2.71 | 0.48 |
| 1:d:300:GLN:NE2 | 1:d:703:TYR:O | 2.45 | 0.48 |
| 1:h:300:GLN:NE2 | 1:h:703:TYR:O | 2.45 | 0.48 |
| 1:i:307:TRP:O | 1:i:426:SER:CB | 2.59 | 0.48 |
| 1:i:487:ARG:HG2 | 1:i:488:GLN:N | 2.27 | 0.48 |
| 1:v:300:GLN:NE2 | 1:v:703:TYR:O | 2.45 | 0.48 |
| 1:w:586:LEU:HD21 | 1:x:490:ARG:CZ | 2.44 | 0.48 |
| 1:x:439:PRO:HB3 | 1:y:381:LEU:HD21 | 1.95 | 0.48 |
| 1:A:382:THR:HG22 | 1:A:383:LEU:N | 2.29 | 0.47 |
| 1:C:254:ASN:C | 1:C:256:HIS:N | 2.71 | 0.47 |
| 1:C:382:THR:HG22 | 1:C:383:LEU:N | 2.29 | 0.47 |
| 1:F:287:PHE:CE1 | 1:F:621:TRP:HH2 | 2.32 | 0.47 |
| 1:M:416:TYR:OH | 1:M:644:HIS:O | 2.27 | 0.47 |
| 1:V:609:TRP:NE1 | 1:e:629:GLY:CA | 2.58 | 0.47 |
| 1:W:329:ASN:O | 1:W:332:THR:OG1 | 2.31 | 0.47 |
| 1:n:426:SER:OG | 1:n:731:THR:O | 2.31 | 0.47 |
| 1:o:382:THR:HG22 | 1:o:383:LEU:N | 2.29 | 0.47 |
| 1:q:585:ASN:OD1 | 1:q:594:ILE:N | 2.45 | 0.47 |
| 1:z:300:GLN:NE2 | 1:z:703:TYR:O | 2.45 | 0.47 |
| 1:2:300:GLN:NE2 | 1:2:703:TYR:O | 2.45 | 0.47 |
| 1:4:287:PHE:CE1 | 1:4:621:TRP:HH2 | 2.32 | 0.47 |
| 1:4:426:SER:OG | 1:4:731:THR:O | 2.31 | 0.47 |
| 1:N:416:TYR:OH | 1:N:644:HIS:O | 2.27 | 0.47 |
| 1:R:585:ASN:OD1 | 1:R:594:ILE:N | 2.45 | 0.47 |
| 1:R:629:GLY:CA | 1:U:609:TRP:NE1 | 2.58 | 0.47 |
| 1:Y:300:GLN:NE2 | 1:Y:703:TYR:O | 2.45 | 0.47 |
| 1:Y:426:SER:OG | 1:Y:731:THR:O | 2.30 | 0.47 |
| 1:b:287:PHE:CE1 | 1:b:621:TRP:HH2 | 2.32 | 0.47 |
| 1:h:585:ASN:OD1 | 1:h:594:ILE:N | 2.45 | 0.47 |
| 1:l:300:GLN:NE2 | 1:l:703:TYR:O | 2.45 | 0.47 |
| 1:n:287:PHE:CE1 | 1:n:621:TRP:HH2 | 2.32 | 0.47 |
| 1:q:232:ASP:HB3 | 1:y:402:PRO:CG | 2.44 | 0.47 |
| 1:r:300:GLN:NE2 | 1:r:703:TYR:O | 2.45 | 0.47 |
| 1:v:585:ASN:OD1 | 1:v:594:ILE:N | 2.45 | 0.47 |
| 1:w:438:ASN:HB2 | 1:x:356:VAL:CG2 | 2.44 | 0.47 |
| 1:6:287:PHE:CE1 | 1:6:621:TRP:HH2 | 2.32 | 0.47 |
| 1:B:287:PHE:CE1 | 1:B:621:TRP:HH2 | 2.32 | 0.47 |
| 1:C:485:CYS:HB2 | 1:C:573:PRO:HG3 | 1.97 | 0.47 |
| 1:D:329:ASN:O | 1:D:332:THR:OG1 | 2.31 | 0.47 |
| 1:D:485:CYS:HB2 | 1:D:573:PRO:HG3 | 1.97 | 0.47 |
| 1:G:300:GLN:NE2 | 1:G:703:TYR:O | 2.45 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:287:PHE:CE1 | 1:H:621:TRP:HH2 | 2.32 | 0.47 |
| 1:H:429:HIS:HD2 | 1:H:610:GLN:OE1 | 1.94 | 0.47 |
| 1:K:485:CYS:HB2 | 1:K:573:PRO:HG3 | 1.97 | 0.47 |
| 1:L:254:ASN:C | 1:L:256:HIS:N | 2.71 | 0.47 |
| 1:L:485:CYS:HB2 | 1:L:573:PRO:HG3 | 1.97 | 0.47 |
| 1:O:485:CYS:HB2 | 1:O:573:PRO:HG3 | 1.97 | 0.47 |
| 1:g:287:PHE:CE1 | 1:g:621:TRP:HH2 | 2.32 | 0.47 |
| 1:m:287:PHE:CE1 | 1:m:621:TRP:HH2 | 2.32 | 0.47 |
| 1:o:287:PHE:CE1 | 1:o:621:TRP:HH2 | 2.32 | 0.47 |
| 1:q:329:ASN:O | 1:q:332:THR:OG1 | 2.31 | 0.47 |
| 1:s:287:PHE:CE1 | 1:s:621:TRP:HH2 | 2.32 | 0.47 |
| 1:t:609:TRP:CD1 | 1:u:629:GLY:CA | 2.85 | 0.47 |
| 1:y:416:TYR:OH | 1:y:644:HIS:O | 2.27 | 0.47 |
| 1:z:287:PHE:CE1 | 1:z:621:TRP:HH2 | 2.32 | 0.47 |
| 1:z:382:THR:HG22 | 1:z:383:LEU:N | 2.29 | 0.47 |
| 1:1:609:TRP:CD1 | 1:2:629:GLY:CA | 2.85 | 0.47 |
| 1:3:300:GLN:NE2 | 1:3:703:TYR:O | 2.45 | 0.47 |
| 1:3:485:CYS:HB2 | 1:3:573:PRO:HG3 | 1.97 | 0.47 |
| 1:A:287:PHE:CE1 | 1:A:621:TRP:HH2 | 2.32 | 0.47 |
| 1:B:485:CYS:HB2 | 1:B:573:PRO:HG3 | 1.97 | 0.47 |
| 1:J:416:TYR:OH | 1:J:644:HIS:O | 2.27 | 0.47 |
| 1:J:485:CYS:HB2 | 1:J:573:PRO:HG3 | 1.97 | 0.47 |
| 1:K:636:LEU:HD11 | 1:8:481:LEU:CD1 | 2.45 | 0.47 |
| 1:M:485:CYS:HB2 | 1:M:573:PRO:HG3 | 1.97 | 0.47 |
| 1:P:426:SER:OG | 1:P:731:THR:O | 2.31 | 0.47 |
| 1:T:416:TYR:OH | 1:T:644:HIS:O | 2.27 | 0.47 |
| 1:X:307:TRP:O | 1:X:426:SER:CB | 2.59 | 0.47 |
| 1:Z:287:PHE:CE1 | 1:Z:621:TRP:HH2 | 2.32 | 0.47 |
| 1:Z:382:THR:HG22 | 1:Z:383:LEU:N | 2.29 | 0.47 |
| 1:a:416:TYR:OH | 1:a:644:HIS:O | 2.27 | 0.47 |
| 1:b:485:CYS:HB2 | 1:b:573:PRO:HG3 | 1.97 | 0.47 |
| 1:b:585:ASN:OD1 | 1:b:594:ILE:N | 2.45 | 0.47 |
| 1:e:254:ASN:C | 1:e:256:HIS:N | 2.71 | 0.47 |
| 1:e:382:THR:HG22 | 1:e:383:LEU:N | 2.29 | 0.47 |
| 1:f:254:ASN:C | 1:f:256:HIS:N | 2.71 | 0.47 |
| 1:i:287:PHE:CE1 | 1:i:621:TRP:HH2 | 2.32 | 0.47 |
| 1:j:254:ASN:C | 1:j:256:HIS:N | 2.71 | 0.47 |
| 1:j:287:PHE:CE1 | 1:j:621:TRP:HH2 | 2.32 | 0.47 |
| 1:l:287:PHE:CE1 | 1:l:621:TRP:HH2 | 2.32 | 0.47 |
| 1:n:485:CYS:HB2 | 1:n:573:PRO:HG3 | 1.97 | 0.47 |
| 1:p:300:GLN:NE2 | 1:p:703:TYR:O | 2.45 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:p:382:THR:HG22 | 1:p:383:LEU:N | 2.29 | 0.47 |
| 1:r:287:PHE:CE1 | 1:r:621:TRP:HH2 | 2.32 | 0.47 |
| 1:w:382:THR:HG22 | 1:w:383:LEU:N | 2.29 | 0.47 |
| 1:x:307:TRP:O | 1:x:426:SER:CB | 2.59 | 0.47 |
| 1:x:585:ASN:OD1 | 1:x:594:ILE:N | 2.45 | 0.47 |
| 1:1:416:TYR:OH | 1:1:644:HIS:O | 2.27 | 0.47 |
| 1:4:485:CYS:HB2 | 1:4:573:PRO:HG3 | 1.97 | 0.47 |
| 1:6:426:SER:OG | 1:6:731:THR:O | 2.31 | 0.47 |
| 1:7:287:PHE:CE1 | 1:7:621:TRP:HH2 | 2.32 | 0.47 |
| 1:D:636:LEU:HD11 | 1:P:481:LEU:CD1 | 2.45 | 0.47 |
| 1:E:287:PHE:CE1 | 1:E:621:TRP:HH2 | 2.32 | 0.47 |
| 1:F:426:SER:OG | 1:F:731:THR:O | 2.31 | 0.47 |
| 1:M:585:ASN:OD1 | 1:M:594:ILE:N | 2.45 | 0.47 |
| 1:O:300:GLN:NE2 | 1:O:703:TYR:O | 2.45 | 0.47 |
| 1:R:307:TRP:O | 1:R:426:SER:CB | 2.59 | 0.47 |
| 1:U:434:ASP:OD1 | 1:U:434:ASP:N | 2.41 | 0.47 |
| 1:Y:287:PHE:CE1 | 1:Y:621:TRP:HH2 | 2.32 | 0.47 |
| 1:f:287:PHE:CE1 | 1:f:621:TRP:HH2 | 2.32 | 0.47 |
| 1:h:254:ASN:C | 1:h:256:HIS:N | 2.71 | 0.47 |
| 1:h:287:PHE:CE1 | 1:h:621:TRP:HH2 | 2.32 | 0.47 |
| 1:h:429:HIS:HD2 | 1:h:610:GLN:OE1 | 1.94 | 0.47 |
| 1:k:254:ASN:C | 1:k:256:HIS:N | 2.71 | 0.47 |
| 1:l:329:ASN:O | 1:l:332:THR:OG1 | 2.31 | 0.47 |
| 1:q:485:CYS:HB2 | 1:q:573:PRO:HG3 | 1.96 | 0.47 |
| 1:r:426:SER:OG | 1:r:731:THR:O | 2.30 | 0.47 |
| 1:s:429:HIS:HD2 | 1:s:610:GLN:OE1 | 1.94 | 0.47 |
| 1:t:307:TRP:O | 1:t:426:SER:CB | 2.59 | 0.47 |
| 1:v:434:ASP:OD1 | 1:v:434:ASP:N | 2.41 | 0.47 |
| 1:w:586:LEU:HD11 | 1:x:490:ARG:NE | 2.30 | 0.47 |
| 1:8:426:SER:OG | 1:8:731:THR:O | 2.31 | 0.47 |
| 1:A:383:LEU:HG | 1:I:430:SER:O | 2.15 | 0.47 |
| 1:D:416:TYR:OH | 1:D:644:HIS:O | 2.27 | 0.47 |
| 1:G:382:THR:HG22 | 1:G:383:LEU:N | 2.29 | 0.47 |
| 1:I:287:PHE:CE1 | 1:I:621:TRP:HH2 | 2.32 | 0.47 |
| 1:R:609:TRP:CD1 | 1:S:629:GLY:CA | 2.85 | 0.47 |
| 1:W:426:SER:OG | 1:W:731:THR:O | 2.31 | 0.47 |
| 1:W:485:CYS:HB2 | 1:W:573:PRO:HG3 | 1.97 | 0.47 |
| 1:X:585:ASN:OD1 | 1:X:594:ILE:N | 2.45 | 0.47 |
| 1:i:485:CYS:HB2 | 1:i:573:PRO:HG3 | 1.97 | 0.47 |
| 1:j:426:SER:OG | 1:j:731:THR:O | 2.31 | 0.47 |
| 1:l:382:THR:HG22 | 1:l:383:LEU:N | 2.29 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:382:THR:HG22 | 1:m:383:LEU:N | 2.29 | 0.47 |
| 1:p:485:CYS:HB2 | 1:p:573:PRO:HG3 | 1.97 | 0.47 |
| 1:w:254:ASN:C | 1:w:256:HIS:N | 2.71 | 0.47 |
| 1:x:254:ASN:C | 1:x:256:HIS:N | 2.71 | 0.47 |
| 1:A:430:SER:O | 1:G:383:LEU:HG | 2.15 | 0.47 |
| 1:A:481:LEU:CD1 | 1:G:636:LEU:HD11 | 2.45 | 0.47 |
| 1:B:254:ASN:C | 1:B:256:HIS:N | 2.71 | 0.47 |
| 1:C:287:PHE:CE1 | 1:C:621:TRP:HH2 | 2.32 | 0.47 |
| 1:D:254:ASN:C | 1:D:256:HIS:N | 2.71 | 0.47 |
| 1:F:434:ASP:OD1 | 1:F:434:ASP:N | 2.41 | 0.47 |
| 1:F:485:CYS:HB2 | 1:F:573:PRO:HG3 | 1.97 | 0.47 |
| 1:G:485:CYS:HB2 | 1:G:573:PRO:HG3 | 1.97 | 0.47 |
| 1:H:383:LEU:HG | 1:Y:430:SER:O | 2.15 | 0.47 |
| 1:J:585:ASN:OD1 | 1:J:594:ILE:N | 2.45 | 0.47 |
| 1:K:416:TYR:OH | 1:K:644:HIS:O | 2.27 | 0.47 |
| 1:L:287:PHE:CE1 | 1:L:621:TRP:HH2 | 2.32 | 0.47 |
| 1:N:307:TRP:O | 1:N:426:SER:CB | 2.59 | 0.47 |
| 1:P:254:ASN:C | 1:P:256:HIS:N | 2.71 | 0.47 |
| 1:T:609:TRP:CD1 | 1:d:629:GLY:CA | 2.85 | 0.47 |
| 1:U:287:PHE:CE1 | 1:U:621:TRP:HH2 | 2.32 | 0.47 |
| 1:V:416:TYR:OH | 1:V:644:HIS:O | 2.27 | 0.47 |
| 1:V:438:ASN:HB2 | 1:e:356:VAL:CG2 | 2.45 | 0.47 |
| 1:V:481:LEU:CD1 | 1:e:636:LEU:HD11 | 2.45 | 0.47 |
| 1:X:254:ASN:C | 1:X:256:HIS:N | 2.71 | 0.47 |
| 1:Y:485:CYS:HB2 | 1:Y:573:PRO:HG3 | 1.97 | 0.47 |
| 1:a:300:GLN:NE2 | 1:a:703:TYR:O | 2.45 | 0.47 |
| 1:a:307:TRP:O | 1:a:426:SER:CB | 2.59 | 0.47 |
| 1:c:254:ASN:C | 1:c:256:HIS:N | 2.71 | 0.47 |
| 1:c:287:PHE:CE1 | 1:c:621:TRP:HH2 | 2.32 | 0.47 |
| 1:e:307:TRP:O | 1:e:426:SER:CB | 2.59 | 0.47 |
| 1:f:429:HIS:HD2 | 1:f:610:GLN:OE1 | 1.94 | 0.47 |
| 1:g:485:CYS:HB2 | 1:g:573:PRO:HG3 | 1.97 | 0.47 |
| 1:j:429:HIS:HD2 | 1:j:610:GLN:OE1 | 1.94 | 0.47 |
| 1:k:287:PHE:CE1 | 1:k:621:TRP:HH2 | 2.32 | 0.47 |
| 1:k:429:HIS:HD2 | 1:k:610:GLN:OE1 | 1.94 | 0.47 |
| 1:q:426:SER:OG | 1:q:731:THR:O | 2.31 | 0.47 |
| 1:r:430:SER:O | 1:s:383:LEU:HG | 2.15 | 0.47 |
| 1:r:485:CYS:HB2 | 1:r:573:PRO:HG3 | 1.97 | 0.47 |
| 1:v:287:PHE:CE1 | 1:v:621:TRP:HH2 | 2.32 | 0.47 |
| 1:w:307:TRP:O | 1:w:426:SER:CB | 2.59 | 0.47 |
| 1:w:451:THR:HG21 | 1:x:503:PHE:CE2 | 2.50 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:6:485:CYS:HB2 | 1:6:573:PRO:HG3 | 1.97 | 0.47 |
| 1:D:238:ASP:OD1 | 1:D:239:ARG:N | 2.48 | 0.47 |
| 1:E:609:TRP:NE1 | 1:Q:629:GLY:CA | 2.58 | 0.47 |
| 1:F:383:LEU:HG | 1:Q:430:SER:O | 2.15 | 0.47 |
| 1:G:307:TRP:O | 1:G:426:SER:CB | 2.59 | 0.47 |
| 1:K:254:ASN:C | 1:K:256:HIS:N | 2.71 | 0.47 |
| 1:N:300:GLN:NE2 | 1:N:703:TYR:O | 2.45 | 0.47 |
| 1:S:287:PHE:CE1 | 1:S:621:TRP:HH2 | 2.32 | 0.47 |
| 1:T:300:GLN:NE2 | 1:T:703:TYR:O | 2.45 | 0.47 |
| 1:V:485:CYS:HB2 | 1:V:573:PRO:HG3 | 1.97 | 0.47 |
| 1:X:564:SER:OG | 1:X:566:GLU:HG2 | 2.15 | 0.47 |
| 1:b:254:ASN:C | 1:b:256:HIS:N | 2.71 | 0.47 |
| 1:c:481:LEU:CD1 | 1:o:636:LEU:HD11 | 2.45 | 0.47 |
| 1:c:629:GLY:CA | 1:p:609:TRP:CD1 | 2.85 | 0.47 |
| 1:d:481:LEU:CD1 | 1:l:636:LEU:HD11 | 2.45 | 0.47 |
| 1:f:426:SER:OG | 1:f:731:THR:O | 2.31 | 0.47 |
| 1:j:485:CYS:HB2 | 1:j:573:PRO:HG3 | 1.97 | 0.47 |
| 1:l:585:ASN:OD1 | 1:l:594:ILE:N | 2.45 | 0.47 |
| 1:o:430:SER:O | 1:p:383:LEU:HG | 2.15 | 0.47 |
| 1:o:481:LEU:CD1 | 1:p:636:LEU:HD11 | 2.45 | 0.47 |
| 1:5:238:ASP:OD1 | 1:5:239:ARG:N | 2.48 | 0.47 |
| 1:5:430:SER:O | 1:6:383:LEU:HG | 2.15 | 0.47 |
| 1:8:485:CYS:HB2 | 1:8:573:PRO:HG3 | 1.97 | 0.47 |
| 1:E:485:CYS:HB2 | 1:E:573:PRO:HG3 | 1.97 | 0.47 |
| 1:I:254:ASN:C | 1:I:256:HIS:N | 2.71 | 0.47 |
| 1:I:585:ASN:OD1 | 1:I:594:ILE:N | 2.45 | 0.47 |
| 1:K:238:ASP:OD1 | 1:K:239:ARG:N | 2.48 | 0.47 |
| 1:K:300:GLN:NE2 | 1:K:703:TYR:O | 2.45 | 0.47 |
| 1:P:287:PHE:CE1 | 1:P:621:TRP:HH2 | 2.32 | 0.47 |
| 1:P:485:CYS:HB2 | 1:P:573:PRO:HG3 | 1.97 | 0.47 |
| 1:Q:238:ASP:OD1 | 1:Q:239:ARG:N | 2.48 | 0.47 |
| 1:U:564:SER:OG | 1:U:566:GLU:HG2 | 2.15 | 0.47 |
| 1:X:287:PHE:CE1 | 1:X:621:TRP:HH2 | 2.32 | 0.47 |
| 1:X:636:LEU:HD11 | 1:e:481:LEU:CD1 | 2.45 | 0.47 |
| 1:Y:564:SER:OG | 1:Y:566:GLU:HG2 | 2.15 | 0.47 |
| 1:d:287:PHE:CE1 | 1:d:621:TRP:HH2 | 2.32 | 0.47 |
| 1:e:287:PHE:CE1 | 1:e:621:TRP:HH2 | 2.32 | 0.47 |
| 1:p:307:TRP:O | 1:p:426:SER:CB | 2.59 | 0.47 |
| 1:r:564:SER:OG | 1:r:566:GLU:HG2 | 2.15 | 0.47 |
| 1:u:485:CYS:HB2 | 1:u:573:PRO:HG3 | 1.97 | 0.47 |
| 1:w:425:SER:HB3 | 1:x:628:ASP:OD1 | 2.13 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:x:287:PHE:CE1 | 1:x:621:TRP:HH2 | 2.32 | 0.47 |
| 1:x:564:SER:OG | 1:x:566:GLU:HG2 | 2.15 | 0.47 |
| 1:y:238:ASP:OD1 | 1:y:239:ARG:N | 2.48 | 0.47 |
| 1:y:287:PHE:CE1 | 1:y:621:TRP:HH2 | 2.32 | 0.47 |
| 1:y:485:CYS:HB2 | 1:y:573:PRO:HG3 | 1.97 | 0.47 |
| 1:z:636:LEU:HD11 | 1:2:481:LEU:CD1 | 2.45 | 0.47 |
| 1:2:287:PHE:CE1 | 1:2:621:TRP:HH2 | 2.32 | 0.47 |
| 1:2:328:GLN:NE2 | 1:2:333:LYS:HG3 | 2.24 | 0.47 |
| 1:2:564:SER:OG | 1:2:566:GLU:HG2 | 2.15 | 0.47 |
| 1:7:485:CYS:HB2 | 1:7:573:PRO:HG3 | 1.97 | 0.47 |
| 1:B:636:LEU:HD11 | 1:L:481:LEU:CD1 | 2.45 | 0.47 |
| 1:C:238:ASP:OD1 | 1:C:239:ARG:N | 2.48 | 0.47 |
| 1:C:609:TRP:CD1 | 1:C:609:TRP:C | 2.93 | 0.47 |
| 1:D:382:THR:HG22 | 1:D:383:LEU:N | 2.29 | 0.47 |
| 1:F:238:ASP:OD1 | 1:F:239:ARG:N | 2.48 | 0.47 |
| 1:F:254:ASN:C | 1:F:256:HIS:N | 2.71 | 0.47 |
| 1:I:564:SER:OG | 1:I:566:GLU:HG2 | 2.15 | 0.47 |
| 1:J:287:PHE:CE1 | 1:J:621:TRP:HH2 | 2.32 | 0.47 |
| 1:K:307:TRP:O | 1:K:426:SER:CB | 2.59 | 0.47 |
| 1:K:564:SER:OG | 1:K:566:GLU:HG2 | 2.15 | 0.47 |
| 1:L:238:ASP:OD1 | 1:L:239:ARG:N | 2.48 | 0.47 |
| 1:L:609:TRP:CD1 | 1:L:609:TRP:C | 2.93 | 0.47 |
| 1:M:287:PHE:CE1 | 1:M:621:TRP:HH2 | 2.32 | 0.47 |
| 1:O:383:LEU:HG | 1:n:430:SER:O | 2.15 | 0.47 |
| 1:R:383:LEU:HG | 1:U:430:SER:O | 2.15 | 0.47 |
| 1:S:485:CYS:HB2 | 1:S:573:PRO:HG3 | 1.97 | 0.47 |
| 1:V:238:ASP:OD1 | 1:V:239:ARG:N | 2.48 | 0.47 |
| 1:V:287:PHE:CE1 | 1:V:621:TRP:HH2 | 2.32 | 0.47 |
| 1:V:636:LEU:HD11 | 1:X:481:LEU:CD1 | 2.45 | 0.47 |
| 1:W:481:LEU:CD1 | 1:Y:636:LEU:HD11 | 2.45 | 0.47 |
| 1:X:238:ASP:OD1 | 1:X:239:ARG:N | 2.48 | 0.47 |
| 1:Z:564:SER:OG | 1:Z:566:GLU:HG2 | 2.15 | 0.47 |
| 1:c:430:SER:O | 1:o:383:LEU:HG | 2.15 | 0.47 |
| 1:c:564:SER:OG | 1:c:566:GLU:HG2 | 2.15 | 0.47 |
| 1:c:585:ASN:OD1 | 1:c:594:ILE:N | 2.45 | 0.47 |
| 1:d:564:SER:OG | 1:d:566:GLU:HG2 | 2.15 | 0.47 |
| 1:f:485:CYS:HB2 | 1:f:573:PRO:HG3 | 1.97 | 0.47 |
| 1:l:485:CYS:HB2 | 1:l:573:PRO:HG3 | 1.97 | 0.47 |
| 1:m:564:SER:OG | 1:m:566:GLU:HG2 | 2.15 | 0.47 |
| 1:p:429:HIS:HD2 | 1:p:610:GLN:OE1 | 1.94 | 0.47 |
| 1:q:481:LEU:CD1 | 1:r:636:LEU:HD11 | 2.45 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:t:383:LEU:HG | 1:v:430:SER:O | 2.16 | 0.47 |
| 1:u:287:PHE:CE1 | 1:u:621:TRP:HH2 | 2.32 | 0.47 |
| 1:v:564:SER:OG | 1:v:566:GLU:HG2 | 2.15 | 0.47 |
| 1:w:287:PHE:CE1 | 1:w:621:TRP:HH2 | 2.32 | 0.47 |
| 1:x:238:ASP:OD1 | 1:x:239:ARG:N | 2.48 | 0.47 |
| 1:x:609:TRP:NE1 | 1:y:629:GLY:CA | 2.57 | 0.47 |
| 1:z:356:VAL:CG2 | 1:2:438:ASN:HB2 | 2.45 | 0.47 |
| 1:3:287:PHE:CE1 | 1:3:621:TRP:HH2 | 2.32 | 0.47 |
| 1:6:254:ASN:C | 1:6:256:HIS:N | 2.71 | 0.47 |
| 1:8:287:PHE:CE1 | 1:8:621:TRP:HH2 | 2.32 | 0.47 |
| 1:A:585:ASN:OD1 | 1:A:594:ILE:N | 2.45 | 0.46 |
| 1:C:481:LEU:CD1 | 1:b:636:LEU:HD11 | 2.45 | 0.46 |
| 1:D:564:SER:OG | 1:D:566:GLU:HG2 | 2.15 | 0.46 |
| 1:G:430:SER:O | 1:I:383:LEU:HG | 2.16 | 0.46 |
| 1:H:430:SER:O | 1:W:383:LEU:HG | 2.15 | 0.46 |
| 1:H:481:LEU:CD1 | 1:W:636:LEU:HD11 | 2.46 | 0.46 |
| 1:I:485:CYS:HB2 | 1:I:573:PRO:HG3 | 1.97 | 0.46 |
| 1:R:287:PHE:CE1 | 1:R:621:TRP:HH2 | 2.32 | 0.46 |
| 1:S:430:SER:O | 1:U:383:LEU:HG | 2.15 | 0.46 |
| 1:Z:383:LEU:HG | 1:3:430:SER:O | 2.15 | 0.46 |
| 1:c:383:LEU:HG | 1:p:430:SER:O | 2.16 | 0.46 |
| 1:d:438:ASN:HB2 | 1:l:356:VAL:CG2 | 2.46 | 0.46 |
| 1:e:564:SER:OG | 1:e:566:GLU:HG2 | 2.15 | 0.46 |
| 1:e:609:TRP:CD1 | 1:e:609:TRP:C | 2.93 | 0.46 |
| 1:k:485:CYS:HB2 | 1:k:573:PRO:HG3 | 1.96 | 0.46 |
| 1:q:636:LEU:HD11 | 1:s:481:LEU:CD1 | 2.46 | 0.46 |
| 1:r:238:ASP:OD1 | 1:r:239:ARG:N | 2.48 | 0.46 |
| 1:s:416:TYR:OH | 1:s:644:HIS:O | 2.27 | 0.46 |
| 1:t:300:GLN:NE2 | 1:t:703:TYR:O | 2.45 | 0.46 |
| 1:w:430:SER:O | 1:x:383:LEU:HG | 2.15 | 0.46 |
| 1:w:487:ARG:HD2 | 1:y:583:ALA:O | 2.15 | 0.46 |
| 1:z:485:CYS:HB2 | 1:z:573:PRO:HG3 | 1.97 | 0.46 |
| 1:z:585:ASN:OD1 | 1:z:594:ILE:N | 2.45 | 0.46 |
| 1:1:300:GLN:NE2 | 1:1:703:TYR:O | 2.45 | 0.46 |
| 1:3:383:LEU:HG | 1:4:430:SER:O | 2.15 | 0.46 |
| 1:5:481:LEU:CD1 | 1:6:636:LEU:HD11 | 2.45 | 0.46 |
| 1:5:629:GLY:CA | 1:7:609:TRP:NE1 | 2.58 | 0.46 |
| 1:6:238:ASP:OD1 | 1:6:239:ARG:N | 2.48 | 0.46 |
| 1:A:636:LEU:HD11 | 1:I:481:LEU:CD1 | 2.46 | 0.46 |
| 1:D:300:GLN:NE2 | 1:D:703:TYR:O | 2.45 | 0.46 |
| 1:E:383:LEU:HG | 1:F:430:SER:O | 2.15 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:636:LEU:HD11 | 1:Q:481:LEU:CD1 | 2.45 | 0.46 |
| 1:G:609:TRP:CD1 | 1:I:629:GLY:CA | 2.85 | 0.46 |
| 1:K:382:THR:HG22 | 1:K:383:LEU:N | 2.29 | 0.46 |
| 1:O:287:PHE:CE1 | 1:O:621:TRP:HH2 | 2.32 | 0.46 |
| 1:O:430:SER:O | 1:m:383:LEU:HG | 2.15 | 0.46 |
| 1:R:238:ASP:OD1 | 1:R:239:ARG:N | 2.48 | 0.46 |
| 1:R:485:CYS:HB2 | 1:R:573:PRO:HG3 | 1.97 | 0.46 |
| 1:S:564:SER:OG | 1:S:566:GLU:HG2 | 2.15 | 0.46 |
| 1:T:329:ASN:O | 1:T:332:THR:OG1 | 2.30 | 0.46 |
| 1:Z:307:TRP:O | 1:Z:426:SER:CB | 2.59 | 0.46 |
| 1:a:238:ASP:OD1 | 1:a:239:ARG:N | 2.48 | 0.46 |
| 1:a:564:SER:OG | 1:a:566:GLU:HG2 | 2.15 | 0.46 |
| 1:c:485:CYS:HB2 | 1:c:573:PRO:HG3 | 1.97 | 0.46 |
| 1:d:238:ASP:OD1 | 1:d:239:ARG:N | 2.48 | 0.46 |
| 1:f:481:LEU:CD1 | 1:h:636:LEU:HD11 | 2.45 | 0.46 |
| 1:g:383:LEU:HG | 1:h:430:SER:O | 2.15 | 0.46 |
| 1:g:564:SER:OG | 1:g:566:GLU:HG2 | 2.15 | 0.46 |
| 1:j:481:LEU:CD1 | 1:k:636:LEU:HD11 | 2.45 | 0.46 |
| 1:n:238:ASP:OD1 | 1:n:239:ARG:N | 2.48 | 0.46 |
| 1:q:383:LEU:HG | 1:s:430:SER:O | 2.15 | 0.46 |
| 1:r:609:TRP:CD1 | 1:r:609:TRP:C | 2.93 | 0.46 |
| 1:t:238:ASP:OD1 | 1:t:239:ARG:N | 2.48 | 0.46 |
| 1:t:485:CYS:HB2 | 1:t:573:PRO:HG3 | 1.97 | 0.46 |
| 1:u:564:SER:OG | 1:u:566:GLU:HG2 | 2.15 | 0.46 |
| 1:w:564:SER:OG | 1:w:566:GLU:HG2 | 2.15 | 0.46 |
| 1:w:609:TRP:CD1 | 1:w:609:TRP:C | 2.93 | 0.46 |
| 1:4:238:ASP:OD1 | 1:4:239:ARG:N | 2.48 | 0.46 |
| 1:5:564:SER:OG | 1:5:566:GLU:HG2 | 2.15 | 0.46 |
| 1:6:430:SER:O | 1:7:383:LEU:HG | 2.15 | 0.46 |
| 1:8:382:THR:HG22 | 1:8:383:LEU:N | 2.29 | 0.46 |
| 1:A:438:ASN:HB2 | 1:G:356:VAL:CG2 | 2.46 | 0.46 |
| 1:A:485:CYS:HB2 | 1:A:573:PRO:HG3 | 1.97 | 0.46 |
| 1:B:383:LEU:HG | 1:L:430:SER:O | 2.15 | 0.46 |
| 1:C:564:SER:OG | 1:C:566:GLU:HG2 | 2.15 | 0.46 |
| 1:D:307:TRP:O | 1:D:426:SER:CB | 2.59 | 0.46 |
| 1:G:429:HIS:HD2 | 1:G:610:GLN:OE1 | 1.94 | 0.46 |
| 1:G:481:LEU:CD1 | 1:I:636:LEU:HD11 | 2.45 | 0.46 |
| 1:G:585:ASN:OD1 | 1:G:594:ILE:N | 2.45 | 0.46 |
| 1:L:564:SER:OG | 1:L:566:GLU:HG2 | 2.15 | 0.46 |
| 1:N:238:ASP:OD1 | 1:N:239:ARG:N | 2.48 | 0.46 |
| 1:O:609:TRP:CD1 | 1:O:609:TRP:C | 2.93 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:382:THR:HG22 | 1:P:383:LEU:N | 2.29 | 0.46 |
| 1:Q:564:SER:OG | 1:Q:566:GLU:HG2 | 2.15 | 0.46 |
| 1:Q:609:TRP:CD1 | 1:Q:609:TRP:C | 2.93 | 0.46 |
| 1:S:398:LEU:C | 1:S:400:TYR:H | 2.24 | 0.46 |
| 1:T:356:VAL:CG2 | 1:l:438:ASN:HB2 | 2.46 | 0.46 |
| 1:Y:238:ASP:OD1 | 1:Y:239:ARG:N | 2.48 | 0.46 |
| 1:Y:609:TRP:CD1 | 1:Y:609:TRP:C | 2.93 | 0.46 |
| 1:Z:429:HIS:HD2 | 1:Z:610:GLN:OE1 | 1.94 | 0.46 |
| 1:b:238:ASP:OD1 | 1:b:239:ARG:N | 2.48 | 0.46 |
| 1:c:636:LEU:HD11 | 1:p:481:LEU:CD1 | 2.45 | 0.46 |
| 1:e:238:ASP:OD1 | 1:e:239:ARG:N | 2.48 | 0.46 |
| 1:f:609:TRP:CD1 | 1:f:609:TRP:C | 2.93 | 0.46 |
| 1:g:398:LEU:C | 1:g:400:TYR:H | 2.24 | 0.46 |
| 1:h:485:CYS:HB2 | 1:h:573:PRO:HG3 | 1.97 | 0.46 |
| 1:i:398:LEU:C | 1:i:400:TYR:H | 2.24 | 0.46 |
| 1:i:430:SER:O | 1:j:383:LEU:HG | 2.15 | 0.46 |
| 1:i:564:SER:OG | 1:i:566:GLU:HG2 | 2.15 | 0.46 |
| 1:j:609:TRP:CD1 | 1:j:609:TRP:C | 2.93 | 0.46 |
| 1:m:307:TRP:O | 1:m:426:SER:CB | 2.59 | 0.46 |
| 1:o:485:CYS:HB2 | 1:o:573:PRO:HG3 | 1.97 | 0.46 |
| 1:o:585:ASN:OD1 | 1:o:594:ILE:N | 2.45 | 0.46 |
| 1:p:287:PHE:CE1 | 1:p:621:TRP:HH2 | 2.32 | 0.46 |
| 1:q:609:TRP:NE1 | 1:r:629:GLY:CA | 2.58 | 0.46 |
| 1:u:430:SER:O | 1:v:383:LEU:HG | 2.16 | 0.46 |
| 1:w:238:ASP:OD1 | 1:w:239:ARG:N | 2.48 | 0.46 |
| 1:x:485:CYS:HB2 | 1:x:573:PRO:HG3 | 1.97 | 0.46 |
| 1:z:438:ASN:HB2 | 1:1:356:VAL:CG2 | 2.46 | 0.46 |
| 1:1:485:CYS:HB2 | 1:1:573:PRO:HG3 | 1.97 | 0.46 |
| 1:3:609:TRP:CD1 | 1:3:609:TRP:C | 2.93 | 0.46 |
| 1:5:609:TRP:CD1 | 1:5:609:TRP:C | 2.93 | 0.46 |
| 1:B:238:ASP:OD1 | 1:B:239:ARG:N | 2.48 | 0.46 |
| 1:B:329:ASN:O | 1:B:332:THR:OG1 | 2.31 | 0.46 |
| 1:B:356:VAL:CG2 | 1:L:438:ASN:HB2 | 2.46 | 0.46 |
| 1:C:383:LEU:HG | 1:M:430:SER:O | 2.16 | 0.46 |
| 1:C:430:SER:O | 1:b:383:LEU:HG | 2.15 | 0.46 |
| 1:C:438:ASN:HB2 | 1:b:356:VAL:CG2 | 2.46 | 0.46 |
| 1:E:238:ASP:OD1 | 1:E:239:ARG:N | 2.48 | 0.46 |
| 1:E:636:LEU:HD11 | 1:F:481:LEU:CD1 | 2.45 | 0.46 |
| 1:G:287:PHE:CE1 | 1:G:621:TRP:HH2 | 2.32 | 0.46 |
| 1:H:609:TRP:CD1 | 1:H:609:TRP:C | 2.93 | 0.46 |
| 1:J:430:SER:O | 1:L:383:LEU:HG | 2.16 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:585:ASN:OD1 | 1:L:594:ILE:N | 2.45 | 0.46 |
| 1:N:564:SER:OG | 1:N:566:GLU:HG2 | 2.15 | 0.46 |
| 1:O:398:LEU:C | 1:O:400:TYR:H | 2.24 | 0.46 |
| 1:R:398:LEU:C | 1:R:400:TYR:H | 2.24 | 0.46 |
| 1:T:254:ASN:C | 1:T:256:HIS:N | 2.71 | 0.46 |
| 1:T:485:CYS:HB2 | 1:T:573:PRO:HG3 | 1.97 | 0.46 |
| 1:W:438:ASN:HB2 | 1:Y:356:VAL:CG2 | 2.46 | 0.46 |
| 1:X:383:LEU:HG | 1:e:430:SER:O | 2.15 | 0.46 |
| 1:X:485:CYS:HB2 | 1:X:573:PRO:HG3 | 1.97 | 0.46 |
| 1:a:485:CYS:HB2 | 1:a:573:PRO:HG3 | 1.97 | 0.46 |
| 1:d:485:CYS:HB2 | 1:d:573:PRO:HG3 | 1.97 | 0.46 |
| 1:g:238:ASP:OD1 | 1:g:239:ARG:N | 2.48 | 0.46 |
| 1:i:238:ASP:OD1 | 1:i:239:ARG:N | 2.48 | 0.46 |
| 1:i:383:LEU:HG | 1:k:430:SER:O | 2.15 | 0.46 |
| 1:j:430:SER:O | 1:k:383:LEU:HG | 2.15 | 0.46 |
| 1:m:429:HIS:HD2 | 1:m:610:GLN:OE1 | 1.94 | 0.46 |
| 1:p:585:ASN:OD1 | 1:p:594:ILE:N | 2.45 | 0.46 |
| 1:q:254:ASN:C | 1:q:256:HIS:N | 2.71 | 0.46 |
| 1:q:398:LEU:C | 1:q:400:TYR:H | 2.24 | 0.46 |
| 1:q:438:ASN:HB2 | 1:r:356:VAL:CG2 | 2.46 | 0.46 |
| 1:t:287:PHE:CE1 | 1:t:621:TRP:HH2 | 2.32 | 0.46 |
| 1:u:398:LEU:C | 1:u:400:TYR:H | 2.24 | 0.46 |
| 1:w:383:LEU:HG | 1:y:430:SER:O | 2.16 | 0.46 |
| 1:2:238:ASP:OD1 | 1:2:239:ARG:N | 2.48 | 0.46 |
| 1:5:287:PHE:CE1 | 1:5:621:TRP:HH2 | 2.32 | 0.46 |
| 1:5:356:VAL:CG2 | 1:7:438:ASN:HB2 | 2.46 | 0.46 |
| 1:A:434:ASP:OD1 | 1:A:434:ASP:N | 2.41 | 0.46 |
| 1:A:609:TRP:CD1 | 1:A:609:TRP:C | 2.93 | 0.46 |
| 1:B:438:ASN:HB2 | 1:J:356:VAL:CG2 | 2.46 | 0.46 |
| 1:D:356:VAL:CG2 | 1:P:438:ASN:HB2 | 2.45 | 0.46 |
| 1:E:356:VAL:CG2 | 1:F:438:ASN:HB2 | 2.46 | 0.46 |
| 1:E:438:ASN:HB2 | 1:Q:356:VAL:CG2 | 2.46 | 0.46 |
| 1:H:416:TYR:OH | 1:H:644:HIS:O | 2.27 | 0.46 |
| 1:M:356:VAL:CG2 | 1:b:438:ASN:HB2 | 2.46 | 0.46 |
| 1:N:485:CYS:HB2 | 1:N:573:PRO:HG3 | 1.97 | 0.46 |
| 1:O:356:VAL:CG2 | 1:n:438:ASN:HB2 | 2.46 | 0.46 |
| 1:Q:287:PHE:CE1 | 1:Q:621:TRP:HH2 | 2.32 | 0.46 |
| 1:S:429:HIS:HD2 | 1:S:610:GLN:OE1 | 1.94 | 0.46 |
| 1:T:481:LEU:CD1 | 1:d:636:LEU:HD11 | 2.45 | 0.46 |
| 1:U:238:ASP:OD1 | 1:U:239:ARG:N | 2.48 | 0.46 |
| 1:W:254:ASN:C | 1:W:256:HIS:N | 2.71 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:398:LEU:C | 1:W:400:TYR:H | 2.24 | 0.46 |
| 1:W:429:HIS:HD2 | 1:W:610:GLN:OE1 | 1.94 | 0.46 |
| 1:X:398:LEU:C | 1:X:400:TYR:H | 2.24 | 0.46 |
| 1:b:564:SER:OG | 1:b:566:GLU:HG2 | 2.15 | 0.46 |
| 1:c:629:GLY:CA | 1:p:609:TRP:NE1 | 2.58 | 0.46 |
| 1:f:383:LEU:HG | 1:g:430:SER:O | 2.15 | 0.46 |
| 1:f:430:SER:O | 1:h:383:LEU:HG | 2.16 | 0.46 |
| 1:g:585:ASN:OD1 | 1:g:594:ILE:N | 2.45 | 0.46 |
| 1:h:564:SER:OG | 1:h:566:GLU:HG2 | 2.15 | 0.46 |
| 1:i:636:LEU:HD11 | 1:k:481:LEU:CD1 | 2.45 | 0.46 |
| 1:j:564:SER:OG | 1:j:566:GLU:HG2 | 2.15 | 0.46 |
| 1:m:485:CYS:HB2 | 1:m:573:PRO:HG3 | 1.97 | 0.46 |
| 1:n:564:SER:OG | 1:n:566:GLU:HG2 | 2.15 | 0.46 |
| 1:o:438:ASN:HB2 | 1:p:356:VAL:CG2 | 2.46 | 0.46 |
| 1:q:429:HIS:HD2 | 1:q:610:GLN:OE1 | 1.94 | 0.46 |
| 1:s:382:THR:HG22 | 1:s:383:LEU:N | 2.29 | 0.46 |
| 1:s:609:TRP:CD1 | 1:s:609:TRP:C | 2.93 | 0.46 |
| 1:t:398:LEU:C | 1:t:400:TYR:H | 2.24 | 0.46 |
| 1:v:238:ASP:OD1 | 1:v:239:ARG:N | 2.48 | 0.46 |
| 1:1:254:ASN:C | 1:1:256:HIS:N | 2.71 | 0.46 |
| 1:1:481:LEU:CD1 | 1:2:636:LEU:HD11 | 2.45 | 0.46 |
| 1:2:426:SER:OG | 1:2:731:THR:O | 2.31 | 0.46 |
| 1:2:485:CYS:HB2 | 1:2:573:PRO:HG3 | 1.97 | 0.46 |
| 1:3:356:VAL:CG2 | 1:4:438:ASN:HB2 | 2.46 | 0.46 |
| 1:3:398:LEU:C | 1:3:400:TYR:H | 2.24 | 0.46 |
| 1:6:481:LEU:CD1 | 1:7:636:LEU:HD11 | 2.45 | 0.46 |
| 1:7:238:ASP:OD1 | 1:7:239:ARG:N | 2.48 | 0.46 |
| 1:A:238:ASP:OD1 | 1:A:239:ARG:N | 2.48 | 0.46 |
| 1:A:426:SER:OG | 1:A:731:THR:O | 2.31 | 0.46 |
| 1:B:564:SER:OG | 1:B:566:GLU:HG2 | 2.15 | 0.46 |
| 1:C:585:ASN:OD1 | 1:C:594:ILE:N | 2.45 | 0.46 |
| 1:H:398:LEU:C | 1:H:400:TYR:H | 2.24 | 0.46 |
| 1:J:609:TRP:CD1 | 1:J:609:TRP:C | 2.93 | 0.46 |
| 1:K:356:VAL:CG2 | 1:8:438:ASN:HB2 | 2.45 | 0.46 |
| 1:M:609:TRP:CD1 | 1:M:609:TRP:C | 2.93 | 0.46 |
| 1:N:481:LEU:CD1 | 1:P:636:LEU:HD11 | 2.45 | 0.46 |
| 1:O:238:ASP:OD1 | 1:O:239:ARG:N | 2.48 | 0.46 |
| 1:R:481:LEU:CD1 | 1:S:636:LEU:HD11 | 2.45 | 0.46 |
| 1:S:481:LEU:CD1 | 1:U:636:LEU:HD11 | 2.45 | 0.46 |
| 1:Z:438:ASN:HB2 | 1:4:356:VAL:CG2 | 2.46 | 0.46 |
| 1:f:356:VAL:CG2 | 1:g:438:ASN:HB2 | 2.46 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:f:564:SER:OG | 1:f:566:GLU:HG2 | 2.15 | 0.46 |
| 1:f:636:LEU:HD11 | 1:g:481:LEU:CD1 | 2.45 | 0.46 |
| 1:g:636:LEU:HD11 | 1:h:481:LEU:CD1 | 2.45 | 0.46 |
| 1:h:238:ASP:OD1 | 1:h:239:ARG:N | 2.48 | 0.46 |
| 1:i:481:LEU:CD1 | 1:j:636:LEU:HD11 | 2.45 | 0.46 |
| 1:i:609:TRP:CD1 | 1:i:609:TRP:C | 2.93 | 0.46 |
| 1:k:238:ASP:OD1 | 1:k:239:ARG:N | 2.48 | 0.46 |
| 1:k:564:SER:OG | 1:k:566:GLU:HG2 | 2.15 | 0.46 |
| 1:m:438:ASN:HB2 | 1:n:356:VAL:CG2 | 2.46 | 0.46 |
| 1:o:238:ASP:OD1 | 1:o:239:ARG:N | 2.48 | 0.46 |
| 1:o:609:TRP:CD1 | 1:o:609:TRP:C | 2.93 | 0.46 |
| 1:s:398:LEU:C | 1:s:400:TYR:H | 2.24 | 0.46 |
| 1:t:430:SER:O | 1:u:383:LEU:HG | 2.15 | 0.46 |
| 1:2:329:ASN:O | 1:2:332:THR:OG1 | 2.31 | 0.46 |
| 1:3:238:ASP:OD1 | 1:3:239:ARG:N | 2.48 | 0.46 |
| 1:4:564:SER:OG | 1:4:566:GLU:HG2 | 2.15 | 0.46 |
| 1:6:429:HIS:HD2 | 1:6:610:GLN:OE1 | 1.94 | 0.46 |
| 1:6:438:ASN:HB2 | 1:7:356:VAL:CG2 | 2.46 | 0.46 |
| 1:6:585:ASN:OD1 | 1:6:594:ILE:N | 2.45 | 0.46 |
| 1:D:438:ASN:HB2 | 1:N:356:VAL:CG2 | 2.46 | 0.46 |
| 1:G:438:ASN:HB2 | 1:I:356:VAL:CG2 | 2.46 | 0.46 |
| 1:H:382:THR:HG22 | 1:H:383:LEU:N | 2.29 | 0.46 |
| 1:H:426:SER:OG | 1:H:731:THR:O | 2.31 | 0.46 |
| 1:K:481:LEU:CD1 | 1:a:636:LEU:HD11 | 2.45 | 0.46 |
| 1:O:481:LEU:CD1 | 1:m:636:LEU:HD11 | 2.45 | 0.46 |
| 1:R:430:SER:O | 1:S:383:LEU:HG | 2.15 | 0.46 |
| 1:S:438:ASN:HB2 | 1:U:356:VAL:CG2 | 2.46 | 0.46 |
| 1:T:438:ASN:HB2 | 1:d:356:VAL:CG2 | 2.46 | 0.46 |
| 1:U:398:LEU:C | 1:U:400:TYR:H | 2.24 | 0.46 |
| 1:V:356:VAL:CG2 | 1:X:438:ASN:HB2 | 2.46 | 0.46 |
| 1:Y:398:LEU:C | 1:Y:400:TYR:H | 2.24 | 0.46 |
| 1:Z:238:ASP:OD1 | 1:Z:239:ARG:N | 2.48 | 0.46 |
| 1:Z:485:CYS:HB2 | 1:Z:573:PRO:HG3 | 1.97 | 0.46 |
| 1:Z:636:LEU:HD11 | 1:3:481:LEU:CD1 | 2.45 | 0.46 |
| 1:a:481:LEU:CD1 | 1:8:636:LEU:HD11 | 2.45 | 0.46 |
| 1:e:485:CYS:HB2 | 1:e:573:PRO:HG3 | 1.97 | 0.46 |
| 1:f:609:TRP:NE1 | 1:h:629:GLY:CA | 2.58 | 0.46 |
| 1:g:254:ASN:C | 1:g:256:HIS:N | 2.71 | 0.46 |
| 1:g:609:TRP:CD1 | 1:g:609:TRP:C | 2.93 | 0.46 |
| 1:j:232:ASP:HB3 | 1:x:402:PRO:CG | 2.46 | 0.46 |
| 1:j:609:TRP:NE1 | 1:k:629:GLY:CA | 2.58 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:481:LEU:CD1 | 1:n:636:LEU:HD11 | 2.45 | 0.46 |
| 1:n:398:LEU:C | 1:n:400:TYR:H | 2.24 | 0.46 |
| 1:r:382:THR:HG22 | 1:r:383:LEU:N | 2.29 | 0.46 |
| 1:r:398:LEU:C | 1:r:400:TYR:H | 2.24 | 0.46 |
| 1:s:238:ASP:OD1 | 1:s:239:ARG:N | 2.48 | 0.46 |
| 1:s:254:ASN:C | 1:s:256:HIS:N | 2.71 | 0.46 |
| 1:u:438:ASN:HB2 | 1:v:356:VAL:CG2 | 2.46 | 0.46 |
| 1:u:481:LEU:CD1 | 1:v:636:LEU:HD11 | 2.45 | 0.46 |
| 1:y:609:TRP:CD1 | 1:y:609:TRP:C | 2.94 | 0.46 |
| 1:1:430:SER:O | 1:2:383:LEU:HG | 2.15 | 0.46 |
| 1:1:438:ASN:HB2 | 1:2:356:VAL:CG2 | 2.46 | 0.46 |
| 1:4:398:LEU:C | 1:4:400:TYR:H | 2.24 | 0.46 |
| 1:D:481:LEU:CD1 | 1:N:636:LEU:HD11 | 2.45 | 0.46 |
| 1:E:398:LEU:C | 1:E:400:TYR:H | 2.24 | 0.46 |
| 1:F:356:VAL:CG2 | 1:Q:438:ASN:HB2 | 2.46 | 0.46 |
| 1:H:564:SER:OG | 1:H:566:GLU:HG2 | 2.15 | 0.46 |
| 1:J:438:ASN:HB2 | 1:L:356:VAL:CG2 | 2.46 | 0.46 |
| 1:O:636:LEU:HD11 | 1:n:481:LEU:CD1 | 2.46 | 0.46 |
| 1:Q:398:LEU:C | 1:Q:400:TYR:H | 2.24 | 0.46 |
| 1:R:438:ASN:HB2 | 1:S:356:VAL:CG2 | 2.46 | 0.46 |
| 1:R:609:TRP:CD1 | 1:R:609:TRP:C | 2.93 | 0.46 |
| 1:T:430:SER:O | 1:d:383:LEU:HG | 2.15 | 0.46 |
| 1:V:564:SER:OG | 1:V:566:GLU:HG2 | 2.15 | 0.46 |
| 1:V:609:TRP:CD1 | 1:V:609:TRP:C | 2.94 | 0.46 |
| 1:W:430:SER:O | 1:Y:383:LEU:HG | 2.15 | 0.46 |
| 1:Z:481:LEU:CD1 | 1:4:636:LEU:HD11 | 2.45 | 0.46 |
| 1:Z:609:TRP:CD1 | 1:Z:609:TRP:C | 2.93 | 0.46 |
| 1:d:329:ASN:O | 1:d:332:THR:OG1 | 2.31 | 0.46 |
| 1:d:398:LEU:C | 1:d:400:TYR:H | 2.24 | 0.46 |
| 1:d:426:SER:OG | 1:d:731:THR:O | 2.31 | 0.46 |
| 1:i:585:ASN:OD1 | 1:i:594:ILE:N | 2.45 | 0.46 |
| 1:m:238:ASP:OD1 | 1:m:239:ARG:N | 2.48 | 0.46 |
| 1:m:609:TRP:CD1 | 1:m:609:TRP:C | 2.93 | 0.46 |
| 1:o:426:SER:OG | 1:o:731:THR:O | 2.31 | 0.46 |
| 1:o:434:ASP:OD1 | 1:o:434:ASP:N | 2.41 | 0.46 |
| 1:o:564:SER:OG | 1:o:566:GLU:HG2 | 2.15 | 0.46 |
| 1:p:238:ASP:OD1 | 1:p:239:ARG:N | 2.48 | 0.46 |
| 1:q:238:ASP:OD1 | 1:q:239:ARG:N | 2.48 | 0.46 |
| 1:s:426:SER:OG | 1:s:731:THR:O | 2.31 | 0.46 |
| 1:t:609:TRP:CD1 | 1:t:609:TRP:C | 2.93 | 0.46 |
| 1:u:429:HIS:HD2 | 1:u:610:GLN:OE1 | 1.94 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:v:398:LEU:C | 1:v:400:TYR:H | 2.24 | 0.46 |
| 1:w:485:CYS:HB2 | 1:w:573:PRO:HG3 | 1.97 | 0.46 |
| 1:x:398:LEU:C | 1:x:400:TYR:H | 2.24 | 0.46 |
| 1:z:238:ASP:OD1 | 1:z:239:ARG:N | 2.48 | 0.46 |
| 1:3:307:TRP:O | 1:3:426:SER:CB | 2.59 | 0.46 |
| 1:5:398:LEU:C | 1:5:400:TYR:H | 2.24 | 0.46 |
| 1:5:438:ASN:HB2 | 1:6:356:VAL:CG2 | 2.46 | 0.46 |
| 1:6:398:LEU:C | 1:6:400:TYR:H | 2.24 | 0.46 |
| 1:7:254:ASN:C | 1:7:256:HIS:N | 2.71 | 0.46 |
| 1:7:398:LEU:C | 1:7:400:TYR:H | 2.24 | 0.46 |
| 1:7:564:SER:OG | 1:7:566:GLU:HG2 | 2.15 | 0.46 |
| 1:A:564:SER:OG | 1:A:566:GLU:HG2 | 2.15 | 0.46 |
| 1:B:426:SER:OG | 1:B:731:THR:O | 2.31 | 0.46 |
| 1:C:356:VAL:CG2 | 1:M:438:ASN:HB2 | 2.46 | 0.46 |
| 1:C:434:ASP:OD1 | 1:C:434:ASP:N | 2.41 | 0.46 |
| 1:D:383:LEU:HG | 1:P:430:SER:O | 2.16 | 0.46 |
| 1:E:254:ASN:C | 1:E:256:HIS:N | 2.71 | 0.46 |
| 1:E:481:LEU:CD1 | 1:Q:636:LEU:HD11 | 2.45 | 0.46 |
| 1:F:429:HIS:HD2 | 1:F:610:GLN:OE1 | 1.94 | 0.46 |
| 1:G:238:ASP:OD1 | 1:G:239:ARG:N | 2.48 | 0.46 |
| 1:G:398:LEU:C | 1:G:400:TYR:H | 2.24 | 0.46 |
| 1:H:238:ASP:OD1 | 1:H:239:ARG:N | 2.48 | 0.46 |
| 1:H:254:ASN:C | 1:H:256:HIS:N | 2.71 | 0.46 |
| 1:H:636:LEU:HD11 | 1:Y:481:LEU:CD1 | 2.45 | 0.46 |
| 1:K:383:LEU:HG | 1:8:430:SER:O | 2.16 | 0.46 |
| 1:K:402:PRO:CG | 1:7:232:ASP:HB3 | 2.46 | 0.46 |
| 1:K:609:TRP:CD1 | 1:K:609:TRP:C | 2.93 | 0.46 |
| 1:L:434:ASP:OD1 | 1:L:434:ASP:N | 2.41 | 0.46 |
| 1:M:254:ASN:C | 1:M:256:HIS:N | 2.71 | 0.46 |
| 1:Q:485:CYS:HB2 | 1:Q:573:PRO:HG3 | 1.97 | 0.46 |
| 1:R:356:VAL:CG2 | 1:U:438:ASN:HB2 | 2.46 | 0.46 |
| 1:S:416:TYR:OH | 1:S:644:HIS:O | 2.27 | 0.46 |
| 1:V:434:ASP:OD1 | 1:V:434:ASP:N | 2.41 | 0.46 |
| 1:W:609:TRP:NE1 | 1:Y:629:GLY:CA | 2.58 | 0.46 |
| 1:Y:382:THR:HG22 | 1:Y:383:LEU:N | 2.29 | 0.46 |
| 1:c:356:VAL:CG2 | 1:p:438:ASN:HB2 | 2.46 | 0.46 |
| 1:e:398:LEU:C | 1:e:400:TYR:H | 2.24 | 0.46 |
| 1:f:238:ASP:OD1 | 1:f:239:ARG:N | 2.48 | 0.46 |
| 1:i:438:ASN:HB2 | 1:j:356:VAL:CG2 | 2.46 | 0.46 |
| 1:j:238:ASP:OD1 | 1:j:239:ARG:N | 2.48 | 0.46 |
| 1:j:307:TRP:O | 1:j:426:SER:CB | 2.59 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:382:THR:HG22 | 1:j:383:LEU:N | 2.29 | 0.46 |
| 1:l:238:ASP:OD1 | 1:l:239:ARG:N | 2.48 | 0.46 |
| 1:p:329:ASN:O | 1:p:332:THR:OG1 | 2.31 | 0.46 |
| 1:p:398:LEU:C | 1:p:400:TYR:H | 2.24 | 0.46 |
| 1:t:356:VAL:CG2 | 1:v:438:ASN:HB2 | 2.46 | 0.46 |
| 1:t:438:ASN:HB2 | 1:u:356:VAL:CG2 | 2.46 | 0.46 |
| 1:t:481:LEU:CD1 | 1:u:636:LEU:HD11 | 2.45 | 0.46 |
| 1:u:307:TRP:CE2 | 1:u:692:GLU:HG2 | 2.51 | 0.46 |
| 1:v:307:TRP:CE2 | 1:v:692:GLU:HG2 | 2.51 | 0.46 |
| 1:v:473:MET:HE3 | 1:v:473:MET:HB2 | 1.81 | 0.46 |
| 1:w:426:SER:OG | 1:w:731:THR:O | 2.31 | 0.46 |
| 1:w:490:ARG:NE | 1:y:586:LEU:HD11 | 2.31 | 0.46 |
| 1:y:564:SER:OG | 1:y:566:GLU:HG2 | 2.15 | 0.46 |
| 1:2:398:LEU:C | 1:2:400:TYR:H | 2.24 | 0.46 |
| 1:3:636:LEU:HD11 | 1:4:481:LEU:CD1 | 2.46 | 0.46 |
| 1:5:485:CYS:HB2 | 1:5:573:PRO:HG3 | 1.97 | 0.46 |
| 1:5:636:LEU:HD11 | 1:7:481:LEU:CD1 | 2.45 | 0.46 |
| 1:8:307:TRP:O | 1:8:426:SER:CB | 2.59 | 0.46 |
| 1:8:564:SER:OG | 1:8:566:GLU:HG2 | 2.15 | 0.46 |
| 1:B:430:SER:O | 1:J:383:LEU:HG | 2.15 | 0.46 |
| 1:D:609:TRP:CD1 | 1:D:609:TRP:C | 2.94 | 0.46 |
| 1:E:564:SER:OG | 1:E:566:GLU:HG2 | 2.15 | 0.46 |
| 1:G:609:TRP:CD1 | 1:G:609:TRP:C | 2.93 | 0.46 |
| 1:H:307:TRP:CE2 | 1:H:692:GLU:HG2 | 2.51 | 0.46 |
| 1:H:485:CYS:HB2 | 1:H:573:PRO:HG3 | 1.97 | 0.46 |
| 1:H:585:ASN:OD1 | 1:H:594:ILE:N | 2.45 | 0.46 |
| 1:K:430:SER:O | 1:a:383:LEU:HG | 2.15 | 0.46 |
| 1:K:438:ASN:HB2 | 1:a:356:VAL:CG2 | 2.46 | 0.46 |
| 1:M:238:ASP:OD1 | 1:M:239:ARG:N | 2.48 | 0.46 |
| 1:M:398:LEU:C | 1:M:400:TYR:H | 2.24 | 0.46 |
| 1:M:636:LEU:HD11 | 1:b:481:LEU:CD1 | 2.45 | 0.46 |
| 1:N:429:HIS:HD2 | 1:N:610:GLN:OE1 | 1.94 | 0.46 |
| 1:O:307:TRP:O | 1:O:426:SER:CB | 2.59 | 0.46 |
| 1:O:564:SER:OG | 1:O:566:GLU:HG2 | 2.15 | 0.46 |
| 1:P:238:ASP:OD1 | 1:P:239:ARG:N | 2.48 | 0.46 |
| 1:P:564:SER:OG | 1:P:566:GLU:HG2 | 2.15 | 0.46 |
| 1:T:238:ASP:OD1 | 1:T:239:ARG:N | 2.48 | 0.46 |
| 1:T:609:TRP:CD1 | 1:T:609:TRP:C | 2.93 | 0.46 |
| 1:U:307:TRP:CE2 | 1:U:692:GLU:HG2 | 2.51 | 0.46 |
| 1:V:629:GLY:CA | 1:X:609:TRP:NE1 | 2.58 | 0.46 |
| 1:W:238:ASP:OD1 | 1:W:239:ARG:N | 2.48 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:307:TRP:CE2 | 1:W:692:GLU:HG2 | 2.51 | 0.46 |
| 1:W:382:THR:HG22 | 1:W:383:LEU:N | 2.29 | 0.46 |
| 1:Z:307:TRP:CE2 | 1:Z:692:GLU:HG2 | 2.51 | 0.46 |
| 1:Z:356:VAL:CG2 | 1:3:438:ASN:HB2 | 2.46 | 0.46 |
| 1:Z:398:LEU:C | 1:Z:400:TYR:H | 2.24 | 0.46 |
| 1:a:329:ASN:O | 1:a:332:THR:OG1 | 2.31 | 0.46 |
| 1:a:429:HIS:HD2 | 1:a:610:GLN:OE1 | 1.94 | 0.46 |
| 1:f:382:THR:HG22 | 1:f:383:LEU:N | 2.29 | 0.46 |
| 1:i:254:ASN:C | 1:i:256:HIS:N | 2.71 | 0.46 |
| 1:k:402:PRO:CG | 1:w:232:ASP:HB3 | 2.43 | 0.46 |
| 1:m:398:LEU:C | 1:m:400:TYR:H | 2.24 | 0.46 |
| 1:n:300:GLN:NE2 | 1:n:703:TYR:O | 2.45 | 0.46 |
| 1:n:307:TRP:CE2 | 1:n:692:GLU:HG2 | 2.51 | 0.46 |
| 1:q:430:SER:O | 1:r:383:LEU:HG | 2.15 | 0.46 |
| 1:r:481:LEU:CD1 | 1:s:636:LEU:HD11 | 2.45 | 0.46 |
| 1:s:307:TRP:CE2 | 1:s:692:GLU:HG2 | 2.51 | 0.46 |
| 1:s:485:CYS:HB2 | 1:s:573:PRO:HG3 | 1.97 | 0.46 |
| 1:s:564:SER:OG | 1:s:566:GLU:HG2 | 2.15 | 0.46 |
| 1:w:398:LEU:C | 1:w:400:TYR:H | 2.24 | 0.46 |
| 1:x:307:TRP:CE2 | 1:x:692:GLU:HG2 | 2.51 | 0.46 |
| 1:4:300:GLN:NE2 | 1:4:703:TYR:O | 2.45 | 0.46 |
| 1:7:609:TRP:CD1 | 1:7:609:TRP:C | 2.94 | 0.46 |
| 1:A:307:TRP:CE2 | 1:A:692:GLU:HG2 | 2.52 | 0.45 |
| 1:B:481:LEU:CD1 | 1:J:636:LEU:HD11 | 2.45 | 0.45 |
| 1:E:609:TRP:CD1 | 1:E:609:TRP:C | 2.94 | 0.45 |
| 1:F:258:TYR:OH | 1:F:399:GLU:OE1 | 2.22 | 0.45 |
| 1:F:398:LEU:C | 1:F:400:TYR:H | 2.24 | 0.45 |
| 1:F:609:TRP:CD1 | 1:F:609:TRP:C | 2.93 | 0.45 |
| 1:G:609:TRP:NE1 | 1:I:629:GLY:CA | 2.58 | 0.45 |
| 1:J:238:ASP:OD1 | 1:J:239:ARG:N | 2.48 | 0.45 |
| 1:J:609:TRP:NE1 | 1:L:629:GLY:CA | 2.58 | 0.45 |
| 1:J:616:LEU:HD22 | 1:J:729:ILE:HD12 | 1.99 | 0.45 |
| 1:L:307:TRP:CE2 | 1:L:692:GLU:HG2 | 2.51 | 0.45 |
| 1:M:383:LEU:HG | 1:b:430:SER:O | 2.15 | 0.45 |
| 1:M:426:SER:OG | 1:M:731:THR:O | 2.31 | 0.45 |
| 1:M:564:SER:OG | 1:M:566:GLU:HG2 | 2.15 | 0.45 |
| 1:O:438:ASN:HB2 | 1:m:356:VAL:CG2 | 2.46 | 0.45 |
| 1:P:232:ASP:HB3 | 1:Q:402:PRO:CG | 2.46 | 0.45 |
| 1:S:238:ASP:OD1 | 1:S:239:ARG:N | 2.48 | 0.45 |
| 1:V:402:PRO:CG | 1:W:232:ASP:HB3 | 2.46 | 0.45 |
| 1:V:430:SER:O | 1:e:383:LEU:HG | 2.16 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:307:TRP:CE2 | 1:X:692:GLU:HG2 | 2.52 | 0.45 |
| 1:b:426:SER:OG | 1:b:731:THR:O | 2.31 | 0.45 |
| 1:c:416:TYR:OH | 1:c:644:HIS:O | 2.27 | 0.45 |
| 1:d:430:SER:O | 1:l:383:LEU:HG | 2.16 | 0.45 |
| 1:f:438:ASN:HB2 | 1:h:356:VAL:CG2 | 2.46 | 0.45 |
| 1:m:307:TRP:CE2 | 1:m:692:GLU:HG2 | 2.51 | 0.45 |
| 1:o:307:TRP:CE2 | 1:o:692:GLU:HG2 | 2.52 | 0.45 |
| 1:o:329:ASN:O | 1:o:332:THR:OG1 | 2.30 | 0.45 |
| 1:q:307:TRP:CE2 | 1:q:692:GLU:HG2 | 2.51 | 0.45 |
| 1:t:636:LEU:HD11 | 1:v:481:LEU:CD1 | 2.45 | 0.45 |
| 1:v:485:CYS:HB2 | 1:v:573:PRO:HG3 | 1.97 | 0.45 |
| 1:1:564:SER:OG | 1:1:566:GLU:HG2 | 2.15 | 0.45 |
| 1:1:609:TRP:CD1 | 1:1:609:TRP:C | 2.93 | 0.45 |
| 1:2:609:TRP:CD1 | 1:2:609:TRP:C | 2.93 | 0.45 |
| 1:4:307:TRP:CE2 | 1:4:692:GLU:HG2 | 2.51 | 0.45 |
| 1:5:402:PRO:CG | 1:8:232:ASP:HB3 | 2.46 | 0.45 |
| 1:6:609:TRP:CD1 | 1:6:609:TRP:C | 2.93 | 0.45 |
| 1:8:238:ASP:OD1 | 1:8:239:ARG:N | 2.48 | 0.45 |
| 1:A:290:PHE:O | 1:A:293:HIS:N | 2.47 | 0.45 |
| 1:A:329:ASN:O | 1:A:332:THR:OG1 | 2.31 | 0.45 |
| 1:B:307:TRP:CE2 | 1:B:692:GLU:HG2 | 2.51 | 0.45 |
| 1:B:609:TRP:CD1 | 1:B:609:TRP:C | 2.93 | 0.45 |
| 1:C:307:TRP:CE2 | 1:C:692:GLU:HG2 | 2.51 | 0.45 |
| 1:D:430:SER:O | 1:N:383:LEU:HG | 2.15 | 0.45 |
| 1:F:564:SER:OG | 1:F:566:GLU:HG2 | 2.15 | 0.45 |
| 1:G:564:SER:OG | 1:G:566:GLU:HG2 | 2.15 | 0.45 |
| 1:J:254:ASN:C | 1:J:256:HIS:N | 2.71 | 0.45 |
| 1:J:398:LEU:C | 1:J:400:TYR:H | 2.24 | 0.45 |
| 1:J:564:SER:OG | 1:J:566:GLU:HG2 | 2.15 | 0.45 |
| 1:P:609:TRP:CD1 | 1:P:609:TRP:C | 2.93 | 0.45 |
| 1:Q:426:SER:OG | 1:Q:731:THR:O | 2.31 | 0.45 |
| 1:R:382:THR:HG22 | 1:R:383:LEU:N | 2.29 | 0.45 |
| 1:R:402:PRO:CG | 1:V:232:ASP:HB3 | 2.46 | 0.45 |
| 1:S:307:TRP:CE2 | 1:S:692:GLU:HG2 | 2.52 | 0.45 |
| 1:S:382:THR:HG22 | 1:S:383:LEU:N | 2.29 | 0.45 |
| 1:U:427:TYR:O | 1:U:427:TYR:HD1 | 2.00 | 0.45 |
| 1:U:485:CYS:HB2 | 1:U:573:PRO:HG3 | 1.97 | 0.45 |
| 1:V:586:LEU:HD21 | 1:e:490:ARG:NH1 | 2.31 | 0.45 |
| 1:Y:616:LEU:HD22 | 1:Y:729:ILE:HD12 | 1.99 | 0.45 |
| 1:Z:430:SER:O | 1:4:383:LEU:HG | 2.15 | 0.45 |
| 1:b:307:TRP:CE2 | 1:b:692:GLU:HG2 | 2.51 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:609:TRP:CD1 | 1:b:609:TRP:C | 2.93 | 0.45 |
| 1:c:609:TRP:CD1 | 1:c:609:TRP:C | 2.93 | 0.45 |
| 1:d:609:TRP:CD1 | 1:d:609:TRP:C | 2.93 | 0.45 |
| 1:f:307:TRP:O | 1:f:426:SER:CB | 2.59 | 0.45 |
| 1:f:629:GLY:CA | 1:g:609:TRP:CD1 | 2.86 | 0.45 |
| 1:g:356:VAL:CG2 | 1:h:438:ASN:HB2 | 2.46 | 0.45 |
| 1:g:616:LEU:HD22 | 1:g:729:ILE:HD12 | 1.99 | 0.45 |
| 1:i:616:LEU:HD22 | 1:i:729:ILE:HD12 | 1.99 | 0.45 |
| 1:j:307:TRP:CE2 | 1:j:692:GLU:HG2 | 2.51 | 0.45 |
| 1:k:307:TRP:CE2 | 1:k:692:GLU:HG2 | 2.51 | 0.45 |
| 1:o:290:PHE:O | 1:o:293:HIS:N | 2.47 | 0.45 |
| 1:p:564:SER:OG | 1:p:566:GLU:HG2 | 2.15 | 0.45 |
| 1:p:609:TRP:CD1 | 1:p:609:TRP:C | 2.93 | 0.45 |
| 1:t:564:SER:OG | 1:t:566:GLU:HG2 | 2.15 | 0.45 |
| 1:u:238:ASP:OD1 | 1:u:239:ARG:N | 2.48 | 0.45 |
| 1:v:609:TRP:CD1 | 1:v:609:TRP:C | 2.93 | 0.45 |
| 1:x:258:TYR:OH | 1:x:399:GLU:OE1 | 2.22 | 0.45 |
| 1:1:238:ASP:OD1 | 1:1:239:ARG:N | 2.48 | 0.45 |
| 1:3:564:SER:OG | 1:3:566:GLU:HG2 | 2.15 | 0.45 |
| 1:3:585:ASN:OD1 | 1:3:594:ILE:N | 2.45 | 0.45 |
| 1:6:564:SER:OG | 1:6:566:GLU:HG2 | 2.15 | 0.45 |
| 1:C:636:LEU:HD11 | 1:M:481:LEU:CD1 | 2.45 | 0.45 |
| 1:D:307:TRP:CE2 | 1:D:692:GLU:HG2 | 2.52 | 0.45 |
| 1:D:427:TYR:O | 1:D:427:TYR:HD1 | 2.00 | 0.45 |
| 1:D:554:ASN:HB3 | 1:P:464:LEU:HD23 | 1.98 | 0.45 |
| 1:G:427:TYR:O | 1:G:427:TYR:HD1 | 2.00 | 0.45 |
| 1:H:356:VAL:CG2 | 1:Y:438:ASN:HB2 | 2.46 | 0.45 |
| 1:I:609:TRP:CD1 | 1:I:609:TRP:C | 2.93 | 0.45 |
| 1:K:427:TYR:HD1 | 1:K:427:TYR:O | 2.00 | 0.45 |
| 1:K:435:ARG:HD3 | 1:K:435:ARG:HA | 1.79 | 0.45 |
| 1:K:490:ARG:NH1 | 1:8:586:LEU:HD21 | 2.31 | 0.45 |
| 1:M:616:LEU:HD22 | 1:M:729:ILE:HD12 | 1.99 | 0.45 |
| 1:N:329:ASN:O | 1:N:332:THR:OG1 | 2.31 | 0.45 |
| 1:N:382:THR:HG22 | 1:N:383:LEU:N | 2.29 | 0.45 |
| 1:N:398:LEU:C | 1:N:400:TYR:H | 2.24 | 0.45 |
| 1:N:609:TRP:CD1 | 1:N:609:TRP:C | 2.93 | 0.45 |
| 1:P:307:TRP:O | 1:P:426:SER:CB | 2.59 | 0.45 |
| 1:R:636:LEU:HD11 | 1:U:481:LEU:CD1 | 2.45 | 0.45 |
| 1:T:383:LEU:HG | 1:l:430:SER:O | 2.15 | 0.45 |
| 1:T:564:SER:OG | 1:T:566:GLU:HG2 | 2.15 | 0.45 |
| 1:T:636:LEU:HD11 | 1:l:481:LEU:CD1 | 2.45 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:258:TYR:OH | 1:X:399:GLU:OE1 | 2.22 | 0.45 |
| 1:a:382:THR:HG22 | 1:a:383:LEU:N | 2.29 | 0.45 |
| 1:a:430:SER:O | 1:8:383:LEU:HG | 2.16 | 0.45 |
| 1:a:609:TRP:CD1 | 1:a:609:TRP:C | 2.93 | 0.45 |
| 1:d:427:TYR:O | 1:d:427:TYR:HD1 | 2.00 | 0.45 |
| 1:e:427:TYR:O | 1:e:427:TYR:HD1 | 2.00 | 0.45 |
| 1:f:307:TRP:CE2 | 1:f:692:GLU:HG2 | 2.52 | 0.45 |
| 1:j:398:LEU:C | 1:j:400:TYR:H | 2.24 | 0.45 |
| 1:l:307:TRP:CE2 | 1:l:692:GLU:HG2 | 2.51 | 0.45 |
| 1:l:564:SER:OG | 1:l:566:GLU:HG2 | 2.15 | 0.45 |
| 1:l:609:TRP:CD1 | 1:l:609:TRP:C | 2.93 | 0.45 |
| 1:p:427:TYR:O | 1:p:427:TYR:HD1 | 2.00 | 0.45 |
| 1:q:382:THR:HG22 | 1:q:383:LEU:N | 2.29 | 0.45 |
| 1:r:616:LEU:HD22 | 1:r:729:ILE:HD12 | 1.99 | 0.45 |
| 1:v:402:PRO:CG | 1:1:232:ASP:HB3 | 2.47 | 0.45 |
| 1:v:427:TYR:HD1 | 1:v:427:TYR:O | 2.00 | 0.45 |
| 1:x:464:LEU:HD23 | 1:y:554:ASN:HB3 | 1.98 | 0.45 |
| 1:y:398:LEU:C | 1:y:400:TYR:H | 2.24 | 0.45 |
| 1:z:383:LEU:HG | 1:2:430:SER:O | 2.16 | 0.45 |
| 1:z:398:LEU:C | 1:z:400:TYR:H | 2.24 | 0.45 |
| 1:z:481:LEU:CD1 | 1:1:636:LEU:HD11 | 2.45 | 0.45 |
| 1:2:427:TYR:O | 1:2:427:TYR:HD1 | 2.00 | 0.45 |
| 1:4:382:THR:HG22 | 1:4:383:LEU:N | 2.29 | 0.45 |
| 1:5:383:LEU:HG | 1:7:430:SER:O | 2.15 | 0.45 |
| 1:6:258:TYR:OH | 1:6:399:GLU:OE1 | 2.22 | 0.45 |
| 1:8:398:LEU:C | 1:8:400:TYR:H | 2.24 | 0.45 |
| 1:D:435:ARG:HD3 | 1:D:435:ARG:HA | 1.79 | 0.45 |
| 1:D:473:MET:HE3 | 1:D:473:MET:HB2 | 1.81 | 0.45 |
| 1:D:490:ARG:NH1 | 1:P:586:LEU:HD21 | 2.31 | 0.45 |
| 1:D:616:LEU:HD22 | 1:D:729:ILE:HD12 | 1.99 | 0.45 |
| 1:H:438:ASN:HB2 | 1:W:356:VAL:CG2 | 2.46 | 0.45 |
| 1:J:426:SER:OG | 1:J:731:THR:O | 2.31 | 0.45 |
| 1:J:481:LEU:CD1 | 1:L:636:LEU:HD11 | 2.45 | 0.45 |
| 1:K:307:TRP:CE2 | 1:K:692:GLU:HG2 | 2.52 | 0.45 |
| 1:K:616:LEU:HD22 | 1:K:729:ILE:HD12 | 1.99 | 0.45 |
| 1:N:430:SER:O | 1:P:383:LEU:HG | 2.16 | 0.45 |
| 1:N:438:ASN:HB2 | 1:P:356:VAL:CG2 | 2.46 | 0.45 |
| 1:O:616:LEU:HD22 | 1:O:729:ILE:HD12 | 1.99 | 0.45 |
| 1:R:307:TRP:CE2 | 1:R:692:GLU:HG2 | 2.52 | 0.45 |
| 1:R:564:SER:OG | 1:R:566:GLU:HG2 | 2.15 | 0.45 |
| 1:S:616:LEU:HD22 | 1:S:729:ILE:HD12 | 1.99 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:426:SER:OG | 1:U:731:THR:O | 2.31 | 0.45 |
| 1:U:473:MET:HE3 | 1:U:473:MET:HB2 | 1.81 | 0.45 |
| 1:U:609:TRP:CD1 | 1:U:609:TRP:C | 2.94 | 0.45 |
| 1:V:398:LEU:C | 1:V:400:TYR:H | 2.24 | 0.45 |
| 1:W:609:TRP:CD1 | 1:W:609:TRP:C | 2.93 | 0.45 |
| 1:X:356:VAL:CG2 | 1:e:438:ASN:HB2 | 2.46 | 0.45 |
| 1:X:609:TRP:CD1 | 1:X:609:TRP:C | 2.93 | 0.45 |
| 1:a:527:ALA:O | 1:a:575:ALA:N | 2.45 | 0.45 |
| 1:c:438:ASN:HB2 | 1:o:356:VAL:CG2 | 2.46 | 0.45 |
| 1:d:429:HIS:HD2 | 1:d:610:GLN:OE1 | 1.94 | 0.45 |
| 1:e:435:ARG:HD3 | 1:e:435:ARG:HA | 1.79 | 0.45 |
| 1:g:341:SER:HB3 | 1:g:675:GLN:NE2 | 2.32 | 0.45 |
| 1:h:307:TRP:CE2 | 1:h:692:GLU:HG2 | 2.52 | 0.45 |
| 1:i:356:VAL:CG2 | 1:k:438:ASN:HB2 | 2.46 | 0.45 |
| 1:j:438:ASN:HB2 | 1:k:356:VAL:CG2 | 2.46 | 0.45 |
| 1:l:254:ASN:C | 1:l:256:HIS:N | 2.71 | 0.45 |
| 1:l:402:PRO:CG | 1:n:232:ASP:HB3 | 2.46 | 0.45 |
| 1:n:435:ARG:HD3 | 1:n:435:ARG:HA | 1.79 | 0.45 |
| 1:o:300:GLN:NE2 | 1:o:703:TYR:O | 2.45 | 0.45 |
| 1:q:609:TRP:CD1 | 1:q:609:TRP:C | 2.93 | 0.45 |
| 1:r:438:ASN:HB2 | 1:s:356:VAL:CG2 | 2.46 | 0.45 |
| 1:t:232:ASP:HB3 | 1:6:402:PRO:CG | 2.47 | 0.45 |
| 1:u:382:THR:HG22 | 1:u:383:LEU:N | 2.29 | 0.45 |
| 1:u:616:LEU:HD22 | 1:u:729:ILE:HD12 | 1.99 | 0.45 |
| 1:w:427:TYR:O | 1:w:427:TYR:HD1 | 2.00 | 0.45 |
| 1:z:254:ASN:C | 1:z:256:HIS:N | 2.71 | 0.45 |
| 1:z:307:TRP:CE2 | 1:z:692:GLU:HG2 | 2.52 | 0.45 |
| 1:5:426:SER:OG | 1:5:731:THR:O | 2.31 | 0.45 |
| 1:8:609:TRP:CD1 | 1:8:609:TRP:C | 2.94 | 0.45 |
| 1:A:356:VAL:CG2 | 1:I:438:ASN:HB2 | 2.46 | 0.45 |
| 1:A:586:LEU:HD21 | 1:G:490:ARG:NH1 | 2.32 | 0.45 |
| 1:E:430:SER:O | 1:Q:383:LEU:HG | 2.15 | 0.45 |
| 1:F:402:PRO:CG | 1:R:232:ASP:HB3 | 2.47 | 0.45 |
| 1:K:554:ASN:HB3 | 1:8:464:LEU:HD23 | 1.98 | 0.45 |
| 1:N:307:TRP:CE2 | 1:N:692:GLU:HG2 | 2.51 | 0.45 |
| 1:O:585:ASN:OD1 | 1:O:594:ILE:N | 2.45 | 0.45 |
| 1:P:527:ALA:O | 1:P:575:ALA:N | 2.45 | 0.45 |
| 1:Q:427:TYR:O | 1:Q:427:TYR:HD1 | 2.00 | 0.45 |
| 1:R:341:SER:HB3 | 1:R:675:GLN:NE2 | 2.32 | 0.45 |
| 1:T:232:ASP:HB3 | 1:U:402:PRO:CG | 2.47 | 0.45 |
| 1:a:254:ASN:C | 1:a:256:HIS:N | 2.71 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:a:438:ASN:HB2 | 1:8:356:VAL:CG2 | 2.46 | 0.45 |
| 1:a:616:LEU:HD22 | 1:a:729:ILE:HD12 | 1.99 | 0.45 |
| 1:h:398:LEU:C | 1:h:400:TYR:H | 2.24 | 0.45 |
| 1:i:341:SER:HB3 | 1:i:675:GLN:NE2 | 2.32 | 0.45 |
| 1:k:527:ALA:O | 1:k:575:ALA:N | 2.45 | 0.45 |
| 1:l:398:LEU:C | 1:l:400:TYR:H | 2.24 | 0.45 |
| 1:m:430:SER:O | 1:n:383:LEU:HG | 2.15 | 0.45 |
| 1:m:616:LEU:HD22 | 1:m:729:ILE:HD12 | 1.99 | 0.45 |
| 1:n:382:THR:HG22 | 1:n:383:LEU:N | 2.29 | 0.45 |
| 1:q:356:VAL:CG2 | 1:s:438:ASN:HB2 | 2.46 | 0.45 |
| 1:t:307:TRP:CE2 | 1:t:692:GLU:HG2 | 2.52 | 0.45 |
| 1:t:382:THR:HG22 | 1:t:383:LEU:N | 2.29 | 0.45 |
| 1:x:609:TRP:CD1 | 1:x:609:TRP:C | 2.93 | 0.45 |
| 1:y:616:LEU:HD22 | 1:y:729:ILE:HD12 | 1.99 | 0.45 |
| 1:z:564:SER:OG | 1:z:566:GLU:HG2 | 2.15 | 0.45 |
| 1:z:609:TRP:CD1 | 1:z:609:TRP:C | 2.93 | 0.45 |
| 1:3:616:LEU:HD22 | 1:3:729:ILE:HD12 | 1.99 | 0.45 |
| 1:A:629:GLY:CA | 1:I:609:TRP:NE1 | 2.59 | 0.45 |
| 1:B:398:LEU:C | 1:B:400:TYR:H | 2.24 | 0.45 |
| 1:C:629:GLY:CA | 1:M:609:TRP:NE1 | 2.58 | 0.45 |
| 1:F:341:SER:HB3 | 1:F:675:GLN:NE2 | 2.32 | 0.45 |
| 1:H:427:TYR:O | 1:H:427:TYR:HD1 | 2.00 | 0.45 |
| 1:K:609:TRP:CD1 | 1:a:629:GLY:CA | 2.85 | 0.45 |
| 1:N:254:ASN:C | 1:N:256:HIS:N | 2.71 | 0.45 |
| 1:O:341:SER:HB3 | 1:O:675:GLN:NE2 | 2.32 | 0.45 |
| 1:P:616:LEU:HD22 | 1:P:729:ILE:HD12 | 1.99 | 0.45 |
| 1:S:232:ASP:HB3 | 1:d:402:PRO:CG | 2.47 | 0.45 |
| 1:S:427:TYR:HD1 | 1:S:427:TYR:O | 2.00 | 0.45 |
| 1:V:426:SER:OG | 1:V:731:THR:O | 2.31 | 0.45 |
| 1:V:427:TYR:HD1 | 1:V:427:TYR:O | 2.00 | 0.45 |
| 1:V:616:LEU:HD22 | 1:V:729:ILE:HD12 | 1.99 | 0.45 |
| 1:X:402:PRO:CG | 1:f:232:ASP:HB3 | 2.46 | 0.45 |
| 1:Z:427:TYR:O | 1:Z:427:TYR:HD1 | 2.00 | 0.45 |
| 1:Z:616:LEU:HD22 | 1:Z:729:ILE:HD12 | 1.99 | 0.45 |
| 1:a:307:TRP:CE2 | 1:a:692:GLU:HG2 | 2.51 | 0.45 |
| 1:b:232:ASP:HB3 | 1:o:402:PRO:CG | 2.47 | 0.45 |
| 1:b:398:LEU:C | 1:b:400:TYR:H | 2.24 | 0.45 |
| 1:e:527:ALA:O | 1:e:575:ALA:N | 2.45 | 0.45 |
| 1:f:398:LEU:C | 1:f:400:TYR:H | 2.24 | 0.45 |
| 1:f:586:LEU:HD21 | 1:h:490:ARG:NH1 | 2.32 | 0.45 |
| 1:i:609:TRP:CD1 | 1:j:629:GLY:CA | 2.86 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:l:341:SER:HB3 | 1:l:675:GLN:NE2 | 2.32 | 0.45 |
| 1:l:616:LEU:HD22 | 1:l:729:ILE:HD12 | 1.99 | 0.45 |
| 1:n:427:TYR:HD1 | 1:n:427:TYR:O | 2.00 | 0.45 |
| 1:o:398:LEU:C | 1:o:400:TYR:H | 2.24 | 0.45 |
| 1:t:290:PHE:O | 1:t:293:HIS:N | 2.47 | 0.45 |
| 1:t:341:SER:HB3 | 1:t:675:GLN:NE2 | 2.32 | 0.45 |
| 1:w:381:LEU:HD21 | 1:y:439:PRO:HB3 | 1.99 | 0.45 |
| 1:w:435:ARG:HD3 | 1:w:435:ARG:HA | 1.79 | 0.45 |
| 1:y:427:TYR:HD1 | 1:y:427:TYR:O | 2.00 | 0.45 |
| 1:z:402:PRO:CG | 1:4:232:ASP:HB3 | 2.47 | 0.45 |
| 1:z:430:SER:O | 1:1:383:LEU:HG | 2.16 | 0.45 |
| 1:z:616:LEU:HD22 | 1:z:729:ILE:HD12 | 1.99 | 0.45 |
| 1:1:382:THR:HG22 | 1:1:383:LEU:N | 2.29 | 0.45 |
| 1:2:429:HIS:HD2 | 1:2:610:GLN:OE1 | 1.95 | 0.45 |
| 1:3:341:SER:HB3 | 1:3:675:GLN:NE2 | 2.32 | 0.45 |
| 1:4:427:TYR:O | 1:4:427:TYR:HD1 | 2.00 | 0.45 |
| 1:4:609:TRP:CD1 | 1:4:609:TRP:C | 2.93 | 0.45 |
| 1:5:427:TYR:O | 1:5:427:TYR:HD1 | 2.00 | 0.45 |
| 1:6:341:SER:HB3 | 1:6:675:GLN:NE2 | 2.32 | 0.45 |
| 1:A:300:GLN:NE2 | 1:A:703:TYR:O | 2.45 | 0.45 |
| 1:A:341:SER:HB3 | 1:A:675:GLN:NE2 | 2.32 | 0.45 |
| 1:A:398:LEU:C | 1:A:400:TYR:H | 2.24 | 0.45 |
| 1:A:527:ALA:O | 1:A:575:ALA:N | 2.45 | 0.45 |
| 1:E:427:TYR:O | 1:E:427:TYR:CD1 | 2.70 | 0.45 |
| 1:F:616:LEU:HD22 | 1:F:729:ILE:HD12 | 1.99 | 0.45 |
| 1:G:616:LEU:HD22 | 1:G:729:ILE:HD12 | 1.99 | 0.45 |
| 1:K:586:LEU:HD21 | 1:a:490:ARG:NH1 | 2.32 | 0.45 |
| 1:L:232:ASP:HB3 | 1:b:402:PRO:CG | 2.46 | 0.45 |
| 1:N:427:TYR:HD1 | 1:N:427:TYR:O | 2.00 | 0.45 |
| 1:N:585:ASN:OD1 | 1:N:594:ILE:N | 2.45 | 0.45 |
| 1:N:616:LEU:HD22 | 1:N:729:ILE:HD12 | 1.99 | 0.45 |
| 1:Q:382:THR:HG22 | 1:Q:383:LEU:N | 2.29 | 0.45 |
| 1:T:382:THR:HG22 | 1:T:383:LEU:N | 2.29 | 0.45 |
| 1:U:342:THR:HG22 | 1:U:407:ARG:CG | 2.47 | 0.45 |
| 1:Z:341:SER:HB3 | 1:Z:675:GLN:NE2 | 2.32 | 0.45 |
| 1:c:490:ARG:NH1 | 1:p:586:LEU:HD21 | 2.32 | 0.45 |
| 1:c:616:LEU:HD22 | 1:c:729:ILE:HD12 | 1.99 | 0.45 |
| 1:d:307:TRP:CE2 | 1:d:692:GLU:HG2 | 2.52 | 0.45 |
| 1:f:427:TYR:HD1 | 1:f:427:TYR:O | 2.00 | 0.45 |
| 1:g:490:ARG:NH1 | 1:h:586:LEU:HD21 | 2.32 | 0.45 |
| 1:h:382:THR:HG22 | 1:h:383:LEU:N | 2.29 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:427:TYR:O | 1:j:427:TYR:HD1 | 2.00 | 0.45 |
| 1:k:427:TYR:O | 1:k:427:TYR:HD1 | 2.00 | 0.45 |
| 1:m:427:TYR:O | 1:m:427:TYR:HD1 | 2.00 | 0.45 |
| 1:p:616:LEU:HD22 | 1:p:729:ILE:HD12 | 1.99 | 0.45 |
| 1:s:427:TYR:O | 1:s:427:TYR:HD1 | 2.00 | 0.45 |
| 1:u:232:ASP:HB3 | 1:2:402:PRO:CG | 2.47 | 0.45 |
| 1:v:342:THR:HG22 | 1:v:407:ARG:CG | 2.47 | 0.45 |
| 1:v:426:SER:OG | 1:v:731:THR:O | 2.31 | 0.45 |
| 1:v:435:ARG:HD3 | 1:v:435:ARG:HA | 1.79 | 0.45 |
| 1:w:616:LEU:HD22 | 1:w:729:ILE:HD12 | 1.99 | 0.45 |
| 1:y:426:SER:OG | 1:y:731:THR:O | 2.31 | 0.45 |
| 1:3:527:ALA:O | 1:3:575:ALA:N | 2.45 | 0.45 |
| 1:7:427:TYR:O | 1:7:427:TYR:CD1 | 2.70 | 0.45 |
| 1:7:616:LEU:HD22 | 1:7:729:ILE:HD12 | 1.99 | 0.45 |
| 1:8:616:LEU:HD22 | 1:8:729:ILE:HD12 | 1.99 | 0.45 |
| 1:B:402:PRO:CG | 1:C:232:ASP:HB3 | 2.46 | 0.45 |
| 1:B:629:GLY:CA | 1:L:609:TRP:CD1 | 2.85 | 0.45 |
| 1:C:427:TYR:O | 1:C:427:TYR:CD1 | 2.70 | 0.45 |
| 1:D:342:THR:HG22 | 1:D:407:ARG:CG | 2.47 | 0.45 |
| 1:D:586:LEU:HD21 | 1:N:490:ARG:NH1 | 2.32 | 0.45 |
| 1:E:307:TRP:CE2 | 1:E:692:GLU:HG2 | 2.51 | 0.45 |
| 1:E:616:LEU:HD22 | 1:E:729:ILE:HD12 | 1.99 | 0.45 |
| 1:F:342:THR:HG22 | 1:F:407:ARG:CG | 2.47 | 0.45 |
| 1:F:473:MET:HE3 | 1:F:473:MET:HB2 | 1.81 | 0.45 |
| 1:F:490:ARG:NH1 | 1:Q:586:LEU:HD21 | 2.32 | 0.45 |
| 1:G:254:ASN:C | 1:G:256:HIS:N | 2.71 | 0.45 |
| 1:G:586:LEU:HD21 | 1:I:490:ARG:NH1 | 2.32 | 0.45 |
| 1:I:616:LEU:HD22 | 1:I:729:ILE:HD12 | 1.99 | 0.45 |
| 1:K:342:THR:HG22 | 1:K:407:ARG:CG | 2.47 | 0.45 |
| 1:L:427:TYR:CD1 | 1:L:427:TYR:O | 2.70 | 0.45 |
| 1:O:427:TYR:CD1 | 1:O:427:TYR:O | 2.70 | 0.45 |
| 1:P:307:TRP:CE2 | 1:P:692:GLU:HG2 | 2.51 | 0.45 |
| 1:Q:232:ASP:HB3 | 1:S:402:PRO:CG | 2.47 | 0.45 |
| 1:R:290:PHE:O | 1:R:293:HIS:N | 2.47 | 0.45 |
| 1:S:220:ASP:OD1 | 1:S:220:ASP:N | 2.50 | 0.45 |
| 1:T:427:TYR:O | 1:T:427:TYR:HD1 | 2.00 | 0.45 |
| 1:U:621:TRP:CH2 | 1:U:646:PRO:HG2 | 2.52 | 0.45 |
| 1:V:383:LEU:HG | 1:X:430:SER:O | 2.16 | 0.45 |
| 1:X:342:THR:HG22 | 1:X:407:ARG:CG | 2.47 | 0.45 |
| 1:X:621:TRP:CH2 | 1:X:646:PRO:HG2 | 2.52 | 0.45 |
| 1:Z:220:ASP:OD1 | 1:Z:220:ASP:N | 2.50 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:a:398:LEU:C | 1:a:400:TYR:H | 2.24 | 0.45 |
| 1:a:427:TYR:HD1 | 1:a:427:TYR:O | 2.00 | 0.45 |
| 1:c:238:ASP:OD1 | 1:c:239:ARG:N | 2.48 | 0.45 |
| 1:c:402:PRO:CG | 1:s:232:ASP:HB3 | 2.47 | 0.45 |
| 1:c:609:TRP:NE1 | 1:o:629:GLY:CA | 2.58 | 0.45 |
| 1:d:586:LEU:HD21 | 1:l:490:ARG:NH1 | 2.32 | 0.45 |
| 1:e:616:LEU:HD22 | 1:e:729:ILE:HD12 | 1.99 | 0.45 |
| 1:f:341:SER:HB3 | 1:f:675:GLN:NE2 | 2.32 | 0.45 |
| 1:g:307:TRP:CE2 | 1:g:692:GLU:HG2 | 2.51 | 0.45 |
| 1:h:427:TYR:O | 1:h:427:TYR:HD1 | 2.00 | 0.45 |
| 1:j:586:LEU:HD21 | 1:k:490:ARG:NH1 | 2.32 | 0.45 |
| 1:j:704:THR:HB | 1:w:702:GLN:HB2 | 1.99 | 0.45 |
| 1:k:609:TRP:CD1 | 1:k:609:TRP:C | 2.93 | 0.45 |
| 1:l:427:TYR:CD1 | 1:l:427:TYR:O | 2.70 | 0.45 |
| 1:l:621:TRP:CH2 | 1:l:646:PRO:HG2 | 2.52 | 0.45 |
| 1:m:220:ASP:OD1 | 1:m:220:ASP:N | 2.50 | 0.45 |
| 1:m:341:SER:HB3 | 1:m:675:GLN:NE2 | 2.32 | 0.45 |
| 1:n:609:TRP:CD1 | 1:n:609:TRP:C | 2.93 | 0.45 |
| 1:n:616:LEU:HD22 | 1:n:729:ILE:HD12 | 1.99 | 0.45 |
| 1:q:564:SER:OG | 1:q:566:GLU:HG2 | 2.15 | 0.45 |
| 1:u:220:ASP:OD1 | 1:u:220:ASP:N | 2.50 | 0.45 |
| 1:u:427:TYR:O | 1:u:427:TYR:HD1 | 2.00 | 0.45 |
| 1:v:621:TRP:CH2 | 1:v:646:PRO:HG2 | 2.52 | 0.45 |
| 1:w:527:ALA:O | 1:w:575:ALA:N | 2.45 | 0.45 |
| 1:x:342:THR:HG22 | 1:x:407:ARG:CG | 2.47 | 0.45 |
| 1:1:427:TYR:O | 1:1:427:TYR:HD1 | 2.00 | 0.45 |
| 1:2:307:TRP:CE2 | 1:2:692:GLU:HG2 | 2.52 | 0.45 |
| 1:3:427:TYR:O | 1:3:427:TYR:CD1 | 2.70 | 0.45 |
| 1:5:382:THR:HG22 | 1:5:383:LEU:N | 2.29 | 0.45 |
| 1:6:342:THR:HG22 | 1:6:407:ARG:CG | 2.47 | 0.45 |
| 1:6:473:MET:HE3 | 1:6:473:MET:HB2 | 1.81 | 0.45 |
| 1:6:616:LEU:HD22 | 1:6:729:ILE:HD12 | 1.99 | 0.45 |
| 1:6:621:TRP:CH2 | 1:6:646:PRO:HG2 | 2.52 | 0.45 |
| 1:8:307:TRP:CE2 | 1:8:692:GLU:HG2 | 2.51 | 0.45 |
| 1:8:527:ALA:O | 1:8:575:ALA:N | 2.45 | 0.45 |
| 1:F:621:TRP:CH2 | 1:F:646:PRO:HG2 | 2.52 | 0.45 |
| 1:H:224:SER:OG | 1:H:225:SER:N | 2.50 | 0.45 |
| 1:H:232:ASP:HB3 | 1:I:402:PRO:CG | 2.46 | 0.45 |
| 1:H:609:TRP:CD1 | 1:W:629:GLY:CA | 2.85 | 0.45 |
| 1:I:238:ASP:OD1 | 1:I:239:ARG:N | 2.48 | 0.45 |
| 1:I:307:TRP:CE2 | 1:I:692:GLU:HG2 | 2.51 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:621:TRP:CH2 | 1:J:646:PRO:HG2 | 2.52 | 0.45 |
| 1:K:329:ASN:CA | 1:K:330:GLU:OE1 | 2.65 | 0.45 |
| 1:L:621:TRP:CH2 | 1:L:646:PRO:HG2 | 2.52 | 0.45 |
| 1:O:435:ARG:HD3 | 1:O:435:ARG:HA | 1.79 | 0.45 |
| 1:O:527:ALA:O | 1:O:575:ALA:N | 2.45 | 0.45 |
| 1:P:224:SER:OG | 1:P:225:SER:N | 2.50 | 0.45 |
| 1:P:329:ASN:CA | 1:P:330:GLU:OE1 | 2.65 | 0.45 |
| 1:Q:307:TRP:CE2 | 1:Q:692:GLU:HG2 | 2.52 | 0.45 |
| 1:Q:342:THR:HG22 | 1:Q:407:ARG:CG | 2.47 | 0.45 |
| 1:T:342:THR:HG22 | 1:T:407:ARG:CG | 2.47 | 0.45 |
| 1:W:564:SER:OG | 1:W:566:GLU:HG2 | 2.15 | 0.45 |
| 1:Y:224:SER:OG | 1:Y:225:SER:N | 2.50 | 0.45 |
| 1:Y:341:SER:HB3 | 1:Y:675:GLN:NE2 | 2.32 | 0.45 |
| 1:b:258:TYR:OH | 1:b:399:GLU:OE1 | 2.22 | 0.45 |
| 1:c:342:THR:HG22 | 1:c:407:ARG:CG | 2.47 | 0.45 |
| 1:c:586:LEU:HD21 | 1:o:490:ARG:NH1 | 2.32 | 0.45 |
| 1:e:224:SER:OG | 1:e:225:SER:N | 2.50 | 0.45 |
| 1:e:427:TYR:O | 1:e:427:TYR:CD1 | 2.70 | 0.45 |
| 1:h:527:ALA:O | 1:h:575:ALA:N | 2.45 | 0.45 |
| 1:h:609:TRP:CD1 | 1:h:609:TRP:C | 2.93 | 0.45 |
| 1:i:342:THR:HG22 | 1:i:407:ARG:CG | 2.47 | 0.45 |
| 1:i:490:ARG:NH1 | 1:k:586:LEU:HD21 | 2.32 | 0.45 |
| 1:j:341:SER:HB3 | 1:j:675:GLN:NE2 | 2.32 | 0.45 |
| 1:k:382:THR:HG22 | 1:k:383:LEU:N | 2.29 | 0.45 |
| 1:k:398:LEU:C | 1:k:400:TYR:H | 2.24 | 0.45 |
| 1:k:621:TRP:CH2 | 1:k:646:PRO:HG2 | 2.52 | 0.45 |
| 1:n:427:TYR:O | 1:n:427:TYR:CD1 | 2.70 | 0.45 |
| 1:n:621:TRP:CH2 | 1:n:646:PRO:HG2 | 2.52 | 0.45 |
| 1:r:224:SER:OG | 1:r:225:SER:N | 2.50 | 0.45 |
| 1:s:224:SER:OG | 1:s:225:SER:N | 2.50 | 0.45 |
| 1:s:329:ASN:CA | 1:s:330:GLU:OE1 | 2.65 | 0.45 |
| 1:u:402:PRO:CG | 1:5:232:ASP:HB3 | 2.47 | 0.45 |
| 1:w:224:SER:OG | 1:w:225:SER:N | 2.50 | 0.45 |
| 1:w:307:TRP:CE2 | 1:w:692:GLU:HG2 | 2.51 | 0.45 |
| 1:w:427:TYR:O | 1:w:427:TYR:CD1 | 2.70 | 0.45 |
| 1:w:480:TRP:CH2 | 1:x:624:ILE:HG12 | 2.52 | 0.45 |
| 1:x:586:LEU:HD21 | 1:y:490:ARG:NH1 | 2.32 | 0.45 |
| 1:x:621:TRP:CH2 | 1:x:646:PRO:HG2 | 2.52 | 0.45 |
| 1:z:427:TYR:CD1 | 1:z:427:TYR:O | 2.70 | 0.45 |
| 1:z:490:ARG:NH1 | 1:2:586:LEU:HD21 | 2.32 | 0.45 |
| 1:z:621:TRP:CH2 | 1:z:646:PRO:HG2 | 2.52 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:342:THR:HG22 | 1:1:407:ARG:CG | 2.47 | 0.45 |
| 1:3:435:ARG:HD3 | 1:3:435:ARG:HA | 1.79 | 0.45 |
| 1:4:427:TYR:O | 1:4:427:TYR:CD1 | 2.70 | 0.45 |
| 1:4:616:LEU:HD22 | 1:4:729:ILE:HD12 | 1.99 | 0.45 |
| 1:5:342:THR:HG22 | 1:5:407:ARG:CG | 2.47 | 0.45 |
| 1:5:586:LEU:HD21 | 1:6:490:ARG:NH1 | 2.32 | 0.45 |
| 1:6:244:SER:C | 1:6:245:THR:HG1 | 2.23 | 0.45 |
| 1:7:307:TRP:CE2 | 1:7:692:GLU:HG2 | 2.51 | 0.45 |
| 1:8:224:SER:OG | 1:8:225:SER:N | 2.50 | 0.45 |
| 1:8:329:ASN:CA | 1:8:330:GLU:OE1 | 2.65 | 0.45 |
| 1:A:427:TYR:O | 1:A:427:TYR:HD1 | 2.00 | 0.45 |
| 1:B:586:LEU:HD21 | 1:J:490:ARG:NH1 | 2.32 | 0.45 |
| 1:C:224:SER:OG | 1:C:225:SER:N | 2.50 | 0.45 |
| 1:C:290:PHE:O | 1:C:293:HIS:N | 2.47 | 0.45 |
| 1:C:621:TRP:CH2 | 1:C:646:PRO:HG2 | 2.52 | 0.45 |
| 1:D:329:ASN:CA | 1:D:330:GLU:OE1 | 2.65 | 0.45 |
| 1:D:609:TRP:CD1 | 1:N:629:GLY:CA | 2.85 | 0.45 |
| 1:E:326:VAL:HG21 | 1:E:333:LYS:HZ2 | 1.80 | 0.45 |
| 1:F:609:TRP:CD1 | 1:F:609:TRP:O | 2.71 | 0.45 |
| 1:H:220:ASP:OD1 | 1:H:220:ASP:N | 2.50 | 0.45 |
| 1:H:329:ASN:CA | 1:H:330:GLU:OE1 | 2.65 | 0.45 |
| 1:H:616:LEU:HD22 | 1:H:729:ILE:HD12 | 1.99 | 0.45 |
| 1:I:398:LEU:C | 1:I:400:TYR:H | 2.24 | 0.45 |
| 1:I:427:TYR:O | 1:I:427:TYR:HD1 | 2.00 | 0.45 |
| 1:J:586:LEU:HD21 | 1:L:490:ARG:NH1 | 2.32 | 0.45 |
| 1:K:473:MET:HE3 | 1:K:473:MET:HB2 | 1.81 | 0.45 |
| 1:L:224:SER:OG | 1:L:225:SER:N | 2.50 | 0.45 |
| 1:M:490:ARG:NH1 | 1:b:586:LEU:HD21 | 2.32 | 0.45 |
| 1:M:527:ALA:O | 1:M:575:ALA:N | 2.45 | 0.45 |
| 1:M:621:TRP:CH2 | 1:M:646:PRO:HG2 | 2.52 | 0.45 |
| 1:O:586:LEU:HD21 | 1:m:490:ARG:NH1 | 2.32 | 0.45 |
| 1:P:398:LEU:C | 1:P:400:TYR:H | 2.24 | 0.45 |
| 1:P:427:TYR:O | 1:P:427:TYR:HD1 | 2.00 | 0.45 |
| 1:Q:224:SER:OG | 1:Q:225:SER:N | 2.50 | 0.45 |
| 1:T:220:ASP:OD1 | 1:T:220:ASP:N | 2.50 | 0.45 |
| 1:T:307:TRP:CE2 | 1:T:692:GLU:HG2 | 2.52 | 0.45 |
| 1:T:453:SER:OG | 1:T:458:GLN:O | 2.36 | 0.45 |
| 1:T:586:LEU:HD21 | 1:d:490:ARG:NH1 | 2.32 | 0.45 |
| 1:W:586:LEU:HD21 | 1:Y:490:ARG:NH1 | 2.32 | 0.45 |
| 1:Y:621:TRP:CH2 | 1:Y:646:PRO:HG2 | 2.52 | 0.45 |
| 1:a:585:ASN:OD1 | 1:a:594:ILE:N | 2.45 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:c:307:TRP:CE2 | 1:c:692:GLU:HG2 | 2.51 | 0.45 |
| 1:c:398:LEU:C | 1:c:400:TYR:H | 2.24 | 0.45 |
| 1:e:307:TRP:CE2 | 1:e:692:GLU:HG2 | 2.52 | 0.45 |
| 1:g:427:TYR:CD1 | 1:g:427:TYR:O | 2.70 | 0.45 |
| 1:g:427:TYR:O | 1:g:427:TYR:HD1 | 2.00 | 0.45 |
| 1:h:427:TYR:O | 1:h:427:TYR:CD1 | 2.70 | 0.45 |
| 1:h:621:TRP:CH2 | 1:h:646:PRO:HG2 | 2.52 | 0.45 |
| 1:i:307:TRP:CE2 | 1:i:692:GLU:HG2 | 2.51 | 0.45 |
| 1:k:427:TYR:O | 1:k:427:TYR:CD1 | 2.70 | 0.45 |
| 1:n:329:ASN:CA | 1:n:330:GLU:OE1 | 2.65 | 0.45 |
| 1:o:427:TYR:O | 1:o:427:TYR:HD1 | 2.00 | 0.45 |
| 1:q:341:SER:HB3 | 1:q:675:GLN:NE2 | 2.32 | 0.45 |
| 1:r:341:SER:HB3 | 1:r:675:GLN:NE2 | 2.32 | 0.45 |
| 1:s:220:ASP:OD1 | 1:s:220:ASP:N | 2.50 | 0.45 |
| 1:s:616:LEU:HD22 | 1:s:729:ILE:HD12 | 1.99 | 0.45 |
| 1:x:430:SER:O | 1:y:383:LEU:HG | 2.17 | 0.45 |
| 1:x:609:TRP:CD1 | 1:x:609:TRP:O | 2.70 | 0.45 |
| 1:1:427:TYR:O | 1:1:427:TYR:CD1 | 2.70 | 0.45 |
| 1:1:453:SER:OG | 1:1:458:GLN:O | 2.36 | 0.45 |
| 1:4:329:ASN:CA | 1:4:330:GLU:OE1 | 2.65 | 0.45 |
| 1:4:621:TRP:CH2 | 1:4:646:PRO:HG2 | 2.52 | 0.45 |
| 1:5:224:SER:OG | 1:5:225:SER:N | 2.50 | 0.45 |
| 1:8:427:TYR:HD1 | 1:8:427:TYR:O | 2.00 | 0.45 |
| 1:8:453:SER:OG | 1:8:458:GLN:O | 2.35 | 0.45 |
| 1:A:342:THR:HG22 | 1:A:407:ARG:CG | 2.47 | 0.44 |
| 1:A:464:LEU:HD23 | 1:G:554:ASN:HB3 | 1.99 | 0.44 |
| 1:B:340:THR:CB | 1:B:407:ARG:HH21 | 2.20 | 0.44 |
| 1:B:427:TYR:O | 1:B:427:TYR:CD1 | 2.70 | 0.44 |
| 1:C:490:ARG:NH1 | 1:M:586:LEU:HD21 | 2.32 | 0.44 |
| 1:D:609:TRP:NE1 | 1:N:629:GLY:CA | 2.58 | 0.44 |
| 1:E:427:TYR:O | 1:E:427:TYR:HD1 | 2.00 | 0.44 |
| 1:E:621:TRP:CH2 | 1:E:646:PRO:HG2 | 2.52 | 0.44 |
| 1:F:427:TYR:O | 1:F:427:TYR:CD1 | 2.70 | 0.44 |
| 1:H:490:ARG:NH1 | 1:Y:586:LEU:HD21 | 2.32 | 0.44 |
| 1:K:398:LEU:C | 1:K:400:TYR:H | 2.24 | 0.44 |
| 1:L:290:PHE:O | 1:L:293:HIS:N | 2.47 | 0.44 |
| 1:P:453:SER:OG | 1:P:458:GLN:O | 2.36 | 0.44 |
| 1:Q:609:TRP:CD1 | 1:Q:609:TRP:O | 2.70 | 0.44 |
| 1:R:329:ASN:CA | 1:R:330:GLU:OE1 | 2.65 | 0.44 |
| 1:R:609:TRP:CD1 | 1:R:609:TRP:O | 2.70 | 0.44 |
| 1:S:621:TRP:CH2 | 1:S:646:PRO:HG2 | 2.52 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:427:TYR:O | 1:T:427:TYR:CD1 | 2.70 | 0.44 |
| 1:V:427:TYR:O | 1:V:427:TYR:CD1 | 2.70 | 0.44 |
| 1:V:464:LEU:HD23 | 1:e:554:ASN:HB3 | 1.98 | 0.44 |
| 1:W:341:SER:HB3 | 1:W:675:GLN:NE2 | 2.32 | 0.44 |
| 1:X:609:TRP:CD1 | 1:X:609:TRP:O | 2.70 | 0.44 |
| 1:X:626:HIS:CD2 | 1:e:736:ARG:NH2 | 2.79 | 0.44 |
| 1:Y:435:ARG:HD3 | 1:Y:435:ARG:HA | 1.79 | 0.44 |
| 1:Y:609:TRP:CD1 | 1:Y:609:TRP:O | 2.71 | 0.44 |
| 1:Z:427:TYR:O | 1:Z:427:TYR:CD1 | 2.70 | 0.44 |
| 1:Z:490:ARG:NH1 | 1:3:586:LEU:HD21 | 2.32 | 0.44 |
| 1:b:609:TRP:CD1 | 1:b:609:TRP:O | 2.70 | 0.44 |
| 1:c:427:TYR:O | 1:c:427:TYR:CD1 | 2.70 | 0.44 |
| 1:c:427:TYR:O | 1:c:427:TYR:HD1 | 2.00 | 0.44 |
| 1:e:300:GLN:NE2 | 1:e:703:TYR:O | 2.45 | 0.44 |
| 1:f:616:LEU:HD22 | 1:f:729:ILE:HD12 | 1.99 | 0.44 |
| 1:g:342:THR:HG22 | 1:g:407:ARG:CG | 2.47 | 0.44 |
| 1:g:426:SER:O | 1:g:732:ARG:HA | 2.18 | 0.44 |
| 1:g:453:SER:OG | 1:g:458:GLN:O | 2.36 | 0.44 |
| 1:h:434:ASP:OD1 | 1:h:434:ASP:N | 2.41 | 0.44 |
| 1:i:224:SER:OG | 1:i:225:SER:N | 2.50 | 0.44 |
| 1:i:427:TYR:O | 1:i:427:TYR:CD1 | 2.70 | 0.44 |
| 1:i:453:SER:OG | 1:i:458:GLN:O | 2.36 | 0.44 |
| 1:j:453:SER:OG | 1:j:458:GLN:O | 2.36 | 0.44 |
| 1:j:609:TRP:CD1 | 1:j:609:TRP:O | 2.70 | 0.44 |
| 1:j:616:LEU:HD22 | 1:j:729:ILE:HD12 | 1.99 | 0.44 |
| 1:m:427:TYR:O | 1:m:427:TYR:CD1 | 2.70 | 0.44 |
| 1:o:342:THR:HG22 | 1:o:407:ARG:CG | 2.47 | 0.44 |
| 1:o:527:ALA:O | 1:o:575:ALA:N | 2.45 | 0.44 |
| 1:r:329:ASN:CA | 1:r:330:GLU:OE1 | 2.65 | 0.44 |
| 1:r:586:LEU:HD21 | 1:s:490:ARG:NH1 | 2.32 | 0.44 |
| 1:r:609:TRP:CD1 | 1:r:609:TRP:O | 2.71 | 0.44 |
| 1:r:621:TRP:CH2 | 1:r:646:PRO:HG2 | 2.52 | 0.44 |
| 1:t:329:ASN:CA | 1:t:330:GLU:OE1 | 2.65 | 0.44 |
| 1:u:621:TRP:CH2 | 1:u:646:PRO:HG2 | 2.52 | 0.44 |
| 1:v:220:ASP:OD1 | 1:v:220:ASP:N | 2.50 | 0.44 |
| 1:y:427:TYR:O | 1:y:427:TYR:CD1 | 2.70 | 0.44 |
| 1:1:220:ASP:OD1 | 1:1:220:ASP:N | 2.50 | 0.44 |
| 1:1:307:TRP:CE2 | 1:1:692:GLU:HG2 | 2.52 | 0.44 |
| 1:1:586:LEU:HD21 | 1:2:490:ARG:NH1 | 2.32 | 0.44 |
| 1:2:585:ASN:OD1 | 1:2:594:ILE:N | 2.45 | 0.44 |
| 1:5:307:TRP:CE2 | 1:5:692:GLU:HG2 | 2.52 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:609:TRP:CD1 | 1:5:609:TRP:O | 2.70 | 0.44 |
| 1:5:616:LEU:HD22 | 1:5:729:ILE:HD12 | 1.99 | 0.44 |
| 1:6:427:TYR:CD1 | 1:6:427:TYR:O | 2.70 | 0.44 |
| 1:6:609:TRP:CD1 | 1:6:609:TRP:O | 2.71 | 0.44 |
| 1:7:427:TYR:O | 1:7:427:TYR:HD1 | 2.00 | 0.44 |
| 1:A:490:ARG:NH1 | 1:I:586:LEU:HD21 | 2.33 | 0.44 |
| 1:B:427:TYR:O | 1:B:427:TYR:HD1 | 2.00 | 0.44 |
| 1:B:453:SER:OG | 1:B:458:GLN:O | 2.36 | 0.44 |
| 1:B:609:TRP:CD1 | 1:B:609:TRP:O | 2.70 | 0.44 |
| 1:D:398:LEU:C | 1:D:400:TYR:H | 2.24 | 0.44 |
| 1:G:224:SER:OG | 1:G:225:SER:N | 2.50 | 0.44 |
| 1:G:307:TRP:CE2 | 1:G:692:GLU:HG2 | 2.52 | 0.44 |
| 1:H:429:HIS:CE1 | 1:W:627:THR:HG22 | 2.52 | 0.44 |
| 1:I:220:ASP:OD1 | 1:I:220:ASP:N | 2.50 | 0.44 |
| 1:I:329:ASN:CA | 1:I:330:GLU:OE1 | 2.65 | 0.44 |
| 1:I:427:TYR:O | 1:I:427:TYR:CD1 | 2.70 | 0.44 |
| 1:J:341:SER:HB3 | 1:J:675:GLN:NE2 | 2.32 | 0.44 |
| 1:J:527:ALA:O | 1:J:575:ALA:N | 2.45 | 0.44 |
| 1:K:426:SER:OG | 1:K:731:THR:O | 2.31 | 0.44 |
| 1:K:585:ASN:OD1 | 1:K:594:ILE:N | 2.45 | 0.44 |
| 1:L:329:ASN:O | 1:L:332:THR:OG1 | 2.31 | 0.44 |
| 1:M:402:PRO:CG | 1:c:232:ASP:HB3 | 2.47 | 0.44 |
| 1:N:621:TRP:CH2 | 1:N:646:PRO:HG2 | 2.52 | 0.44 |
| 1:R:427:TYR:O | 1:R:427:TYR:CD1 | 2.70 | 0.44 |
| 1:T:429:HIS:CE1 | 1:d:627:THR:HG22 | 2.53 | 0.44 |
| 1:U:220:ASP:OD1 | 1:U:220:ASP:N | 2.50 | 0.44 |
| 1:U:616:LEU:HD22 | 1:U:729:ILE:HD12 | 1.99 | 0.44 |
| 1:X:490:ARG:NH1 | 1:e:586:LEU:HD21 | 2.32 | 0.44 |
| 1:Y:329:ASN:CA | 1:Y:330:GLU:OE1 | 2.65 | 0.44 |
| 1:a:621:TRP:CH2 | 1:a:646:PRO:HG2 | 2.52 | 0.44 |
| 1:b:341:SER:HB3 | 1:b:675:GLN:NE2 | 2.32 | 0.44 |
| 1:b:427:TYR:CD1 | 1:b:427:TYR:O | 2.70 | 0.44 |
| 1:c:329:ASN:CA | 1:c:330:GLU:OE1 | 2.65 | 0.44 |
| 1:d:224:SER:OG | 1:d:225:SER:N | 2.50 | 0.44 |
| 1:d:427:TYR:O | 1:d:427:TYR:CD1 | 2.70 | 0.44 |
| 1:d:464:LEU:HD23 | 1:l:554:ASN:HB3 | 2.00 | 0.44 |
| 1:e:609:TRP:CD1 | 1:e:609:TRP:O | 2.70 | 0.44 |
| 1:g:224:SER:OG | 1:g:225:SER:N | 2.50 | 0.44 |
| 1:i:426:SER:O | 1:i:732:ARG:HA | 2.18 | 0.44 |
| 1:i:427:TYR:O | 1:i:427:TYR:HD1 | 2.00 | 0.44 |
| 1:k:340:THR:HB | 1:w:322:GLN:HB3 | 1.99 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:k:434:ASP:OD1 | 1:k:434:ASP:N | 2.41 | 0.44 |
| 1:o:586:LEU:HD21 | 1:p:490:ARG:NH1 | 2.32 | 0.44 |
| 1:p:307:TRP:CE2 | 1:p:692:GLU:HG2 | 2.52 | 0.44 |
| 1:p:329:ASN:CA | 1:p:330:GLU:OE1 | 2.65 | 0.44 |
| 1:q:586:LEU:HD21 | 1:r:490:ARG:NH1 | 2.32 | 0.44 |
| 1:r:342:THR:HG22 | 1:r:407:ARG:CG | 2.47 | 0.44 |
| 1:t:427:TYR:CD1 | 1:t:427:TYR:O | 2.70 | 0.44 |
| 1:t:609:TRP:CD1 | 1:t:609:TRP:O | 2.71 | 0.44 |
| 1:u:736:ARG:NH2 | 1:v:626:HIS:CD2 | 2.79 | 0.44 |
| 1:v:609:TRP:CD1 | 1:v:609:TRP:O | 2.70 | 0.44 |
| 1:v:616:LEU:HD22 | 1:v:729:ILE:HD12 | 1.99 | 0.44 |
| 1:w:609:TRP:CD1 | 1:w:609:TRP:O | 2.71 | 0.44 |
| 1:x:427:TYR:O | 1:x:427:TYR:CD1 | 2.70 | 0.44 |
| 1:z:554:ASN:HB3 | 1:2:464:LEU:HD23 | 2.00 | 0.44 |
| 1:1:429:HIS:CE1 | 1:2:627:THR:HG22 | 2.53 | 0.44 |
| 1:2:224:SER:OG | 1:2:225:SER:N | 2.50 | 0.44 |
| 1:2:427:TYR:O | 1:2:427:TYR:CD1 | 2.70 | 0.44 |
| 1:2:435:ARG:HD3 | 1:2:435:ARG:HA | 1.79 | 0.44 |
| 1:5:627:THR:HG22 | 1:7:429:HIS:CE1 | 2.53 | 0.44 |
| 1:6:224:SER:OG | 1:6:225:SER:N | 2.50 | 0.44 |
| 1:7:621:TRP:CH2 | 1:7:646:PRO:HG2 | 2.52 | 0.44 |
| 1:A:554:ASN:HB3 | 1:I:464:LEU:HD23 | 2.00 | 0.44 |
| 1:A:616:LEU:HD22 | 1:A:729:ILE:HD12 | 1.99 | 0.44 |
| 1:B:554:ASN:HB3 | 1:L:464:LEU:HD23 | 2.00 | 0.44 |
| 1:C:464:LEU:HD23 | 1:b:554:ASN:HB3 | 2.00 | 0.44 |
| 1:C:609:TRP:CD1 | 1:C:609:TRP:O | 2.71 | 0.44 |
| 1:C:609:TRP:CD1 | 1:b:629:GLY:CA | 2.85 | 0.44 |
| 1:D:427:TYR:O | 1:D:427:TYR:CD1 | 2.70 | 0.44 |
| 1:E:429:HIS:CE1 | 1:Q:627:THR:HG22 | 2.53 | 0.44 |
| 1:G:329:ASN:CA | 1:G:330:GLU:OE1 | 2.65 | 0.44 |
| 1:I:232:ASP:HB3 | 1:J:402:PRO:CG | 2.47 | 0.44 |
| 1:J:220:ASP:OD1 | 1:J:220:ASP:N | 2.50 | 0.44 |
| 1:K:427:TYR:O | 1:K:427:TYR:CD1 | 2.70 | 0.44 |
| 1:L:426:SER:O | 1:L:732:ARG:HA | 2.18 | 0.44 |
| 1:M:341:SER:HB3 | 1:M:675:GLN:NE2 | 2.32 | 0.44 |
| 1:N:453:SER:OG | 1:N:458:GLN:O | 2.36 | 0.44 |
| 1:P:342:THR:HG22 | 1:P:407:ARG:CG | 2.47 | 0.44 |
| 1:Q:427:TYR:O | 1:Q:427:TYR:CD1 | 2.70 | 0.44 |
| 1:Q:616:LEU:HD22 | 1:Q:729:ILE:HD12 | 1.99 | 0.44 |
| 1:R:426:SER:O | 1:R:732:ARG:HA | 2.18 | 0.44 |
| 1:T:490:ARG:NH1 | 1:l:586:LEU:HD21 | 2.32 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:609:TRP:CD1 | 1:T:609:TRP:O | 2.70 | 0.44 |
| 1:U:609:TRP:CD1 | 1:U:609:TRP:O | 2.71 | 0.44 |
| 1:V:621:TRP:CH2 | 1:V:646:PRO:HG2 | 2.52 | 0.44 |
| 1:X:427:TYR:O | 1:X:427:TYR:CD1 | 2.70 | 0.44 |
| 1:X:554:ASN:HB3 | 1:e:464:LEU:HD23 | 2.00 | 0.44 |
| 1:Y:342:THR:HG22 | 1:Y:407:ARG:CG | 2.47 | 0.44 |
| 1:Z:426:SER:O | 1:Z:732:ARG:HA | 2.18 | 0.44 |
| 1:b:427:TYR:O | 1:b:427:TYR:HD1 | 2.00 | 0.44 |
| 1:b:453:SER:OG | 1:b:458:GLN:O | 2.36 | 0.44 |
| 1:c:220:ASP:OD1 | 1:c:220:ASP:N | 2.50 | 0.44 |
| 1:f:426:SER:O | 1:f:732:ARG:HA | 2.18 | 0.44 |
| 1:f:453:SER:OG | 1:f:458:GLN:O | 2.36 | 0.44 |
| 1:f:609:TRP:CD1 | 1:f:609:TRP:O | 2.70 | 0.44 |
| 1:j:426:SER:O | 1:j:732:ARG:HA | 2.18 | 0.44 |
| 1:m:426:SER:O | 1:m:732:ARG:HA | 2.18 | 0.44 |
| 1:p:224:SER:OG | 1:p:225:SER:N | 2.50 | 0.44 |
| 1:q:627:THR:HG22 | 1:s:429:HIS:CE1 | 2.53 | 0.44 |
| 1:r:402:PRO:CG | 1:x:232:ASP:HB3 | 2.46 | 0.44 |
| 1:s:341:SER:HB3 | 1:s:675:GLN:NE2 | 2.32 | 0.44 |
| 1:t:426:SER:O | 1:t:732:ARG:HA | 2.18 | 0.44 |
| 1:u:426:SER:O | 1:u:732:ARG:HA | 2.18 | 0.44 |
| 1:u:609:TRP:CD1 | 1:u:609:TRP:C | 2.93 | 0.44 |
| 1:w:300:GLN:NE2 | 1:w:703:TYR:O | 2.45 | 0.44 |
| 1:x:426:SER:O | 1:x:732:ARG:HA | 2.18 | 0.44 |
| 1:x:453:SER:OG | 1:x:458:GLN:O | 2.35 | 0.44 |
| 1:y:307:TRP:CE2 | 1:y:692:GLU:HG2 | 2.52 | 0.44 |
| 1:y:621:TRP:CH2 | 1:y:646:PRO:HG2 | 2.52 | 0.44 |
| 1:z:224:SER:OG | 1:z:225:SER:N | 2.50 | 0.44 |
| 1:z:434:ASP:OD1 | 1:z:434:ASP:N | 2.41 | 0.44 |
| 1:3:307:TRP:CE2 | 1:3:692:GLU:HG2 | 2.51 | 0.44 |
| 1:3:426:SER:O | 1:3:732:ARG:HA | 2.18 | 0.44 |
| 1:4:342:THR:HG22 | 1:4:407:ARG:CG | 2.47 | 0.44 |
| 1:5:427:TYR:O | 1:5:427:TYR:CD1 | 2.70 | 0.44 |
| 1:8:342:THR:HG22 | 1:8:407:ARG:CG | 2.47 | 0.44 |
| 1:A:402:PRO:CG | 1:B:232:ASP:HB3 | 2.47 | 0.44 |
| 1:B:258:TYR:OH | 1:B:399:GLU:OE1 | 2.22 | 0.44 |
| 1:B:341:SER:HB3 | 1:B:675:GLN:NE2 | 2.32 | 0.44 |
| 1:B:429:HIS:CE1 | 1:J:627:THR:HG22 | 2.53 | 0.44 |
| 1:B:616:LEU:HD22 | 1:B:729:ILE:HD12 | 1.99 | 0.44 |
| 1:C:426:SER:O | 1:C:732:ARG:HA | 2.18 | 0.44 |
| 1:C:453:SER:OG | 1:C:458:GLN:O | 2.36 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:224:SER:OG | 1:E:225:SER:N | 2.50 | 0.44 |
| 1:F:244:SER:C | 1:F:245:THR:HG1 | 2.24 | 0.44 |
| 1:F:329:ASN:CA | 1:F:330:GLU:OE1 | 2.65 | 0.44 |
| 1:F:382:THR:HG22 | 1:F:383:LEU:N | 2.29 | 0.44 |
| 1:G:427:TYR:O | 1:G:427:TYR:CD1 | 2.70 | 0.44 |
| 1:H:341:SER:HB3 | 1:H:675:GLN:NE2 | 2.32 | 0.44 |
| 1:J:427:TYR:O | 1:J:427:TYR:CD1 | 2.70 | 0.44 |
| 1:L:609:TRP:CD1 | 1:L:609:TRP:O | 2.71 | 0.44 |
| 1:M:220:ASP:OD1 | 1:M:220:ASP:N | 2.50 | 0.44 |
| 1:M:427:TYR:O | 1:M:427:TYR:CD1 | 2.70 | 0.44 |
| 1:M:627:THR:HG22 | 1:b:429:HIS:CE1 | 2.53 | 0.44 |
| 1:O:307:TRP:CE2 | 1:O:692:GLU:HG2 | 2.51 | 0.44 |
| 1:O:426:SER:O | 1:O:732:ARG:HA | 2.18 | 0.44 |
| 1:O:427:TYR:O | 1:O:427:TYR:HD1 | 2.00 | 0.44 |
| 1:P:427:TYR:O | 1:P:427:TYR:CD1 | 2.70 | 0.44 |
| 1:R:427:TYR:O | 1:R:427:TYR:HD1 | 2.00 | 0.44 |
| 1:S:609:TRP:CD1 | 1:S:609:TRP:C | 2.93 | 0.44 |
| 1:T:398:LEU:C | 1:T:400:TYR:H | 2.24 | 0.44 |
| 1:U:435:ARG:HD3 | 1:U:435:ARG:HA | 1.79 | 0.44 |
| 1:V:307:TRP:CE2 | 1:V:692:GLU:HG2 | 2.51 | 0.44 |
| 1:V:342:THR:HG22 | 1:V:407:ARG:CG | 2.47 | 0.44 |
| 1:X:224:SER:OG | 1:X:225:SER:N | 2.50 | 0.44 |
| 1:X:426:SER:O | 1:X:732:ARG:HA | 2.18 | 0.44 |
| 1:X:453:SER:OG | 1:X:458:GLN:O | 2.36 | 0.44 |
| 1:Z:621:TRP:CH2 | 1:Z:646:PRO:HG2 | 2.52 | 0.44 |
| 1:a:453:SER:OG | 1:a:458:GLN:O | 2.36 | 0.44 |
| 1:b:224:SER:OG | 1:b:225:SER:N | 2.50 | 0.44 |
| 1:b:616:LEU:HD22 | 1:b:729:ILE:HD12 | 1.99 | 0.44 |
| 1:c:464:LEU:HD23 | 1:o:554:ASN:HB3 | 2.00 | 0.44 |
| 1:d:453:SER:OG | 1:d:458:GLN:O | 2.36 | 0.44 |
| 1:d:585:ASN:OD1 | 1:d:594:ILE:N | 2.45 | 0.44 |
| 1:f:220:ASP:OD1 | 1:f:220:ASP:N | 2.50 | 0.44 |
| 1:f:342:THR:HG22 | 1:f:407:ARG:CG | 2.47 | 0.44 |
| 1:f:402:PRO:CG | 1:z:232:ASP:HB3 | 2.47 | 0.44 |
| 1:h:329:ASN:CA | 1:h:330:GLU:OE1 | 2.65 | 0.44 |
| 1:i:429:HIS:CE1 | 1:j:627:THR:HG22 | 2.53 | 0.44 |
| 1:k:329:ASN:CA | 1:k:330:GLU:OE1 | 2.65 | 0.44 |
| 1:k:453:SER:OG | 1:k:458:GLN:O | 2.36 | 0.44 |
| 1:l:224:SER:OG | 1:l:225:SER:N | 2.50 | 0.44 |
| 1:l:329:ASN:CA | 1:l:330:GLU:OE1 | 2.65 | 0.44 |
| 1:m:621:TRP:CH2 | 1:m:646:PRO:HG2 | 2.52 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:n:342:THR:HG22 | 1:n:407:ARG:CG | 2.47 | 0.44 |
| 1:o:220:ASP:OD1 | 1:o:220:ASP:N | 2.50 | 0.44 |
| 1:o:224:SER:OG | 1:o:225:SER:N | 2.50 | 0.44 |
| 1:o:329:ASN:CA | 1:o:330:GLU:OE1 | 2.65 | 0.44 |
| 1:o:616:LEU:HD22 | 1:o:729:ILE:HD12 | 1.99 | 0.44 |
| 1:p:621:TRP:CH2 | 1:p:646:PRO:HG2 | 2.52 | 0.44 |
| 1:q:616:LEU:HD22 | 1:q:729:ILE:HD12 | 1.99 | 0.44 |
| 1:q:629:GLY:CA | 1:s:609:TRP:CD1 | 2.85 | 0.44 |
| 1:r:307:TRP:CE2 | 1:r:692:GLU:HG2 | 2.51 | 0.44 |
| 1:u:341:SER:HB3 | 1:u:675:GLN:NE2 | 2.32 | 0.44 |
| 1:x:426:SER:OG | 1:x:731:THR:O | 2.31 | 0.44 |
| 1:y:342:THR:HG22 | 1:y:407:ARG:CG | 2.47 | 0.44 |
| 1:y:609:TRP:CD1 | 1:y:609:TRP:O | 2.70 | 0.44 |
| 1:1:398:LEU:C | 1:1:400:TYR:H | 2.24 | 0.44 |
| 1:1:609:TRP:CD1 | 1:1:609:TRP:O | 2.70 | 0.44 |
| 1:4:609:TRP:CD1 | 1:4:609:TRP:O | 2.71 | 0.44 |
| 1:6:329:ASN:CA | 1:6:330:GLU:OE1 | 2.65 | 0.44 |
| 1:8:427:TYR:O | 1:8:427:TYR:CD1 | 2.70 | 0.44 |
| 1:A:220:ASP:OD1 | 1:A:220:ASP:N | 2.50 | 0.44 |
| 1:A:224:SER:OG | 1:A:225:SER:N | 2.50 | 0.44 |
| 1:A:329:ASN:CA | 1:A:330:GLU:OE1 | 2.65 | 0.44 |
| 1:B:224:SER:OG | 1:B:225:SER:N | 2.50 | 0.44 |
| 1:B:300:GLN:NE2 | 1:B:703:TYR:O | 2.45 | 0.44 |
| 1:B:329:ASN:CA | 1:B:330:GLU:OE1 | 2.65 | 0.44 |
| 1:C:736:ARG:NH2 | 1:b:626:HIS:CD2 | 2.79 | 0.44 |
| 1:D:426:SER:OG | 1:D:731:THR:O | 2.31 | 0.44 |
| 1:D:585:ASN:OD1 | 1:D:594:ILE:N | 2.45 | 0.44 |
| 1:E:429:HIS:HD2 | 1:E:610:GLN:OE1 | 1.94 | 0.44 |
| 1:G:453:SER:OG | 1:G:458:GLN:O | 2.36 | 0.44 |
| 1:G:621:TRP:CH2 | 1:G:646:PRO:HG2 | 2.52 | 0.44 |
| 1:I:621:TRP:CH2 | 1:I:646:PRO:HG2 | 2.52 | 0.44 |
| 1:L:453:SER:OG | 1:L:458:GLN:O | 2.36 | 0.44 |
| 1:O:429:HIS:CE1 | 1:m:627:THR:HG22 | 2.53 | 0.44 |
| 1:P:426:SER:O | 1:P:732:ARG:HA | 2.18 | 0.44 |
| 1:Q:300:GLN:NE2 | 1:Q:703:TYR:O | 2.45 | 0.44 |
| 1:R:616:LEU:HD22 | 1:R:729:ILE:HD12 | 1.99 | 0.44 |
| 1:S:341:SER:HB3 | 1:S:675:GLN:NE2 | 2.32 | 0.44 |
| 1:S:426:SER:O | 1:S:732:ARG:HA | 2.18 | 0.44 |
| 1:S:427:TYR:O | 1:S:427:TYR:CD1 | 2.70 | 0.44 |
| 1:S:609:TRP:CD1 | 1:S:609:TRP:O | 2.71 | 0.44 |
| 1:S:736:ARG:NH2 | 1:U:626:HIS:CD2 | 2.79 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:220:ASP:OD1 | 1:V:220:ASP:N | 2.50 | 0.44 |
| 1:V:341:SER:HB3 | 1:V:675:GLN:NE2 | 2.32 | 0.44 |
| 1:V:609:TRP:CD1 | 1:V:609:TRP:O | 2.71 | 0.44 |
| 1:W:616:LEU:HD22 | 1:W:729:ILE:HD12 | 1.99 | 0.44 |
| 1:X:220:ASP:OD1 | 1:X:220:ASP:N | 2.50 | 0.44 |
| 1:X:473:MET:HB2 | 1:X:473:MET:HE3 | 1.81 | 0.44 |
| 1:Y:427:TYR:CD1 | 1:Y:427:TYR:O | 2.70 | 0.44 |
| 1:Z:586:LEU:HD21 | 1:4:490:ARG:NH1 | 2.32 | 0.44 |
| 1:Z:627:THR:HG22 | 1:3:429:HIS:CE1 | 2.53 | 0.44 |
| 1:a:426:SER:O | 1:a:732:ARG:HA | 2.18 | 0.44 |
| 1:a:609:TRP:CD1 | 1:a:609:TRP:O | 2.70 | 0.44 |
| 1:b:220:ASP:OD1 | 1:b:220:ASP:N | 2.50 | 0.44 |
| 1:b:329:ASN:CA | 1:b:330:GLU:OE1 | 2.65 | 0.44 |
| 1:b:340:THR:CB | 1:b:407:ARG:HH21 | 2.20 | 0.44 |
| 1:d:220:ASP:OD1 | 1:d:220:ASP:N | 2.50 | 0.44 |
| 1:d:426:SER:O | 1:d:732:ARG:HA | 2.18 | 0.44 |
| 1:d:435:ARG:HD3 | 1:d:435:ARG:HA | 1.79 | 0.44 |
| 1:f:224:SER:OG | 1:f:225:SER:N | 2.50 | 0.44 |
| 1:f:490:ARG:NH1 | 1:g:586:LEU:HD21 | 2.32 | 0.44 |
| 1:f:627:THR:HG22 | 1:g:429:HIS:CE1 | 2.53 | 0.44 |
| 1:h:341:SER:HB3 | 1:h:675:GLN:NE2 | 2.32 | 0.44 |
| 1:h:453:SER:OG | 1:h:458:GLN:O | 2.36 | 0.44 |
| 1:i:586:LEU:HD21 | 1:j:490:ARG:NH1 | 2.32 | 0.44 |
| 1:j:220:ASP:OD1 | 1:j:220:ASP:N | 2.50 | 0.44 |
| 1:j:224:SER:OG | 1:j:225:SER:N | 2.50 | 0.44 |
| 1:j:329:ASN:CA | 1:j:330:GLU:OE1 | 2.65 | 0.44 |
| 1:j:342:THR:HG22 | 1:j:407:ARG:CG | 2.47 | 0.44 |
| 1:k:341:SER:HB3 | 1:k:675:GLN:NE2 | 2.32 | 0.44 |
| 1:l:434:ASP:OD1 | 1:l:434:ASP:N | 2.41 | 0.44 |
| 1:l:453:SER:OG | 1:l:458:GLN:O | 2.35 | 0.44 |
| 1:m:300:GLN:NE2 | 1:m:703:TYR:O | 2.45 | 0.44 |
| 1:m:329:ASN:CA | 1:m:330:GLU:OE1 | 2.65 | 0.44 |
| 1:m:586:LEU:HD21 | 1:n:490:ARG:NH1 | 2.32 | 0.44 |
| 1:n:609:TRP:CD1 | 1:n:609:TRP:O | 2.71 | 0.44 |
| 1:p:427:TYR:O | 1:p:427:TYR:CD1 | 2.70 | 0.44 |
| 1:p:453:SER:OG | 1:p:458:GLN:O | 2.36 | 0.44 |
| 1:p:609:TRP:CD1 | 1:p:609:TRP:O | 2.71 | 0.44 |
| 1:q:329:ASN:CA | 1:q:330:GLU:OE1 | 2.65 | 0.44 |
| 1:q:427:TYR:HD1 | 1:q:427:TYR:O | 2.00 | 0.44 |
| 1:s:609:TRP:CD1 | 1:s:609:TRP:O | 2.70 | 0.44 |
| 1:s:621:TRP:CH2 | 1:s:646:PRO:HG2 | 2.52 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:w:356:VAL:CG2 | 1:y:438:ASN:HB2 | 2.48 | 0.44 |
| 1:x:224:SER:OG | 1:x:225:SER:N | 2.50 | 0.44 |
| 1:y:290:PHE:O | 1:y:293:HIS:N | 2.47 | 0.44 |
| 1:y:341:SER:HB3 | 1:y:675:GLN:NE2 | 2.32 | 0.44 |
| 1:z:453:SER:OG | 1:z:458:GLN:O | 2.35 | 0.44 |
| 1:z:473:MET:HE3 | 1:z:473:MET:HB2 | 1.81 | 0.44 |
| 1:z:586:LEU:HD21 | 1:1:490:ARG:NH1 | 2.32 | 0.44 |
| 1:2:220:ASP:OD1 | 1:2:220:ASP:N | 2.50 | 0.44 |
| 1:2:426:SER:O | 1:2:732:ARG:HA | 2.18 | 0.44 |
| 1:2:453:SER:OG | 1:2:458:GLN:O | 2.36 | 0.44 |
| 1:2:621:TRP:CH2 | 1:2:646:PRO:HG2 | 2.52 | 0.44 |
| 1:5:220:ASP:OD1 | 1:5:220:ASP:N | 2.50 | 0.44 |
| 1:5:453:SER:OG | 1:5:458:GLN:O | 2.35 | 0.44 |
| 1:6:382:THR:HG22 | 1:6:383:LEU:N | 2.29 | 0.44 |
| 1:7:224:SER:OG | 1:7:225:SER:N | 2.50 | 0.44 |
| 1:8:426:SER:O | 1:8:732:ARG:HA | 2.18 | 0.44 |
| 1:A:435:ARG:HD3 | 1:A:435:ARG:HA | 1.79 | 0.44 |
| 1:A:621:TRP:CH2 | 1:A:646:PRO:HG2 | 2.52 | 0.44 |
| 1:B:220:ASP:OD1 | 1:B:220:ASP:N | 2.50 | 0.44 |
| 1:B:490:ARG:NH1 | 1:L:586:LEU:HD21 | 2.32 | 0.44 |
| 1:B:621:TRP:CH2 | 1:B:646:PRO:HG2 | 2.52 | 0.44 |
| 1:C:554:ASN:HB3 | 1:M:464:LEU:HD23 | 2.00 | 0.44 |
| 1:D:487:ARG:HD2 | 1:P:583:ALA:O | 2.17 | 0.44 |
| 1:E:453:SER:OG | 1:E:458:GLN:O | 2.36 | 0.44 |
| 1:F:307:TRP:CE2 | 1:F:692:GLU:HG2 | 2.52 | 0.44 |
| 1:G:583:ALA:O | 1:I:487:ARG:HD2 | 2.18 | 0.44 |
| 1:G:609:TRP:CD1 | 1:G:609:TRP:O | 2.71 | 0.44 |
| 1:H:609:TRP:CD1 | 1:H:609:TRP:O | 2.71 | 0.44 |
| 1:J:329:ASN:CA | 1:J:330:GLU:OE1 | 2.65 | 0.44 |
| 1:J:342:THR:HG22 | 1:J:407:ARG:CG | 2.47 | 0.44 |
| 1:K:487:ARG:HD2 | 1:8:583:ALA:O | 2.18 | 0.44 |
| 1:K:609:TRP:NE1 | 1:a:629:GLY:CA | 2.58 | 0.44 |
| 1:K:626:HIS:CD2 | 1:8:736:ARG:NH2 | 2.79 | 0.44 |
| 1:M:232:ASP:HB3 | 1:N:402:PRO:CG | 2.46 | 0.44 |
| 1:M:290:PHE:O | 1:M:293:HIS:N | 2.47 | 0.44 |
| 1:M:307:TRP:CE2 | 1:M:692:GLU:HG2 | 2.52 | 0.44 |
| 1:M:329:ASN:CA | 1:M:330:GLU:OE1 | 2.65 | 0.44 |
| 1:M:342:THR:HG22 | 1:M:407:ARG:CG | 2.47 | 0.44 |
| 1:N:609:TRP:CD1 | 1:N:609:TRP:O | 2.71 | 0.44 |
| 1:Q:220:ASP:OD1 | 1:Q:220:ASP:N | 2.50 | 0.44 |
| 1:Q:453:SER:OG | 1:Q:458:GLN:O | 2.35 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:453:SER:OG | 1:S:458:GLN:O | 2.35 | 0.44 |
| 1:T:426:SER:O | 1:T:732:ARG:HA | 2.18 | 0.44 |
| 1:U:426:SER:O | 1:U:732:ARG:HA | 2.18 | 0.44 |
| 1:V:224:SER:OG | 1:V:225:SER:N | 2.50 | 0.44 |
| 1:V:490:ARG:NH1 | 1:X:586:LEU:HD21 | 2.33 | 0.44 |
| 1:W:427:TYR:O | 1:W:427:TYR:HD1 | 2.00 | 0.44 |
| 1:X:426:SER:OG | 1:X:731:THR:O | 2.31 | 0.44 |
| 1:Y:307:TRP:CE2 | 1:Y:692:GLU:HG2 | 2.51 | 0.44 |
| 1:Z:300:GLN:NE2 | 1:Z:703:TYR:O | 2.45 | 0.44 |
| 1:Z:329:ASN:CA | 1:Z:330:GLU:OE1 | 2.65 | 0.44 |
| 1:Z:429:HIS:CE1 | 1:4:627:THR:HG22 | 2.53 | 0.44 |
| 1:Z:583:ALA:O | 1:4:487:ARG:HD2 | 2.18 | 0.44 |
| 1:c:429:HIS:CE1 | 1:o:627:THR:HG22 | 2.53 | 0.44 |
| 1:d:621:TRP:CH2 | 1:d:646:PRO:HG2 | 2.52 | 0.44 |
| 1:f:329:ASN:CA | 1:f:330:GLU:OE1 | 2.65 | 0.44 |
| 1:f:621:TRP:CH2 | 1:f:646:PRO:HG2 | 2.52 | 0.44 |
| 1:i:329:ASN:CA | 1:i:330:GLU:OE1 | 2.65 | 0.44 |
| 1:j:402:PRO:CG | 1:l:232:ASP:HB3 | 2.47 | 0.44 |
| 1:j:621:TRP:CH2 | 1:j:646:PRO:HG2 | 2.52 | 0.44 |
| 1:l:527:ALA:O | 1:l:575:ALA:N | 2.45 | 0.44 |
| 1:l:609:TRP:CD1 | 1:l:609:TRP:O | 2.71 | 0.44 |
| 1:m:583:ALA:O | 1:n:487:ARG:HD2 | 2.18 | 0.44 |
| 1:n:585:ASN:OD1 | 1:n:594:ILE:N | 2.45 | 0.44 |
| 1:q:220:ASP:OD1 | 1:q:220:ASP:N | 2.50 | 0.44 |
| 1:q:429:HIS:CE1 | 1:r:627:THR:HG22 | 2.53 | 0.44 |
| 1:r:427:TYR:CD1 | 1:r:427:TYR:O | 2.70 | 0.44 |
| 1:s:426:SER:O | 1:s:732:ARG:HA | 2.18 | 0.44 |
| 1:t:427:TYR:O | 1:t:427:TYR:HD1 | 2.00 | 0.44 |
| 1:t:627:THR:HG22 | 1:v:429:HIS:CE1 | 2.53 | 0.44 |
| 1:u:427:TYR:O | 1:u:427:TYR:CD1 | 2.70 | 0.44 |
| 1:u:453:SER:OG | 1:u:458:GLN:O | 2.35 | 0.44 |
| 1:u:609:TRP:CD1 | 1:u:609:TRP:O | 2.71 | 0.44 |
| 1:x:220:ASP:OD1 | 1:x:220:ASP:N | 2.50 | 0.44 |
| 1:y:220:ASP:OD1 | 1:y:220:ASP:N | 2.50 | 0.44 |
| 1:y:426:SER:O | 1:y:732:ARG:HA | 2.18 | 0.44 |
| 1:z:329:ASN:CA | 1:z:330:GLU:OE1 | 2.65 | 0.44 |
| 1:z:427:TYR:O | 1:z:427:TYR:HD1 | 2.00 | 0.44 |
| 1:z:609:TRP:CD1 | 1:z:609:TRP:O | 2.71 | 0.44 |
| 1:1:426:SER:O | 1:1:732:ARG:HA | 2.18 | 0.44 |
| 1:3:427:TYR:O | 1:3:427:TYR:HD1 | 2.00 | 0.44 |
| 1:5:621:TRP:CH2 | 1:5:646:PRO:HG2 | 2.52 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:6:307:TRP:CE2 | 1:6:692:GLU:HG2 | 2.52 | 0.44 |
| 1:7:453:SER:OG | 1:7:458:GLN:O | 2.36 | 0.44 |
| 1:A:232:ASP:HB3 | 1:E:402:PRO:CG | 2.46 | 0.44 |
| 1:A:427:TYR:O | 1:A:427:TYR:CD1 | 2.70 | 0.44 |
| 1:C:586:LEU:HD21 | 1:b:490:ARG:NH1 | 2.32 | 0.44 |
| 1:D:609:TRP:CD1 | 1:D:609:TRP:O | 2.71 | 0.44 |
| 1:D:621:TRP:CH2 | 1:D:646:PRO:HG2 | 2.52 | 0.44 |
| 1:E:464:LEU:HD23 | 1:Q:554:ASN:HB3 | 2.00 | 0.44 |
| 1:H:426:SER:O | 1:H:732:ARG:HA | 2.18 | 0.44 |
| 1:H:427:TYR:O | 1:H:427:TYR:CD1 | 2.70 | 0.44 |
| 1:H:586:LEU:HD21 | 1:W:490:ARG:NH1 | 2.33 | 0.44 |
| 1:J:307:TRP:CE2 | 1:J:692:GLU:HG2 | 2.52 | 0.44 |
| 1:J:464:LEU:HD23 | 1:L:554:ASN:HB3 | 2.00 | 0.44 |
| 1:K:329:ASN:O | 1:K:332:THR:OG1 | 2.31 | 0.44 |
| 1:K:609:TRP:CD1 | 1:K:609:TRP:O | 2.70 | 0.44 |
| 1:K:621:TRP:CH2 | 1:K:646:PRO:HG2 | 2.52 | 0.44 |
| 1:N:426:SER:O | 1:N:732:ARG:HA | 2.18 | 0.44 |
| 1:N:429:HIS:CE1 | 1:P:627:THR:HG22 | 2.53 | 0.44 |
| 1:O:426:SER:OG | 1:O:731:THR:O | 2.31 | 0.44 |
| 1:Q:621:TRP:CH2 | 1:Q:646:PRO:HG2 | 2.52 | 0.44 |
| 1:R:627:THR:HG22 | 1:U:429:HIS:CE1 | 2.53 | 0.44 |
| 1:T:609:TRP:NE1 | 1:d:629:GLY:CA | 2.59 | 0.44 |
| 1:U:453:SER:OG | 1:U:458:GLN:O | 2.36 | 0.44 |
| 1:V:290:PHE:O | 1:V:293:HIS:N | 2.47 | 0.44 |
| 1:V:426:SER:O | 1:V:732:ARG:HA | 2.18 | 0.44 |
| 1:W:220:ASP:OD1 | 1:W:220:ASP:N | 2.50 | 0.44 |
| 1:W:329:ASN:CA | 1:W:330:GLU:OE1 | 2.65 | 0.44 |
| 1:W:429:HIS:CE1 | 1:Y:627:THR:HG22 | 2.53 | 0.44 |
| 1:W:609:TRP:CD1 | 1:W:609:TRP:O | 2.70 | 0.44 |
| 1:W:621:TRP:CH2 | 1:W:646:PRO:HG2 | 2.52 | 0.44 |
| 1:X:232:ASP:HB3 | 1:Y:402:PRO:CG | 2.46 | 0.44 |
| 1:Y:427:TYR:O | 1:Y:427:TYR:HD1 | 2.00 | 0.44 |
| 1:Z:464:LEU:HD23 | 1:4:554:ASN:HB3 | 2.00 | 0.44 |
| 1:a:429:HIS:CE1 | 1:8:627:THR:HG22 | 2.53 | 0.44 |
| 1:b:621:TRP:CH2 | 1:b:646:PRO:HG2 | 2.52 | 0.44 |
| 1:c:487:ARG:HD2 | 1:p:583:ALA:O | 2.18 | 0.44 |
| 1:c:621:TRP:CH2 | 1:c:646:PRO:HG2 | 2.52 | 0.44 |
| 1:d:609:TRP:CD1 | 1:d:609:TRP:O | 2.71 | 0.44 |
| 1:l:427:TYR:O | 1:l:427:TYR:HD1 | 2.00 | 0.44 |
| 1:m:258:TYR:OH | 1:m:399:GLU:OE1 | 2.22 | 0.44 |
| 1:m:429:HIS:CE1 | 1:n:627:THR:HG22 | 2.53 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:464:LEU:HD23 | 1:n:554:ASN:HB3 | 2.00 | 0.44 |
| 1:n:426:SER:O | 1:n:732:ARG:HA | 2.18 | 0.44 |
| 1:o:427:TYR:O | 1:o:427:TYR:CD1 | 2.70 | 0.44 |
| 1:o:621:TRP:CH2 | 1:o:646:PRO:HG2 | 2.52 | 0.44 |
| 1:q:322:GLN:HB3 | 1:y:340:THR:HB | 1.99 | 0.44 |
| 1:q:609:TRP:CD1 | 1:q:609:TRP:O | 2.71 | 0.44 |
| 1:q:621:TRP:CH2 | 1:q:646:PRO:HG2 | 2.52 | 0.44 |
| 1:r:427:TYR:O | 1:r:427:TYR:HD1 | 2.00 | 0.44 |
| 1:s:427:TYR:O | 1:s:427:TYR:CD1 | 2.70 | 0.44 |
| 1:t:616:LEU:HD22 | 1:t:729:ILE:HD12 | 1.99 | 0.44 |
| 1:v:426:SER:O | 1:v:732:ARG:HA | 2.18 | 0.44 |
| 1:w:341:SER:HB3 | 1:w:675:GLN:NE2 | 2.32 | 0.44 |
| 1:w:621:TRP:CH2 | 1:w:646:PRO:HG2 | 2.52 | 0.44 |
| 1:2:609:TRP:CD1 | 1:2:609:TRP:O | 2.71 | 0.44 |
| 1:3:627:THR:HG22 | 1:4:429:HIS:CE1 | 2.52 | 0.44 |
| 1:4:426:SER:O | 1:4:732:ARG:HA | 2.18 | 0.44 |
| 1:4:585:ASN:OD1 | 1:4:594:ILE:N | 2.45 | 0.44 |
| 1:5:554:ASN:HB3 | 1:7:464:LEU:HD23 | 2.00 | 0.44 |
| 1:7:426:SER:O | 1:7:732:ARG:HA | 2.18 | 0.44 |
| 1:B:627:THR:HG22 | 1:L:429:HIS:CE1 | 2.53 | 0.44 |
| 1:C:429:HIS:CE1 | 1:b:627:THR:HG22 | 2.53 | 0.44 |
| 1:D:224:SER:OG | 1:D:225:SER:N | 2.50 | 0.44 |
| 1:D:453:SER:OG | 1:D:458:GLN:O | 2.36 | 0.44 |
| 1:D:583:ALA:O | 1:N:487:ARG:HD2 | 2.18 | 0.44 |
| 1:E:341:SER:HB3 | 1:E:675:GLN:NE2 | 2.32 | 0.44 |
| 1:E:426:SER:O | 1:E:732:ARG:HA | 2.18 | 0.44 |
| 1:E:627:THR:HG22 | 1:F:429:HIS:CE1 | 2.53 | 0.44 |
| 1:F:453:SER:OG | 1:F:458:GLN:O | 2.35 | 0.44 |
| 1:G:426:SER:O | 1:G:732:ARG:HA | 2.18 | 0.44 |
| 1:G:464:LEU:HD23 | 1:I:554:ASN:HB3 | 2.00 | 0.44 |
| 1:H:453:SER:OG | 1:H:458:GLN:O | 2.36 | 0.44 |
| 1:H:464:LEU:HD23 | 1:W:554:ASN:HB3 | 2.00 | 0.44 |
| 1:H:621:TRP:CH2 | 1:H:646:PRO:HG2 | 2.52 | 0.44 |
| 1:J:232:ASP:HB3 | 1:a:402:PRO:CG | 2.46 | 0.44 |
| 1:J:522:PRO:O | 1:J:541:GLY:HA2 | 2.18 | 0.44 |
| 1:M:522:PRO:O | 1:M:541:GLY:HA2 | 2.18 | 0.44 |
| 1:N:224:SER:OG | 1:N:225:SER:N | 2.50 | 0.44 |
| 1:O:224:SER:OG | 1:O:225:SER:N | 2.50 | 0.44 |
| 1:O:627:THR:HG22 | 1:n:429:HIS:CE1 | 2.53 | 0.44 |
| 1:P:621:TRP:CH2 | 1:P:646:PRO:HG2 | 2.52 | 0.44 |
| 1:Q:522:PRO:O | 1:Q:541:GLY:HA2 | 2.18 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:586:LEU:HD21 | 1:U:490:ARG:NH1 | 2.32 | 0.44 |
| 1:T:224:SER:OG | 1:T:225:SER:N | 2.50 | 0.44 |
| 1:T:621:TRP:CH2 | 1:T:646:PRO:HG2 | 2.52 | 0.44 |
| 1:V:554:ASN:HB3 | 1:X:464:LEU:HD23 | 1.99 | 0.44 |
| 1:W:427:TYR:O | 1:W:427:TYR:CD1 | 2.70 | 0.44 |
| 1:X:627:THR:HG22 | 1:e:429:HIS:CE1 | 2.53 | 0.44 |
| 1:a:220:ASP:OD1 | 1:a:220:ASP:N | 2.50 | 0.44 |
| 1:a:427:TYR:O | 1:a:427:TYR:CD1 | 2.70 | 0.44 |
| 1:d:342:THR:HG22 | 1:d:407:ARG:CG | 2.47 | 0.44 |
| 1:d:583:ALA:O | 1:l:487:ARG:HD2 | 2.18 | 0.44 |
| 1:e:341:SER:HB3 | 1:e:675:GLN:NE2 | 2.32 | 0.44 |
| 1:e:342:THR:HG22 | 1:e:407:ARG:CG | 2.47 | 0.44 |
| 1:e:429:HIS:HD2 | 1:e:610:GLN:OE1 | 1.94 | 0.44 |
| 1:e:621:TRP:CH2 | 1:e:646:PRO:HG2 | 2.52 | 0.44 |
| 1:f:435:ARG:HD3 | 1:f:435:ARG:HA | 1.79 | 0.44 |
| 1:f:583:ALA:O | 1:h:487:ARG:HD2 | 2.18 | 0.44 |
| 1:g:329:ASN:CA | 1:g:330:GLU:OE1 | 2.65 | 0.44 |
| 1:h:220:ASP:OD1 | 1:h:220:ASP:N | 2.50 | 0.44 |
| 1:h:616:LEU:HD22 | 1:h:729:ILE:HD12 | 1.99 | 0.44 |
| 1:i:621:TRP:CH2 | 1:i:646:PRO:HG2 | 2.52 | 0.44 |
| 1:n:429:HIS:HD2 | 1:n:610:GLN:OE1 | 1.94 | 0.44 |
| 1:o:609:TRP:CD1 | 1:o:609:TRP:O | 2.70 | 0.44 |
| 1:r:435:ARG:HD3 | 1:r:435:ARG:HA | 1.79 | 0.44 |
| 1:v:382:THR:HG22 | 1:v:383:LEU:N | 2.29 | 0.44 |
| 1:v:453:SER:OG | 1:v:458:GLN:O | 2.36 | 0.44 |
| 1:x:616:LEU:HD22 | 1:x:729:ILE:HD12 | 1.99 | 0.44 |
| 1:y:224:SER:OG | 1:y:225:SER:N | 2.50 | 0.44 |
| 1:z:342:THR:HG22 | 1:z:407:ARG:CG | 2.47 | 0.44 |
| 1:1:585:ASN:OD1 | 1:1:594:ILE:N | 2.45 | 0.44 |
| 1:2:329:ASN:CA | 1:2:330:GLU:OE1 | 2.65 | 0.44 |
| 1:3:224:SER:OG | 1:3:225:SER:N | 2.50 | 0.44 |
| 1:3:434:ASP:OD1 | 1:3:434:ASP:N | 2.41 | 0.44 |
| 1:5:522:PRO:O | 1:5:541:GLY:HA2 | 2.18 | 0.44 |
| 1:6:453:SER:OG | 1:6:458:GLN:O | 2.35 | 0.44 |
| 1:A:627:THR:HG22 | 1:I:429:HIS:CE1 | 2.53 | 0.44 |
| 1:C:398:LEU:C | 1:C:400:TYR:H | 2.24 | 0.44 |
| 1:C:435:ARG:HA | 1:C:435:ARG:HD3 | 1.79 | 0.44 |
| 1:C:627:THR:HG22 | 1:M:429:HIS:CE1 | 2.53 | 0.44 |
| 1:E:490:ARG:NH1 | 1:F:586:LEU:HD21 | 2.32 | 0.44 |
| 1:F:427:TYR:O | 1:F:427:TYR:HD1 | 2.00 | 0.44 |
| 1:H:487:ARG:HD2 | 1:Y:583:ALA:O | 2.18 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:341:SER:HB3 | 1:I:675:GLN:NE2 | 2.32 | 0.44 |
| 1:I:426:SER:O | 1:I:732:ARG:HA | 2.18 | 0.44 |
| 1:J:290:PHE:O | 1:J:293:HIS:N | 2.47 | 0.44 |
| 1:K:224:SER:OG | 1:K:225:SER:N | 2.50 | 0.44 |
| 1:K:583:ALA:O | 1:a:487:ARG:HD2 | 2.18 | 0.44 |
| 1:L:398:LEU:C | 1:L:400:TYR:H | 2.24 | 0.44 |
| 1:M:329:ASN:O | 1:M:332:THR:OG1 | 2.30 | 0.44 |
| 1:N:220:ASP:OD1 | 1:N:220:ASP:N | 2.50 | 0.44 |
| 1:N:427:TYR:O | 1:N:427:TYR:CD1 | 2.70 | 0.44 |
| 1:O:464:LEU:HD23 | 1:m:554:ASN:HB3 | 2.00 | 0.44 |
| 1:Q:585:ASN:OD1 | 1:Q:594:ILE:N | 2.45 | 0.44 |
| 1:R:224:SER:OG | 1:R:225:SER:N | 2.50 | 0.44 |
| 1:R:453:SER:OG | 1:R:458:GLN:O | 2.36 | 0.44 |
| 1:T:585:ASN:OD1 | 1:T:594:ILE:N | 2.45 | 0.44 |
| 1:T:616:LEU:HD22 | 1:T:729:ILE:HD12 | 1.99 | 0.44 |
| 1:U:427:TYR:O | 1:U:427:TYR:CD1 | 2.70 | 0.44 |
| 1:V:627:THR:HG22 | 1:X:429:HIS:CE1 | 2.53 | 0.44 |
| 1:X:427:TYR:O | 1:X:427:TYR:HD1 | 2.00 | 0.44 |
| 1:X:487:ARG:HD2 | 1:e:583:ALA:O | 2.18 | 0.44 |
| 1:X:616:LEU:HD22 | 1:X:729:ILE:HD12 | 1.99 | 0.44 |
| 1:Z:554:ASN:HB3 | 1:3:464:LEU:HD23 | 2.00 | 0.44 |
| 1:a:224:SER:OG | 1:a:225:SER:N | 2.50 | 0.44 |
| 1:a:522:PRO:O | 1:a:541:GLY:HA2 | 2.18 | 0.44 |
| 1:b:522:PRO:O | 1:b:541:GLY:HA2 | 2.18 | 0.44 |
| 1:c:554:ASN:HB3 | 1:p:464:LEU:HD23 | 2.00 | 0.44 |
| 1:c:627:THR:HG22 | 1:p:429:HIS:CE1 | 2.53 | 0.44 |
| 1:d:329:ASN:CA | 1:d:330:GLU:OE1 | 2.65 | 0.44 |
| 1:g:627:THR:HG22 | 1:h:429:HIS:CE1 | 2.53 | 0.44 |
| 1:i:382:THR:HG22 | 1:i:383:LEU:N | 2.29 | 0.44 |
| 1:i:609:TRP:CD1 | 1:i:609:TRP:O | 2.70 | 0.44 |
| 1:i:627:THR:HG22 | 1:k:429:HIS:CE1 | 2.53 | 0.44 |
| 1:j:427:TYR:O | 1:j:427:TYR:CD1 | 2.70 | 0.44 |
| 1:j:583:ALA:O | 1:k:487:ARG:HD2 | 2.18 | 0.44 |
| 1:k:224:SER:OG | 1:k:225:SER:N | 2.50 | 0.44 |
| 1:k:616:LEU:HD22 | 1:k:729:ILE:HD12 | 1.99 | 0.44 |
| 1:o:435:ARG:HD3 | 1:o:435:ARG:HA | 1.79 | 0.44 |
| 1:p:426:SER:O | 1:p:732:ARG:HA | 2.18 | 0.44 |
| 1:q:427:TYR:O | 1:q:427:TYR:CD1 | 2.70 | 0.44 |
| 1:q:490:ARG:NH1 | 1:s:586:LEU:HD21 | 2.33 | 0.44 |
| 1:r:583:ALA:O | 1:s:487:ARG:HD2 | 2.18 | 0.44 |
| 1:s:453:SER:OG | 1:s:458:GLN:O | 2.36 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:t:453:SER:OG | 1:t:458:GLN:O | 2.35 | 0.44 |
| 1:u:586:LEU:HD21 | 1:v:490:ARG:NH1 | 2.33 | 0.44 |
| 1:w:342:THR:HG22 | 1:w:407:ARG:CG | 2.47 | 0.44 |
| 1:z:527:ALA:O | 1:z:575:ALA:N | 2.45 | 0.44 |
| 1:1:224:SER:OG | 1:1:225:SER:N | 2.50 | 0.44 |
| 1:1:616:LEU:HD22 | 1:1:729:ILE:HD12 | 1.99 | 0.44 |
| 1:1:621:TRP:CH2 | 1:1:646:PRO:HG2 | 2.52 | 0.44 |
| 1:2:342:THR:HG22 | 1:2:407:ARG:CG | 2.47 | 0.44 |
| 1:3:322:GLN:HB3 | 1:8:340:THR:HB | 2.00 | 0.44 |
| 1:3:426:SER:OG | 1:3:731:THR:O | 2.31 | 0.44 |
| 1:6:427:TYR:O | 1:6:427:TYR:HD1 | 2.00 | 0.44 |
| 1:6:429:HIS:CE1 | 1:7:627:THR:HG22 | 2.53 | 0.44 |
| 1:6:586:LEU:HD21 | 1:7:490:ARG:NH1 | 2.32 | 0.44 |
| 1:7:341:SER:HB3 | 1:7:675:GLN:NE2 | 2.32 | 0.44 |
| 1:7:429:HIS:HD2 | 1:7:610:GLN:OE1 | 1.94 | 0.44 |
| 1:A:453:SER:OG | 1:A:458:GLN:O | 2.36 | 0.43 |
| 1:A:609:TRP:CD1 | 1:A:609:TRP:O | 2.70 | 0.43 |
| 1:B:522:PRO:O | 1:B:541:GLY:HA2 | 2.18 | 0.43 |
| 1:C:616:LEU:HD22 | 1:C:729:ILE:HD12 | 1.99 | 0.43 |
| 1:D:429:HIS:CE1 | 1:N:627:THR:HG22 | 2.53 | 0.43 |
| 1:D:464:LEU:HD23 | 1:N:554:ASN:HB3 | 2.00 | 0.43 |
| 1:D:626:HIS:CD2 | 1:P:736:ARG:NH2 | 2.79 | 0.43 |
| 1:G:429:HIS:CE1 | 1:I:627:THR:HG22 | 2.53 | 0.43 |
| 1:J:429:HIS:CE1 | 1:L:627:THR:HG22 | 2.53 | 0.43 |
| 1:K:453:SER:OG | 1:K:458:GLN:O | 2.36 | 0.43 |
| 1:L:429:HIS:HD2 | 1:L:610:GLN:OE1 | 1.94 | 0.43 |
| 1:N:329:ASN:CA | 1:N:330:GLU:OE1 | 2.65 | 0.43 |
| 1:N:464:LEU:HD23 | 1:P:554:ASN:HB3 | 1.99 | 0.43 |
| 1:N:522:PRO:O | 1:N:541:GLY:HA2 | 2.18 | 0.43 |
| 1:O:220:ASP:OD1 | 1:O:220:ASP:N | 2.50 | 0.43 |
| 1:O:322:GLN:HB3 | 1:P:340:THR:HB | 2.00 | 0.43 |
| 1:R:426:SER:OG | 1:R:731:THR:O | 2.31 | 0.43 |
| 1:R:429:HIS:CE1 | 1:S:627:THR:HG22 | 2.53 | 0.43 |
| 1:T:522:PRO:O | 1:T:541:GLY:HA2 | 2.18 | 0.43 |
| 1:U:224:SER:OG | 1:U:225:SER:N | 2.50 | 0.43 |
| 1:U:307:TRP:O | 1:U:426:SER:CB | 2.59 | 0.43 |
| 1:U:382:THR:HG22 | 1:U:383:LEU:N | 2.29 | 0.43 |
| 1:V:583:ALA:O | 1:e:487:ARG:HD2 | 2.18 | 0.43 |
| 1:X:341:SER:HB3 | 1:X:675:GLN:NE2 | 2.32 | 0.43 |
| 1:a:464:LEU:HD23 | 1:8:554:ASN:HB3 | 1.99 | 0.43 |
| 1:c:426:SER:O | 1:c:732:ARG:HA | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:f:427:TYR:O | 1:f:427:TYR:CD1 | 2.70 | 0.43 |
| 1:g:382:THR:HG22 | 1:g:383:LEU:N | 2.29 | 0.43 |
| 1:g:609:TRP:CD1 | 1:g:609:TRP:O | 2.70 | 0.43 |
| 1:g:621:TRP:CH2 | 1:g:646:PRO:HG2 | 2.52 | 0.43 |
| 1:h:224:SER:OG | 1:h:225:SER:N | 2.50 | 0.43 |
| 1:j:290:PHE:O | 1:j:293:HIS:N | 2.47 | 0.43 |
| 1:k:585:ASN:OD1 | 1:k:594:ILE:N | 2.45 | 0.43 |
| 1:l:342:THR:HG22 | 1:l:407:ARG:CG | 2.47 | 0.43 |
| 1:l:473:MET:HE3 | 1:l:473:MET:HB2 | 1.81 | 0.43 |
| 1:m:232:ASP:HB3 | 1:s:402:PRO:CG | 2.46 | 0.43 |
| 1:n:522:PRO:O | 1:n:541:GLY:HA2 | 2.18 | 0.43 |
| 1:o:232:ASP:HB3 | 1:7:402:PRO:CG | 2.47 | 0.43 |
| 1:p:232:ASP:HB3 | 1:q:402:PRO:CG | 2.46 | 0.43 |
| 1:q:554:ASN:HB3 | 1:s:464:LEU:HD23 | 2.00 | 0.43 |
| 1:s:522:PRO:O | 1:s:541:GLY:HA2 | 2.18 | 0.43 |
| 1:t:224:SER:OG | 1:t:225:SER:N | 2.50 | 0.43 |
| 1:t:487:ARG:HD2 | 1:v:583:ALA:O | 2.18 | 0.43 |
| 1:t:527:ALA:O | 1:t:575:ALA:N | 2.45 | 0.43 |
| 1:t:626:HIS:CD2 | 1:v:736:ARG:NH2 | 2.79 | 0.43 |
| 1:u:224:SER:OG | 1:u:225:SER:N | 2.50 | 0.43 |
| 1:v:224:SER:OG | 1:v:225:SER:N | 2.50 | 0.43 |
| 1:w:329:ASN:CA | 1:w:330:GLU:OE1 | 2.65 | 0.43 |
| 1:z:487:ARG:HD2 | 1:2:583:ALA:O | 2.18 | 0.43 |
| 1:z:627:THR:HG22 | 1:2:429:HIS:CE1 | 2.53 | 0.43 |
| 1:1:522:PRO:O | 1:1:541:GLY:HA2 | 2.18 | 0.43 |
| 1:2:616:LEU:HD22 | 1:2:729:ILE:HD12 | 1.99 | 0.43 |
| 1:3:220:ASP:OD1 | 1:3:220:ASP:N | 2.50 | 0.43 |
| 1:3:621:TRP:CH2 | 1:3:646:PRO:HG2 | 2.52 | 0.43 |
| 1:4:429:HIS:HD2 | 1:4:610:GLN:OE1 | 1.94 | 0.43 |
| 1:8:609:TRP:CD1 | 1:8:609:TRP:O | 2.71 | 0.43 |
| 1:8:621:TRP:CH2 | 1:8:646:PRO:HG2 | 2.52 | 0.43 |
| 1:B:464:LEU:HD23 | 1:J:554:ASN:HB3 | 2.00 | 0.43 |
| 1:C:427:TYR:O | 1:C:427:TYR:HD1 | 2.00 | 0.43 |
| 1:E:583:ALA:O | 1:Q:487:ARG:HD2 | 2.18 | 0.43 |
| 1:F:426:SER:O | 1:F:732:ARG:HA | 2.18 | 0.43 |
| 1:F:627:THR:HG22 | 1:Q:429:HIS:CE1 | 2.53 | 0.43 |
| 1:G:452:GLN:HE21 | 1:G:459:GLY:HA3 | 1.84 | 0.43 |
| 1:H:402:PRO:CG | 1:Z:232:ASP:HB3 | 2.46 | 0.43 |
| 1:H:522:PRO:O | 1:H:541:GLY:HA2 | 2.18 | 0.43 |
| 1:K:429:HIS:CE1 | 1:a:627:THR:HG22 | 2.53 | 0.43 |
| 1:K:464:LEU:HD23 | 1:a:554:ASN:HB3 | 2.00 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:341:SER:HB3 | 1:L:675:GLN:NE2 | 2.32 | 0.43 |
| 1:M:427:TYR:O | 1:M:427:TYR:HD1 | 2.00 | 0.43 |
| 1:M:429:HIS:HD2 | 1:M:610:GLN:OE1 | 1.94 | 0.43 |
| 1:N:586:LEU:HD21 | 1:P:490:ARG:NH1 | 2.33 | 0.43 |
| 1:O:278:TYR:CE2 | 1:O:395:PHE:HD1 | 2.37 | 0.43 |
| 1:O:621:TRP:CH2 | 1:O:646:PRO:HG2 | 2.52 | 0.43 |
| 1:O:629:GLY:CA | 1:n:609:TRP:NE1 | 2.59 | 0.43 |
| 1:R:452:GLN:HE21 | 1:R:459:GLY:HA3 | 1.84 | 0.43 |
| 1:R:487:ARG:HD2 | 1:U:583:ALA:O | 2.18 | 0.43 |
| 1:R:621:TRP:CH2 | 1:R:646:PRO:HG2 | 2.52 | 0.43 |
| 1:S:429:HIS:CE1 | 1:U:627:THR:HG22 | 2.53 | 0.43 |
| 1:S:527:ALA:O | 1:S:575:ALA:N | 2.45 | 0.43 |
| 1:V:453:SER:OG | 1:V:458:GLN:O | 2.35 | 0.43 |
| 1:W:224:SER:OG | 1:W:225:SER:N | 2.50 | 0.43 |
| 1:W:522:PRO:O | 1:W:541:GLY:HA2 | 2.18 | 0.43 |
| 1:X:435:ARG:HD3 | 1:X:435:ARG:HA | 1.79 | 0.43 |
| 1:a:329:ASN:CA | 1:a:330:GLU:OE1 | 2.65 | 0.43 |
| 1:a:586:LEU:HD21 | 1:8:490:ARG:NH1 | 2.33 | 0.43 |
| 1:c:341:SER:HB3 | 1:c:675:GLN:NE2 | 2.32 | 0.43 |
| 1:d:429:HIS:CE1 | 1:l:627:THR:HG22 | 2.53 | 0.43 |
| 1:d:616:LEU:HD22 | 1:d:729:ILE:HD12 | 1.99 | 0.43 |
| 1:e:329:ASN:CA | 1:e:330:GLU:OE1 | 2.65 | 0.43 |
| 1:f:290:PHE:O | 1:f:293:HIS:N | 2.47 | 0.43 |
| 1:g:522:PRO:O | 1:g:541:GLY:HA2 | 2.18 | 0.43 |
| 1:i:522:PRO:O | 1:i:541:GLY:HA2 | 2.18 | 0.43 |
| 1:m:342:THR:HG22 | 1:m:407:ARG:CG | 2.47 | 0.43 |
| 1:o:453:SER:OG | 1:o:458:GLN:O | 2.36 | 0.43 |
| 1:o:464:LEU:HD23 | 1:p:554:ASN:HB3 | 2.00 | 0.43 |
| 1:p:452:GLN:HE21 | 1:p:459:GLY:HA3 | 1.84 | 0.43 |
| 1:q:453:SER:OG | 1:q:458:GLN:O | 2.36 | 0.43 |
| 1:r:609:TRP:CD1 | 1:s:629:GLY:CA | 2.85 | 0.43 |
| 1:t:429:HIS:CE1 | 1:u:627:THR:HG22 | 2.53 | 0.43 |
| 1:t:621:TRP:CH2 | 1:t:646:PRO:HG2 | 2.52 | 0.43 |
| 1:u:329:ASN:CA | 1:u:330:GLU:OE1 | 2.65 | 0.43 |
| 1:u:429:HIS:CE1 | 1:v:627:THR:HG22 | 2.53 | 0.43 |
| 1:v:427:TYR:O | 1:v:427:TYR:CD1 | 2.70 | 0.43 |
| 1:v:429:HIS:HD2 | 1:v:610:GLN:OE1 | 1.94 | 0.43 |
| 1:w:586:LEU:HD11 | 1:x:490:ARG:CZ | 2.48 | 0.43 |
| 1:x:341:SER:HB3 | 1:x:675:GLN:NE2 | 2.32 | 0.43 |
| 1:x:427:TYR:O | 1:x:427:TYR:HD1 | 2.00 | 0.43 |
| 1:4:522:PRO:O | 1:4:541:GLY:HA2 | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:429:HIS:CE1 | 1:6:627:THR:HG22 | 2.53 | 0.43 |
| 1:5:487:ARG:HD2 | 1:7:583:ALA:O | 2.18 | 0.43 |
| 1:6:464:LEU:HD23 | 1:7:554:ASN:HB3 | 2.00 | 0.43 |
| 1:8:278:TYR:CE2 | 1:8:395:PHE:HD1 | 2.37 | 0.43 |
| 1:D:278:TYR:CE2 | 1:D:395:PHE:HD1 | 2.37 | 0.43 |
| 1:E:554:ASN:HB3 | 1:F:464:LEU:HD23 | 2.00 | 0.43 |
| 1:E:609:TRP:CD1 | 1:E:609:TRP:O | 2.71 | 0.43 |
| 1:F:224:SER:OG | 1:F:225:SER:N | 2.50 | 0.43 |
| 1:F:487:ARG:HD2 | 1:Q:583:ALA:O | 2.18 | 0.43 |
| 1:G:232:ASP:HB3 | 1:W:402:PRO:CG | 2.46 | 0.43 |
| 1:H:629:GLY:CA | 1:Y:609:TRP:CD1 | 2.85 | 0.43 |
| 1:K:278:TYR:CE2 | 1:K:395:PHE:HD1 | 2.37 | 0.43 |
| 1:L:435:ARG:HA | 1:L:435:ARG:HD3 | 1.79 | 0.43 |
| 1:L:616:LEU:HD22 | 1:L:729:ILE:HD12 | 1.99 | 0.43 |
| 1:M:290:PHE:HE2 | 1:M:614:VAL:HB | 1.84 | 0.43 |
| 1:M:453:SER:OG | 1:M:458:GLN:O | 2.36 | 0.43 |
| 1:M:554:ASN:HB3 | 1:b:464:LEU:HD23 | 2.00 | 0.43 |
| 1:O:490:ARG:NH1 | 1:n:586:LEU:HD21 | 2.33 | 0.43 |
| 1:P:278:TYR:CE2 | 1:P:395:PHE:HD1 | 2.37 | 0.43 |
| 1:P:609:TRP:CD1 | 1:P:609:TRP:O | 2.71 | 0.43 |
| 1:R:340:THR:O | 1:R:407:ARG:CZ | 2.67 | 0.43 |
| 1:R:522:PRO:O | 1:R:541:GLY:HA2 | 2.18 | 0.43 |
| 1:R:527:ALA:O | 1:R:575:ALA:N | 2.45 | 0.43 |
| 1:R:626:HIS:CD2 | 1:U:736:ARG:NH2 | 2.79 | 0.43 |
| 1:S:224:SER:OG | 1:S:225:SER:N | 2.50 | 0.43 |
| 1:S:278:TYR:CE2 | 1:S:395:PHE:HD1 | 2.37 | 0.43 |
| 1:S:329:ASN:CA | 1:S:330:GLU:OE1 | 2.65 | 0.43 |
| 1:S:340:THR:O | 1:S:407:ARG:CZ | 2.67 | 0.43 |
| 1:X:340:THR:O | 1:X:407:ARG:CZ | 2.67 | 0.43 |
| 1:Z:224:SER:OG | 1:Z:225:SER:N | 2.50 | 0.43 |
| 1:Z:278:TYR:CE2 | 1:Z:395:PHE:HD1 | 2.37 | 0.43 |
| 1:Z:609:TRP:CD1 | 1:Z:609:TRP:O | 2.71 | 0.43 |
| 1:b:329:ASN:O | 1:b:332:THR:OG1 | 2.31 | 0.43 |
| 1:b:340:THR:O | 1:b:407:ARG:CZ | 2.67 | 0.43 |
| 1:m:224:SER:OG | 1:m:225:SER:N | 2.50 | 0.43 |
| 1:m:278:TYR:CE2 | 1:m:395:PHE:HD1 | 2.36 | 0.43 |
| 1:m:609:TRP:CD1 | 1:m:609:TRP:O | 2.71 | 0.43 |
| 1:n:224:SER:OG | 1:n:225:SER:N | 2.50 | 0.43 |
| 1:n:290:PHE:HE2 | 1:n:614:VAL:HB | 1.84 | 0.43 |
| 1:p:434:ASP:OD1 | 1:p:434:ASP:N | 2.41 | 0.43 |
| 1:q:522:PRO:O | 1:q:541:GLY:HA2 | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:r:453:SER:OG | 1:r:458:GLN:O | 2.36 | 0.43 |
| 1:s:452:GLN:HE21 | 1:s:459:GLY:HA3 | 1.84 | 0.43 |
| 1:t:522:PRO:O | 1:t:541:GLY:HA2 | 2.18 | 0.43 |
| 1:u:290:PHE:O | 1:u:293:HIS:N | 2.47 | 0.43 |
| 1:u:340:THR:O | 1:u:407:ARG:CZ | 2.67 | 0.43 |
| 1:u:527:ALA:O | 1:u:575:ALA:N | 2.45 | 0.43 |
| 1:v:307:TRP:O | 1:v:426:SER:CB | 2.59 | 0.43 |
| 1:v:702:GLN:HB2 | 1:y:704:THR:HB | 2.00 | 0.43 |
| 1:w:340:THR:O | 1:w:407:ARG:CZ | 2.67 | 0.43 |
| 1:w:426:SER:O | 1:w:732:ARG:HA | 2.18 | 0.43 |
| 1:w:429:HIS:HD2 | 1:w:610:GLN:OE1 | 1.94 | 0.43 |
| 1:w:453:SER:OG | 1:w:458:GLN:O | 2.35 | 0.43 |
| 1:w:490:ARG:CZ | 1:y:586:LEU:HD11 | 2.48 | 0.43 |
| 1:x:340:THR:O | 1:x:407:ARG:CZ | 2.67 | 0.43 |
| 1:x:435:ARG:HD3 | 1:x:435:ARG:HA | 1.79 | 0.43 |
| 1:x:438:ASN:HB2 | 1:y:356:VAL:CG2 | 2.48 | 0.43 |
| 1:x:452:GLN:HE21 | 1:x:459:GLY:HA3 | 1.84 | 0.43 |
| 1:x:586:LEU:HD21 | 1:y:490:ARG:CZ | 2.48 | 0.43 |
| 1:1:609:TRP:NE1 | 1:2:629:GLY:CA | 2.59 | 0.43 |
| 1:2:452:GLN:HE21 | 1:2:459:GLY:HA3 | 1.84 | 0.43 |
| 1:3:278:TYR:CE2 | 1:3:395:PHE:HD1 | 2.37 | 0.43 |
| 1:4:290:PHE:HE2 | 1:4:614:VAL:HB | 1.84 | 0.43 |
| 1:5:278:TYR:CE2 | 1:5:395:PHE:HD1 | 2.37 | 0.43 |
| 1:5:585:ASN:OD1 | 1:5:594:ILE:N | 2.45 | 0.43 |
| 1:6:426:SER:O | 1:6:732:ARG:HA | 2.18 | 0.43 |
| 1:B:340:THR:O | 1:B:407:ARG:CZ | 2.67 | 0.43 |
| 1:C:340:THR:HB | 1:D:322:GLN:HB3 | 2.00 | 0.43 |
| 1:C:341:SER:HB3 | 1:C:675:GLN:NE2 | 2.32 | 0.43 |
| 1:C:429:HIS:HD2 | 1:C:610:GLN:OE1 | 1.94 | 0.43 |
| 1:E:342:THR:HG22 | 1:E:407:ARG:CG | 2.47 | 0.43 |
| 1:H:342:THR:HG22 | 1:H:407:ARG:CG | 2.47 | 0.43 |
| 1:H:452:GLN:HE21 | 1:H:459:GLY:HA3 | 1.84 | 0.43 |
| 1:H:554:ASN:HB3 | 1:Y:464:LEU:HD23 | 2.00 | 0.43 |
| 1:J:278:TYR:CE2 | 1:J:395:PHE:HD1 | 2.37 | 0.43 |
| 1:J:290:PHE:HE2 | 1:J:614:VAL:HB | 1.84 | 0.43 |
| 1:J:427:TYR:O | 1:J:427:TYR:HD1 | 2.00 | 0.43 |
| 1:J:453:SER:OG | 1:J:458:GLN:O | 2.36 | 0.43 |
| 1:K:627:THR:HG22 | 1:8:429:HIS:CE1 | 2.53 | 0.43 |
| 1:L:427:TYR:O | 1:L:427:TYR:HD1 | 2.00 | 0.43 |
| 1:L:452:GLN:HE21 | 1:L:459:GLY:HA3 | 1.84 | 0.43 |
| 1:M:224:SER:OG | 1:M:225:SER:N | 2.50 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:278:TYR:CE2 | 1:M:395:PHE:HD1 | 2.37 | 0.43 |
| 1:N:290:PHE:HE2 | 1:N:614:VAL:HB | 1.84 | 0.43 |
| 1:O:452:GLN:HE21 | 1:O:459:GLY:HA3 | 1.84 | 0.43 |
| 1:O:453:SER:OG | 1:O:458:GLN:O | 2.36 | 0.43 |
| 1:O:487:ARG:HD2 | 1:n:583:ALA:O | 2.19 | 0.43 |
| 1:Q:278:TYR:CE2 | 1:Q:395:PHE:HD1 | 2.37 | 0.43 |
| 1:Q:426:SER:O | 1:Q:732:ARG:HA | 2.18 | 0.43 |
| 1:Q:452:GLN:HE21 | 1:Q:459:GLY:HA3 | 1.84 | 0.43 |
| 1:R:464:LEU:HD23 | 1:S:554:ASN:HB3 | 2.00 | 0.43 |
| 1:R:490:ARG:NH1 | 1:U:586:LEU:HD21 | 2.32 | 0.43 |
| 1:R:554:ASN:HB3 | 1:U:464:LEU:HD23 | 2.00 | 0.43 |
| 1:R:586:LEU:HD21 | 1:S:490:ARG:NH1 | 2.32 | 0.43 |
| 1:S:290:PHE:O | 1:S:293:HIS:N | 2.47 | 0.43 |
| 1:S:329:ASN:O | 1:S:332:THR:OG1 | 2.31 | 0.43 |
| 1:S:452:GLN:HE21 | 1:S:459:GLY:HA3 | 1.84 | 0.43 |
| 1:T:736:ARG:NH2 | 1:d:626:HIS:CD2 | 2.79 | 0.43 |
| 1:U:429:HIS:HD2 | 1:U:610:GLN:OE1 | 1.94 | 0.43 |
| 1:V:340:THR:O | 1:V:407:ARG:CZ | 2.67 | 0.43 |
| 1:W:426:SER:O | 1:W:732:ARG:HA | 2.18 | 0.43 |
| 1:W:453:SER:OG | 1:W:458:GLN:O | 2.36 | 0.43 |
| 1:W:527:ALA:O | 1:W:575:ALA:N | 2.45 | 0.43 |
| 1:X:452:GLN:HE21 | 1:X:459:GLY:HA3 | 1.84 | 0.43 |
| 1:Y:453:SER:OG | 1:Y:458:GLN:O | 2.35 | 0.43 |
| 1:Z:342:THR:HG22 | 1:Z:407:ARG:CG | 2.47 | 0.43 |
| 1:Z:426:SER:OG | 1:Z:731:THR:O | 2.30 | 0.43 |
| 1:a:290:PHE:HE2 | 1:a:614:VAL:HB | 1.84 | 0.43 |
| 1:d:452:GLN:HE21 | 1:d:459:GLY:HA3 | 1.84 | 0.43 |
| 1:e:340:THR:O | 1:e:407:ARG:CZ | 2.67 | 0.43 |
| 1:e:426:SER:O | 1:e:732:ARG:HA | 2.18 | 0.43 |
| 1:f:522:PRO:O | 1:f:541:GLY:HA2 | 2.18 | 0.43 |
| 1:j:522:PRO:O | 1:j:541:GLY:HA2 | 2.18 | 0.43 |
| 1:k:426:SER:O | 1:k:732:ARG:HA | 2.18 | 0.43 |
| 1:k:609:TRP:CD1 | 1:k:609:TRP:O | 2.71 | 0.43 |
| 1:l:290:PHE:O | 1:l:293:HIS:N | 2.47 | 0.43 |
| 1:n:452:GLN:HE21 | 1:n:459:GLY:HA3 | 1.84 | 0.43 |
| 1:o:429:HIS:CE1 | 1:p:627:THR:HG22 | 2.53 | 0.43 |
| 1:q:224:SER:OG | 1:q:225:SER:N | 2.50 | 0.43 |
| 1:q:527:ALA:O | 1:q:575:ALA:N | 2.45 | 0.43 |
| 1:r:464:LEU:HD23 | 1:s:554:ASN:HB3 | 2.00 | 0.43 |
| 1:s:290:PHE:O | 1:s:293:HIS:N | 2.47 | 0.43 |
| 1:t:340:THR:O | 1:t:407:ARG:CZ | 2.67 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:t:452:GLN:HE21 | 1:t:459:GLY:HA3 | 1.84 | 0.43 |
| 1:t:554:ASN:HB3 | 1:v:464:LEU:HD23 | 2.00 | 0.43 |
| 1:u:278:TYR:CE2 | 1:u:395:PHE:HD1 | 2.37 | 0.43 |
| 1:u:452:GLN:HE21 | 1:u:459:GLY:HA3 | 1.84 | 0.43 |
| 1:w:629:GLY:CA | 1:y:609:TRP:CD1 | 2.88 | 0.43 |
| 1:y:340:THR:O | 1:y:407:ARG:CZ | 2.67 | 0.43 |
| 1:y:453:SER:OG | 1:y:458:GLN:O | 2.36 | 0.43 |
| 1:3:452:GLN:HE21 | 1:3:459:GLY:HA3 | 1.84 | 0.43 |
| 1:3:490:ARG:NH1 | 1:4:586:LEU:HD21 | 2.33 | 0.43 |
| 1:3:609:TRP:CD1 | 1:3:609:TRP:O | 2.70 | 0.43 |
| 1:4:224:SER:OG | 1:4:225:SER:N | 2.50 | 0.43 |
| 1:4:452:GLN:HE21 | 1:4:459:GLY:HA3 | 1.84 | 0.43 |
| 1:A:278:TYR:CE2 | 1:A:395:PHE:HD1 | 2.37 | 0.43 |
| 1:C:220:ASP:OD1 | 1:C:220:ASP:N | 2.50 | 0.43 |
| 1:C:278:TYR:CE2 | 1:C:395:PHE:HD1 | 2.37 | 0.43 |
| 1:C:340:THR:O | 1:C:407:ARG:CZ | 2.67 | 0.43 |
| 1:C:452:GLN:HE21 | 1:C:459:GLY:HA3 | 1.84 | 0.43 |
| 1:C:487:ARG:HD2 | 1:M:583:ALA:O | 2.18 | 0.43 |
| 1:C:522:PRO:O | 1:C:541:GLY:HA2 | 2.18 | 0.43 |
| 1:E:522:PRO:O | 1:E:541:GLY:HA2 | 2.18 | 0.43 |
| 1:E:586:LEU:HD21 | 1:Q:490:ARG:NH1 | 2.32 | 0.43 |
| 1:F:220:ASP:OD1 | 1:F:220:ASP:N | 2.50 | 0.43 |
| 1:J:224:SER:OG | 1:J:225:SER:N | 2.50 | 0.43 |
| 1:J:583:ALA:O | 1:L:487:ARG:HD2 | 2.18 | 0.43 |
| 1:K:322:GLN:HB3 | 1:L:340:THR:HB | 2.00 | 0.43 |
| 1:L:278:TYR:CE2 | 1:L:395:PHE:HD1 | 2.37 | 0.43 |
| 1:L:340:THR:O | 1:L:407:ARG:CZ | 2.67 | 0.43 |
| 1:N:278:TYR:CE2 | 1:N:395:PHE:HD1 | 2.36 | 0.43 |
| 1:P:329:ASN:O | 1:P:332:THR:OG1 | 2.31 | 0.43 |
| 1:R:278:TYR:CE2 | 1:R:395:PHE:HD1 | 2.37 | 0.43 |
| 1:U:522:PRO:O | 1:U:541:GLY:HA2 | 2.18 | 0.43 |
| 1:V:522:PRO:O | 1:V:541:GLY:HA2 | 2.18 | 0.43 |
| 1:X:322:GLN:HB3 | 1:Y:340:THR:HB | 2.01 | 0.43 |
| 1:b:426:SER:O | 1:b:732:ARG:HA | 2.18 | 0.43 |
| 1:c:609:TRP:CD1 | 1:c:609:TRP:O | 2.71 | 0.43 |
| 1:e:322:GLN:HB3 | 1:h:340:THR:HB | 2.00 | 0.43 |
| 1:e:453:SER:OG | 1:e:458:GLN:O | 2.36 | 0.43 |
| 1:f:290:PHE:HE2 | 1:f:614:VAL:HB | 1.84 | 0.43 |
| 1:g:340:THR:O | 1:g:407:ARG:CZ | 2.67 | 0.43 |
| 1:h:340:THR:O | 1:h:407:ARG:CZ | 2.67 | 0.43 |
| 1:h:426:SER:O | 1:h:732:ARG:HA | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:h:609:TRP:CD1 | 1:h:609:TRP:O | 2.71 | 0.43 |
| 1:i:583:ALA:O | 1:j:487:ARG:HD2 | 2.19 | 0.43 |
| 1:j:435:ARG:HA | 1:j:435:ARG:HD3 | 1.79 | 0.43 |
| 1:k:340:THR:O | 1:k:407:ARG:CZ | 2.67 | 0.43 |
| 1:l:290:PHE:HE2 | 1:l:614:VAL:HB | 1.84 | 0.43 |
| 1:l:426:SER:O | 1:l:732:ARG:HA | 2.18 | 0.43 |
| 1:n:453:SER:OG | 1:n:458:GLN:O | 2.35 | 0.43 |
| 1:o:278:TYR:CE2 | 1:o:395:PHE:HD1 | 2.37 | 0.43 |
| 1:o:426:SER:O | 1:o:732:ARG:HA | 2.18 | 0.43 |
| 1:p:340:THR:O | 1:p:407:ARG:CZ | 2.67 | 0.43 |
| 1:r:340:THR:HB | 1:x:322:GLN:HB3 | 2.01 | 0.43 |
| 1:r:429:HIS:CE1 | 1:s:627:THR:HG22 | 2.53 | 0.43 |
| 1:s:342:THR:HG22 | 1:s:407:ARG:CG | 2.47 | 0.43 |
| 1:t:278:TYR:CE2 | 1:t:395:PHE:HD1 | 2.37 | 0.43 |
| 1:t:464:LEU:HD23 | 1:u:554:ASN:HB3 | 2.00 | 0.43 |
| 1:t:490:ARG:NH1 | 1:v:586:LEU:HD21 | 2.32 | 0.43 |
| 1:w:220:ASP:OD1 | 1:w:220:ASP:N | 2.50 | 0.43 |
| 1:y:522:PRO:O | 1:y:541:GLY:HA2 | 2.18 | 0.43 |
| 1:z:290:PHE:HE2 | 1:z:614:VAL:HB | 1.84 | 0.43 |
| 1:z:426:SER:O | 1:z:732:ARG:HA | 2.18 | 0.43 |
| 1:1:452:GLN:HE21 | 1:1:459:GLY:HA3 | 1.84 | 0.43 |
| 1:1:736:ARG:NH2 | 1:2:626:HIS:CD2 | 2.79 | 0.43 |
| 1:3:453:SER:OG | 1:3:458:GLN:O | 2.36 | 0.43 |
| 1:4:453:SER:OG | 1:4:458:GLN:O | 2.36 | 0.43 |
| 1:5:426:SER:O | 1:5:732:ARG:HA | 2.18 | 0.43 |
| 1:5:452:GLN:HE21 | 1:5:459:GLY:HA3 | 1.84 | 0.43 |
| 1:5:490:ARG:NH1 | 1:7:586:LEU:HD21 | 2.32 | 0.43 |
| 1:5:583:ALA:O | 1:6:487:ARG:HD2 | 2.18 | 0.43 |
| 1:6:220:ASP:OD1 | 1:6:220:ASP:N | 2.50 | 0.43 |
| 1:7:342:THR:HG22 | 1:7:407:ARG:CG | 2.47 | 0.43 |
| 1:7:609:TRP:CD1 | 1:7:609:TRP:O | 2.71 | 0.43 |
| 1:A:426:SER:O | 1:A:732:ARG:HA | 2.18 | 0.43 |
| 1:A:522:PRO:O | 1:A:541:GLY:HA2 | 2.18 | 0.43 |
| 1:B:426:SER:O | 1:B:732:ARG:HA | 2.18 | 0.43 |
| 1:B:487:ARG:HD2 | 1:L:583:ALA:O | 2.18 | 0.43 |
| 1:C:583:ALA:O | 1:b:487:ARG:HD2 | 2.18 | 0.43 |
| 1:C:629:GLY:CA | 1:M:609:TRP:CD1 | 2.85 | 0.43 |
| 1:D:627:THR:HG22 | 1:P:429:HIS:CE1 | 2.53 | 0.43 |
| 1:E:248:TRP:HB3 | 1:E:373:PHE:CZ | 2.54 | 0.43 |
| 1:E:487:ARG:HD2 | 1:F:583:ALA:O | 2.18 | 0.43 |
| 1:F:522:PRO:O | 1:F:541:GLY:HA2 | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:340:THR:O | 1:G:407:ARG:CZ | 2.67 | 0.43 |
| 1:H:627:THR:HG22 | 1:Y:429:HIS:CE1 | 2.53 | 0.43 |
| 1:I:522:PRO:O | 1:I:541:GLY:HA2 | 2.18 | 0.43 |
| 1:J:429:HIS:HD2 | 1:J:610:GLN:OE1 | 1.94 | 0.43 |
| 1:L:220:ASP:OD1 | 1:L:220:ASP:N | 2.50 | 0.43 |
| 1:L:522:PRO:O | 1:L:541:GLY:HA2 | 2.18 | 0.43 |
| 1:M:609:TRP:CD1 | 1:M:609:TRP:O | 2.70 | 0.43 |
| 1:O:609:TRP:CD1 | 1:O:609:TRP:O | 2.71 | 0.43 |
| 1:S:342:THR:HG22 | 1:S:407:ARG:CG | 2.47 | 0.43 |
| 1:T:452:GLN:HE21 | 1:T:459:GLY:HA3 | 1.84 | 0.43 |
| 1:T:627:THR:HG22 | 1:l:429:HIS:CE1 | 2.53 | 0.43 |
| 1:U:278:TYR:CE2 | 1:U:395:PHE:HD1 | 2.37 | 0.43 |
| 1:V:278:TYR:CE2 | 1:V:395:PHE:HD1 | 2.37 | 0.43 |
| 1:V:473:MET:HB2 | 1:V:473:MET:HE3 | 1.81 | 0.43 |
| 1:Z:453:SER:OG | 1:Z:458:GLN:O | 2.35 | 0.43 |
| 1:c:522:PRO:O | 1:c:541:GLY:HA2 | 2.18 | 0.43 |
| 1:d:290:PHE:O | 1:d:293:HIS:N | 2.47 | 0.43 |
| 1:e:220:ASP:OD1 | 1:e:220:ASP:N | 2.50 | 0.43 |
| 1:e:264:GLY:HA2 | 1:e:387:SER:HB3 | 2.01 | 0.43 |
| 1:f:452:GLN:HE21 | 1:f:459:GLY:HA3 | 1.84 | 0.43 |
| 1:f:554:ASN:HB3 | 1:g:464:LEU:HD23 | 2.00 | 0.43 |
| 1:i:340:THR:O | 1:i:407:ARG:CZ | 2.67 | 0.43 |
| 1:j:290:PHE:HE2 | 1:j:614:VAL:HB | 1.84 | 0.43 |
| 1:m:453:SER:OG | 1:m:458:GLN:O | 2.35 | 0.43 |
| 1:n:220:ASP:OD1 | 1:n:220:ASP:N | 2.50 | 0.43 |
| 1:n:402:PRO:CG | 1:r:232:ASP:HB3 | 2.46 | 0.43 |
| 1:o:264:GLY:HA2 | 1:o:387:SER:HB3 | 2.01 | 0.43 |
| 1:r:426:SER:O | 1:r:732:ARG:HA | 2.18 | 0.43 |
| 1:t:402:PRO:CG | 1:y:232:ASP:HB3 | 2.49 | 0.43 |
| 1:w:329:ASN:O | 1:w:332:THR:OG1 | 2.30 | 0.43 |
| 1:y:278:TYR:CE2 | 1:y:395:PHE:HD1 | 2.37 | 0.43 |
| 1:y:452:GLN:HE21 | 1:y:459:GLY:HA3 | 1.84 | 0.43 |
| 1:y:473:MET:HB2 | 1:y:473:MET:HE3 | 1.81 | 0.43 |
| 1:z:429:HIS:CE1 | 1:1:627:THR:HG22 | 2.53 | 0.43 |
| 1:z:609:TRP:NE1 | 1:1:629:GLY:CA | 2.58 | 0.43 |
| 1:2:290:PHE:O | 1:2:293:HIS:N | 2.47 | 0.43 |
| 1:3:487:ARG:HD2 | 1:4:583:ALA:O | 2.19 | 0.43 |
| 1:7:248:TRP:HB3 | 1:7:373:PHE:CZ | 2.54 | 0.43 |
| 1:7:522:PRO:O | 1:7:541:GLY:HA2 | 2.18 | 0.43 |
| 1:A:264:GLY:HA2 | 1:A:387:SER:HB3 | 2.01 | 0.43 |
| 1:B:429:HIS:HD2 | 1:B:610:GLN:OE1 | 1.94 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:342:THR:HG22 | 1:C:407:ARG:CG | 2.47 | 0.43 |
| 1:D:340:THR:O | 1:D:407:ARG:CZ | 2.67 | 0.43 |
| 1:G:434:ASP:OD1 | 1:G:434:ASP:N | 2.41 | 0.43 |
| 1:H:264:GLY:HA2 | 1:H:387:SER:HB3 | 2.01 | 0.43 |
| 1:I:453:SER:OG | 1:I:458:GLN:O | 2.35 | 0.43 |
| 1:I:609:TRP:CD1 | 1:I:609:TRP:O | 2.71 | 0.43 |
| 1:J:609:TRP:CD1 | 1:J:609:TRP:O | 2.70 | 0.43 |
| 1:K:452:GLN:HE21 | 1:K:459:GLY:HA3 | 1.84 | 0.43 |
| 1:N:248:TRP:HB3 | 1:N:373:PHE:CZ | 2.54 | 0.43 |
| 1:O:264:GLY:HA2 | 1:O:387:SER:HB3 | 2.01 | 0.43 |
| 1:O:554:ASN:HB3 | 1:n:464:LEU:HD23 | 2.00 | 0.43 |
| 1:T:278:TYR:CE2 | 1:T:395:PHE:HD1 | 2.37 | 0.43 |
| 1:W:278:TYR:CE2 | 1:W:395:PHE:HD1 | 2.37 | 0.43 |
| 1:X:248:TRP:HB3 | 1:X:373:PHE:CZ | 2.54 | 0.43 |
| 1:X:340:THR:O | 1:X:407:ARG:NE | 2.52 | 0.43 |
| 1:Y:278:TYR:CE2 | 1:Y:395:PHE:HD1 | 2.37 | 0.43 |
| 1:Y:426:SER:O | 1:Y:732:ARG:HA | 2.18 | 0.43 |
| 1:Z:522:PRO:O | 1:Z:541:GLY:HA2 | 2.18 | 0.43 |
| 1:a:248:TRP:HB3 | 1:a:373:PHE:CZ | 2.54 | 0.43 |
| 1:a:278:TYR:CE2 | 1:a:395:PHE:HD1 | 2.37 | 0.43 |
| 1:c:453:SER:OG | 1:c:458:GLN:O | 2.35 | 0.43 |
| 1:e:232:ASP:HB3 | 1:h:402:PRO:CG | 2.46 | 0.43 |
| 1:e:329:ASN:O | 1:e:332:THR:OG1 | 2.31 | 0.43 |
| 1:f:487:ARG:HD2 | 1:g:583:ALA:O | 2.19 | 0.43 |
| 1:g:340:THR:HB | 1:k:322:GLN:HB3 | 2.01 | 0.43 |
| 1:i:278:TYR:CE2 | 1:i:395:PHE:HD1 | 2.37 | 0.43 |
| 1:i:487:ARG:HD2 | 1:k:583:ALA:O | 2.18 | 0.43 |
| 1:j:429:HIS:CE1 | 1:k:627:THR:HG22 | 2.53 | 0.43 |
| 1:j:452:GLN:HE21 | 1:j:459:GLY:HA3 | 1.84 | 0.43 |
| 1:l:278:TYR:CE2 | 1:l:395:PHE:HD1 | 2.37 | 0.43 |
| 1:o:522:PRO:O | 1:o:541:GLY:HA2 | 2.18 | 0.43 |
| 1:p:290:PHE:O | 1:p:293:HIS:N | 2.47 | 0.43 |
| 1:q:426:SER:O | 1:q:732:ARG:HA | 2.18 | 0.43 |
| 1:s:264:GLY:HA2 | 1:s:387:SER:HB3 | 2.01 | 0.43 |
| 1:t:586:LEU:HD21 | 1:u:490:ARG:NH1 | 2.32 | 0.43 |
| 1:u:342:THR:HG22 | 1:u:407:ARG:CG | 2.47 | 0.43 |
| 1:v:522:PRO:O | 1:v:541:GLY:HA2 | 2.18 | 0.43 |
| 1:w:264:GLY:HA2 | 1:w:387:SER:HB3 | 2.01 | 0.43 |
| 1:w:452:GLN:HE21 | 1:w:459:GLY:HA3 | 1.84 | 0.43 |
| 1:x:248:TRP:HB3 | 1:x:373:PHE:CZ | 2.54 | 0.43 |
| 1:y:329:ASN:CA | 1:y:330:GLU:OE1 | 2.65 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:y:340:THR:O | 1:y:407:ARG:NE | 2.52 | 0.43 |
| 1:z:290:PHE:O | 1:z:293:HIS:N | 2.47 | 0.43 |
| 1:1:278:TYR:CE2 | 1:1:395:PHE:HD1 | 2.37 | 0.43 |
| 1:2:297:ARG:HG3 | 1:2:301:ARG:NH1 | 2.34 | 0.43 |
| 1:2:341:SER:HB3 | 1:2:675:GLN:NE2 | 2.32 | 0.43 |
| 1:3:248:TRP:HB3 | 1:3:373:PHE:CZ | 2.54 | 0.43 |
| 1:3:264:GLY:HA2 | 1:3:387:SER:HB3 | 2.01 | 0.43 |
| 1:4:220:ASP:OD1 | 1:4:220:ASP:N | 2.50 | 0.43 |
| 1:4:278:TYR:CE2 | 1:4:395:PHE:HD1 | 2.37 | 0.43 |
| 1:6:522:PRO:O | 1:6:541:GLY:HA2 | 2.18 | 0.43 |
| 1:A:297:ARG:HG3 | 1:A:301:ARG:NH1 | 2.34 | 0.43 |
| 1:A:340:THR:O | 1:A:407:ARG:NE | 2.52 | 0.43 |
| 1:B:435:ARG:HD3 | 1:B:435:ARG:HA | 1.79 | 0.43 |
| 1:D:452:GLN:HE21 | 1:D:459:GLY:HA3 | 1.84 | 0.43 |
| 1:D:490:ARG:CZ | 1:P:586:LEU:HD21 | 2.49 | 0.43 |
| 1:E:340:THR:O | 1:E:407:ARG:NE | 2.52 | 0.43 |
| 1:G:290:PHE:O | 1:G:293:HIS:N | 2.47 | 0.43 |
| 1:H:290:PHE:O | 1:H:293:HIS:N | 2.47 | 0.43 |
| 1:H:340:THR:O | 1:H:407:ARG:CZ | 2.67 | 0.43 |
| 1:I:278:TYR:CE2 | 1:I:395:PHE:HD1 | 2.37 | 0.43 |
| 1:K:340:THR:O | 1:K:407:ARG:CZ | 2.67 | 0.43 |
| 1:L:342:THR:HG22 | 1:L:407:ARG:CG | 2.47 | 0.43 |
| 1:M:473:MET:HE3 | 1:M:473:MET:HB2 | 1.81 | 0.43 |
| 1:N:340:THR:O | 1:N:407:ARG:NE | 2.52 | 0.43 |
| 1:N:426:SER:OG | 1:N:731:THR:O | 2.31 | 0.43 |
| 1:P:290:PHE:O | 1:P:293:HIS:N | 2.47 | 0.43 |
| 1:Q:329:ASN:CA | 1:Q:330:GLU:OE1 | 2.65 | 0.43 |
| 1:Q:568:ILE:HD12 | 1:Q:572:ASN:HD22 | 1.84 | 0.43 |
| 1:R:429:HIS:HD2 | 1:R:610:GLN:OE1 | 1.94 | 0.43 |
| 1:S:297:ARG:HG3 | 1:S:301:ARG:NH1 | 2.34 | 0.43 |
| 1:T:297:ARG:HG3 | 1:T:301:ARG:NH1 | 2.34 | 0.43 |
| 1:T:340:THR:O | 1:T:407:ARG:CZ | 2.67 | 0.43 |
| 1:V:329:ASN:CA | 1:V:330:GLU:OE1 | 2.65 | 0.43 |
| 1:V:340:THR:HB | 1:W:322:GLN:HB3 | 2.00 | 0.43 |
| 1:V:340:THR:O | 1:V:407:ARG:NE | 2.52 | 0.43 |
| 1:V:452:GLN:HE21 | 1:V:459:GLY:HA3 | 1.84 | 0.43 |
| 1:Y:232:ASP:HB3 | 1:4:402:PRO:CG | 2.46 | 0.43 |
| 1:a:297:ARG:HG3 | 1:a:301:ARG:NH1 | 2.34 | 0.43 |
| 1:b:429:HIS:HD2 | 1:b:610:GLN:OE1 | 1.94 | 0.43 |
| 1:c:278:TYR:CE2 | 1:c:395:PHE:HD1 | 2.37 | 0.43 |
| 1:d:297:ARG:HG3 | 1:d:301:ARG:NH1 | 2.34 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:d:341:SER:HB3 | 1:d:675:GLN:NE2 | 2.32 | 0.43 |
| 1:e:452:GLN:HE21 | 1:e:459:GLY:HA3 | 1.84 | 0.43 |
| 1:g:278:TYR:CE2 | 1:g:395:PHE:HD1 | 2.37 | 0.43 |
| 1:g:487:ARG:HD2 | 1:h:583:ALA:O | 2.18 | 0.43 |
| 1:h:322:GLN:HB3 | 1:i:340:THR:HB | 2.01 | 0.43 |
| 1:i:464:LEU:HD23 | 1:j:554:ASN:HB3 | 2.00 | 0.43 |
| 1:l:248:TRP:HB3 | 1:l:373:PHE:CZ | 2.54 | 0.43 |
| 1:l:452:GLN:HE21 | 1:l:459:GLY:HA3 | 1.84 | 0.43 |
| 1:m:426:SER:OG | 1:m:731:THR:O | 2.30 | 0.43 |
| 1:n:278:TYR:CE2 | 1:n:395:PHE:HD1 | 2.37 | 0.43 |
| 1:n:340:THR:O | 1:n:407:ARG:CZ | 2.67 | 0.43 |
| 1:o:340:THR:O | 1:o:407:ARG:NE | 2.52 | 0.43 |
| 1:q:278:TYR:CE2 | 1:q:395:PHE:HD1 | 2.37 | 0.43 |
| 1:q:342:THR:HG22 | 1:q:407:ARG:CG | 2.47 | 0.43 |
| 1:q:487:ARG:HD2 | 1:s:583:ALA:O | 2.19 | 0.43 |
| 1:r:278:TYR:CE2 | 1:r:395:PHE:HD1 | 2.37 | 0.43 |
| 1:s:278:TYR:CE2 | 1:s:395:PHE:HD1 | 2.37 | 0.43 |
| 1:t:429:HIS:HD2 | 1:t:610:GLN:OE1 | 1.94 | 0.43 |
| 1:v:278:TYR:CE2 | 1:v:395:PHE:HD1 | 2.37 | 0.43 |
| 1:x:340:THR:O | 1:x:407:ARG:NE | 2.52 | 0.43 |
| 1:z:452:GLN:HE21 | 1:z:459:GLY:HA3 | 1.84 | 0.43 |
| 1:1:297:ARG:HG3 | 1:1:301:ARG:NH1 | 2.34 | 0.43 |
| 1:3:342:THR:HG22 | 1:3:407:ARG:CG | 2.47 | 0.43 |
| 1:3:554:ASN:HB3 | 1:4:464:LEU:HD23 | 2.00 | 0.43 |
| 1:4:341:SER:HB3 | 1:4:675:GLN:NE2 | 2.32 | 0.43 |
| 1:6:583:ALA:O | 1:7:487:ARG:HD2 | 2.18 | 0.43 |
| 1:8:568:ILE:HD12 | 1:8:572:ASN:HD22 | 1.84 | 0.43 |
| 1:B:568:ILE:HD12 | 1:B:572:ASN:HD22 | 1.84 | 0.43 |
| 1:C:473:MET:HE3 | 1:C:473:MET:HB2 | 1.81 | 0.43 |
| 1:E:297:ARG:HG3 | 1:E:301:ARG:NH1 | 2.34 | 0.43 |
| 1:F:340:THR:O | 1:F:407:ARG:NE | 2.52 | 0.43 |
| 1:G:278:TYR:CE2 | 1:G:395:PHE:HD1 | 2.37 | 0.43 |
| 1:H:248:TRP:HB3 | 1:H:373:PHE:CZ | 2.54 | 0.43 |
| 1:H:278:TYR:CE2 | 1:H:395:PHE:HD1 | 2.37 | 0.43 |
| 1:H:583:ALA:O | 1:W:487:ARG:HD2 | 2.19 | 0.43 |
| 1:I:248:TRP:HB3 | 1:I:373:PHE:CZ | 2.54 | 0.43 |
| 1:I:340:THR:O | 1:I:407:ARG:CZ | 2.67 | 0.43 |
| 1:J:473:MET:HE3 | 1:J:473:MET:HB2 | 1.81 | 0.43 |
| 1:K:490:ARG:CZ | 1:8:586:LEU:HD21 | 2.49 | 0.43 |
| 1:M:435:ARG:HD3 | 1:M:435:ARG:HA | 1.79 | 0.43 |
| 1:N:232:ASP:HB3 | 1:m:402:PRO:CG | 2.46 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:297:ARG:HG3 | 1:N:301:ARG:NH1 | 2.34 | 0.43 |
| 1:O:248:TRP:HB3 | 1:O:373:PHE:CZ | 2.54 | 0.43 |
| 1:O:340:THR:O | 1:O:407:ARG:NE | 2.52 | 0.43 |
| 1:R:583:ALA:O | 1:S:487:ARG:HD2 | 2.18 | 0.43 |
| 1:T:329:ASN:CA | 1:T:330:GLU:OE1 | 2.65 | 0.43 |
| 1:T:340:THR:O | 1:T:407:ARG:NE | 2.52 | 0.43 |
| 1:T:464:LEU:HD23 | 1:d:554:ASN:HB3 | 2.00 | 0.43 |
| 1:T:554:ASN:HB3 | 1:l:464:LEU:HD23 | 2.00 | 0.43 |
| 1:T:629:GLY:CA | 1:l:609:TRP:NE1 | 2.58 | 0.43 |
| 1:U:568:ILE:HD12 | 1:U:572:ASN:HD22 | 1.84 | 0.43 |
| 1:V:487:ARG:HD2 | 1:X:583:ALA:O | 2.19 | 0.43 |
| 1:W:248:TRP:HB3 | 1:W:373:PHE:CZ | 2.54 | 0.43 |
| 1:W:342:THR:HG22 | 1:W:407:ARG:CG | 2.47 | 0.43 |
| 1:Z:248:TRP:HB3 | 1:Z:373:PHE:CZ | 2.54 | 0.43 |
| 1:Z:736:ARG:NH2 | 1:4:626:HIS:CD2 | 2.79 | 0.43 |
| 1:a:340:THR:O | 1:a:407:ARG:NE | 2.52 | 0.43 |
| 1:a:568:ILE:HD12 | 1:a:572:ASN:HD22 | 1.84 | 0.43 |
| 1:b:248:TRP:HB3 | 1:b:373:PHE:CZ | 2.54 | 0.43 |
| 1:b:297:ARG:HG3 | 1:b:301:ARG:NH1 | 2.34 | 0.43 |
| 1:b:452:GLN:HE21 | 1:b:459:GLY:HA3 | 1.84 | 0.43 |
| 1:b:568:ILE:HD12 | 1:b:572:ASN:HD22 | 1.84 | 0.43 |
| 1:c:248:TRP:HB3 | 1:c:373:PHE:CZ | 2.54 | 0.43 |
| 1:c:340:THR:O | 1:c:407:ARG:CZ | 2.67 | 0.43 |
| 1:c:583:ALA:O | 1:o:487:ARG:HD2 | 2.18 | 0.43 |
| 1:e:585:ASN:OD1 | 1:e:594:ILE:N | 2.45 | 0.43 |
| 1:f:429:HIS:CE1 | 1:h:627:THR:HG22 | 2.53 | 0.43 |
| 1:f:568:ILE:HD12 | 1:f:572:ASN:HD22 | 1.84 | 0.43 |
| 1:g:340:THR:O | 1:g:407:ARG:NE | 2.52 | 0.43 |
| 1:g:554:ASN:HB3 | 1:h:464:LEU:HD23 | 2.00 | 0.43 |
| 1:h:342:THR:HG22 | 1:h:407:ARG:CG | 2.47 | 0.43 |
| 1:i:554:ASN:HB3 | 1:k:464:LEU:HD23 | 2.00 | 0.43 |
| 1:j:568:ILE:HD12 | 1:j:572:ASN:HD22 | 1.84 | 0.43 |
| 1:k:568:ILE:HD12 | 1:k:572:ASN:HD22 | 1.84 | 0.43 |
| 1:m:248:TRP:HB3 | 1:m:373:PHE:CZ | 2.54 | 0.43 |
| 1:m:522:PRO:O | 1:m:541:GLY:HA2 | 2.18 | 0.43 |
| 1:m:585:ASN:OD1 | 1:m:594:ILE:N | 2.45 | 0.43 |
| 1:o:297:ARG:HG3 | 1:o:301:ARG:NH1 | 2.34 | 0.43 |
| 1:p:278:TYR:CE2 | 1:p:395:PHE:HD1 | 2.37 | 0.43 |
| 1:p:435:ARG:HD3 | 1:p:435:ARG:HA | 1.79 | 0.43 |
| 1:q:248:TRP:HB3 | 1:q:373:PHE:CZ | 2.54 | 0.43 |
| 1:q:264:GLY:HA2 | 1:q:387:SER:HB3 | 2.01 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:q:464:LEU:HD23 | 1:r:554:ASN:HB3 | 2.00 | 0.43 |
| 1:s:248:TRP:HB3 | 1:s:373:PHE:CZ | 2.54 | 0.43 |
| 1:s:340:THR:O | 1:s:407:ARG:CZ | 2.67 | 0.43 |
| 1:u:297:ARG:HG3 | 1:u:301:ARG:NH1 | 2.34 | 0.43 |
| 1:v:568:ILE:HD12 | 1:v:572:ASN:HD22 | 1.84 | 0.43 |
| 1:w:585:ASN:OD1 | 1:w:594:ILE:N | 2.45 | 0.43 |
| 1:w:627:THR:HG22 | 1:y:429:HIS:CE1 | 2.53 | 0.43 |
| 1:x:429:HIS:CE1 | 1:y:627:THR:HG22 | 2.54 | 0.43 |
| 1:x:522:PRO:O | 1:x:541:GLY:HA2 | 2.18 | 0.43 |
| 1:x:583:ALA:O | 1:y:487:ARG:HD2 | 2.19 | 0.43 |
| 1:z:248:TRP:HB3 | 1:z:373:PHE:CZ | 2.54 | 0.43 |
| 1:z:278:TYR:CE2 | 1:z:395:PHE:HD1 | 2.37 | 0.43 |
| 1:1:464:LEU:HD23 | 1:2:554:ASN:HB3 | 2.00 | 0.43 |
| 1:1:527:ALA:O | 1:1:575:ALA:N | 2.45 | 0.43 |
| 1:4:340:THR:O | 1:4:407:ARG:CZ | 2.67 | 0.43 |
| 1:5:329:ASN:CA | 1:5:330:GLU:OE1 | 2.65 | 0.43 |
| 1:5:568:ILE:HD12 | 1:5:572:ASN:HD22 | 1.84 | 0.43 |
| 1:6:340:THR:O | 1:6:407:ARG:NE | 2.52 | 0.43 |
| 1:7:297:ARG:HG3 | 1:7:301:ARG:NH1 | 2.34 | 0.43 |
| 1:7:329:ASN:CA | 1:7:330:GLU:OE1 | 2.65 | 0.43 |
| 1:7:452:GLN:HE21 | 1:7:459:GLY:HA3 | 1.84 | 0.43 |
| 1:8:220:ASP:OD1 | 1:8:220:ASP:N | 2.50 | 0.43 |
| 1:A:583:ALA:O | 1:G:487:ARG:HD2 | 2.18 | 0.43 |
| 1:B:248:TRP:HB3 | 1:B:373:PHE:CZ | 2.54 | 0.43 |
| 1:B:264:GLY:HA2 | 1:B:387:SER:HB3 | 2.01 | 0.43 |
| 1:B:297:ARG:HG3 | 1:B:301:ARG:NH1 | 2.34 | 0.43 |
| 1:B:452:GLN:HE21 | 1:B:459:GLY:HA3 | 1.84 | 0.43 |
| 1:D:426:SER:O | 1:D:732:ARG:HA | 2.18 | 0.43 |
| 1:D:522:PRO:O | 1:D:541:GLY:HA2 | 2.18 | 0.43 |
| 1:E:329:ASN:CA | 1:E:330:GLU:OE1 | 2.65 | 0.43 |
| 1:E:452:GLN:HE21 | 1:E:459:GLY:HA3 | 1.84 | 0.43 |
| 1:F:248:TRP:HB3 | 1:F:373:PHE:CZ | 2.54 | 0.43 |
| 1:F:264:GLY:HA2 | 1:F:387:SER:HB3 | 2.01 | 0.43 |
| 1:F:278:TYR:CE2 | 1:F:395:PHE:HD1 | 2.37 | 0.43 |
| 1:F:297:ARG:HG3 | 1:F:301:ARG:NH1 | 2.34 | 0.43 |
| 1:F:568:ILE:HD12 | 1:F:572:ASN:HD22 | 1.84 | 0.43 |
| 1:G:264:GLY:HA2 | 1:G:387:SER:HB3 | 2.01 | 0.43 |
| 1:G:342:THR:HG22 | 1:G:407:ARG:CG | 2.47 | 0.43 |
| 1:H:329:ASN:O | 1:H:332:THR:OG1 | 2.31 | 0.43 |
| 1:J:248:TRP:HB3 | 1:J:373:PHE:CZ | 2.54 | 0.43 |
| 1:J:297:ARG:HG3 | 1:J:301:ARG:NH1 | 2.34 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:322:GLN:HB3 | 1:a:340:THR:HB | 2.01 | 0.43 |
| 1:J:426:SER:O | 1:J:732:ARG:HA | 2.18 | 0.43 |
| 1:J:435:ARG:HD3 | 1:J:435:ARG:HA | 1.79 | 0.43 |
| 1:J:568:ILE:HD12 | 1:J:572:ASN:HD22 | 1.84 | 0.43 |
| 1:K:264:GLY:HA2 | 1:K:387:SER:HB3 | 2.01 | 0.43 |
| 1:K:522:PRO:O | 1:K:541:GLY:HA2 | 2.18 | 0.43 |
| 1:L:264:GLY:HA2 | 1:L:387:SER:HB3 | 2.01 | 0.43 |
| 1:L:340:THR:O | 1:L:407:ARG:NE | 2.52 | 0.43 |
| 1:L:473:MET:HE3 | 1:L:473:MET:HB2 | 1.81 | 0.43 |
| 1:M:248:TRP:HB3 | 1:M:373:PHE:CZ | 2.54 | 0.43 |
| 1:M:297:ARG:HG3 | 1:M:301:ARG:NH1 | 2.34 | 0.43 |
| 1:N:568:ILE:HD12 | 1:N:572:ASN:HD22 | 1.84 | 0.43 |
| 1:N:583:ALA:O | 1:P:487:ARG:HD2 | 2.19 | 0.43 |
| 1:O:340:THR:O | 1:O:407:ARG:CZ | 2.67 | 0.43 |
| 1:O:342:THR:HG22 | 1:O:407:ARG:CG | 2.47 | 0.43 |
| 1:O:473:MET:HB2 | 1:O:473:MET:HE3 | 1.81 | 0.43 |
| 1:O:511:TYR:HD2 | 1:O:520:VAL:HG22 | 1.84 | 0.43 |
| 1:O:522:PRO:O | 1:O:541:GLY:HA2 | 2.18 | 0.43 |
| 1:P:220:ASP:OD1 | 1:P:220:ASP:N | 2.50 | 0.43 |
| 1:P:248:TRP:HB3 | 1:P:373:PHE:CZ | 2.54 | 0.43 |
| 1:P:473:MET:HE3 | 1:P:473:MET:HB2 | 1.81 | 0.43 |
| 1:P:522:PRO:O | 1:P:541:GLY:HA2 | 2.18 | 0.43 |
| 1:Q:264:GLY:HA2 | 1:Q:387:SER:HB3 | 2.01 | 0.43 |
| 1:Q:340:THR:O | 1:Q:407:ARG:NE | 2.52 | 0.43 |
| 1:R:340:THR:O | 1:R:407:ARG:NE | 2.52 | 0.43 |
| 1:S:522:PRO:O | 1:S:541:GLY:HA2 | 2.18 | 0.43 |
| 1:S:583:ALA:O | 1:U:487:ARG:HD2 | 2.18 | 0.43 |
| 1:T:341:SER:HB3 | 1:T:675:GLN:NE2 | 2.32 | 0.43 |
| 1:V:297:ARG:HG3 | 1:V:301:ARG:NH1 | 2.34 | 0.43 |
| 1:W:464:LEU:HD23 | 1:Y:554:ASN:HB3 | 2.00 | 0.43 |
| 1:X:522:PRO:O | 1:X:541:GLY:HA2 | 2.18 | 0.43 |
| 1:Y:290:PHE:HE2 | 1:Y:614:VAL:HB | 1.84 | 0.43 |
| 1:b:264:GLY:HA2 | 1:b:387:SER:HB3 | 2.01 | 0.43 |
| 1:b:342:THR:HG22 | 1:b:407:ARG:CG | 2.47 | 0.43 |
| 1:b:473:MET:HE3 | 1:b:473:MET:HB2 | 1.81 | 0.43 |
| 1:e:297:ARG:HG3 | 1:e:301:ARG:NH1 | 2.34 | 0.43 |
| 1:e:522:PRO:O | 1:e:541:GLY:HA2 | 2.18 | 0.43 |
| 1:f:736:ARG:NH2 | 1:h:626:HIS:CD2 | 2.79 | 0.43 |
| 1:i:340:THR:O | 1:i:407:ARG:NE | 2.52 | 0.43 |
| 1:k:342:THR:HG22 | 1:k:407:ARG:CG | 2.47 | 0.43 |
| 1:l:340:THR:O | 1:l:407:ARG:CZ | 2.67 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:434:ASP:N | 1:m:434:ASP:OD1 | 2.41 | 0.43 |
| 1:m:736:ARG:NH2 | 1:n:626:HIS:CD2 | 2.79 | 0.43 |
| 1:p:264:GLY:HA2 | 1:p:387:SER:HB3 | 2.01 | 0.43 |
| 1:p:522:PRO:O | 1:p:541:GLY:HA2 | 2.18 | 0.43 |
| 1:r:290:PHE:HE2 | 1:r:614:VAL:HB | 1.84 | 0.43 |
| 1:r:340:THR:O | 1:r:407:ARG:CZ | 2.67 | 0.43 |
| 1:r:522:PRO:O | 1:r:541:GLY:HA2 | 2.18 | 0.43 |
| 1:t:340:THR:O | 1:t:407:ARG:NE | 2.52 | 0.43 |
| 1:u:426:SER:OG | 1:u:731:THR:O | 2.31 | 0.43 |
| 1:v:264:GLY:HA2 | 1:v:387:SER:HB3 | 2.01 | 0.43 |
| 1:w:522:PRO:O | 1:w:541:GLY:HA2 | 2.18 | 0.43 |
| 1:z:464:LEU:HD23 | 1:1:554:ASN:HB3 | 2.00 | 0.43 |
| 1:1:329:ASN:CA | 1:1:330:GLU:OE1 | 2.65 | 0.43 |
| 1:1:340:THR:O | 1:1:407:ARG:CZ | 2.67 | 0.43 |
| 1:1:340:THR:O | 1:1:407:ARG:NE | 2.52 | 0.43 |
| 1:2:278:TYR:CE2 | 1:2:395:PHE:HD1 | 2.37 | 0.43 |
| 1:3:340:THR:O | 1:3:407:ARG:NE | 2.52 | 0.43 |
| 1:3:511:TYR:HD2 | 1:3:520:VAL:HG22 | 1.84 | 0.43 |
| 1:3:522:PRO:O | 1:3:541:GLY:HA2 | 2.18 | 0.43 |
| 1:4:340:THR:O | 1:4:407:ARG:NE | 2.52 | 0.43 |
| 1:5:264:GLY:HA2 | 1:5:387:SER:HB3 | 2.01 | 0.43 |
| 1:5:340:THR:O | 1:5:407:ARG:NE | 2.52 | 0.43 |
| 1:6:248:TRP:HB3 | 1:6:373:PHE:CZ | 2.54 | 0.43 |
| 1:6:264:GLY:HA2 | 1:6:387:SER:HB3 | 2.01 | 0.43 |
| 1:6:297:ARG:HG3 | 1:6:301:ARG:NH1 | 2.34 | 0.43 |
| 1:6:568:ILE:HD12 | 1:6:572:ASN:HD22 | 1.84 | 0.43 |
| 1:7:340:THR:O | 1:7:407:ARG:NE | 2.52 | 0.43 |
| 1:8:473:MET:HE3 | 1:8:473:MET:HB2 | 1.81 | 0.43 |
| 1:8:522:PRO:O | 1:8:541:GLY:HA2 | 2.18 | 0.43 |
| 1:8:585:ASN:OD1 | 1:8:594:ILE:N | 2.45 | 0.43 |
| 1:A:340:THR:O | 1:A:407:ARG:CZ | 2.67 | 0.42 |
| 1:A:487:ARG:HD2 | 1:I:583:ALA:O | 2.19 | 0.42 |
| 1:A:609:TRP:NE1 | 1:G:629:GLY:CA | 2.58 | 0.42 |
| 1:C:264:GLY:HA2 | 1:C:387:SER:HB3 | 2.01 | 0.42 |
| 1:C:329:ASN:CA | 1:C:330:GLU:OE1 | 2.65 | 0.42 |
| 1:D:568:ILE:HD12 | 1:D:572:ASN:HD22 | 1.84 | 0.42 |
| 1:F:452:GLN:HE21 | 1:F:459:GLY:HA3 | 1.84 | 0.42 |
| 1:G:322:GLN:HB3 | 1:W:340:THR:HB | 2.01 | 0.42 |
| 1:G:522:PRO:O | 1:G:541:GLY:HA2 | 2.18 | 0.42 |
| 1:I:297:ARG:HG3 | 1:I:301:ARG:NH1 | 2.34 | 0.42 |
| 1:J:340:THR:O | 1:J:407:ARG:NE | 2.52 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:609:TRP:CD1 | 1:L:629:GLY:CA | 2.85 | 0.42 |
| 1:K:248:TRP:HB3 | 1:K:373:PHE:CZ | 2.54 | 0.42 |
| 1:K:568:ILE:HD12 | 1:K:572:ASN:HD22 | 1.84 | 0.42 |
| 1:L:329:ASN:CA | 1:L:330:GLU:OE1 | 2.65 | 0.42 |
| 1:M:340:THR:O | 1:M:407:ARG:NE | 2.52 | 0.42 |
| 1:M:426:SER:O | 1:M:732:ARG:HA | 2.18 | 0.42 |
| 1:M:568:ILE:HD12 | 1:M:572:ASN:HD22 | 1.84 | 0.42 |
| 1:N:340:THR:O | 1:N:407:ARG:CZ | 2.67 | 0.42 |
| 1:O:583:ALA:O | 1:m:487:ARG:HD2 | 2.18 | 0.42 |
| 1:P:568:ILE:HD12 | 1:P:572:ASN:HD22 | 1.84 | 0.42 |
| 1:P:585:ASN:OD1 | 1:P:594:ILE:N | 2.45 | 0.42 |
| 1:S:426:SER:OG | 1:S:731:THR:O | 2.31 | 0.42 |
| 1:U:264:GLY:HA2 | 1:U:387:SER:HB3 | 2.01 | 0.42 |
| 1:V:264:GLY:HA2 | 1:V:387:SER:HB3 | 2.01 | 0.42 |
| 1:W:264:GLY:HA2 | 1:W:387:SER:HB3 | 2.01 | 0.42 |
| 1:Y:340:THR:O | 1:Y:407:ARG:CZ | 2.67 | 0.42 |
| 1:Z:402:PRO:CG | 1:a:232:ASP:HB3 | 2.46 | 0.42 |
| 1:Z:487:ARG:HD2 | 1:3:583:ALA:O | 2.18 | 0.42 |
| 1:Z:585:ASN:OD1 | 1:Z:594:ILE:N | 2.45 | 0.42 |
| 1:a:340:THR:O | 1:a:407:ARG:CZ | 2.67 | 0.42 |
| 1:a:341:SER:HB3 | 1:a:675:GLN:NE2 | 2.32 | 0.42 |
| 1:a:583:ALA:O | 1:8:487:ARG:HD2 | 2.19 | 0.42 |
| 1:c:297:ARG:HG3 | 1:c:301:ARG:NH1 | 2.34 | 0.42 |
| 1:c:340:THR:O | 1:c:407:ARG:NE | 2.52 | 0.42 |
| 1:d:278:TYR:CE2 | 1:d:395:PHE:HD1 | 2.37 | 0.42 |
| 1:e:568:ILE:HD12 | 1:e:572:ASN:HD22 | 1.84 | 0.42 |
| 1:h:568:ILE:HD12 | 1:h:572:ASN:HD22 | 1.84 | 0.42 |
| 1:i:297:ARG:HG3 | 1:i:301:ARG:NH1 | 2.34 | 0.42 |
| 1:i:511:TYR:HD2 | 1:i:520:VAL:HG22 | 1.84 | 0.42 |
| 1:k:297:ARG:HG3 | 1:k:301:ARG:NH1 | 2.34 | 0.42 |
| 1:n:297:ARG:HG3 | 1:n:301:ARG:NH1 | 2.34 | 0.42 |
| 1:n:340:THR:O | 1:n:407:ARG:NE | 2.52 | 0.42 |
| 1:n:341:SER:HB3 | 1:n:675:GLN:NE2 | 2.32 | 0.42 |
| 1:o:340:THR:O | 1:o:407:ARG:CZ | 2.67 | 0.42 |
| 1:p:342:THR:HG22 | 1:p:407:ARG:CG | 2.47 | 0.42 |
| 1:q:583:ALA:O | 1:r:487:ARG:HD2 | 2.18 | 0.42 |
| 1:r:297:ARG:HG3 | 1:r:301:ARG:NH1 | 2.34 | 0.42 |
| 1:u:522:PRO:O | 1:u:541:GLY:HA2 | 2.18 | 0.42 |
| 1:u:583:ALA:O | 1:v:487:ARG:HD2 | 2.18 | 0.42 |
| 1:x:290:PHE:O | 1:x:293:HIS:N | 2.47 | 0.42 |
| 1:y:297:ARG:HG3 | 1:y:301:ARG:NH1 | 2.34 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:y:511:TYR:HD2 | 1:y:520:VAL:HG22 | 1.84 | 0.42 |
| 1:z:340:THR:O | 1:z:407:ARG:CZ | 2.67 | 0.42 |
| 1:2:248:TRP:HB3 | 1:2:373:PHE:CZ | 2.54 | 0.42 |
| 1:4:297:ARG:HG3 | 1:4:301:ARG:NH1 | 2.34 | 0.42 |
| 1:7:568:ILE:HD12 | 1:7:572:ASN:HD22 | 1.84 | 0.42 |
| 1:8:290:PHE:O | 1:8:293:HIS:N | 2.47 | 0.42 |
| 1:8:297:ARG:HG3 | 1:8:301:ARG:NH1 | 2.34 | 0.42 |
| 1:A:322:GLN:HB3 | 1:E:340:THR:HB | 2.01 | 0.42 |
| 1:C:340:THR:O | 1:C:407:ARG:NE | 2.52 | 0.42 |
| 1:D:248:TRP:HB3 | 1:D:373:PHE:CZ | 2.54 | 0.42 |
| 1:D:264:GLY:HA2 | 1:D:387:SER:HB3 | 2.01 | 0.42 |
| 1:E:568:ILE:HD12 | 1:E:572:ASN:HD22 | 1.84 | 0.42 |
| 1:E:629:GLY:CA | 1:F:609:TRP:NE1 | 2.58 | 0.42 |
| 1:F:340:THR:O | 1:F:407:ARG:CZ | 2.67 | 0.42 |
| 1:G:511:TYR:HD2 | 1:G:520:VAL:HG22 | 1.84 | 0.42 |
| 1:I:340:THR:O | 1:I:407:ARG:NE | 2.52 | 0.42 |
| 1:K:426:SER:O | 1:K:732:ARG:HA | 2.18 | 0.42 |
| 1:M:322:GLN:HB3 | 1:N:340:THR:HB | 2.01 | 0.42 |
| 1:N:511:TYR:HD2 | 1:N:520:VAL:HG22 | 1.84 | 0.42 |
| 1:P:297:ARG:HG3 | 1:P:301:ARG:NH1 | 2.34 | 0.42 |
| 1:Q:297:ARG:HG3 | 1:Q:301:ARG:NH1 | 2.34 | 0.42 |
| 1:S:264:GLY:HA2 | 1:S:387:SER:HB3 | 2.01 | 0.42 |
| 1:S:340:THR:O | 1:S:407:ARG:NE | 2.52 | 0.42 |
| 1:T:487:ARG:HD2 | 1:l:583:ALA:O | 2.18 | 0.42 |
| 1:T:527:ALA:O | 1:T:575:ALA:N | 2.45 | 0.42 |
| 1:V:248:TRP:HB3 | 1:V:373:PHE:CZ | 2.54 | 0.42 |
| 1:V:429:HIS:CE1 | 1:e:627:THR:HG22 | 2.53 | 0.42 |
| 1:W:511:TYR:HD2 | 1:W:520:VAL:HG22 | 1.84 | 0.42 |
| 1:Y:248:TRP:HB3 | 1:Y:373:PHE:CZ | 2.54 | 0.42 |
| 1:Y:297:ARG:HG3 | 1:Y:301:ARG:NH1 | 2.34 | 0.42 |
| 1:Y:522:PRO:O | 1:Y:541:GLY:HA2 | 2.18 | 0.42 |
| 1:a:511:TYR:HD2 | 1:a:520:VAL:HG22 | 1.84 | 0.42 |
| 1:d:248:TRP:HB3 | 1:d:373:PHE:CZ | 2.54 | 0.42 |
| 1:e:278:TYR:CE2 | 1:e:395:PHE:HD1 | 2.37 | 0.42 |
| 1:f:278:TYR:CE2 | 1:f:395:PHE:HD1 | 2.37 | 0.42 |
| 1:g:297:ARG:HG3 | 1:g:301:ARG:NH1 | 2.34 | 0.42 |
| 1:h:232:ASP:HB3 | 1:i:402:PRO:CG | 2.46 | 0.42 |
| 1:h:297:ARG:HG3 | 1:h:301:ARG:NH1 | 2.34 | 0.42 |
| 1:j:322:GLN:CB | 1:x:340:THR:HB | 2.49 | 0.42 |
| 1:k:407:ARG:CD | 1:w:224:SER:O | 2.68 | 0.42 |
| 1:m:290:PHE:O | 1:m:293:HIS:N | 2.47 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:n:340:THR:HB | 1:r:322:GLN:HB3 | 2.01 | 0.42 |
| 1:n:511:TYR:HD2 | 1:n:520:VAL:HG22 | 1.84 | 0.42 |
| 1:q:511:TYR:HD2 | 1:q:520:VAL:HG22 | 1.84 | 0.42 |
| 1:r:264:GLY:HA2 | 1:r:387:SER:HB3 | 2.01 | 0.42 |
| 1:t:583:ALA:O | 1:u:487:ARG:HD2 | 2.18 | 0.42 |
| 1:u:340:THR:O | 1:u:407:ARG:NE | 2.52 | 0.42 |
| 1:v:452:GLN:HE21 | 1:v:459:GLY:HA3 | 1.84 | 0.42 |
| 1:w:278:TYR:CE2 | 1:w:395:PHE:HD1 | 2.37 | 0.42 |
| 1:w:297:ARG:HG3 | 1:w:301:ARG:NH1 | 2.34 | 0.42 |
| 1:y:248:TRP:HB3 | 1:y:373:PHE:CZ | 2.54 | 0.42 |
| 1:y:264:GLY:HA2 | 1:y:387:SER:HB3 | 2.01 | 0.42 |
| 1:1:341:SER:HB3 | 1:1:675:GLN:NE2 | 2.32 | 0.42 |
| 1:1:429:HIS:HD2 | 1:1:610:GLN:OE1 | 1.94 | 0.42 |
| 1:3:340:THR:O | 1:3:407:ARG:CZ | 2.67 | 0.42 |
| 1:3:473:MET:HB2 | 1:3:473:MET:HE3 | 1.81 | 0.42 |
| 1:5:341:SER:HB3 | 1:5:675:GLN:NE2 | 2.32 | 0.42 |
| 1:5:511:TYR:HD2 | 1:5:520:VAL:HG22 | 1.84 | 0.42 |
| 1:6:278:TYR:CE2 | 1:6:395:PHE:HD1 | 2.37 | 0.42 |
| 1:6:340:THR:O | 1:6:407:ARG:CZ | 2.67 | 0.42 |
| 1:7:278:TYR:CE2 | 1:7:395:PHE:HD1 | 2.37 | 0.42 |
| 1:8:248:TRP:HB3 | 1:8:373:PHE:CZ | 2.54 | 0.42 |
| 1:B:278:TYR:CE2 | 1:B:395:PHE:HD1 | 2.37 | 0.42 |
| 1:B:342:THR:HG22 | 1:B:407:ARG:CG | 2.47 | 0.42 |
| 1:E:278:TYR:CE2 | 1:E:395:PHE:HD1 | 2.37 | 0.42 |
| 1:M:629:GLY:CA | 1:b:609:TRP:CD1 | 2.86 | 0.42 |
| 1:O:340:THR:HB | 1:d:322:GLN:HB3 | 2.01 | 0.42 |
| 1:O:568:ILE:HD12 | 1:O:572:ASN:HD22 | 1.84 | 0.42 |
| 1:P:452:GLN:HE21 | 1:P:459:GLY:HA3 | 1.84 | 0.42 |
| 1:Q:511:TYR:HD2 | 1:Q:520:VAL:HG22 | 1.84 | 0.42 |
| 1:R:297:ARG:HG3 | 1:R:301:ARG:NH1 | 2.34 | 0.42 |
| 1:T:568:ILE:HD12 | 1:T:572:ASN:HD22 | 1.84 | 0.42 |
| 1:U:232:ASP:HB3 | 1:e:402:PRO:CG | 2.46 | 0.42 |
| 1:U:452:GLN:HE21 | 1:U:459:GLY:HA3 | 1.84 | 0.42 |
| 1:V:511:TYR:HD2 | 1:V:520:VAL:HG22 | 1.85 | 0.42 |
| 1:W:583:ALA:O | 1:Y:487:ARG:HD2 | 2.18 | 0.42 |
| 1:X:290:PHE:O | 1:X:293:HIS:N | 2.47 | 0.42 |
| 1:Y:322:GLN:HB3 | 1:4:340:THR:HB | 2.01 | 0.42 |
| 1:Z:340:THR:O | 1:Z:407:ARG:CZ | 2.67 | 0.42 |
| 1:Z:434:ASP:N | 1:Z:434:ASP:OD1 | 2.41 | 0.42 |
| 1:Z:452:GLN:HE21 | 1:Z:459:GLY:HA3 | 1.84 | 0.42 |
| 1:Z:568:ILE:HD12 | 1:Z:572:ASN:HD22 | 1.84 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:a:452:GLN:HE21 | 1:a:459:GLY:HA3 | 1.84 | 0.42 |
| 1:b:278:TYR:CE2 | 1:b:395:PHE:HD1 | 2.37 | 0.42 |
| 1:d:522:PRO:O | 1:d:541:GLY:HA2 | 2.18 | 0.42 |
| 1:f:319:PHE:CE1 | 1:f:680:GLN:HB2 | 2.55 | 0.42 |
| 1:g:452:GLN:HE21 | 1:g:459:GLY:HA3 | 1.84 | 0.42 |
| 1:g:511:TYR:HD2 | 1:g:520:VAL:HG22 | 1.84 | 0.42 |
| 1:h:248:TRP:HB3 | 1:h:373:PHE:CZ | 2.54 | 0.42 |
| 1:i:220:ASP:OD1 | 1:i:220:ASP:N | 2.50 | 0.42 |
| 1:i:248:TRP:HB3 | 1:i:373:PHE:CZ | 2.54 | 0.42 |
| 1:i:452:GLN:HE21 | 1:i:459:GLY:HA3 | 1.84 | 0.42 |
| 1:j:278:TYR:CE2 | 1:j:395:PHE:HD1 | 2.37 | 0.42 |
| 1:k:522:PRO:O | 1:k:541:GLY:HA2 | 2.18 | 0.42 |
| 1:m:340:THR:O | 1:m:407:ARG:CZ | 2.67 | 0.42 |
| 1:m:340:THR:O | 1:m:407:ARG:NE | 2.52 | 0.42 |
| 1:n:248:TRP:HB3 | 1:n:373:PHE:CZ | 2.54 | 0.42 |
| 1:n:568:ILE:HD12 | 1:n:572:ASN:HD22 | 1.84 | 0.42 |
| 1:p:322:GLN:HB3 | 1:q:340:THR:HB | 2.01 | 0.42 |
| 1:p:511:TYR:HD2 | 1:p:520:VAL:HG22 | 1.84 | 0.42 |
| 1:q:340:THR:O | 1:q:407:ARG:NE | 2.52 | 0.42 |
| 1:s:329:ASN:O | 1:s:332:THR:OG1 | 2.31 | 0.42 |
| 1:t:220:ASP:OD1 | 1:t:220:ASP:N | 2.50 | 0.42 |
| 1:t:297:ARG:HG3 | 1:t:301:ARG:NH1 | 2.34 | 0.42 |
| 1:u:264:GLY:HA2 | 1:u:387:SER:HB3 | 2.01 | 0.42 |
| 1:w:568:ILE:HD12 | 1:w:572:ASN:HD22 | 1.84 | 0.42 |
| 1:1:248:TRP:HB3 | 1:1:373:PHE:CZ | 2.54 | 0.42 |
| 1:2:322:GLN:HB3 | 1:3:340:THR:HB | 2.01 | 0.42 |
| 1:2:522:PRO:O | 1:2:541:GLY:HA2 | 2.18 | 0.42 |
| 1:4:511:TYR:HD2 | 1:4:520:VAL:HG22 | 1.84 | 0.42 |
| 1:4:568:ILE:HD12 | 1:4:572:ASN:HD22 | 1.84 | 0.42 |
| 1:5:248:TRP:HB3 | 1:5:373:PHE:CZ | 2.54 | 0.42 |
| 1:5:297:ARG:HG3 | 1:5:301:ARG:NH1 | 2.34 | 0.42 |
| 1:5:464:LEU:HD23 | 1:6:554:ASN:HB3 | 2.00 | 0.42 |
| 1:6:452:GLN:HE21 | 1:6:459:GLY:HA3 | 1.84 | 0.42 |
| 1:A:290:PHE:HE2 | 1:A:614:VAL:HB | 1.84 | 0.42 |
| 1:B:609:TRP:CD1 | 1:J:629:GLY:CA | 2.86 | 0.42 |
| 1:F:554:ASN:HB3 | 1:Q:464:LEU:HD23 | 2.00 | 0.42 |
| 1:G:220:ASP:OD1 | 1:G:220:ASP:N | 2.50 | 0.42 |
| 1:H:319:PHE:CE1 | 1:H:680:GLN:HB2 | 2.55 | 0.42 |
| 1:H:340:THR:O | 1:H:407:ARG:NE | 2.52 | 0.42 |
| 1:H:568:ILE:HD12 | 1:H:572:ASN:HD22 | 1.84 | 0.42 |
| 1:J:264:GLY:HA2 | 1:J:387:SER:HB3 | 2.01 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:322:GLN:HB3 | 1:b:340:THR:HB | 2.01 | 0.42 |
| 1:M:264:GLY:HA2 | 1:M:387:SER:HB3 | 2.01 | 0.42 |
| 1:N:319:PHE:CE1 | 1:N:680:GLN:HB2 | 2.55 | 0.42 |
| 1:N:341:SER:HB3 | 1:N:675:GLN:NE2 | 2.32 | 0.42 |
| 1:Q:248:TRP:HB3 | 1:Q:373:PHE:CZ | 2.54 | 0.42 |
| 1:Q:341:SER:HB3 | 1:Q:675:GLN:NE2 | 2.32 | 0.42 |
| 1:R:220:ASP:OD1 | 1:R:220:ASP:N | 2.50 | 0.42 |
| 1:S:248:TRP:HB3 | 1:S:373:PHE:CZ | 2.54 | 0.42 |
| 1:S:319:PHE:CE1 | 1:S:680:GLN:HB2 | 2.55 | 0.42 |
| 1:T:248:TRP:HB3 | 1:T:373:PHE:CZ | 2.54 | 0.42 |
| 1:T:402:PRO:CG | 1:i:232:ASP:HB3 | 2.47 | 0.42 |
| 1:V:586:LEU:HD21 | 1:e:490:ARG:CZ | 2.49 | 0.42 |
| 1:Y:264:GLY:HA2 | 1:Y:387:SER:HB3 | 2.01 | 0.42 |
| 1:Y:340:THR:O | 1:Y:407:ARG:NE | 2.52 | 0.42 |
| 1:Z:340:THR:O | 1:Z:407:ARG:NE | 2.52 | 0.42 |
| 1:a:319:PHE:CE1 | 1:a:680:GLN:HB2 | 2.55 | 0.42 |
| 1:c:435:ARG:HD3 | 1:c:435:ARG:HA | 1.79 | 0.42 |
| 1:f:340:THR:HB | 1:z:322:GLN:HB3 | 2.02 | 0.42 |
| 1:f:464:LEU:HD23 | 1:h:554:ASN:HB3 | 2.00 | 0.42 |
| 1:g:248:TRP:HB3 | 1:g:373:PHE:CZ | 2.54 | 0.42 |
| 1:h:511:TYR:HD2 | 1:h:520:VAL:HG22 | 1.84 | 0.42 |
| 1:j:319:PHE:CE1 | 1:j:680:GLN:HB2 | 2.55 | 0.42 |
| 1:j:322:GLN:HB3 | 1:x:340:THR:HB | 2.00 | 0.42 |
| 1:j:736:ARG:NH2 | 1:k:626:HIS:CD2 | 2.79 | 0.42 |
| 1:k:248:TRP:HB3 | 1:k:373:PHE:CZ | 2.54 | 0.42 |
| 1:k:511:TYR:HD2 | 1:k:520:VAL:HG22 | 1.84 | 0.42 |
| 1:l:568:ILE:HD12 | 1:l:572:ASN:HD22 | 1.84 | 0.42 |
| 1:m:450:ARG:HG2 | 1:m:452:GLN:H | 1.85 | 0.42 |
| 1:m:568:ILE:HD12 | 1:m:572:ASN:HD22 | 1.84 | 0.42 |
| 1:o:248:TRP:HB3 | 1:o:373:PHE:CZ | 2.54 | 0.42 |
| 1:o:583:ALA:O | 1:p:487:ARG:HD2 | 2.18 | 0.42 |
| 1:p:220:ASP:OD1 | 1:p:220:ASP:N | 2.50 | 0.42 |
| 1:r:248:TRP:HB3 | 1:r:373:PHE:CZ | 2.54 | 0.42 |
| 1:s:319:PHE:CE1 | 1:s:680:GLN:HB2 | 2.55 | 0.42 |
| 1:s:340:THR:O | 1:s:407:ARG:NE | 2.52 | 0.42 |
| 1:u:319:PHE:CE1 | 1:u:680:GLN:HB2 | 2.55 | 0.42 |
| 1:u:464:LEU:HD23 | 1:v:554:ASN:HB3 | 2.00 | 0.42 |
| 1:y:319:PHE:CE1 | 1:y:680:GLN:HB2 | 2.55 | 0.42 |
| 1:1:568:ILE:HD12 | 1:1:572:ASN:HD22 | 1.84 | 0.42 |
| 1:1:583:ALA:O | 1:2:487:ARG:HD2 | 2.18 | 0.42 |
| 1:4:248:TRP:HB3 | 1:4:373:PHE:CZ | 2.54 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:6:609:TRP:NE1 | 1:7:629:GLY:CA | 2.58 | 0.42 |
| 1:7:290:PHE:HE2 | 1:7:614:VAL:HB | 1.84 | 0.42 |
| 1:A:248:TRP:HB3 | 1:A:373:PHE:CZ | 2.54 | 0.42 |
| 1:A:322:GLN:CB | 1:E:340:THR:HB | 2.50 | 0.42 |
| 1:A:429:HIS:CE1 | 1:G:627:THR:HG22 | 2.54 | 0.42 |
| 1:A:586:LEU:HD21 | 1:G:490:ARG:CZ | 2.50 | 0.42 |
| 1:B:340:THR:HB | 1:C:322:GLN:HB3 | 2.01 | 0.42 |
| 1:B:583:ALA:O | 1:J:487:ARG:HD2 | 2.19 | 0.42 |
| 1:C:248:TRP:HB3 | 1:C:373:PHE:CZ | 2.54 | 0.42 |
| 1:D:297:ARG:HG3 | 1:D:301:ARG:NH1 | 2.34 | 0.42 |
| 1:D:340:THR:HB | 1:E:322:GLN:HB3 | 2.01 | 0.42 |
| 1:E:290:PHE:HE2 | 1:E:614:VAL:HB | 1.84 | 0.42 |
| 1:G:297:ARG:HG3 | 1:G:301:ARG:NH1 | 2.34 | 0.42 |
| 1:G:435:ARG:HD3 | 1:G:435:ARG:HA | 1.79 | 0.42 |
| 1:H:322:GLN:CB | 1:I:340:THR:HB | 2.50 | 0.42 |
| 1:J:340:THR:O | 1:J:407:ARG:CZ | 2.67 | 0.42 |
| 1:K:341:SER:HB3 | 1:K:675:GLN:NE2 | 2.32 | 0.42 |
| 1:M:487:ARG:HD2 | 1:b:583:ALA:O | 2.19 | 0.42 |
| 1:N:452:GLN:HE21 | 1:N:459:GLY:HA3 | 1.84 | 0.42 |
| 1:O:232:ASP:HB3 | 1:P:402:PRO:CG | 2.46 | 0.42 |
| 1:O:319:PHE:CE1 | 1:O:680:GLN:HB2 | 2.55 | 0.42 |
| 1:R:248:TRP:HB3 | 1:R:373:PHE:CZ | 2.54 | 0.42 |
| 1:T:583:ALA:O | 1:d:487:ARG:HD2 | 2.18 | 0.42 |
| 1:V:568:ILE:HD12 | 1:V:572:ASN:HD22 | 1.84 | 0.42 |
| 1:W:340:THR:O | 1:W:407:ARG:NE | 2.52 | 0.42 |
| 1:W:450:ARG:HG2 | 1:W:452:GLN:H | 1.85 | 0.42 |
| 1:X:329:ASN:CA | 1:X:330:GLU:OE1 | 2.65 | 0.42 |
| 1:Y:568:ILE:HD12 | 1:Y:572:ASN:HD22 | 1.84 | 0.42 |
| 1:Z:290:PHE:O | 1:Z:293:HIS:N | 2.47 | 0.42 |
| 1:Z:340:THR:HB | 1:a:322:GLN:HB3 | 2.01 | 0.42 |
| 1:Z:450:ARG:HG2 | 1:Z:452:GLN:H | 1.85 | 0.42 |
| 1:b:435:ARG:HA | 1:b:435:ARG:HD3 | 1.79 | 0.42 |
| 1:c:340:THR:HB | 1:s:322:GLN:CB | 2.50 | 0.42 |
| 1:c:473:MET:HE3 | 1:c:473:MET:HB2 | 1.81 | 0.42 |
| 1:e:704:THR:HB | 1:f:702:GLN:HB2 | 2.02 | 0.42 |
| 1:g:220:ASP:OD1 | 1:g:220:ASP:N | 2.50 | 0.42 |
| 1:g:232:ASP:HB3 | 1:1:402:PRO:CG | 2.47 | 0.42 |
| 1:g:402:PRO:CG | 1:k:232:ASP:HB3 | 2.46 | 0.42 |
| 1:h:340:THR:O | 1:h:407:ARG:NE | 2.52 | 0.42 |
| 1:h:522:PRO:O | 1:h:541:GLY:HA2 | 2.18 | 0.42 |
| 1:i:736:ARG:NH2 | 1:j:626:HIS:CD2 | 2.79 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:248:TRP:HB3 | 1:j:373:PHE:CZ | 2.54 | 0.42 |
| 1:k:409:GLY:N | 1:w:223:GLY:O | 2.50 | 0.42 |
| 1:l:319:PHE:CE1 | 1:l:680:GLN:HB2 | 2.55 | 0.42 |
| 1:l:340:THR:HB | 1:n:322:GLN:CB | 2.50 | 0.42 |
| 1:l:340:THR:HB | 1:n:322:GLN:HB3 | 2.01 | 0.42 |
| 1:m:452:GLN:HE21 | 1:m:459:GLY:HA3 | 1.84 | 0.42 |
| 1:p:297:ARG:HG3 | 1:p:301:ARG:NH1 | 2.34 | 0.42 |
| 1:r:568:ILE:HD12 | 1:r:572:ASN:HD22 | 1.84 | 0.42 |
| 1:u:248:TRP:HB3 | 1:u:373:PHE:CZ | 2.54 | 0.42 |
| 1:v:329:ASN:CA | 1:v:330:GLU:OE1 | 2.65 | 0.42 |
| 1:w:319:PHE:CE1 | 1:w:680:GLN:HB2 | 2.55 | 0.42 |
| 1:w:503:PHE:CE2 | 1:y:451:THR:HG21 | 2.54 | 0.42 |
| 1:z:319:PHE:CE1 | 1:z:680:GLN:HB2 | 2.55 | 0.42 |
| 1:z:340:THR:HB | 1:4:322:GLN:CB | 2.50 | 0.42 |
| 1:z:583:ALA:O | 1:1:487:ARG:HD2 | 2.18 | 0.42 |
| 1:2:450:ARG:HG2 | 1:2:452:GLN:H | 1.85 | 0.42 |
| 1:3:319:PHE:CE1 | 1:3:680:GLN:HB2 | 2.55 | 0.42 |
| 1:3:568:ILE:HD12 | 1:3:572:ASN:HD22 | 1.84 | 0.42 |
| 1:A:568:ILE:HD12 | 1:A:572:ASN:HD22 | 1.84 | 0.42 |
| 1:D:341:SER:HB3 | 1:D:675:GLN:NE2 | 2.32 | 0.42 |
| 1:D:450:ARG:HG2 | 1:D:452:GLN:H | 1.85 | 0.42 |
| 1:D:704:THR:HB | 1:M:702:GLN:HB2 | 2.02 | 0.42 |
| 1:E:312:LYS:HA | 1:E:312:LYS:HD2 | 1.90 | 0.42 |
| 1:J:702:GLN:HB2 | 1:K:704:THR:HB | 2.02 | 0.42 |
| 1:K:297:ARG:HG3 | 1:K:301:ARG:NH1 | 2.34 | 0.42 |
| 1:K:340:THR:HB | 1:7:322:GLN:HB3 | 2.01 | 0.42 |
| 1:K:429:HIS:HD2 | 1:K:610:GLN:OE1 | 1.94 | 0.42 |
| 1:L:248:TRP:HB3 | 1:L:373:PHE:CZ | 2.54 | 0.42 |
| 1:M:340:THR:O | 1:M:407:ARG:CZ | 2.67 | 0.42 |
| 1:N:322:GLN:HB3 | 1:m:340:THR:HB | 2.01 | 0.42 |
| 1:O:322:GLN:CB | 1:P:340:THR:HB | 2.49 | 0.42 |
| 1:O:402:PRO:CG | 1:d:232:ASP:HB3 | 2.46 | 0.42 |
| 1:P:340:THR:O | 1:P:407:ARG:CZ | 2.67 | 0.42 |
| 1:S:322:GLN:CB | 1:d:340:THR:HB | 2.50 | 0.42 |
| 1:S:464:LEU:HD23 | 1:U:554:ASN:HB3 | 2.00 | 0.42 |
| 1:T:264:GLY:HA2 | 1:T:387:SER:HB3 | 2.01 | 0.42 |
| 1:U:297:ARG:HG3 | 1:U:301:ARG:NH1 | 2.34 | 0.42 |
| 1:U:329:ASN:CA | 1:U:330:GLU:OE1 | 2.65 | 0.42 |
| 1:V:319:PHE:CE1 | 1:V:680:GLN:HB2 | 2.55 | 0.42 |
| 1:X:297:ARG:HG3 | 1:X:301:ARG:NH1 | 2.34 | 0.42 |
| 1:Y:452:GLN:HE21 | 1:Y:459:GLY:HA3 | 1.84 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:c:290:PHE:O | 1:c:293:HIS:N | 2.47 | 0.42 |
| 1:d:340:THR:O | 1:d:407:ARG:NE | 2.52 | 0.42 |
| 1:d:450:ARG:HG2 | 1:d:452:GLN:H | 1.85 | 0.42 |
| 1:e:319:PHE:CE1 | 1:e:680:GLN:HB2 | 2.55 | 0.42 |
| 1:e:322:GLN:CB | 1:h:340:THR:HB | 2.49 | 0.42 |
| 1:f:248:TRP:HB3 | 1:f:373:PHE:CZ | 2.54 | 0.42 |
| 1:f:297:ARG:HG3 | 1:f:301:ARG:NH1 | 2.34 | 0.42 |
| 1:g:290:PHE:O | 1:g:293:HIS:N | 2.47 | 0.42 |
| 1:j:297:ARG:HG3 | 1:j:301:ARG:NH1 | 2.34 | 0.42 |
| 1:k:340:THR:O | 1:k:407:ARG:NE | 2.52 | 0.42 |
| 1:m:264:GLY:HA2 | 1:m:387:SER:HB3 | 2.01 | 0.42 |
| 1:n:319:PHE:CE1 | 1:n:680:GLN:HB2 | 2.55 | 0.42 |
| 1:o:290:PHE:HE2 | 1:o:614:VAL:HB | 1.84 | 0.42 |
| 1:q:450:ARG:HG2 | 1:q:452:GLN:H | 1.85 | 0.42 |
| 1:q:568:ILE:HD12 | 1:q:572:ASN:HD22 | 1.84 | 0.42 |
| 1:r:340:THR:O | 1:r:407:ARG:NE | 2.52 | 0.42 |
| 1:s:568:ILE:HD12 | 1:s:572:ASN:HD22 | 1.84 | 0.42 |
| 1:t:248:TRP:HB3 | 1:t:373:PHE:CZ | 2.54 | 0.42 |
| 1:t:656:VAL:HG11 | 1:y:324:LYS:HE3 | 2.01 | 0.42 |
| 1:u:322:GLN:CB | 1:2:340:THR:HB | 2.50 | 0.42 |
| 1:u:435:ARG:HD3 | 1:u:435:ARG:HA | 1.80 | 0.42 |
| 1:v:297:ARG:HG3 | 1:v:301:ARG:NH1 | 2.34 | 0.42 |
| 1:v:340:THR:HB | 1:1:322:GLN:HB3 | 2.01 | 0.42 |
| 1:v:340:THR:O | 1:v:407:ARG:CZ | 2.67 | 0.42 |
| 1:w:248:TRP:HB3 | 1:w:373:PHE:CZ | 2.54 | 0.42 |
| 1:z:435:ARG:HD3 | 1:z:435:ARG:HA | 1.79 | 0.42 |
| 1:z:522:PRO:O | 1:z:541:GLY:HA2 | 2.18 | 0.42 |
| 1:z:568:ILE:HD12 | 1:z:572:ASN:HD22 | 1.84 | 0.42 |
| 1:1:264:GLY:HA2 | 1:1:387:SER:HB3 | 2.01 | 0.42 |
| 1:2:232:ASP:HB3 | 1:3:402:PRO:CG | 2.46 | 0.42 |
| 1:2:319:PHE:CE1 | 1:2:680:GLN:HB2 | 2.55 | 0.42 |
| 1:2:340:THR:O | 1:2:407:ARG:NE | 2.52 | 0.42 |
| 1:4:319:PHE:CE1 | 1:4:680:GLN:HB2 | 2.55 | 0.42 |
| 1:7:426:SER:OG | 1:7:731:THR:O | 2.31 | 0.42 |
| 1:8:452:GLN:HE21 | 1:8:459:GLY:HA3 | 1.84 | 0.42 |
| 1:B:473:MET:HE3 | 1:B:473:MET:HB2 | 1.81 | 0.42 |
| 1:C:319:PHE:CE1 | 1:C:680:GLN:HB2 | 2.55 | 0.42 |
| 1:F:232:ASP:HB3 | 1:G:402:PRO:CG | 2.47 | 0.42 |
| 1:H:297:ARG:HG3 | 1:H:301:ARG:NH1 | 2.34 | 0.42 |
| 1:I:256:HIS:CD2 | 1:I:655:PRO:HB3 | 2.55 | 0.42 |
| 1:I:473:MET:HE3 | 1:I:473:MET:HB2 | 1.81 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:290:PHE:HE2 | 1:K:614:VAL:HB | 1.84 | 0.42 |
| 1:L:297:ARG:HG3 | 1:L:301:ARG:NH1 | 2.34 | 0.42 |
| 1:N:322:GLN:CB | 1:m:340:THR:HB | 2.50 | 0.42 |
| 1:N:326:VAL:HG21 | 1:N:333:LYS:HZ2 | 1.85 | 0.42 |
| 1:O:700:GLU:HB2 | 1:O:702:GLN:HE21 | 1.85 | 0.42 |
| 1:P:330:GLU:N | 1:P:330:GLU:CD | 2.78 | 0.42 |
| 1:P:434:ASP:N | 1:P:434:ASP:OD1 | 2.41 | 0.42 |
| 1:Q:340:THR:O | 1:Q:407:ARG:CZ | 2.67 | 0.42 |
| 1:R:568:ILE:HD12 | 1:R:572:ASN:HD22 | 1.84 | 0.42 |
| 1:S:450:ARG:HG2 | 1:S:452:GLN:H | 1.85 | 0.42 |
| 1:T:322:GLN:HB3 | 1:U:340:THR:HB | 2.01 | 0.42 |
| 1:T:429:HIS:HD2 | 1:T:610:GLN:OE1 | 1.94 | 0.42 |
| 1:T:629:GLY:CA | 1:l:609:TRP:CD1 | 2.85 | 0.42 |
| 1:T:700:GLU:HB2 | 1:T:702:GLN:HE21 | 1.85 | 0.42 |
| 1:U:290:PHE:O | 1:U:293:HIS:N | 2.47 | 0.42 |
| 1:V:435:ARG:HD3 | 1:V:435:ARG:HA | 1.79 | 0.42 |
| 1:V:700:GLU:HB2 | 1:V:702:GLN:HE21 | 1.85 | 0.42 |
| 1:W:568:ILE:HD12 | 1:W:572:ASN:HD22 | 1.84 | 0.42 |
| 1:X:278:TYR:CE2 | 1:X:395:PHE:HD1 | 2.37 | 0.42 |
| 1:X:290:PHE:HE2 | 1:X:614:VAL:HB | 1.84 | 0.42 |
| 1:X:319:PHE:CE1 | 1:X:680:GLN:HB2 | 2.55 | 0.42 |
| 1:Z:340:THR:HB | 1:a:322:GLN:CB | 2.50 | 0.42 |
| 1:Z:700:GLU:HB2 | 1:Z:702:GLN:HE21 | 1.85 | 0.42 |
| 1:b:340:THR:O | 1:b:407:ARG:NE | 2.52 | 0.42 |
| 1:d:256:HIS:CD2 | 1:d:655:PRO:HB3 | 2.55 | 0.42 |
| 1:d:319:PHE:CE1 | 1:d:680:GLN:HB2 | 2.55 | 0.42 |
| 1:d:340:THR:O | 1:d:407:ARG:CZ | 2.67 | 0.42 |
| 1:e:248:TRP:HB3 | 1:e:373:PHE:CZ | 2.54 | 0.42 |
| 1:f:626:HIS:CD2 | 1:g:736:ARG:NH2 | 2.79 | 0.42 |
| 1:j:464:LEU:HD23 | 1:k:554:ASN:HB3 | 2.00 | 0.42 |
| 1:l:511:TYR:HD2 | 1:l:520:VAL:HG22 | 1.84 | 0.42 |
| 1:m:700:GLU:HB2 | 1:m:702:GLN:HE21 | 1.85 | 0.42 |
| 1:n:450:ARG:HG2 | 1:n:452:GLN:H | 1.85 | 0.42 |
| 1:o:322:GLN:CB | 1:7:340:THR:HB | 2.50 | 0.42 |
| 1:o:322:GLN:HB3 | 1:7:340:THR:HB | 2.01 | 0.42 |
| 1:o:568:ILE:HD12 | 1:o:572:ASN:HD22 | 1.84 | 0.42 |
| 1:o:704:THR:HB | 1:6:702:GLN:HB2 | 2.02 | 0.42 |
| 1:p:402:PRO:CG | 1:6:232:ASP:HB3 | 2.47 | 0.42 |
| 1:q:256:HIS:CD2 | 1:q:655:PRO:HB3 | 2.55 | 0.42 |
| 1:r:452:GLN:HE21 | 1:r:459:GLY:HA3 | 1.84 | 0.42 |
| 1:t:568:ILE:HD12 | 1:t:572:ASN:HD22 | 1.84 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:u:450:ARG:HG2 | 1:u:452:GLN:H | 1.85 | 0.42 |
| 1:v:248:TRP:HB3 | 1:v:373:PHE:CZ | 2.54 | 0.42 |
| 1:x:297:ARG:HG3 | 1:x:301:ARG:NH1 | 2.34 | 0.42 |
| 1:x:329:ASN:CA | 1:x:330:GLU:OE1 | 2.65 | 0.42 |
| 1:x:450:ARG:HG2 | 1:x:452:GLN:H | 1.85 | 0.42 |
| 1:y:568:ILE:HD12 | 1:y:572:ASN:HD22 | 1.84 | 0.42 |
| 1:z:490:ARG:CZ | 1:2:586:LEU:HD21 | 2.50 | 0.42 |
| 1:z:511:TYR:HD2 | 1:z:520:VAL:HG22 | 1.84 | 0.42 |
| 1:1:700:GLU:HB2 | 1:1:702:GLN:HE21 | 1.85 | 0.42 |
| 1:2:340:THR:O | 1:2:407:ARG:CZ | 2.67 | 0.42 |
| 1:3:322:GLN:CB | 1:8:340:THR:HB | 2.49 | 0.42 |
| 1:3:700:GLU:HB2 | 1:3:702:GLN:HE21 | 1.85 | 0.42 |
| 1:5:340:THR:O | 1:5:407:ARG:CZ | 2.67 | 0.42 |
| 1:7:264:GLY:HA2 | 1:7:387:SER:HB3 | 2.01 | 0.42 |
| 1:8:341:SER:HB3 | 1:8:675:GLN:NE2 | 2.32 | 0.42 |
| 1:A:450:ARG:HG2 | 1:A:452:GLN:H | 1.85 | 0.42 |
| 1:A:700:GLU:HB2 | 1:A:702:GLN:HE21 | 1.85 | 0.42 |
| 1:C:256:HIS:CD2 | 1:C:655:PRO:HB3 | 2.55 | 0.42 |
| 1:C:297:ARG:HG3 | 1:C:301:ARG:NH1 | 2.34 | 0.42 |
| 1:C:571:THR:HG22 | 1:C:608:VAL:O | 2.20 | 0.42 |
| 1:E:256:HIS:CD2 | 1:E:655:PRO:HB3 | 2.55 | 0.42 |
| 1:E:264:GLY:HA2 | 1:E:387:SER:HB3 | 2.01 | 0.42 |
| 1:E:340:THR:O | 1:E:407:ARG:CZ | 2.67 | 0.42 |
| 1:H:322:GLN:HB3 | 1:I:340:THR:HB | 2.01 | 0.42 |
| 1:L:319:PHE:CE1 | 1:L:680:GLN:HB2 | 2.55 | 0.42 |
| 1:L:450:ARG:HG2 | 1:L:452:GLN:H | 1.85 | 0.42 |
| 1:L:571:THR:HG22 | 1:L:608:VAL:O | 2.20 | 0.42 |
| 1:M:452:GLN:HE21 | 1:M:459:GLY:HA3 | 1.84 | 0.42 |
| 1:N:421:VAL:CG2 | 1:N:422:PRO:HD2 | 2.50 | 0.42 |
| 1:O:297:ARG:HG3 | 1:O:301:ARG:NH1 | 2.34 | 0.42 |
| 1:O:330:GLU:N | 1:O:330:GLU:CD | 2.78 | 0.42 |
| 1:O:429:HIS:HD2 | 1:O:610:GLN:OE1 | 1.94 | 0.42 |
| 1:P:341:SER:HB3 | 1:P:675:GLN:NE2 | 2.32 | 0.42 |
| 1:Q:256:HIS:CD2 | 1:Q:655:PRO:HB3 | 2.55 | 0.42 |
| 1:S:435:ARG:HD3 | 1:S:435:ARG:HA | 1.80 | 0.42 |
| 1:S:571:THR:HG22 | 1:S:608:VAL:O | 2.20 | 0.42 |
| 1:S:609:TRP:NE1 | 1:U:629:GLY:CA | 2.58 | 0.42 |
| 1:T:342:THR:HG22 | 1:T:407:ARG:HA | 2.02 | 0.42 |
| 1:T:626:HIS:CD2 | 1:l:736:ARG:NH2 | 2.79 | 0.42 |
| 1:U:248:TRP:HB3 | 1:U:373:PHE:CZ | 2.54 | 0.42 |
| 1:U:340:THR:O | 1:U:407:ARG:CZ | 2.67 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:340:THR:HB | 1:W:322:GLN:CB | 2.49 | 0.42 |
| 1:W:256:HIS:CD2 | 1:W:655:PRO:HB3 | 2.55 | 0.42 |
| 1:W:297:ARG:HG3 | 1:W:301:ARG:NH1 | 2.34 | 0.42 |
| 1:W:700:GLU:HB2 | 1:W:702:GLN:HE21 | 1.85 | 0.42 |
| 1:X:450:ARG:HG2 | 1:X:452:GLN:H | 1.85 | 0.42 |
| 1:Y:319:PHE:CE1 | 1:Y:680:GLN:HB2 | 2.55 | 0.42 |
| 1:Y:434:ASP:OD1 | 1:Y:434:ASP:N | 2.41 | 0.42 |
| 1:Z:264:GLY:HA2 | 1:Z:387:SER:HB3 | 2.01 | 0.42 |
| 1:Z:297:ARG:HG3 | 1:Z:301:ARG:NH1 | 2.34 | 0.42 |
| 1:c:256:HIS:CD2 | 1:c:655:PRO:HB3 | 2.55 | 0.42 |
| 1:d:586:LEU:HD21 | 1:l:490:ARG:CZ | 2.50 | 0.42 |
| 1:d:700:GLU:HB2 | 1:d:702:GLN:HE21 | 1.85 | 0.42 |
| 1:e:421:VAL:CG2 | 1:e:422:PRO:HD2 | 2.50 | 0.42 |
| 1:g:256:HIS:CD2 | 1:g:655:PRO:HB3 | 2.55 | 0.42 |
| 1:h:278:TYR:CE2 | 1:h:395:PHE:HD1 | 2.37 | 0.42 |
| 1:i:290:PHE:O | 1:i:293:HIS:N | 2.47 | 0.42 |
| 1:j:340:THR:O | 1:j:407:ARG:NE | 2.52 | 0.42 |
| 1:k:256:HIS:CD2 | 1:k:655:PRO:HB3 | 2.55 | 0.42 |
| 1:l:264:GLY:HA2 | 1:l:387:SER:HB3 | 2.01 | 0.42 |
| 1:l:522:PRO:O | 1:l:541:GLY:HA2 | 2.18 | 0.42 |
| 1:m:527:ALA:O | 1:m:575:ALA:N | 2.45 | 0.42 |
| 1:o:256:HIS:CD2 | 1:o:655:PRO:HB3 | 2.55 | 0.42 |
| 1:o:609:TRP:NE1 | 1:p:629:GLY:CA | 2.59 | 0.42 |
| 1:q:700:GLU:HB2 | 1:q:702:GLN:HE21 | 1.85 | 0.42 |
| 1:t:511:TYR:HD2 | 1:t:520:VAL:HG22 | 1.84 | 0.42 |
| 1:u:571:THR:HG22 | 1:u:608:VAL:O | 2.20 | 0.42 |
| 1:w:421:VAL:CG2 | 1:w:422:PRO:HD2 | 2.50 | 0.42 |
| 1:w:629:GLY:CA | 1:y:609:TRP:NE1 | 2.60 | 0.42 |
| 1:x:278:TYR:CE2 | 1:x:395:PHE:HD1 | 2.37 | 0.42 |
| 1:x:319:PHE:CE1 | 1:x:680:GLN:HB2 | 2.55 | 0.42 |
| 1:x:511:TYR:HD2 | 1:x:520:VAL:HG22 | 1.84 | 0.42 |
| 1:y:700:GLU:HB2 | 1:y:702:GLN:HE21 | 1.85 | 0.42 |
| 1:z:340:THR:O | 1:z:407:ARG:NE | 2.52 | 0.42 |
| 1:2:256:HIS:CD2 | 1:2:655:PRO:HB3 | 2.55 | 0.42 |
| 1:2:568:ILE:HD12 | 1:2:572:ASN:HD22 | 1.84 | 0.42 |
| 1:2:700:GLU:HB2 | 1:2:702:GLN:HE21 | 1.85 | 0.42 |
| 1:3:232:ASP:HB3 | 1:8:402:PRO:CG | 2.46 | 0.42 |
| 1:3:330:GLU:N | 1:3:330:GLU:CD | 2.78 | 0.42 |
| 1:4:450:ARG:HG2 | 1:4:452:GLN:H | 1.85 | 0.42 |
| 1:5:319:PHE:CE1 | 1:5:680:GLN:HB2 | 2.55 | 0.42 |
| 1:7:256:HIS:CD2 | 1:7:655:PRO:HB3 | 2.55 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:8:330:GLU:N | 1:8:330:GLU:CD | 2.78 | 0.42 |
| 1:8:340:THR:O | 1:8:407:ARG:CZ | 2.67 | 0.42 |
| 1:B:256:HIS:CD2 | 1:B:655:PRO:HB3 | 2.55 | 0.42 |
| 1:B:340:THR:O | 1:B:407:ARG:NE | 2.52 | 0.42 |
| 1:B:490:ARG:CZ | 1:L:586:LEU:HD21 | 2.50 | 0.42 |
| 1:B:571:THR:HG22 | 1:B:608:VAL:O | 2.20 | 0.42 |
| 1:C:450:ARG:HG2 | 1:C:452:GLN:H | 1.85 | 0.42 |
| 1:D:290:PHE:HE2 | 1:D:614:VAL:HB | 1.84 | 0.42 |
| 1:D:340:THR:O | 1:D:407:ARG:NE | 2.52 | 0.42 |
| 1:D:511:TYR:HD2 | 1:D:520:VAL:HG22 | 1.84 | 0.42 |
| 1:E:290:PHE:O | 1:E:293:HIS:N | 2.47 | 0.42 |
| 1:E:421:VAL:CG2 | 1:E:422:PRO:HD2 | 2.50 | 0.42 |
| 1:E:511:TYR:HD2 | 1:E:520:VAL:HG22 | 1.84 | 0.42 |
| 1:E:702:GLN:HB2 | 1:P:704:THR:HB | 2.02 | 0.42 |
| 1:G:319:PHE:CE1 | 1:G:680:GLN:HB2 | 2.55 | 0.42 |
| 1:G:571:THR:HG22 | 1:G:608:VAL:O | 2.20 | 0.42 |
| 1:H:571:THR:HG22 | 1:H:608:VAL:O | 2.20 | 0.42 |
| 1:I:290:PHE:O | 1:I:293:HIS:N | 2.47 | 0.42 |
| 1:K:322:GLN:CB | 1:L:340:THR:HB | 2.49 | 0.42 |
| 1:K:450:ARG:HG2 | 1:K:452:GLN:H | 1.85 | 0.42 |
| 1:K:586:LEU:HD21 | 1:a:490:ARG:CZ | 2.50 | 0.42 |
| 1:L:256:HIS:CD2 | 1:L:655:PRO:HB3 | 2.55 | 0.42 |
| 1:M:342:THR:HG22 | 1:M:407:ARG:HA | 2.02 | 0.42 |
| 1:O:329:ASN:CA | 1:O:330:GLU:OE1 | 2.65 | 0.42 |
| 1:Q:319:PHE:CE1 | 1:Q:680:GLN:HB2 | 2.55 | 0.42 |
| 1:R:319:PHE:CE1 | 1:R:680:GLN:HB2 | 2.55 | 0.42 |
| 1:R:342:THR:HG22 | 1:R:407:ARG:CG | 2.47 | 0.42 |
| 1:R:511:TYR:HD2 | 1:R:520:VAL:HG22 | 1.84 | 0.42 |
| 1:T:511:TYR:HD2 | 1:T:520:VAL:HG22 | 1.84 | 0.42 |
| 1:U:322:GLN:HB3 | 1:e:340:THR:HB | 2.01 | 0.42 |
| 1:U:340:THR:O | 1:U:407:ARG:NE | 2.52 | 0.42 |
| 1:U:342:THR:HG22 | 1:U:407:ARG:HA | 2.02 | 0.42 |
| 1:X:256:HIS:CD2 | 1:X:655:PRO:HB3 | 2.55 | 0.42 |
| 1:X:264:GLY:HA2 | 1:X:387:SER:HB3 | 2.01 | 0.42 |
| 1:X:322:GLN:CB | 1:Y:340:THR:HB | 2.50 | 0.42 |
| 1:X:330:GLU:N | 1:X:330:GLU:CD | 2.78 | 0.42 |
| 1:X:490:ARG:CZ | 1:e:586:LEU:HD21 | 2.50 | 0.42 |
| 1:Y:256:HIS:CD2 | 1:Y:655:PRO:HB3 | 2.55 | 0.42 |
| 1:Z:527:ALA:O | 1:Z:575:ALA:N | 2.45 | 0.42 |
| 1:Z:571:THR:HG22 | 1:Z:608:VAL:O | 2.20 | 0.42 |
| 1:a:421:VAL:CG2 | 1:a:422:PRO:HD2 | 2.50 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:a:450:ARG:HG2 | 1:a:452:GLN:H | 1.85 | 0.42 |
| 1:a:571:THR:HG22 | 1:a:608:VAL:O | 2.20 | 0.42 |
| 1:c:571:THR:HG22 | 1:c:608:VAL:O | 2.20 | 0.42 |
| 1:d:264:GLY:HA2 | 1:d:387:SER:HB3 | 2.01 | 0.42 |
| 1:e:340:THR:O | 1:e:407:ARG:NE | 2.52 | 0.42 |
| 1:e:342:THR:HG22 | 1:e:407:ARG:HA | 2.02 | 0.42 |
| 1:f:473:MET:HE3 | 1:f:473:MET:HB2 | 1.81 | 0.42 |
| 1:f:484:PRO:HD2 | 1:f:609:TRP:CE3 | 2.55 | 0.42 |
| 1:h:256:HIS:CD2 | 1:h:655:PRO:HB3 | 2.55 | 0.42 |
| 1:h:571:THR:HG22 | 1:h:608:VAL:O | 2.20 | 0.42 |
| 1:i:256:HIS:CD2 | 1:i:655:PRO:HB3 | 2.55 | 0.42 |
| 1:i:264:GLY:HA2 | 1:i:387:SER:HB3 | 2.01 | 0.42 |
| 1:j:340:THR:HB | 1:l:322:GLN:HB3 | 2.02 | 0.42 |
| 1:k:319:PHE:CE1 | 1:k:680:GLN:HB2 | 2.55 | 0.42 |
| 1:l:340:THR:O | 1:l:407:ARG:NE | 2.52 | 0.42 |
| 1:m:297:ARG:HG3 | 1:m:301:ARG:NH1 | 2.34 | 0.42 |
| 1:m:571:THR:HG22 | 1:m:608:VAL:O | 2.20 | 0.42 |
| 1:o:450:ARG:HG2 | 1:o:452:GLN:H | 1.85 | 0.42 |
| 1:o:700:GLU:HB2 | 1:o:702:GLN:HE21 | 1.85 | 0.42 |
| 1:p:248:TRP:HB3 | 1:p:373:PHE:CZ | 2.54 | 0.42 |
| 1:p:319:PHE:CE1 | 1:p:680:GLN:HB2 | 2.55 | 0.42 |
| 1:p:340:THR:O | 1:p:407:ARG:NE | 2.52 | 0.42 |
| 1:q:297:ARG:HG3 | 1:q:301:ARG:NH1 | 2.34 | 0.42 |
| 1:r:220:ASP:OD1 | 1:r:220:ASP:N | 2.50 | 0.42 |
| 1:r:256:HIS:CD2 | 1:r:655:PRO:HB3 | 2.55 | 0.42 |
| 1:r:319:PHE:CE1 | 1:r:680:GLN:HB2 | 2.55 | 0.42 |
| 1:r:511:TYR:HD2 | 1:r:520:VAL:HG22 | 1.84 | 0.42 |
| 1:s:297:ARG:HG3 | 1:s:301:ARG:NH1 | 2.34 | 0.42 |
| 1:t:319:PHE:CE1 | 1:t:680:GLN:HB2 | 2.55 | 0.42 |
| 1:u:511:TYR:HD2 | 1:u:520:VAL:HG22 | 1.85 | 0.42 |
| 1:w:340:THR:O | 1:w:407:ARG:NE | 2.52 | 0.42 |
| 1:w:342:THR:HG22 | 1:w:407:ARG:HA | 2.02 | 0.42 |
| 1:x:256:HIS:CD2 | 1:x:655:PRO:HB3 | 2.55 | 0.42 |
| 1:x:264:GLY:HA2 | 1:x:387:SER:HB3 | 2.01 | 0.42 |
| 1:x:290:PHE:HE2 | 1:x:614:VAL:HB | 1.84 | 0.42 |
| 1:z:264:GLY:HA2 | 1:z:387:SER:HB3 | 2.01 | 0.42 |
| 1:z:340:THR:HB | 1:4:322:GLN:HB3 | 2.01 | 0.42 |
| 1:z:421:VAL:CG2 | 1:z:422:PRO:HD2 | 2.50 | 0.42 |
| 1:z:609:TRP:CD1 | 1:1:629:GLY:CA | 2.85 | 0.42 |
| 1:2:264:GLY:HA2 | 1:2:387:SER:HB3 | 2.01 | 0.42 |
| 1:3:297:ARG:HG3 | 1:3:301:ARG:NH1 | 2.34 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:429:HIS:HD2 | 1:3:610:GLN:OE1 | 1.94 | 0.42 |
| 1:3:571:THR:HG22 | 1:3:608:VAL:O | 2.20 | 0.42 |
| 1:5:256:HIS:CD2 | 1:5:655:PRO:HB3 | 2.55 | 0.42 |
| 1:6:700:GLU:HB2 | 1:6:702:GLN:HE21 | 1.85 | 0.42 |
| 1:7:290:PHE:O | 1:7:293:HIS:N | 2.47 | 0.42 |
| 1:7:319:PHE:CE1 | 1:7:680:GLN:HB2 | 2.55 | 0.42 |
| 1:7:340:THR:O | 1:7:407:ARG:CZ | 2.67 | 0.42 |
| 1:7:421:VAL:CG2 | 1:7:422:PRO:HD2 | 2.50 | 0.42 |
| 1:7:511:TYR:HD2 | 1:7:520:VAL:HG22 | 1.84 | 0.42 |
| 1:A:256:HIS:CD2 | 1:A:655:PRO:HB3 | 2.55 | 0.42 |
| 1:A:319:PHE:CE1 | 1:A:680:GLN:HB2 | 2.55 | 0.42 |
| 1:B:319:PHE:CE1 | 1:B:680:GLN:HB2 | 2.55 | 0.42 |
| 1:C:340:THR:HB | 1:D:322:GLN:CB | 2.49 | 0.42 |
| 1:C:342:THR:HG22 | 1:C:407:ARG:HA | 2.02 | 0.42 |
| 1:C:586:LEU:HD21 | 1:b:490:ARG:CZ | 2.50 | 0.42 |
| 1:D:429:HIS:HD2 | 1:D:610:GLN:OE1 | 1.94 | 0.42 |
| 1:E:319:PHE:CE1 | 1:E:680:GLN:HB2 | 2.55 | 0.42 |
| 1:E:571:THR:HG22 | 1:E:608:VAL:O | 2.20 | 0.42 |
| 1:F:322:GLN:HB3 | 1:G:340:THR:HB | 2.01 | 0.42 |
| 1:F:700:GLU:HB2 | 1:F:702:GLN:HE21 | 1.85 | 0.42 |
| 1:G:248:TRP:HB3 | 1:G:373:PHE:CZ | 2.54 | 0.42 |
| 1:G:290:PHE:HE2 | 1:G:614:VAL:HB | 1.84 | 0.42 |
| 1:G:322:GLN:CB | 1:W:340:THR:HB | 2.50 | 0.42 |
| 1:G:340:THR:O | 1:G:407:ARG:NE | 2.52 | 0.42 |
| 1:G:342:THR:HG22 | 1:G:407:ARG:HA | 2.02 | 0.42 |
| 1:I:264:GLY:HA2 | 1:I:387:SER:HB3 | 2.01 | 0.42 |
| 1:I:571:THR:HG22 | 1:I:608:VAL:O | 2.20 | 0.42 |
| 1:J:322:GLN:CB | 1:a:340:THR:HB | 2.50 | 0.42 |
| 1:J:342:THR:HG22 | 1:J:407:ARG:HA | 2.02 | 0.42 |
| 1:J:511:TYR:HD2 | 1:J:520:VAL:HG22 | 1.84 | 0.42 |
| 1:K:340:THR:O | 1:K:407:ARG:NE | 2.52 | 0.42 |
| 1:L:342:THR:HG22 | 1:L:407:ARG:HA | 2.02 | 0.42 |
| 1:L:511:TYR:HD2 | 1:L:520:VAL:HG22 | 1.84 | 0.42 |
| 1:L:568:ILE:HD12 | 1:L:572:ASN:HD22 | 1.84 | 0.42 |
| 1:M:319:PHE:CE1 | 1:M:680:GLN:HB2 | 2.55 | 0.42 |
| 1:M:421:VAL:CG2 | 1:M:422:PRO:HD2 | 2.50 | 0.42 |
| 1:M:511:TYR:HD2 | 1:M:520:VAL:HG22 | 1.84 | 0.42 |
| 1:N:256:HIS:CD2 | 1:N:655:PRO:HB3 | 2.55 | 0.42 |
| 1:N:450:ARG:HG2 | 1:N:452:GLN:H | 1.85 | 0.42 |
| 1:N:571:THR:HG22 | 1:N:608:VAL:O | 2.20 | 0.42 |
| 1:O:484:PRO:HD2 | 1:O:609:TRP:CE3 | 2.55 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:571:THR:HG22 | 1:O:608:VAL:O | 2.20 | 0.42 |
| 1:O:586:LEU:HD21 | 1:m:490:ARG:CZ | 2.50 | 0.42 |
| 1:P:340:THR:O | 1:P:407:ARG:NE | 2.52 | 0.42 |
| 1:R:340:THR:HB | 1:V:322:GLN:CB | 2.50 | 0.42 |
| 1:S:511:TYR:HD2 | 1:S:520:VAL:HG22 | 1.85 | 0.42 |
| 1:S:702:GLN:HB2 | 1:T:704:THR:HB | 2.02 | 0.42 |
| 1:U:421:VAL:CG2 | 1:U:422:PRO:HD2 | 2.50 | 0.42 |
| 1:X:340:THR:HB | 1:f:322:GLN:CB | 2.50 | 0.42 |
| 1:X:511:TYR:HD2 | 1:X:520:VAL:HG22 | 1.84 | 0.42 |
| 1:Y:421:VAL:CG2 | 1:Y:422:PRO:HD2 | 2.50 | 0.42 |
| 1:Y:511:TYR:HD2 | 1:Y:520:VAL:HG22 | 1.84 | 0.42 |
| 1:Z:490:ARG:CZ | 1:3:586:LEU:HD21 | 2.50 | 0.42 |
| 1:a:256:HIS:CD2 | 1:a:655:PRO:HB3 | 2.55 | 0.42 |
| 1:b:256:HIS:CD2 | 1:b:655:PRO:HB3 | 2.55 | 0.42 |
| 1:b:319:PHE:CE1 | 1:b:680:GLN:HB2 | 2.55 | 0.42 |
| 1:b:322:GLN:HB3 | 1:o:340:THR:HB | 2.01 | 0.42 |
| 1:b:421:VAL:CG2 | 1:b:422:PRO:HD2 | 2.50 | 0.42 |
| 1:b:571:THR:HG22 | 1:b:608:VAL:O | 2.20 | 0.42 |
| 1:c:264:GLY:HA2 | 1:c:387:SER:HB3 | 2.01 | 0.42 |
| 1:c:656:VAL:HG11 | 1:s:324:LYS:HE3 | 2.02 | 0.42 |
| 1:d:484:PRO:HD2 | 1:d:609:TRP:CE3 | 2.55 | 0.42 |
| 1:d:568:ILE:HD12 | 1:d:572:ASN:HD22 | 1.84 | 0.42 |
| 1:d:571:THR:HG22 | 1:d:608:VAL:O | 2.20 | 0.42 |
| 1:e:571:THR:HG22 | 1:e:608:VAL:O | 2.20 | 0.42 |
| 1:f:340:THR:O | 1:f:407:ARG:NE | 2.52 | 0.42 |
| 1:f:490:ARG:CZ | 1:g:586:LEU:HD21 | 2.50 | 0.42 |
| 1:f:511:TYR:HD2 | 1:f:520:VAL:HG22 | 1.84 | 0.42 |
| 1:g:264:GLY:HA2 | 1:g:387:SER:HB3 | 2.01 | 0.42 |
| 1:h:319:PHE:CE1 | 1:h:680:GLN:HB2 | 2.55 | 0.42 |
| 1:h:421:VAL:CG2 | 1:h:422:PRO:HD2 | 2.50 | 0.42 |
| 1:h:450:ARG:HG2 | 1:h:452:GLN:H | 1.85 | 0.42 |
| 1:i:586:LEU:HD21 | 1:j:490:ARG:CZ | 2.50 | 0.42 |
| 1:j:324:LYS:HE3 | 1:x:656:VAL:HG11 | 2.02 | 0.42 |
| 1:j:484:PRO:HD2 | 1:j:609:TRP:CE3 | 2.55 | 0.42 |
| 1:j:511:TYR:HD2 | 1:j:520:VAL:HG22 | 1.84 | 0.42 |
| 1:k:340:THR:HB | 1:w:322:GLN:NE2 | 2.14 | 0.42 |
| 1:l:330:GLU:N | 1:l:330:GLU:CD | 2.78 | 0.42 |
| 1:l:421:VAL:CG2 | 1:l:422:PRO:HD2 | 2.50 | 0.42 |
| 1:l:450:ARG:HG2 | 1:l:452:GLN:H | 1.85 | 0.42 |
| 1:n:342:THR:HG22 | 1:n:407:ARG:HA | 2.02 | 0.42 |
| 1:o:319:PHE:CE1 | 1:o:680:GLN:HB2 | 2.55 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:o:324:LYS:HE3 | 1:7:656:VAL:HG11 | 2.02 | 0.42 |
| 1:p:342:THR:HG22 | 1:p:407:ARG:HA | 2.02 | 0.42 |
| 1:p:571:THR:HG22 | 1:p:608:VAL:O | 2.20 | 0.42 |
| 1:r:340:THR:HB | 1:x:322:GLN:CB | 2.50 | 0.42 |
| 1:s:571:THR:HG22 | 1:s:608:VAL:O | 2.20 | 0.42 |
| 1:t:256:HIS:CD2 | 1:t:655:PRO:HB3 | 2.55 | 0.42 |
| 1:t:700:GLU:HB2 | 1:t:702:GLN:HE21 | 1.85 | 0.42 |
| 1:v:290:PHE:O | 1:v:293:HIS:N | 2.47 | 0.42 |
| 1:v:340:THR:O | 1:v:407:ARG:NE | 2.52 | 0.42 |
| 1:v:342:THR:HG22 | 1:v:407:ARG:HA | 2.02 | 0.42 |
| 1:w:571:THR:HG22 | 1:w:608:VAL:O | 2.20 | 0.42 |
| 1:x:330:GLU:N | 1:x:330:GLU:CD | 2.78 | 0.42 |
| 1:x:695:LYS:HB3 | 1:y:401:PHE:HE1 | 1.85 | 0.42 |
| 1:y:435:ARG:HA | 1:y:435:ARG:HD3 | 1.79 | 0.42 |
| 1:1:342:THR:HG22 | 1:1:407:ARG:HA | 2.02 | 0.42 |
| 1:1:511:TYR:HD2 | 1:1:520:VAL:HG22 | 1.84 | 0.42 |
| 1:2:484:PRO:HD2 | 1:2:609:TRP:CE3 | 2.55 | 0.42 |
| 1:4:342:THR:HG22 | 1:4:407:ARG:HA | 2.02 | 0.42 |
| 1:7:702:GLN:HB2 | 1:8:704:THR:HB | 2.02 | 0.42 |
| 1:8:434:ASP:N | 1:8:434:ASP:OD1 | 2.41 | 0.42 |
| 1:A:421:VAL:CG2 | 1:A:422:PRO:HD2 | 2.50 | 0.41 |
| 1:B:421:VAL:CG2 | 1:B:422:PRO:HD2 | 2.50 | 0.41 |
| 1:C:402:PRO:CG | 1:D:232:ASP:HB3 | 2.46 | 0.41 |
| 1:C:568:ILE:HD12 | 1:C:572:ASN:HD22 | 1.84 | 0.41 |
| 1:D:484:PRO:HD2 | 1:D:609:TRP:CE3 | 2.55 | 0.41 |
| 1:D:586:LEU:HD21 | 1:N:490:ARG:CZ | 2.50 | 0.41 |
| 1:E:700:GLU:HB2 | 1:E:702:GLN:HE21 | 1.85 | 0.41 |
| 1:G:324:LYS:HE3 | 1:W:656:VAL:HG11 | 2.02 | 0.41 |
| 1:G:568:ILE:HD12 | 1:G:572:ASN:HD22 | 1.84 | 0.41 |
| 1:H:324:LYS:HE3 | 1:I:656:VAL:HG11 | 2.02 | 0.41 |
| 1:H:342:THR:HG22 | 1:H:407:ARG:HA | 2.02 | 0.41 |
| 1:I:319:PHE:CE1 | 1:I:680:GLN:HB2 | 2.55 | 0.41 |
| 1:I:435:ARG:HA | 1:I:435:ARG:HD3 | 1.79 | 0.41 |
| 1:I:450:ARG:HG2 | 1:I:452:GLN:H | 1.85 | 0.41 |
| 1:J:319:PHE:CE1 | 1:J:680:GLN:HB2 | 2.55 | 0.41 |
| 1:J:421:VAL:CG2 | 1:J:422:PRO:HD2 | 2.50 | 0.41 |
| 1:J:452:GLN:HE21 | 1:J:459:GLY:HA3 | 1.84 | 0.41 |
| 1:K:484:PRO:HD2 | 1:K:609:TRP:CE3 | 2.55 | 0.41 |
| 1:K:511:TYR:HD2 | 1:K:520:VAL:HG22 | 1.84 | 0.41 |
| 1:M:322:GLN:CB | 1:N:340:THR:HB | 2.50 | 0.41 |
| 1:O:290:PHE:HE2 | 1:O:614:VAL:HB | 1.84 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:450:ARG:HG2 | 1:P:452:GLN:H | 1.85 | 0.41 |
| 1:Q:322:GLN:CB | 1:S:340:THR:HB | 2.50 | 0.41 |
| 1:S:256:HIS:CD2 | 1:S:655:PRO:HB3 | 2.55 | 0.41 |
| 1:T:473:MET:HE3 | 1:T:473:MET:HB2 | 1.81 | 0.41 |
| 1:U:382:THR:HG21 | 1:U:394:SER:N | 2.35 | 0.41 |
| 1:V:330:GLU:N | 1:V:330:GLU:CD | 2.78 | 0.41 |
| 1:W:340:THR:O | 1:W:407:ARG:CZ | 2.67 | 0.41 |
| 1:W:421:VAL:CG2 | 1:W:422:PRO:HD2 | 2.50 | 0.41 |
| 1:X:324:LYS:HE3 | 1:Y:656:VAL:HG11 | 2.02 | 0.41 |
| 1:X:329:ASN:O | 1:X:332:THR:OG1 | 2.31 | 0.41 |
| 1:X:568:ILE:HD12 | 1:X:572:ASN:HD22 | 1.84 | 0.41 |
| 1:Y:220:ASP:OD1 | 1:Y:220:ASP:N | 2.50 | 0.41 |
| 1:Y:342:THR:HG22 | 1:Y:407:ARG:HA | 2.02 | 0.41 |
| 1:Z:256:HIS:CD2 | 1:Z:655:PRO:HB3 | 2.55 | 0.41 |
| 1:Z:421:VAL:CG2 | 1:Z:422:PRO:HD2 | 2.50 | 0.41 |
| 1:a:264:GLY:HA2 | 1:a:387:SER:HB3 | 2.01 | 0.41 |
| 1:b:450:ARG:HG2 | 1:b:452:GLN:H | 1.85 | 0.41 |
| 1:b:511:TYR:HD2 | 1:b:520:VAL:HG22 | 1.84 | 0.41 |
| 1:c:340:THR:HB | 1:s:322:GLN:HB3 | 2.01 | 0.41 |
| 1:c:450:ARG:HG2 | 1:c:452:GLN:H | 1.85 | 0.41 |
| 1:c:586:LEU:HD21 | 1:o:490:ARG:CZ | 2.50 | 0.41 |
| 1:e:324:LYS:HE3 | 1:h:656:VAL:HG11 | 2.02 | 0.41 |
| 1:k:264:GLY:HA2 | 1:k:387:SER:HB3 | 2.01 | 0.41 |
| 1:k:278:TYR:CE2 | 1:k:395:PHE:HD1 | 2.37 | 0.41 |
| 1:k:450:ARG:HG2 | 1:k:452:GLN:H | 1.85 | 0.41 |
| 1:k:571:THR:HG22 | 1:k:608:VAL:O | 2.20 | 0.41 |
| 1:l:342:THR:HG22 | 1:l:407:ARG:HA | 2.02 | 0.41 |
| 1:m:322:GLN:HB3 | 1:s:340:THR:HB | 2.01 | 0.41 |
| 1:m:421:VAL:CG2 | 1:m:422:PRO:HD2 | 2.50 | 0.41 |
| 1:o:342:THR:HG22 | 1:o:407:ARG:HA | 2.02 | 0.41 |
| 1:o:381:LEU:HD23 | 1:o:381:LEU:HA | 1.90 | 0.41 |
| 1:o:586:LEU:HD21 | 1:p:490:ARG:CZ | 2.50 | 0.41 |
| 1:p:322:GLN:CB | 1:q:340:THR:HB | 2.50 | 0.41 |
| 1:p:324:LYS:HE3 | 1:q:656:VAL:HG11 | 2.02 | 0.41 |
| 1:q:421:VAL:CG2 | 1:q:422:PRO:HD2 | 2.50 | 0.41 |
| 1:r:421:VAL:CG2 | 1:r:422:PRO:HD2 | 2.50 | 0.41 |
| 1:s:342:THR:HG22 | 1:s:407:ARG:HA | 2.02 | 0.41 |
| 1:s:511:TYR:HD2 | 1:s:520:VAL:HG22 | 1.84 | 0.41 |
| 1:t:450:ARG:HG2 | 1:t:452:GLN:H | 1.85 | 0.41 |
| 1:t:702:GLN:HB2 | 1:5:704:THR:HB | 2.03 | 0.41 |
| 1:u:256:HIS:CD2 | 1:u:655:PRO:HB3 | 2.55 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:u:342:THR:HG22 | 1:u:407:ARG:HA | 2.02 | 0.41 |
| 1:u:702:GLN:HB2 | 1:1:704:THR:HB | 2.02 | 0.41 |
| 1:u:704:THR:HB | 1:1:702:GLN:HB2 | 2.02 | 0.41 |
| 1:v:421:VAL:CG2 | 1:v:422:PRO:HD2 | 2.50 | 0.41 |
| 1:x:328:GLN:HE22 | 1:x:333:LYS:CG | 2.30 | 0.41 |
| 1:x:568:ILE:HD12 | 1:x:572:ASN:HD22 | 1.84 | 0.41 |
| 1:y:256:HIS:CD2 | 1:y:655:PRO:HB3 | 2.55 | 0.41 |
| 1:y:330:GLU:N | 1:y:330:GLU:CD | 2.78 | 0.41 |
| 1:z:342:THR:HG22 | 1:z:407:ARG:HA | 2.02 | 0.41 |
| 1:z:450:ARG:HG2 | 1:z:452:GLN:H | 1.85 | 0.41 |
| 1:1:319:PHE:CE1 | 1:1:680:GLN:HB2 | 2.55 | 0.41 |
| 1:2:527:ALA:O | 1:2:575:ALA:N | 2.45 | 0.41 |
| 1:2:571:THR:HG22 | 1:2:608:VAL:O | 2.20 | 0.41 |
| 1:3:484:PRO:HD2 | 1:3:609:TRP:CE3 | 2.55 | 0.41 |
| 1:5:381:LEU:HD23 | 1:5:381:LEU:HA | 1.90 | 0.41 |
| 1:7:312:LYS:HA | 1:7:312:LYS:HD2 | 1.90 | 0.41 |
| 1:7:571:THR:HG22 | 1:7:608:VAL:O | 2.20 | 0.41 |
| 1:8:450:ARG:HG2 | 1:8:452:GLN:H | 1.85 | 0.41 |
| 1:A:342:THR:HG22 | 1:A:407:ARG:HA | 2.02 | 0.41 |
| 1:A:490:ARG:CZ | 1:I:586:LEU:HD21 | 2.50 | 0.41 |
| 1:B:342:THR:HG22 | 1:B:407:ARG:HA | 2.02 | 0.41 |
| 1:B:450:ARG:HG2 | 1:B:452:GLN:H | 1.85 | 0.41 |
| 1:C:511:TYR:HD2 | 1:C:520:VAL:HG22 | 1.84 | 0.41 |
| 1:E:220:ASP:OD1 | 1:E:220:ASP:N | 2.50 | 0.41 |
| 1:G:382:THR:HG21 | 1:G:394:SER:N | 2.36 | 0.41 |
| 1:G:421:VAL:CG2 | 1:G:422:PRO:HD2 | 2.50 | 0.41 |
| 1:H:340:THR:HB | 1:Z:322:GLN:HB3 | 2.01 | 0.41 |
| 1:H:511:TYR:HD2 | 1:H:520:VAL:HG22 | 1.84 | 0.41 |
| 1:I:421:VAL:CG2 | 1:I:422:PRO:HD2 | 2.50 | 0.41 |
| 1:K:220:ASP:OD1 | 1:K:220:ASP:N | 2.50 | 0.41 |
| 1:O:256:HIS:CD2 | 1:O:655:PRO:HB3 | 2.55 | 0.41 |
| 1:O:312:LYS:HA | 1:O:312:LYS:HD2 | 1.90 | 0.41 |
| 1:P:511:TYR:HD2 | 1:P:520:VAL:HG22 | 1.84 | 0.41 |
| 1:Q:290:PHE:O | 1:Q:293:HIS:N | 2.47 | 0.41 |
| 1:R:256:HIS:CD2 | 1:R:655:PRO:HB3 | 2.55 | 0.41 |
| 1:R:340:THR:HB | 1:V:322:GLN:HB3 | 2.01 | 0.41 |
| 1:R:450:ARG:HG2 | 1:R:452:GLN:H | 1.85 | 0.41 |
| 1:R:700:GLU:HB2 | 1:R:702:GLN:HE21 | 1.85 | 0.41 |
| 1:S:342:THR:HG22 | 1:S:407:ARG:HA | 2.02 | 0.41 |
| 1:S:484:PRO:HD2 | 1:S:609:TRP:CE3 | 2.55 | 0.41 |
| 1:S:704:THR:HB | 1:T:702:GLN:HB2 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:319:PHE:CE1 | 1:T:680:GLN:HB2 | 2.55 | 0.41 |
| 1:U:700:GLU:HB2 | 1:U:702:GLN:HE21 | 1.85 | 0.41 |
| 1:W:328:GLN:HE22 | 1:W:333:LYS:CG | 2.30 | 0.41 |
| 1:X:328:GLN:HE22 | 1:X:333:LYS:CG | 2.30 | 0.41 |
| 1:X:512:HIS:CE1 | 1:X:515:GLY:HA2 | 2.56 | 0.41 |
| 1:Z:511:TYR:HD2 | 1:Z:520:VAL:HG22 | 1.84 | 0.41 |
| 1:b:342:THR:HG22 | 1:b:407:ARG:HA | 2.02 | 0.41 |
| 1:c:319:PHE:CE1 | 1:c:680:GLN:HB2 | 2.55 | 0.41 |
| 1:e:330:GLU:N | 1:e:330:GLU:CD | 2.78 | 0.41 |
| 1:g:328:GLN:HE22 | 1:g:333:LYS:CG | 2.30 | 0.41 |
| 1:k:421:VAL:CG2 | 1:k:422:PRO:HD2 | 2.50 | 0.41 |
| 1:l:435:ARG:HD3 | 1:l:435:ARG:HA | 1.79 | 0.41 |
| 1:o:341:SER:HB3 | 1:o:675:GLN:NE2 | 2.32 | 0.41 |
| 1:o:421:VAL:CG2 | 1:o:422:PRO:HD2 | 2.50 | 0.41 |
| 1:p:290:PHE:HE2 | 1:p:614:VAL:HB | 1.84 | 0.41 |
| 1:p:340:THR:HB | 1:6:322:GLN:HB3 | 2.01 | 0.41 |
| 1:p:382:THR:HG21 | 1:p:394:SER:N | 2.36 | 0.41 |
| 1:p:421:VAL:CG2 | 1:p:422:PRO:HD2 | 2.50 | 0.41 |
| 1:p:656:VAL:HG11 | 1:6:324:LYS:HE3 | 2.02 | 0.41 |
| 1:q:340:THR:O | 1:q:407:ARG:CZ | 2.67 | 0.41 |
| 1:q:452:GLN:HE21 | 1:q:459:GLY:HA3 | 1.83 | 0.41 |
| 1:r:342:THR:HG22 | 1:r:407:ARG:HA | 2.02 | 0.41 |
| 1:r:382:THR:HG21 | 1:r:394:SER:N | 2.35 | 0.41 |
| 1:u:340:THR:HB | 1:5:322:GLN:CB | 2.50 | 0.41 |
| 1:u:484:PRO:HD2 | 1:u:609:TRP:CE3 | 2.55 | 0.41 |
| 1:w:700:GLU:HB2 | 1:w:702:GLN:HE21 | 1.85 | 0.41 |
| 1:x:512:HIS:CE1 | 1:x:515:GLY:HA2 | 2.56 | 0.41 |
| 1:z:330:GLU:N | 1:z:330:GLU:CD | 2.78 | 0.41 |
| 1:z:700:GLU:HB2 | 1:z:702:GLN:HE21 | 1.85 | 0.41 |
| 1:3:256:HIS:CD2 | 1:3:655:PRO:HB3 | 2.55 | 0.41 |
| 1:3:290:PHE:HE2 | 1:3:614:VAL:HB | 1.84 | 0.41 |
| 1:3:329:ASN:CA | 1:3:330:GLU:OE1 | 2.65 | 0.41 |
| 1:5:340:THR:HB | 1:8:322:GLN:CB | 2.50 | 0.41 |
| 1:6:571:THR:HG22 | 1:6:608:VAL:O | 2.20 | 0.41 |
| 1:7:700:GLU:HB2 | 1:7:702:GLN:HE21 | 1.85 | 0.41 |
| 1:8:256:HIS:CD2 | 1:8:655:PRO:HB3 | 2.55 | 0.41 |
| 1:8:328:GLN:HE22 | 1:8:333:LYS:CG | 2.30 | 0.41 |
| 1:8:340:THR:O | 1:8:407:ARG:NE | 2.52 | 0.41 |
| 1:A:324:LYS:HE3 | 1:E:656:VAL:HG11 | 2.02 | 0.41 |
| 1:A:330:GLU:N | 1:A:330:GLU:CD | 2.78 | 0.41 |
| 1:A:511:TYR:HD2 | 1:A:520:VAL:HG22 | 1.84 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:704:THR:HB | 1:F:702:GLN:HB2 | 2.03 | 0.41 |
| 1:C:381:LEU:HD23 | 1:C:381:LEU:HA | 1.90 | 0.41 |
| 1:C:512:HIS:CE1 | 1:C:515:GLY:HA2 | 2.56 | 0.41 |
| 1:D:220:ASP:OD1 | 1:D:220:ASP:N | 2.50 | 0.41 |
| 1:E:253:TYR:HB2 | 1:E:281:PRO:O | 2.21 | 0.41 |
| 1:E:484:PRO:HD2 | 1:E:609:TRP:CE3 | 2.56 | 0.41 |
| 1:F:340:THR:HB | 1:R:322:GLN:CB | 2.50 | 0.41 |
| 1:F:490:ARG:CZ | 1:Q:586:LEU:HD21 | 2.50 | 0.41 |
| 1:F:571:THR:HG22 | 1:F:608:VAL:O | 2.20 | 0.41 |
| 1:G:341:SER:HB3 | 1:G:675:GLN:NE2 | 2.32 | 0.41 |
| 1:H:253:TYR:HB2 | 1:H:281:PRO:O | 2.21 | 0.41 |
| 1:H:256:HIS:CD2 | 1:H:655:PRO:HB3 | 2.55 | 0.41 |
| 1:I:511:TYR:HD2 | 1:I:520:VAL:HG22 | 1.84 | 0.41 |
| 1:J:571:THR:HG22 | 1:J:608:VAL:O | 2.20 | 0.41 |
| 1:L:382:THR:HG21 | 1:L:394:SER:N | 2.35 | 0.41 |
| 1:M:256:HIS:CD2 | 1:M:655:PRO:HB3 | 2.55 | 0.41 |
| 1:M:571:THR:HG22 | 1:M:608:VAL:O | 2.20 | 0.41 |
| 1:N:702:GLN:HB2 | 1:O:704:THR:HB | 2.02 | 0.41 |
| 1:O:450:ARG:HG2 | 1:O:452:GLN:H | 1.85 | 0.41 |
| 1:P:256:HIS:CD2 | 1:P:655:PRO:HB3 | 2.55 | 0.41 |
| 1:P:322:GLN:CB | 1:Q:340:THR:HB | 2.50 | 0.41 |
| 1:P:328:GLN:HE22 | 1:P:333:LYS:CG | 2.30 | 0.41 |
| 1:P:700:GLU:HB2 | 1:P:702:GLN:HE21 | 1.85 | 0.41 |
| 1:Q:381:LEU:HD23 | 1:Q:381:LEU:HA | 1.90 | 0.41 |
| 1:Q:450:ARG:HG2 | 1:Q:452:GLN:H | 1.85 | 0.41 |
| 1:Q:484:PRO:HD2 | 1:Q:609:TRP:CE3 | 2.55 | 0.41 |
| 1:Q:704:THR:HB | 1:R:702:GLN:HB2 | 2.03 | 0.41 |
| 1:R:659:ASP:OD1 | 1:R:659:ASP:N | 2.54 | 0.41 |
| 1:U:253:TYR:HB2 | 1:U:281:PRO:O | 2.21 | 0.41 |
| 1:U:322:GLN:CB | 1:e:340:THR:HB | 2.50 | 0.41 |
| 1:V:256:HIS:CD2 | 1:V:655:PRO:HB3 | 2.55 | 0.41 |
| 1:V:571:THR:HG22 | 1:V:608:VAL:O | 2.20 | 0.41 |
| 1:W:452:GLN:HE21 | 1:W:459:GLY:HA3 | 1.84 | 0.41 |
| 1:X:340:THR:HB | 1:f:322:GLN:HB3 | 2.01 | 0.41 |
| 1:X:342:THR:HG22 | 1:X:407:ARG:HA | 2.02 | 0.41 |
| 1:Y:382:THR:HG21 | 1:Y:394:SER:N | 2.36 | 0.41 |
| 1:a:702:GLN:HB2 | 1:3:704:THR:HB | 2.03 | 0.41 |
| 1:c:421:VAL:CG2 | 1:c:422:PRO:HD2 | 2.50 | 0.41 |
| 1:c:452:GLN:HE21 | 1:c:459:GLY:HA3 | 1.84 | 0.41 |
| 1:c:511:TYR:HD2 | 1:c:520:VAL:HG22 | 1.84 | 0.41 |
| 1:e:256:HIS:CD2 | 1:e:655:PRO:HB3 | 2.55 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:e:290:PHE:HE2 | 1:e:614:VAL:HB | 1.84 | 0.41 |
| 1:e:484:PRO:HD2 | 1:e:609:TRP:CE3 | 2.55 | 0.41 |
| 1:e:512:HIS:CE1 | 1:e:515:GLY:HA2 | 2.56 | 0.41 |
| 1:e:700:GLU:HB2 | 1:e:702:GLN:HE21 | 1.85 | 0.41 |
| 1:f:264:GLY:HA2 | 1:f:387:SER:HB3 | 2.01 | 0.41 |
| 1:f:340:THR:HB | 1:z:322:GLN:CB | 2.50 | 0.41 |
| 1:f:659:ASP:OD1 | 1:f:659:ASP:N | 2.54 | 0.41 |
| 1:h:253:TYR:HB2 | 1:h:281:PRO:O | 2.21 | 0.41 |
| 1:h:264:GLY:HA2 | 1:h:387:SER:HB3 | 2.01 | 0.41 |
| 1:j:264:GLY:HA2 | 1:j:387:SER:HB3 | 2.01 | 0.41 |
| 1:j:473:MET:HE3 | 1:j:473:MET:HB2 | 1.81 | 0.41 |
| 1:j:512:HIS:CE1 | 1:j:515:GLY:HA2 | 2.56 | 0.41 |
| 1:k:290:PHE:O | 1:k:293:HIS:N | 2.47 | 0.41 |
| 1:l:256:HIS:CD2 | 1:l:655:PRO:HB3 | 2.55 | 0.41 |
| 1:l:297:ARG:HG3 | 1:l:301:ARG:NH1 | 2.34 | 0.41 |
| 1:l:700:GLU:HB2 | 1:l:702:GLN:HE21 | 1.85 | 0.41 |
| 1:m:256:HIS:CD2 | 1:m:655:PRO:HB3 | 2.55 | 0.41 |
| 1:m:511:TYR:HD2 | 1:m:520:VAL:HG22 | 1.84 | 0.41 |
| 1:n:264:GLY:HA2 | 1:n:387:SER:HB3 | 2.01 | 0.41 |
| 1:o:330:GLU:N | 1:o:330:GLU:CD | 2.78 | 0.41 |
| 1:p:568:ILE:HD12 | 1:p:572:ASN:HD22 | 1.84 | 0.41 |
| 1:q:328:GLN:HE22 | 1:q:333:LYS:CG | 2.30 | 0.41 |
| 1:q:702:GLN:HB2 | 1:x:704:THR:HB | 2.02 | 0.41 |
| 1:s:253:TYR:HB2 | 1:s:281:PRO:O | 2.21 | 0.41 |
| 1:s:256:HIS:CD2 | 1:s:655:PRO:HB3 | 2.55 | 0.41 |
| 1:s:450:ARG:HG2 | 1:s:452:GLN:H | 1.85 | 0.41 |
| 1:t:312:LYS:HA | 1:t:312:LYS:HD2 | 1.90 | 0.41 |
| 1:t:342:THR:HG22 | 1:t:407:ARG:CG | 2.47 | 0.41 |
| 1:t:659:ASP:OD1 | 1:t:659:ASP:N | 2.54 | 0.41 |
| 1:u:568:ILE:HD12 | 1:u:572:ASN:HD22 | 1.84 | 0.41 |
| 1:v:253:TYR:HB2 | 1:v:281:PRO:O | 2.21 | 0.41 |
| 1:v:382:THR:HG21 | 1:v:394:SER:N | 2.36 | 0.41 |
| 1:v:700:GLU:HB2 | 1:v:702:GLN:HE21 | 1.85 | 0.41 |
| 1:w:256:HIS:CD2 | 1:w:655:PRO:HB3 | 2.55 | 0.41 |
| 1:w:330:GLU:N | 1:w:330:GLU:CD | 2.78 | 0.41 |
| 1:w:512:HIS:CE1 | 1:w:515:GLY:HA2 | 2.56 | 0.41 |
| 1:x:342:THR:HG22 | 1:x:407:ARG:HA | 2.02 | 0.41 |
| 1:y:571:THR:HG22 | 1:y:608:VAL:O | 2.20 | 0.41 |
| 1:z:253:TYR:HB2 | 1:z:281:PRO:O | 2.21 | 0.41 |
| 1:z:297:ARG:HG3 | 1:z:301:ARG:NH1 | 2.34 | 0.41 |
| 1:z:341:SER:HB3 | 1:z:675:GLN:NE2 | 2.32 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2:511:TYR:HD2 | 1:2:520:VAL:HG22 | 1.84 | 0.41 |
| 1:4:421:VAL:CG2 | 1:4:422:PRO:HD2 | 2.50 | 0.41 |
| 1:5:450:ARG:HG2 | 1:5:452:GLN:H | 1.85 | 0.41 |
| 1:5:484:PRO:HD2 | 1:5:609:TRP:CE3 | 2.55 | 0.41 |
| 1:7:253:TYR:HB2 | 1:7:281:PRO:O | 2.21 | 0.41 |
| 1:7:435:ARG:HA | 1:7:435:ARG:HD3 | 1.79 | 0.41 |
| 1:7:484:PRO:HD2 | 1:7:609:TRP:CE3 | 2.55 | 0.41 |
| 1:8:700:GLU:HB2 | 1:8:702:GLN:HE21 | 1.85 | 0.41 |
| 1:B:511:TYR:HD2 | 1:B:520:VAL:HG22 | 1.84 | 0.41 |
| 1:C:700:GLU:HB2 | 1:C:702:GLN:HE21 | 1.85 | 0.41 |
| 1:D:319:PHE:CE1 | 1:D:680:GLN:HB2 | 2.55 | 0.41 |
| 1:D:421:VAL:CG2 | 1:D:422:PRO:HD2 | 2.50 | 0.41 |
| 1:E:586:LEU:HD21 | 1:Q:490:ARG:CZ | 2.51 | 0.41 |
| 1:F:324:LYS:HE3 | 1:G:656:VAL:HG11 | 2.02 | 0.41 |
| 1:G:256:HIS:CD2 | 1:G:655:PRO:HB3 | 2.55 | 0.41 |
| 1:H:450:ARG:HG2 | 1:H:452:GLN:H | 1.85 | 0.41 |
| 1:H:512:HIS:CE1 | 1:H:515:GLY:HA2 | 2.56 | 0.41 |
| 1:I:568:ILE:HD12 | 1:I:572:ASN:HD22 | 1.84 | 0.41 |
| 1:J:256:HIS:CD2 | 1:J:655:PRO:HB3 | 2.55 | 0.41 |
| 1:K:232:ASP:HB3 | 1:L:402:PRO:CG | 2.46 | 0.41 |
| 1:K:659:ASP:OD1 | 1:K:659:ASP:N | 2.54 | 0.41 |
| 1:L:512:HIS:CE1 | 1:L:515:GLY:HA2 | 2.56 | 0.41 |
| 1:N:264:GLY:HA2 | 1:N:387:SER:HB3 | 2.01 | 0.41 |
| 1:P:421:VAL:CG2 | 1:P:422:PRO:HD2 | 2.50 | 0.41 |
| 1:P:659:ASP:N | 1:P:659:ASP:OD1 | 2.54 | 0.41 |
| 1:R:312:LYS:HA | 1:R:312:LYS:HD2 | 1.90 | 0.41 |
| 1:S:382:THR:HG21 | 1:S:394:SER:N | 2.36 | 0.41 |
| 1:S:586:LEU:HD21 | 1:U:490:ARG:CZ | 2.50 | 0.41 |
| 1:T:340:THR:HB | 1:i:322:GLN:HB3 | 2.01 | 0.41 |
| 1:T:571:THR:HG22 | 1:T:608:VAL:O | 2.20 | 0.41 |
| 1:U:511:TYR:HD2 | 1:U:520:VAL:HG22 | 1.84 | 0.41 |
| 1:V:490:ARG:CZ | 1:X:586:LEU:HD21 | 2.50 | 0.41 |
| 1:Y:659:ASP:OD1 | 1:Y:659:ASP:N | 2.54 | 0.41 |
| 1:Z:253:TYR:HB2 | 1:Z:281:PRO:O | 2.21 | 0.41 |
| 1:Z:656:VAL:HG11 | 1:a:324:LYS:HE3 | 2.02 | 0.41 |
| 1:d:421:VAL:CG2 | 1:d:422:PRO:HD2 | 2.50 | 0.41 |
| 1:d:511:TYR:HD2 | 1:d:520:VAL:HG22 | 1.84 | 0.41 |
| 1:d:527:ALA:O | 1:d:575:ALA:N | 2.45 | 0.41 |
| 1:f:421:VAL:CG2 | 1:f:422:PRO:HD2 | 2.50 | 0.41 |
| 1:f:586:LEU:HD21 | 1:h:490:ARG:CZ | 2.50 | 0.41 |
| 1:g:340:THR:HB | 1:k:322:GLN:CB | 2.50 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:i:429:HIS:HD2 | 1:i:610:GLN:OE1 | 1.94 | 0.41 |
| 1:i:571:THR:HG22 | 1:i:608:VAL:O | 2.20 | 0.41 |
| 1:j:421:VAL:CG2 | 1:j:422:PRO:HD2 | 2.50 | 0.41 |
| 1:j:659:ASP:OD1 | 1:j:659:ASP:N | 2.54 | 0.41 |
| 1:k:253:TYR:HB2 | 1:k:281:PRO:O | 2.21 | 0.41 |
| 1:k:452:GLN:HE21 | 1:k:459:GLY:HA3 | 1.84 | 0.41 |
| 1:l:253:TYR:HB2 | 1:l:281:PRO:O | 2.21 | 0.41 |
| 1:m:253:TYR:HB2 | 1:m:281:PRO:O | 2.21 | 0.41 |
| 1:m:586:LEU:HD21 | 1:n:490:ARG:CZ | 2.50 | 0.41 |
| 1:o:452:GLN:HE21 | 1:o:459:GLY:HA3 | 1.84 | 0.41 |
| 1:p:256:HIS:CD2 | 1:p:655:PRO:HB3 | 2.55 | 0.41 |
| 1:p:341:SER:HB3 | 1:p:675:GLN:NE2 | 2.32 | 0.41 |
| 1:q:571:THR:HG22 | 1:q:608:VAL:O | 2.20 | 0.41 |
| 1:r:434:ASP:OD1 | 1:r:434:ASP:N | 2.41 | 0.41 |
| 1:r:659:ASP:OD1 | 1:r:659:ASP:N | 2.54 | 0.41 |
| 1:s:512:HIS:CE1 | 1:s:515:GLY:HA2 | 2.56 | 0.41 |
| 1:s:585:ASN:OD1 | 1:s:594:ILE:N | 2.45 | 0.41 |
| 1:t:473:MET:HB2 | 1:t:473:MET:HE3 | 1.81 | 0.41 |
| 1:u:290:PHE:HE2 | 1:u:614:VAL:HB | 1.84 | 0.41 |
| 1:u:382:THR:HG21 | 1:u:394:SER:N | 2.36 | 0.41 |
| 1:u:586:LEU:HD21 | 1:v:490:ARG:CZ | 2.51 | 0.41 |
| 1:v:340:THR:HB | 1:1:322:GLN:CB | 2.50 | 0.41 |
| 1:v:341:SER:HB3 | 1:v:675:GLN:NE2 | 2.32 | 0.41 |
| 1:z:429:HIS:NE2 | 1:z:610:GLN:CD | 2.79 | 0.41 |
| 1:2:253:TYR:HB2 | 1:2:281:PRO:O | 2.21 | 0.41 |
| 1:2:421:VAL:CG2 | 1:2:422:PRO:HD2 | 2.50 | 0.41 |
| 1:3:450:ARG:HG2 | 1:3:452:GLN:H | 1.85 | 0.41 |
| 1:4:264:GLY:HA2 | 1:4:387:SER:HB3 | 2.01 | 0.41 |
| 1:5:586:LEU:HD21 | 1:6:490:ARG:CZ | 2.50 | 0.41 |
| 1:6:511:TYR:HD2 | 1:6:520:VAL:HG22 | 1.85 | 0.41 |
| 1:7:220:ASP:OD1 | 1:7:220:ASP:N | 2.50 | 0.41 |
| 1:8:253:TYR:HB2 | 1:8:281:PRO:O | 2.21 | 0.41 |
| 1:8:264:GLY:HA2 | 1:8:387:SER:HB3 | 2.01 | 0.41 |
| 1:8:511:TYR:HD2 | 1:8:520:VAL:HG22 | 1.85 | 0.41 |
| 1:A:452:GLN:HE21 | 1:A:459:GLY:HA3 | 1.84 | 0.41 |
| 1:A:512:HIS:CE1 | 1:A:515:GLY:HA2 | 2.56 | 0.41 |
| 1:A:571:THR:HG22 | 1:A:608:VAL:O | 2.20 | 0.41 |
| 1:C:290:PHE:HE2 | 1:C:614:VAL:HB | 1.84 | 0.41 |
| 1:D:256:HIS:CD2 | 1:D:655:PRO:HB3 | 2.55 | 0.41 |
| 1:D:659:ASP:OD1 | 1:D:659:ASP:N | 2.54 | 0.41 |
| 1:E:450:ARG:HG2 | 1:E:452:GLN:H | 1.85 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:429:HIS:NE2 | 1:F:610:GLN:CD | 2.79 | 0.41 |
| 1:H:344:GLN:HG2 | 1:H:405:MET:HG2 | 2.03 | 0.41 |
| 1:H:421:VAL:CG2 | 1:H:422:PRO:HD2 | 2.50 | 0.41 |
| 1:I:452:GLN:HE21 | 1:I:459:GLY:HA3 | 1.84 | 0.41 |
| 1:J:344:GLN:HG2 | 1:J:405:MET:HG2 | 2.03 | 0.41 |
| 1:J:429:HIS:NE2 | 1:J:610:GLN:CD | 2.79 | 0.41 |
| 1:K:319:PHE:CE1 | 1:K:680:GLN:HB2 | 2.55 | 0.41 |
| 1:K:421:VAL:CG2 | 1:K:422:PRO:HD2 | 2.50 | 0.41 |
| 1:L:421:VAL:CG2 | 1:L:422:PRO:HD2 | 2.50 | 0.41 |
| 1:M:700:GLU:HB2 | 1:M:702:GLN:HE21 | 1.85 | 0.41 |
| 1:O:253:TYR:HB2 | 1:O:281:PRO:O | 2.21 | 0.41 |
| 1:O:342:THR:HG22 | 1:O:407:ARG:HA | 2.02 | 0.41 |
| 1:P:253:TYR:HB2 | 1:P:281:PRO:O | 2.21 | 0.41 |
| 1:P:264:GLY:HA2 | 1:P:387:SER:HB3 | 2.01 | 0.41 |
| 1:P:322:GLN:HB3 | 1:Q:340:THR:HB | 2.01 | 0.41 |
| 1:Q:421:VAL:CG2 | 1:Q:422:PRO:HD2 | 2.50 | 0.41 |
| 1:S:290:PHE:HE2 | 1:S:614:VAL:HB | 1.84 | 0.41 |
| 1:S:322:GLN:HB3 | 1:d:340:THR:HB | 2.01 | 0.41 |
| 1:S:568:ILE:HD12 | 1:S:572:ASN:HD22 | 1.84 | 0.41 |
| 1:T:322:GLN:CB | 1:U:340:THR:HB | 2.50 | 0.41 |
| 1:T:421:VAL:CG2 | 1:T:422:PRO:HD2 | 2.50 | 0.41 |
| 1:U:702:GLN:HB2 | 1:V:704:THR:HB | 2.02 | 0.41 |
| 1:W:319:PHE:CE1 | 1:W:680:GLN:HB2 | 2.55 | 0.41 |
| 1:W:571:THR:HG22 | 1:W:608:VAL:O | 2.20 | 0.41 |
| 1:W:659:ASP:OD1 | 1:W:659:ASP:N | 2.54 | 0.41 |
| 1:X:656:VAL:HG11 | 1:f:324:LYS:HE3 | 2.03 | 0.41 |
| 1:Y:571:THR:HG22 | 1:Y:608:VAL:O | 2.20 | 0.41 |
| 1:a:342:THR:HG22 | 1:a:407:ARG:CG | 2.47 | 0.41 |
| 1:c:342:THR:HG22 | 1:c:407:ARG:HA | 2.02 | 0.41 |
| 1:d:253:TYR:HB2 | 1:d:281:PRO:O | 2.21 | 0.41 |
| 1:e:511:TYR:HD2 | 1:e:520:VAL:HG22 | 1.84 | 0.41 |
| 1:f:253:TYR:HB2 | 1:f:281:PRO:O | 2.21 | 0.41 |
| 1:f:340:THR:O | 1:f:407:ARG:CZ | 2.67 | 0.41 |
| 1:f:512:HIS:CE1 | 1:f:515:GLY:HA2 | 2.56 | 0.41 |
| 1:g:319:PHE:CE1 | 1:g:680:GLN:HB2 | 2.55 | 0.41 |
| 1:g:421:VAL:CG2 | 1:g:422:PRO:HD2 | 2.50 | 0.41 |
| 1:g:571:THR:HG22 | 1:g:608:VAL:O | 2.20 | 0.41 |
| 1:g:700:GLU:HB2 | 1:g:702:GLN:HE21 | 1.85 | 0.41 |
| 1:h:322:GLN:CB | 1:i:340:THR:HB | 2.50 | 0.41 |
| 1:h:452:GLN:HE21 | 1:h:459:GLY:HA3 | 1.84 | 0.41 |
| 1:h:700:GLU:HB2 | 1:h:702:GLN:HE21 | 1.85 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:i:319:PHE:CE1 | 1:i:680:GLN:HB2 | 2.55 | 0.41 |
| 1:i:328:GLN:HE22 | 1:i:333:LYS:CG | 2.30 | 0.41 |
| 1:j:340:THR:O | 1:j:407:ARG:CZ | 2.67 | 0.41 |
| 1:k:330:GLU:N | 1:k:330:GLU:CD | 2.78 | 0.41 |
| 1:k:700:GLU:HB2 | 1:k:702:GLN:HE21 | 1.85 | 0.41 |
| 1:l:429:HIS:NE2 | 1:l:610:GLN:CD | 2.79 | 0.41 |
| 1:n:421:VAL:CG2 | 1:n:422:PRO:HD2 | 2.50 | 0.41 |
| 1:n:659:ASP:N | 1:n:659:ASP:OD1 | 2.54 | 0.41 |
| 1:o:511:TYR:HD2 | 1:o:520:VAL:HG22 | 1.84 | 0.41 |
| 1:o:512:HIS:CE1 | 1:o:515:GLY:HA2 | 2.56 | 0.41 |
| 1:p:450:ARG:HG2 | 1:p:452:GLN:H | 1.85 | 0.41 |
| 1:q:319:PHE:CE1 | 1:q:680:GLN:HB2 | 2.55 | 0.41 |
| 1:r:571:THR:HG22 | 1:r:608:VAL:O | 2.20 | 0.41 |
| 1:s:344:GLN:HG2 | 1:s:405:MET:HG2 | 2.03 | 0.41 |
| 1:s:421:VAL:CG2 | 1:s:422:PRO:HD2 | 2.50 | 0.41 |
| 1:t:571:THR:HG22 | 1:t:608:VAL:O | 2.20 | 0.41 |
| 1:w:290:PHE:HE2 | 1:w:614:VAL:HB | 1.84 | 0.41 |
| 1:w:484:PRO:HD2 | 1:w:609:TRP:CE3 | 2.55 | 0.41 |
| 1:w:511:TYR:HD2 | 1:w:520:VAL:HG22 | 1.85 | 0.41 |
| 1:x:329:ASN:O | 1:x:332:THR:OG1 | 2.31 | 0.41 |
| 1:y:344:GLN:HG2 | 1:y:405:MET:HG2 | 2.03 | 0.41 |
| 1:y:450:ARG:HG2 | 1:y:452:GLN:H | 1.85 | 0.41 |
| 1:z:256:HIS:CD2 | 1:z:655:PRO:HB3 | 2.55 | 0.41 |
| 1:1:421:VAL:CG2 | 1:1:422:PRO:HD2 | 2.50 | 0.41 |
| 1:1:571:THR:HG22 | 1:1:608:VAL:O | 2.20 | 0.41 |
| 1:3:253:TYR:HB2 | 1:3:281:PRO:O | 2.21 | 0.41 |
| 1:4:571:THR:HG22 | 1:4:608:VAL:O | 2.20 | 0.41 |
| 1:5:290:PHE:O | 1:5:293:HIS:N | 2.47 | 0.41 |
| 1:5:340:THR:HB | 1:8:322:GLN:HB3 | 2.01 | 0.41 |
| 1:5:490:ARG:CZ | 1:7:586:LEU:HD21 | 2.51 | 0.41 |
| 1:6:290:PHE:HE2 | 1:6:614:VAL:HB | 1.84 | 0.41 |
| 1:7:450:ARG:HG2 | 1:7:452:GLN:H | 1.85 | 0.41 |
| 1:8:421:VAL:CG2 | 1:8:422:PRO:HD2 | 2.50 | 0.41 |
| 1:A:381:LEU:HD23 | 1:A:381:LEU:HA | 1.90 | 0.41 |
| 1:C:253:TYR:HB2 | 1:C:281:PRO:O | 2.21 | 0.41 |
| 1:C:421:VAL:CG2 | 1:C:422:PRO:HD2 | 2.50 | 0.41 |
| 1:E:512:HIS:CE1 | 1:E:515:GLY:HA2 | 2.56 | 0.41 |
| 1:F:290:PHE:HE2 | 1:F:614:VAL:HB | 1.84 | 0.41 |
| 1:F:511:TYR:HD2 | 1:F:520:VAL:HG22 | 1.85 | 0.41 |
| 1:G:450:ARG:HG2 | 1:G:452:GLN:H | 1.85 | 0.41 |
| 1:H:290:PHE:HE2 | 1:H:614:VAL:HB | 1.84 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:224:SER:OG | 1:I:225:SER:N | 2.50 | 0.41 |
| 1:I:342:THR:HG22 | 1:I:407:ARG:HA | 2.02 | 0.41 |
| 1:K:256:HIS:CD2 | 1:K:655:PRO:HB3 | 2.55 | 0.41 |
| 1:L:253:TYR:HB2 | 1:L:281:PRO:O | 2.21 | 0.41 |
| 1:L:700:GLU:HB2 | 1:L:702:GLN:HE21 | 1.85 | 0.41 |
| 1:M:344:GLN:HG2 | 1:M:405:MET:HG2 | 2.03 | 0.41 |
| 1:M:429:HIS:NE2 | 1:M:610:GLN:CD | 2.79 | 0.41 |
| 1:N:324:LYS:HE3 | 1:m:656:VAL:HG11 | 2.02 | 0.41 |
| 1:N:342:THR:HG22 | 1:N:407:ARG:HA | 2.02 | 0.41 |
| 1:Q:322:GLN:HB3 | 1:S:340:THR:HB | 2.01 | 0.41 |
| 1:R:344:GLN:HG2 | 1:R:405:MET:HG2 | 2.03 | 0.41 |
| 1:R:571:THR:HG22 | 1:R:608:VAL:O | 2.20 | 0.41 |
| 1:S:512:HIS:CE1 | 1:S:515:GLY:HA2 | 2.56 | 0.41 |
| 1:T:429:HIS:NE2 | 1:T:610:GLN:CD | 2.79 | 0.41 |
| 1:U:341:SER:HB3 | 1:U:675:GLN:NE2 | 2.32 | 0.41 |
| 1:V:344:GLN:HG2 | 1:V:405:MET:HG2 | 2.03 | 0.41 |
| 1:V:450:ARG:HG2 | 1:V:452:GLN:H | 1.85 | 0.41 |
| 1:Z:586:LEU:HD21 | 1:4:490:ARG:CZ | 2.50 | 0.41 |
| 1:a:342:THR:HG22 | 1:a:407:ARG:HA | 2.02 | 0.41 |
| 1:c:568:ILE:HD12 | 1:c:572:ASN:HD22 | 1.84 | 0.41 |
| 1:c:700:GLU:HB2 | 1:c:702:GLN:HE21 | 1.85 | 0.41 |
| 1:d:736:ARG:NH2 | 1:l:626:HIS:CD2 | 2.79 | 0.41 |
| 1:e:659:ASP:N | 1:e:659:ASP:OD1 | 2.54 | 0.41 |
| 1:g:322:GLN:HB3 | 1:1:340:THR:HB | 2.01 | 0.41 |
| 1:g:512:HIS:CE1 | 1:g:515:GLY:HA2 | 2.56 | 0.41 |
| 1:g:527:ALA:O | 1:g:575:ALA:N | 2.45 | 0.41 |
| 1:h:290:PHE:O | 1:h:293:HIS:N | 2.47 | 0.41 |
| 1:h:659:ASP:OD1 | 1:h:659:ASP:N | 2.54 | 0.41 |
| 1:i:421:VAL:CG2 | 1:i:422:PRO:HD2 | 2.50 | 0.41 |
| 1:i:512:HIS:CE1 | 1:i:515:GLY:HA2 | 2.56 | 0.41 |
| 1:i:568:ILE:HD12 | 1:i:572:ASN:HD22 | 1.84 | 0.41 |
| 1:i:700:GLU:HB2 | 1:i:702:GLN:HE21 | 1.85 | 0.41 |
| 1:j:253:TYR:HB2 | 1:j:281:PRO:O | 2.21 | 0.41 |
| 1:j:344:GLN:HG2 | 1:j:405:MET:HG2 | 2.03 | 0.41 |
| 1:k:402:PRO:HG3 | 1:w:232:ASP:CB | 2.48 | 0.41 |
| 1:k:512:HIS:CE1 | 1:k:515:GLY:HA2 | 2.56 | 0.41 |
| 1:n:571:THR:HG22 | 1:n:608:VAL:O | 2.20 | 0.41 |
| 1:o:571:THR:HG22 | 1:o:608:VAL:O | 2.20 | 0.41 |
| 1:q:322:GLN:CB | 1:y:340:THR:HB | 2.49 | 0.41 |
| 1:q:659:ASP:OD1 | 1:q:659:ASP:N | 2.54 | 0.41 |
| 1:r:512:HIS:CE1 | 1:r:515:GLY:HA2 | 2.56 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:r:656:VAL:HG11 | 1:x:324:LYS:HE3 | 2.03 | 0.41 |
| 1:r:700:GLU:HB2 | 1:r:702:GLN:HE21 | 1.85 | 0.41 |
| 1:t:344:GLN:HG2 | 1:t:405:MET:HG2 | 2.03 | 0.41 |
| 1:u:253:TYR:HB2 | 1:u:281:PRO:O | 2.21 | 0.41 |
| 1:u:322:GLN:HB3 | 1:2:340:THR:HB | 2.01 | 0.41 |
| 1:u:340:THR:HB | 1:5:322:GLN:HB3 | 2.01 | 0.41 |
| 1:u:512:HIS:CE1 | 1:u:515:GLY:HA2 | 2.56 | 0.41 |
| 1:w:438:ASN:HB2 | 1:x:356:VAL:HG21 | 2.02 | 0.41 |
| 1:x:473:MET:HB2 | 1:x:473:MET:HE3 | 1.81 | 0.41 |
| 1:y:381:LEU:HD23 | 1:y:381:LEU:HA | 1.90 | 0.41 |
| 1:y:421:VAL:CG2 | 1:y:422:PRO:HD2 | 2.50 | 0.41 |
| 1:z:220:ASP:OD1 | 1:z:220:ASP:N | 2.50 | 0.41 |
| 1:z:429:HIS:HD2 | 1:z:610:GLN:OE1 | 1.94 | 0.41 |
| 1:3:312:LYS:HA | 1:3:312:LYS:HD2 | 1.90 | 0.41 |
| 1:3:342:THR:HG22 | 1:3:407:ARG:HA | 2.02 | 0.41 |
| 1:3:421:VAL:CG2 | 1:3:422:PRO:HD2 | 2.50 | 0.41 |
| 1:4:659:ASP:N | 1:4:659:ASP:OD1 | 2.54 | 0.41 |
| 1:5:421:VAL:CG2 | 1:5:422:PRO:HD2 | 2.50 | 0.41 |
| 1:6:429:HIS:NE2 | 1:6:610:GLN:CD | 2.79 | 0.41 |
| 1:7:512:HIS:CE1 | 1:7:515:GLY:HA2 | 2.56 | 0.41 |
| 1:8:512:HIS:CE1 | 1:8:515:GLY:HA2 | 2.56 | 0.41 |
| 1:8:659:ASP:OD1 | 1:8:659:ASP:N | 2.54 | 0.41 |
| 1:A:340:THR:HB | 1:B:322:GLN:HB3 | 2.02 | 0.41 |
| 1:B:253:TYR:HB2 | 1:B:281:PRO:O | 2.21 | 0.41 |
| 1:B:429:HIS:NE2 | 1:B:610:GLN:CD | 2.79 | 0.41 |
| 1:B:452:GLN:HG3 | 1:B:459:GLY:O | 2.21 | 0.41 |
| 1:E:342:THR:HG22 | 1:E:407:ARG:HA | 2.02 | 0.41 |
| 1:E:435:ARG:HA | 1:E:435:ARG:HD3 | 1.79 | 0.41 |
| 1:F:256:HIS:CD2 | 1:F:655:PRO:HB3 | 2.55 | 0.41 |
| 1:G:704:THR:HB | 1:H:702:GLN:HB2 | 2.03 | 0.41 |
| 1:H:609:TRP:NE1 | 1:W:629:GLY:CA | 2.58 | 0.41 |
| 1:I:344:GLN:HG2 | 1:I:405:MET:HG2 | 2.03 | 0.41 |
| 1:I:429:HIS:NE2 | 1:I:610:GLN:CD | 2.79 | 0.41 |
| 1:J:700:GLU:HB2 | 1:J:702:GLN:HE21 | 1.85 | 0.41 |
| 1:K:512:HIS:CE1 | 1:K:515:GLY:HA2 | 2.56 | 0.41 |
| 1:L:290:PHE:HE2 | 1:L:614:VAL:HB | 1.84 | 0.41 |
| 1:L:429:HIS:NE2 | 1:L:610:GLN:CD | 2.79 | 0.41 |
| 1:N:253:TYR:HB2 | 1:N:281:PRO:O | 2.21 | 0.41 |
| 1:N:342:THR:HG22 | 1:N:407:ARG:CG | 2.47 | 0.41 |
| 1:O:421:VAL:CG2 | 1:O:422:PRO:HD2 | 2.50 | 0.41 |
| 1:P:571:THR:HG22 | 1:P:608:VAL:O | 2.20 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:253:TYR:HB2 | 1:Q:281:PRO:O | 2.21 | 0.41 |
| 1:Q:429:HIS:NE2 | 1:Q:610:GLN:CD | 2.79 | 0.41 |
| 1:Q:512:HIS:CE1 | 1:Q:515:GLY:HA2 | 2.56 | 0.41 |
| 1:S:253:TYR:HB2 | 1:S:281:PRO:O | 2.21 | 0.41 |
| 1:T:253:TYR:HB2 | 1:T:281:PRO:O | 2.21 | 0.41 |
| 1:T:324:LYS:HE3 | 1:U:656:VAL:HG11 | 2.02 | 0.41 |
| 1:T:512:HIS:CE1 | 1:T:515:GLY:HA2 | 2.56 | 0.41 |
| 1:V:421:VAL:CG2 | 1:V:422:PRO:HD2 | 2.50 | 0.41 |
| 1:V:429:HIS:NE2 | 1:V:610:GLN:CD | 2.79 | 0.41 |
| 1:V:626:HIS:CD2 | 1:X:736:ARG:NH2 | 2.79 | 0.41 |
| 1:X:429:HIS:NE2 | 1:X:610:GLN:CD | 2.79 | 0.41 |
| 1:Y:322:GLN:CB | 1:4:340:THR:HB | 2.51 | 0.41 |
| 1:Z:659:ASP:N | 1:Z:659:ASP:OD1 | 2.54 | 0.41 |
| 1:a:253:TYR:HB2 | 1:a:281:PRO:O | 2.21 | 0.41 |
| 1:b:322:GLN:CB | 1:o:340:THR:HB | 2.50 | 0.41 |
| 1:b:429:HIS:NE2 | 1:b:610:GLN:CD | 2.79 | 0.41 |
| 1:b:452:GLN:HG3 | 1:b:459:GLY:O | 2.21 | 0.41 |
| 1:c:224:SER:OG | 1:c:225:SER:N | 2.50 | 0.41 |
| 1:c:429:HIS:NE2 | 1:c:610:GLN:CD | 2.79 | 0.41 |
| 1:h:330:GLU:N | 1:h:330:GLU:CD | 2.78 | 0.41 |
| 1:h:342:THR:HG22 | 1:h:407:ARG:HA | 2.02 | 0.41 |
| 1:h:512:HIS:CE1 | 1:h:515:GLY:HA2 | 2.56 | 0.41 |
| 1:k:340:THR:HB | 1:w:322:GLN:CB | 2.50 | 0.41 |
| 1:k:382:THR:HG21 | 1:k:394:SER:N | 2.36 | 0.41 |
| 1:k:659:ASP:OD1 | 1:k:659:ASP:N | 2.54 | 0.41 |
| 1:l:452:GLN:HG3 | 1:l:459:GLY:O | 2.21 | 0.41 |
| 1:m:512:HIS:CE1 | 1:m:515:GLY:HA2 | 2.56 | 0.41 |
| 1:n:253:TYR:HB2 | 1:n:281:PRO:O | 2.21 | 0.41 |
| 1:r:344:GLN:HG2 | 1:r:405:MET:HG2 | 2.03 | 0.41 |
| 1:t:322:GLN:CB | 1:6:340:THR:HB | 2.51 | 0.41 |
| 1:t:429:HIS:NE2 | 1:t:610:GLN:CD | 2.79 | 0.41 |
| 1:t:490:ARG:CZ | 1:v:586:LEU:HD21 | 2.51 | 0.41 |
| 1:u:330:GLU:N | 1:u:330:GLU:CD | 2.78 | 0.41 |
| 1:v:319:PHE:CE1 | 1:v:680:GLN:HB2 | 2.55 | 0.41 |
| 1:v:511:TYR:HD2 | 1:v:520:VAL:HG22 | 1.84 | 0.41 |
| 1:v:656:VAL:HG11 | 1:1:324:LYS:HE3 | 2.02 | 0.41 |
| 1:w:381:LEU:HD23 | 1:w:381:LEU:HA | 1.90 | 0.41 |
| 1:w:659:ASP:N | 1:w:659:ASP:OD1 | 2.54 | 0.41 |
| 1:x:429:HIS:NE2 | 1:x:610:GLN:CD | 2.79 | 0.41 |
| 1:z:452:GLN:HG3 | 1:z:459:GLY:O | 2.21 | 0.41 |
| 1:z:571:THR:HG22 | 1:z:608:VAL:O | 2.20 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:z:626:HIS:CD2 | 1:2:736:ARG:NH2 | 2.79 | 0.41 |
| 1:z:656:VAL:HG11 | 1:4:324:LYS:HE3 | 2.02 | 0.41 |
| 1:1:429:HIS:NE2 | 1:1:610:GLN:CD | 2.79 | 0.41 |
| 1:1:473:MET:HE3 | 1:1:473:MET:HB2 | 1.81 | 0.41 |
| 1:2:322:GLN:CB | 1:3:340:THR:HB | 2.50 | 0.41 |
| 1:2:512:HIS:CE1 | 1:2:515:GLY:HA2 | 2.56 | 0.41 |
| 1:2:659:ASP:N | 1:2:659:ASP:OD1 | 2.54 | 0.41 |
| 1:5:253:TYR:HB2 | 1:5:281:PRO:O | 2.21 | 0.41 |
| 1:5:429:HIS:NE2 | 1:5:610:GLN:CD | 2.79 | 0.41 |
| 1:5:512:HIS:CE1 | 1:5:515:GLY:HA2 | 2.56 | 0.41 |
| 1:6:512:HIS:CE1 | 1:6:515:GLY:HA2 | 2.56 | 0.41 |
| 1:8:571:THR:HG22 | 1:8:608:VAL:O | 2.20 | 0.41 |
| 1:C:429:HIS:NE2 | 1:C:610:GLN:CD | 2.79 | 0.41 |
| 1:D:452:GLN:HG3 | 1:D:459:GLY:O | 2.21 | 0.41 |
| 1:F:512:HIS:CE1 | 1:F:515:GLY:HA2 | 2.56 | 0.41 |
| 1:G:429:HIS:NE2 | 1:G:610:GLN:CD | 2.79 | 0.41 |
| 1:H:736:ARG:NH2 | 1:W:626:HIS:CD2 | 2.79 | 0.41 |
| 1:I:512:HIS:CE1 | 1:I:515:GLY:HA2 | 2.56 | 0.41 |
| 1:I:700:GLU:HB2 | 1:I:702:GLN:HE21 | 1.85 | 0.41 |
| 1:K:452:GLN:HG3 | 1:K:459:GLY:O | 2.21 | 0.41 |
| 1:K:700:GLU:HB2 | 1:K:702:GLN:HE21 | 1.85 | 0.41 |
| 1:L:381:LEU:HD23 | 1:L:381:LEU:HA | 1.90 | 0.41 |
| 1:N:249:ALA:O | 1:N:251:PRO:HD3 | 2.21 | 0.41 |
| 1:O:656:VAL:HG11 | 1:d:324:LYS:HE3 | 2.02 | 0.41 |
| 1:P:512:HIS:CE1 | 1:P:515:GLY:HA2 | 2.56 | 0.41 |
| 1:R:264:GLY:HA2 | 1:R:387:SER:HB3 | 2.01 | 0.41 |
| 1:R:429:HIS:NE2 | 1:R:610:GLN:CD | 2.79 | 0.41 |
| 1:R:512:HIS:CE1 | 1:R:515:GLY:HA2 | 2.56 | 0.41 |
| 1:S:585:ASN:OD1 | 1:S:594:ILE:N | 2.45 | 0.41 |
| 1:S:700:GLU:HB2 | 1:S:702:GLN:HE21 | 1.85 | 0.41 |
| 1:T:330:GLU:N | 1:T:330:GLU:CD | 2.78 | 0.41 |
| 1:U:450:ARG:HG2 | 1:U:452:GLN:H | 1.85 | 0.41 |
| 1:V:381:LEU:HD23 | 1:V:381:LEU:HA | 1.90 | 0.41 |
| 1:V:656:VAL:HG11 | 1:W:324:LYS:HE3 | 2.03 | 0.41 |
| 1:W:344:GLN:HG2 | 1:W:405:MET:HG2 | 2.03 | 0.41 |
| 1:X:571:THR:HG22 | 1:X:608:VAL:O | 2.20 | 0.41 |
| 1:Y:344:GLN:HG2 | 1:Y:405:MET:HG2 | 2.03 | 0.41 |
| 1:Y:450:ARG:HG2 | 1:Y:452:GLN:H | 1.85 | 0.41 |
| 1:Y:512:HIS:CE1 | 1:Y:515:GLY:HA2 | 2.56 | 0.41 |
| 1:Y:700:GLU:HB2 | 1:Y:702:GLN:HE21 | 1.85 | 0.41 |
| 1:Z:342:THR:HG22 | 1:Z:407:ARG:HA | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z:512:HIS:CE1 | 1:Z:515:GLY:HA2 | 2.56 | 0.41 |
| 1:a:249:ALA:O | 1:a:251:PRO:HD3 | 2.21 | 0.41 |
| 1:b:253:TYR:HB2 | 1:b:281:PRO:O | 2.21 | 0.41 |
| 1:c:344:GLN:HG2 | 1:c:405:MET:HG2 | 2.03 | 0.41 |
| 1:c:490:ARG:CZ | 1:p:586:LEU:HD21 | 2.50 | 0.41 |
| 1:c:512:HIS:CE1 | 1:c:515:GLY:HA2 | 2.56 | 0.41 |
| 1:d:512:HIS:CE1 | 1:d:515:GLY:HA2 | 2.56 | 0.41 |
| 1:d:659:ASP:N | 1:d:659:ASP:OD1 | 2.54 | 0.41 |
| 1:f:344:GLN:HG2 | 1:f:405:MET:HG2 | 2.03 | 0.41 |
| 1:f:656:VAL:HG11 | 1:z:324:LYS:HE3 | 2.02 | 0.41 |
| 1:g:568:ILE:HD12 | 1:g:572:ASN:HD22 | 1.84 | 0.41 |
| 1:h:344:GLN:HG2 | 1:h:405:MET:HG2 | 2.03 | 0.41 |
| 1:h:382:THR:HG21 | 1:h:394:SER:N | 2.36 | 0.41 |
| 1:i:450:ARG:HG2 | 1:i:452:GLN:H | 1.85 | 0.41 |
| 1:j:586:LEU:HD21 | 1:k:490:ARG:CZ | 2.51 | 0.41 |
| 1:k:342:THR:HG22 | 1:k:407:ARG:HA | 2.02 | 0.41 |
| 1:k:344:GLN:HG2 | 1:k:405:MET:HG2 | 2.03 | 0.41 |
| 1:l:382:THR:HG21 | 1:l:394:SER:N | 2.36 | 0.41 |
| 1:l:429:HIS:HD2 | 1:l:610:GLN:OE1 | 1.94 | 0.41 |
| 1:l:571:THR:HG22 | 1:l:608:VAL:O | 2.20 | 0.41 |
| 1:l:656:VAL:HG11 | 1:n:324:LYS:HE3 | 2.02 | 0.41 |
| 1:m:312:LYS:HA | 1:m:312:LYS:HD2 | 1.90 | 0.41 |
| 1:m:659:ASP:N | 1:m:659:ASP:OD1 | 2.54 | 0.41 |
| 1:n:256:HIS:CD2 | 1:n:655:PRO:HB3 | 2.55 | 0.41 |
| 1:n:340:THR:HB | 1:r:322:GLN:CB | 2.51 | 0.41 |
| 1:n:429:HIS:NE2 | 1:n:610:GLN:CD | 2.79 | 0.41 |
| 1:p:429:HIS:NE2 | 1:p:610:GLN:CD | 2.79 | 0.41 |
| 1:p:704:THR:HB | 1:s:702:GLN:HB2 | 2.03 | 0.41 |
| 1:q:344:GLN:HG2 | 1:q:405:MET:HG2 | 2.03 | 0.41 |
| 1:q:429:HIS:NE2 | 1:q:610:GLN:CD | 2.79 | 0.41 |
| 1:r:609:TRP:NE1 | 1:s:629:GLY:CA | 2.58 | 0.41 |
| 1:t:324:LYS:HE3 | 1:6:656:VAL:HG11 | 2.03 | 0.41 |
| 1:t:512:HIS:CE1 | 1:t:515:GLY:HA2 | 2.56 | 0.41 |
| 1:u:429:HIS:NE2 | 1:u:610:GLN:CD | 2.79 | 0.41 |
| 1:u:656:VAL:HG11 | 1:5:324:LYS:HE3 | 2.03 | 0.41 |
| 1:v:322:GLN:CB | 1:w:340:THR:HB | 2.51 | 0.41 |
| 1:v:324:LYS:HE3 | 1:w:656:VAL:HG11 | 2.03 | 0.41 |
| 1:w:450:ARG:HG2 | 1:w:452:GLN:H | 1.85 | 0.41 |
| 1:y:429:HIS:NE2 | 1:y:610:GLN:CD | 2.79 | 0.41 |
| 1:1:253:TYR:HB2 | 1:1:281:PRO:O | 2.21 | 0.41 |
| 1:1:512:HIS:CE1 | 1:1:515:GLY:HA2 | 2.56 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2:324:LYS:HE3 | 1:3:656:VAL:HG11 | 2.02 | 0.41 |
| 1:4:253:TYR:HB2 | 1:4:281:PRO:O | 2.21 | 0.41 |
| 1:4:256:HIS:CD2 | 1:4:655:PRO:HB3 | 2.55 | 0.41 |
| 1:4:429:HIS:NE2 | 1:4:610:GLN:CD | 2.79 | 0.41 |
| 1:5:290:PHE:HE2 | 1:5:614:VAL:HB | 1.84 | 0.41 |
| 1:6:344:GLN:HG2 | 1:6:405:MET:HG2 | 2.03 | 0.41 |
| 1:7:342:THR:HG22 | 1:7:407:ARG:HA | 2.02 | 0.41 |
| 1:A:270:THR:HG23 | 1:A:272:ASP:H | 1.86 | 0.41 |
| 1:A:340:THR:HB | 1:B:322:GLN:CB | 2.50 | 0.41 |
| 1:A:452:GLN:HG3 | 1:A:459:GLY:O | 2.21 | 0.41 |
| 1:A:484:PRO:HD2 | 1:A:609:TRP:HE3 | 1.86 | 0.41 |
| 1:A:702:GLN:HB2 | 1:F:704:THR:HB | 2.02 | 0.41 |
| 1:B:270:THR:HG23 | 1:B:272:ASP:H | 1.86 | 0.41 |
| 1:B:586:LEU:HD21 | 1:J:490:ARG:CZ | 2.50 | 0.41 |
| 1:D:512:HIS:CE1 | 1:D:515:GLY:HA2 | 2.56 | 0.41 |
| 1:D:700:GLU:HB2 | 1:D:702:GLN:HE21 | 1.85 | 0.41 |
| 1:E:344:GLN:HG2 | 1:E:405:MET:HG2 | 2.03 | 0.41 |
| 1:E:429:HIS:NE2 | 1:E:610:GLN:CD | 2.79 | 0.41 |
| 1:F:249:ALA:O | 1:F:251:PRO:HD3 | 2.21 | 0.41 |
| 1:F:319:PHE:CE1 | 1:F:680:GLN:HB2 | 2.55 | 0.41 |
| 1:F:322:GLN:CB | 1:G:340:THR:HB | 2.50 | 0.41 |
| 1:F:340:THR:HB | 1:R:322:GLN:HB3 | 2.01 | 0.41 |
| 1:F:344:GLN:HG2 | 1:F:405:MET:HG2 | 2.03 | 0.41 |
| 1:F:421:VAL:CG2 | 1:F:422:PRO:HD2 | 2.50 | 0.41 |
| 1:F:450:ARG:HG2 | 1:F:452:GLN:H | 1.85 | 0.41 |
| 1:F:656:VAL:HG11 | 1:R:324:LYS:HE3 | 2.03 | 0.41 |
| 1:G:253:TYR:HB2 | 1:G:281:PRO:O | 2.21 | 0.41 |
| 1:G:330:GLU:N | 1:G:330:GLU:CD | 2.78 | 0.41 |
| 1:G:452:GLN:HG3 | 1:G:459:GLY:O | 2.21 | 0.41 |
| 1:G:586:LEU:HD21 | 1:I:490:ARG:CZ | 2.50 | 0.41 |
| 1:H:586:LEU:HD21 | 1:W:490:ARG:CZ | 2.51 | 0.41 |
| 1:H:626:HIS:CD2 | 1:Y:736:ARG:NH2 | 2.79 | 0.41 |
| 1:I:342:THR:HG22 | 1:I:407:ARG:CG | 2.47 | 0.41 |
| 1:I:485:CYS:HB3 | 1:I:579:TYR:HB2 | 2.03 | 0.41 |
| 1:J:249:ALA:O | 1:J:251:PRO:HD3 | 2.21 | 0.41 |
| 1:J:382:THR:HG21 | 1:J:394:SER:N | 2.35 | 0.41 |
| 1:M:249:ALA:O | 1:M:251:PRO:HD3 | 2.21 | 0.41 |
| 1:M:450:ARG:HG2 | 1:M:452:GLN:H | 1.85 | 0.41 |
| 1:M:490:ARG:CZ | 1:b:586:LEU:HD21 | 2.50 | 0.41 |
| 1:N:429:HIS:NE2 | 1:N:610:GLN:CD | 2.79 | 0.41 |
| 1:N:512:HIS:CE1 | 1:N:515:GLY:HA2 | 2.56 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:586:LEU:HD21 | 1:P:490:ARG:CZ | 2.50 | 0.41 |
| 1:N:700:GLU:HB2 | 1:N:702:GLN:HE21 | 1.85 | 0.41 |
| 1:O:340:THR:HB | 1:d:322:GLN:CB | 2.50 | 0.41 |
| 1:O:490:ARG:CZ | 1:n:586:LEU:HD21 | 2.51 | 0.41 |
| 1:P:319:PHE:CE1 | 1:P:680:GLN:HB2 | 2.55 | 0.41 |
| 1:P:355:TYR:CZ | 1:P:357:LEU:HB2 | 2.56 | 0.41 |
| 1:Q:290:PHE:HE2 | 1:Q:614:VAL:HB | 1.84 | 0.41 |
| 1:Q:324:LYS:HE3 | 1:S:656:VAL:HG11 | 2.03 | 0.41 |
| 1:R:299:TRP:CG | 1:R:616:LEU:HD13 | 2.56 | 0.41 |
| 1:R:342:THR:HG22 | 1:R:407:ARG:HA | 2.02 | 0.41 |
| 1:R:473:MET:HB2 | 1:R:473:MET:HE3 | 1.81 | 0.41 |
| 1:R:490:ARG:CZ | 1:U:586:LEU:HD21 | 2.51 | 0.41 |
| 1:R:586:LEU:HD21 | 1:S:490:ARG:CZ | 2.50 | 0.41 |
| 1:S:330:GLU:N | 1:S:330:GLU:CD | 2.78 | 0.41 |
| 1:S:429:HIS:NE2 | 1:S:610:GLN:CD | 2.79 | 0.41 |
| 1:S:659:ASP:OD1 | 1:S:659:ASP:N | 2.54 | 0.41 |
| 1:T:256:HIS:CD2 | 1:T:655:PRO:HB3 | 2.55 | 0.41 |
| 1:T:340:THR:HB | 1:i:322:GLN:CB | 2.50 | 0.41 |
| 1:T:490:ARG:CZ | 1:l:586:LEU:HD21 | 2.50 | 0.41 |
| 1:T:659:ASP:N | 1:T:659:ASP:OD1 | 2.54 | 0.41 |
| 1:U:270:THR:HG23 | 1:U:272:ASP:H | 1.86 | 0.41 |
| 1:U:319:PHE:CE1 | 1:U:680:GLN:HB2 | 2.55 | 0.41 |
| 1:V:249:ALA:O | 1:V:251:PRO:HD3 | 2.21 | 0.41 |
| 1:V:270:THR:HG23 | 1:V:272:ASP:H | 1.86 | 0.41 |
| 1:V:452:GLN:HG3 | 1:V:459:GLY:O | 2.21 | 0.41 |
| 1:W:249:ALA:O | 1:W:251:PRO:HD3 | 2.21 | 0.41 |
| 1:W:429:HIS:NE2 | 1:W:610:GLN:CD | 2.79 | 0.41 |
| 1:W:702:GLN:HB2 | 1:X:704:THR:HB | 2.02 | 0.41 |
| 1:W:715:PHE:CZ | 1:W:729:ILE:HD11 | 2.56 | 0.41 |
| 1:X:344:GLN:HG2 | 1:X:405:MET:HG2 | 2.03 | 0.41 |
| 1:X:700:GLU:HB2 | 1:X:702:GLN:HE21 | 1.85 | 0.41 |
| 1:Y:290:PHE:O | 1:Y:293:HIS:N | 2.47 | 0.41 |
| 1:Y:299:TRP:CG | 1:Y:616:LEU:HD13 | 2.56 | 0.41 |
| 1:Y:429:HIS:NE2 | 1:Y:610:GLN:CD | 2.79 | 0.41 |
| 1:Z:319:PHE:CE1 | 1:Z:680:GLN:HB2 | 2.55 | 0.41 |
| 1:a:429:HIS:NE2 | 1:a:610:GLN:CD | 2.79 | 0.41 |
| 1:a:512:HIS:CE1 | 1:a:515:GLY:HA2 | 2.56 | 0.41 |
| 1:a:700:GLU:HB2 | 1:a:702:GLN:HE21 | 1.85 | 0.41 |
| 1:b:270:THR:HG23 | 1:b:272:ASP:H | 1.86 | 0.41 |
| 1:b:704:THR:HB | 1:c:702:GLN:HB2 | 2.02 | 0.41 |
| 1:e:249:ALA:O | 1:e:251:PRO:HD3 | 2.21 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:e:381:LEU:HD23 | 1:e:381:LEU:HA | 1.90 | 0.41 |
| 1:e:450:ARG:HG2 | 1:e:452:GLN:H | 1.85 | 0.41 |
| 1:e:715:PHE:CZ | 1:e:729:ILE:HD11 | 2.56 | 0.41 |
| 1:g:342:THR:HG22 | 1:g:407:ARG:HA | 2.02 | 0.41 |
| 1:g:429:HIS:NE2 | 1:g:610:GLN:CD | 2.79 | 0.41 |
| 1:g:429:HIS:HD2 | 1:g:610:GLN:OE1 | 1.94 | 0.41 |
| 1:g:473:MET:HB2 | 1:g:473:MET:HE3 | 1.81 | 0.41 |
| 1:h:429:HIS:NE2 | 1:h:610:GLN:CD | 2.79 | 0.41 |
| 1:i:342:THR:HG22 | 1:i:407:ARG:HA | 2.02 | 0.41 |
| 1:i:429:HIS:NE2 | 1:i:610:GLN:CD | 2.79 | 0.41 |
| 1:i:473:MET:HB2 | 1:i:473:MET:HE3 | 1.81 | 0.41 |
| 1:j:256:HIS:CD2 | 1:j:655:PRO:HB3 | 2.55 | 0.41 |
| 1:j:571:THR:HG22 | 1:j:608:VAL:O | 2.20 | 0.41 |
| 1:j:656:VAL:HG11 | 1:l:324:LYS:HE3 | 2.02 | 0.41 |
| 1:k:429:HIS:NE2 | 1:k:610:GLN:CD | 2.79 | 0.41 |
| 1:l:220:ASP:OD1 | 1:l:220:ASP:N | 2.50 | 0.41 |
| 1:m:319:PHE:CE1 | 1:m:680:GLN:HB2 | 2.55 | 0.41 |
| 1:m:342:THR:HG22 | 1:m:407:ARG:HA | 2.02 | 0.41 |
| 1:n:344:GLN:HG2 | 1:n:405:MET:HG2 | 2.03 | 0.41 |
| 1:o:270:THR:HG23 | 1:o:272:ASP:H | 1.86 | 0.41 |
| 1:o:452:GLN:HG3 | 1:o:459:GLY:O | 2.21 | 0.41 |
| 1:o:485:CYS:HB3 | 1:o:579:TYR:HB2 | 2.03 | 0.41 |
| 1:p:253:TYR:HB2 | 1:p:281:PRO:O | 2.21 | 0.41 |
| 1:p:340:THR:HB | 1:6:322:GLN:CB | 2.50 | 0.41 |
| 1:p:452:GLN:HG3 | 1:p:459:GLY:O | 2.21 | 0.41 |
| 1:p:527:ALA:O | 1:p:575:ALA:N | 2.45 | 0.41 |
| 1:q:249:ALA:O | 1:q:251:PRO:HD3 | 2.21 | 0.41 |
| 1:q:490:ARG:CZ | 1:s:586:LEU:HD21 | 2.51 | 0.41 |
| 1:r:290:PHE:O | 1:r:293:HIS:N | 2.47 | 0.41 |
| 1:r:429:HIS:NE2 | 1:r:610:GLN:CD | 2.79 | 0.41 |
| 1:r:450:ARG:HG2 | 1:r:452:GLN:H | 1.85 | 0.41 |
| 1:r:586:LEU:HD21 | 1:s:490:ARG:CZ | 2.50 | 0.41 |
| 1:t:249:ALA:O | 1:t:251:PRO:HD3 | 2.21 | 0.41 |
| 1:t:264:GLY:HA2 | 1:t:387:SER:HB3 | 2.01 | 0.41 |
| 1:t:299:TRP:CG | 1:t:616:LEU:HD13 | 2.56 | 0.41 |
| 1:t:421:VAL:CG2 | 1:t:422:PRO:HD2 | 2.50 | 0.41 |
| 1:t:586:LEU:HD21 | 1:u:490:ARG:CZ | 2.51 | 0.41 |
| 1:u:324:LYS:HE3 | 1:2:656:VAL:HG11 | 2.02 | 0.41 |
| 1:u:421:VAL:CG2 | 1:u:422:PRO:HD2 | 2.50 | 0.41 |
| 1:u:659:ASP:OD1 | 1:u:659:ASP:N | 2.54 | 0.41 |
| 1:u:700:GLU:HB2 | 1:u:702:GLN:HE21 | 1.85 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:v:270:THR:HG23 | 1:v:272:ASP:H | 1.86 | 0.41 |
| 1:v:450:ARG:HG2 | 1:v:452:GLN:H | 1.85 | 0.41 |
| 1:w:499:ASN:ND2 | 1:y:592:GLY:HA2 | 2.34 | 0.41 |
| 1:w:715:PHE:CZ | 1:w:729:ILE:HD11 | 2.56 | 0.41 |
| 1:x:253:TYR:HB2 | 1:x:281:PRO:O | 2.21 | 0.41 |
| 1:x:344:GLN:HG2 | 1:x:405:MET:HG2 | 2.03 | 0.41 |
| 1:x:571:THR:HG22 | 1:x:608:VAL:O | 2.20 | 0.41 |
| 1:y:270:THR:HG23 | 1:y:272:ASP:H | 1.86 | 0.41 |
| 1:y:290:PHE:HE2 | 1:y:614:VAL:HB | 1.84 | 0.41 |
| 1:y:452:GLN:HG3 | 1:y:459:GLY:O | 2.21 | 0.41 |
| 1:y:484:PRO:HD2 | 1:y:609:TRP:CE3 | 2.55 | 0.41 |
| 1:z:382:THR:HG21 | 1:z:394:SER:N | 2.36 | 0.41 |
| 1:z:586:LEU:HD21 | 1:1:490:ARG:CZ | 2.50 | 0.41 |
| 1:z:736:ARG:NH2 | 1:1:626:HIS:CD2 | 2.79 | 0.41 |
| 1:1:330:GLU:N | 1:1:330:GLU:CD | 2.78 | 0.41 |
| 1:1:450:ARG:HG2 | 1:1:452:GLN:H | 1.85 | 0.41 |
| 1:1:659:ASP:N | 1:1:659:ASP:OD1 | 2.54 | 0.41 |
| 1:3:324:LYS:HE3 | 1:8:656:VAL:HG11 | 2.03 | 0.41 |
| 1:3:490:ARG:CZ | 1:4:586:LEU:HD21 | 2.51 | 0.41 |
| 1:3:512:HIS:CE1 | 1:3:515:GLY:HA2 | 2.56 | 0.41 |
| 1:4:344:GLN:HG2 | 1:4:405:MET:HG2 | 2.03 | 0.41 |
| 1:5:382:THR:HG21 | 1:5:394:SER:N | 2.35 | 0.41 |
| 1:6:249:ALA:O | 1:6:251:PRO:HD3 | 2.21 | 0.41 |
| 1:6:253:TYR:HB2 | 1:6:281:PRO:O | 2.21 | 0.41 |
| 1:6:256:HIS:CD2 | 1:6:655:PRO:HB3 | 2.55 | 0.41 |
| 1:6:319:PHE:CE1 | 1:6:680:GLN:HB2 | 2.55 | 0.41 |
| 1:6:421:VAL:CG2 | 1:6:422:PRO:HD2 | 2.50 | 0.41 |
| 1:7:429:HIS:NE2 | 1:7:610:GLN:CD | 2.79 | 0.41 |
| 1:7:452:GLN:HG3 | 1:7:459:GLY:O | 2.21 | 0.41 |
| 1:8:319:PHE:CE1 | 1:8:680:GLN:HB2 | 2.55 | 0.41 |
| 1:8:355:TYR:CZ | 1:8:357:LEU:HB2 | 2.56 | 0.41 |
| 1:A:355:TYR:CZ | 1:A:357:LEU:HB2 | 2.56 | 0.41 |
| 1:A:484:PRO:HD2 | 1:A:609:TRP:CE3 | 2.55 | 0.41 |
| 1:A:485:CYS:HB3 | 1:A:579:TYR:HB2 | 2.03 | 0.41 |
| 1:B:340:THR:HB | 1:C:322:GLN:CB | 2.50 | 0.41 |
| 1:B:704:THR:HB | 1:I:702:GLN:HB2 | 2.02 | 0.41 |
| 1:C:299:TRP:CG | 1:C:616:LEU:HD13 | 2.56 | 0.41 |
| 1:D:299:TRP:CG | 1:D:616:LEU:HD13 | 2.56 | 0.41 |
| 1:D:340:THR:HB | 1:E:322:GLN:CB | 2.50 | 0.41 |
| 1:D:429:HIS:NE2 | 1:D:610:GLN:CD | 2.79 | 0.41 |
| 1:E:299:TRP:CG | 1:E:616:LEU:HD13 | 2.56 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:452:GLN:HG3 | 1:E:459:GLY:O | 2.21 | 0.41 |
| 1:E:490:ARG:CZ | 1:F:586:LEU:HD21 | 2.50 | 0.41 |
| 1:F:253:TYR:HB2 | 1:F:281:PRO:O | 2.21 | 0.41 |
| 1:G:715:PHE:CZ | 1:G:729:ILE:HD11 | 2.56 | 0.41 |
| 1:I:253:TYR:HB2 | 1:I:281:PRO:O | 2.21 | 0.41 |
| 1:J:450:ARG:HG2 | 1:J:452:GLN:H | 1.85 | 0.41 |
| 1:K:299:TRP:CG | 1:K:616:LEU:HD13 | 2.56 | 0.41 |
| 1:K:340:THR:HB | 1:7:322:GLN:CB | 2.50 | 0.41 |
| 1:L:299:TRP:CG | 1:L:616:LEU:HD13 | 2.56 | 0.41 |
| 1:L:322:GLN:CB | 1:b:340:THR:HB | 2.50 | 0.41 |
| 1:L:344:GLN:HG2 | 1:L:405:MET:HG2 | 2.03 | 0.41 |
| 1:M:382:THR:HG21 | 1:M:394:SER:N | 2.35 | 0.41 |
| 1:N:715:PHE:CZ | 1:N:729:ILE:HD11 | 2.56 | 0.41 |
| 1:O:324:LYS:HE3 | 1:P:656:VAL:HG11 | 2.03 | 0.41 |
| 1:O:512:HIS:CE1 | 1:O:515:GLY:HA2 | 2.56 | 0.41 |
| 1:P:485:CYS:HB3 | 1:P:579:TYR:HB2 | 2.03 | 0.41 |
| 1:Q:342:THR:HG22 | 1:Q:407:ARG:HA | 2.02 | 0.41 |
| 1:Q:702:GLN:HB2 | 1:R:704:THR:HB | 2.02 | 0.41 |
| 1:R:249:ALA:O | 1:R:251:PRO:HD3 | 2.21 | 0.41 |
| 1:R:421:VAL:CG2 | 1:R:422:PRO:HD2 | 2.50 | 0.41 |
| 1:S:244:SER:C | 1:S:245:THR:HG1 | 2.28 | 0.41 |
| 1:S:249:ALA:O | 1:S:251:PRO:HD3 | 2.21 | 0.41 |
| 1:S:324:LYS:HE3 | 1:d:656:VAL:HG11 | 2.02 | 0.41 |
| 1:T:344:GLN:HG2 | 1:T:405:MET:HG2 | 2.03 | 0.41 |
| 1:T:450:ARG:HG2 | 1:T:452:GLN:H | 1.85 | 0.41 |
| 1:T:715:PHE:CZ | 1:T:729:ILE:HD11 | 2.56 | 0.41 |
| 1:U:324:LYS:HE3 | 1:e:656:VAL:HG11 | 2.03 | 0.41 |
| 1:U:429:HIS:NE2 | 1:U:610:GLN:CD | 2.79 | 0.41 |
| 1:V:484:PRO:HD2 | 1:V:609:TRP:CE3 | 2.55 | 0.41 |
| 1:W:270:THR:HG23 | 1:W:272:ASP:H | 1.86 | 0.41 |
| 1:W:342:THR:HG22 | 1:W:407:ARG:HA | 2.02 | 0.41 |
| 1:X:253:TYR:HB2 | 1:X:281:PRO:O | 2.21 | 0.41 |
| 1:Y:330:GLU:N | 1:Y:330:GLU:CD | 2.78 | 0.41 |
| 1:Z:715:PHE:CZ | 1:Z:729:ILE:HD11 | 2.56 | 0.41 |
| 1:a:586:LEU:HD21 | 1:8:490:ARG:CZ | 2.50 | 0.41 |
| 1:b:299:TRP:CG | 1:b:616:LEU:HD13 | 2.56 | 0.41 |
| 1:b:512:HIS:CE1 | 1:b:515:GLY:HA2 | 2.56 | 0.41 |
| 1:c:299:TRP:CG | 1:c:616:LEU:HD13 | 2.56 | 0.41 |
| 1:c:485:CYS:HB3 | 1:c:579:TYR:HB2 | 2.03 | 0.41 |
| 1:d:299:TRP:CG | 1:d:616:LEU:HD13 | 2.56 | 0.41 |
| 1:e:429:HIS:NE2 | 1:e:610:GLN:CD | 2.79 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:e:702:GLN:HB2 | 1:f:704:THR:HB | 2.03 | 0.41 |
| 1:f:256:HIS:CD2 | 1:f:655:PRO:HB3 | 2.55 | 0.41 |
| 1:f:342:THR:HG22 | 1:f:407:ARG:HA | 2.02 | 0.41 |
| 1:f:355:TYR:CZ | 1:f:357:LEU:HB2 | 2.56 | 0.41 |
| 1:f:450:ARG:HG2 | 1:f:452:GLN:H | 1.85 | 0.41 |
| 1:f:452:GLN:HG3 | 1:f:459:GLY:O | 2.21 | 0.41 |
| 1:f:571:THR:HG22 | 1:f:608:VAL:O | 2.20 | 0.41 |
| 1:g:322:GLN:CB | 1:1:340:THR:HB | 2.50 | 0.41 |
| 1:g:450:ARG:HG2 | 1:g:452:GLN:H | 1.85 | 0.41 |
| 1:g:485:CYS:HB3 | 1:g:579:TYR:HB2 | 2.03 | 0.41 |
| 1:g:702:GLN:HB2 | 1:z:704:THR:HB | 2.02 | 0.41 |
| 1:h:324:LYS:HE3 | 1:i:656:VAL:HG11 | 2.03 | 0.41 |
| 1:h:355:TYR:CZ | 1:h:357:LEU:HB2 | 2.56 | 0.41 |
| 1:i:435:ARG:HD3 | 1:i:435:ARG:HA | 1.79 | 0.41 |
| 1:i:485:CYS:HB3 | 1:i:579:TYR:HB2 | 2.03 | 0.41 |
| 1:i:527:ALA:O | 1:i:575:ALA:N | 2.45 | 0.41 |
| 1:i:702:GLN:HB2 | 1:l:704:THR:HB | 2.02 | 0.41 |
| 1:j:340:THR:HB | 1:l:322:GLN:CB | 2.51 | 0.41 |
| 1:j:342:THR:HG22 | 1:j:407:ARG:HA | 2.02 | 0.41 |
| 1:j:450:ARG:HG2 | 1:j:452:GLN:H | 1.85 | 0.41 |
| 1:k:355:TYR:CZ | 1:k:357:LEU:HB2 | 2.56 | 0.41 |
| 1:m:484:PRO:HD2 | 1:m:609:TRP:HE3 | 1.86 | 0.41 |
| 1:m:715:PHE:CZ | 1:m:729:ILE:HD11 | 2.56 | 0.41 |
| 1:n:249:ALA:O | 1:n:251:PRO:HD3 | 2.21 | 0.41 |
| 1:n:299:TRP:CG | 1:n:616:LEU:HD13 | 2.56 | 0.41 |
| 1:n:452:GLN:HG3 | 1:n:459:GLY:O | 2.21 | 0.41 |
| 1:n:700:GLU:HB2 | 1:n:702:GLN:HE21 | 1.85 | 0.41 |
| 1:o:355:TYR:CZ | 1:o:357:LEU:HB2 | 2.56 | 0.41 |
| 1:o:484:PRO:HD2 | 1:o:609:TRP:HE3 | 1.86 | 0.41 |
| 1:p:330:GLU:N | 1:p:330:GLU:CD | 2.78 | 0.41 |
| 1:p:700:GLU:HB2 | 1:p:702:GLN:HE21 | 1.85 | 0.41 |
| 1:p:715:PHE:CZ | 1:p:729:ILE:HD11 | 2.56 | 0.41 |
| 1:q:342:THR:HG22 | 1:q:407:ARG:HA | 2.02 | 0.41 |
| 1:q:473:MET:HE3 | 1:q:473:MET:HB2 | 1.81 | 0.41 |
| 1:q:715:PHE:CZ | 1:q:729:ILE:HD11 | 2.56 | 0.41 |
| 1:r:299:TRP:CG | 1:r:616:LEU:HD13 | 2.56 | 0.41 |
| 1:s:700:GLU:HB2 | 1:s:702:GLN:HE21 | 1.85 | 0.41 |
| 1:t:342:THR:HG22 | 1:t:407:ARG:HA | 2.02 | 0.41 |
| 1:u:249:ALA:O | 1:u:251:PRO:HD3 | 2.21 | 0.41 |
| 1:u:452:GLN:HG3 | 1:u:459:GLY:O | 2.21 | 0.41 |
| 1:v:429:HIS:NE2 | 1:v:610:GLN:CD | 2.79 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:w:249:ALA:O | 1:w:251:PRO:HD3 | 2.21 | 0.41 |
| 1:w:429:HIS:CE1 | 1:x:627:THR:HG22 | 2.56 | 0.41 |
| 1:w:480:TRP:CZ2 | 1:x:624:ILE:HA | 2.56 | 0.41 |
| 1:x:421:VAL:CG2 | 1:x:422:PRO:HD2 | 2.50 | 0.41 |
| 1:x:611:ASN:ND2 | 1:y:628:ASP:HB3 | 2.36 | 0.41 |
| 1:x:700:GLU:HB2 | 1:x:702:GLN:HE21 | 1.85 | 0.41 |
| 1:y:249:ALA:O | 1:y:251:PRO:HD3 | 2.21 | 0.41 |
| 1:z:512:HIS:CE1 | 1:z:515:GLY:HA2 | 2.56 | 0.41 |
| 1:1:256:HIS:CD2 | 1:1:655:PRO:HB3 | 2.55 | 0.41 |
| 1:1:586:LEU:HD21 | 1:2:490:ARG:CZ | 2.50 | 0.41 |
| 1:1:715:PHE:CZ | 1:1:729:ILE:HD11 | 2.56 | 0.41 |
| 1:3:355:TYR:CZ | 1:3:357:LEU:HB2 | 2.56 | 0.41 |
| 1:3:452:GLN:HG3 | 1:3:459:GLY:O | 2.21 | 0.41 |
| 1:4:249:ALA:O | 1:4:251:PRO:HD3 | 2.21 | 0.41 |
| 1:4:299:TRP:CG | 1:4:616:LEU:HD13 | 2.56 | 0.41 |
| 1:4:527:ALA:O | 1:4:575:ALA:N | 2.45 | 0.41 |
| 1:4:700:GLU:HB2 | 1:4:702:GLN:HE21 | 1.85 | 0.41 |
| 1:5:700:GLU:HB2 | 1:5:702:GLN:HE21 | 1.85 | 0.41 |
| 1:6:450:ARG:HG2 | 1:6:452:GLN:H | 1.85 | 0.41 |
| 1:6:452:GLN:HG3 | 1:6:459:GLY:O | 2.21 | 0.41 |
| 1:7:249:ALA:O | 1:7:251:PRO:HD3 | 2.21 | 0.41 |
| 1:7:299:TRP:CG | 1:7:616:LEU:HD13 | 2.56 | 0.41 |
| 1:7:344:GLN:HG2 | 1:7:405:MET:HG2 | 2.03 | 0.41 |
| 1:8:381:LEU:HA | 1:8:381:LEU:HD23 | 1.90 | 0.41 |
| 1:8:485:CYS:HB3 | 1:8:579:TYR:HB2 | 2.03 | 0.41 |
| 1:A:659:ASP:N | 1:A:659:ASP:OD1 | 2.54 | 0.40 |
| 1:B:299:TRP:CG | 1:B:616:LEU:HD13 | 2.56 | 0.40 |
| 1:B:512:HIS:CE1 | 1:B:515:GLY:HA2 | 2.56 | 0.40 |
| 1:C:344:GLN:HG2 | 1:C:405:MET:HG2 | 2.03 | 0.40 |
| 1:D:230:HIS:HB3 | 1:D:232:ASP:OD1 | 2.22 | 0.40 |
| 1:D:656:VAL:HG11 | 1:E:324:LYS:HE3 | 2.03 | 0.40 |
| 1:D:702:GLN:HB2 | 1:M:704:THR:HB | 2.03 | 0.40 |
| 1:E:249:ALA:O | 1:E:251:PRO:HD3 | 2.21 | 0.40 |
| 1:F:299:TRP:CG | 1:F:616:LEU:HD13 | 2.56 | 0.40 |
| 1:F:342:THR:HG22 | 1:F:407:ARG:HA | 2.02 | 0.40 |
| 1:F:452:GLN:HG3 | 1:F:459:GLY:O | 2.21 | 0.40 |
| 1:G:230:HIS:HB3 | 1:G:232:ASP:OD1 | 2.21 | 0.40 |
| 1:G:702:GLN:HB2 | 1:H:704:THR:HB | 2.02 | 0.40 |
| 1:H:355:TYR:CZ | 1:H:357:LEU:HB2 | 2.56 | 0.40 |
| 1:H:429:HIS:NE2 | 1:H:610:GLN:CD | 2.79 | 0.40 |
| 1:H:490:ARG:CZ | 1:Y:586:LEU:HD21 | 2.50 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:299:TRP:CG | 1:I:616:LEU:HD13 | 2.56 | 0.40 |
| 1:I:659:ASP:OD1 | 1:I:659:ASP:N | 2.54 | 0.40 |
| 1:J:230:HIS:HB3 | 1:J:232:ASP:OD1 | 2.22 | 0.40 |
| 1:J:704:THR:HB | 1:K:702:GLN:HB2 | 2.03 | 0.40 |
| 1:K:230:HIS:HB3 | 1:K:232:ASP:OD1 | 2.22 | 0.40 |
| 1:K:656:VAL:HG11 | 1:7:324:LYS:HE3 | 2.03 | 0.40 |
| 1:M:230:HIS:HB3 | 1:M:232:ASP:OD1 | 2.22 | 0.40 |
| 1:M:326:VAL:HG21 | 1:M:333:LYS:NZ | 2.37 | 0.40 |
| 1:N:230:HIS:HB3 | 1:N:232:ASP:OD1 | 2.21 | 0.40 |
| 1:O:249:ALA:O | 1:O:251:PRO:HD3 | 2.21 | 0.40 |
| 1:O:355:TYR:CZ | 1:O:357:LEU:HB2 | 2.56 | 0.40 |
| 1:O:452:GLN:HG3 | 1:O:459:GLY:O | 2.21 | 0.40 |
| 1:P:230:HIS:HB3 | 1:P:232:ASP:OD1 | 2.21 | 0.40 |
| 1:Q:230:HIS:HB3 | 1:Q:232:ASP:OD1 | 2.21 | 0.40 |
| 1:Q:329:ASN:O | 1:Q:332:THR:OG1 | 2.30 | 0.40 |
| 1:Q:382:THR:HG21 | 1:Q:394:SER:N | 2.35 | 0.40 |
| 1:Q:434:ASP:OD1 | 1:Q:434:ASP:N | 2.41 | 0.40 |
| 1:S:452:GLN:HG3 | 1:S:459:GLY:O | 2.21 | 0.40 |
| 1:T:230:HIS:HB3 | 1:T:232:ASP:OD1 | 2.22 | 0.40 |
| 1:T:249:ALA:O | 1:T:251:PRO:HD3 | 2.21 | 0.40 |
| 1:T:586:LEU:HD21 | 1:d:490:ARG:CZ | 2.50 | 0.40 |
| 1:U:512:HIS:CE1 | 1:U:515:GLY:HA2 | 2.56 | 0.40 |
| 1:V:290:PHE:HE2 | 1:V:614:VAL:HB | 1.84 | 0.40 |
| 1:W:355:TYR:CZ | 1:W:357:LEU:HB2 | 2.56 | 0.40 |
| 1:W:512:HIS:CE1 | 1:W:515:GLY:HA2 | 2.56 | 0.40 |
| 1:Y:270:THR:HG23 | 1:Y:272:ASP:H | 1.86 | 0.40 |
| 1:Y:579:TYR:OH | 1:Y:607:MET:CE | 2.67 | 0.40 |
| 1:Z:299:TRP:CG | 1:Z:616:LEU:HD13 | 2.56 | 0.40 |
| 1:Z:312:LYS:HA | 1:Z:312:LYS:HD2 | 1.90 | 0.40 |
| 1:Z:355:TYR:CZ | 1:Z:357:LEU:HB2 | 2.56 | 0.40 |
| 1:Z:429:HIS:NE2 | 1:Z:610:GLN:CD | 2.79 | 0.40 |
| 1:Z:484:PRO:HD2 | 1:Z:609:TRP:HE3 | 1.86 | 0.40 |
| 1:Z:626:HIS:CD2 | 1:3:736:ARG:NH2 | 2.79 | 0.40 |
| 1:a:715:PHE:CZ | 1:a:729:ILE:HD11 | 2.56 | 0.40 |
| 1:c:253:TYR:HB2 | 1:c:281:PRO:O | 2.21 | 0.40 |
| 1:d:429:HIS:NE2 | 1:d:610:GLN:CD | 2.79 | 0.40 |
| 1:d:704:THR:HB | 1:n:702:GLN:HB2 | 2.03 | 0.40 |
| 1:g:330:GLU:N | 1:g:330:GLU:CD | 2.78 | 0.40 |
| 1:g:656:VAL:HG11 | 1:k:324:LYS:HE3 | 2.03 | 0.40 |
| 1:g:659:ASP:N | 1:g:659:ASP:OD1 | 2.54 | 0.40 |
| 1:j:355:TYR:CZ | 1:j:357:LEU:HB2 | 2.56 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:j:452:GLN:HG3 | 1:j:459:GLY:O | 2.21 | 0.40 |
| 1:k:230:HIS:HB3 | 1:k:232:ASP:OD1 | 2.22 | 0.40 |
| 1:k:579:TYR:OH | 1:k:607:MET:CE | 2.67 | 0.40 |
| 1:l:512:HIS:CE1 | 1:l:515:GLY:HA2 | 2.56 | 0.40 |
| 1:l:715:PHE:CZ | 1:l:729:ILE:HD11 | 2.56 | 0.40 |
| 1:m:249:ALA:O | 1:m:251:PRO:HD3 | 2.21 | 0.40 |
| 1:m:299:TRP:CG | 1:m:616:LEU:HD13 | 2.56 | 0.40 |
| 1:m:355:TYR:CZ | 1:m:357:LEU:HB2 | 2.56 | 0.40 |
| 1:m:429:HIS:NE2 | 1:m:610:GLN:CD | 2.79 | 0.40 |
| 1:n:355:TYR:CZ | 1:n:357:LEU:HB2 | 2.56 | 0.40 |
| 1:n:485:CYS:HB3 | 1:n:579:TYR:HB2 | 2.03 | 0.40 |
| 1:n:527:ALA:O | 1:n:575:ALA:N | 2.45 | 0.40 |
| 1:o:659:ASP:N | 1:o:659:ASP:OD1 | 2.54 | 0.40 |
| 1:q:270:THR:HG23 | 1:q:272:ASP:H | 1.86 | 0.40 |
| 1:s:355:TYR:CZ | 1:s:357:LEU:HB2 | 2.56 | 0.40 |
| 1:s:429:HIS:NE2 | 1:s:610:GLN:CD | 2.79 | 0.40 |
| 1:t:322:GLN:HB3 | 1:6:340:THR:HB | 2.02 | 0.40 |
| 1:t:330:GLU:N | 1:t:330:GLU:CD | 2.78 | 0.40 |
| 1:u:585:ASN:OD1 | 1:u:594:ILE:N | 2.45 | 0.40 |
| 1:v:256:HIS:CD2 | 1:v:655:PRO:HB3 | 2.55 | 0.40 |
| 1:v:512:HIS:CE1 | 1:v:515:GLY:HA2 | 2.56 | 0.40 |
| 1:w:429:HIS:NE2 | 1:w:610:GLN:CD | 2.79 | 0.40 |
| 1:w:600:SER:OG | 1:y:601:GLN:NE2 | 2.48 | 0.40 |
| 1:y:230:HIS:HB3 | 1:y:232:ASP:OD1 | 2.21 | 0.40 |
| 1:y:512:HIS:CE1 | 1:y:515:GLY:HA2 | 2.56 | 0.40 |
| 1:z:715:PHE:CZ | 1:z:729:ILE:HD11 | 2.56 | 0.40 |
| 1:1:230:HIS:HB3 | 1:1:232:ASP:OD1 | 2.22 | 0.40 |
| 1:1:249:ALA:O | 1:1:251:PRO:HD3 | 2.21 | 0.40 |
| 1:1:344:GLN:HG2 | 1:1:405:MET:HG2 | 2.03 | 0.40 |
| 1:1:355:TYR:CZ | 1:1:357:LEU:HB2 | 2.56 | 0.40 |
| 1:2:270:THR:HG23 | 1:2:272:ASP:H | 1.86 | 0.40 |
| 1:2:299:TRP:CG | 1:2:616:LEU:HD13 | 2.56 | 0.40 |
| 1:2:429:HIS:NE2 | 1:2:610:GLN:CD | 2.79 | 0.40 |
| 1:2:704:THR:HB | 1:4:702:GLN:HB2 | 2.03 | 0.40 |
| 1:3:249:ALA:O | 1:3:251:PRO:HD3 | 2.21 | 0.40 |
| 1:4:355:TYR:CZ | 1:4:357:LEU:HB2 | 2.56 | 0.40 |
| 1:4:452:GLN:HG3 | 1:4:459:GLY:O | 2.21 | 0.40 |
| 1:5:579:TYR:OH | 1:5:607:MET:CE | 2.68 | 0.40 |
| 1:6:299:TRP:CG | 1:6:616:LEU:HD13 | 2.57 | 0.40 |
| 1:6:342:THR:HG22 | 1:6:407:ARG:HA | 2.02 | 0.40 |
| 1:6:586:LEU:HD21 | 1:7:490:ARG:CZ | 2.50 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:8:230:HIS:HB3 | 1:8:232:ASP:OD1 | 2.21 | 0.40 |
| 1:8:342:THR:HG22 | 1:8:407:ARG:HA | 2.02 | 0.40 |
| 1:A:299:TRP:CG | 1:A:616:LEU:HD13 | 2.56 | 0.40 |
| 1:B:485:CYS:HB3 | 1:B:579:TYR:HB2 | 2.03 | 0.40 |
| 1:C:270:THR:HG23 | 1:C:272:ASP:H | 1.86 | 0.40 |
| 1:C:490:ARG:CZ | 1:M:586:LEU:HD21 | 2.50 | 0.40 |
| 1:D:249:ALA:O | 1:D:251:PRO:HD3 | 2.21 | 0.40 |
| 1:D:715:PHE:CZ | 1:D:729:ILE:HD11 | 2.56 | 0.40 |
| 1:G:484:PRO:HD2 | 1:G:609:TRP:CE3 | 2.55 | 0.40 |
| 1:G:700:GLU:HB2 | 1:G:702:GLN:HE21 | 1.85 | 0.40 |
| 1:H:452:GLN:HG3 | 1:H:459:GLY:O | 2.21 | 0.40 |
| 1:H:700:GLU:HB2 | 1:H:702:GLN:HE21 | 1.85 | 0.40 |
| 1:J:586:LEU:HD21 | 1:L:490:ARG:CZ | 2.50 | 0.40 |
| 1:K:249:ALA:O | 1:K:251:PRO:HD3 | 2.21 | 0.40 |
| 1:K:429:HIS:NE2 | 1:K:610:GLN:CD | 2.79 | 0.40 |
| 1:K:715:PHE:CZ | 1:K:729:ILE:HD11 | 2.56 | 0.40 |
| 1:L:270:THR:HG23 | 1:L:272:ASP:H | 1.86 | 0.40 |
| 1:O:270:THR:HG23 | 1:O:272:ASP:H | 1.86 | 0.40 |
| 1:O:429:HIS:NE2 | 1:O:610:GLN:CD | 2.79 | 0.40 |
| 1:P:342:THR:HG22 | 1:P:407:ARG:HA | 2.02 | 0.40 |
| 1:P:484:PRO:HD2 | 1:P:609:TRP:CE3 | 2.55 | 0.40 |
| 1:Q:700:GLU:HB2 | 1:Q:702:GLN:HE21 | 1.85 | 0.40 |
| 1:Q:715:PHE:CZ | 1:Q:729:ILE:HD11 | 2.56 | 0.40 |
| 1:R:330:GLU:N | 1:R:330:GLU:CD | 2.78 | 0.40 |
| 1:S:344:GLN:HG2 | 1:S:405:MET:HG2 | 2.03 | 0.40 |
| 1:S:355:TYR:CZ | 1:S:357:LEU:HB2 | 2.56 | 0.40 |
| 1:S:421:VAL:CG2 | 1:S:422:PRO:HD2 | 2.50 | 0.40 |
| 1:T:355:TYR:CZ | 1:T:357:LEU:HB2 | 2.56 | 0.40 |
| 1:U:299:TRP:CG | 1:U:616:LEU:HD13 | 2.56 | 0.40 |
| 1:U:571:THR:HG22 | 1:U:608:VAL:O | 2.20 | 0.40 |
| 1:U:659:ASP:OD1 | 1:U:659:ASP:N | 2.54 | 0.40 |
| 1:U:704:THR:HB | 1:V:702:GLN:HB2 | 2.03 | 0.40 |
| 1:V:230:HIS:HB3 | 1:V:232:ASP:OD1 | 2.21 | 0.40 |
| 1:W:586:LEU:HD21 | 1:Y:490:ARG:CZ | 2.50 | 0.40 |
| 1:X:299:TRP:CG | 1:X:616:LEU:HD13 | 2.56 | 0.40 |
| 1:X:484:PRO:HD2 | 1:X:609:TRP:CE3 | 2.56 | 0.40 |
| 1:Y:253:TYR:HB2 | 1:Y:281:PRO:O | 2.21 | 0.40 |
| 1:Y:355:TYR:CZ | 1:Y:357:LEU:HB2 | 2.56 | 0.40 |
| 1:Z:249:ALA:O | 1:Z:251:PRO:HD3 | 2.21 | 0.40 |
| 1:Z:452:GLN:HG3 | 1:Z:459:GLY:O | 2.21 | 0.40 |
| 1:a:230:HIS:HB3 | 1:a:232:ASP:OD1 | 2.22 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:b:485:CYS:HB3 | 1:b:579:TYR:HB2 | 2.03 | 0.40 |
| 1:b:700:GLU:HB2 | 1:b:702:GLN:HE21 | 1.85 | 0.40 |
| 1:c:659:ASP:OD1 | 1:c:659:ASP:N | 2.54 | 0.40 |
| 1:c:736:ARG:NH2 | 1:o:626:HIS:CD2 | 2.79 | 0.40 |
| 1:d:270:THR:HG23 | 1:d:272:ASP:H | 1.86 | 0.40 |
| 1:d:342:THR:HG22 | 1:d:407:ARG:HA | 2.02 | 0.40 |
| 1:f:429:HIS:NE2 | 1:f:610:GLN:CD | 2.79 | 0.40 |
| 1:g:299:TRP:CG | 1:g:616:LEU:HD13 | 2.56 | 0.40 |
| 1:g:626:HIS:CD2 | 1:h:736:ARG:NH2 | 2.79 | 0.40 |
| 1:h:230:HIS:HB3 | 1:h:232:ASP:OD1 | 2.22 | 0.40 |
| 1:h:270:THR:HG23 | 1:h:272:ASP:H | 1.86 | 0.40 |
| 1:h:579:TYR:OH | 1:h:607:MET:CE | 2.68 | 0.40 |
| 1:i:659:ASP:N | 1:i:659:ASP:OD1 | 2.54 | 0.40 |
| 1:k:270:THR:HG23 | 1:k:272:ASP:H | 1.86 | 0.40 |
| 1:l:249:ALA:O | 1:l:251:PRO:HD3 | 2.21 | 0.40 |
| 1:l:299:TRP:CG | 1:l:616:LEU:HD13 | 2.56 | 0.40 |
| 1:m:452:GLN:HG3 | 1:m:459:GLY:O | 2.21 | 0.40 |
| 1:n:382:THR:HG21 | 1:n:394:SER:N | 2.36 | 0.40 |
| 1:o:299:TRP:CG | 1:o:616:LEU:HD13 | 2.56 | 0.40 |
| 1:o:344:GLN:HG2 | 1:o:405:MET:HG2 | 2.03 | 0.40 |
| 1:o:429:HIS:NE2 | 1:o:610:GLN:CD | 2.79 | 0.40 |
| 1:o:484:PRO:HD2 | 1:o:609:TRP:CE3 | 2.55 | 0.40 |
| 1:p:230:HIS:HB3 | 1:p:232:ASP:OD1 | 2.21 | 0.40 |
| 1:p:312:LYS:HA | 1:p:312:LYS:HD2 | 1.90 | 0.40 |
| 1:p:702:GLN:HB2 | 1:s:704:THR:HB | 2.02 | 0.40 |
| 1:q:230:HIS:HB3 | 1:q:232:ASP:OD1 | 2.22 | 0.40 |
| 1:q:355:TYR:CZ | 1:q:357:LEU:HB2 | 2.56 | 0.40 |
| 1:q:485:CYS:HB3 | 1:q:579:TYR:HB2 | 2.03 | 0.40 |
| 1:q:626:HIS:CD2 | 1:s:736:ARG:NH2 | 2.79 | 0.40 |
| 1:r:253:TYR:HB2 | 1:r:281:PRO:O | 2.21 | 0.40 |
| 1:r:330:GLU:N | 1:r:330:GLU:CD | 2.78 | 0.40 |
| 1:r:736:ARG:NH2 | 1:s:626:HIS:CD2 | 2.79 | 0.40 |
| 1:s:452:GLN:HG3 | 1:s:459:GLY:O | 2.21 | 0.40 |
| 1:s:485:CYS:HB3 | 1:s:579:TYR:HB2 | 2.03 | 0.40 |
| 1:t:704:THR:HB | 1:5:702:GLN:HB2 | 2.03 | 0.40 |
| 1:u:270:THR:HG23 | 1:u:272:ASP:H | 1.86 | 0.40 |
| 1:u:355:TYR:CZ | 1:u:357:LEU:HB2 | 2.56 | 0.40 |
| 1:v:299:TRP:CG | 1:v:616:LEU:HD13 | 2.56 | 0.40 |
| 1:v:485:CYS:HB3 | 1:v:579:TYR:HB2 | 2.03 | 0.40 |
| 1:v:659:ASP:OD1 | 1:v:659:ASP:N | 2.54 | 0.40 |
| 1:x:326:VAL:HG21 | 1:x:333:LYS:NZ | 2.37 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:x:355:TYR:CZ | 1:x:357:LEU:HB2 | 2.56 | 0.40 |
| 1:x:484:PRO:HD2 | 1:x:609:TRP:CE3 | 2.55 | 0.40 |
| 1:y:312:LYS:HA | 1:y:312:LYS:HD2 | 1.90 | 0.40 |
| 1:z:249:ALA:O | 1:z:251:PRO:HD3 | 2.21 | 0.40 |
| 1:z:299:TRP:CG | 1:z:616:LEU:HD13 | 2.56 | 0.40 |
| 1:z:484:PRO:HD2 | 1:z:609:TRP:CE3 | 2.55 | 0.40 |
| 1:2:342:THR:HG22 | 1:2:407:ARG:HA | 2.02 | 0.40 |
| 1:3:270:THR:HG23 | 1:3:272:ASP:H | 1.86 | 0.40 |
| 1:4:484:PRO:HD2 | 1:4:609:TRP:HE3 | 1.86 | 0.40 |
| 1:4:485:CYS:HB3 | 1:4:579:TYR:HB2 | 2.03 | 0.40 |
| 1:5:230:HIS:HB3 | 1:5:232:ASP:OD1 | 2.21 | 0.40 |
| 1:5:342:THR:HG22 | 1:5:407:ARG:HA | 2.02 | 0.40 |
| 1:6:270:THR:HG23 | 1:6:272:ASP:H | 1.86 | 0.40 |
| 1:8:484:PRO:HD2 | 1:8:609:TRP:CE3 | 2.55 | 0.40 |
| 1:A:626:HIS:CD2 | 1:I:736:ARG:NH2 | 2.79 | 0.40 |
| 1:B:700:GLU:HB2 | 1:B:702:GLN:HE21 | 1.85 | 0.40 |
| 1:B:702:GLN:HB2 | 1:I:704:THR:HB | 2.02 | 0.40 |
| 1:C:715:PHE:CZ | 1:C:729:ILE:HD11 | 2.56 | 0.40 |
| 1:E:270:THR:HG23 | 1:E:272:ASP:H | 1.86 | 0.40 |
| 1:F:270:THR:HG23 | 1:F:272:ASP:H | 1.86 | 0.40 |
| 1:G:736:ARG:NH2 | 1:I:626:HIS:CD2 | 2.79 | 0.40 |
| 1:H:485:CYS:HB3 | 1:H:579:TYR:HB2 | 2.03 | 0.40 |
| 1:H:629:GLY:CA | 1:Y:609:TRP:NE1 | 2.58 | 0.40 |
| 1:H:659:ASP:OD1 | 1:H:659:ASP:N | 2.54 | 0.40 |
| 1:I:322:GLN:HB3 | 1:J:340:THR:HB | 2.02 | 0.40 |
| 1:I:328:GLN:HE22 | 1:I:333:LYS:CG | 2.30 | 0.40 |
| 1:J:270:THR:HG23 | 1:J:272:ASP:H | 1.86 | 0.40 |
| 1:J:330:GLU:N | 1:J:330:GLU:CD | 2.78 | 0.40 |
| 1:L:715:PHE:CZ | 1:L:729:ILE:HD11 | 2.56 | 0.40 |
| 1:N:270:THR:HG23 | 1:N:272:ASP:H | 1.86 | 0.40 |
| 1:N:704:THR:HB | 1:O:702:GLN:HB2 | 2.02 | 0.40 |
| 1:O:299:TRP:CG | 1:O:616:LEU:HD13 | 2.56 | 0.40 |
| 1:Q:579:TYR:OH | 1:Q:607:MET:CE | 2.68 | 0.40 |
| 1:R:715:PHE:CZ | 1:R:729:ILE:HD11 | 2.56 | 0.40 |
| 1:S:270:THR:HG23 | 1:S:272:ASP:H | 1.86 | 0.40 |
| 1:T:270:THR:HG23 | 1:T:272:ASP:H | 1.86 | 0.40 |
| 1:T:299:TRP:CG | 1:T:616:LEU:HD13 | 2.56 | 0.40 |
| 1:T:656:VAL:HG11 | 1:i:324:LYS:HE3 | 2.03 | 0.40 |
| 1:U:256:HIS:CD2 | 1:U:655:PRO:HB3 | 2.55 | 0.40 |
| 1:U:485:CYS:HB3 | 1:U:579:TYR:HB2 | 2.03 | 0.40 |
| 1:V:312:LYS:HA | 1:V:312:LYS:HD2 | 1.90 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:485:CYS:HB3 | 1:V:579:TYR:HB2 | 2.03 | 0.40 |
| 1:V:512:HIS:CE1 | 1:V:515:GLY:HA2 | 2.56 | 0.40 |
| 1:W:230:HIS:HB3 | 1:W:232:ASP:OD1 | 2.22 | 0.40 |
| 1:X:326:VAL:HG21 | 1:X:333:LYS:NZ | 2.37 | 0.40 |
| 1:X:355:TYR:CZ | 1:X:357:LEU:HB2 | 2.56 | 0.40 |
| 1:X:421:VAL:CG2 | 1:X:422:PRO:HD2 | 2.50 | 0.40 |
| 1:X:452:GLN:HG3 | 1:X:459:GLY:O | 2.21 | 0.40 |
| 1:a:270:THR:HG23 | 1:a:272:ASP:H | 1.86 | 0.40 |
| 1:b:484:PRO:HD2 | 1:b:609:TRP:CE3 | 2.55 | 0.40 |
| 1:b:702:GLN:HB2 | 1:c:704:THR:HB | 2.02 | 0.40 |
| 1:c:328:GLN:HE22 | 1:c:333:LYS:CG | 2.30 | 0.40 |
| 1:f:249:ALA:O | 1:f:251:PRO:HD3 | 2.21 | 0.40 |
| 1:f:700:GLU:HB2 | 1:f:702:GLN:HE21 | 1.85 | 0.40 |
| 1:f:715:PHE:CZ | 1:f:729:ILE:HD11 | 2.56 | 0.40 |
| 1:g:270:THR:HG23 | 1:g:272:ASP:H | 1.86 | 0.40 |
| 1:g:324:LYS:HE3 | 1:1:656:VAL:HG11 | 2.03 | 0.40 |
| 1:h:452:GLN:HG3 | 1:h:459:GLY:O | 2.21 | 0.40 |
| 1:h:715:PHE:CZ | 1:h:729:ILE:HD11 | 2.56 | 0.40 |
| 1:i:299:TRP:CG | 1:i:616:LEU:HD13 | 2.56 | 0.40 |
| 1:i:330:GLU:N | 1:i:330:GLU:CD | 2.78 | 0.40 |
| 1:i:704:THR:HB | 1:l:702:GLN:HB2 | 2.02 | 0.40 |
| 1:j:249:ALA:O | 1:j:251:PRO:HD3 | 2.21 | 0.40 |
| 1:j:429:HIS:NE2 | 1:j:610:GLN:CD | 2.79 | 0.40 |
| 1:j:700:GLU:HB2 | 1:j:702:GLN:HE21 | 1.85 | 0.40 |
| 1:k:435:ARG:HA | 1:k:435:ARG:HD3 | 1.79 | 0.40 |
| 1:l:344:GLN:HG2 | 1:l:405:MET:HG2 | 2.03 | 0.40 |
| 1:l:484:PRO:HD2 | 1:l:609:TRP:CE3 | 2.55 | 0.40 |
| 1:l:485:CYS:HB3 | 1:l:579:TYR:HB2 | 2.03 | 0.40 |
| 1:m:702:GLN:HB2 | 1:r:704:THR:HB | 2.03 | 0.40 |
| 1:n:484:PRO:HD2 | 1:n:609:TRP:HE3 | 1.86 | 0.40 |
| 1:n:512:HIS:CE1 | 1:n:515:GLY:HA2 | 2.56 | 0.40 |
| 1:p:484:PRO:HD2 | 1:p:609:TRP:CE3 | 2.55 | 0.40 |
| 1:q:326:VAL:HG21 | 1:q:333:LYS:NZ | 2.37 | 0.40 |
| 1:q:512:HIS:CE1 | 1:q:515:GLY:HA2 | 2.56 | 0.40 |
| 1:q:586:LEU:HD21 | 1:r:490:ARG:CZ | 2.50 | 0.40 |
| 1:r:270:THR:HG23 | 1:r:272:ASP:H | 1.86 | 0.40 |
| 1:r:355:TYR:CZ | 1:r:357:LEU:HB2 | 2.56 | 0.40 |
| 1:r:579:TYR:OH | 1:r:607:MET:CE | 2.68 | 0.40 |
| 1:s:330:GLU:N | 1:s:330:GLU:CD | 2.78 | 0.40 |
| 1:s:527:ALA:O | 1:s:575:ALA:N | 2.45 | 0.40 |
| 1:s:659:ASP:OD1 | 1:s:659:ASP:N | 2.54 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:t:340:THR:HB | 1:y:322:GLN:CB | 2.52 | 0.40 |
| 1:t:355:TYR:CZ | 1:t:357:LEU:HB2 | 2.56 | 0.40 |
| 1:u:344:GLN:HG2 | 1:u:405:MET:HG2 | 2.03 | 0.40 |
| 1:w:392:ARG:NH2 | 1:y:567:GLU:HG3 | 2.37 | 0.40 |
| 1:x:299:TRP:CG | 1:x:616:LEU:HD13 | 2.56 | 0.40 |
| 1:z:344:GLN:HG2 | 1:z:405:MET:HG2 | 2.03 | 0.40 |
| 1:1:270:THR:HG23 | 1:1:272:ASP:H | 1.86 | 0.40 |
| 1:1:381:LEU:HA | 1:1:381:LEU:HD23 | 1.90 | 0.40 |
| 1:2:330:GLU:N | 1:2:330:GLU:CD | 2.78 | 0.40 |
| 1:3:429:HIS:NE2 | 1:3:610:GLN:CD | 2.79 | 0.40 |
| 1:5:715:PHE:CZ | 1:5:729:ILE:HD11 | 2.56 | 0.40 |
| 1:7:230:HIS:HB3 | 1:7:232:ASP:OD1 | 2.22 | 0.40 |
| 1:A:326:VAL:HG21 | 1:A:333:LYS:HZ2 | 1.86 | 0.40 |
| 1:A:326:VAL:HG21 | 1:A:333:LYS:NZ | 2.37 | 0.40 |
| 1:A:344:GLN:HG2 | 1:A:405:MET:HG2 | 2.03 | 0.40 |
| 1:A:429:HIS:NE2 | 1:A:610:GLN:CD | 2.79 | 0.40 |
| 1:B:484:PRO:HD2 | 1:B:609:TRP:CE3 | 2.55 | 0.40 |
| 1:B:527:ALA:O | 1:B:575:ALA:N | 2.45 | 0.40 |
| 1:B:585:ASN:OD1 | 1:B:594:ILE:N | 2.45 | 0.40 |
| 1:B:626:HIS:CD2 | 1:L:736:ARG:NH2 | 2.79 | 0.40 |
| 1:C:230:HIS:HB3 | 1:C:232:ASP:OD1 | 2.21 | 0.40 |
| 1:C:656:VAL:HG11 | 1:D:324:LYS:HE3 | 2.03 | 0.40 |
| 1:D:342:THR:HG22 | 1:D:407:ARG:HA | 2.02 | 0.40 |
| 1:E:230:HIS:HB3 | 1:E:232:ASP:OD1 | 2.22 | 0.40 |
| 1:E:326:VAL:HG21 | 1:E:333:LYS:NZ | 2.37 | 0.40 |
| 1:E:626:HIS:CD2 | 1:F:736:ARG:NH2 | 2.79 | 0.40 |
| 1:F:659:ASP:N | 1:F:659:ASP:OD1 | 2.54 | 0.40 |
| 1:G:249:ALA:O | 1:G:251:PRO:HD3 | 2.21 | 0.40 |
| 1:G:527:ALA:O | 1:G:575:ALA:N | 2.45 | 0.40 |
| 1:H:330:GLU:N | 1:H:330:GLU:CD | 2.78 | 0.40 |
| 1:H:527:ALA:O | 1:H:575:ALA:N | 2.45 | 0.40 |
| 1:I:322:GLN:CB | 1:J:340:THR:HB | 2.50 | 0.40 |
| 1:K:324:LYS:HE3 | 1:L:656:VAL:HG11 | 2.03 | 0.40 |
| 1:M:340:THR:HB | 1:c:322:GLN:HB3 | 2.02 | 0.40 |
| 1:N:355:TYR:CZ | 1:N:357:LEU:HB2 | 2.56 | 0.40 |
| 1:P:324:LYS:HE3 | 1:Q:656:VAL:HG11 | 2.03 | 0.40 |
| 1:P:326:VAL:HG21 | 1:P:333:LYS:NZ | 2.37 | 0.40 |
| 1:Q:571:THR:HG22 | 1:Q:608:VAL:O | 2.20 | 0.40 |
| 1:R:230:HIS:HB3 | 1:R:232:ASP:OD1 | 2.21 | 0.40 |
| 1:R:270:THR:HG23 | 1:R:272:ASP:H | 1.86 | 0.40 |
| 1:R:656:VAL:HG11 | 1:V:324:LYS:HE3 | 2.03 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:253:TYR:HB2 | 1:W:281:PRO:O | 2.21 | 0.40 |
| 1:W:485:CYS:HB3 | 1:W:579:TYR:HB2 | 2.03 | 0.40 |
| 1:Y:704:THR:HB | 1:Z:702:GLN:HB2 | 2.03 | 0.40 |
| 1:a:355:TYR:CZ | 1:a:357:LEU:HB2 | 2.56 | 0.40 |
| 1:a:381:LEU:HD23 | 1:a:381:LEU:HA | 1.90 | 0.40 |
| 1:a:704:THR:HB | 1:3:702:GLN:HB2 | 2.02 | 0.40 |
| 1:c:230:HIS:HB3 | 1:c:232:ASP:OD1 | 2.22 | 0.40 |
| 1:c:626:HIS:CD2 | 1:p:736:ARG:NH2 | 2.79 | 0.40 |
| 1:d:355:TYR:CZ | 1:d:357:LEU:HB2 | 2.56 | 0.40 |
| 1:e:299:TRP:CG | 1:e:616:LEU:HD13 | 2.56 | 0.40 |
| 1:g:249:ALA:O | 1:g:251:PRO:HD3 | 2.21 | 0.40 |
| 1:g:435:ARG:HD3 | 1:g:435:ARG:HA | 1.79 | 0.40 |
| 1:g:704:THR:HB | 1:z:702:GLN:HB2 | 2.02 | 0.40 |
| 1:h:702:GLN:HB2 | 1:k:704:THR:HB | 2.02 | 0.40 |
| 1:i:249:ALA:O | 1:i:251:PRO:HD3 | 2.21 | 0.40 |
| 1:i:270:THR:HG23 | 1:i:272:ASP:H | 1.86 | 0.40 |
| 1:i:490:ARG:CZ | 1:k:586:LEU:HD21 | 2.50 | 0.40 |
| 1:i:626:HIS:CD2 | 1:k:736:ARG:NH2 | 2.79 | 0.40 |
| 1:j:326:VAL:HG21 | 1:j:333:LYS:NZ | 2.37 | 0.40 |
| 1:k:452:GLN:HG3 | 1:k:459:GLY:O | 2.21 | 0.40 |
| 1:k:715:PHE:CZ | 1:k:729:ILE:HD11 | 2.56 | 0.40 |
| 1:m:322:GLN:CB | 1:s:340:THR:HB | 2.51 | 0.40 |
| 1:o:326:VAL:HG21 | 1:o:333:LYS:NZ | 2.37 | 0.40 |
| 1:p:249:ALA:O | 1:p:251:PRO:HD3 | 2.21 | 0.40 |
| 1:q:382:THR:HG21 | 1:q:394:SER:N | 2.36 | 0.40 |
| 1:q:452:GLN:HG3 | 1:q:459:GLY:O | 2.21 | 0.40 |
| 1:u:715:PHE:CZ | 1:u:729:ILE:HD11 | 2.56 | 0.40 |
| 1:v:249:ALA:O | 1:v:251:PRO:HD3 | 2.21 | 0.40 |
| 1:v:322:GLN:HB3 | 1:w:340:THR:HB | 2.03 | 0.40 |
| 1:v:571:THR:HG22 | 1:v:608:VAL:O | 2.20 | 0.40 |
| 1:x:452:GLN:HG3 | 1:x:459:GLY:O | 2.21 | 0.40 |
| 1:y:485:CYS:HB3 | 1:y:579:TYR:HB2 | 2.03 | 0.40 |
| 1:y:715:PHE:CZ | 1:y:729:ILE:HD11 | 2.56 | 0.40 |
| 1:z:485:CYS:HB3 | 1:z:579:TYR:HB2 | 2.03 | 0.40 |
| 1:1:299:TRP:CG | 1:1:616:LEU:HD13 | 2.56 | 0.40 |
| 1:3:299:TRP:CG | 1:3:616:LEU:HD13 | 2.56 | 0.40 |
| 1:4:382:THR:HG21 | 1:4:394:SER:N | 2.36 | 0.40 |
| 1:4:512:HIS:CE1 | 1:4:515:GLY:HA2 | 2.56 | 0.40 |
| 1:7:270:THR:HG23 | 1:7:272:ASP:H | 1.86 | 0.40 |
| 1:8:429:HIS:NE2 | 1:8:610:GLN:CD | 2.79 | 0.40 |
| 1:8:452:GLN:HG3 | 1:8:459:GLY:O | 2.21 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:249:ALA:O | 1:A:251:PRO:HD3 | 2.21 | 0.40 |
| 1:A:253:TYR:HB2 | 1:A:281:PRO:O | 2.21 | 0.40 |
| 1:B:344:GLN:HG2 | 1:B:405:MET:HG2 | 2.03 | 0.40 |
| 1:D:270:THR:HG23 | 1:D:272:ASP:H | 1.86 | 0.40 |
| 1:D:402:PRO:CG | 1:E:232:ASP:HB3 | 2.46 | 0.40 |
| 1:D:579:TYR:OH | 1:D:607:MET:CE | 2.67 | 0.40 |
| 1:E:704:THR:HB | 1:P:702:GLN:HB2 | 2.03 | 0.40 |
| 1:E:736:ARG:NH2 | 1:Q:626:HIS:CD2 | 2.79 | 0.40 |
| 1:G:270:THR:HG23 | 1:G:272:ASP:H | 1.86 | 0.40 |
| 1:G:344:GLN:HG2 | 1:G:405:MET:HG2 | 2.03 | 0.40 |
| 1:G:579:TYR:OH | 1:G:607:MET:CE | 2.68 | 0.40 |
| 1:H:340:THR:HB | 1:Z:322:GLN:CB | 2.51 | 0.40 |
| 1:I:484:PRO:HD2 | 1:I:609:TRP:CE3 | 2.55 | 0.40 |
| 1:J:512:HIS:CE1 | 1:J:515:GLY:HA2 | 2.56 | 0.40 |
| 1:K:342:THR:HG22 | 1:K:407:ARG:HA | 2.02 | 0.40 |
| 1:K:571:THR:HG22 | 1:K:608:VAL:O | 2.20 | 0.40 |
| 1:L:230:HIS:HB3 | 1:L:232:ASP:OD1 | 2.22 | 0.40 |
| 1:L:659:ASP:OD1 | 1:L:659:ASP:N | 2.54 | 0.40 |
| 1:M:270:THR:HG23 | 1:M:272:ASP:H | 1.86 | 0.40 |
| 1:M:330:GLU:N | 1:M:330:GLU:CD | 2.78 | 0.40 |
| 1:M:340:THR:HB | 1:c:322:GLN:CB | 2.50 | 0.40 |
| 1:M:512:HIS:CE1 | 1:M:515:GLY:HA2 | 2.56 | 0.40 |
| 1:N:452:GLN:HG3 | 1:N:459:GLY:O | 2.21 | 0.40 |
| 1:O:398:LEU:C | 1:O:400:TYR:N | 2.80 | 0.40 |
| 1:O:485:CYS:HB3 | 1:O:579:TYR:HB2 | 2.03 | 0.40 |
| 1:O:736:ARG:NH2 | 1:m:626:HIS:CD2 | 2.79 | 0.40 |
| 1:P:429:HIS:NE2 | 1:P:610:GLN:CD | 2.79 | 0.40 |
| 1:Q:299:TRP:CG | 1:Q:616:LEU:HD13 | 2.56 | 0.40 |
| 1:R:253:TYR:HB2 | 1:R:281:PRO:O | 2.21 | 0.40 |
| 1:R:355:TYR:CZ | 1:R:357:LEU:HB2 | 2.56 | 0.40 |
| 1:R:609:TRP:NE1 | 1:S:629:GLY:CA | 2.58 | 0.40 |
| 1:S:715:PHE:CZ | 1:S:729:ILE:HD11 | 2.56 | 0.40 |
| 1:U:249:ALA:O | 1:U:251:PRO:HD3 | 2.21 | 0.40 |
| 1:V:715:PHE:CZ | 1:V:729:ILE:HD11 | 2.56 | 0.40 |
| 1:W:299:TRP:CG | 1:W:616:LEU:HD13 | 2.56 | 0.40 |
| 1:W:382:THR:HG21 | 1:W:394:SER:N | 2.35 | 0.40 |
| 1:W:484:PRO:HD2 | 1:W:609:TRP:CE3 | 2.55 | 0.40 |
| 1:Y:702:GLN:HB2 | 1:Z:704:THR:HB | 2.03 | 0.40 |
| 1:Z:270:THR:HG23 | 1:Z:272:ASP:H | 1.86 | 0.40 |
| 1:a:382:THR:HG21 | 1:a:394:SER:N | 2.35 | 0.40 |
| 1:b:344:GLN:HG2 | 1:b:405:MET:HG2 | 2.03 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:c:452:GLN:HG3 | 1:c:459:GLY:O | 2.21 | 0.40 |
| 1:c:484:PRO:HD2 | 1:c:609:TRP:CE3 | 2.55 | 0.40 |
| 1:d:330:GLU:N | 1:d:330:GLU:CD | 2.78 | 0.40 |
| 1:g:490:ARG:CZ | 1:h:586:LEU:HD21 | 2.50 | 0.40 |
| 1:g:715:PHE:CZ | 1:g:729:ILE:HD11 | 2.56 | 0.40 |
| 1:i:253:TYR:HB2 | 1:i:281:PRO:O | 2.21 | 0.40 |
| 1:i:715:PHE:CZ | 1:i:729:ILE:HD11 | 2.56 | 0.40 |
| 1:j:715:PHE:CZ | 1:j:729:ILE:HD11 | 2.56 | 0.40 |
| 1:m:704:THR:HB | 1:r:702:GLN:HB2 | 2.03 | 0.40 |
| 1:n:715:PHE:CZ | 1:n:729:ILE:HD11 | 2.56 | 0.40 |
| 1:o:253:TYR:HB2 | 1:o:281:PRO:O | 2.21 | 0.40 |
| 1:o:258:TYR:OH | 1:o:399:GLU:OE1 | 2.22 | 0.40 |
| 1:o:702:GLN:HB2 | 1:6:704:THR:HB | 2.02 | 0.40 |
| 1:p:344:GLN:HG2 | 1:p:405:MET:HG2 | 2.03 | 0.40 |
| 1:p:659:ASP:OD1 | 1:p:659:ASP:N | 2.54 | 0.40 |
| 1:q:253:TYR:HB2 | 1:q:281:PRO:O | 2.21 | 0.40 |
| 1:q:299:TRP:CG | 1:q:616:LEU:HD13 | 2.57 | 0.40 |
| 1:q:484:PRO:HD2 | 1:q:609:TRP:CE3 | 2.56 | 0.40 |
| 1:s:249:ALA:O | 1:s:251:PRO:HD3 | 2.21 | 0.40 |
| 1:s:382:THR:HG21 | 1:s:394:SER:N | 2.36 | 0.40 |
| 1:t:230:HIS:HB3 | 1:t:232:ASP:OD1 | 2.22 | 0.40 |
| 1:t:270:THR:HG23 | 1:t:272:ASP:H | 1.86 | 0.40 |
| 1:t:715:PHE:CZ | 1:t:729:ILE:HD11 | 2.56 | 0.40 |
| 1:w:299:TRP:CG | 1:w:616:LEU:HD13 | 2.56 | 0.40 |
| 1:w:382:THR:HG21 | 1:w:394:SER:N | 2.35 | 0.40 |
| 1:2:355:TYR:CZ | 1:2:357:LEU:HB2 | 2.56 | 0.40 |
| 1:3:398:LEU:C | 1:3:400:TYR:N | 2.80 | 0.40 |
| 1:3:485:CYS:HB3 | 1:3:579:TYR:HB2 | 2.03 | 0.40 |
| 1:4:579:TYR:OH | 1:4:607:MET:CE | 2.68 | 0.40 |
| 1:4:715:PHE:CZ | 1:4:729:ILE:HD11 | 2.56 | 0.40 |
| 1:5:299:TRP:CG | 1:5:616:LEU:HD13 | 2.56 | 0.40 |
| 1:5:452:GLN:HG3 | 1:5:459:GLY:O | 2.21 | 0.40 |
| 1:6:659:ASP:N | 1:6:659:ASP:OD1 | 2.54 | 0.40 |
| 1:7:355:TYR:CZ | 1:7:357:LEU:HB2 | 2.56 | 0.40 |
| 1:8:326:VAL:HG21 | 1:8:333:LYS:NZ | 2.37 | 0.40 |
| 1:8:484:PRO:HD2 | 1:8:609:TRP:HE3 | 1.86 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 oligosaccharides 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.

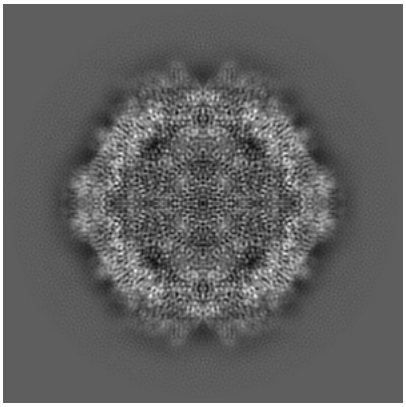
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21017. These allow visual inspection of the internal detail of the map and identification of artifacts.

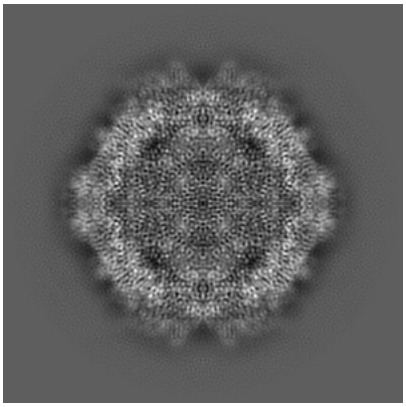
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

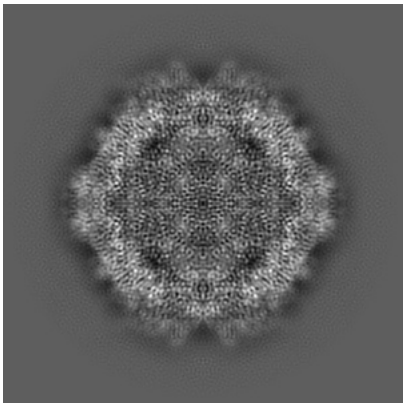
### 6.1.1 Primary map



X



Y

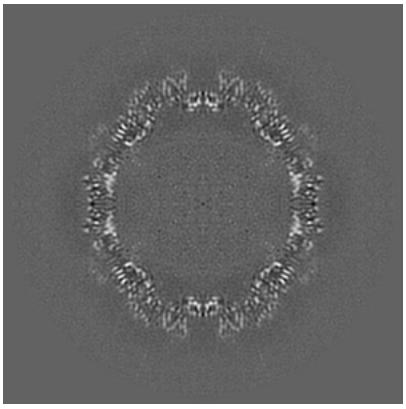


Z

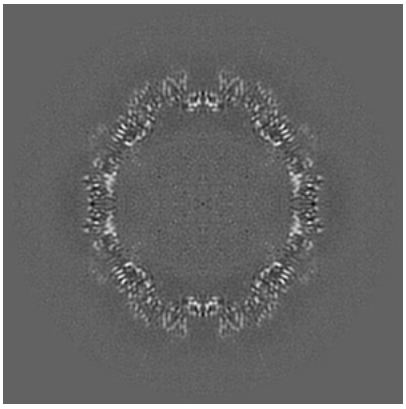
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

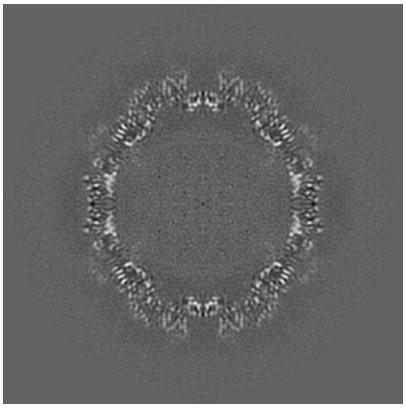
### 6.2.1 Primary map



X Index: 199



Y Index: 199

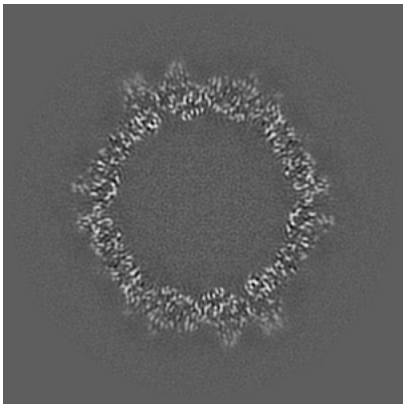


Z Index: 199

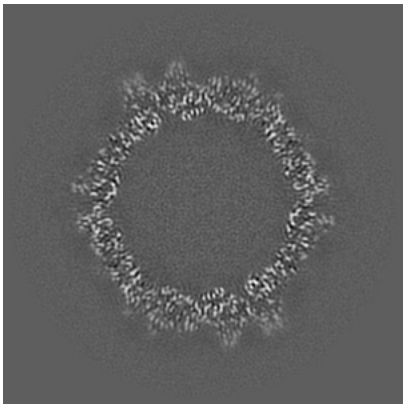
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

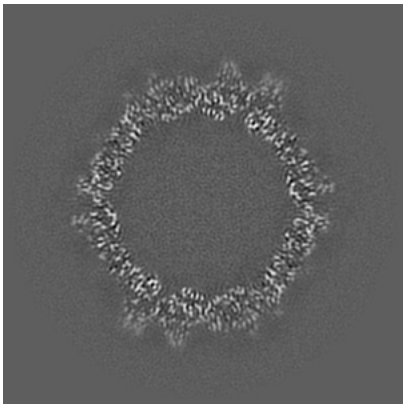
### 6.3.1 Primary map



X Index: 214



Y Index: 214

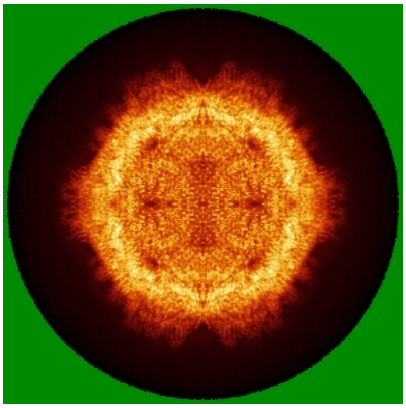


Z Index: 184

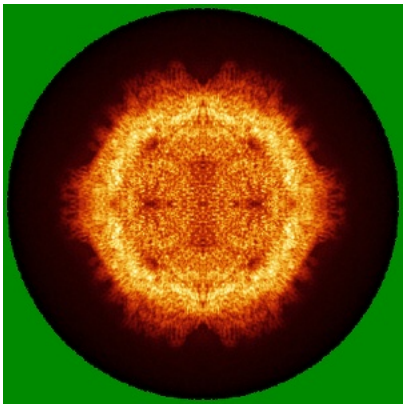
The images above show the largest variance slices of the map in three orthogonal directions.

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

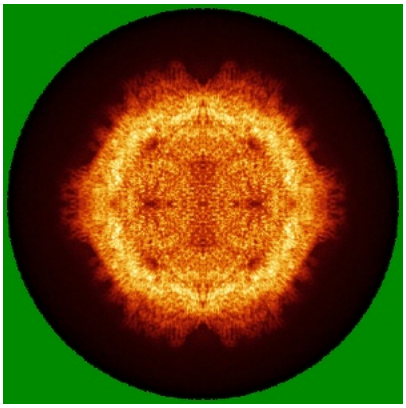
### 6.4.1 Primary map



X



Y

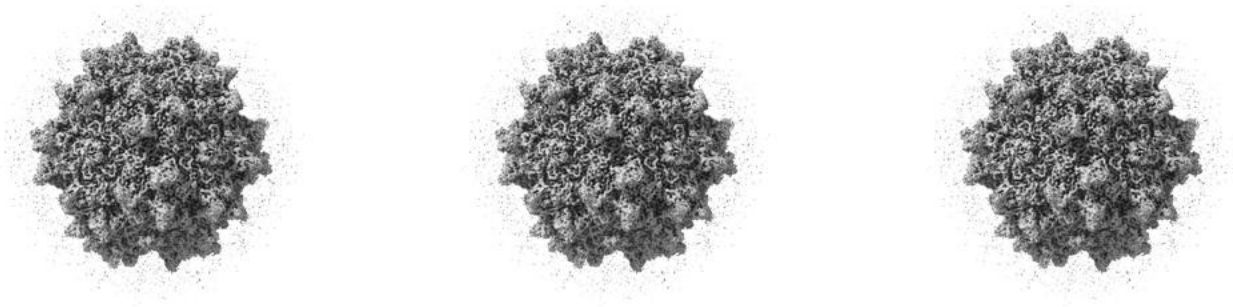


Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

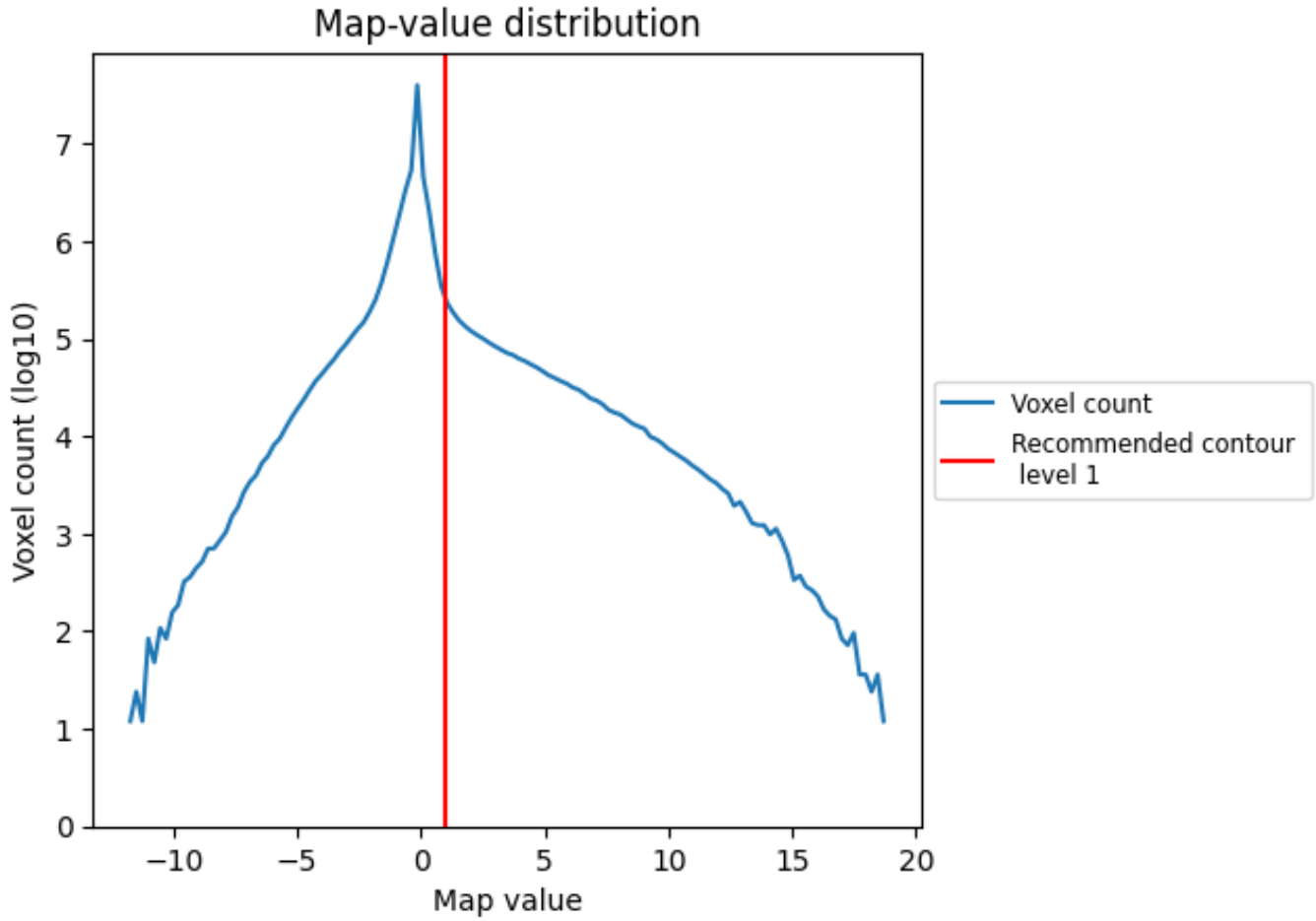
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

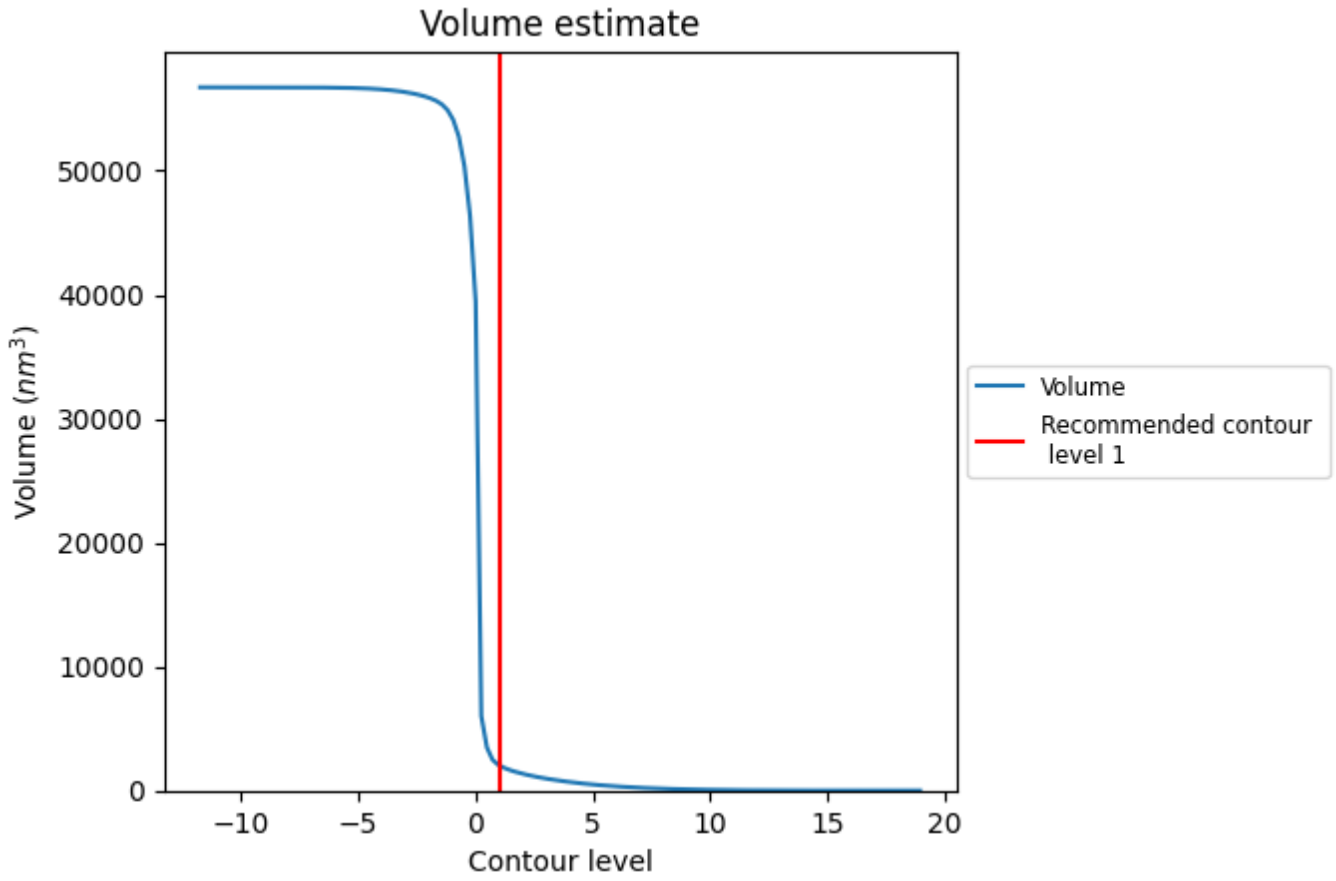
This section contains the results of statistical analysis of the map.

## 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.

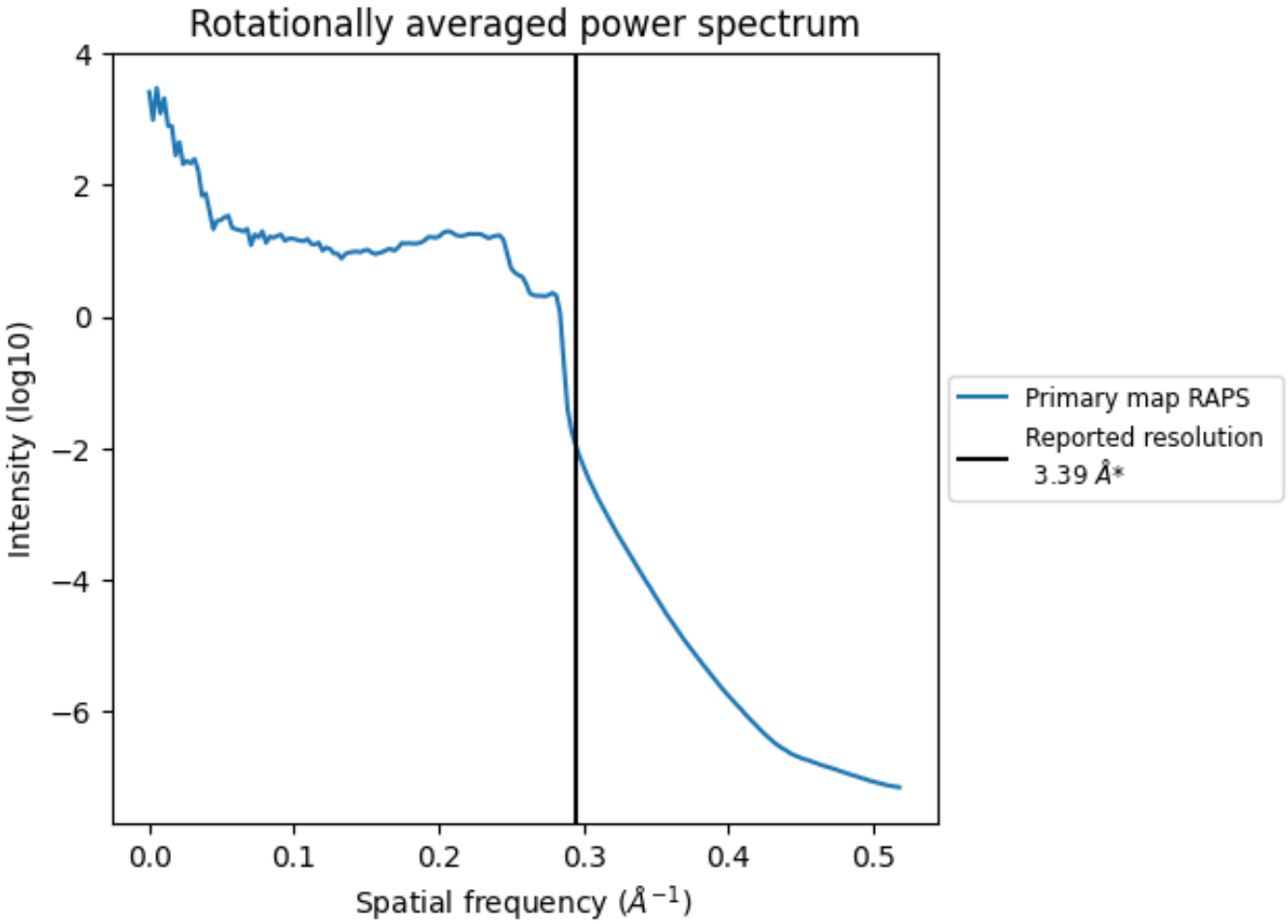
## 7.2 Volume estimate




The volume at the recommended contour level is 2037 $nm^3$; this corresponds to an approximate mass of 1840 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 0.295 Å$^{-1}$

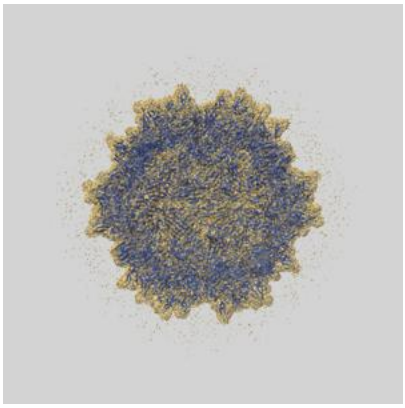
# 8 Fourier-Shell correlation (i)

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

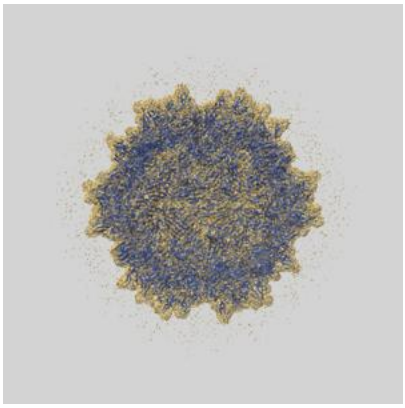
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21017 and PDB model 6V1T. Per-residue inclusion information can be found in section 3 on page 12.

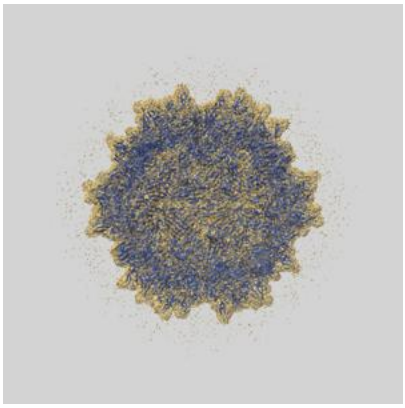
## 9.1 Map-model overlay



X



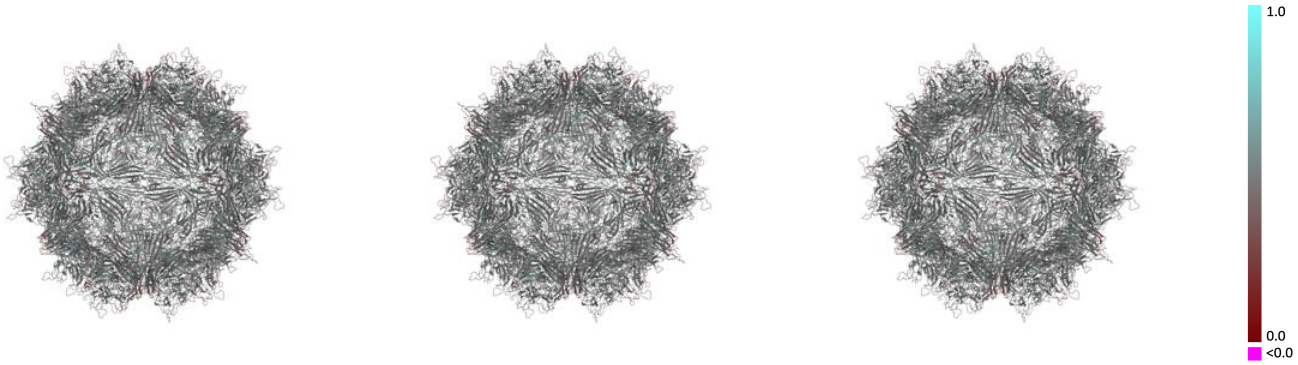
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

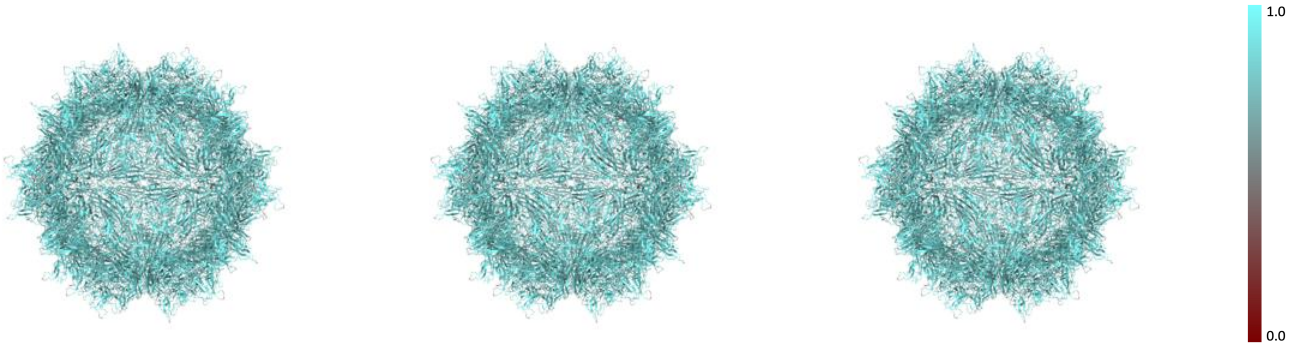
## 9.2 Q-score mapped to coordinate model




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.

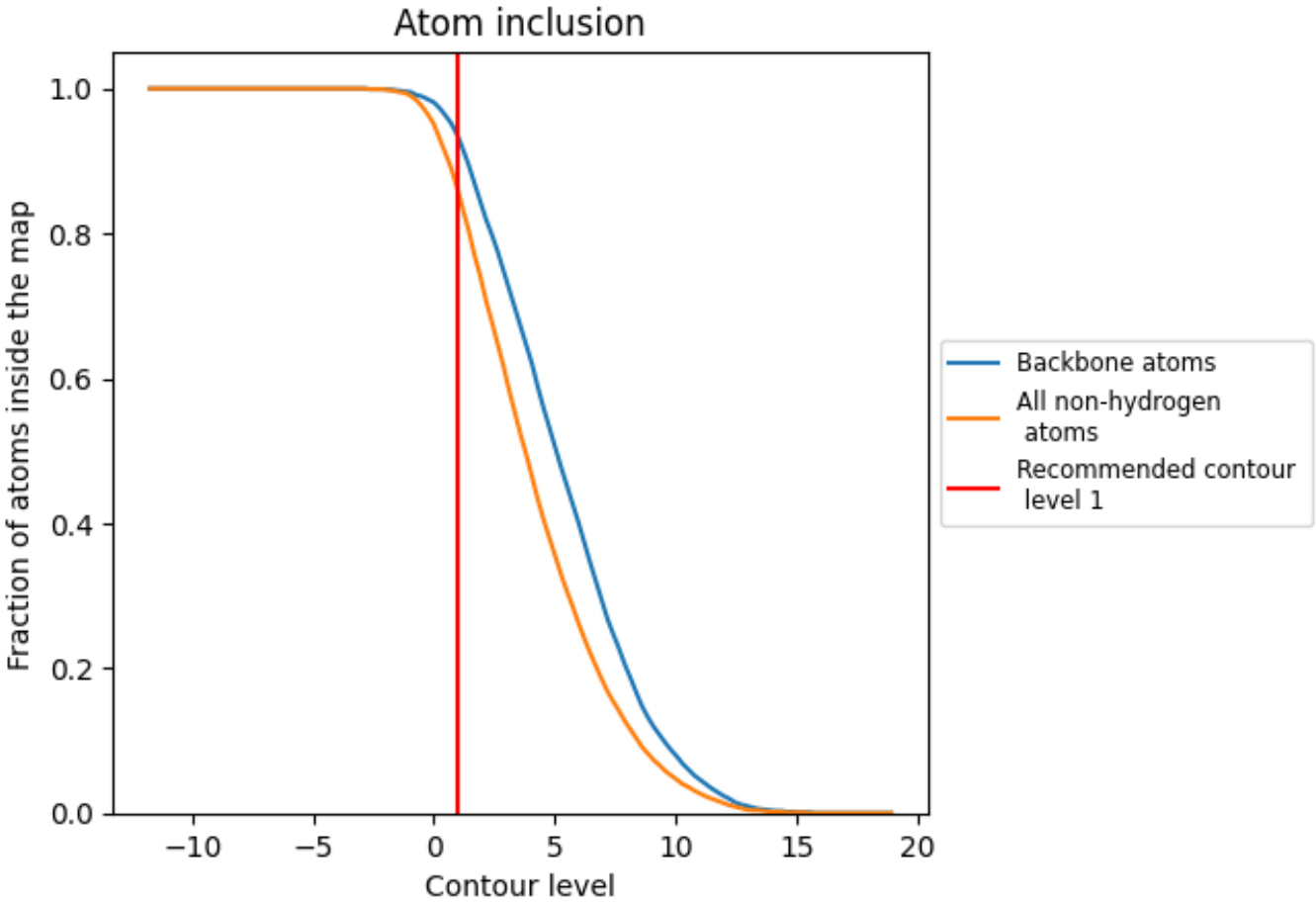
## 9.3 Atom inclusion mapped to coordinate model




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 (1).

## 9.4 Atom inclusion (i)




At the recommended contour level, 93% of all backbone atoms, 86% 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 (1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8590 | 0.4800 |
| 1 | 0.8620 | 0.4810 |
| 2 | 0.8620 | 0.4800 |
| 3 | 0.8590 | 0.4800 |
| 4 | 0.8590 | 0.4800 |
| 5 | 0.8590 | 0.4810 |
| 6 | 0.8600 | 0.4810 |
| 7 | 0.8590 | 0.4800 |
| 8 | 0.8580 | 0.4790 |
| A | 0.8620 | 0.4800 |
| B | 0.8590 | 0.4810 |
| C | 0.8590 | 0.4800 |
| D | 0.8580 | 0.4800 |
| E | 0.8590 | 0.4810 |
| F | 0.8600 | 0.4810 |
| G | 0.8620 | 0.4800 |
| H | 0.8590 | 0.4800 |
| I | 0.8620 | 0.4790 |
| J | 0.8590 | 0.4800 |
| K | 0.8580 | 0.4790 |
| L | 0.8590 | 0.4800 |
| M | 0.8590 | 0.4800 |
| N | 0.8570 | 0.4800 |
| O | 0.8590 | 0.4790 |
| P | 0.8570 | 0.4800 |
| Q | 0.8590 | 0.4790 |
| R | 0.8590 | 0.4800 |
| S | 0.8600 | 0.4810 |
| T | 0.8620 | 0.4790 |
| U | 0.8590 | 0.4810 |
| V | 0.8580 | 0.4800 |
| W | 0.8590 | 0.4780 |
| X | 0.8570 | 0.4800 |
| Y | 0.8590 | 0.4800 |
| Z | 0.8590 | 0.4780 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| a | 0.8570 | 0.4800 |
| b | 0.8590 | 0.4820 |
| c | 0.8620 | 0.4800 |
| d | 0.8620 | 0.4790 |
| e | 0.8580 | 0.4800 |
| f | 0.8590 | 0.4800 |
| g | 0.8590 | 0.4810 |
| h | 0.8590 | 0.4820 |
| i | 0.8590 | 0.4810 |
| j | 0.8600 | 0.4790 |
| k | 0.8590 | 0.4810 |
| l | 0.8620 | 0.4790 |
| m | 0.8590 | 0.4790 |
| n | 0.8590 | 0.4790 |
| o | 0.8620 | 0.4810 |
| p | 0.8620 | 0.4810 |
| q | 0.8590 | 0.4780 |
| r | 0.8590 | 0.4790 |
| s | 0.8590 | 0.4800 |
| t | 0.8590 | 0.4810 |
| u | 0.8600 | 0.4810 |
| v | 0.8590 | 0.4800 |
| w | 0.8590 | 0.4800 |
| x | 0.8580 | 0.4780 |
| y | 0.8570 | 0.4800 |
| z | 0.8620 | 0.4820 |