# Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 02:53 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 9MOF / pdb_00009mof |
| EMDB ID | : | EMD-48458 |
| Title | : | Structure of the bacteriophage T4 portal-neck-tail connector complex |
| Authors | : | Fokine, A.; Zhu, J.; Klose, T.; Vago, F.; Arnaud, C.; Wang, Z.; Khare, B.; Rossmann, M.G.; Chen, Z.; Sun, L.; Fang, Q.; Kuhn, R.; Rao, V.B. |
| Deposited on | : | 2024-12-26 |
| Resolution | : | 3.80 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:

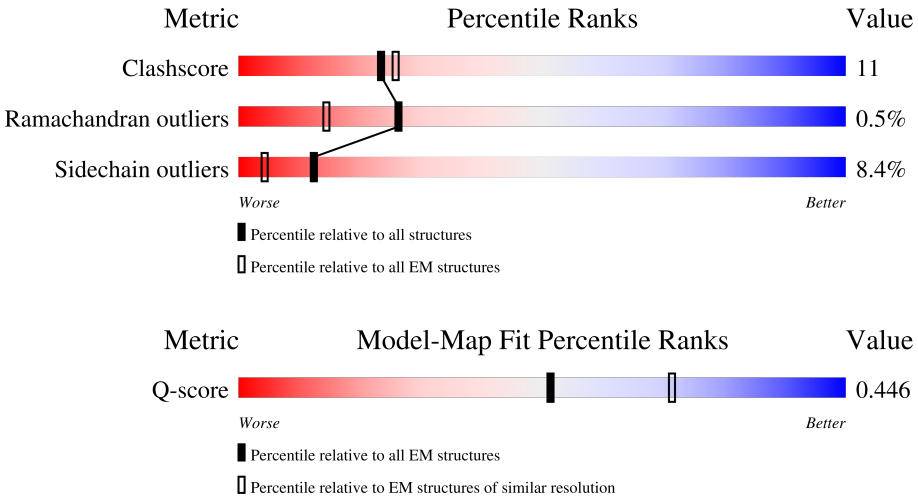
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 10198 ( 3.30 - 4.30 ) |

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 | 0 | 256 | 62% 29% • 5% |
| 1 | k | 256 | 62% 29% 5% 5% |
| 1 | l | 256 | 61% 30% 5% 5% |
| 1 | m | 256 | 58% 32% 5% 5% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | n | 256 | 62% 30% 5% |
| 1 | p | 256 | 59% 31% 5% 5% |
| 2 | 1 | 659 | 12% 66% 31% |
| 2 | 2 | 659 | 13% 68% 29% |
| 2 | 3 | 659 | 11% 69% 27% |
| 2 | 4 | 659 | 10% 68% 28% |
| 2 | 5 | 659 | 10% 68% 29% |
| 2 | AD | 659 | 12% 71% 26% |
| 2 | AK | 659 | 18% 66% 30% |
| 2 | AL | 659 | 19% 68% 27% |
| 2 | AM | 659 | 19% 71% 26% |
| 2 | AN | 659 | 21% 70% 27% |
| 2 | AO | 659 | 22% 69% 28% |
| 2 | AP | 659 | 19% 67% 28% |
| 2 | B1 | 659 | 60% 65% 31% |
| 2 | B2 | 659 | 27% 68% 28% |
| 2 | B3 | 659 | 41% 65% 31% |
| 2 | B4 | 659 | 63% 69% 27% |
| 2 | B5 | 659 | 28% 68% 29% |
| 2 | B6 | 659 | 41% 64% 33% |
| 2 | B7 | 659 | 63% 68% 30% |
| 2 | Bp | 659 | 23% 69% 28% |
| 2 | Bq | 659 | 39% 67% 29% |
| 2 | Br | 659 | 60% 67% 30% |
| 2 | Bs | 659 | 23% 67% 29% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | Bt | 659 | 37% 65% 30% |
| 2 | Bu | 659 | 61% 66% 29% 5% |
| 2 | Bv | 659 | 23% 67% 29% |
| 2 | Bw | 659 | 36% 68% 27% |
| 2 | Bx | 659 | 59% 69% 28% |
| 2 | By | 659 | 24% 69% 27% |
| 2 | Bz | 659 | 39% 67% 29% |
| 3 | 6 | 163 | 65% 30% |
| 3 | 7 | 163 | 61% 33% 5% |
| 3 | 8 | 163 | 60% 34% 6% |
| 3 | 9 | 163 | 57% 37% 5% |
| 3 | AA | 163 | 6% 55% 39% 5% |
| 3 | AE | 163 | 5% 61% 31% 8% |
| 3 | AF | 163 | 7% 56% 36% 7% |
| 3 | AG | 163 | 7% 59% 36% 6% |
| 3 | AH | 163 | 6% 60% 35% 6% |
| 3 | AI | 163 | 7% 61% 36% |
| 3 | AJ | 163 | 8% 63% 29% 7% |
| 3 | BX | 163 | 16% 58% 34% 8% |
| 3 | BY | 163 | 33% 59% 36% 6% |
| 3 | BZ | 163 | 63% 61% 33% 6% |
| 3 | Ba | 163 | 10% 67% 27% 6% |
| 3 | Bb | 163 | 31% 64% 30% 6% |
| 3 | Bc | 163 | 71% 63% 33% |
| 3 | Bd | 163 | 11% 63% 33% 5% |

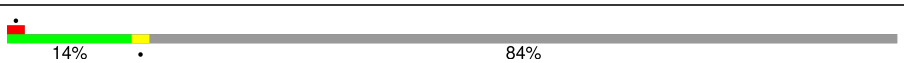
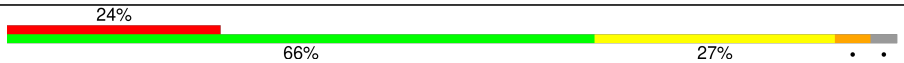
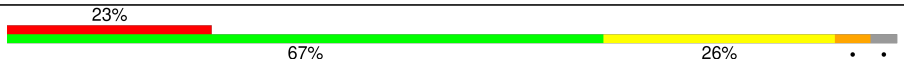
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | Be | 163 | 34% 61% 36% |
| 3 | Bf | 163 | 68% 61% 32% 7% |
| 3 | Bg | 163 | 15% 58% 34% 8% |
| 3 | Bh | 163 | 32% 54% 39% 7% |
| 3 | Bi | 163 | 64% 58% 38% |
| 3 | Bj | 163 | 12% 59% 35% 6% |
| 3 | Bk | 163 | 31% 58% 35% 7% |
| 3 | Bl | 163 | 66% 63% 30% 7% |
| 3 | Bm | 163 | 13% 65% 32% |
| 3 | Bn | 163 | 34% 56% 38% 6% |
| 3 | Bo | 163 | 66% 65% 29% 6% |
| 3 | o | 163 | 61% 32% 7% |
| 4 | A | 487 | 13% 84% |
| 4 | B | 487 | 15% 84% |
| 4 | C | 487 | 14% 84% |
| 4 | D | 487 | 14% 84% |
| 4 | E | 487 | 15% 84% |
| 4 | F | 487 | 14% 84% |
| 4 | G | 487 | 14% 84% |
| 4 | H | 487 | 13% 84% |
| 4 | I | 487 | 14% 84% |
| 4 | J | 487 | 15% 84% |
| 4 | K | 487 | 13% 84% |
| 4 | L | 487 | 13% 84% |
| 4 | M | 487 | 13% 84% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | N | 487 |   |
| 4 | O | 487 |   |
| 4 | P | 487 |   |
| 4 | Q | 487 |   |
| 4 | R | 487 |   |
| 4 | S | 487 |   |
| 4 | T | 487 |   |
| 4 | U | 487 |   |
| 4 | V | 487 |   |
| 4 | W | 487 |   |
| 4 | X | 487 |   |
| 4 | Y | 487 |   |
| 4 | Z | 487 |   |
| 4 | a | 487 |   |
| 4 | b | 487 |   |
| 4 | c | 487 |   |
| 4 | d | 487 |   |
| 4 | e | 487 |   |
| 4 | f | 487 |   |
| 4 | g | 487 |   |
| 4 | h | 487 |   |
| 4 | i | 487 |   |
| 4 | j | 487 |   |
| 5 | A0 | 524 |   |
| 5 | A1 | 524 |   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | A2 | 524 | 26% 65% 28% |
| 5 | A3 | 524 | 23% 58% 33% 6% |
| 5 | Av | 524 | 24% 65% 27% 5% |
| 5 | Ax | 524 | 23% 69% 25% |
| 5 | BA | 524 | 24% 63% 29% 5% |
| 5 | BB | 524 | 21% 60% 30% 7% |
| 5 | BD | 524 | 23% 66% 28% |
| 5 | BF | 524 | 24% 66% 27% |
| 5 | BG | 524 | 23% 66% 24% 5% 5% |
| 5 | BH | 524 | 24% 68% 25% |
| 6 | A4 | 521 | 5% 66% 19% 12% |
| 6 | A5 | 521 | 5% 60% 26% 12% |
| 6 | A7 | 521 | 67% 20% 12% |
| 6 | A8 | 521 | 58% 24% 16% |
| 6 | A9 | 521 | 64% 22% 12% |
| 6 | AV | 521 | 60% 26% 12% |
| 6 | AW | 521 | 6% 65% 20% 12% |
| 6 | AX | 521 | 5% 63% 23% 12% |
| 6 | AZ | 521 | 5% 64% 20% 12% |
| 6 | Ac | 521 | 5% 63% 24% 12% |
| 6 | Ad | 521 | 67% 19% 12% |
| 6 | Ae | 521 | 61% 24% 12% |
| 6 | Af | 521 | 5% 67% 19% 12% |
| 6 | Ag | 521 | 6% 65% 21% 12% |
| 6 | Ah | 521 | 5% 65% 21% 12% |

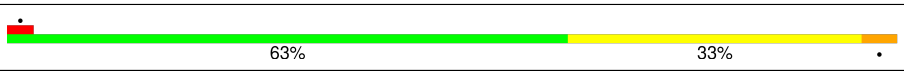
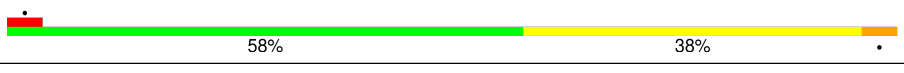
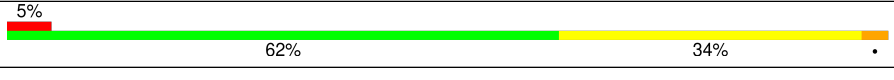
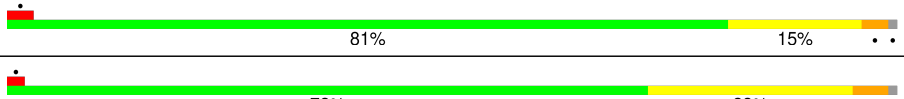
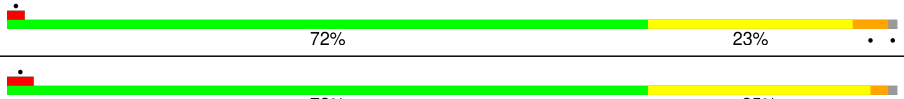
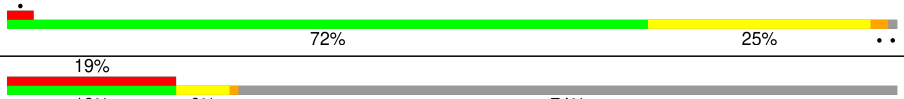
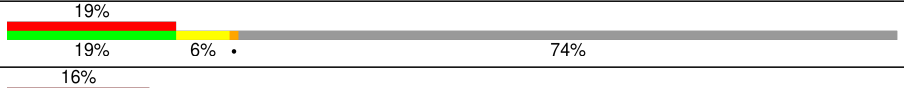
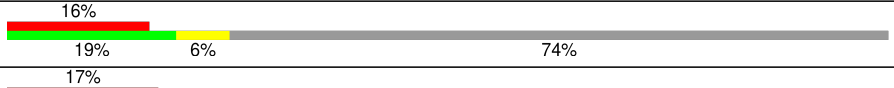
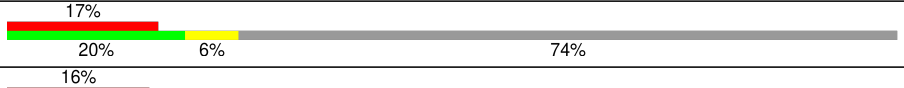
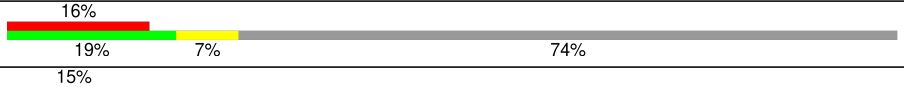
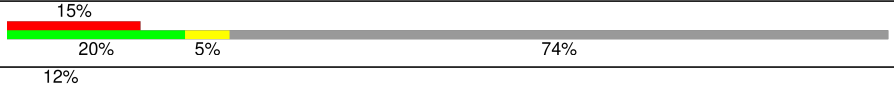
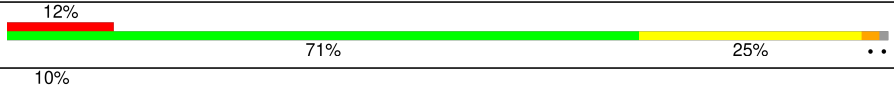
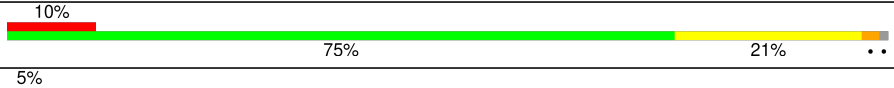
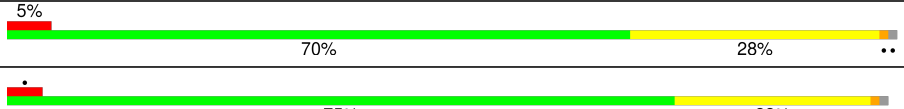
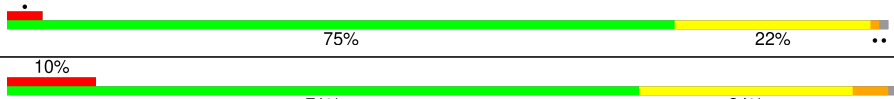
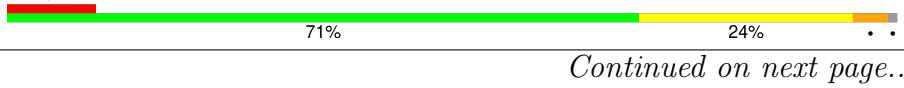
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 6 | Ai | 521 | 7% 69% 18% • 12% |
| 6 | Aj | 521 | 5% 67% 20% • 12% |
| 6 | Ak | 521 | • 64% 23% • 12% |
| 6 | Am | 521 | • 63% 23% • 12% |
| 6 | An | 521 | 5% 61% 22% • 16% |
| 6 | Ao | 521 | • 61% 21% • 16% |
| 6 | Ap | 521 | • 62% 20% • 16% |
| 6 | Au | 521 | • 62% 24% • 12% |
| 6 | Aw | 521 | 6% 66% 20% • 12% |
| 6 | Ay | 521 | • 65% 19% • 12% |
| 6 | Az | 521 | • 64% 22% • 12% |
| 6 | BI | 521 | • 64% 23% • 12% |
| 6 | BJ | 521 | • 57% 26% • 16% |
| 6 | BK | 521 | • 61% 26% • 12% |
| 6 | BM | 521 | • 63% 24% • 12% |
| 7 | A6 | 309 | 7% 69% 27% • |
| 7 | AY | 309 | • 66% 30% • |
| 7 | Aa | 309 | 5% 68% 28% • |
| 7 | Ab | 309 | 5% 69% 26% 5% |
| 7 | Al | 309 | 8% 68% 27% 5% |
| 7 | Aq | 309 | 6% 63% 33% • |
| 7 | Ar | 309 | 5% 62% 27% 5% 6% |
| 7 | As | 309 | 7% 72% 24% • |
| 7 | At | 309 | 13% 67% 25% • • |
| 7 | BC | 309 | 8% 64% 32% • |

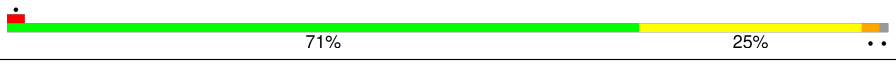
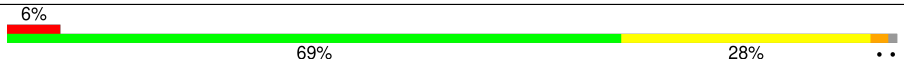
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 7 | BE | 309 |   |
| 7 | BL | 309 |   |
| 8 | AB | 272 |   |
| 8 | q | 272 |   |
| 8 | r | 272 |   |
| 8 | s | 272 |   |
| 8 | t | 272 |   |
| 8 | u | 272 |   |
| 9 | AC | 176 |   |
| 9 | v | 176 |   |
| 9 | w | 176 |   |
| 9 | x | 176 |   |
| 9 | y | 176 |   |
| 9 | z | 176 |   |
| 10 | AQ | 376 |   |
| 10 | AR | 376 |   |
| 10 | AS | 376 |   |
| 10 | AT | 376 |   |
| 10 | AU | 376 |   |
| 11 | BN | 80 |   |
| 11 | BO | 80 |   |
| 11 | BP | 80 |   |
| 11 | BQ | 80 |   |
| 11 | BR | 80 |   |
| 11 | BS | 80 |   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 11 | BT | 80 |   |
| 11 | BU | 80 |   |
| 11 | BV | 80 |   |
| 11 | BW | 80 |   |

# 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 435087 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 gp14, neck protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1993 | 1279 | 323 | 387 | 4 | | |
| 1 | k | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1993 | 1279 | 323 | 387 | 4 | | |
| 1 | l | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1993 | 1279 | 323 | 387 | 4 | | |
| 1 | m | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1993 | 1279 | 323 | 387 | 4 | | |
| 1 | n | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1993 | 1279 | 323 | 387 | 4 | | |
| 1 | p | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1993 | 1279 | 323 | 387 | 4 | | |

- Molecule 2 is a protein called gp18, tail sheath protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 653 | Total | C | N | O | S | 0 | 0 |
| | | | 4985 | 3142 | 839 | 993 | 11 | | |
| 2 | 2 | 653 | Total | C | N | O | S | 0 | 0 |
| | | | 4985 | 3142 | 839 | 993 | 11 | | |
| 2 | 3 | 653 | Total | C | N | O | S | 0 | 0 |
| | | | 4985 | 3142 | 839 | 993 | 11 | | |
| 2 | 4 | 653 | Total | C | N | O | S | 0 | 0 |
| | | | 4985 | 3142 | 839 | 993 | 11 | | |
| 2 | 5 | 653 | Total | C | N | O | S | 0 | 0 |
| | | | 4985 | 3142 | 839 | 993 | 11 | | |
| 2 | AD | 653 | Total | C | N | O | S | 0 | 0 |
| | | | 4985 | 3142 | 839 | 993 | 11 | | |
| 2 | AK | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | AL | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | AM | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | AN | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | AO | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | AP | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | B1 | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | B2 | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | B3 | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | B4 | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | B5 | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | B6 | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | B7 | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bp | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bq | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Br | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bs | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bt | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bu | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bv | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bw | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bx | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | By | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |
| 2 | Bz | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5000 | 3152 | 841 | 996 | 11 | | |

There are 90 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 1 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| 1 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| 1 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| 2 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| 2 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| 2 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| 3 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| 3 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| 3 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| 4 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| 4 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| 4 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| 5 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| 5 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| 5 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| AD | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| AD | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| AD | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| AK | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| AK | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| AK | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| AL | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| AL | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| AL | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| AM | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| AM | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| AM | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| AN | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| AN | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| AN | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| AO | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| AO | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| AO | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| AP | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| AP | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| AP | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| B1 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| B1 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| B1 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| B2 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| B2 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| B2 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B3 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| B3 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| B3 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| B4 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| B4 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| B4 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| B5 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| B5 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| B5 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| B6 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| B6 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| B6 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| B7 | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| B7 | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| B7 | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bp | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bp | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bp | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bq | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bq | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bq | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Br | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Br | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Br | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bs | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bs | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bs | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bt | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bt | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bt | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bu | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bu | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bu | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bv | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bv | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bv | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bw | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bw | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bw | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bx | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bx | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bx | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| By | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| By | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| By | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |
| Bz | 109 | ASN | SER | conflict | UNP A0A7S9SVW9 |
| Bz | 301 | GLY | GLU | conflict | UNP A0A7S9SVW9 |
| Bz | 399 | VAL | ALA | conflict | UNP A0A7S9SVW9 |

- Molecule 3 is a protein called gp19, tail tube protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 6 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 3 | 7 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 3 | 8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 3 | 9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 3 | AA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |
| 3 | AE | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | AF | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | AG | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | AH | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | AI | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | AJ | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | BX | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | BY | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | BZ | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Ba | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bb | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | Bc | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bd | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Be | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bf | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bg | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bh | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bi | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bj | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bk | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bl | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bm | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bn | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | Bo | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 828 | 219 | 253 | 4 | | |
| 3 | o | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 218 | 252 | 3 | | |

- Molecule 4 is a protein called gpwac, fibritin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | A | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | B | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | C | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | D | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | E | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | F | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | G | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | H | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | I | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | J | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | K | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | L | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | M | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | N | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | O | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | P | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | Q | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | R | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | S | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | T | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | U | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | V | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | W | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | X | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | Y | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | Z | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | a | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | b | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | c | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | d | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | e | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | f | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | g | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | h | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | i | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |
| 4 | j | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 601 | 373 | 102 | 125 | 1 | | |

- Molecule 5 is a protein called gp20, portal protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | A0 | 507 | Total | C | N | O | S | 0 | 0 |
| | | | 4140 | 2611 | 717 | 790 | 22 | | |
| 5 | A1 | 507 | Total | C | N | O | S | 0 | 0 |
| | | | 4140 | 2611 | 717 | 790 | 22 | | |
| 5 | A2 | 506 | Total | C | N | O | S | 0 | 0 |
| | | | 4132 | 2607 | 715 | 788 | 22 | | |
| 5 | A3 | 506 | Total | C | N | O | S | 0 | 0 |
| | | | 4132 | 2607 | 715 | 788 | 22 | | |
| 5 | Av | 506 | Total | C | N | O | S | 0 | 0 |
| | | | 4132 | 2607 | 715 | 788 | 22 | | |
| 5 | Ax | 506 | Total | C | N | O | S | 0 | 0 |
| | | | 4132 | 2607 | 715 | 788 | 22 | | |
| 5 | BA | 500 | Total | C | N | O | S | 0 | 0 |
| | | | 4074 | 2571 | 707 | 776 | 20 | | |
| 5 | BB | 488 | Total | C | N | O | S | 0 | 0 |
| | | | 3995 | 2517 | 695 | 761 | 22 | | |
| 5 | BD | 506 | Total | C | N | O | S | 0 | 0 |
| | | | 4132 | 2607 | 715 | 788 | 22 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | BF | 506 | Total | C | N | O | S | 0 | 0 |
| | | | 4132 | 2607 | 715 | 788 | 22 | | |
| 5 | BG | 497 | Total | C | N | O | S | 0 | 0 |
| | | | 4039 | 2549 | 702 | 768 | 20 | | |
| 5 | BH | 506 | Total | C | N | O | S | 0 | 0 |
| | | | 4091 | 2582 | 710 | 779 | 20 | | |

- Molecule 6 is a protein called gp23, major capsid protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | A4 | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | A5 | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | A7 | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | A8 | 440 | Total | C | N | O | S | 0 | 0 |
| | | | 3311 | 2099 | 564 | 633 | 15 | | |
| 6 | A9 | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | AV | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | AW | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | AX | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | AZ | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Ac | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Ad | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Ae | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Af | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Ag | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Ah | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Ai | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | Aj | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Ak | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Am | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | An | 440 | Total | C | N | O | S | 0 | 0 |
| | | | 3311 | 2099 | 564 | 633 | 15 | | |
| 6 | Ao | 437 | Total | C | N | O | S | 0 | 0 |
| | | | 3291 | 2088 | 560 | 628 | 15 | | |
| 6 | Ap | 440 | Total | C | N | O | S | 0 | 0 |
| | | | 3311 | 2099 | 564 | 633 | 15 | | |
| 6 | Au | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Aw | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Ay | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | Az | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | BI | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | BJ | 437 | Total | C | N | O | S | 0 | 0 |
| | | | 3291 | 2088 | 560 | 628 | 15 | | |
| 6 | BK | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |
| 6 | BM | 456 | Total | C | N | O | S | 0 | 0 |
| | | | 3425 | 2167 | 584 | 659 | 15 | | |

- Molecule 7 is a protein called gp13, neck protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | A6 | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1551 | 413 | 461 | 13 | | |
| 7 | AY | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2435 | 1550 | 412 | 460 | 13 | | |
| 7 | Aa | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1551 | 413 | 461 | 13 | | |
| 7 | Ab | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1551 | 413 | 461 | 13 | | |
| 7 | Al | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2435 | 1550 | 412 | 460 | 13 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | Aq | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1551 | 413 | 461 | 13 | | |
| 7 | Ar | 290 | Total | C | N | O | S | 0 | 0 |
| | | | 2310 | 1473 | 389 | 437 | 11 | | |
| 7 | As | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1551 | 413 | 461 | 13 | | |
| 7 | At | 298 | Total | C | N | O | S | 0 | 0 |
| | | | 2371 | 1512 | 402 | 445 | 12 | | |
| 7 | BC | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1551 | 413 | 461 | 13 | | |
| 7 | BE | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1551 | 413 | 461 | 13 | | |
| 7 | BL | 308 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1551 | 413 | 461 | 13 | | |

- Molecule 8 is a protein called gp15, tail terminator protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | AB | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2227 | 1424 | 369 | 425 | 9 | | |
| 8 | q | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2227 | 1424 | 369 | 425 | 9 | | |
| 8 | r | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2227 | 1424 | 369 | 425 | 9 | | |
| 8 | s | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2227 | 1424 | 369 | 425 | 9 | | |
| 8 | t | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2227 | 1424 | 369 | 425 | 9 | | |
| 8 | u | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2227 | 1424 | 369 | 425 | 9 | | |

- Molecule 9 is a protein called gp3, tube terminator protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | AC | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1383 | 890 | 215 | 274 | 4 | | |
| 9 | v | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1383 | 890 | 215 | 274 | 4 | | |
| 9 | w | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1383 | 890 | 215 | 274 | 4 | | |
| 9 | x | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1383 | 890 | 215 | 274 | 4 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | y | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1383 | 890 | 215 | 274 | 4 | | |
| 9 | z | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1383 | 890 | 215 | 274 | 4 | | |

- Molecule 10 is a protein called Hoc, highly immunogenic outer capsid protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | AQ | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 519 | 129 | 152 | 5 | | |
| 10 | AR | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 519 | 129 | 152 | 5 | | |
| 10 | AS | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 519 | 129 | 152 | 5 | | |
| 10 | AT | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 519 | 129 | 152 | 5 | | |
| 10 | AU | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 519 | 129 | 152 | 5 | | |

- Molecule 11 is a protein called Soc, small outer capsid protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 11 | BN | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BO | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BP | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BQ | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BR | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BS | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BT | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BU | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BV | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |
| 11 | BW | 79 | Total | C | N | O | 0 | 0 |
| | | | 636 | 405 | 106 | 125 | | |

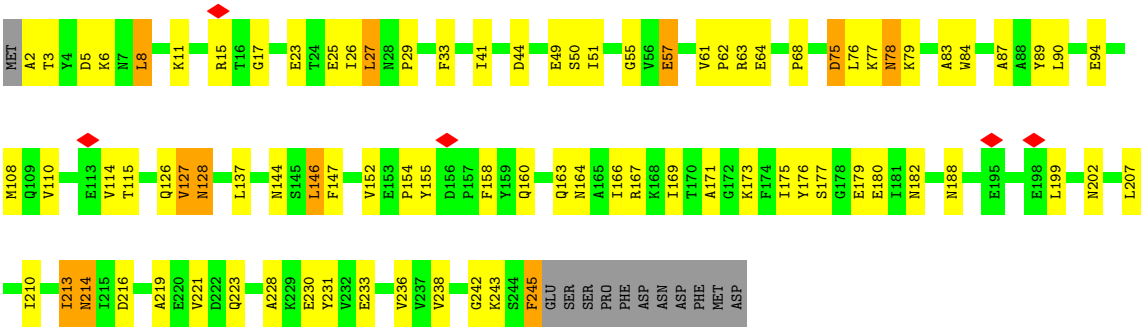
# 3 Residue-property plots (i)

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: gp14, neck protein

Chain 0:

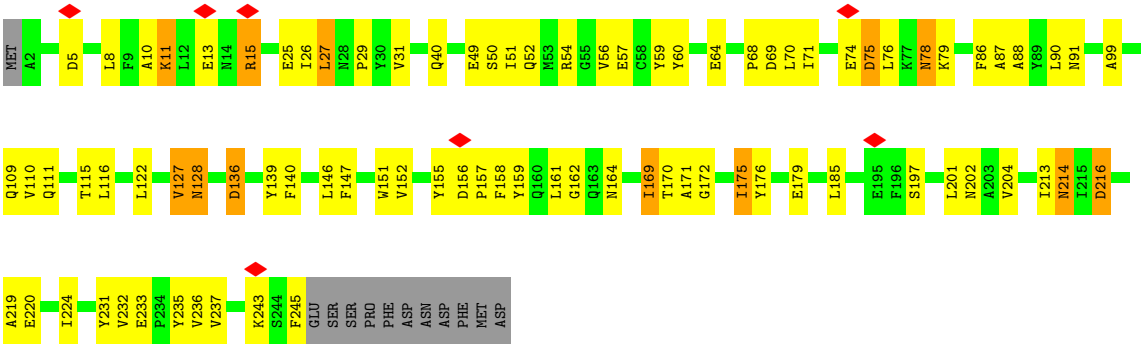



• Molecule 1: gp14, neck protein

Chain k:



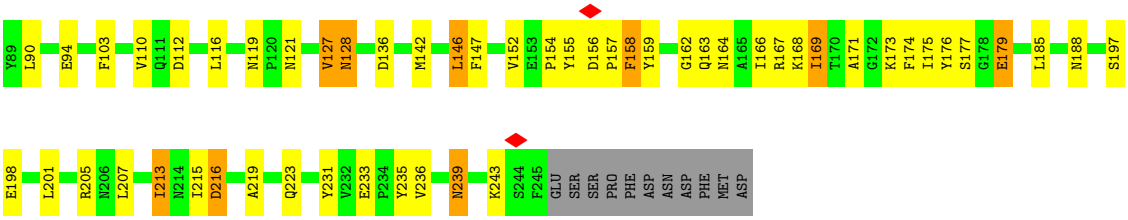




• Molecule 1: gp14, neck protein

Chain l:



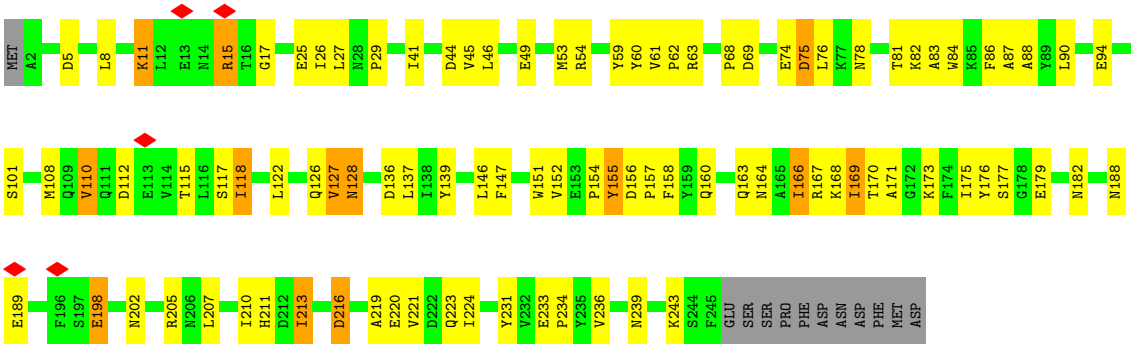



• Molecule 1: gp14, neck protein

Chain m:

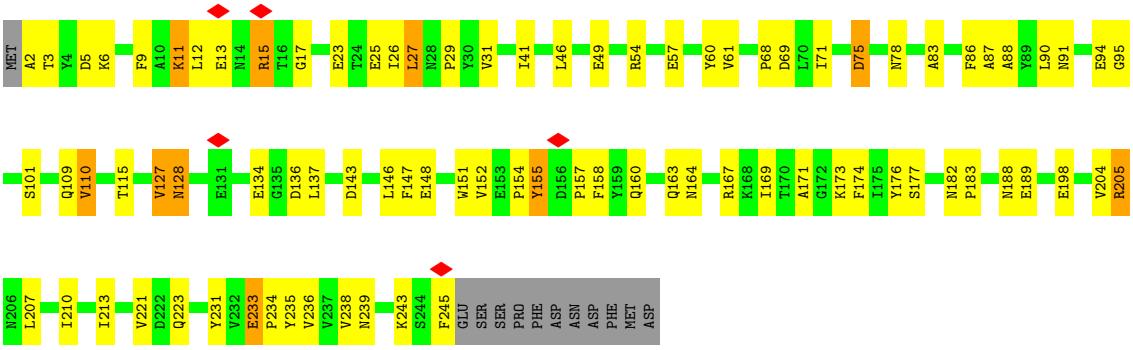



• Molecule 1: gp14, neck protein

Chain n:

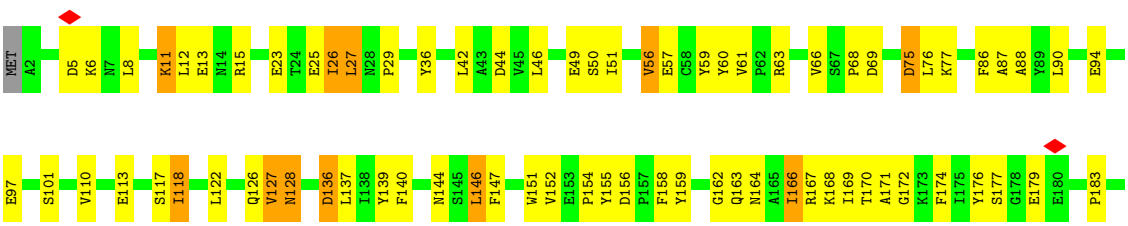



• Molecule 1: gp14, neck protein

Chain p:



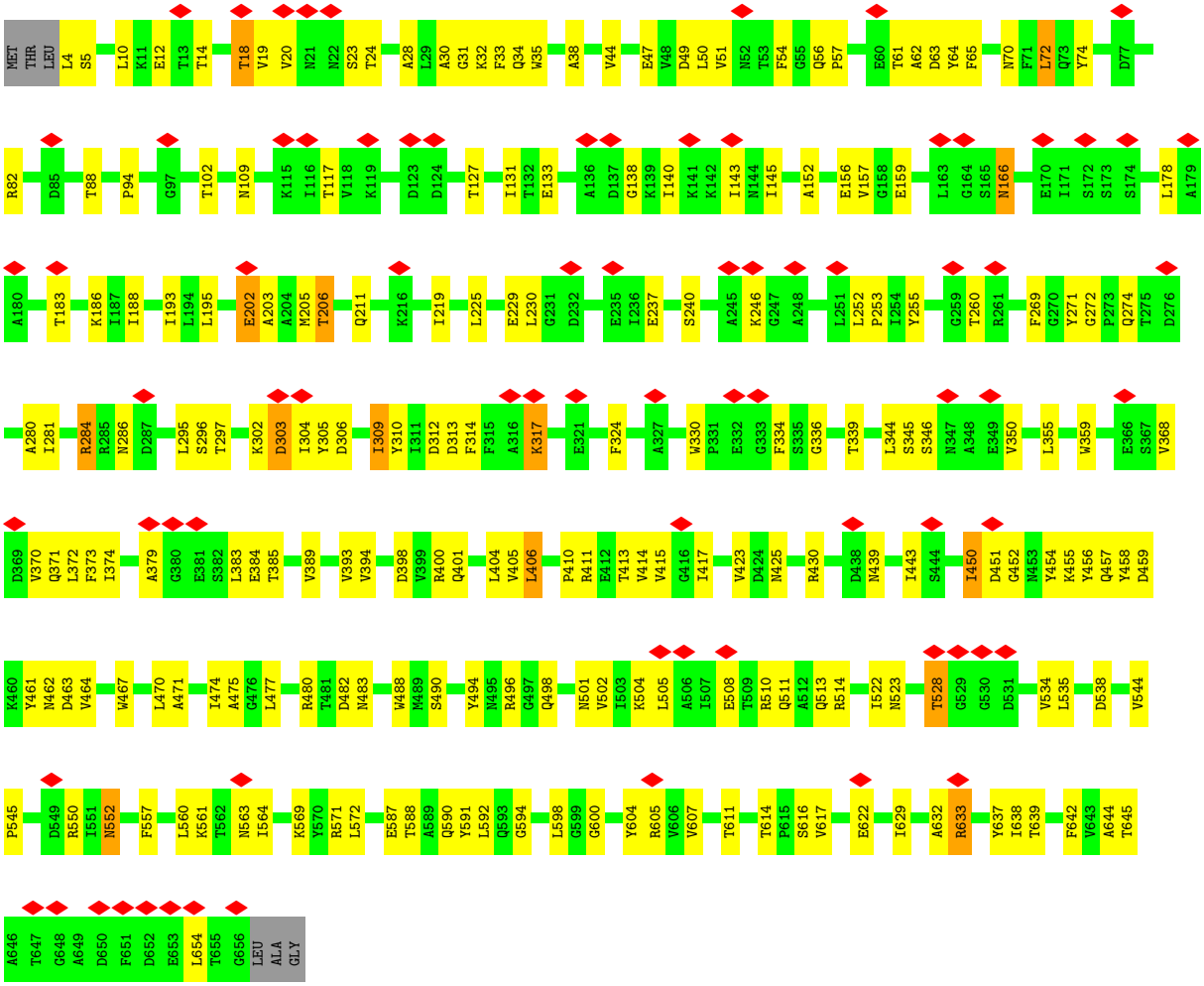






• Molecule 2: gp18, tail sheath protein

Chain 1:

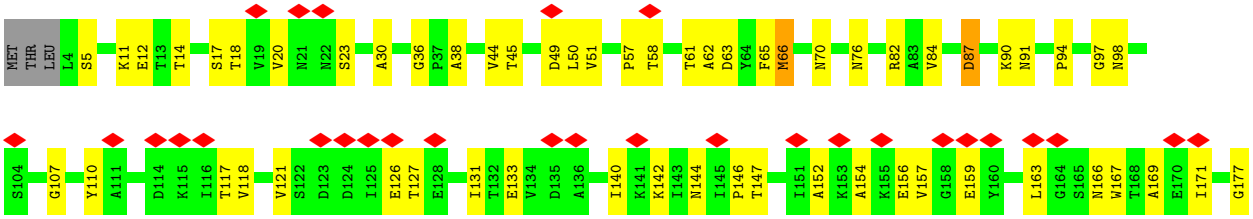


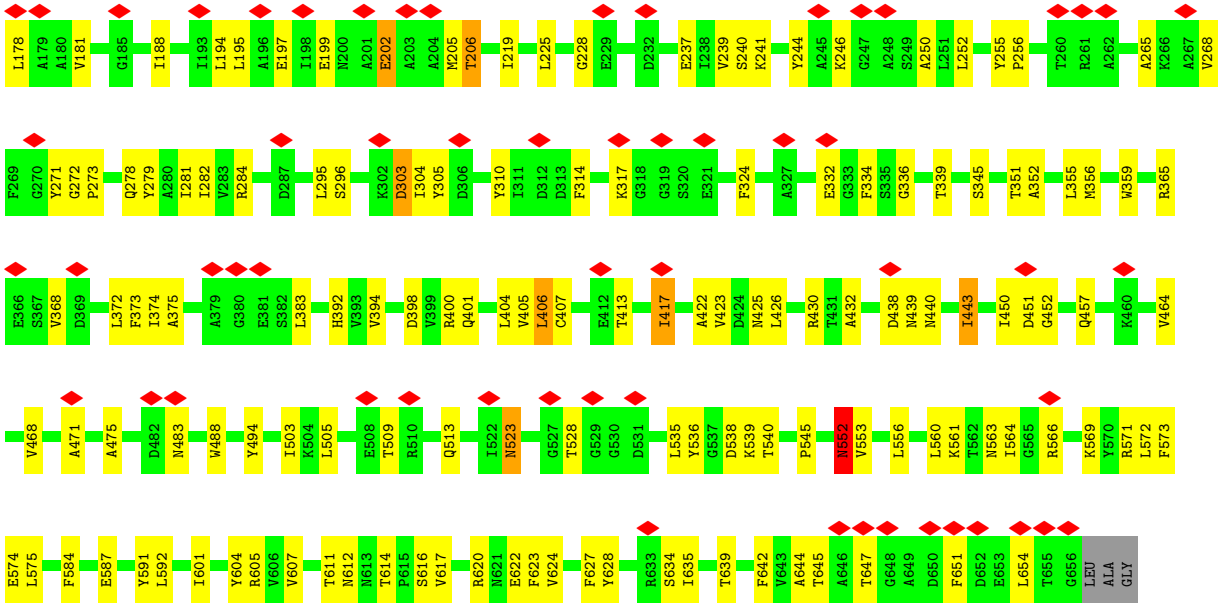




• Molecule 2: gp18, tail sheath protein

Chain 2:



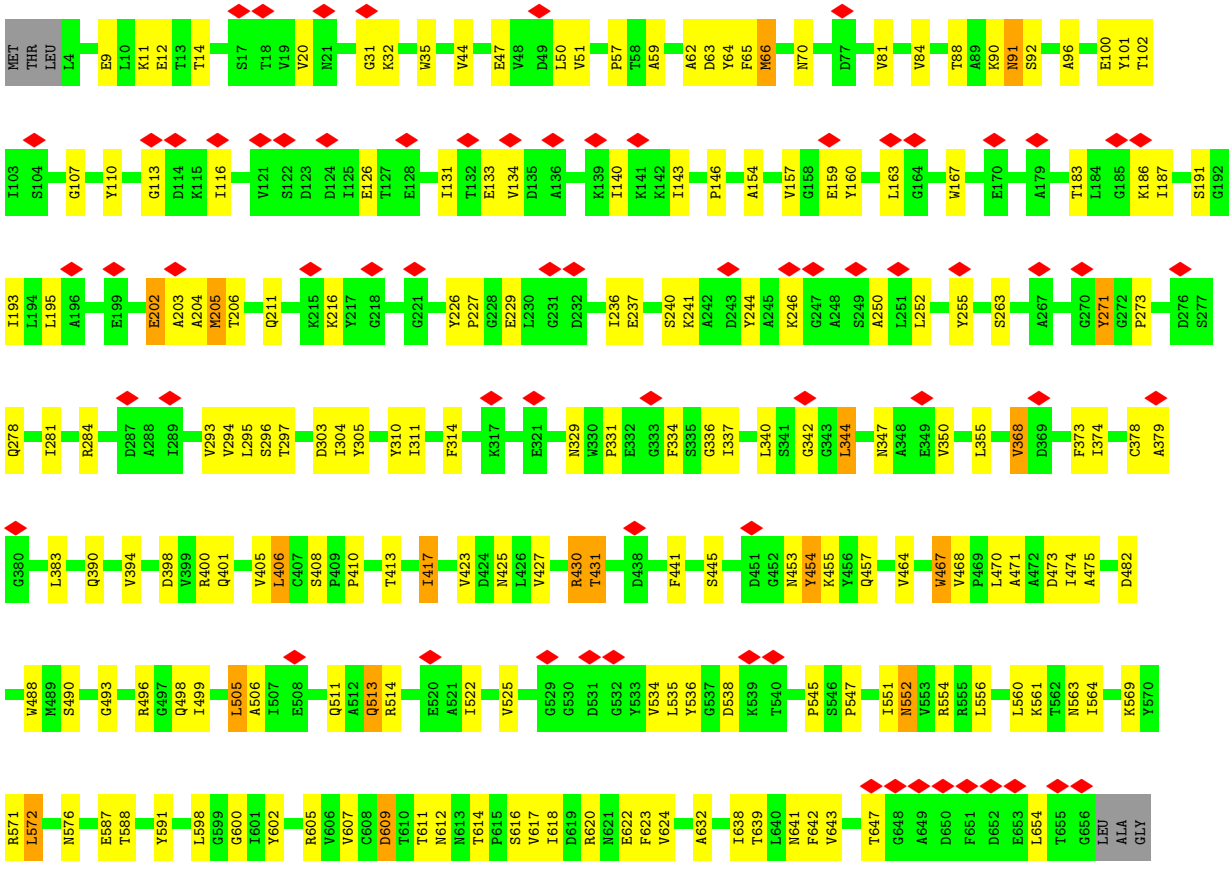





• Molecule 2: gp18, tail sheath protein

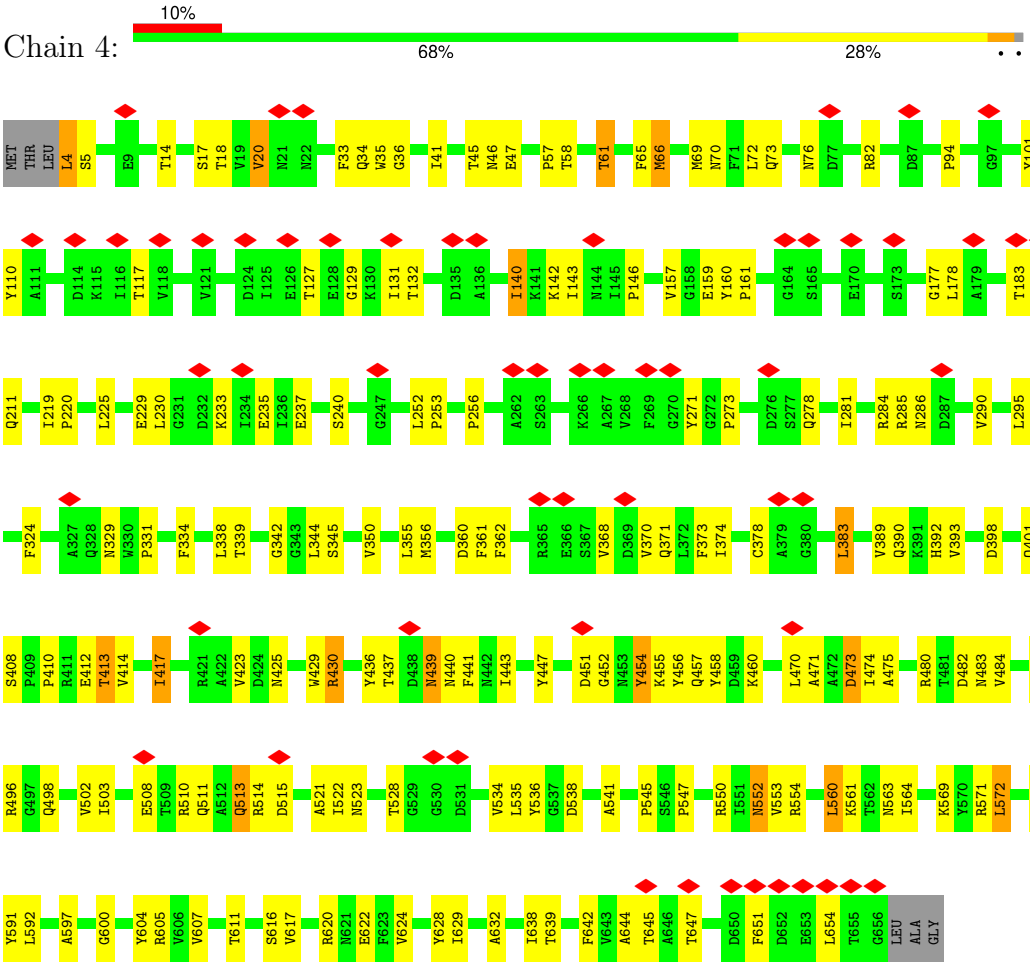
Chain 3:



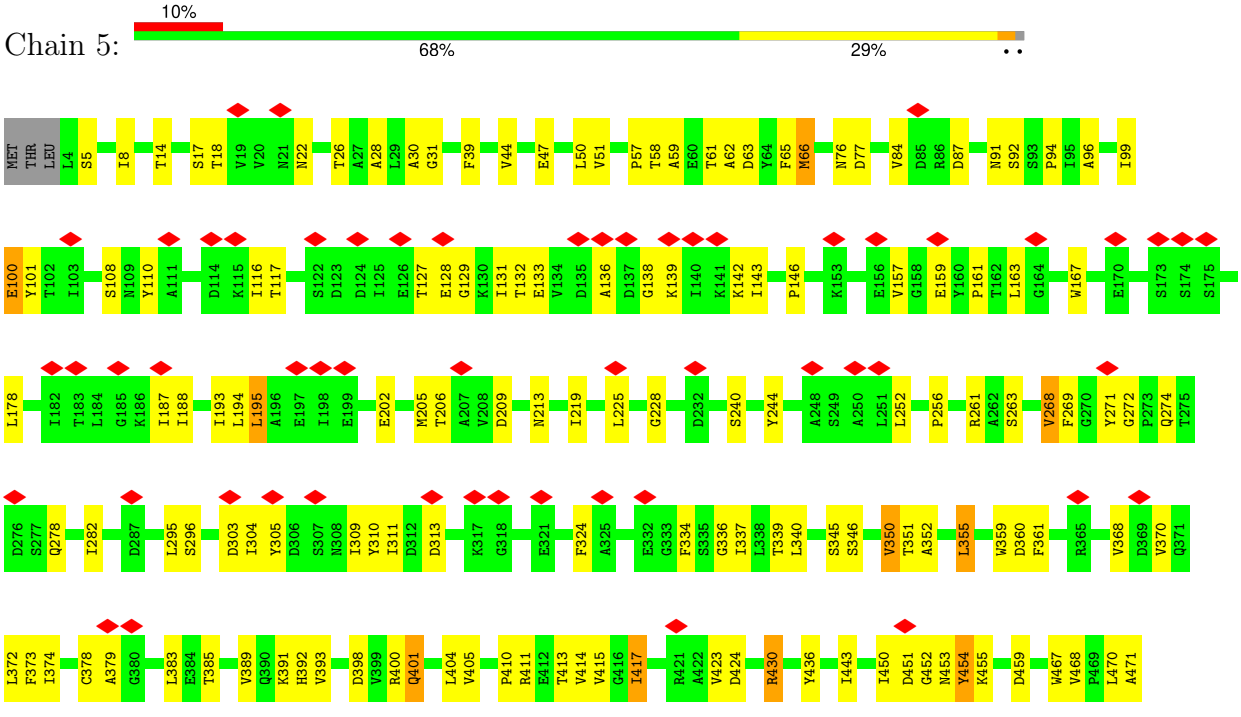
• Molecule 2: gp18, tail sheath protein

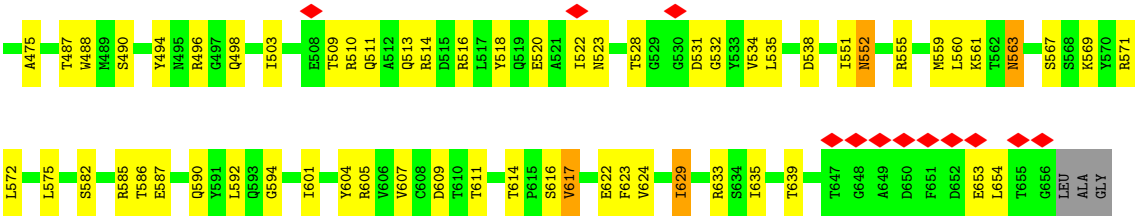
Chain 4:




• Molecule 2: gp18, tail sheath protein

Chain 5:

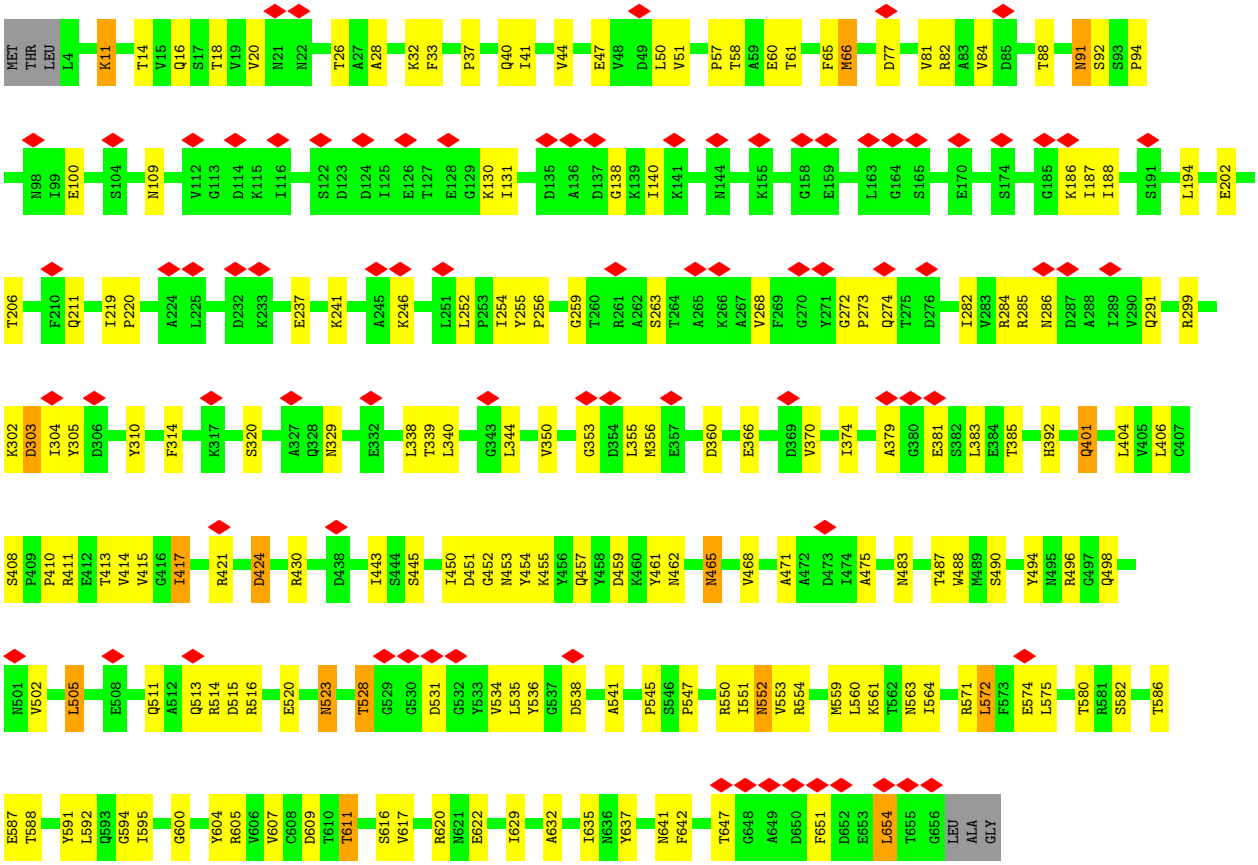





• Molecule 2: gp18, tail sheath protein

Chain AD:

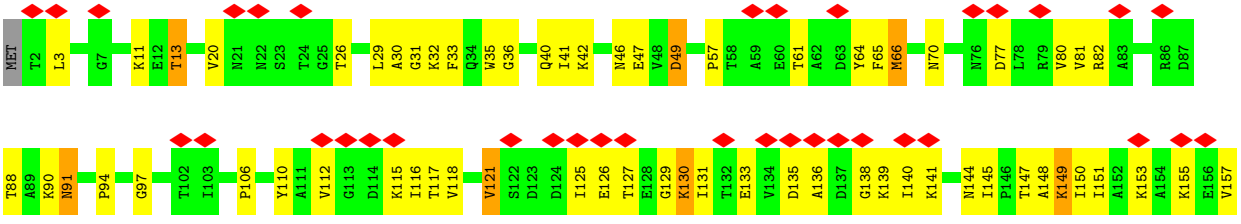


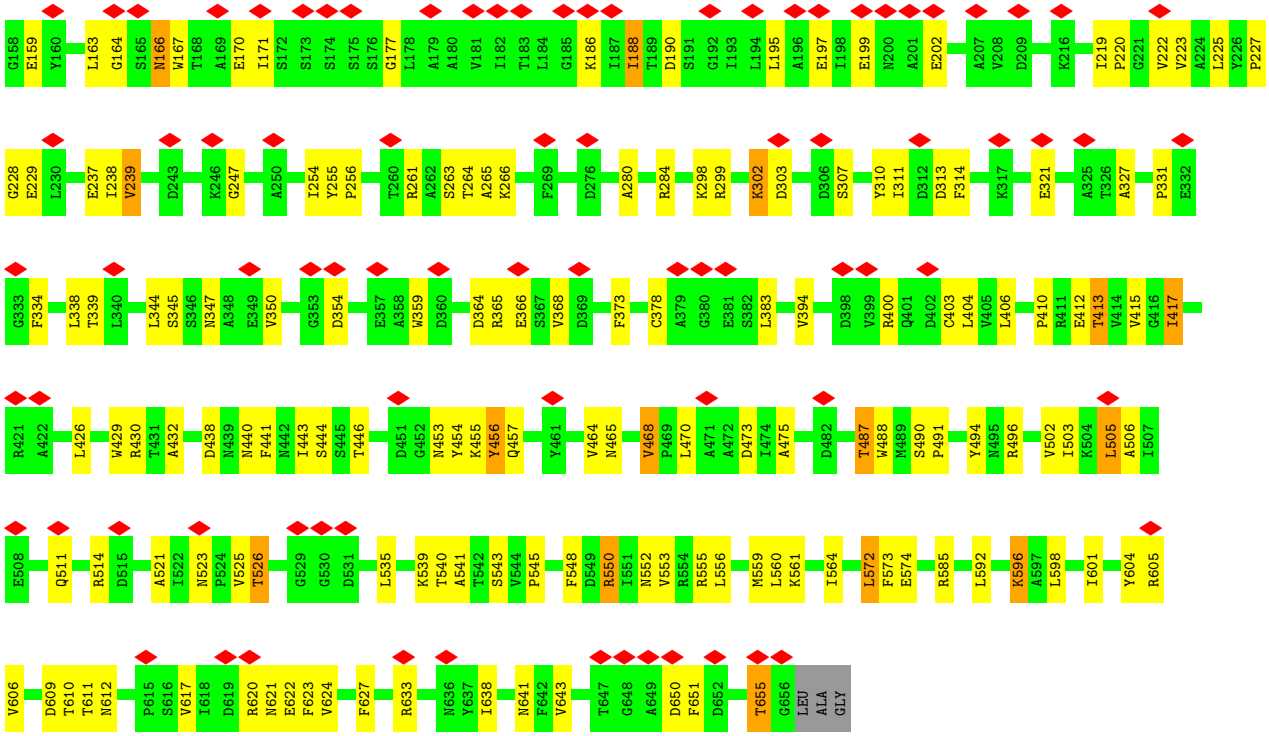




• Molecule 2: gp18, tail sheath protein

Chain AK:



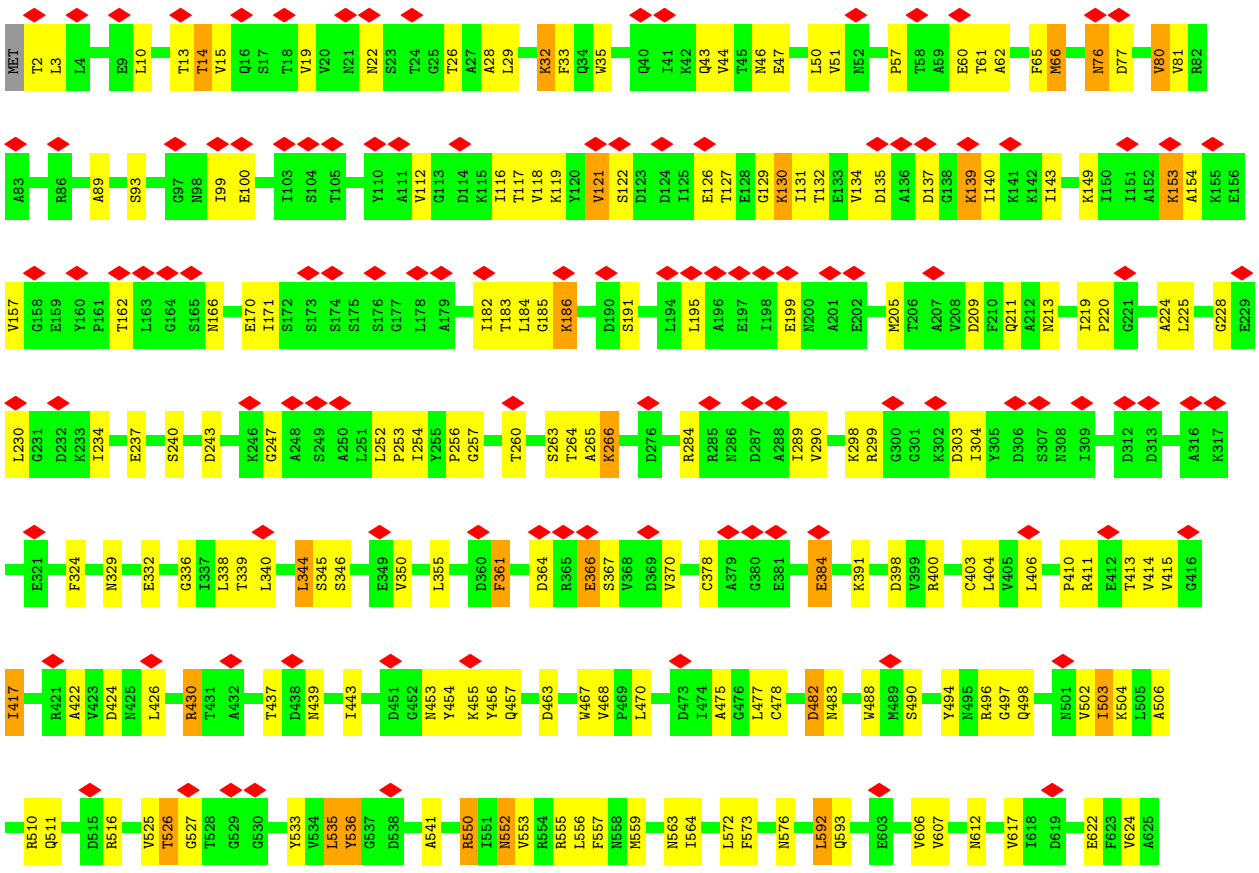



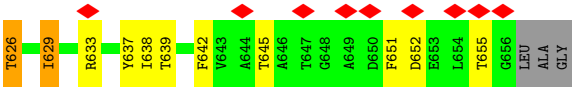


• Molecule 2: gp18, tail sheath protein

Chain AL:





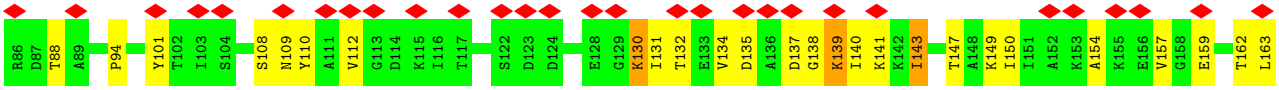

• Molecule 2: gp18, tail sheath protein

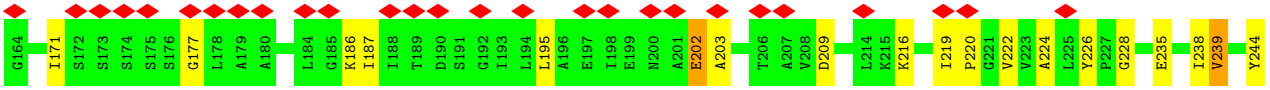
Chain AM:

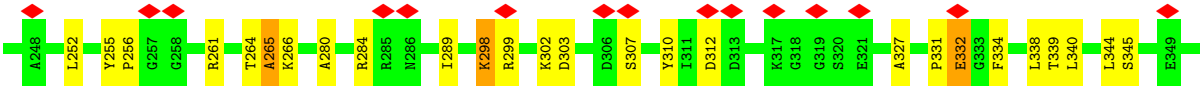


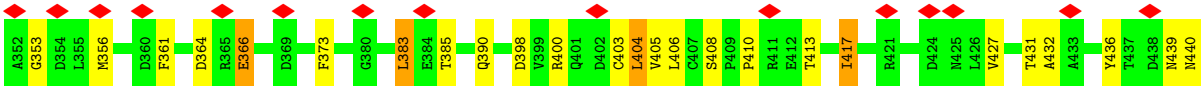


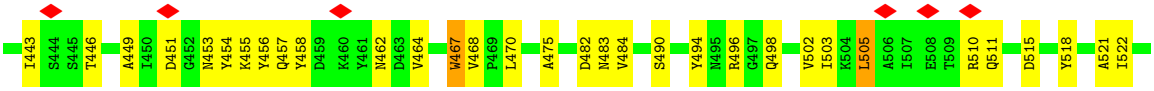


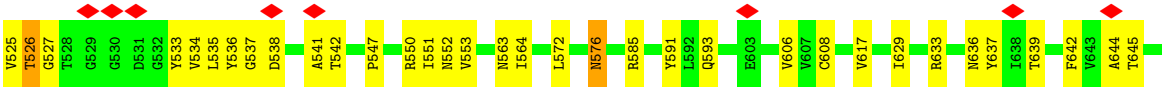


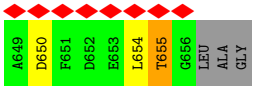



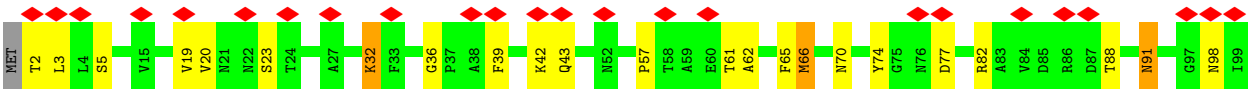



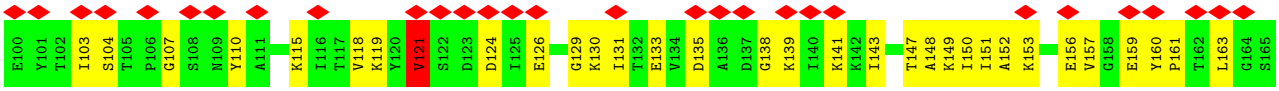



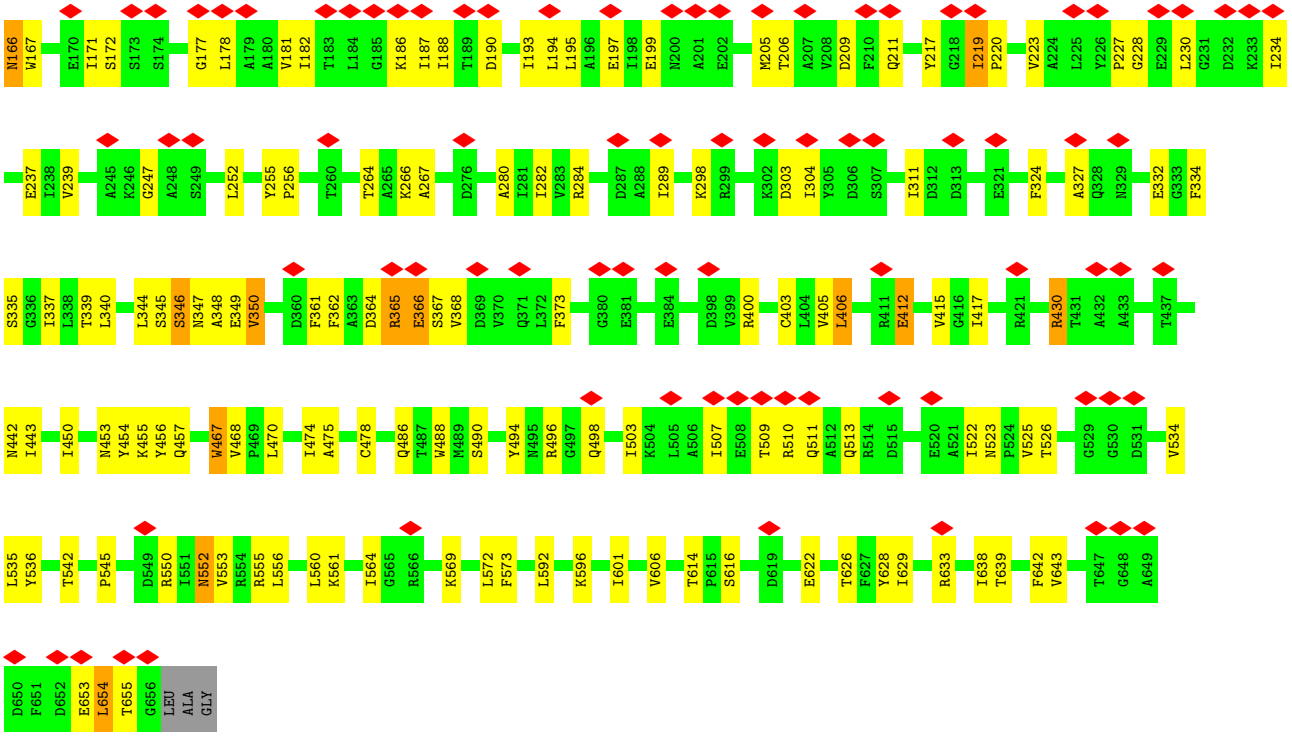

• Molecule 2: gp18, tail sheath protein

Chain AN:



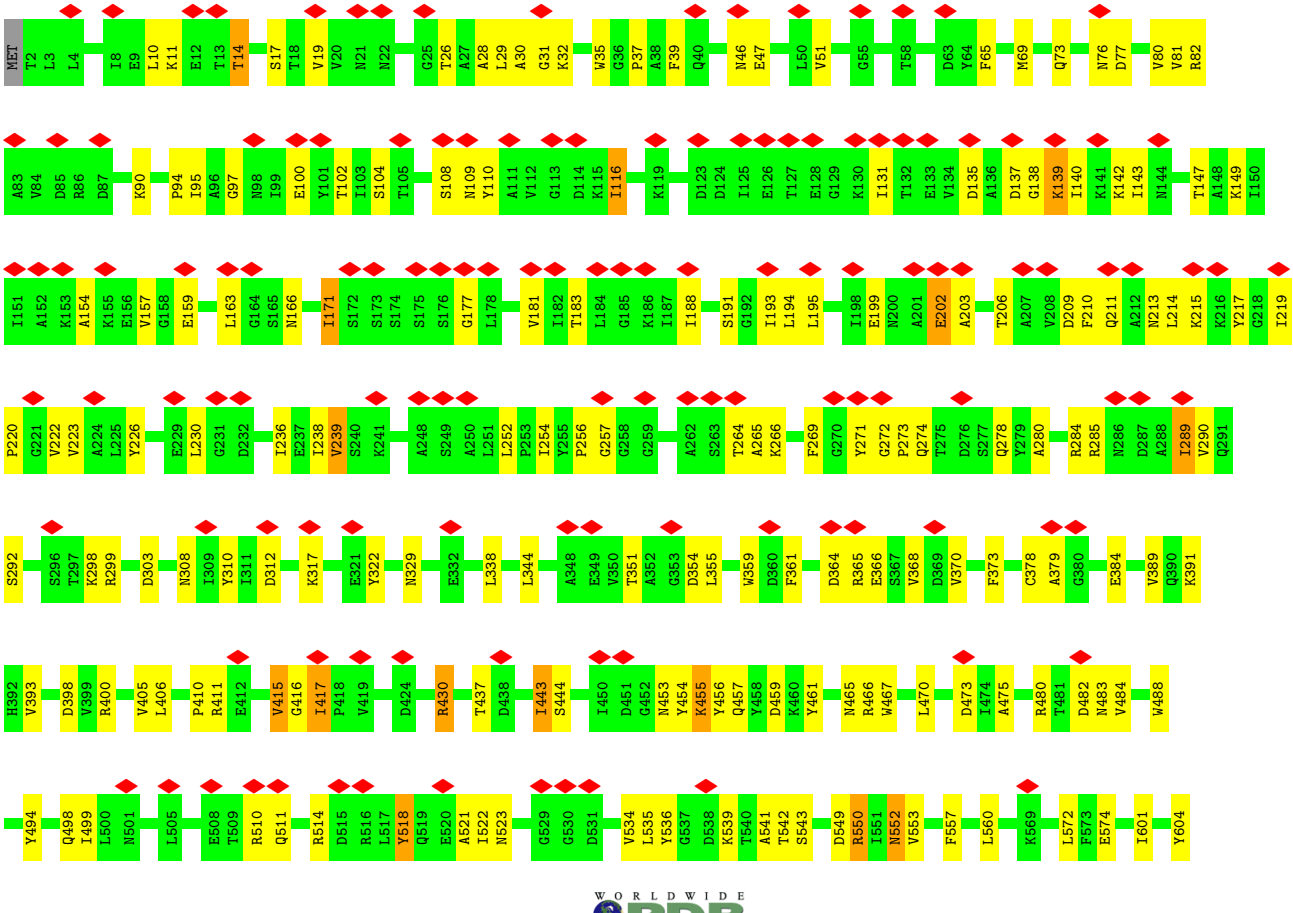



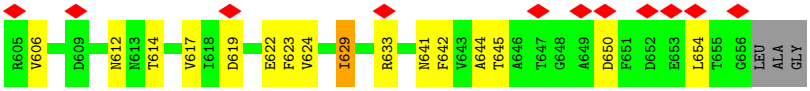


• Molecule 2: gp18, tail sheath protein

Chain AO:



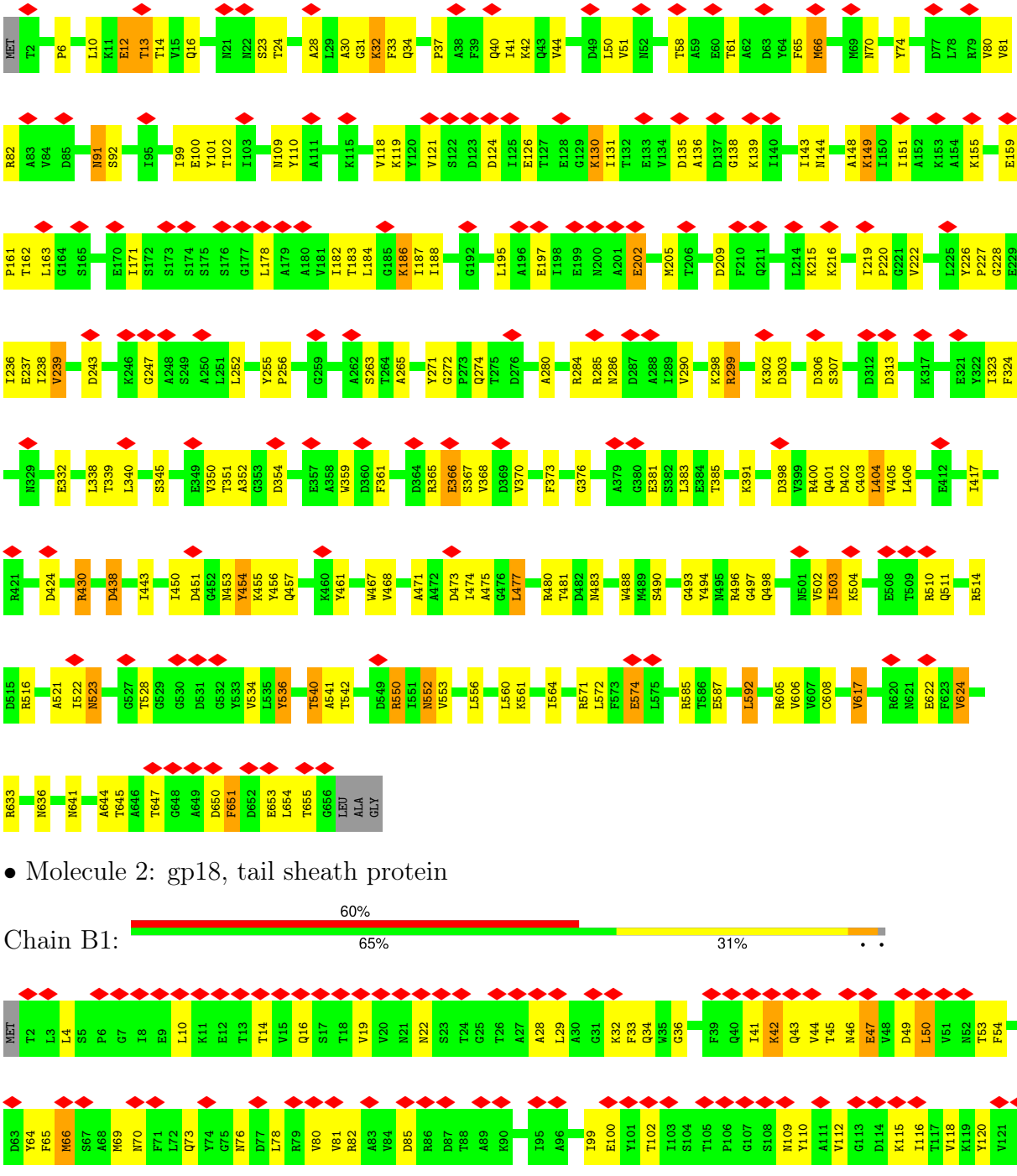






• Molecule 2: gp18, tail sheath protein

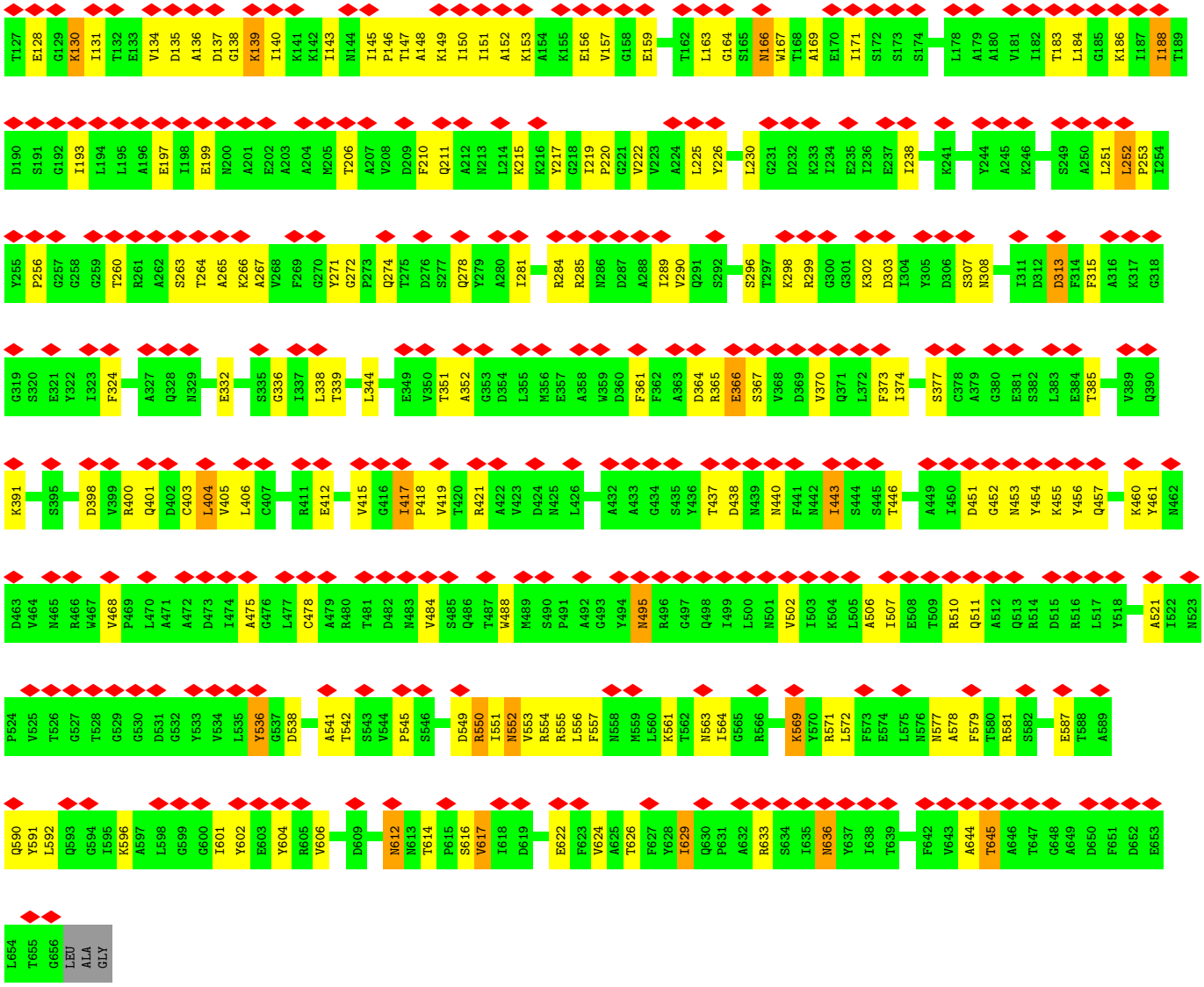
Chain AP:




• Molecule 2: gp18, tail sheath protein

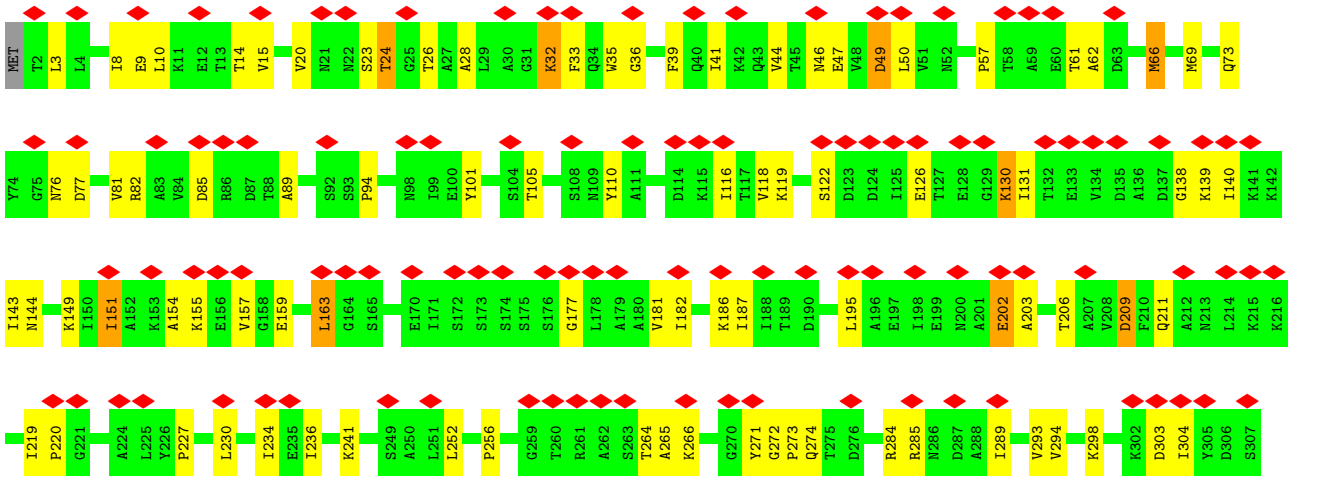
Chain B1:

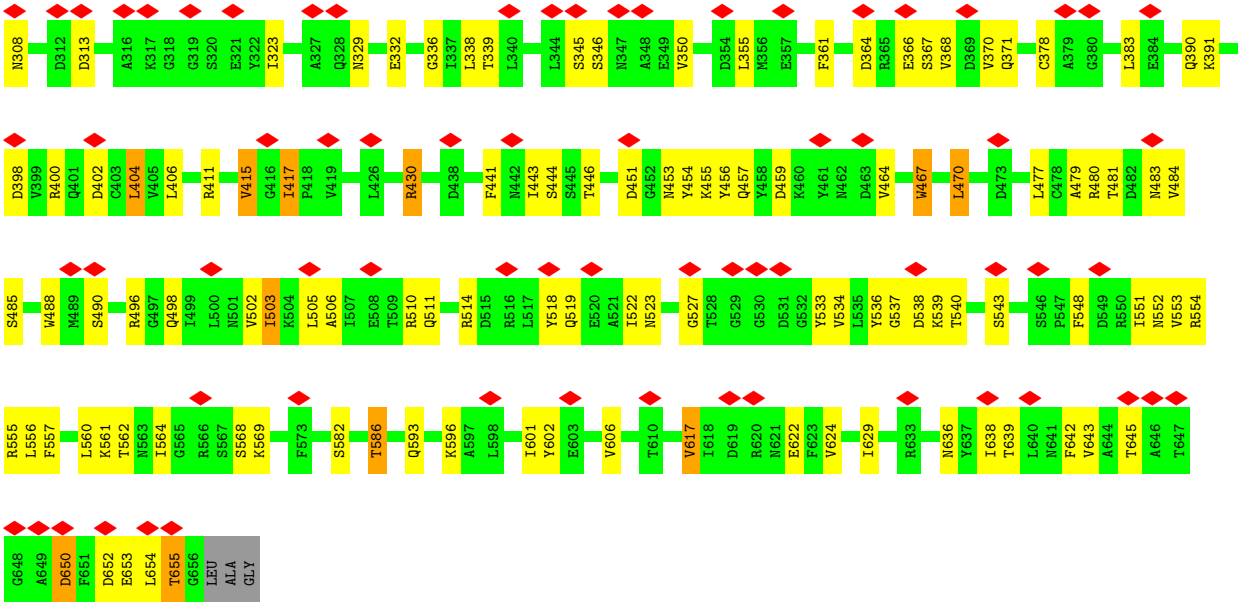


• Molecule 2: gp18, tail sheath protein

Chain B2:



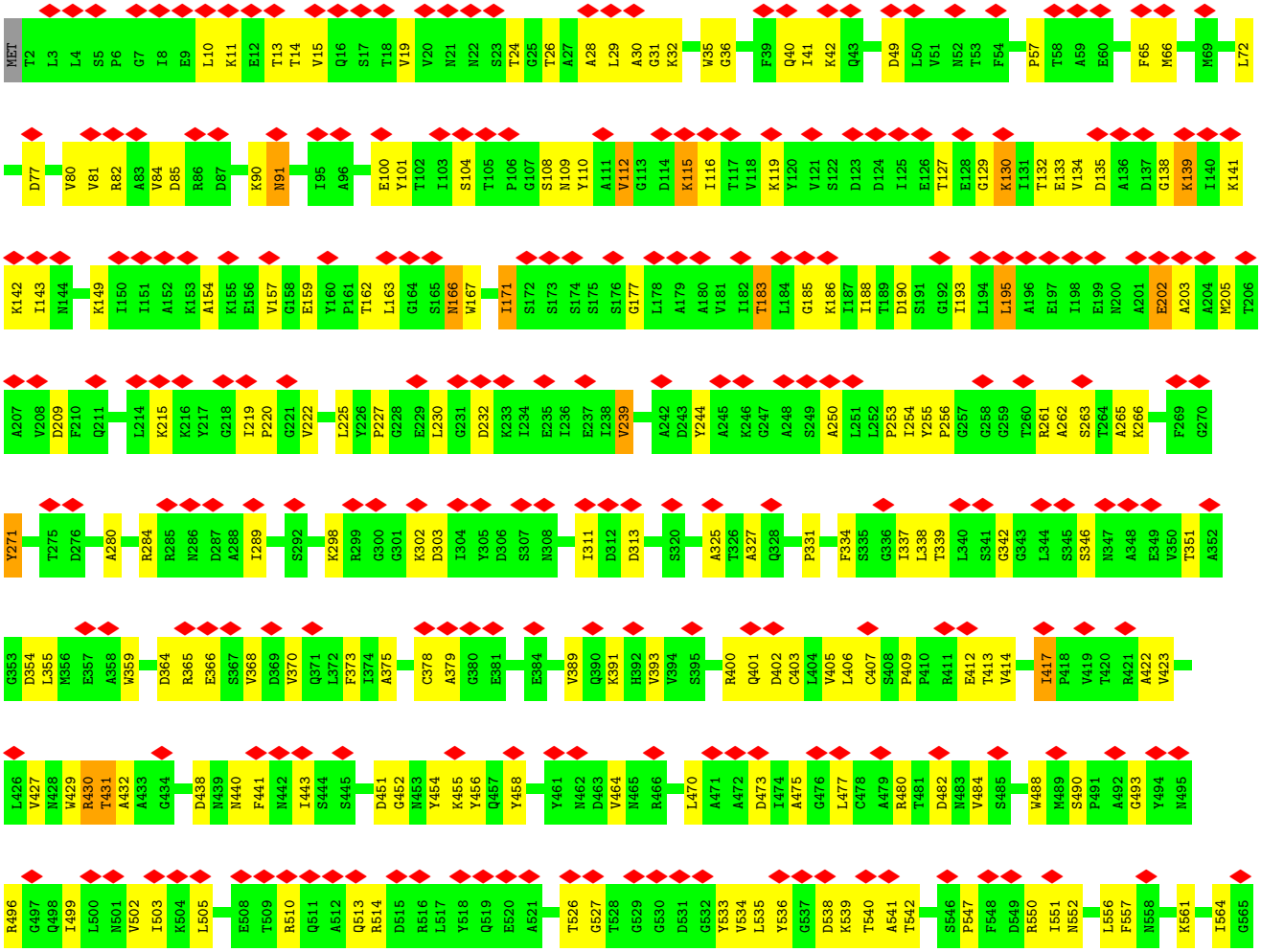



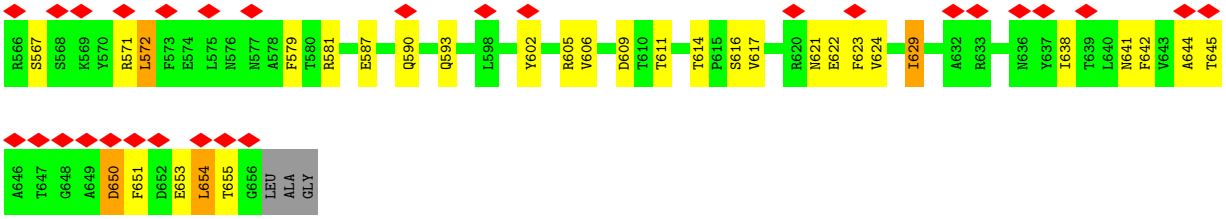


• Molecule 2: gp18, tail sheath protein

Chain B3:



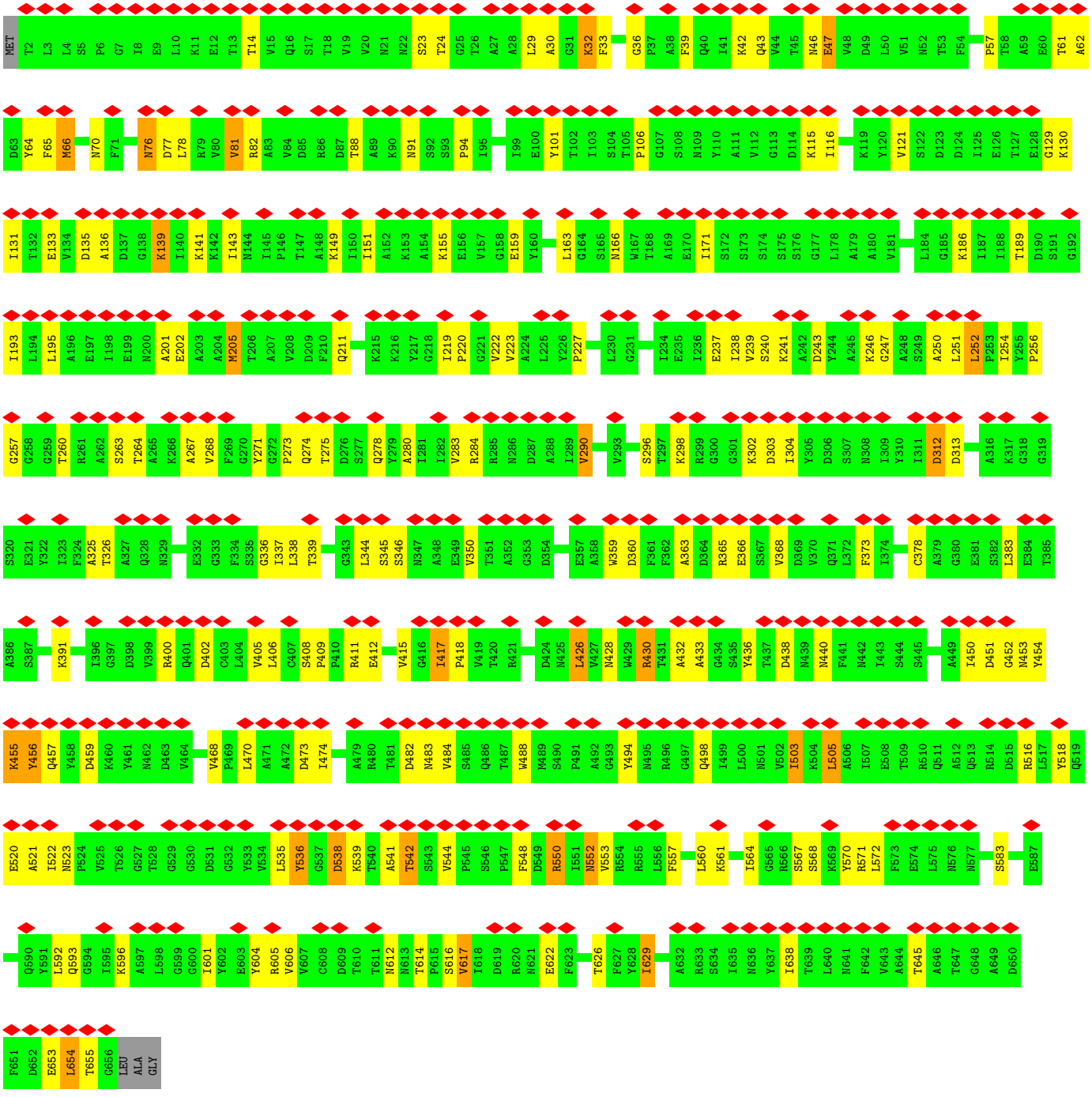






• Molecule 2: gp18, tail sheath protein

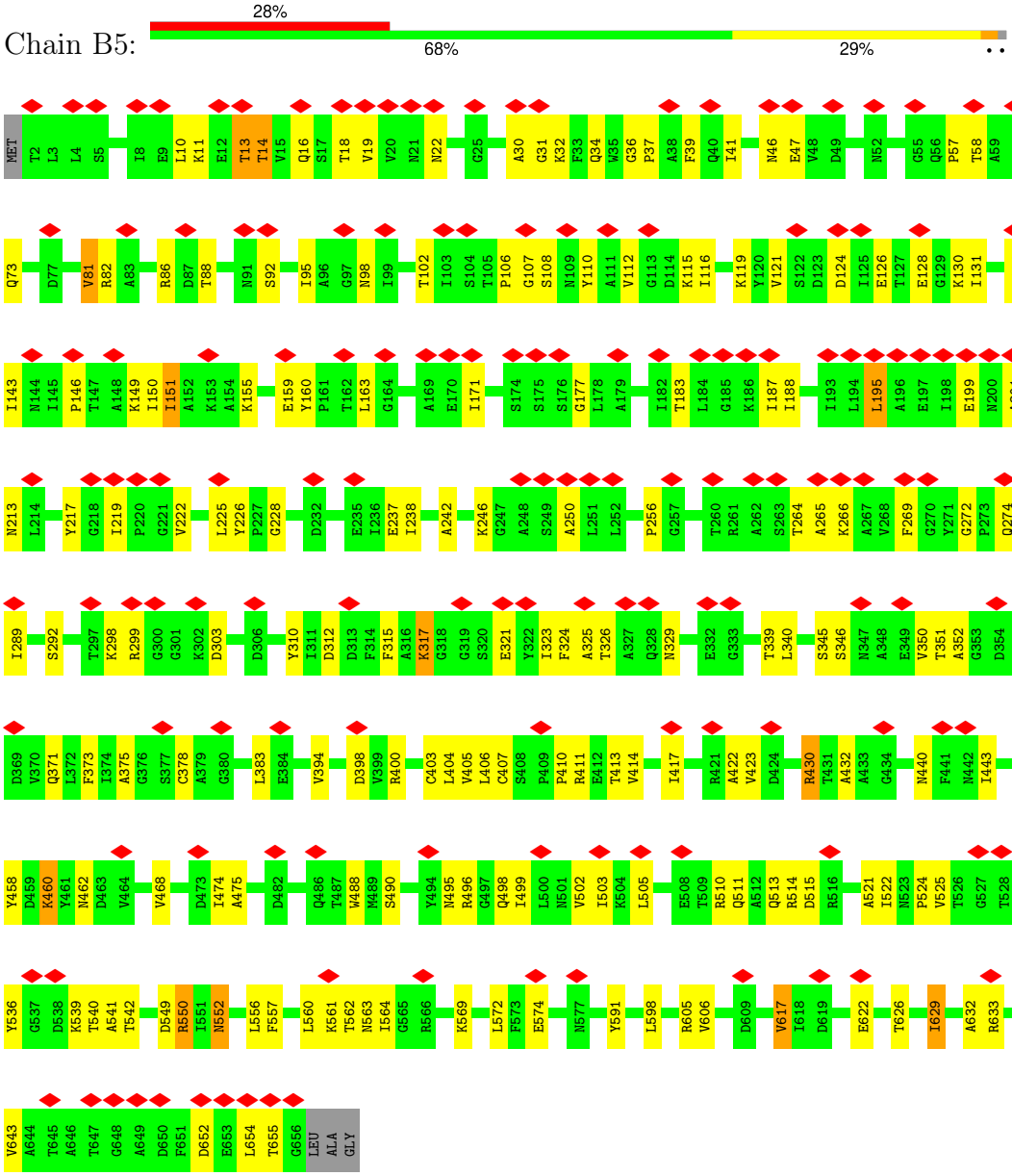
Chain B4:



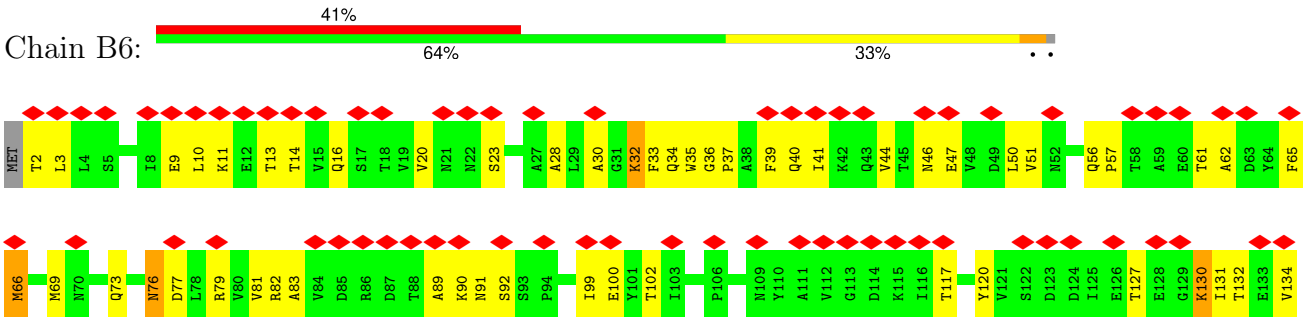
• Molecule 2: gp18, tail sheath protein

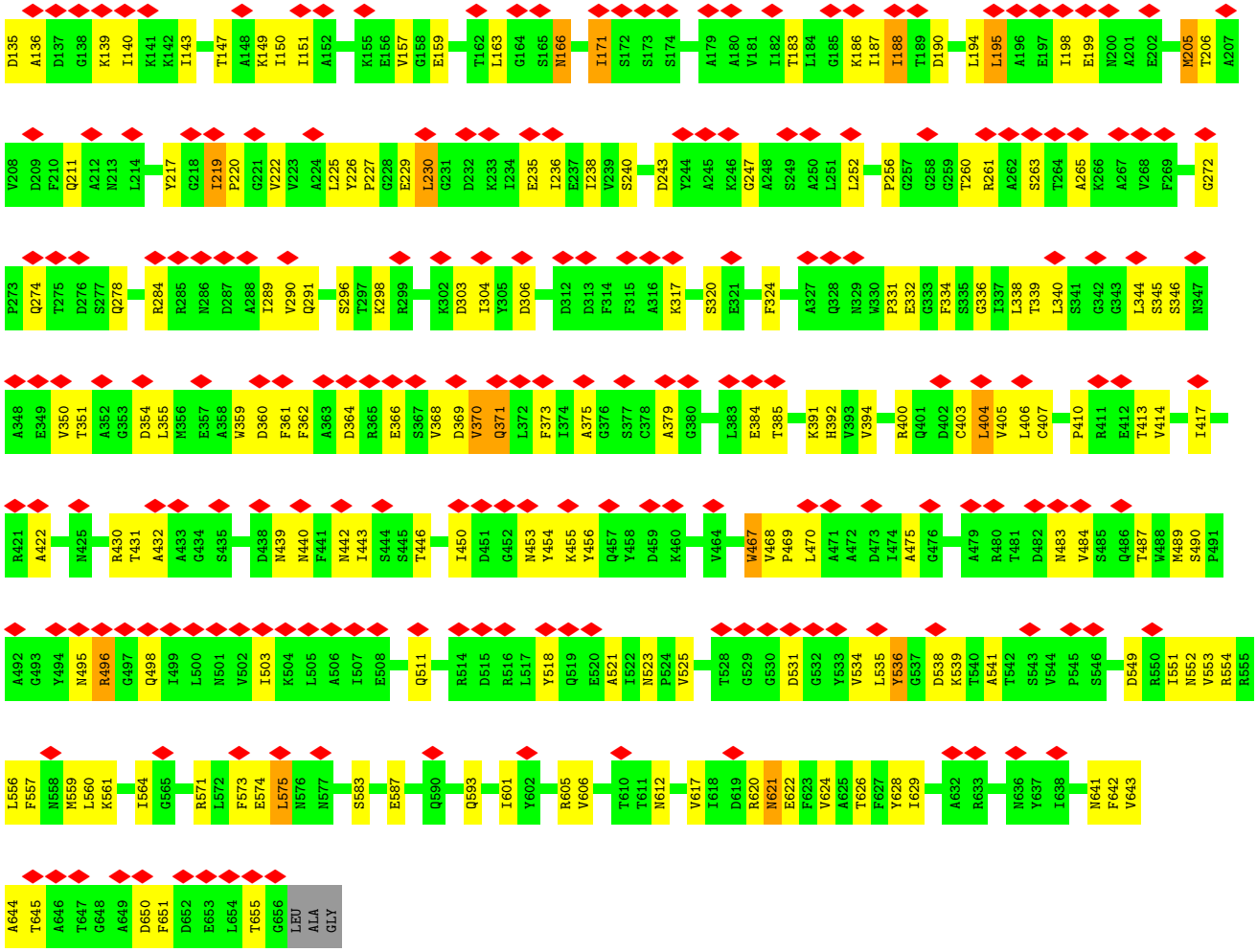
Chain B5:




• Molecule 2: gp18, tail sheath protein

Chain B6:

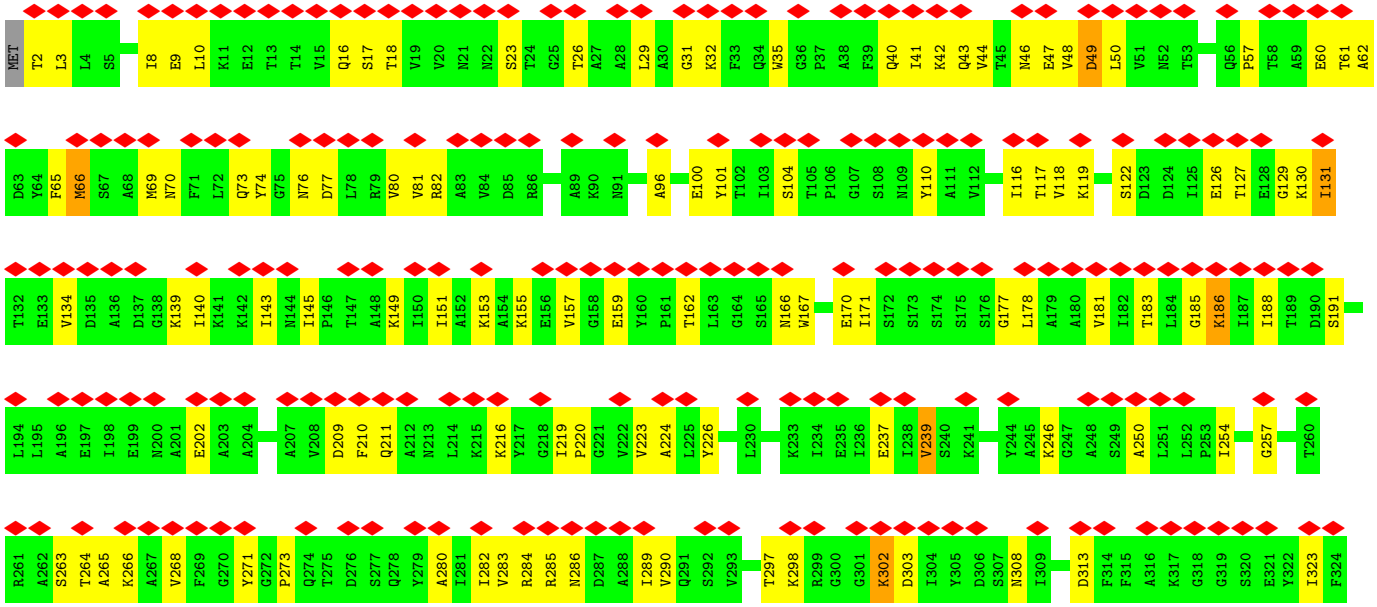


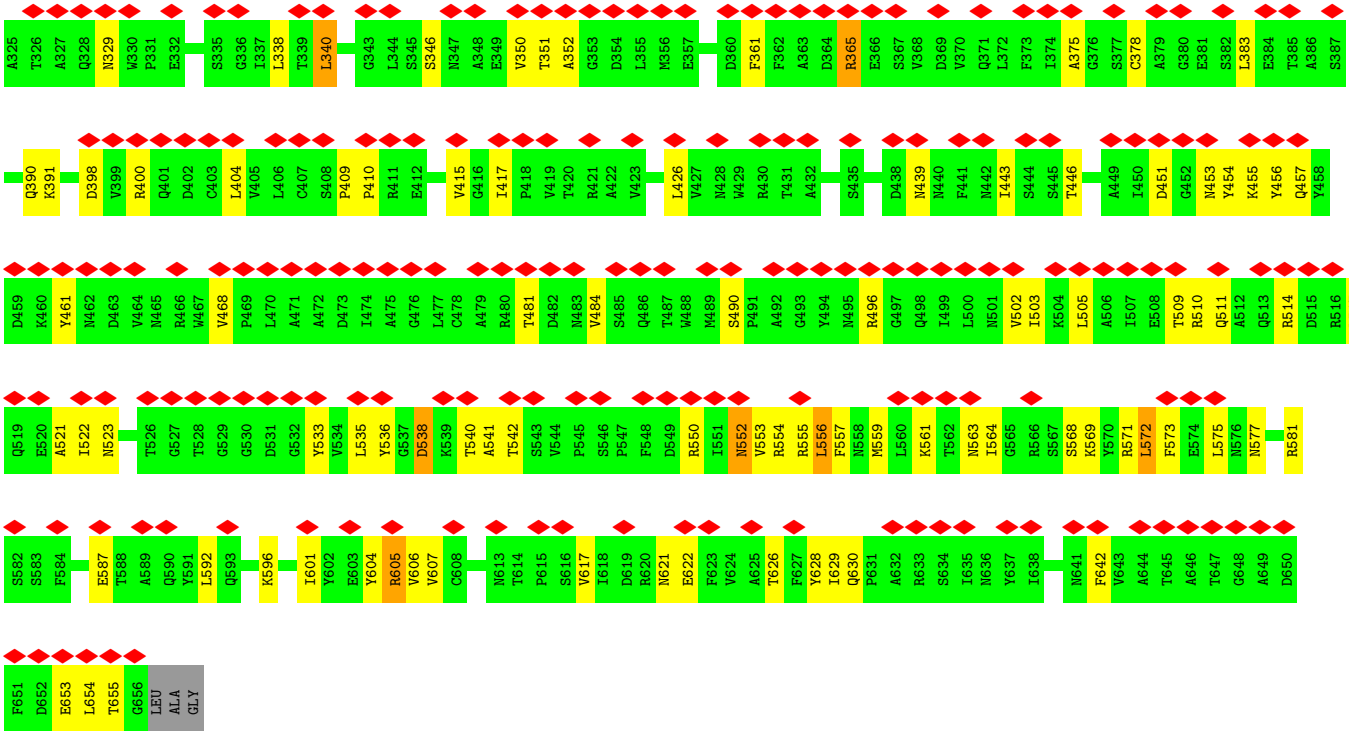


• Molecule 2: gp18, tail sheath protein

Chain B7:



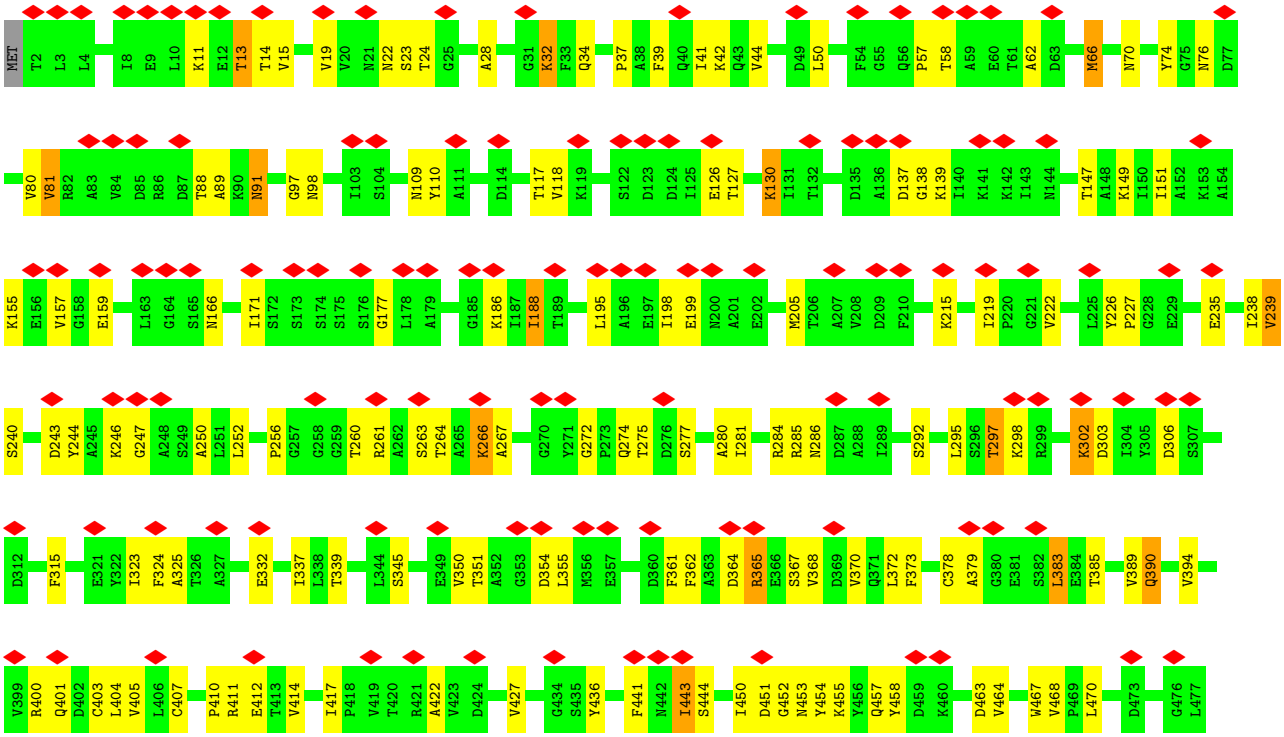



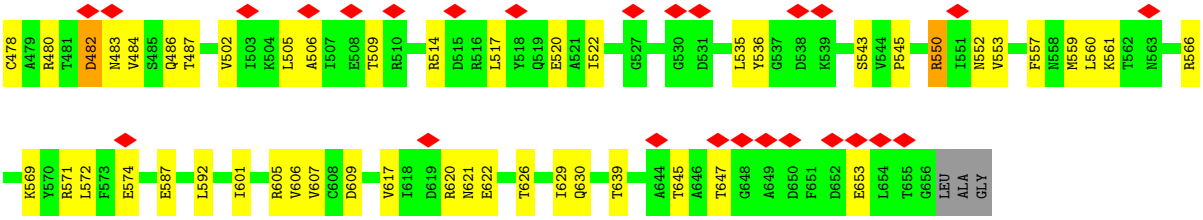



- Molecule 2: gp18, tail sheath protein

Chain Bp:



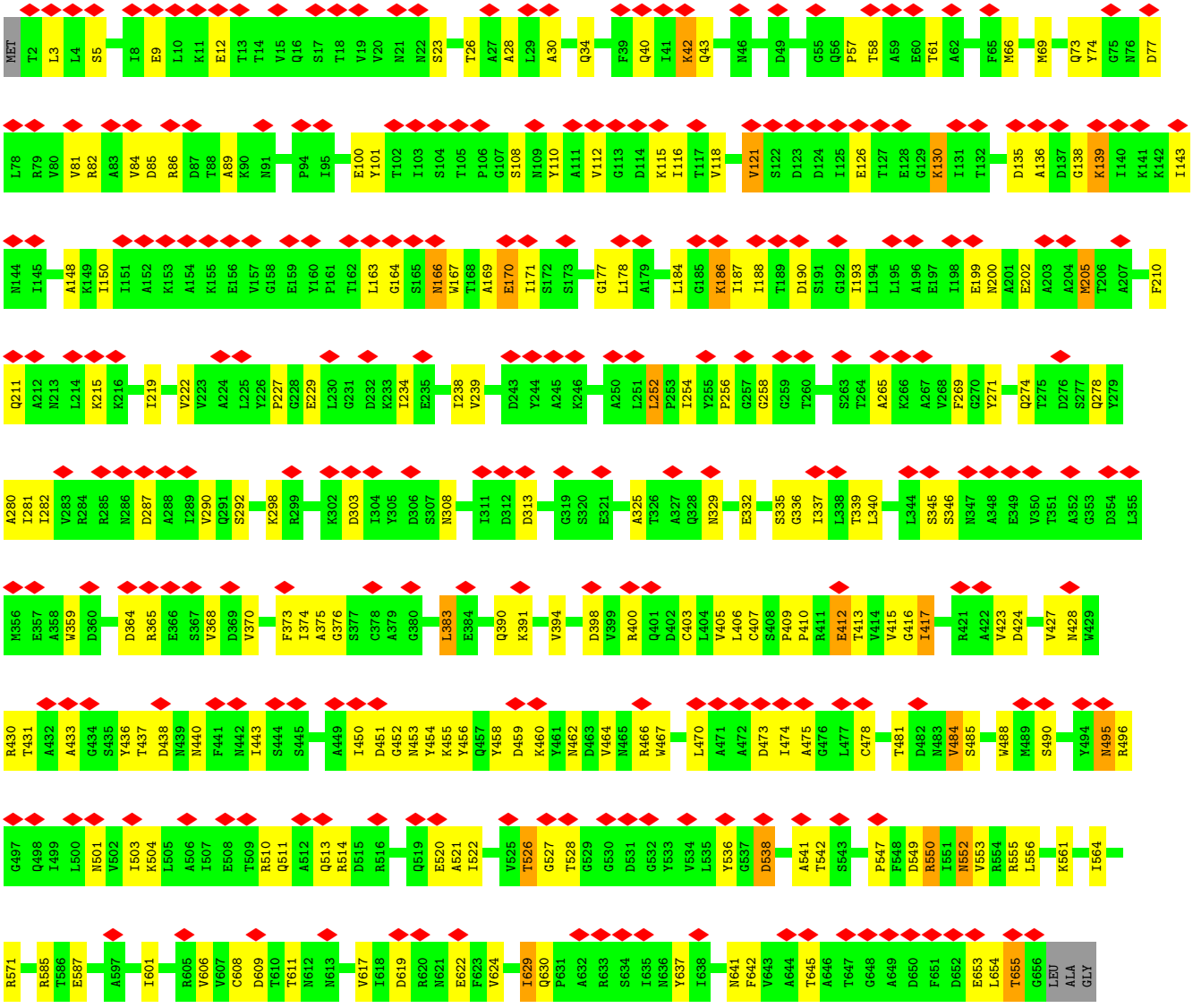





• Molecule 2: gp18, tail sheath protein

Chain Bq:

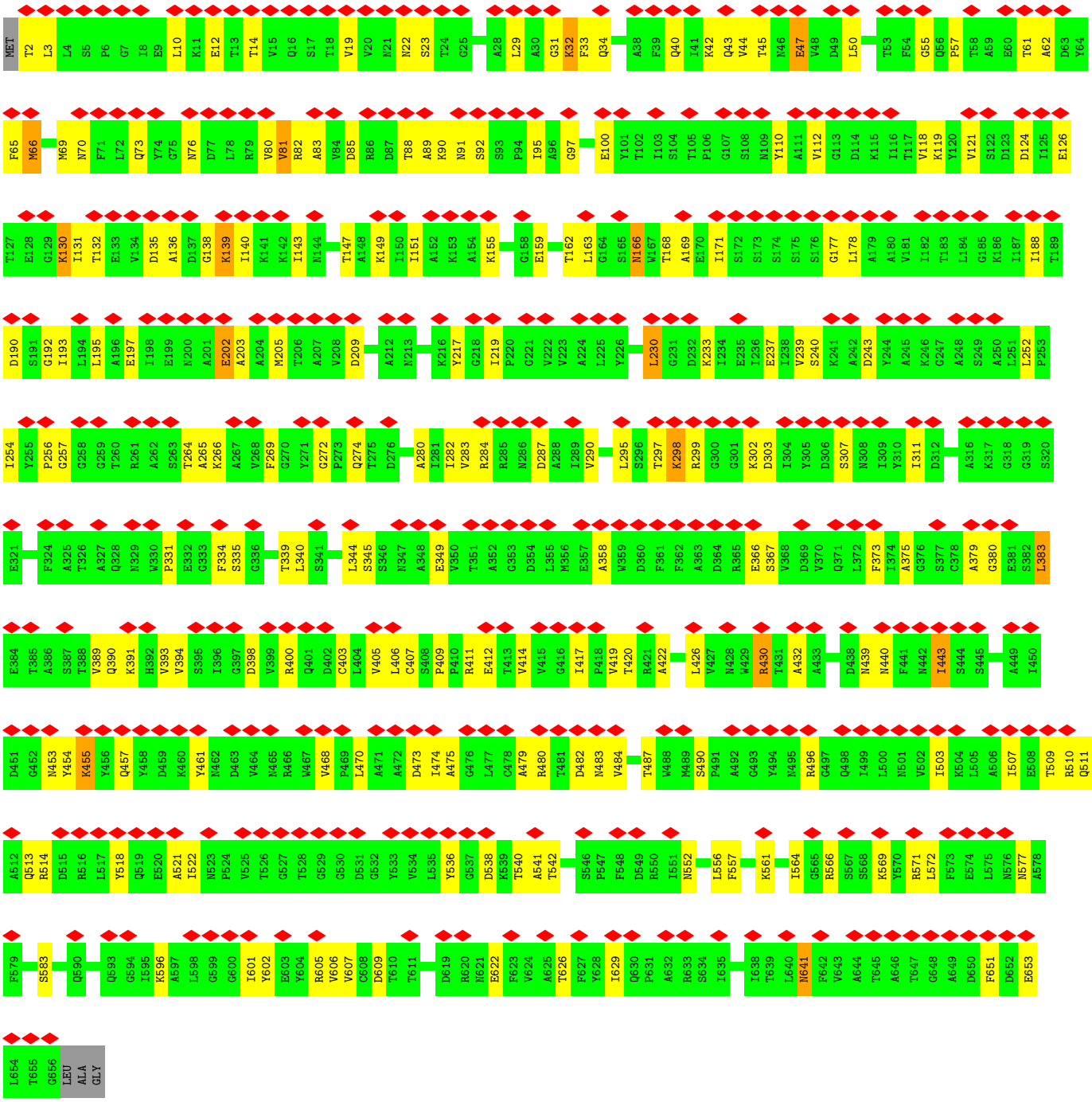


• Molecule 2: gp18, tail sheath protein

Chain Br:

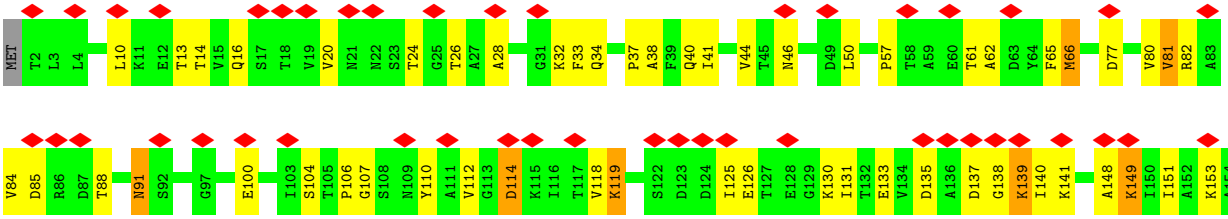


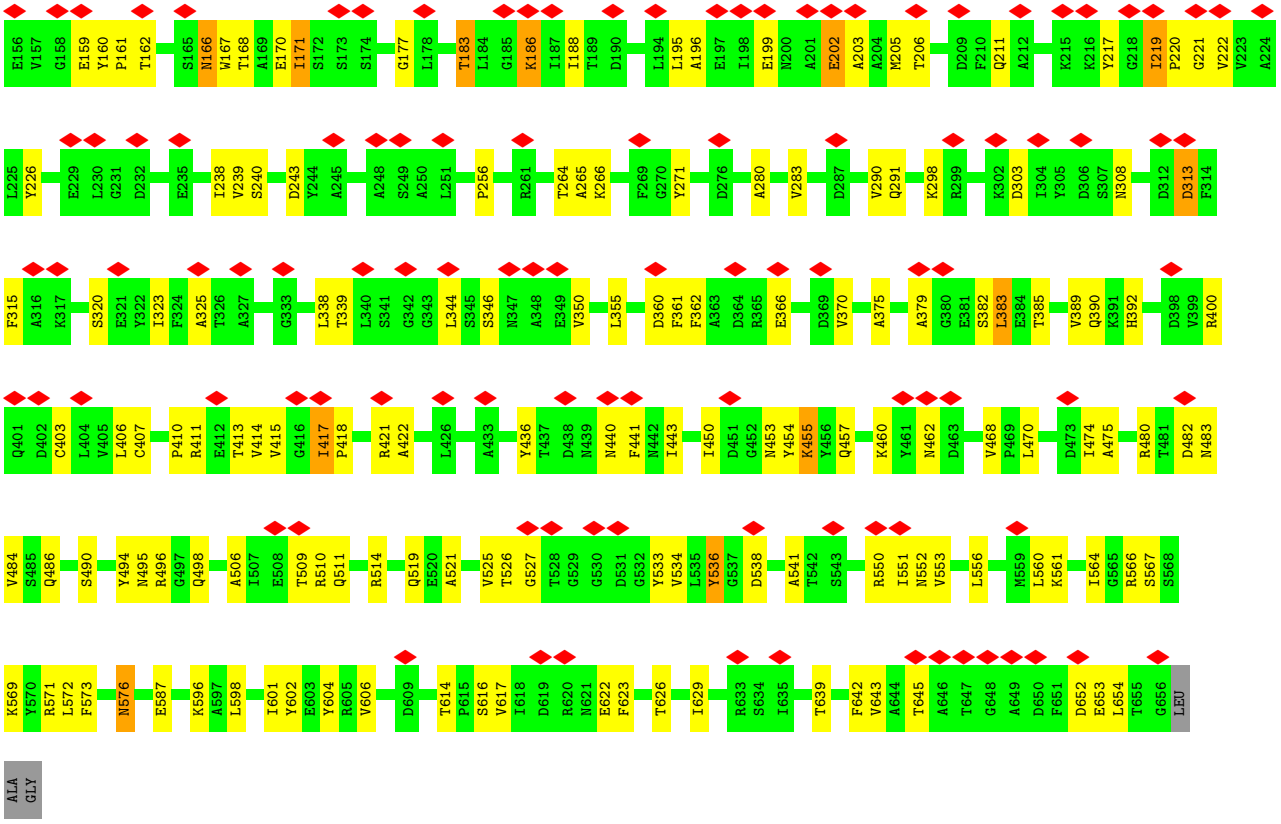


• Molecule 2: gp18, tail sheath protein

Chain Bs:



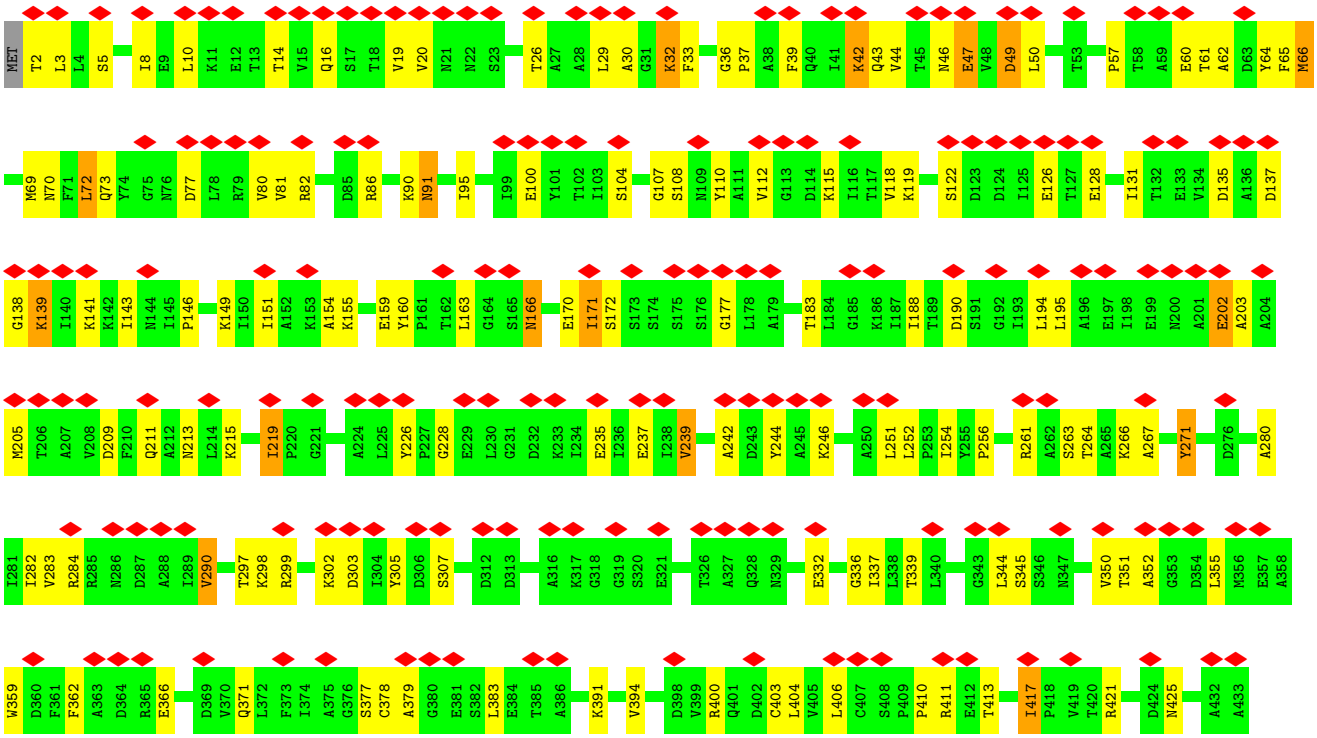



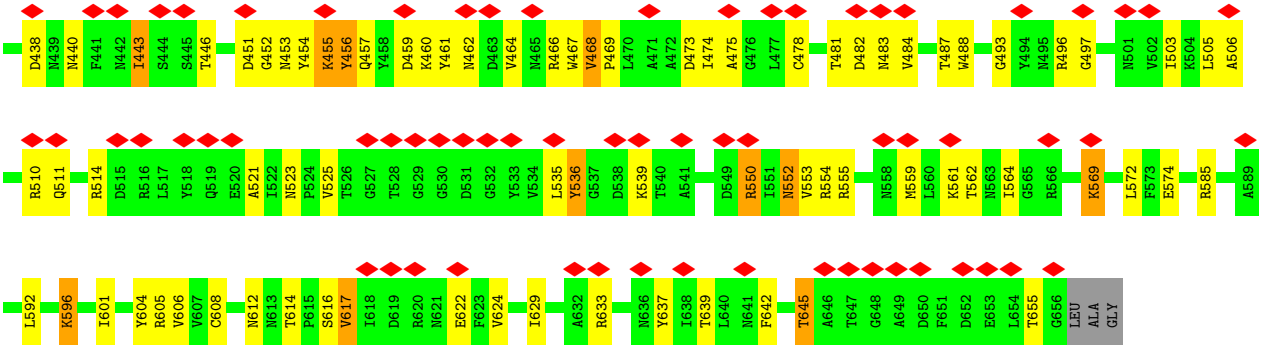



- Molecule 2: gp18, tail sheath protein

Chain Bt:



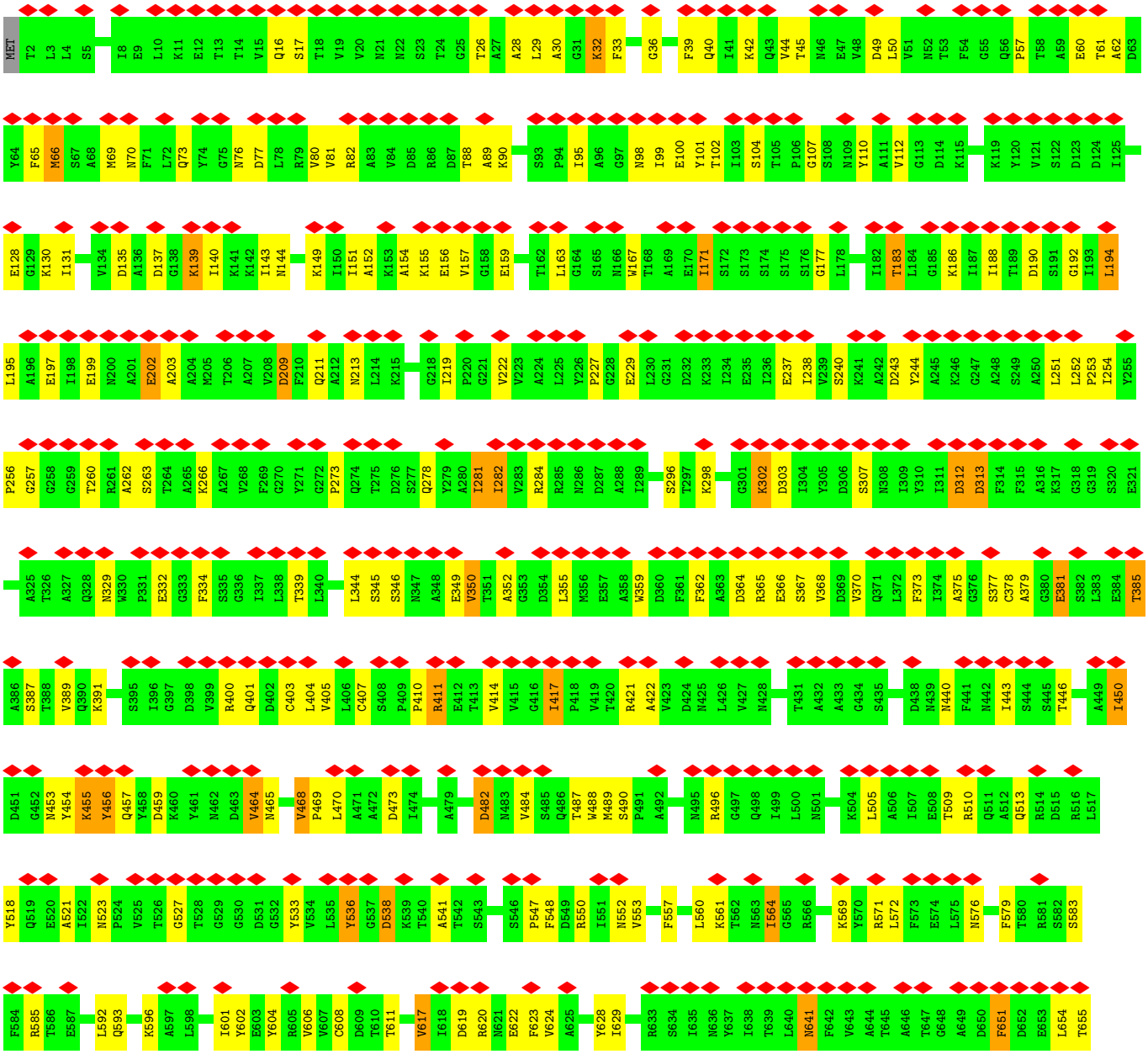






• Molecule 2: gp18, tail sheath protein

Chain Bu:



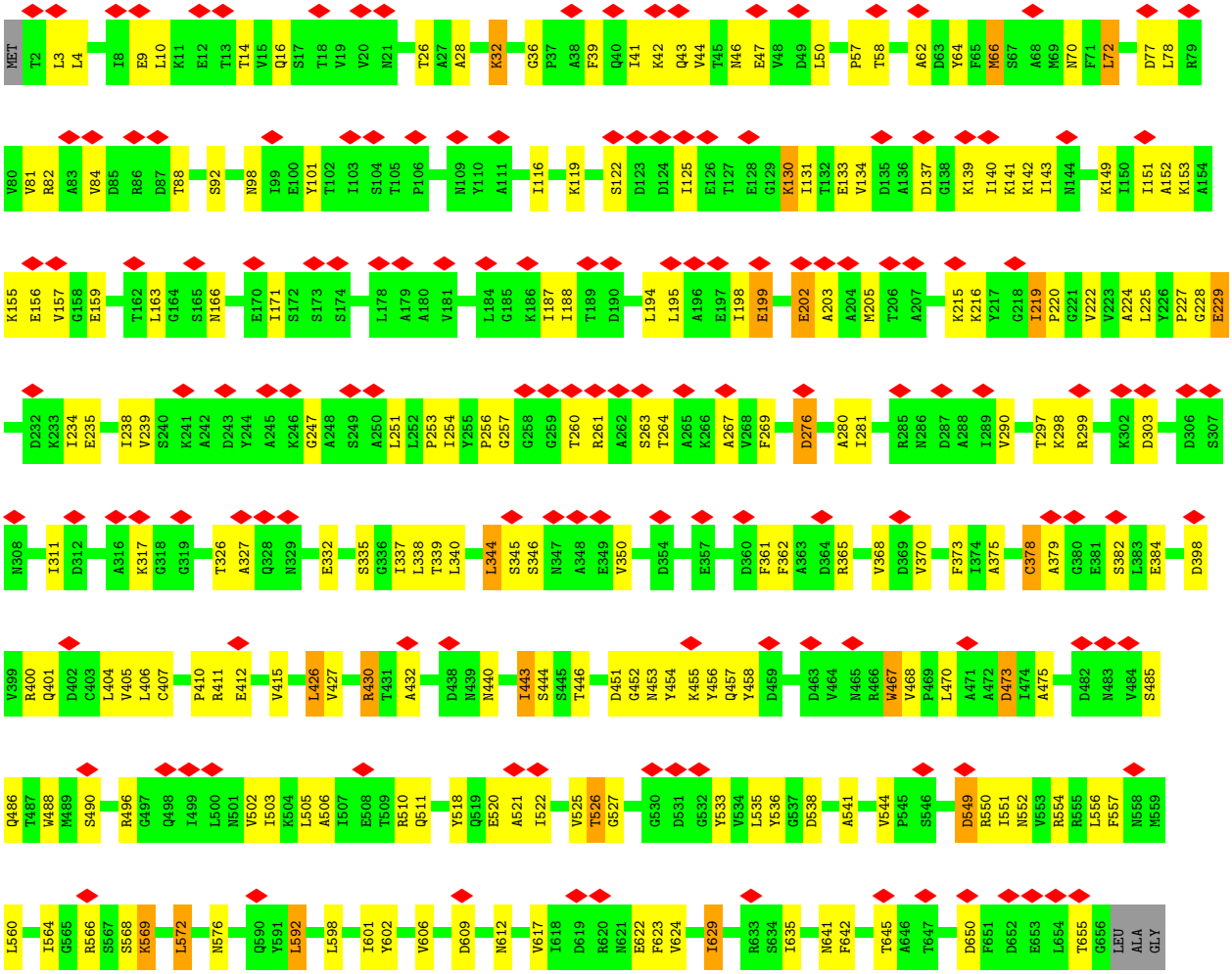






• Molecule 2: gp18, tail sheath protein

Chain Bv:

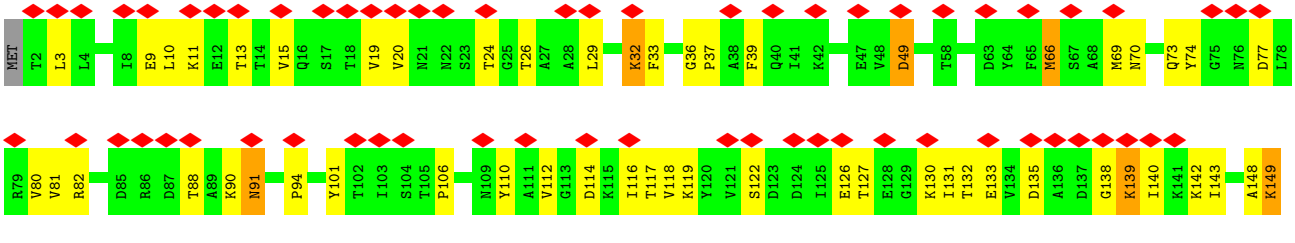


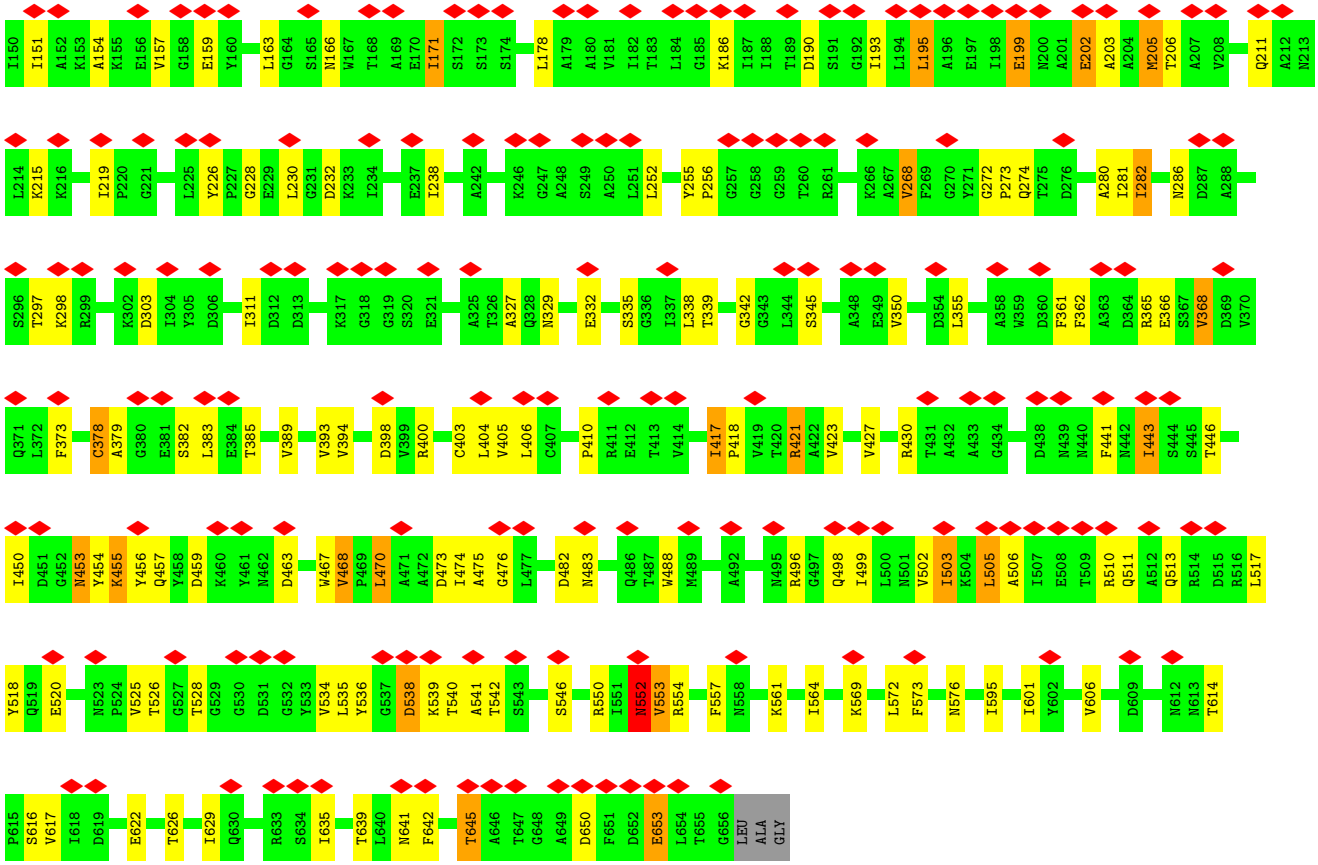




• Molecule 2: gp18, tail sheath protein

Chain Bw:



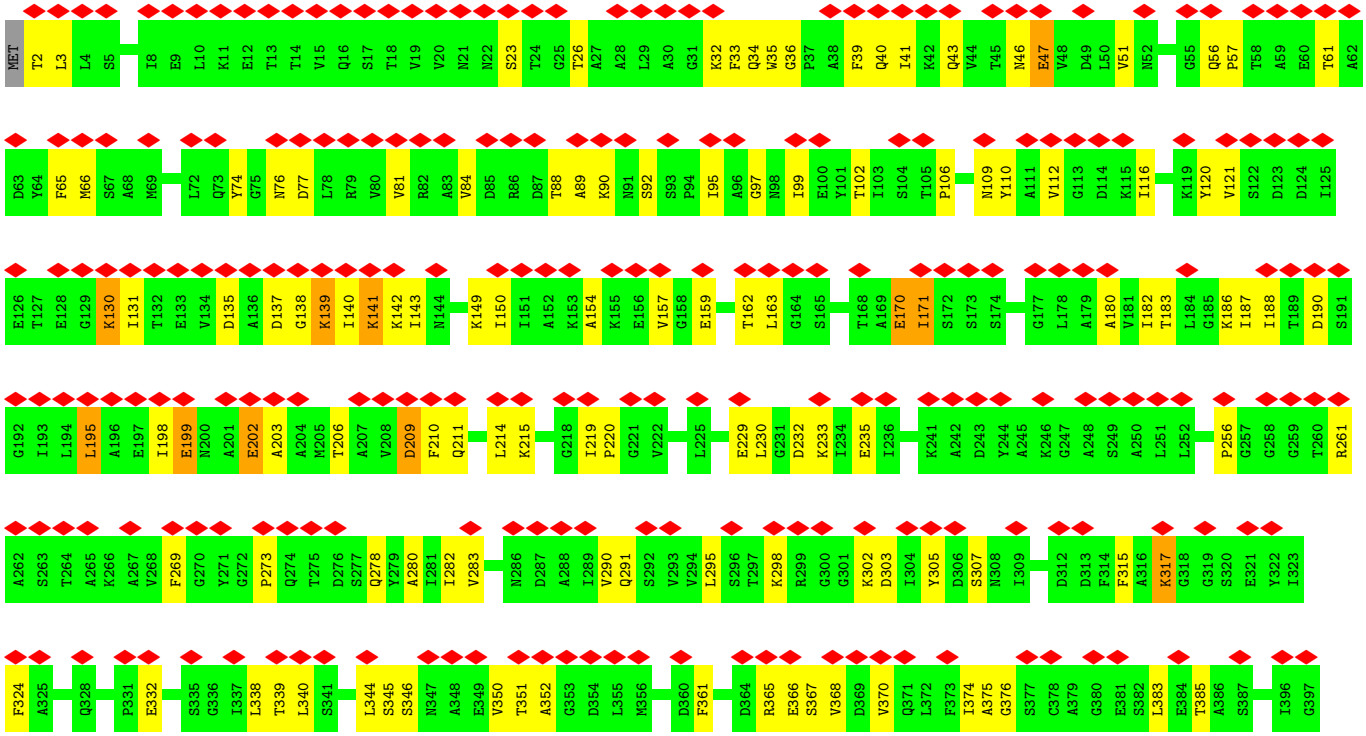



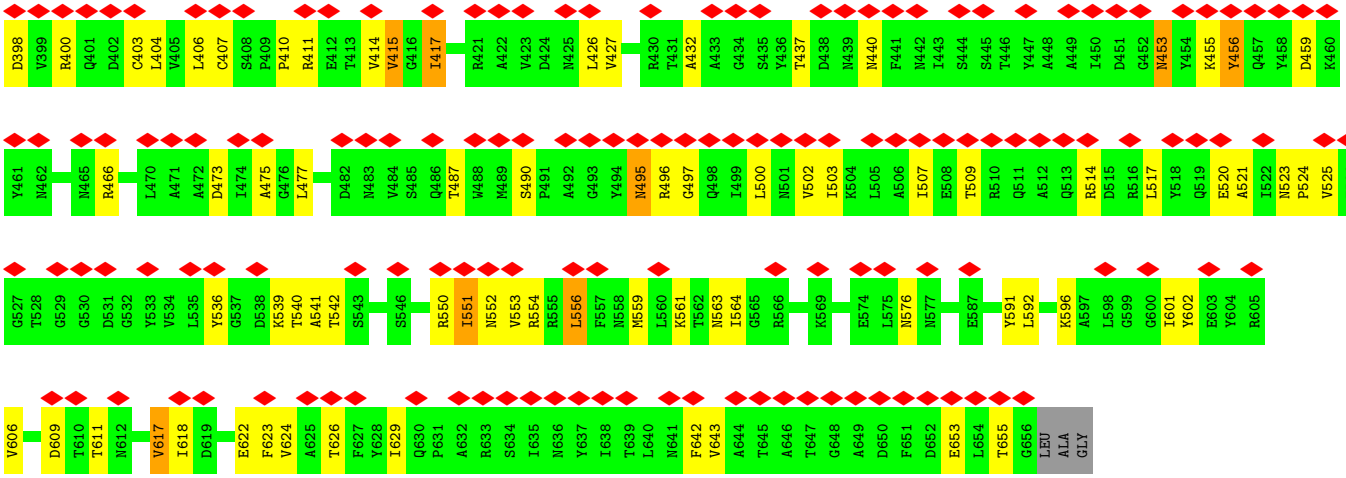



• Molecule 2: gp18, tail sheath protein

Chain Bx:



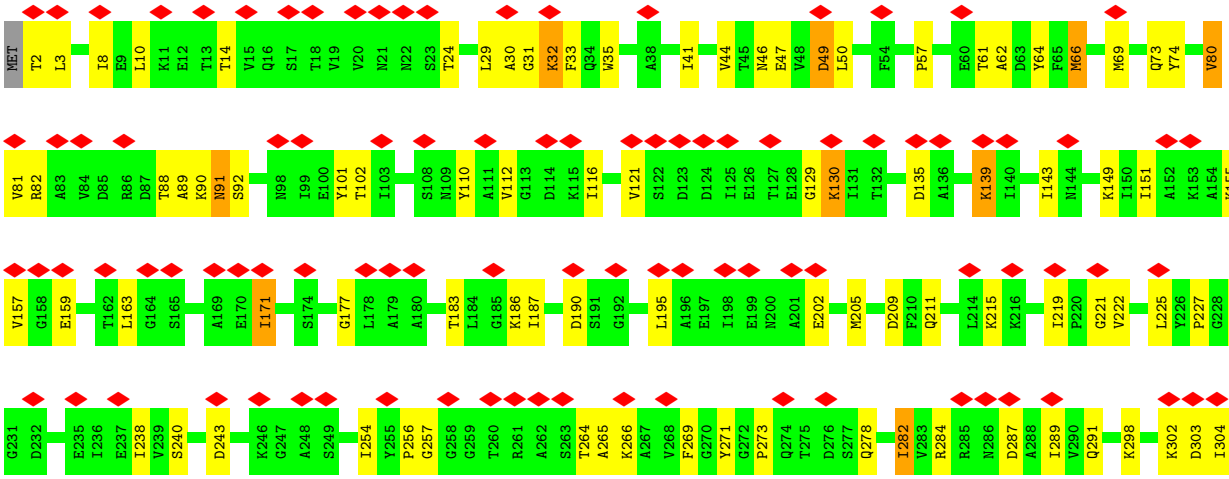






• Molecule 2: gp18, tail sheath protein

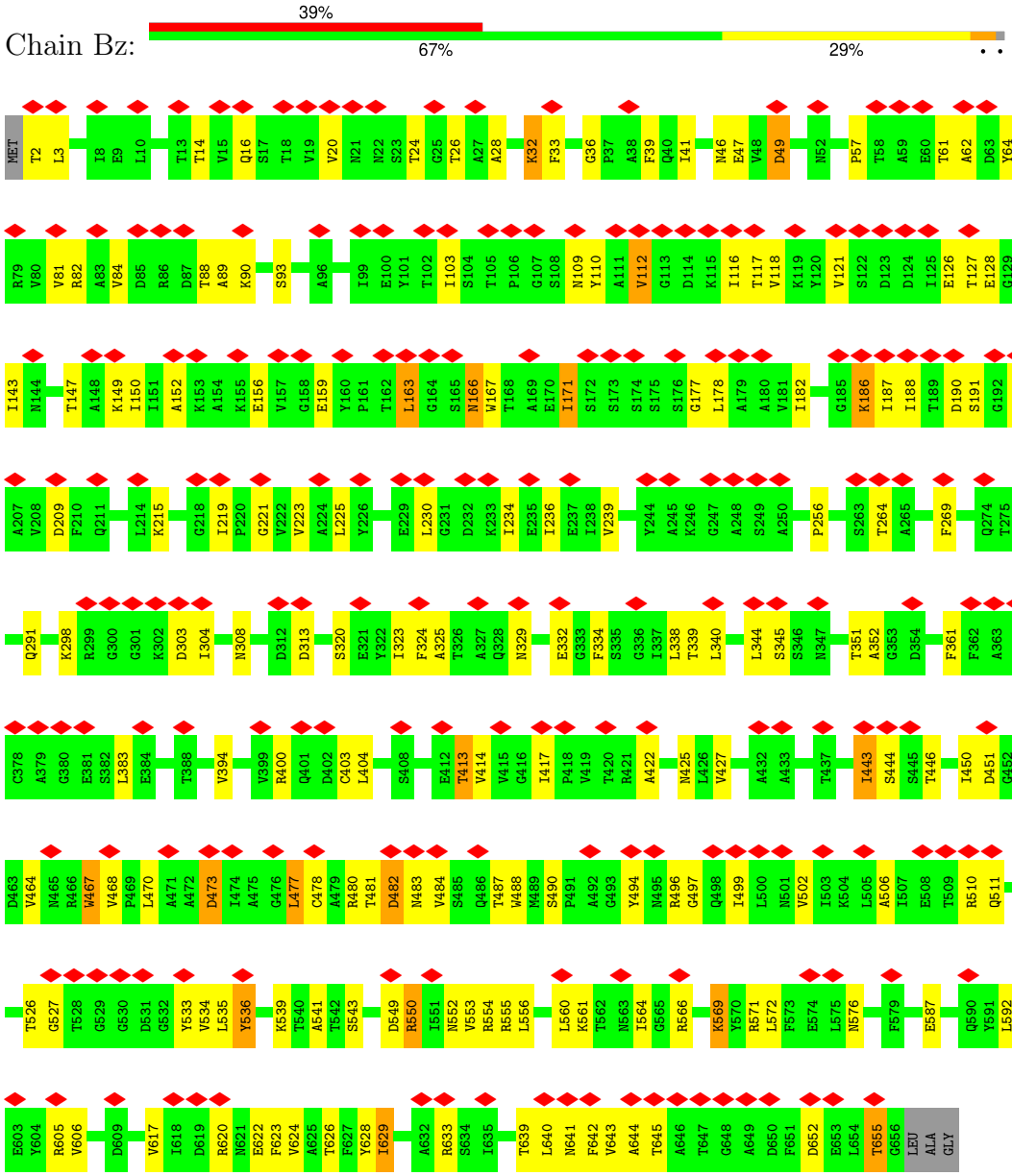
Chain By:



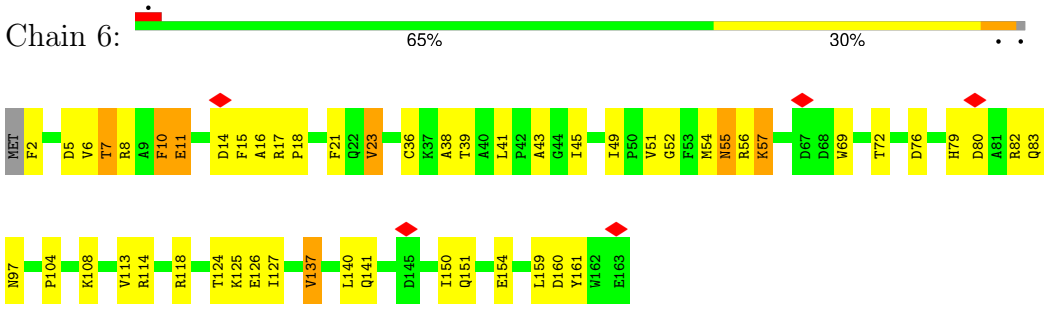

• Molecule 2: gp18, tail sheath protein

Chain Bz:




• Molecule 3: gp19, tail tube protein

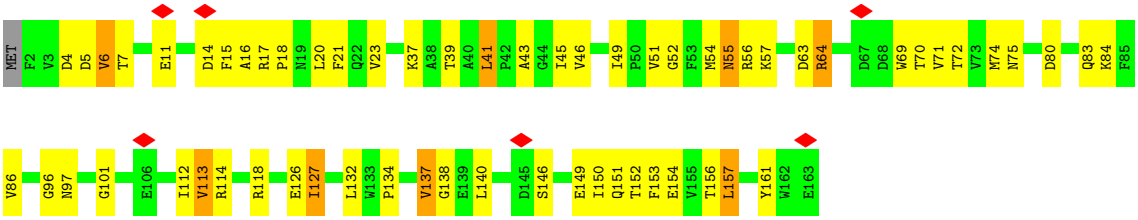
Chain 6:




• Molecule 3: gp19, tail tube protein

Chain 7:

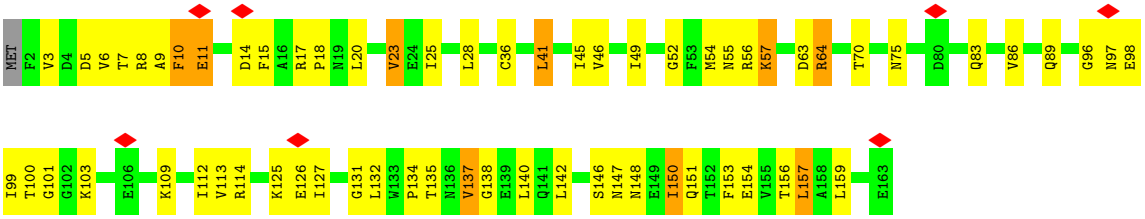





• Molecule 3: gp19, tail tube protein

Chain 8:

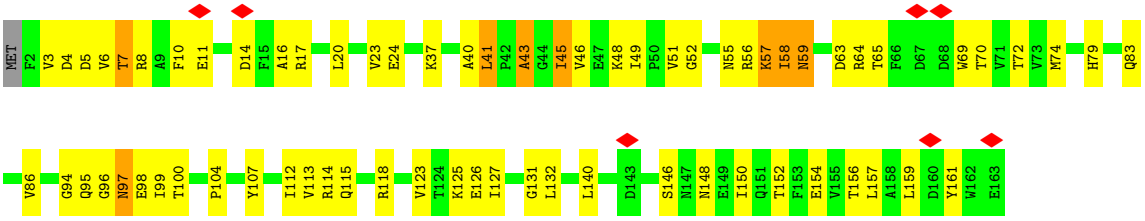



• Molecule 3: gp19, tail tube protein

Chain 9:

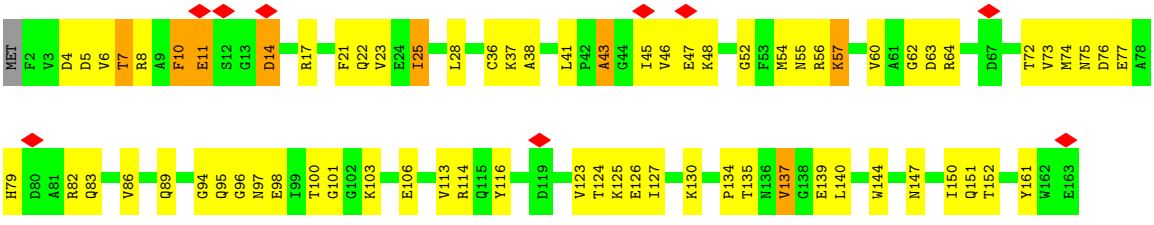



• Molecule 3: gp19, tail tube protein

Chain AA:

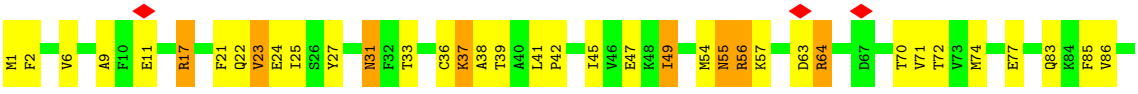


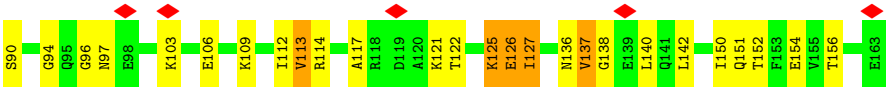




• Molecule 3: gp19, tail tube protein

Chain AE:



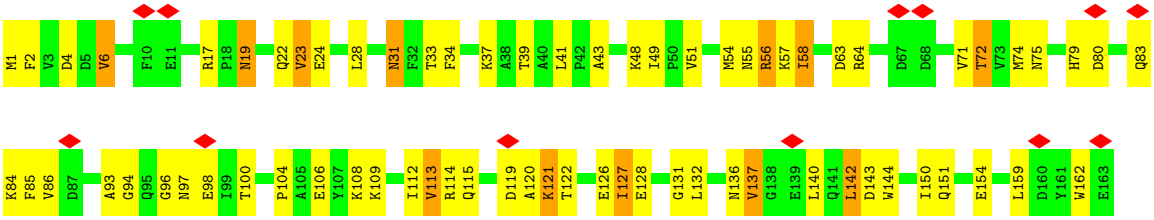






• Molecule 3: gp19, tail tube protein

Chain AF:

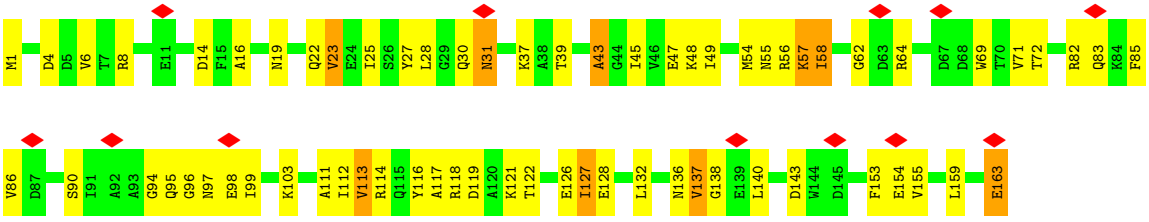



• Molecule 3: gp19, tail tube protein

Chain AG:

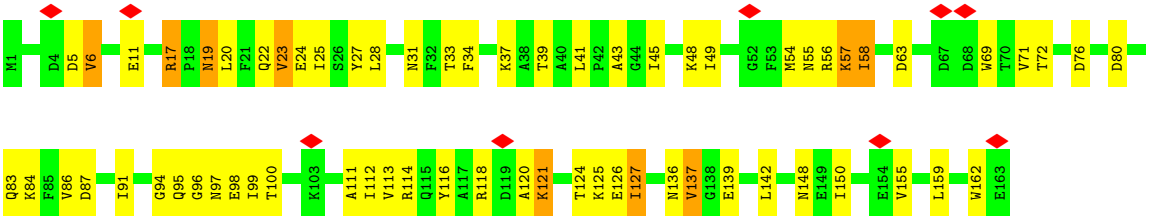



• Molecule 3: gp19, tail tube protein

Chain AH:

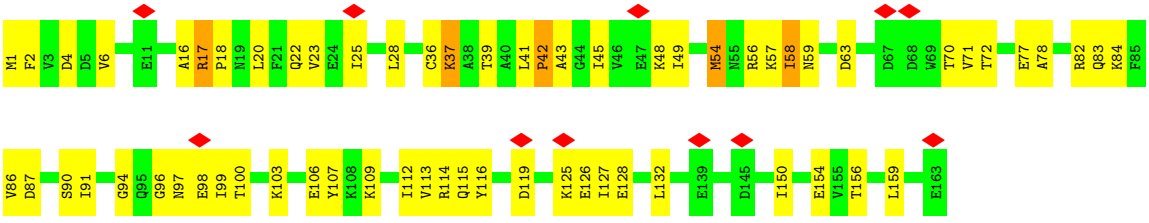



• Molecule 3: gp19, tail tube protein

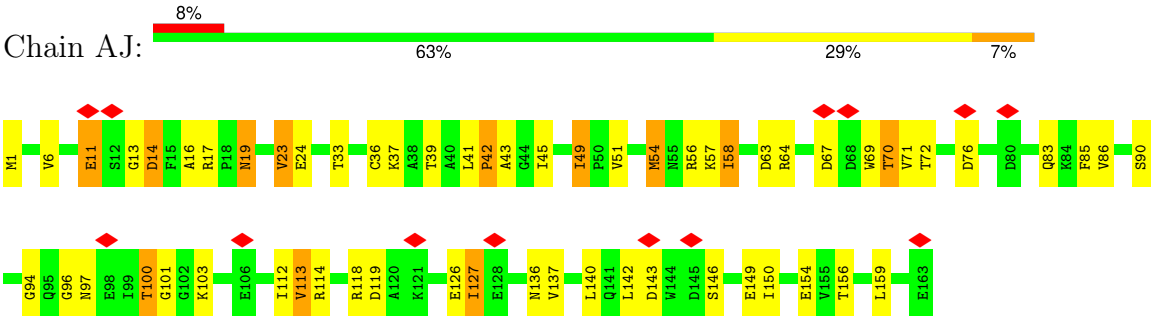
Chain AI:



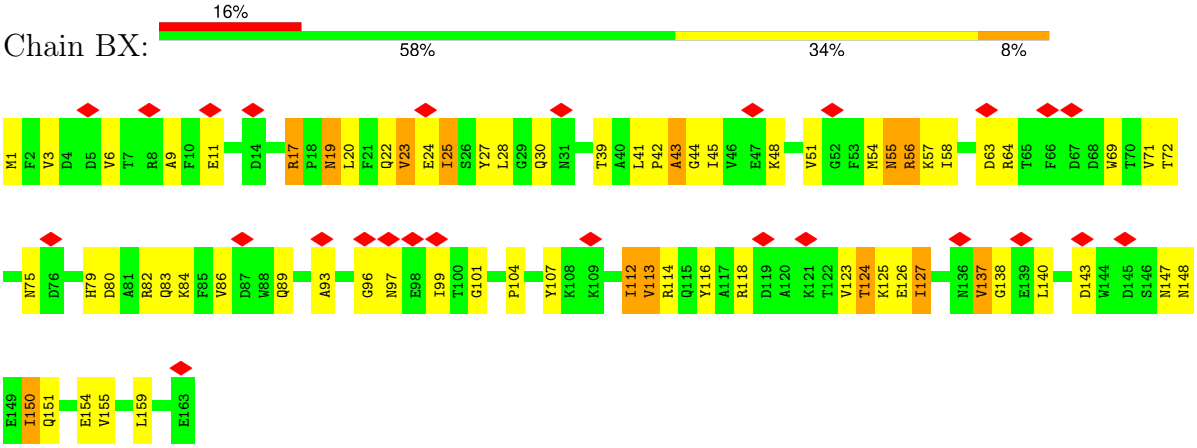

• Molecule 3: gp19, tail tube protein

Chain AJ:



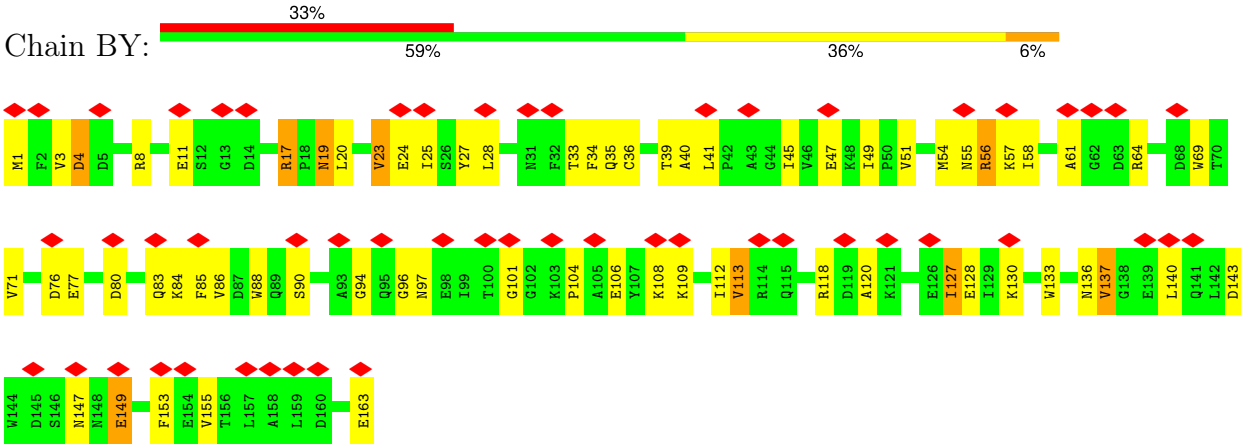

• Molecule 3: gp19, tail tube protein

Chain BX:



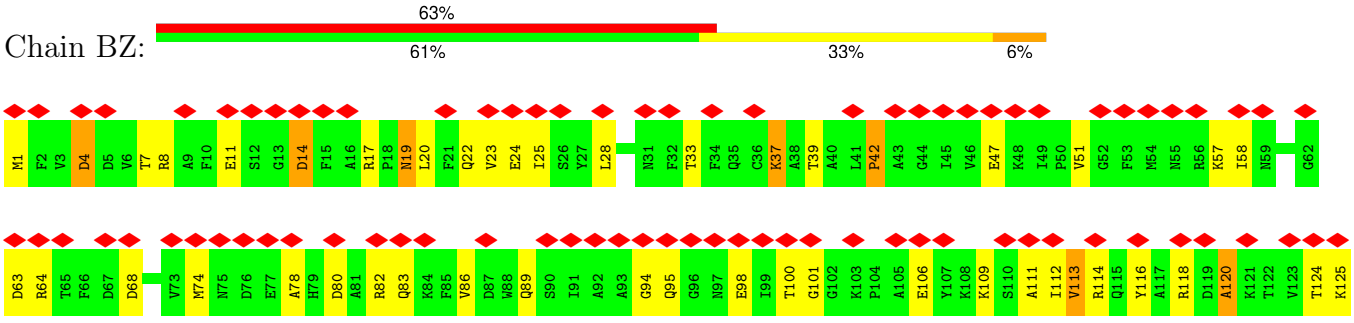

• Molecule 3: gp19, tail tube protein

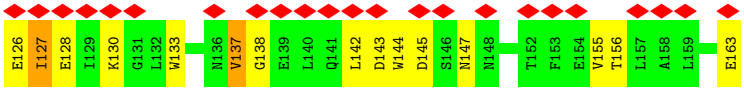
Chain BY:




• Molecule 3: gp19, tail tube protein

Chain BZ:

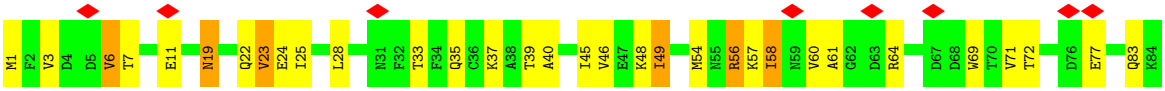


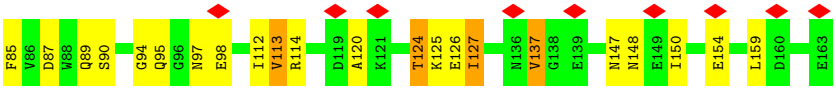



• Molecule 3: gp19, tail tube protein

Chain Ba:



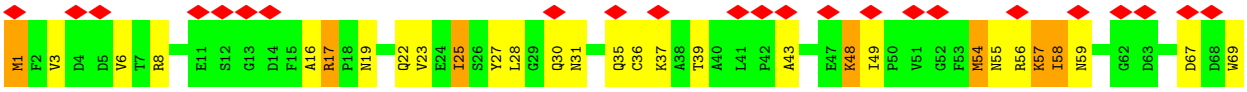



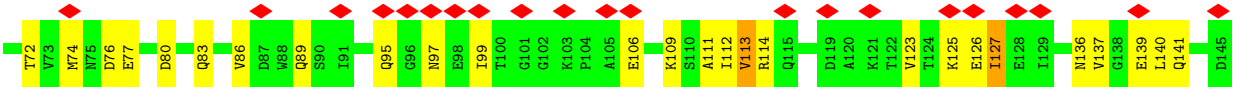



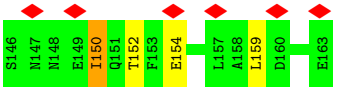

• Molecule 3: gp19, tail tube protein

Chain Bb:



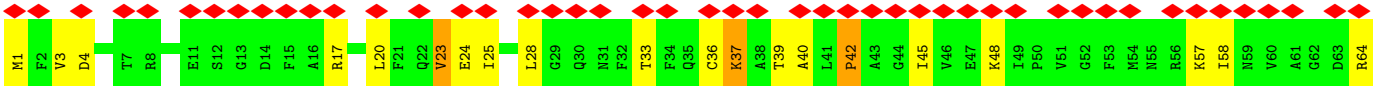



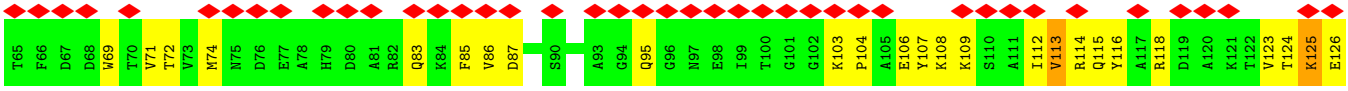




• Molecule 3: gp19, tail tube protein

Chain Bc:



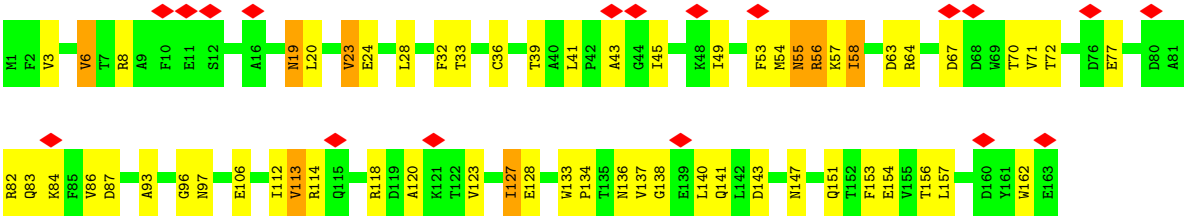




• Molecule 3: gp19, tail tube protein

Chain Bd:

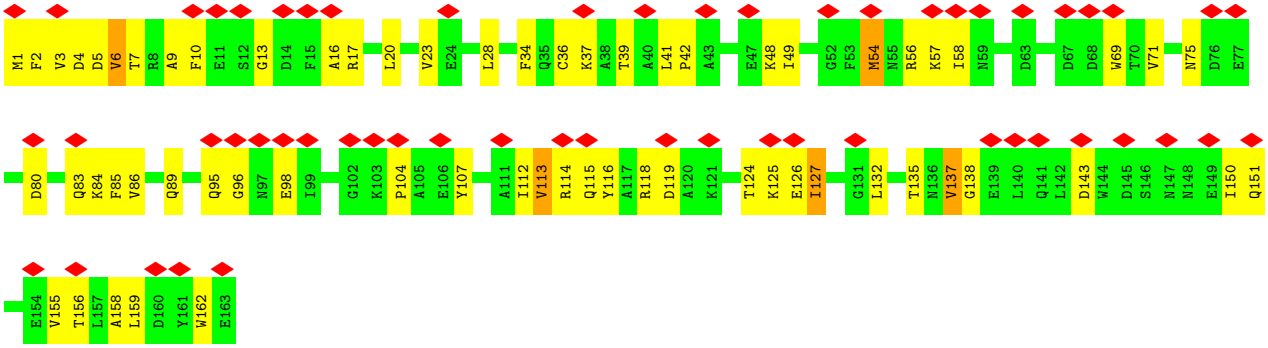





• Molecule 3: gp19, tail tube protein

Chain Be:

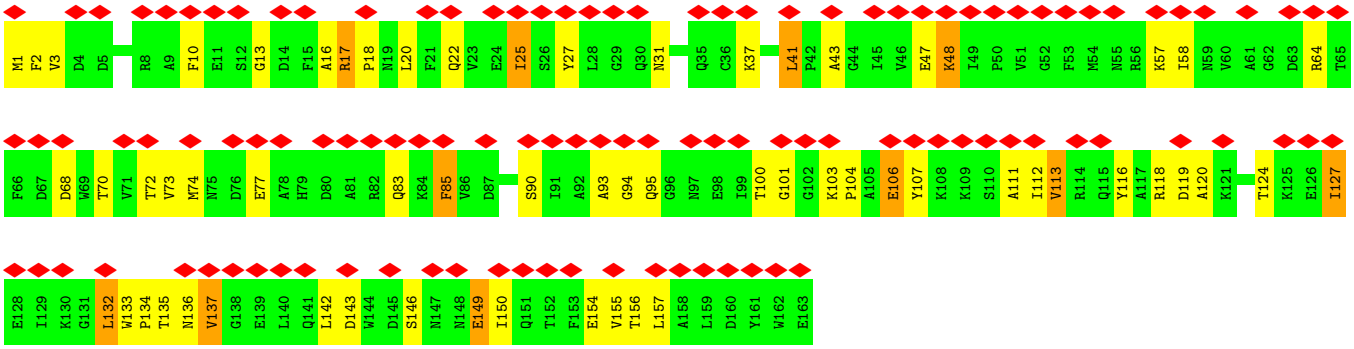



• Molecule 3: gp19, tail tube protein

Chain Bf:

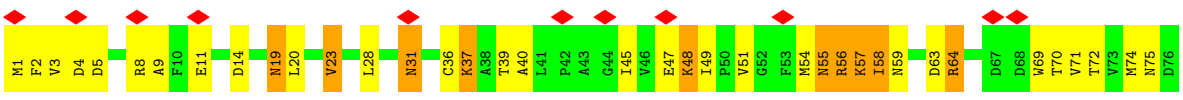


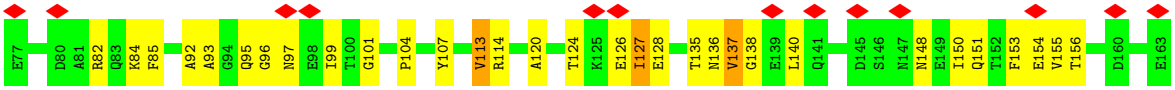




• Molecule 3: gp19, tail tube protein

Chain Bg:

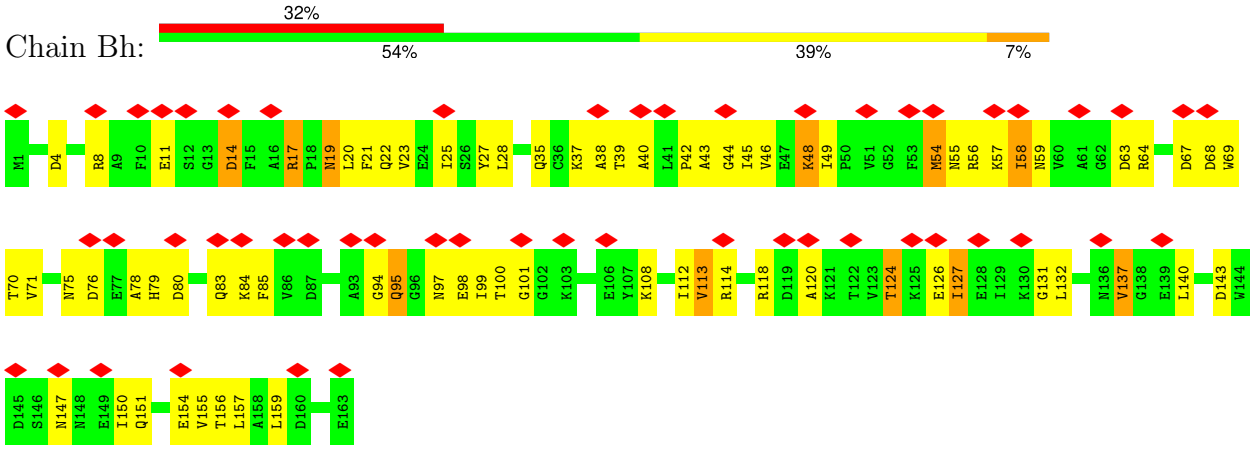


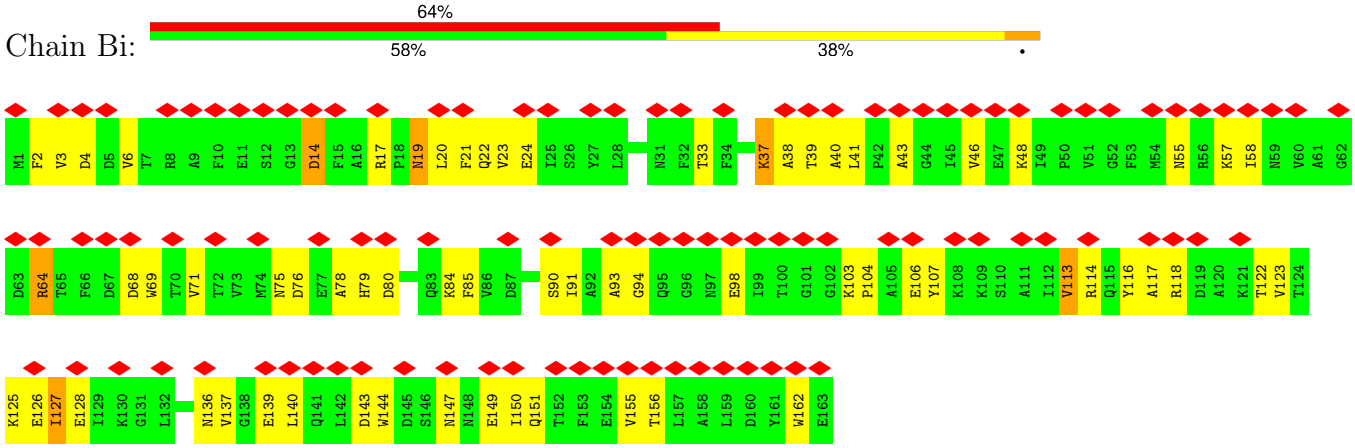

• Molecule 3: gp19, tail tube protein

Chain Bh:



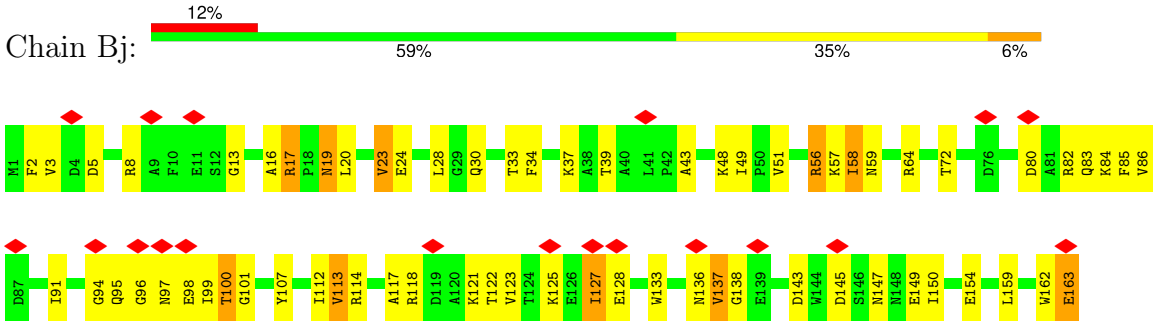

• Molecule 3: gp19, tail tube protein

Chain Bi:



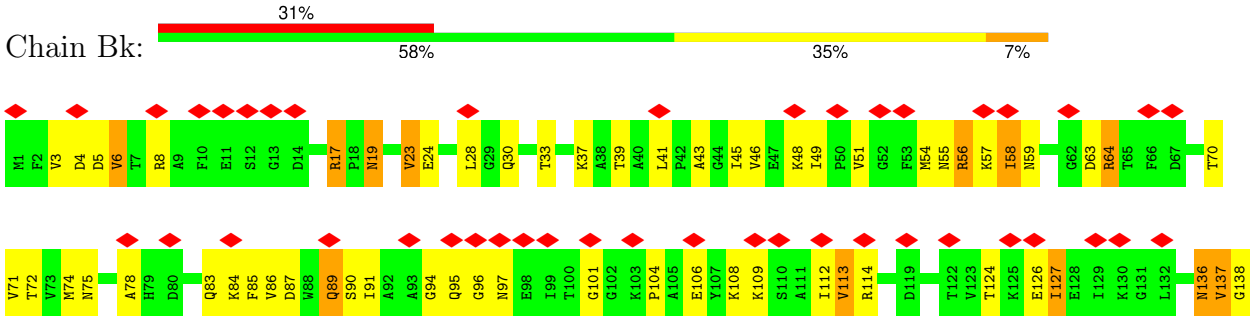

• Molecule 3: gp19, tail tube protein

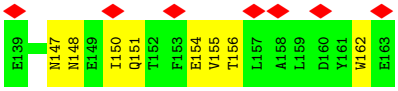
Chain Bj:




• Molecule 3: gp19, tail tube protein

Chain Bk:

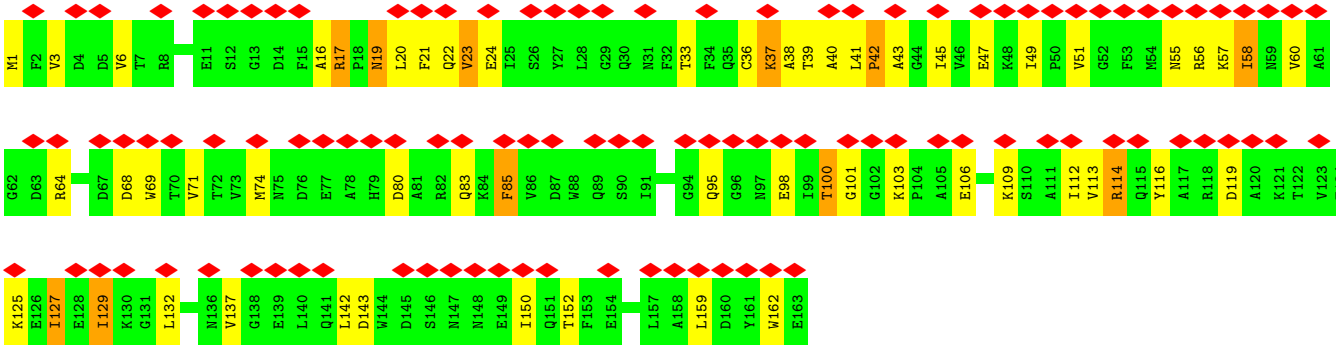





• Molecule 3: gp19, tail tube protein

Chain Bl:

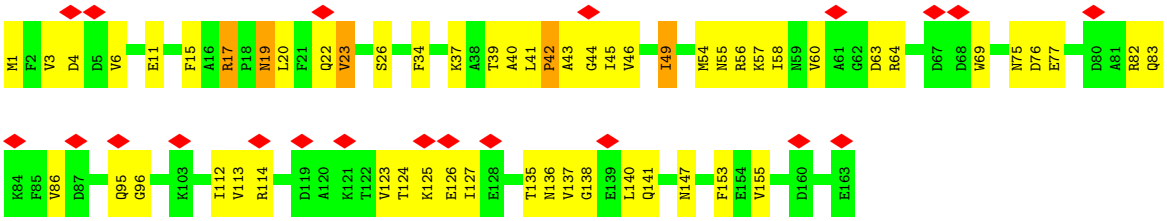



• Molecule 3: gp19, tail tube protein

Chain Bm:

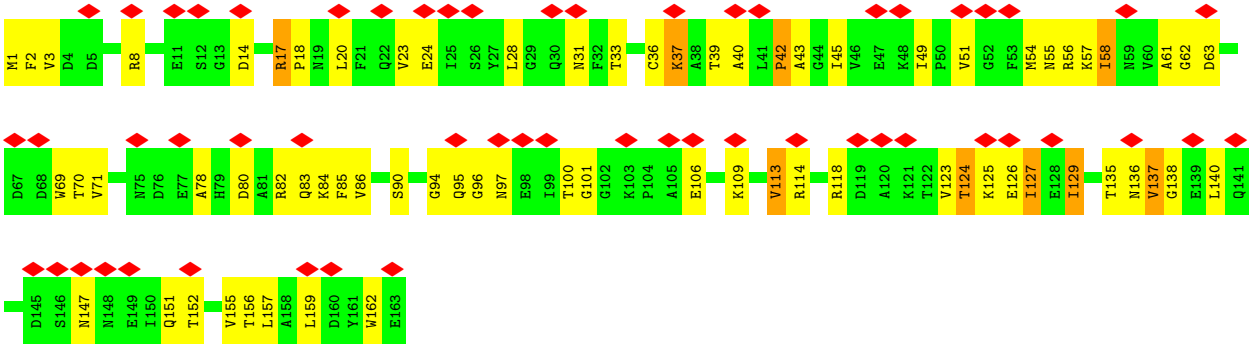



• Molecule 3: gp19, tail tube protein

Chain Bn:

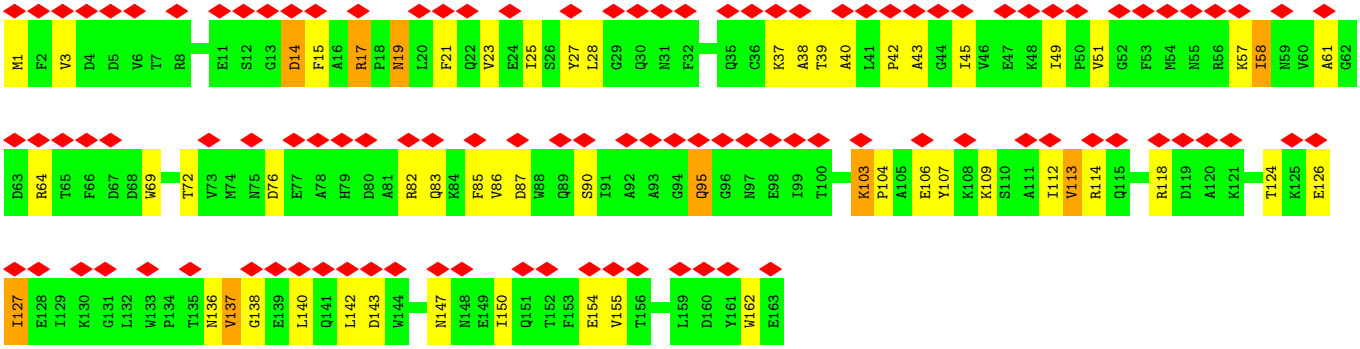



• Molecule 3: gp19, tail tube protein

Chain Bo:

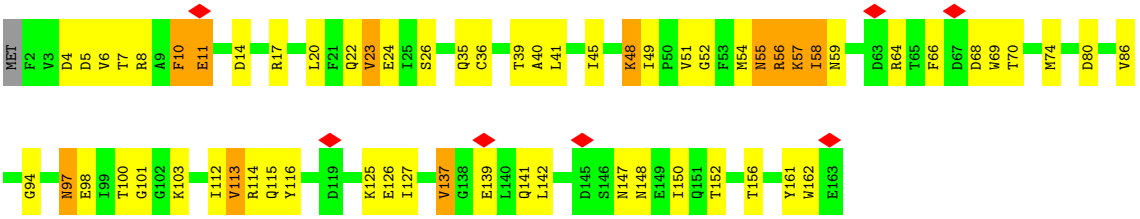





• Molecule 3: gp19, tail tube protein

Chain o:

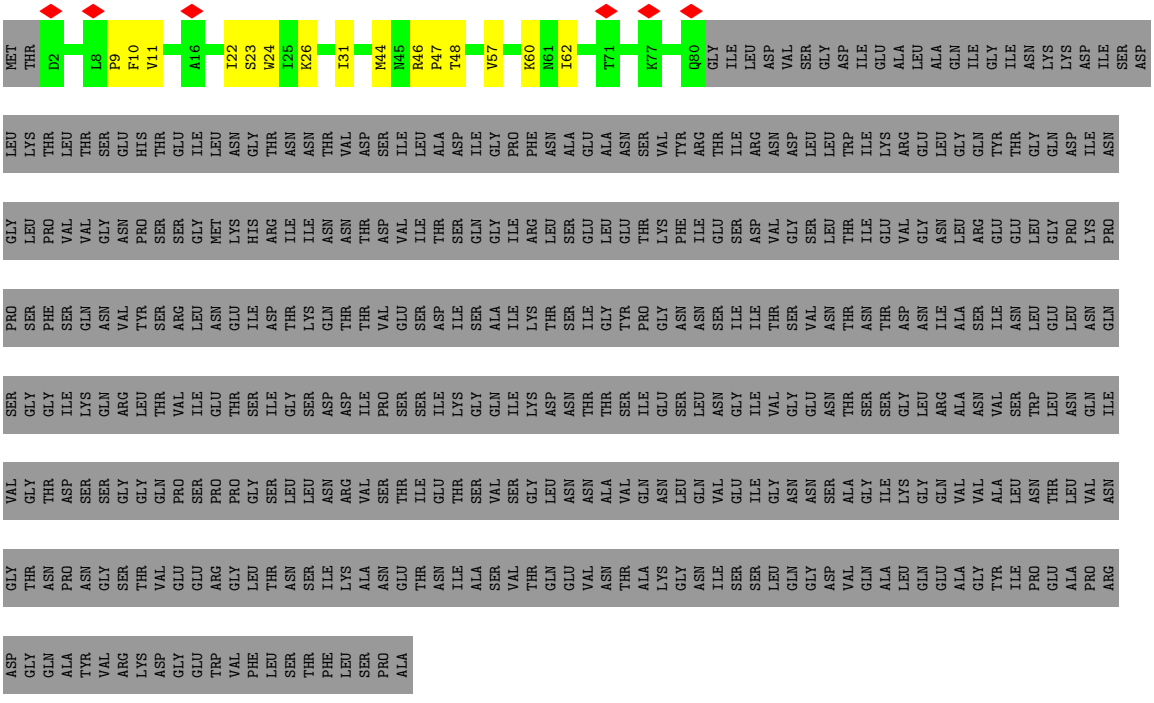



• Molecule 4: gpwac, fibritin

Chain A:

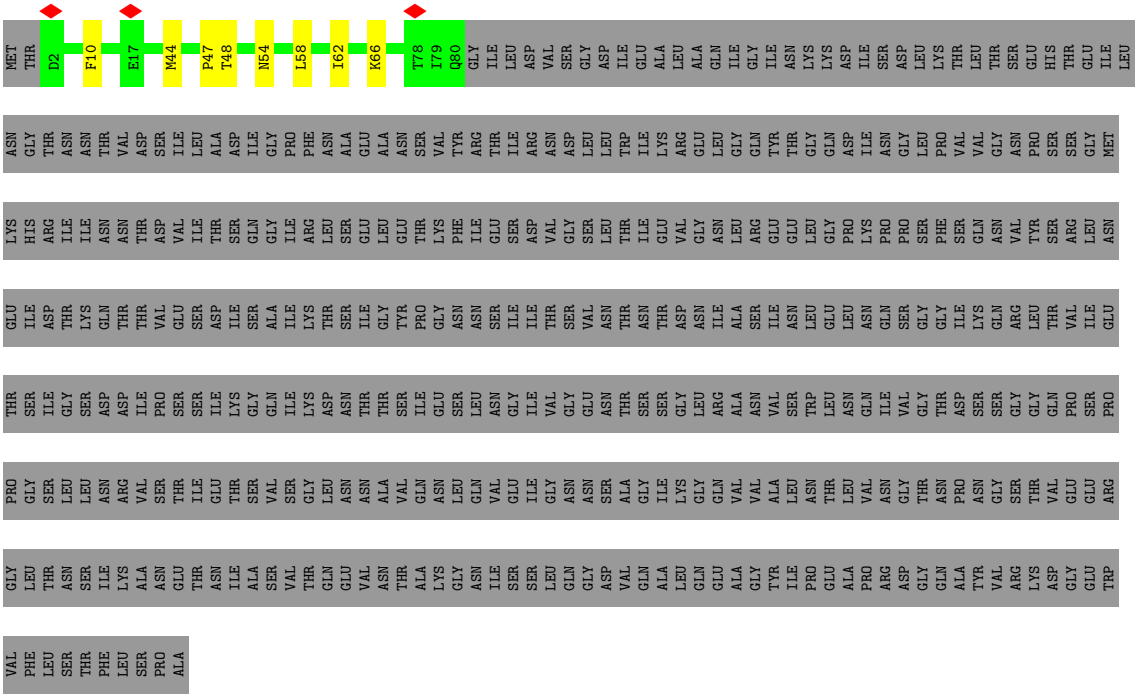



• Molecule 4: gpwac, fibritin

Chain B:

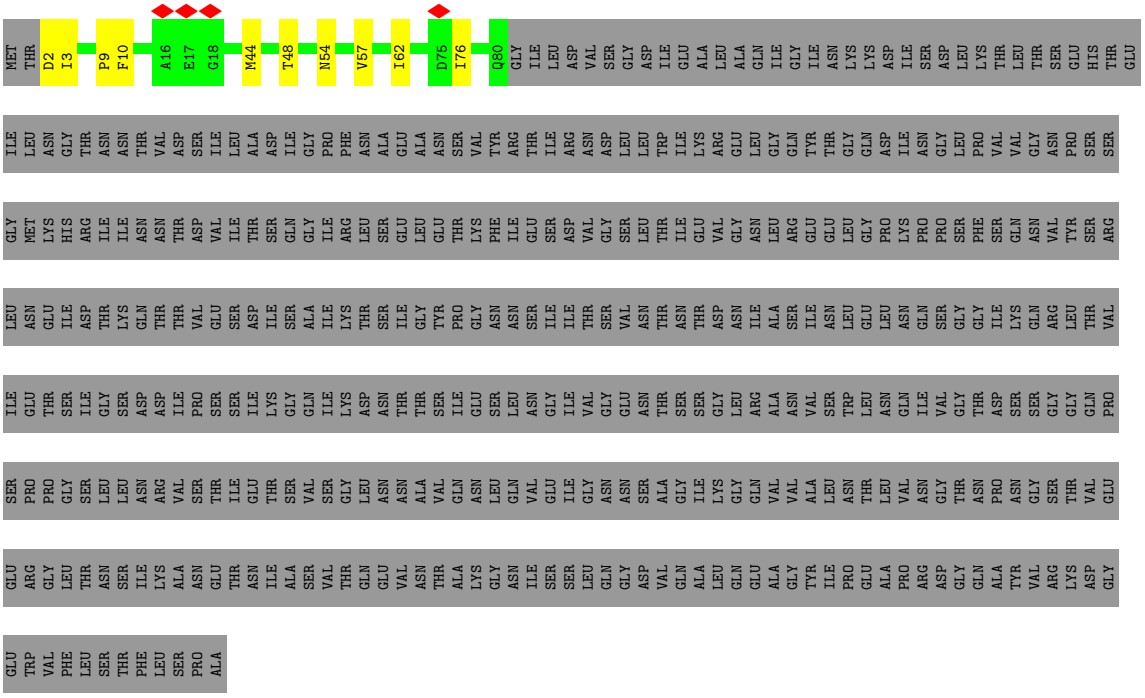





• Molecule 4: gpwac, fibritin

Chain C:

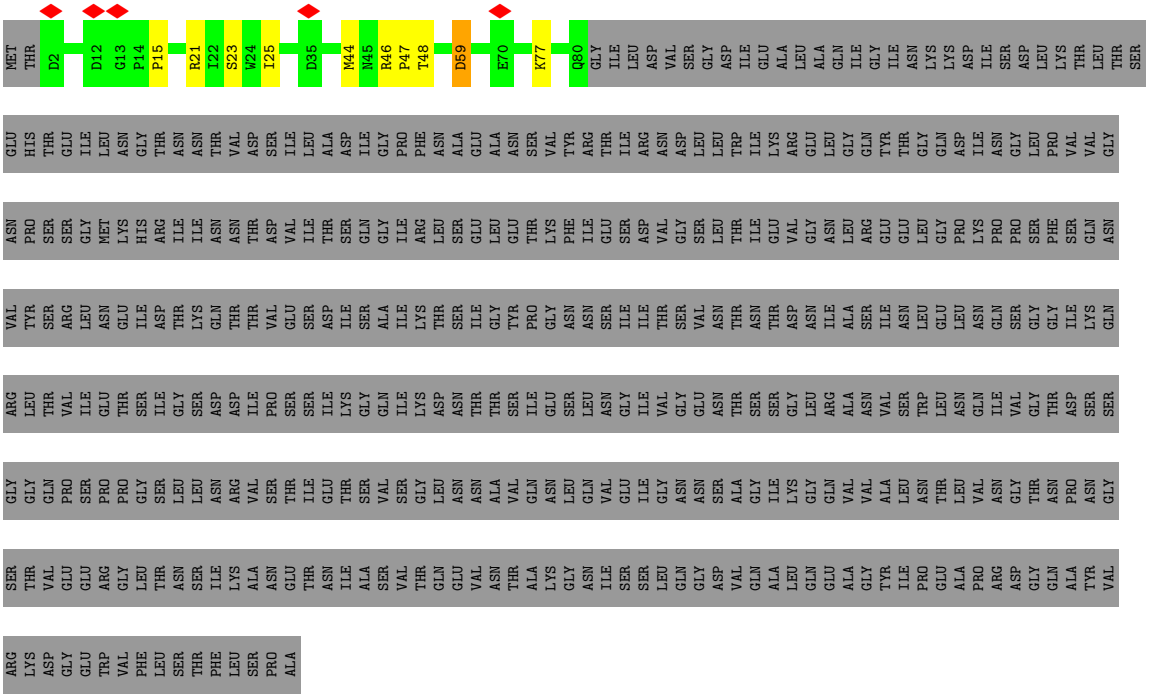



• Molecule 4: gpwac, fibritin

Chain D:

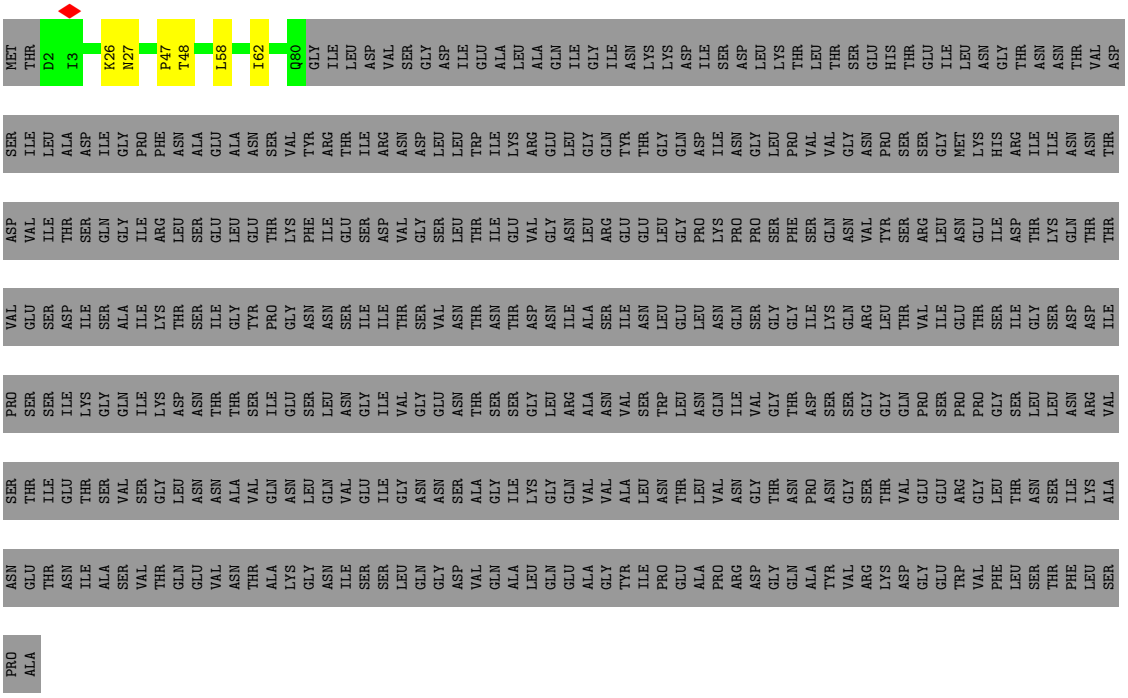





• Molecule 4: gpwac, fibritin

Chain E:

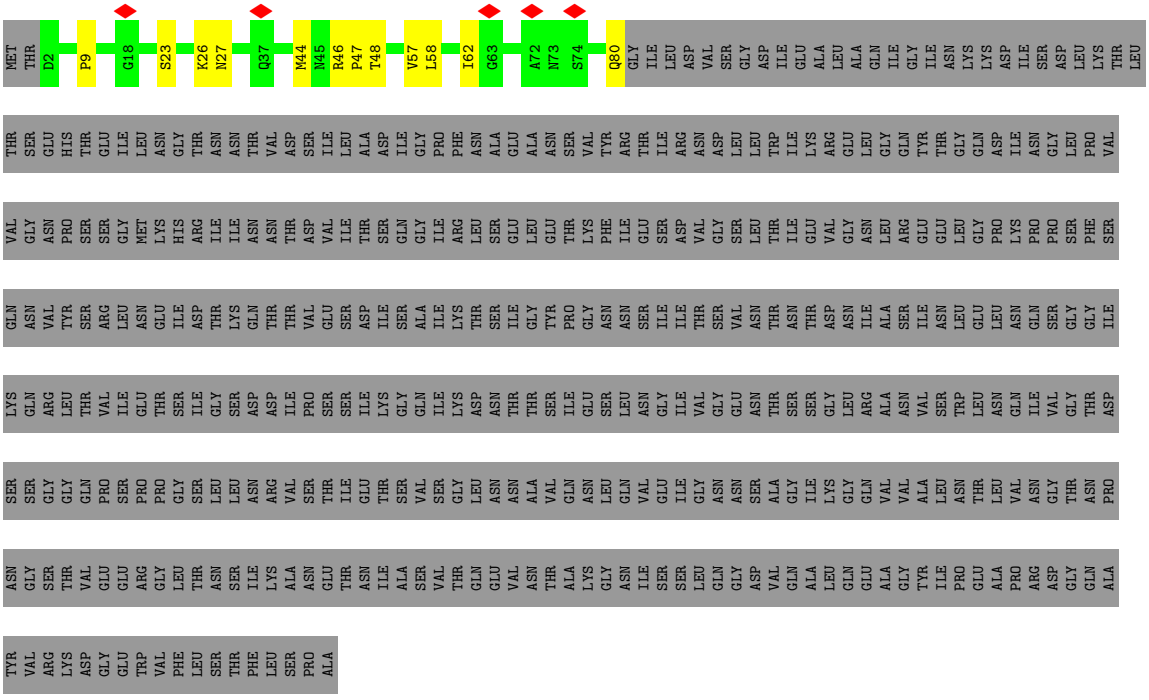



• Molecule 4: gpwac, fibritin

Chain F:

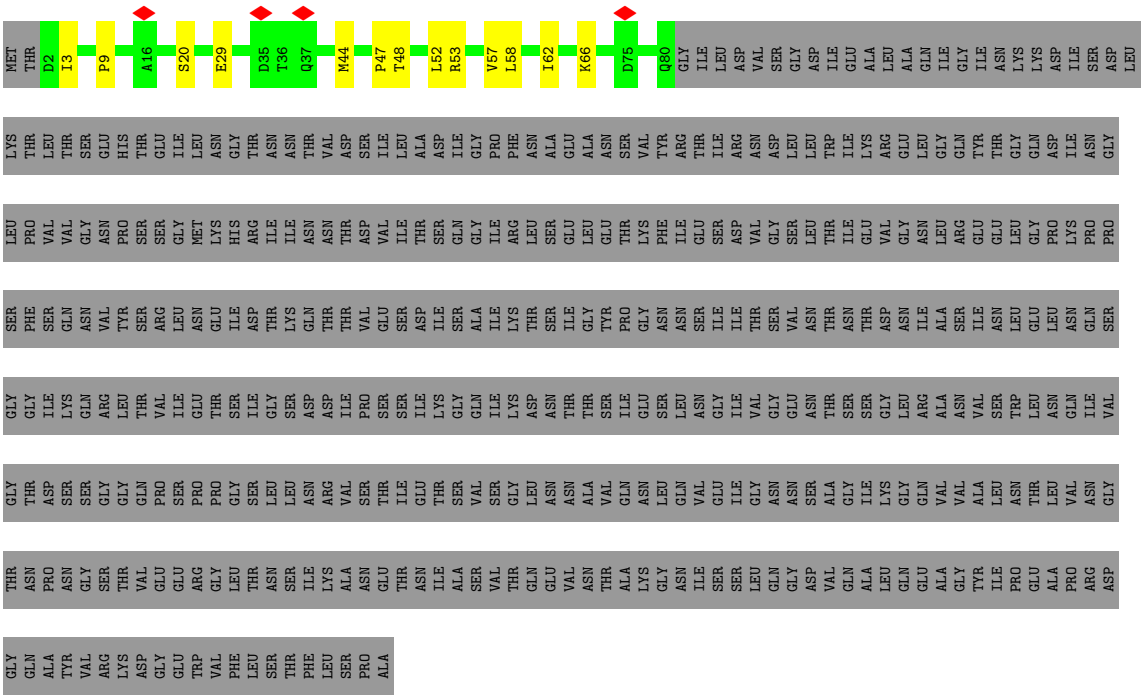





• Molecule 4: gpwac, fibritin

Chain G:

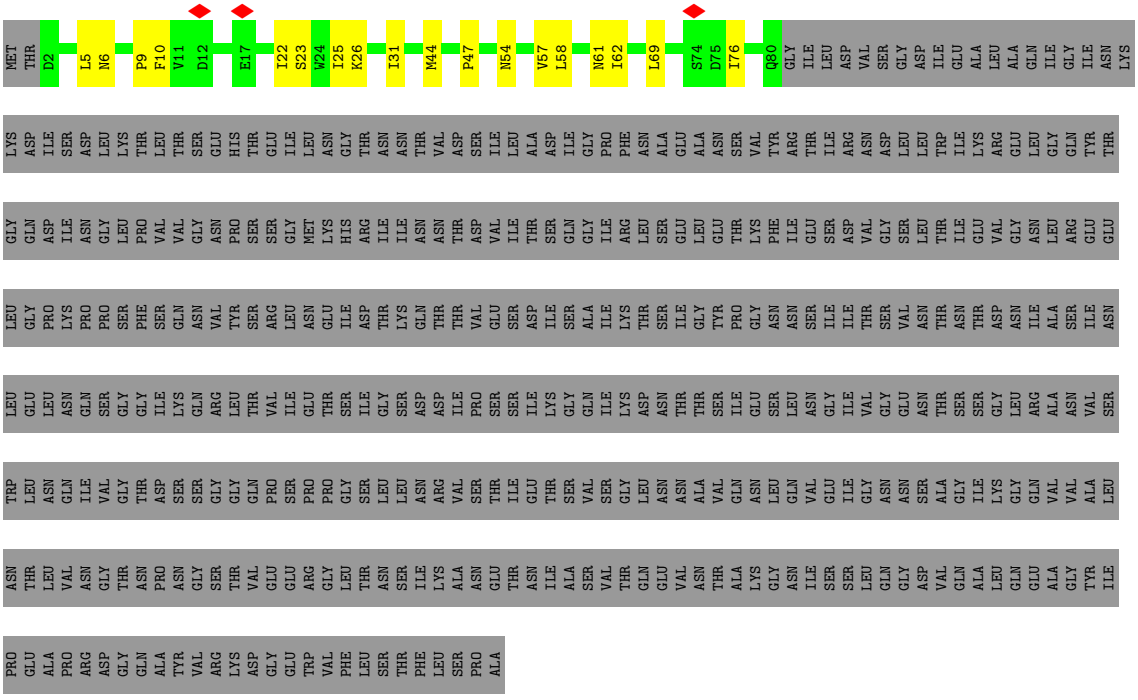



• Molecule 4: gpwac, fibritin

Chain H:

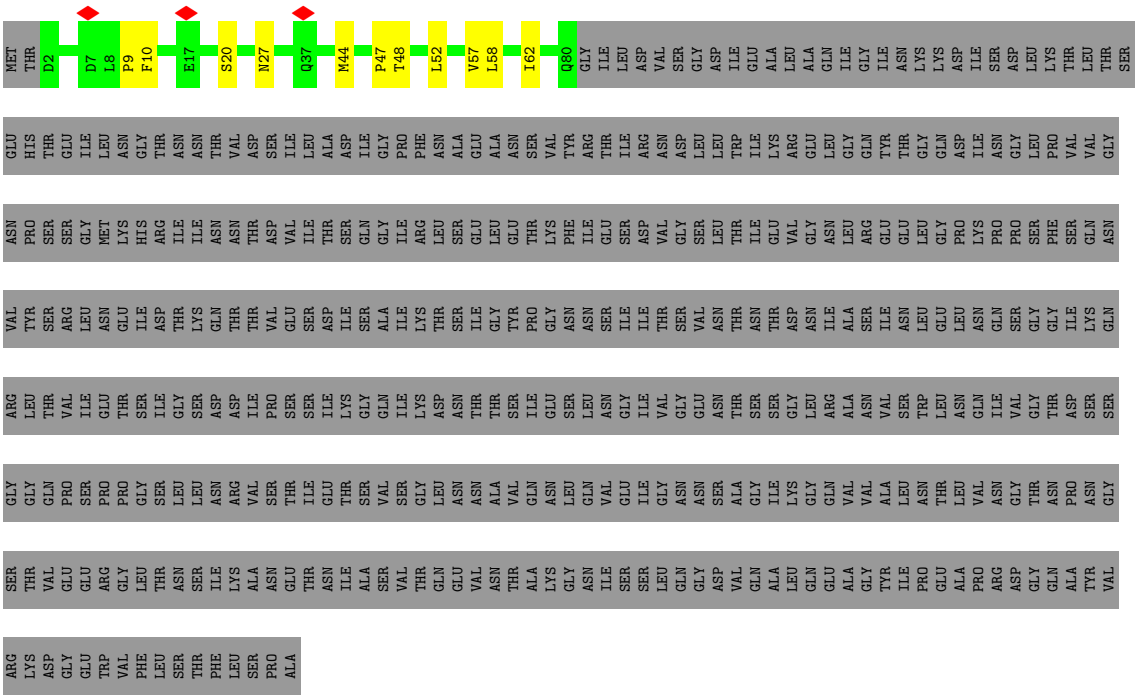





- Molecule 4: gpwac, fibritin

Chain I:

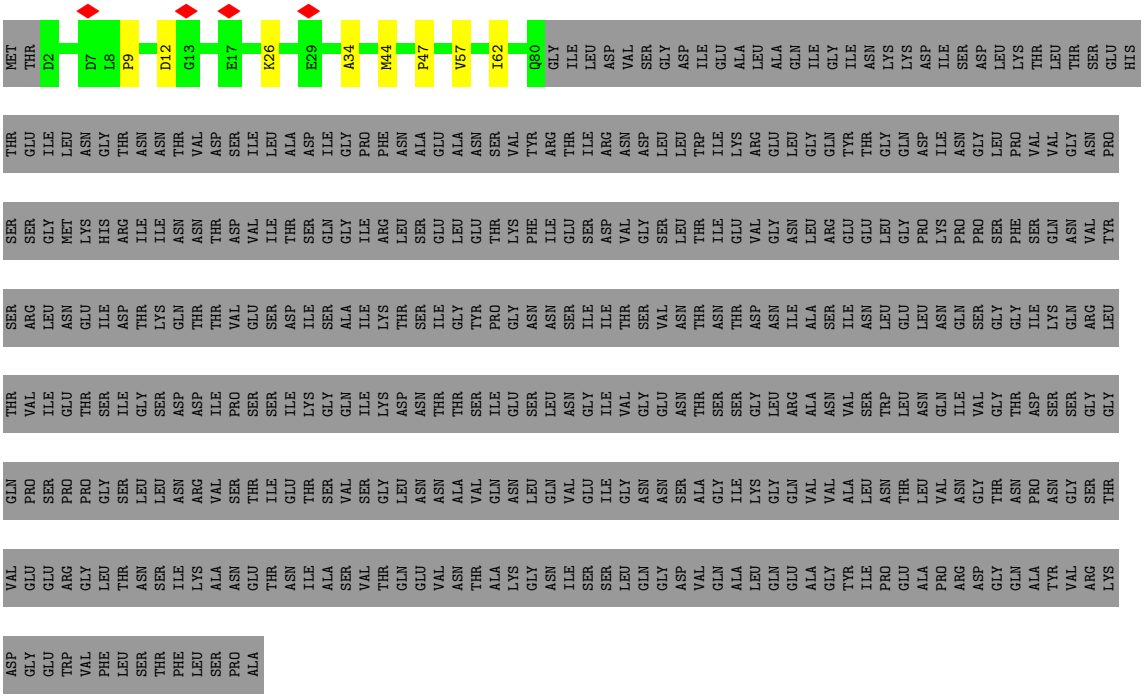



- Molecule 4: gpwac, fibritin

Chain J:

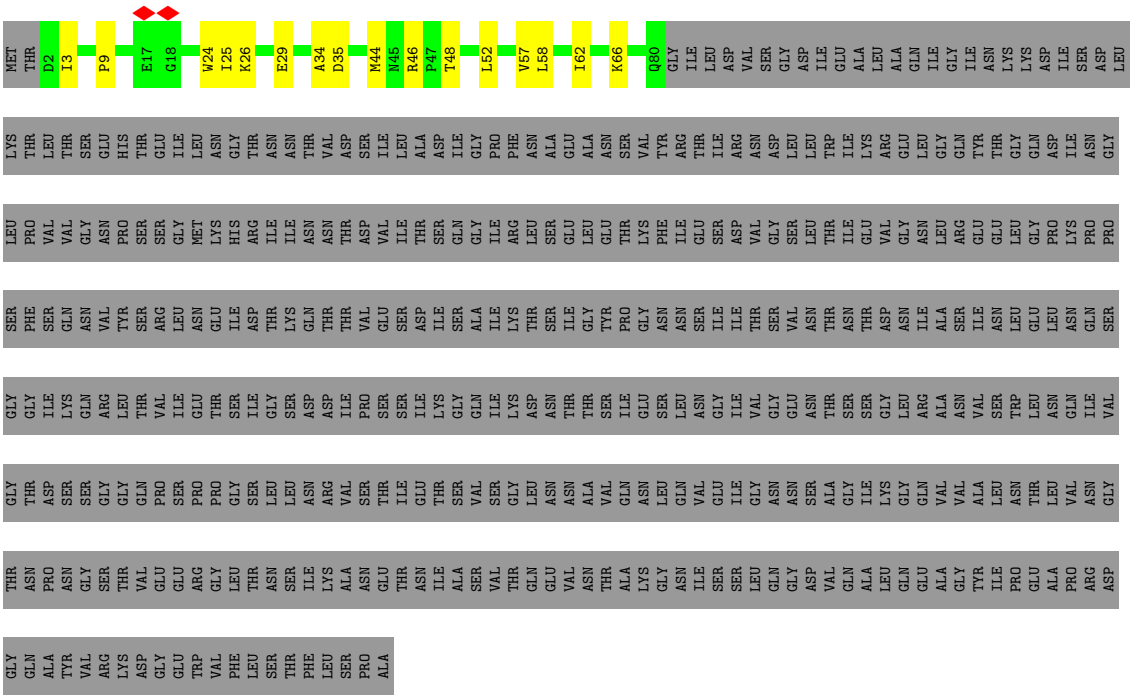





• Molecule 4: gpwac, fibritin

Chain K:

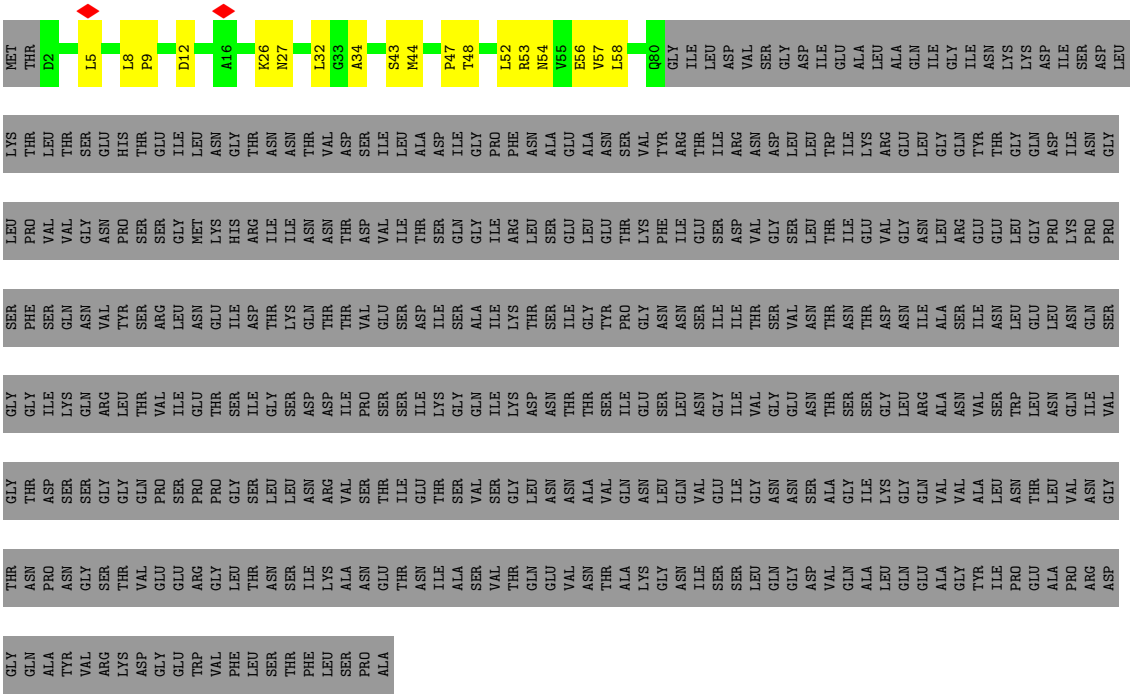



• Molecule 4: gpwac, fibritin

Chain L:

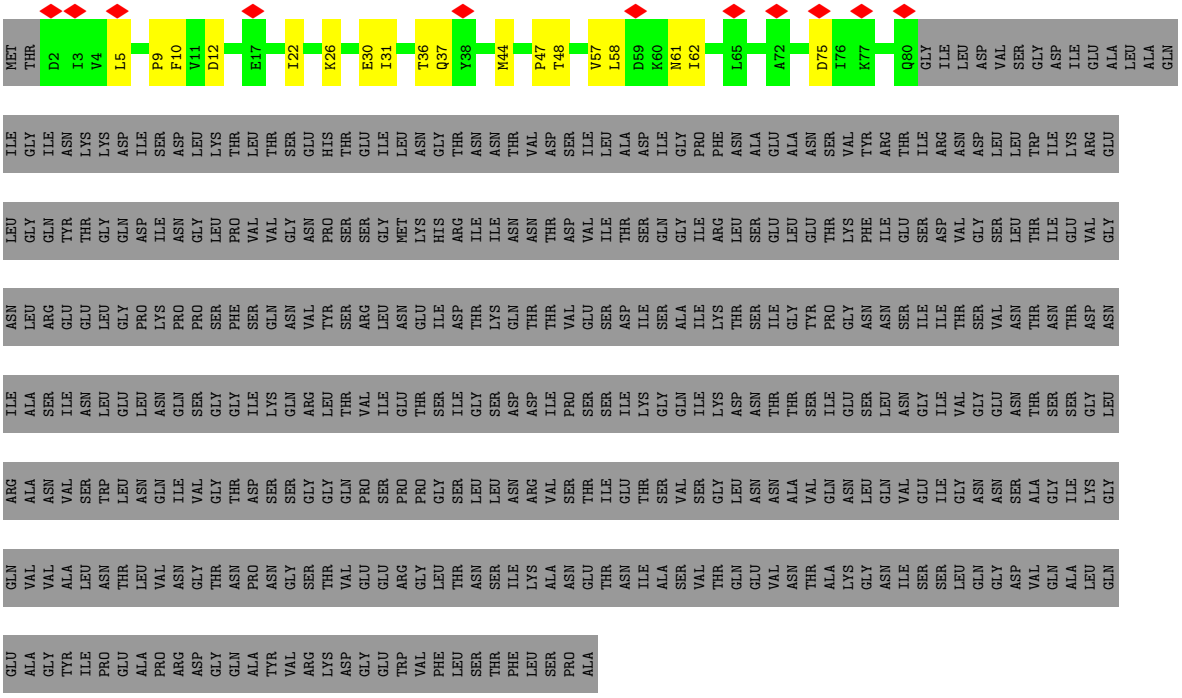





- Molecule 4: gpwac, fibritin

Chain M:

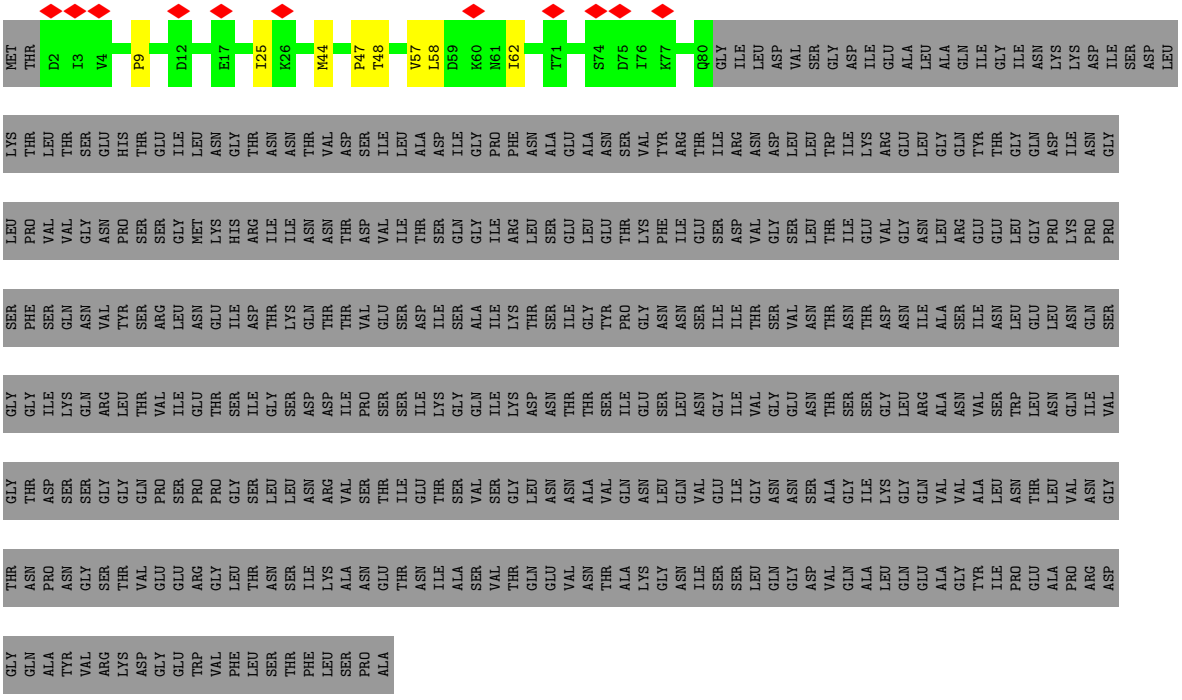



- Molecule 4: gpwac, fibritin

Chain N:

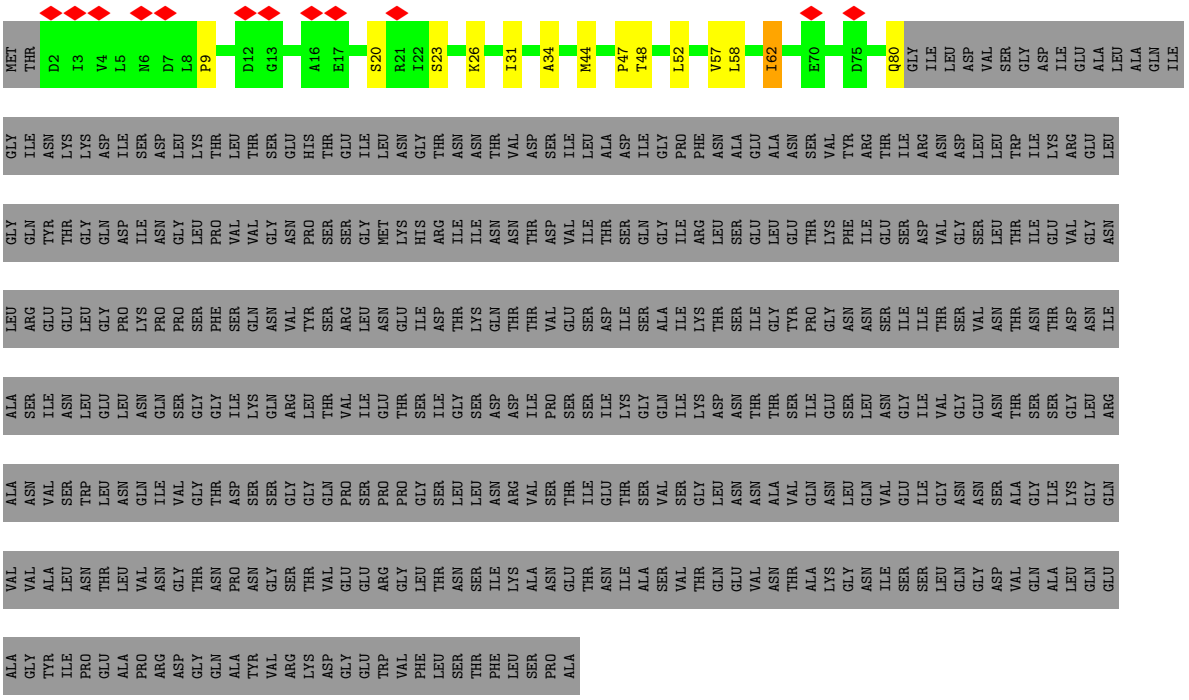





• Molecule 4: gpwac, fibritin

Chain O:

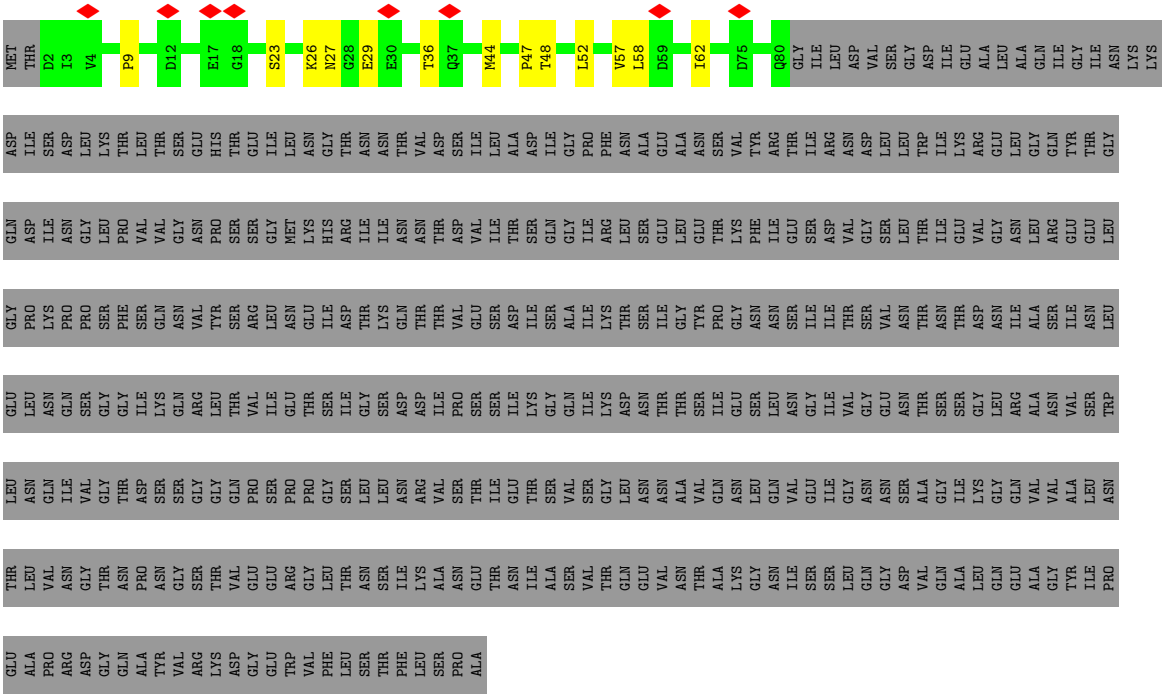


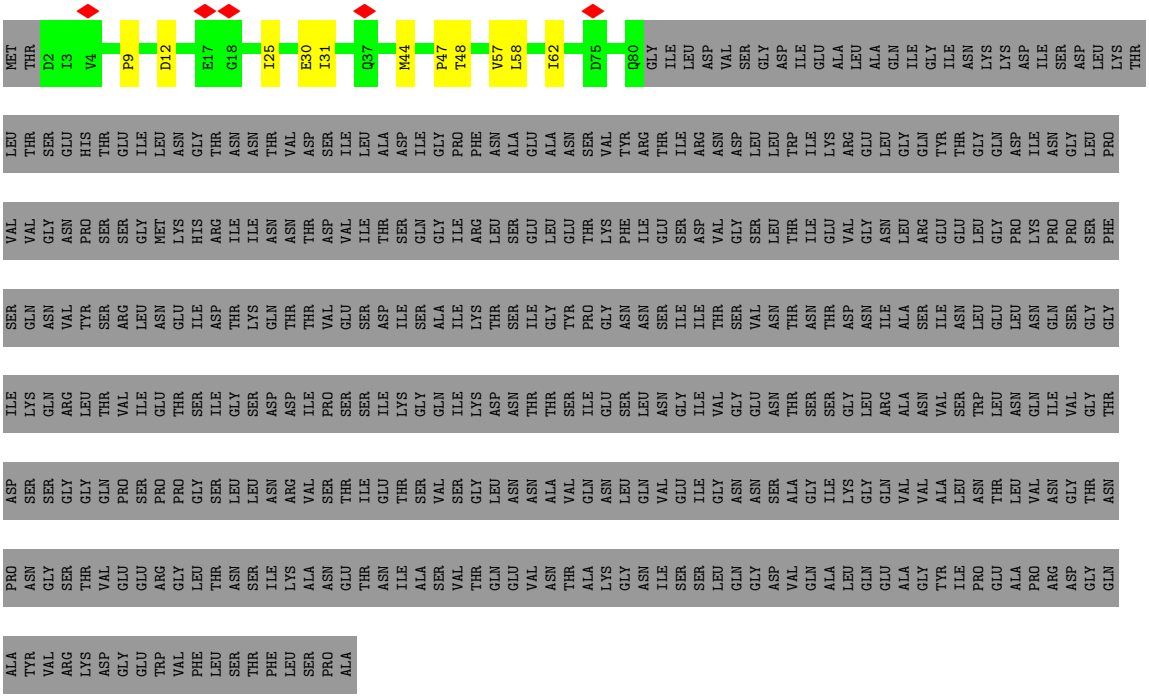




• Molecule 4: gpwac, fibritin

Chain P:



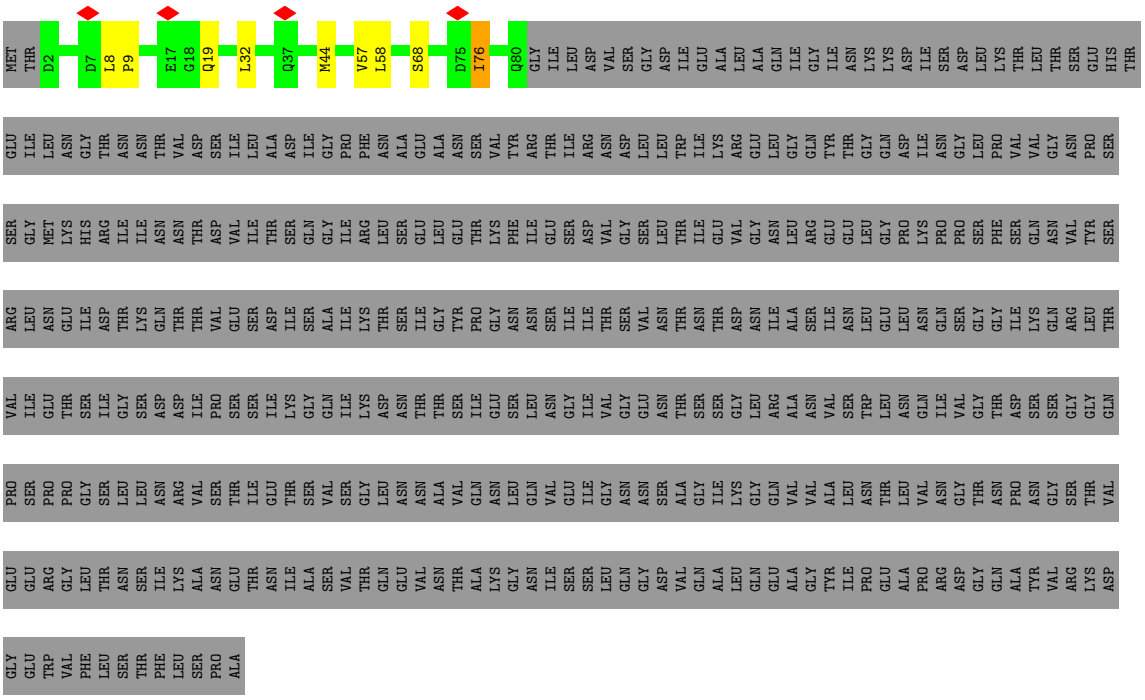

MET THR D2 I3 V4 P9 D12 E17 G18 S23 K26 N27 G28 E29 E30 T36 Q37 M44 P47 T48 L52 V57 L58 D59 I62 D75 Q80 GLY ILE LEU ASP VAL SER GLY ASP ILE LEU ALA LEU GLN ILE GLY ASP ILE GLU ILE LYS ARG GLU LEU GLY GLN ILE GLU ASN LYS LYS
ASP ILE SER ASP LEU LYS THR LEU THR SER GLU HIS THR GLU ILE LEU ASN GLY THR ASN ASN THR VAL ASP SER ILE LEU ALA ASP ILE GLY PRO PHE ASN ALA GLU ALA ASN SER VAL TYR ARG THR ILE ARG ASN ASP LEU LEU TRP ILE LYS ARG GLU LEU GLY GLN TYR THR GLY
GLN ASP ILE ASN GLY LEU PRO VAL VAL GLY ASN PRO SER SER GLY MET LYS HIS ARG ILE ILE ASN ASN THR ASP SER VAL GLY SER LEU THR ILE GLU VAL GLY ASN LEU ARG GLU LEU GLY PRO LYS PRO PRO SER PHE SER
GLY PRO LYS PRO PRO SER PHE SER GLN ASN VAL TYR SER ARG LEU ASN GLU ASP THR LYS GLN THR SER ILE GLY TYR PRO GLY ASN ASN SER ILE ILE THR SER VAL ASN THR ASN THR ASP ASN ILE ALA SER ILE GLN ASN ILE LYS GLN ASP ILE PRO SER SER ILE LYS GLY SER ASP ILE PRO SER SER LEU ASN GLY ILE VAL GLY GLU ASN THR SER ILE GLU GLY TYR PRO GLY ASN ASN SER ILE ILE THR SER VAL ASN THR ASN THR ASP ASN ILE ALA SER ILE GLN ASN ILE LYS GLN




• Molecule 4: gpwac, fibritin

Chain S:

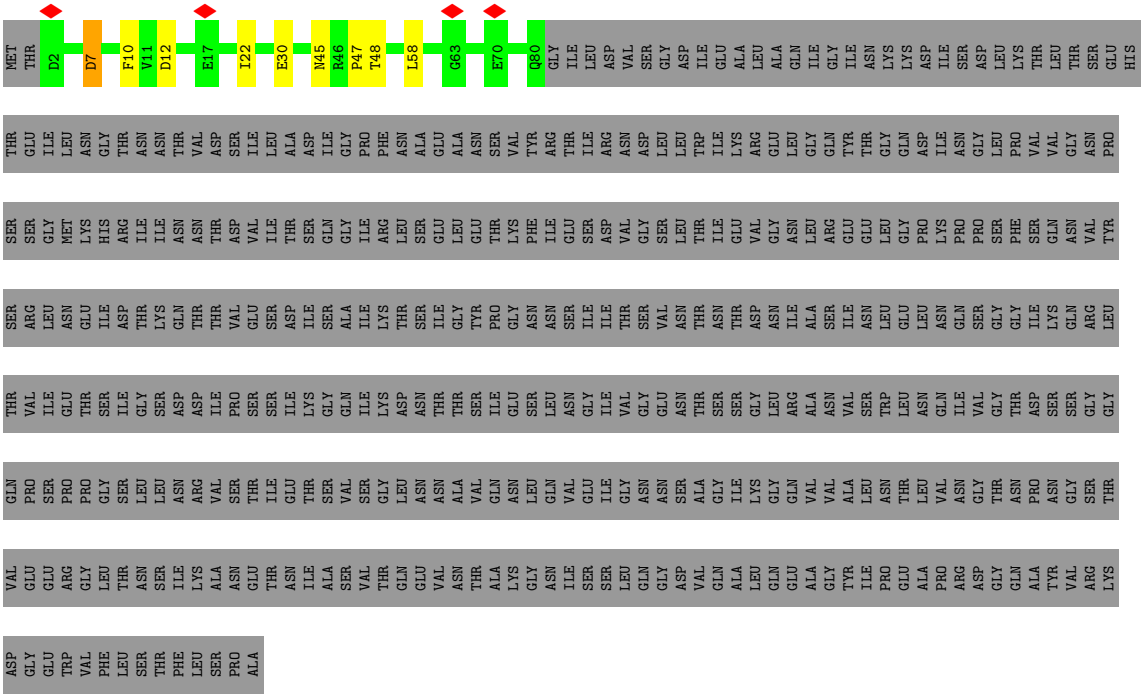



• Molecule 4: gpwac, fibritin

Chain T:

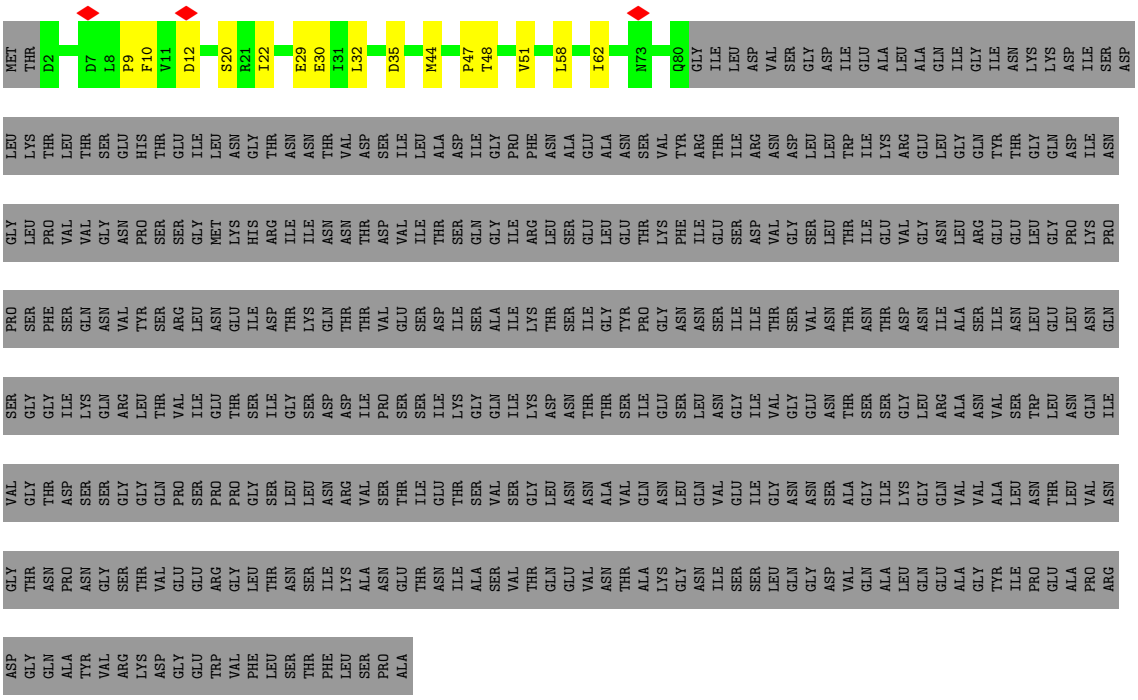





• Molecule 4: gpwac, fibritin

Chain U:

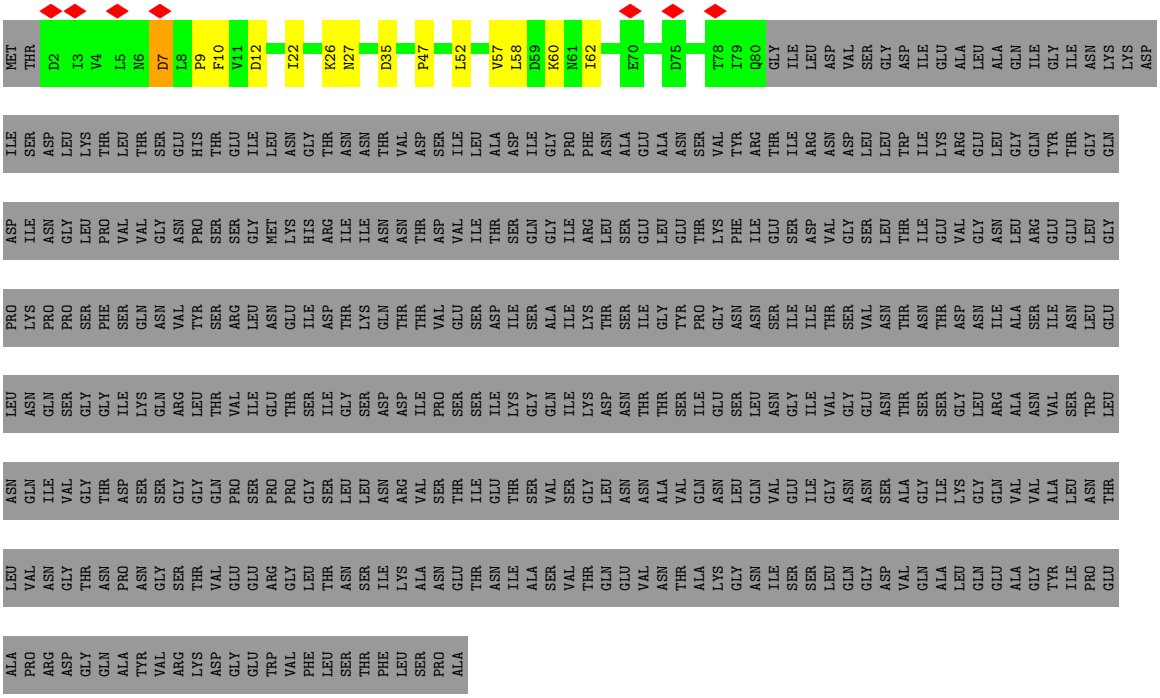



• Molecule 4: gpwac, fibritin

Chain V:

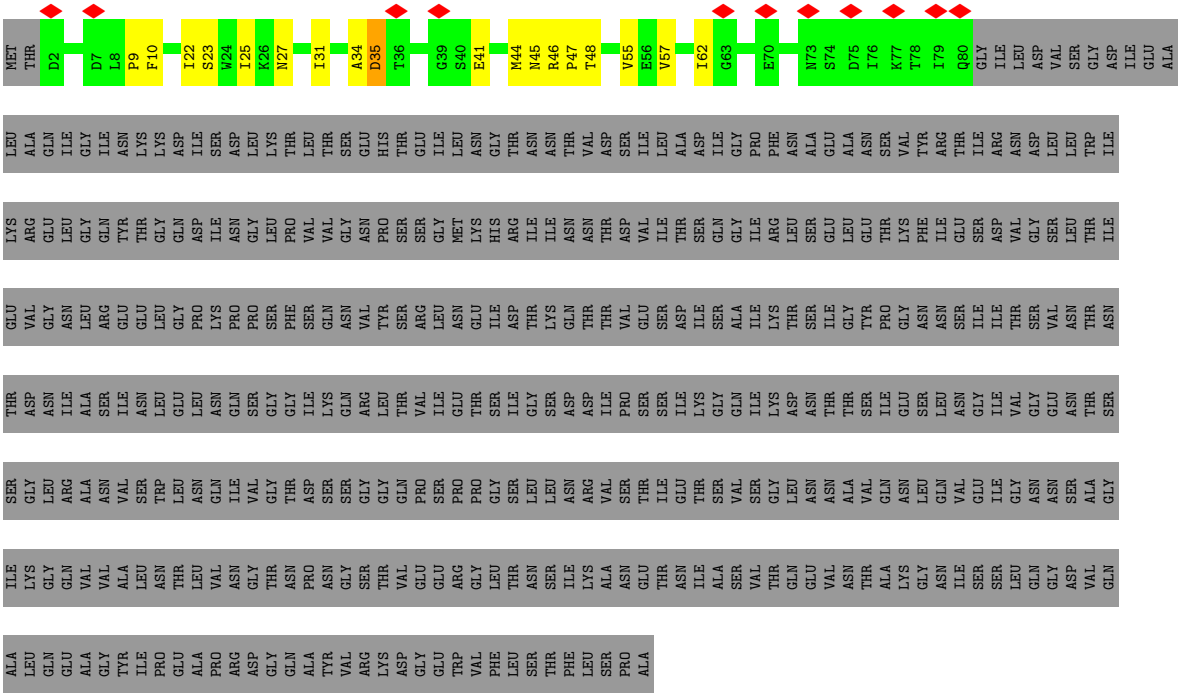





• Molecule 4: gpwac, fibritin

Chain W:

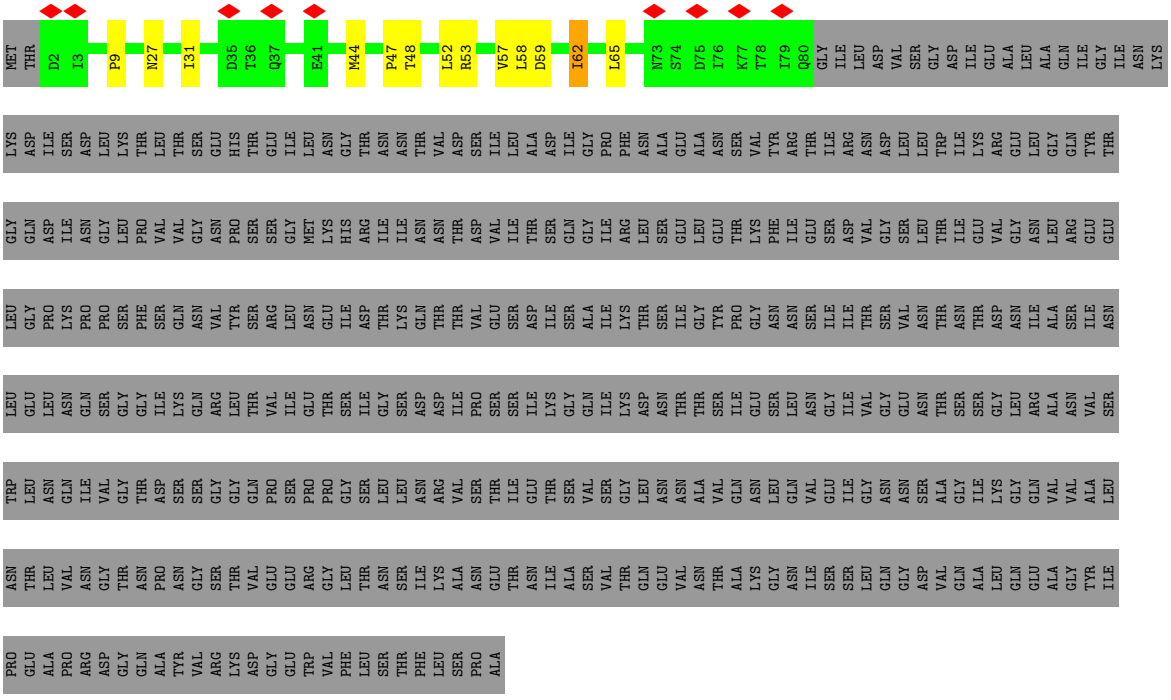



• Molecule 4: gpwac, fibritin

Chain X:

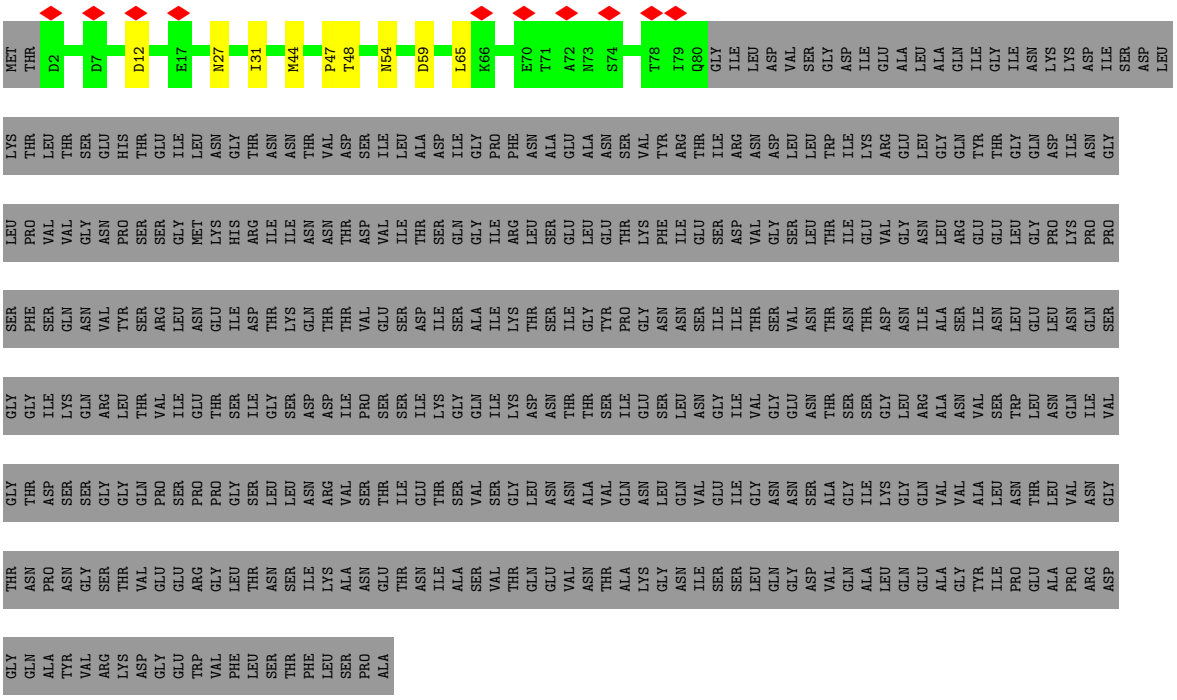





• Molecule 4: gpwac, fibritin

Chain Y:

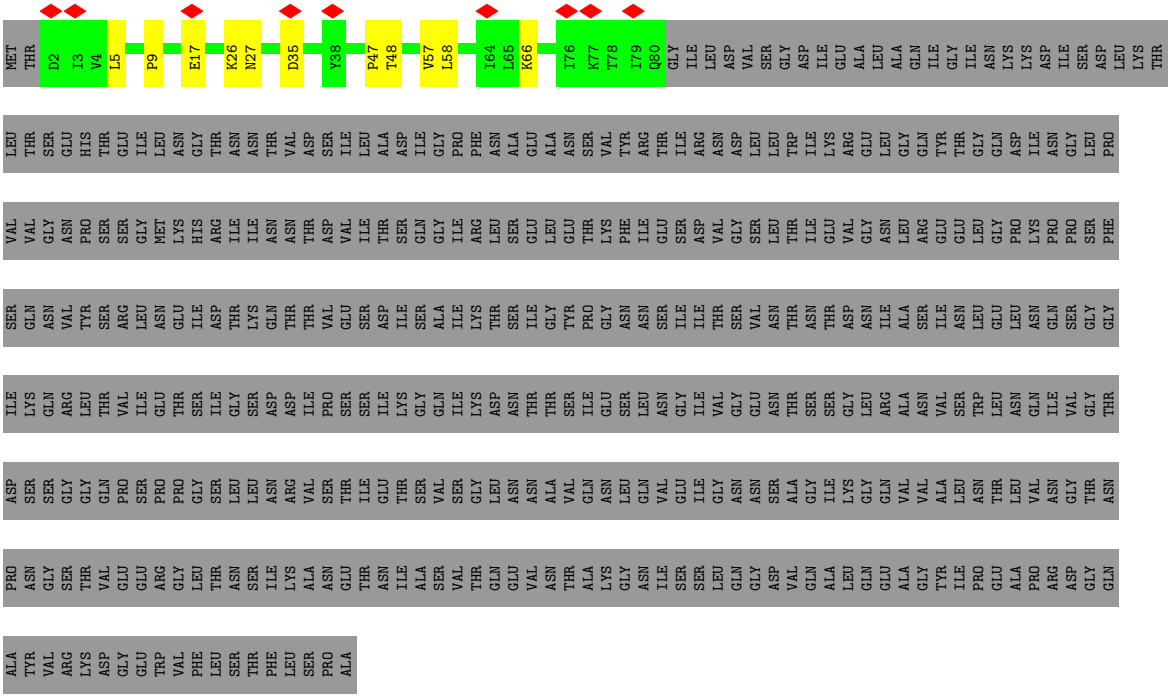



• Molecule 4: gpwac, fibritin

Chain Z:

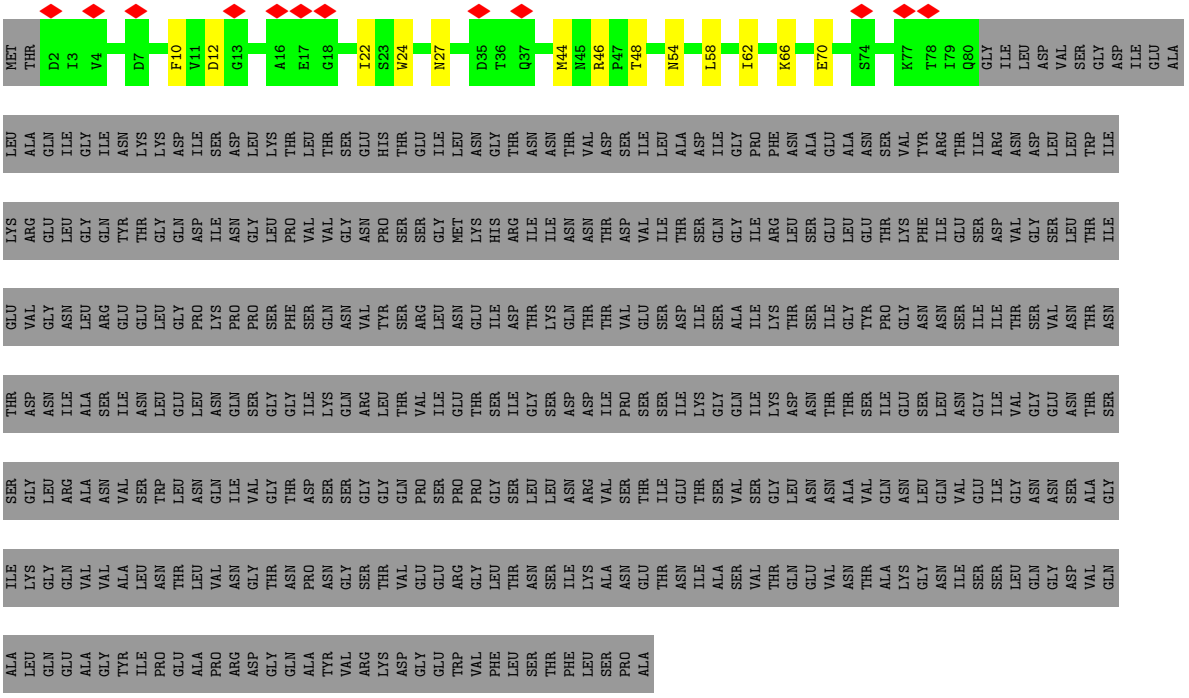





• Molecule 4: gpwac, fibritin

Chain a:

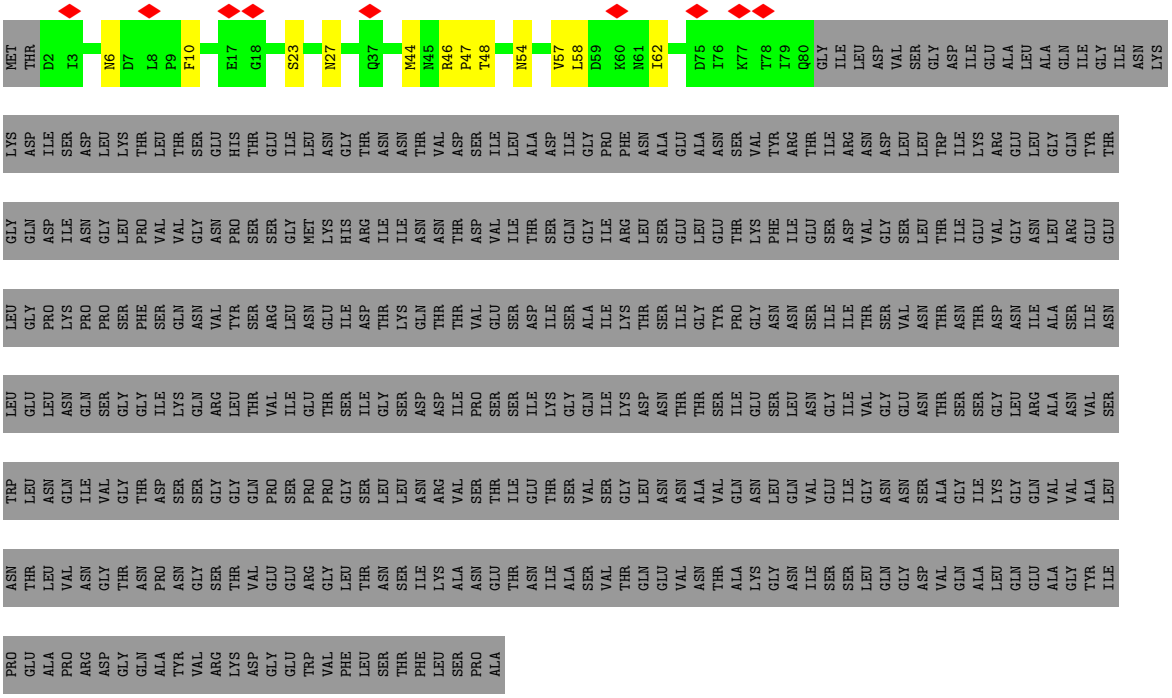



• Molecule 4: gpwac, fibritin

Chain b:

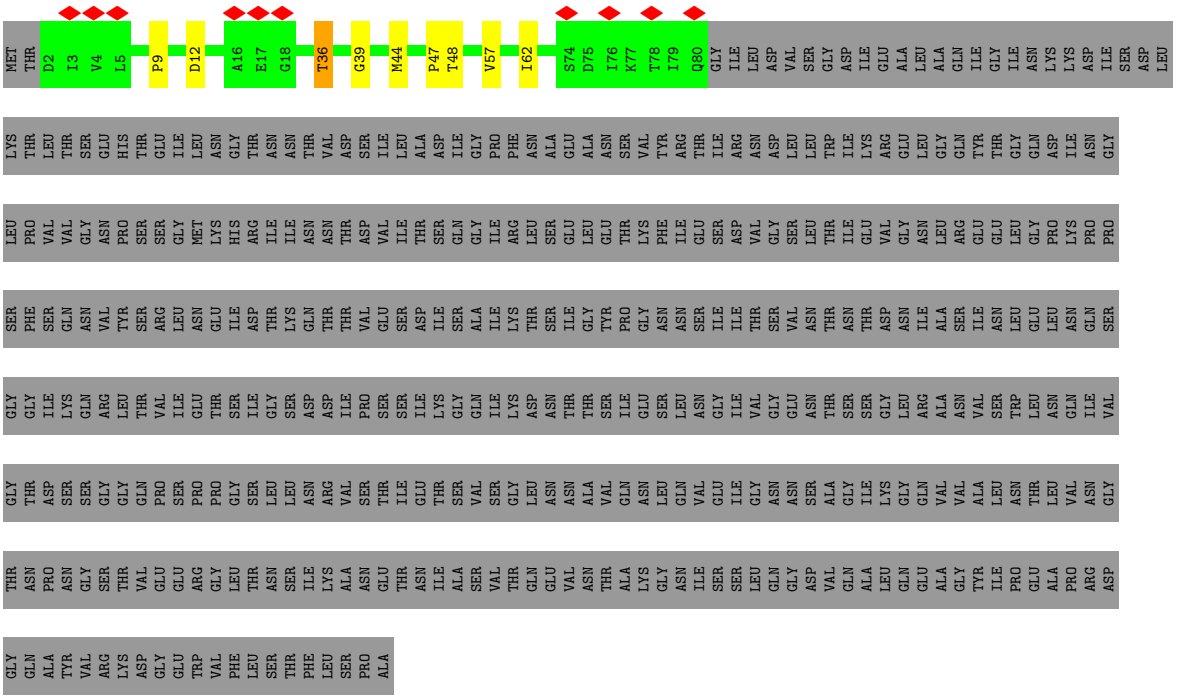





• Molecule 4: gpwac, fibritin

Chain c:

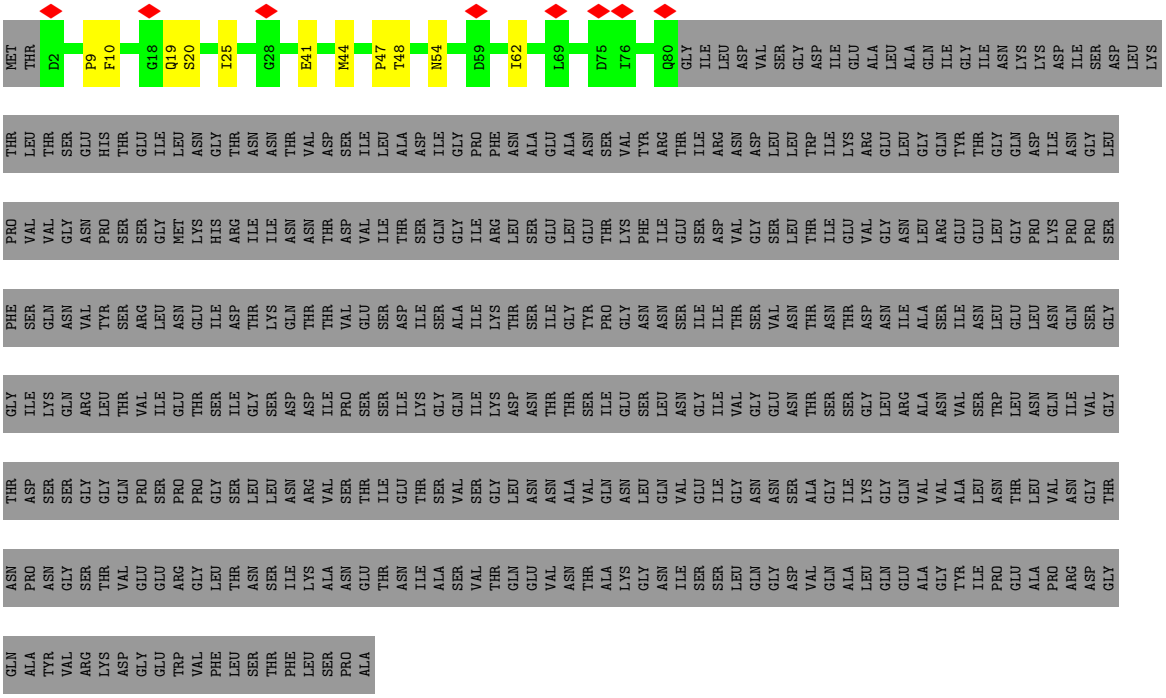



• Molecule 4: gpwac, fibritin

Chain d:

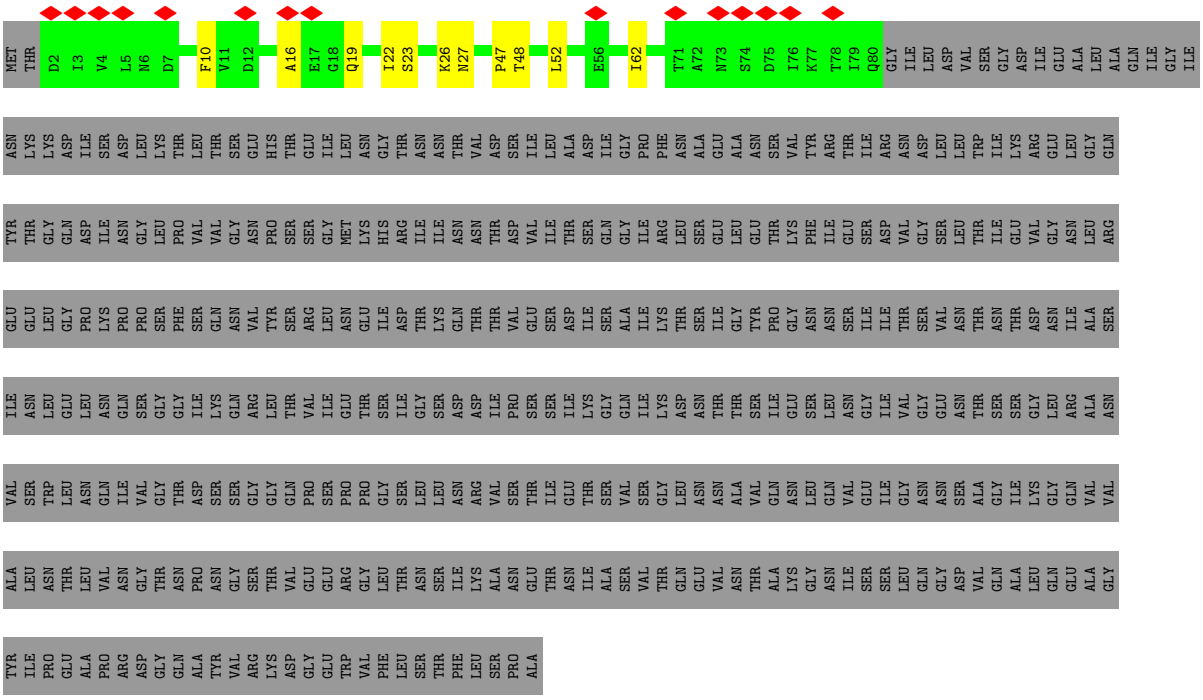





• Molecule 4: gpwac, fibritin

Chain e:

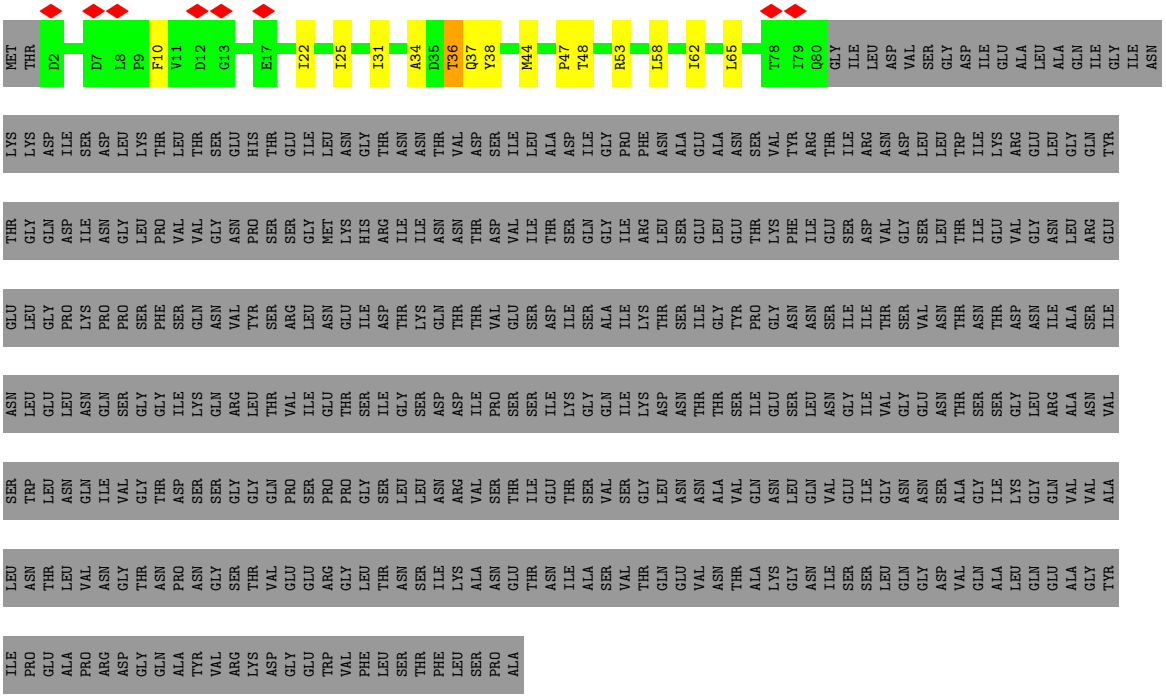



• Molecule 4: gpwac, fibritin

Chain f:

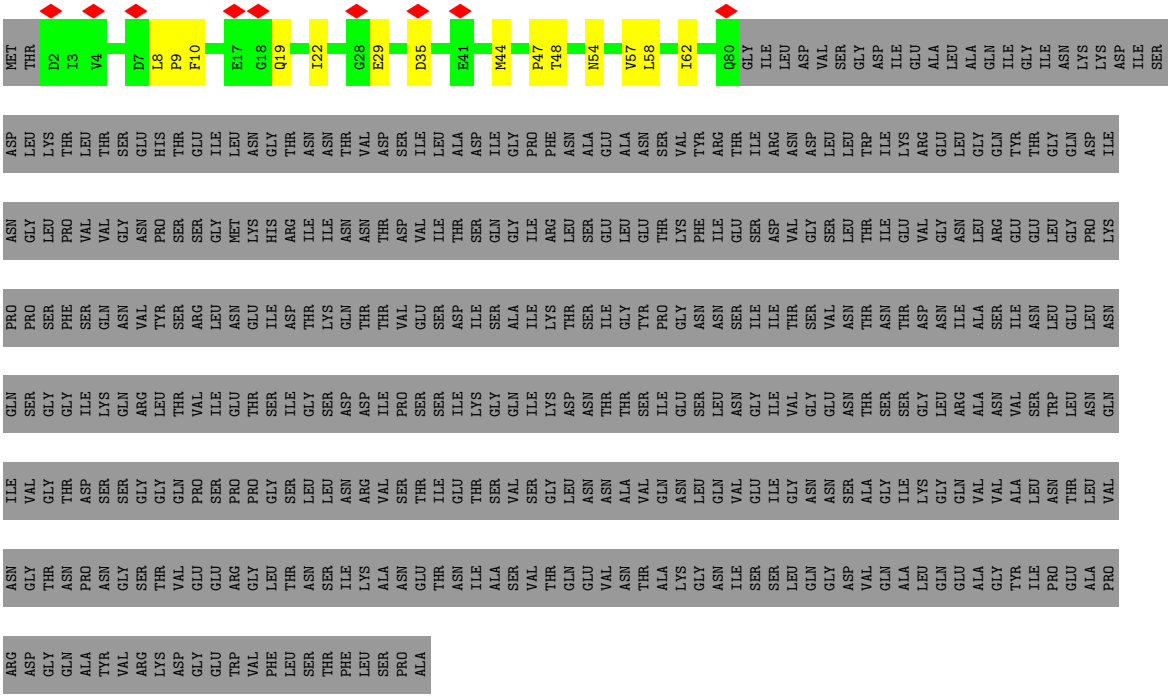





• Molecule 4: gpwac, fibritin

Chain g:

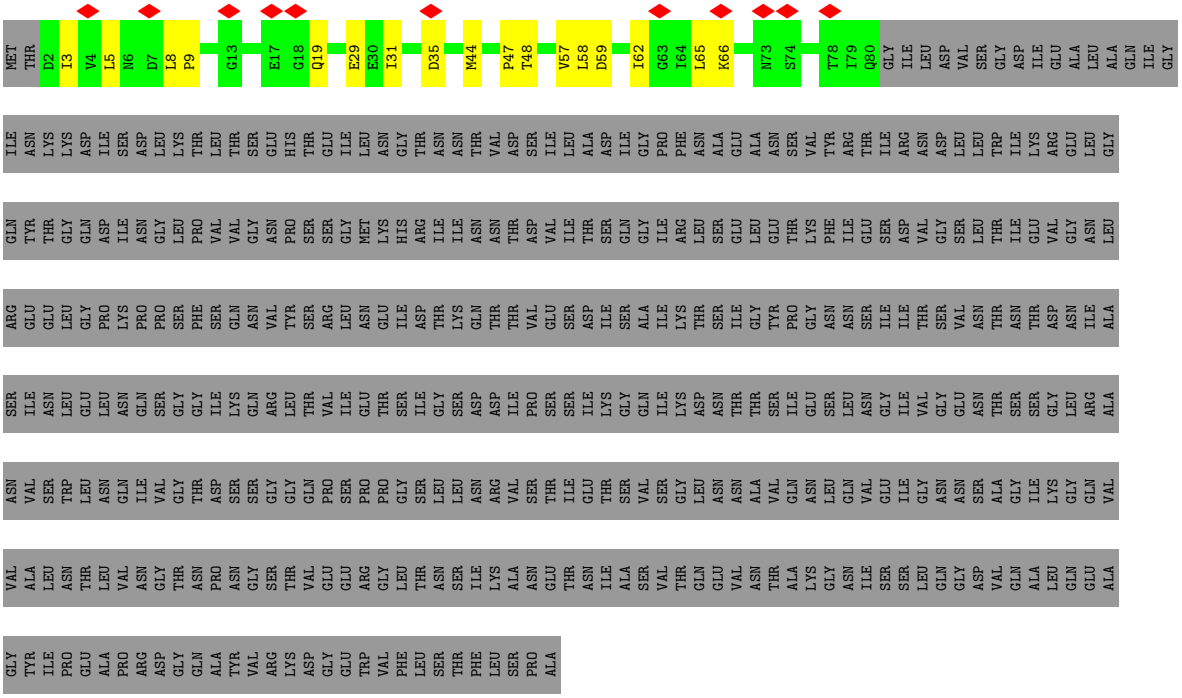



• Molecule 4: gpwac, fibritin

Chain h:

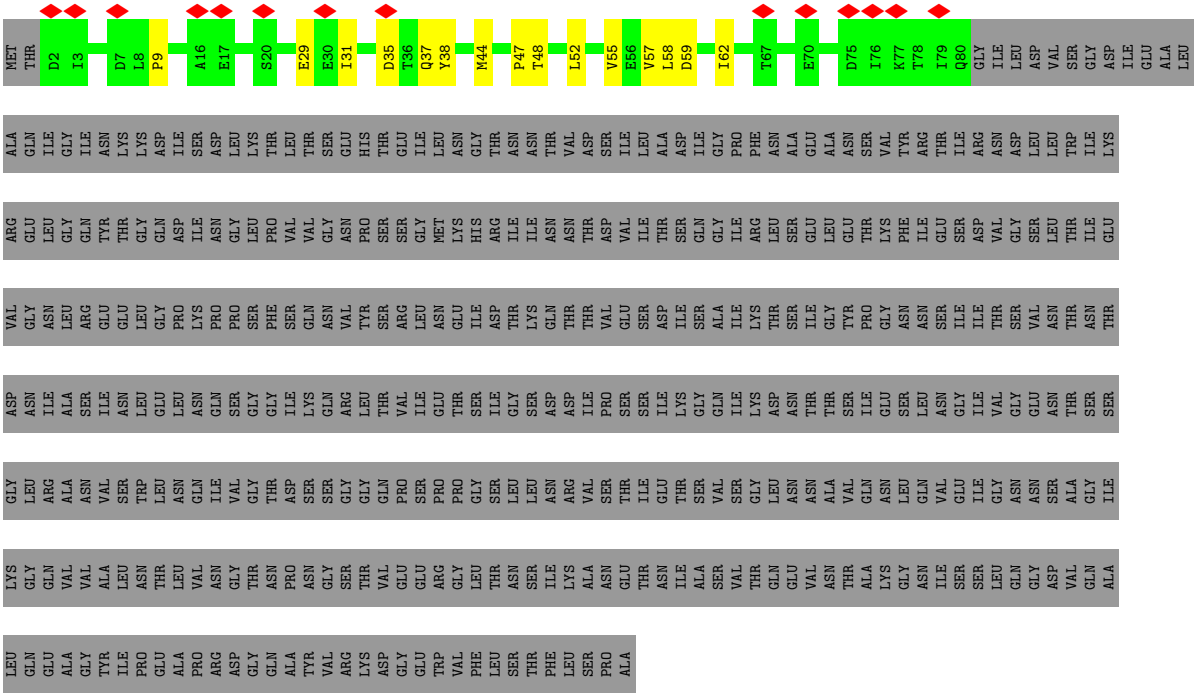





• Molecule 4: gpwac, fibritin

Chain i:

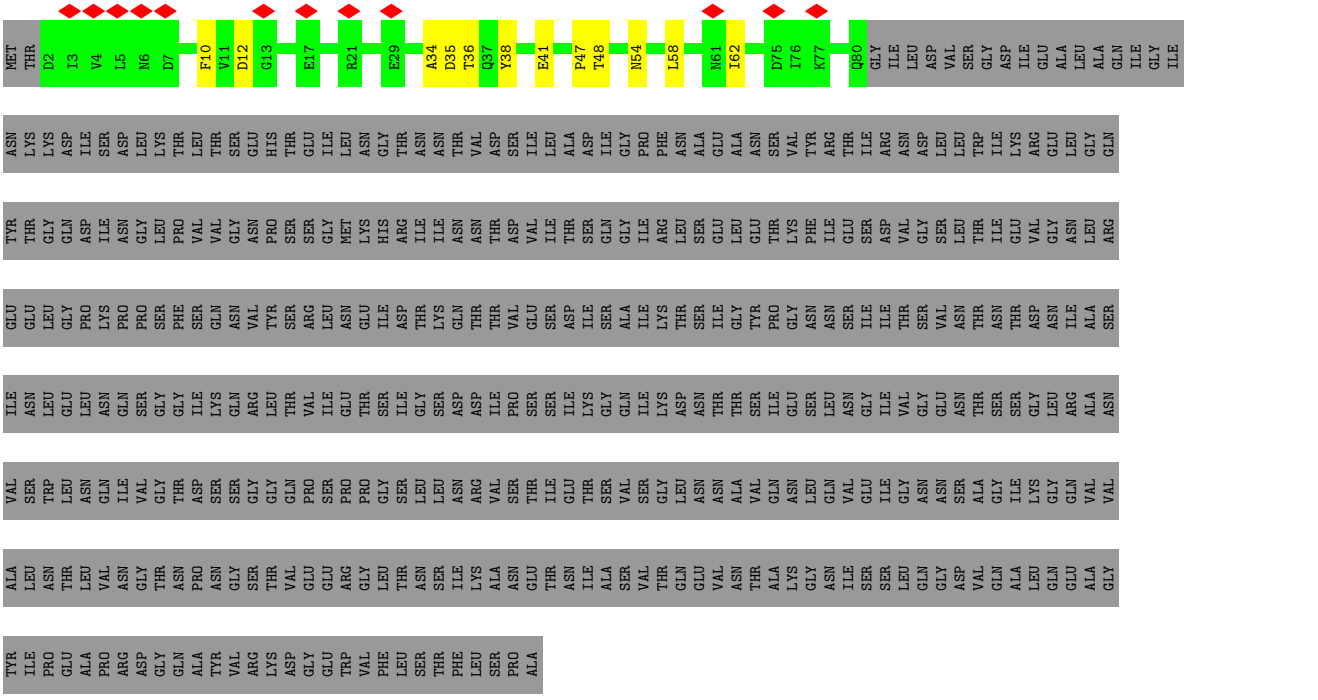



• Molecule 4: gpwac, fibritin

Chain j:

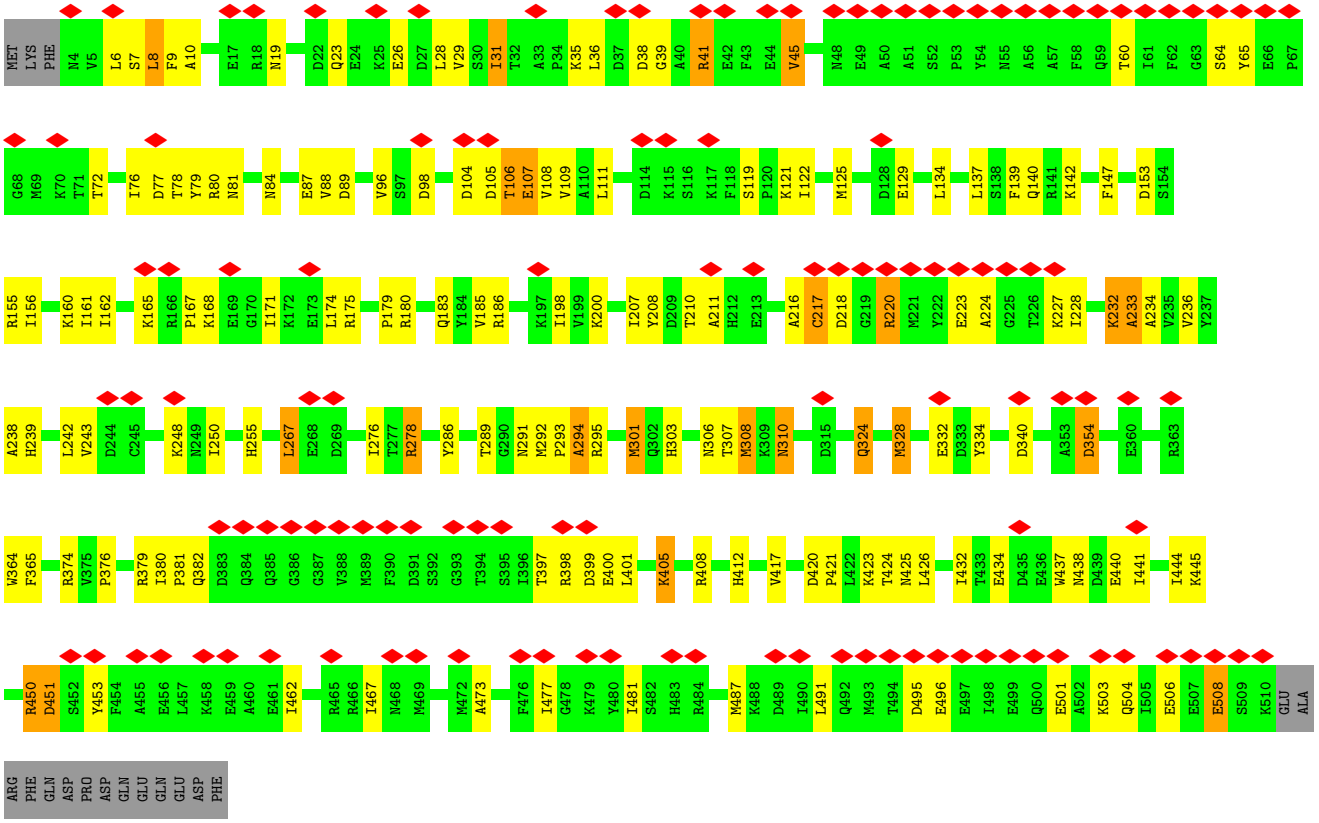




• Molecule 5: gp20, portal protein

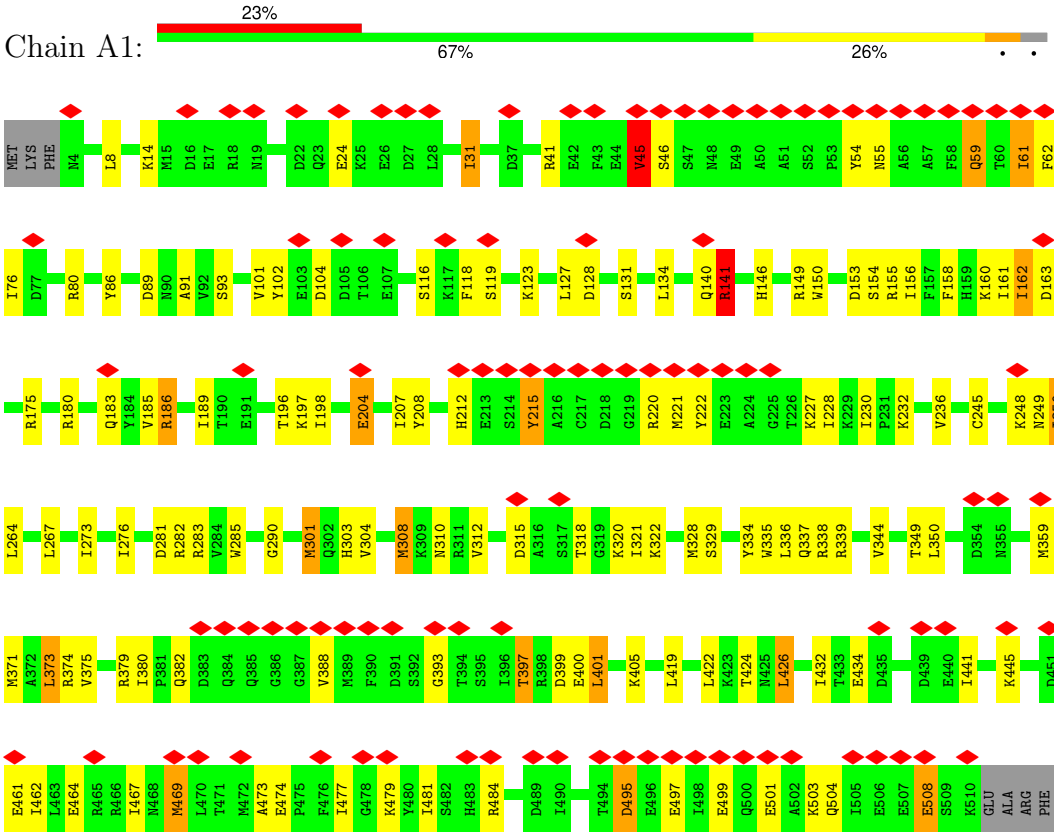
Chain A0:



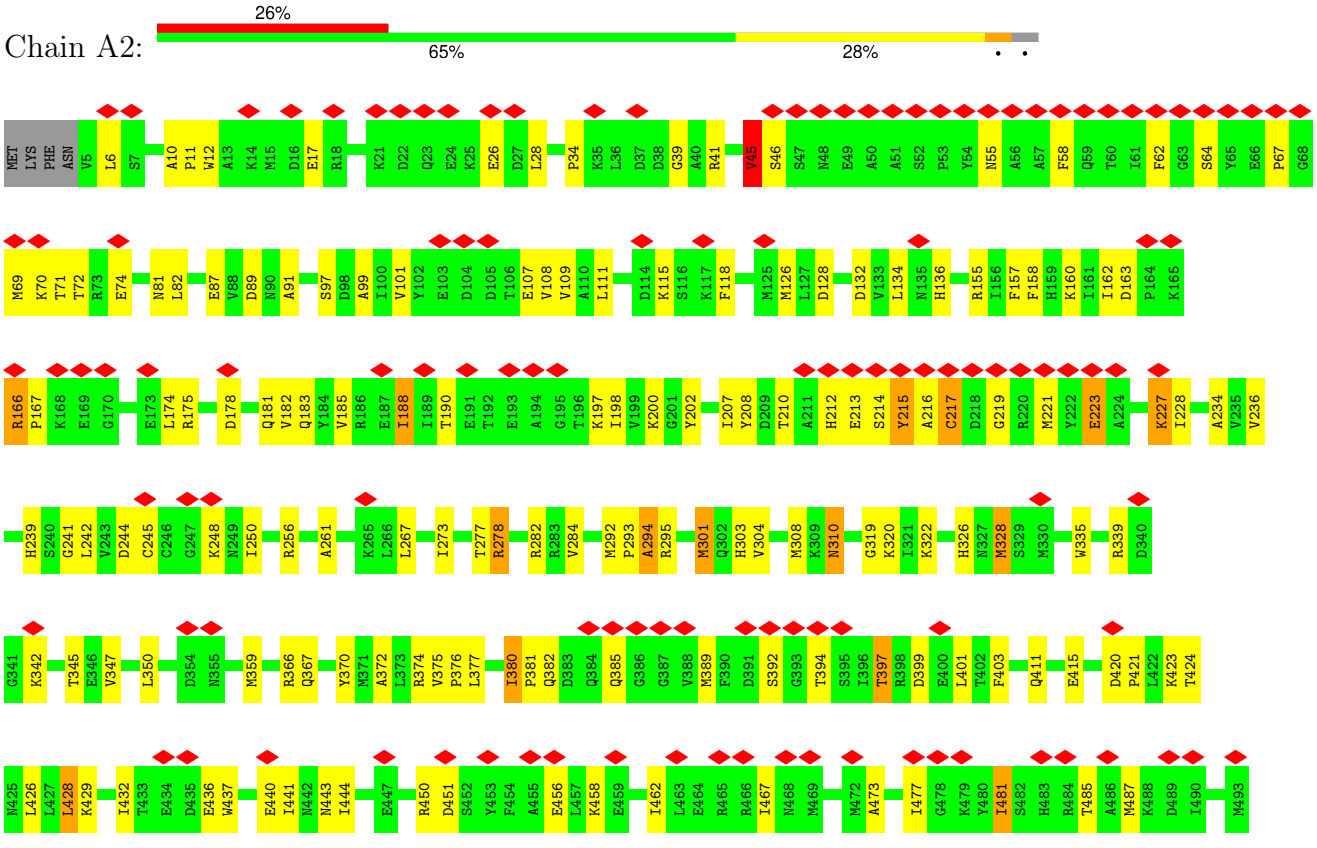
• Molecule 5: gp20, portal protein

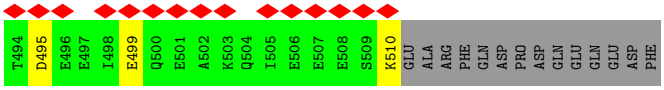
Chain A1:




• Molecule 5: gp20, portal protein

Chain A2:





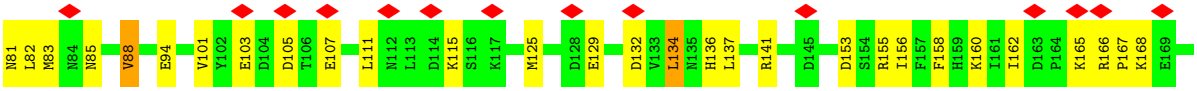

• Molecule 5: gp20, portal protein

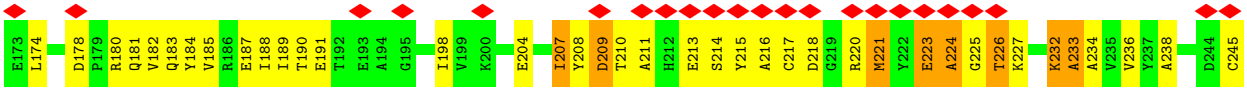
Chain A3:

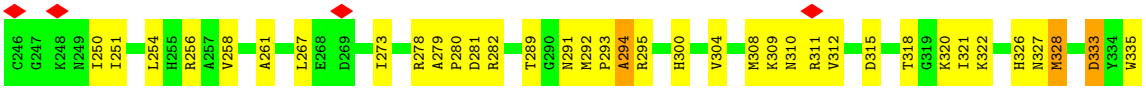


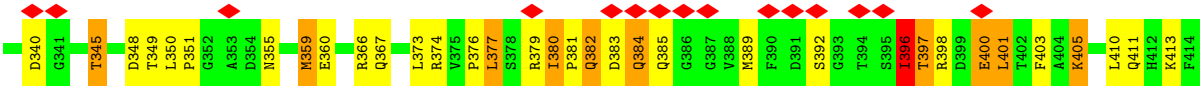


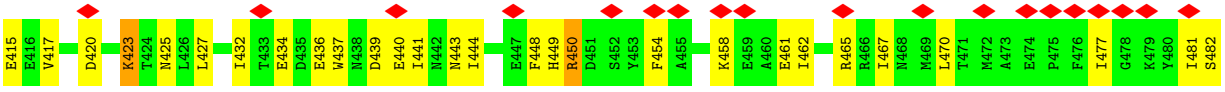


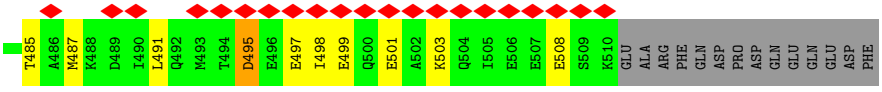


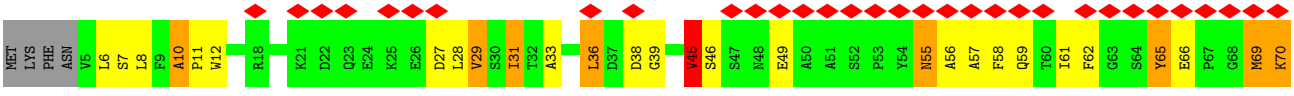



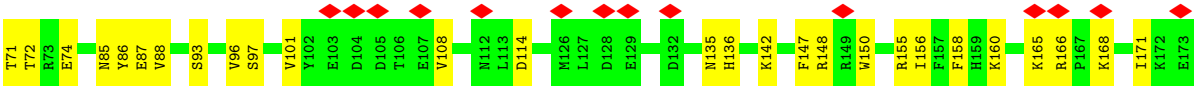




• Molecule 5: gp20, portal protein

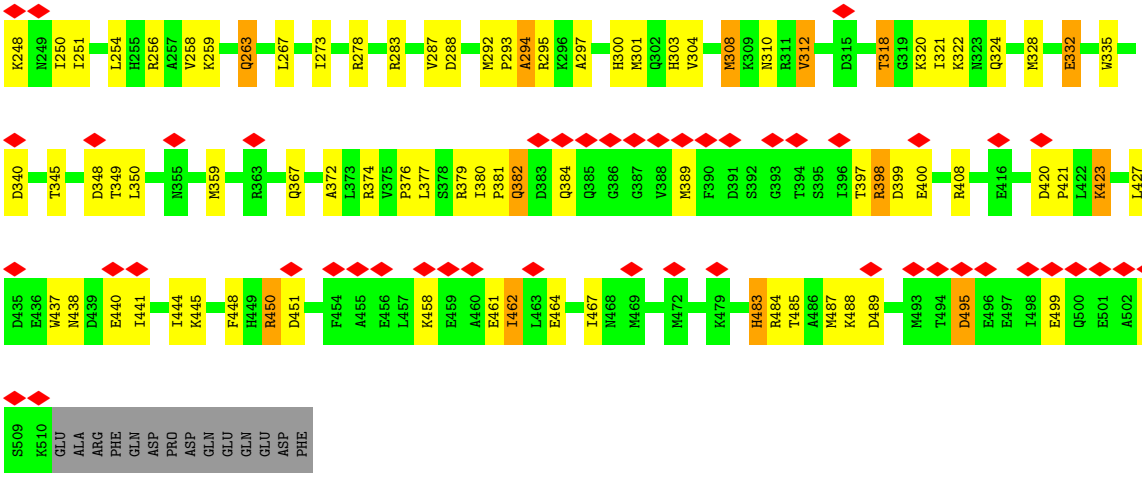
Chain Av:



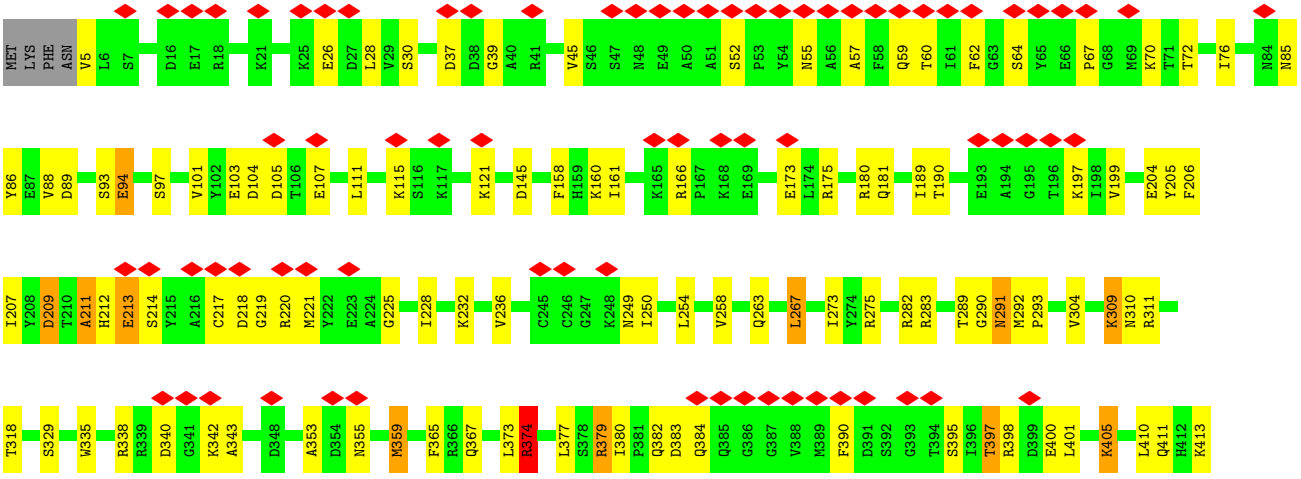



• Molecule 5: gp20, portal protein

Chain Ax:

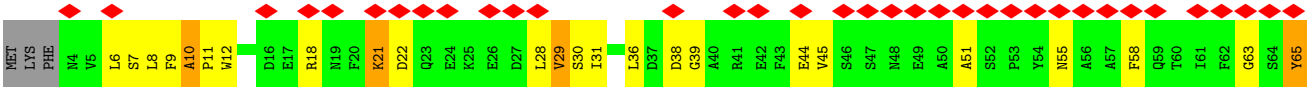


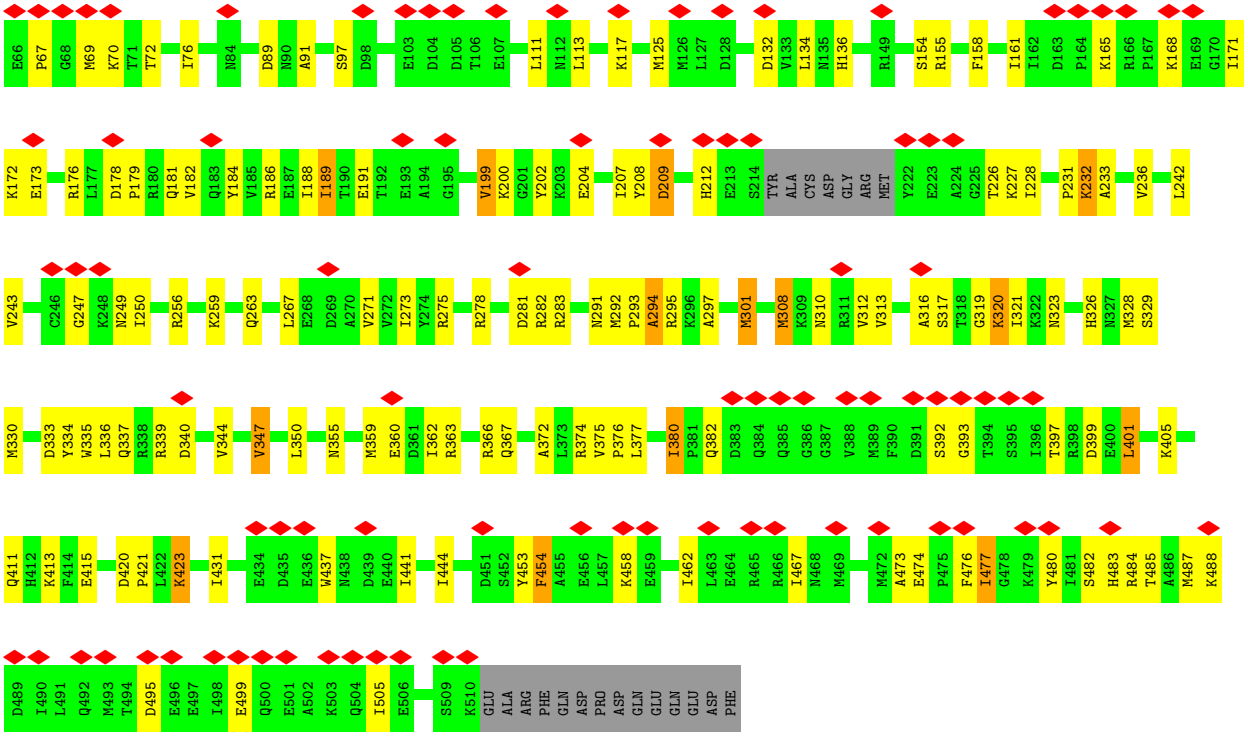




• Molecule 5: gp20, portal protein

Chain BA:



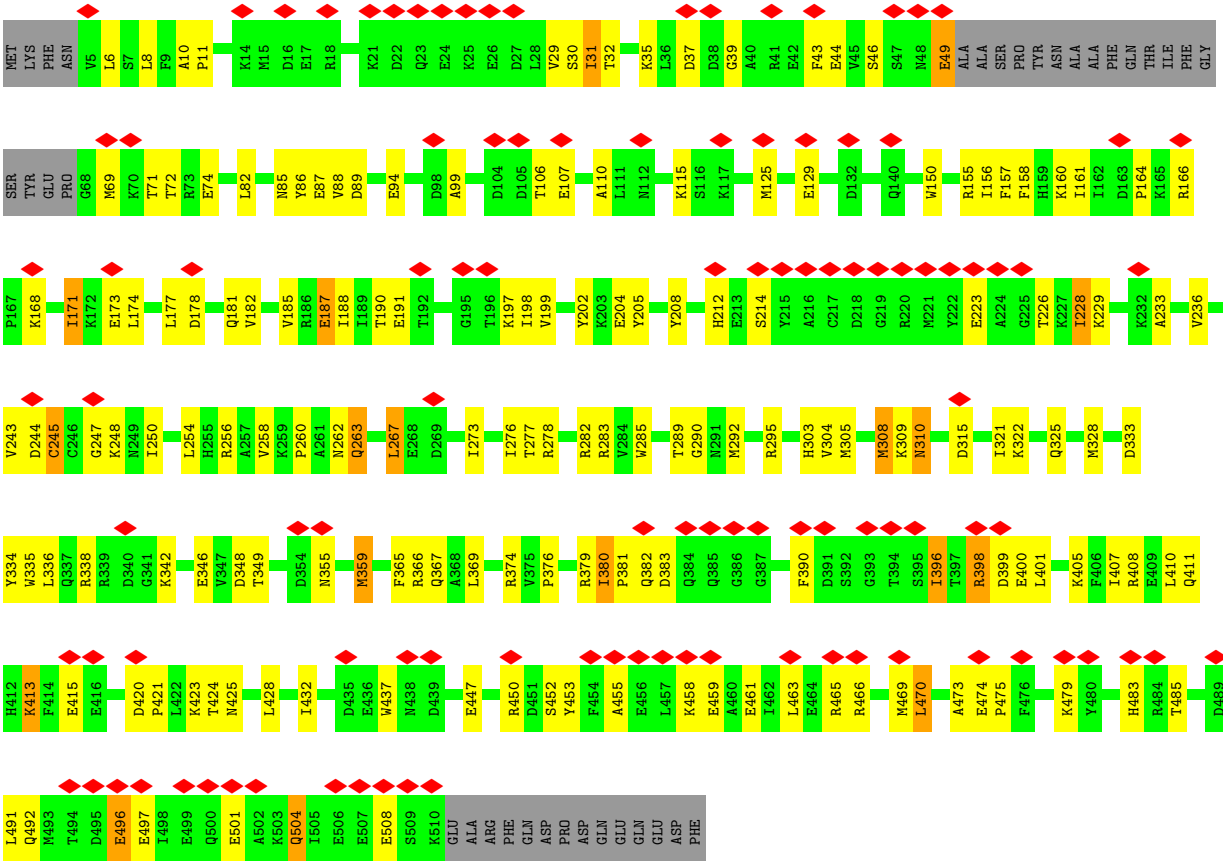





• Molecule 5: gp20, portal protein

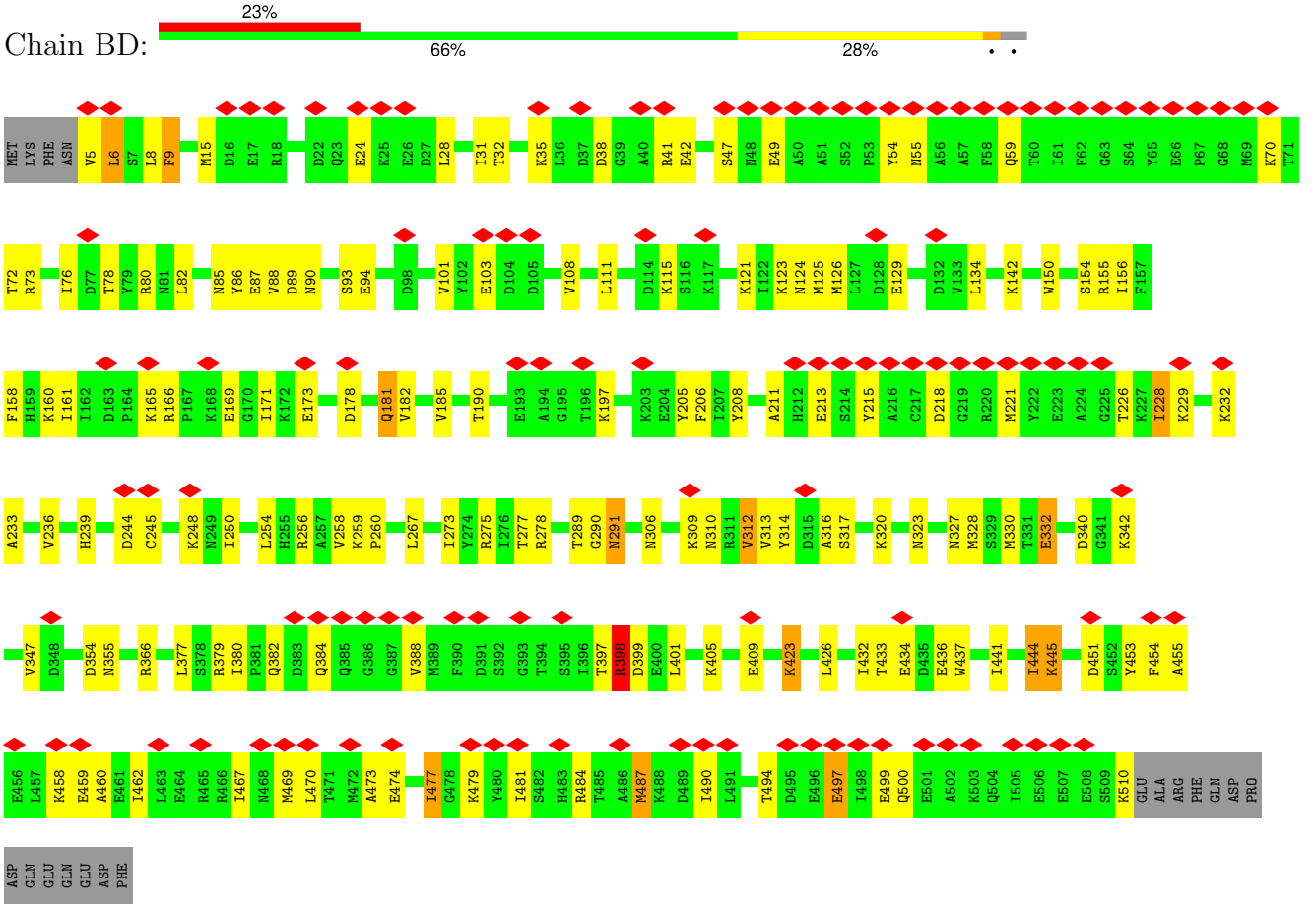
Chain BB:



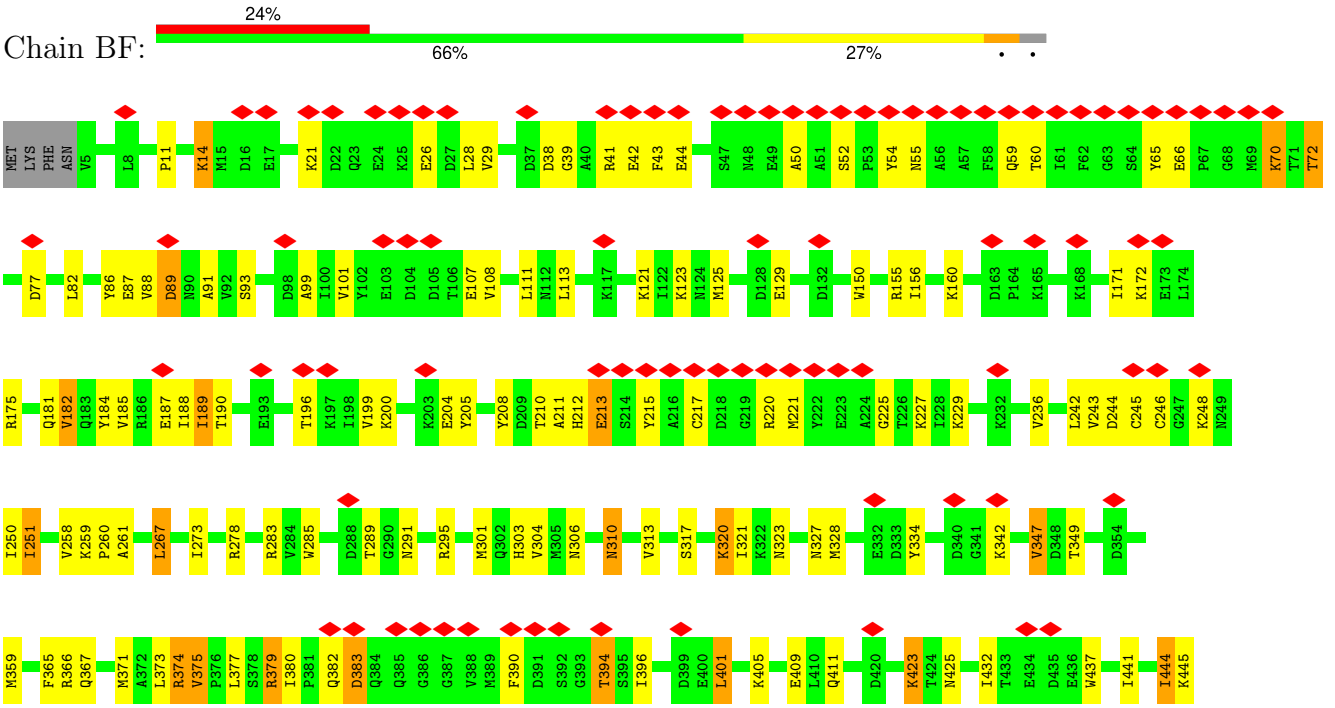
• Molecule 5: gp20, portal protein

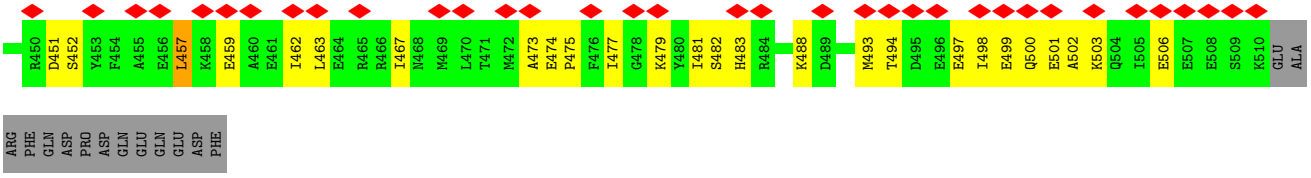
Chain BD:




• Molecule 5: gp20, portal protein

Chain BF:






• Molecule 5: gp20, portal protein

Chain BG:

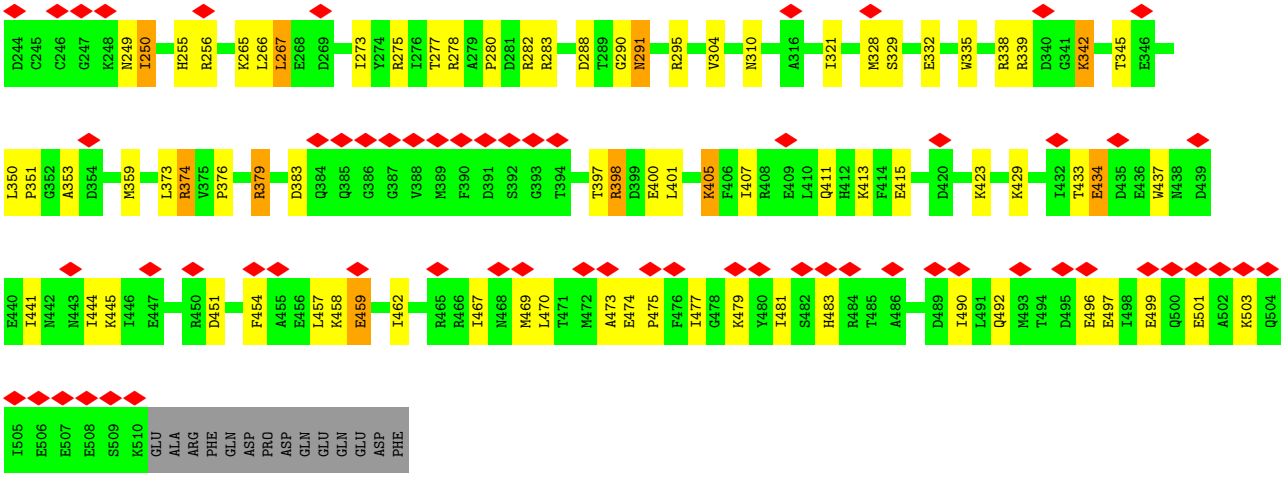






• Molecule 5: gp20, portal protein

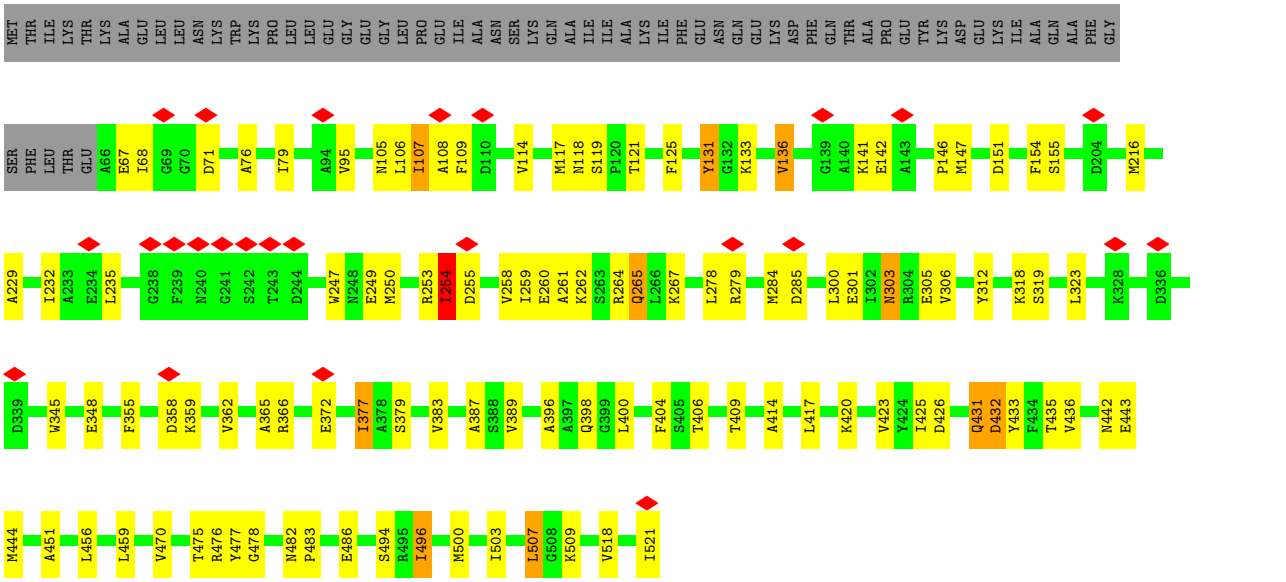
Chain BH:




• Molecule 6: gp23, major capsid protein

Chain A4:

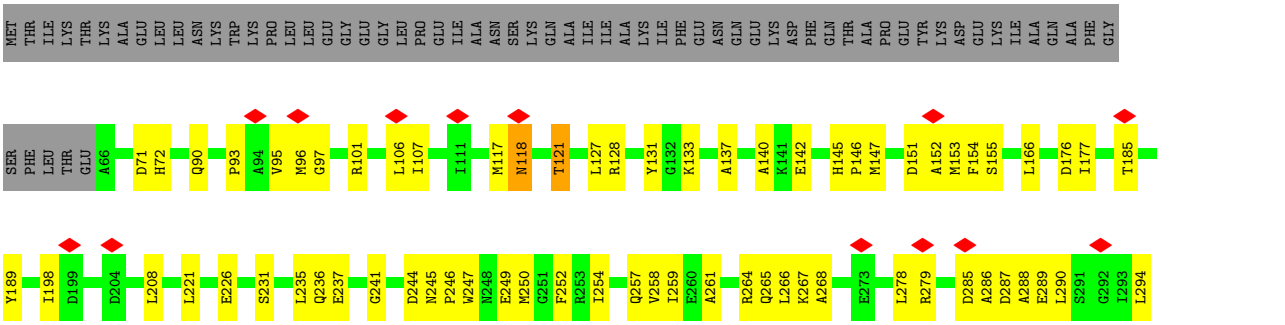


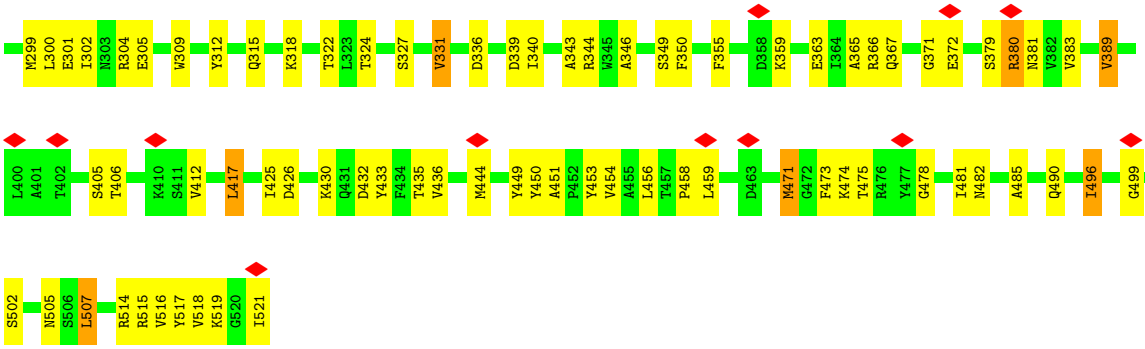




• Molecule 6: gp23, major capsid protein

Chain A5:



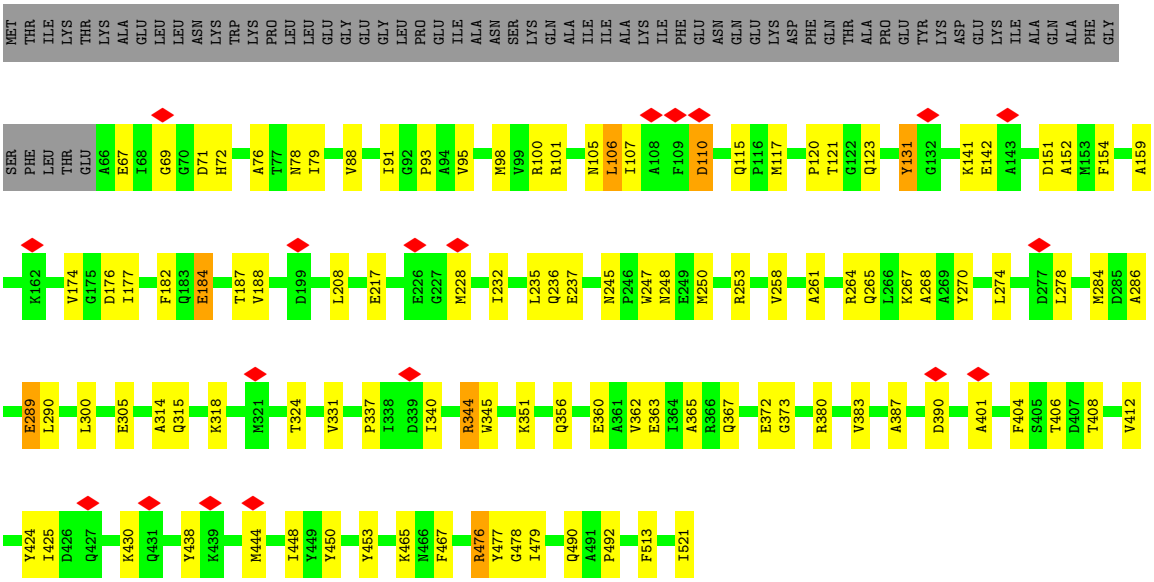






• Molecule 6: gp23, major capsid protein

Chain A7:

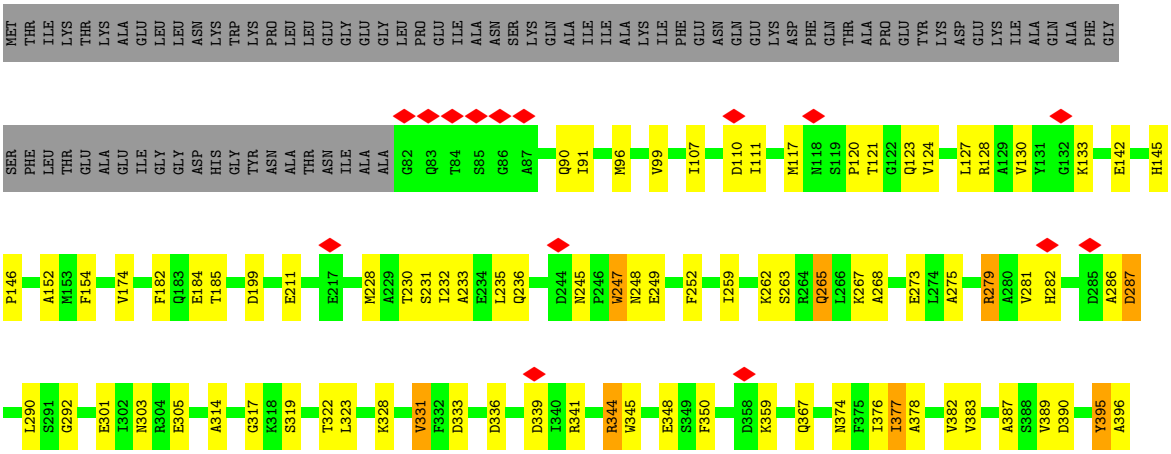


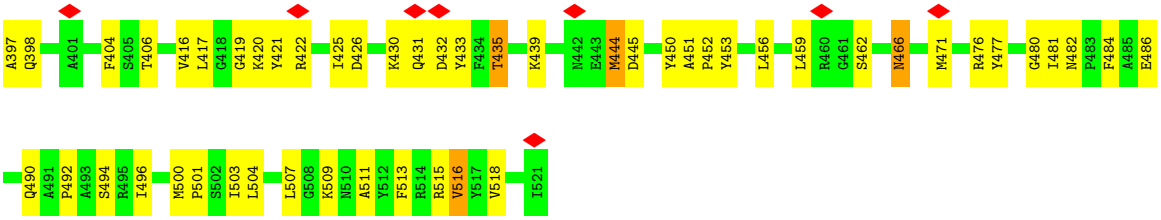




• Molecule 6: gp23, major capsid protein

Chain A8:

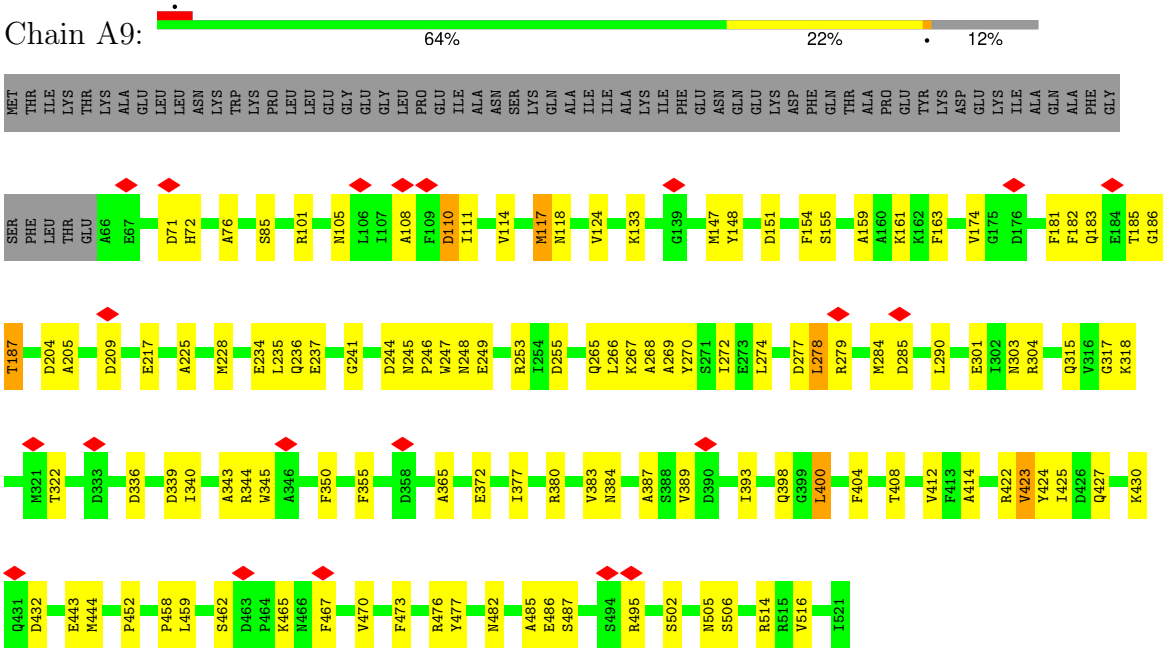




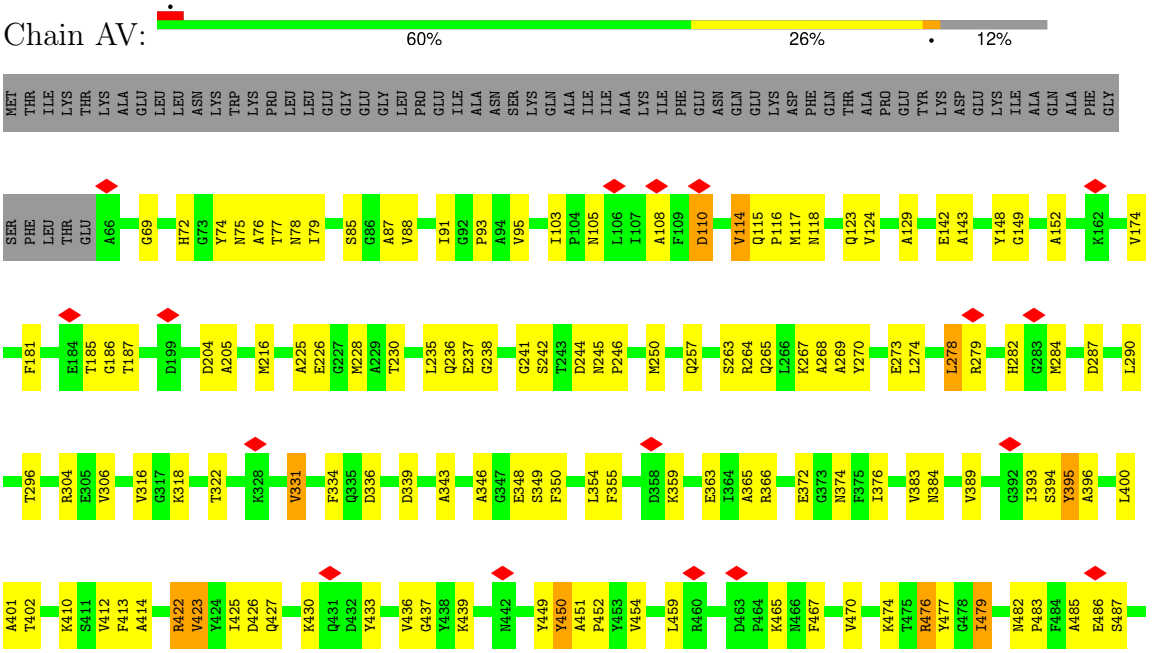

• Molecule 6: gp23, major capsid protein

Chain A9:




• Molecule 6: gp23, major capsid protein

Chain AV:

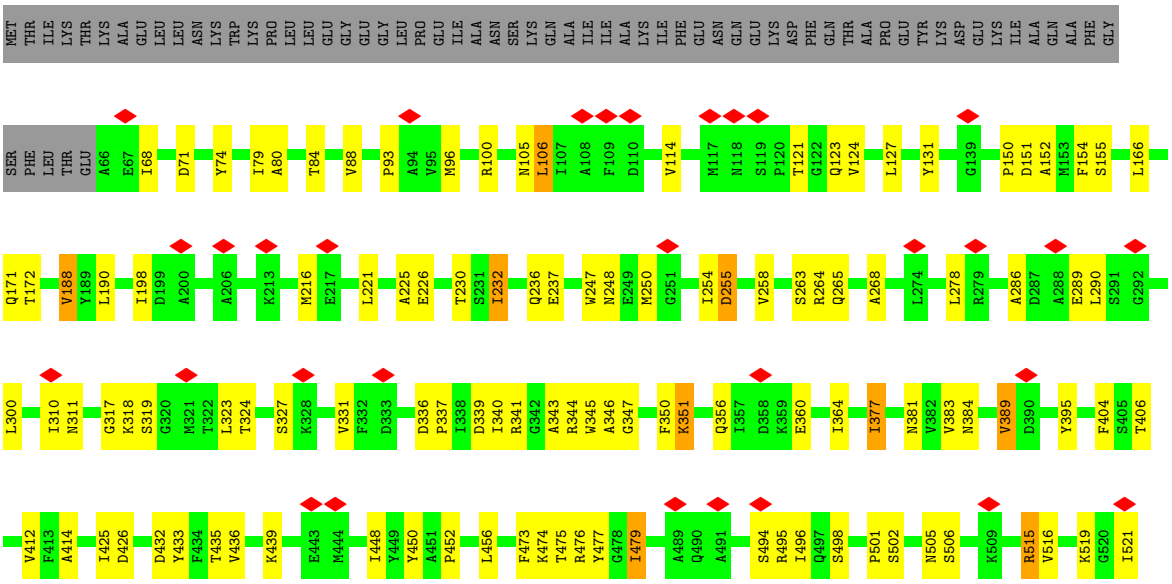





• Molecule 6: gp23, major capsid protein

Chain AW:

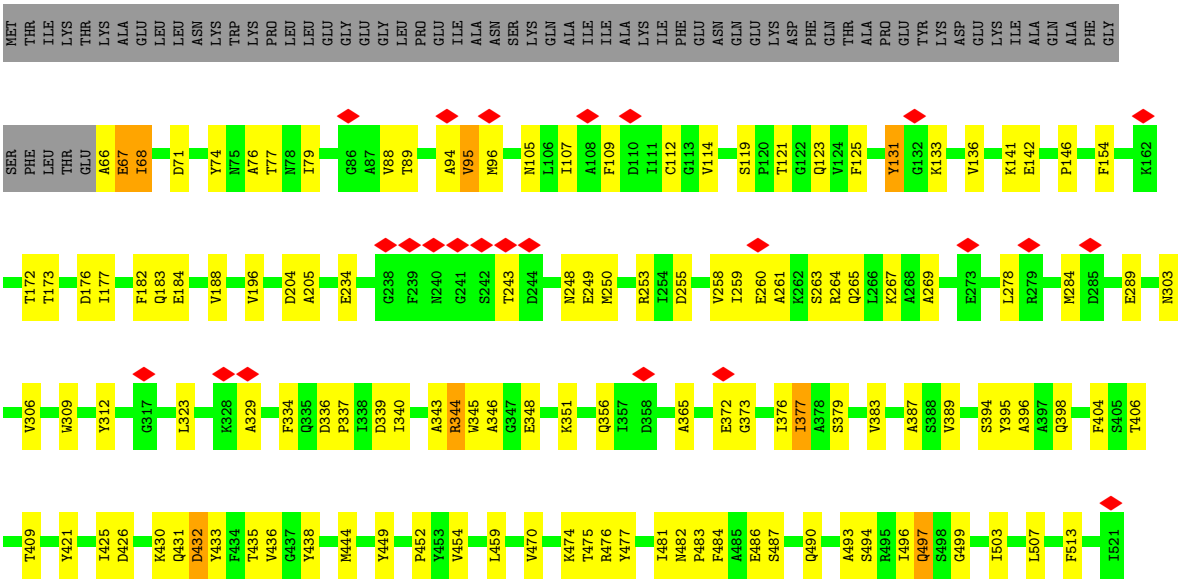



• Molecule 6: gp23, major capsid protein

Chain AX:

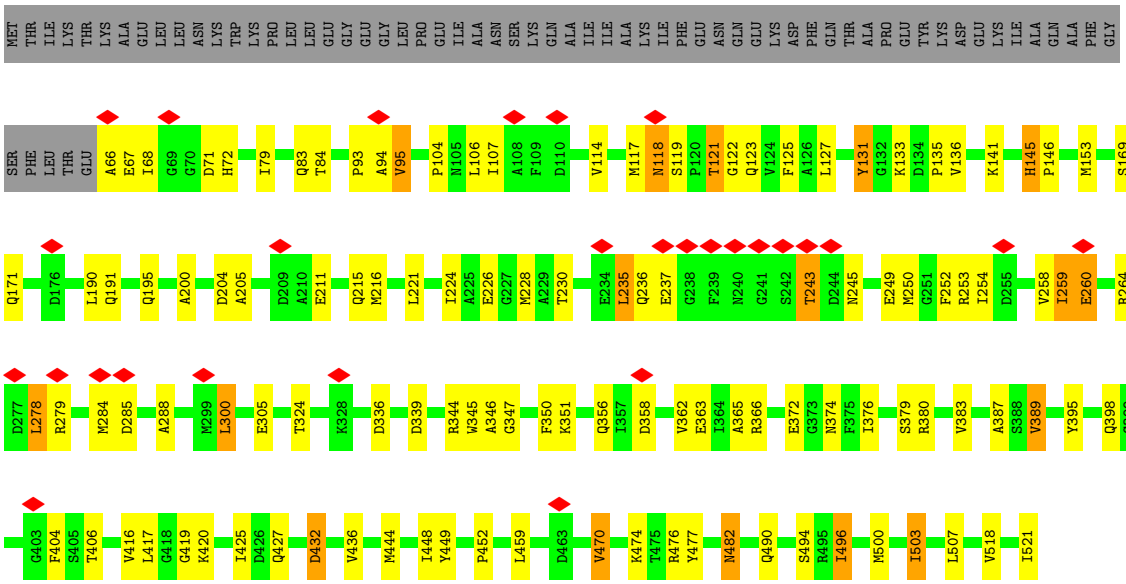



• Molecule 6: gp23, major capsid protein

Chain AZ:

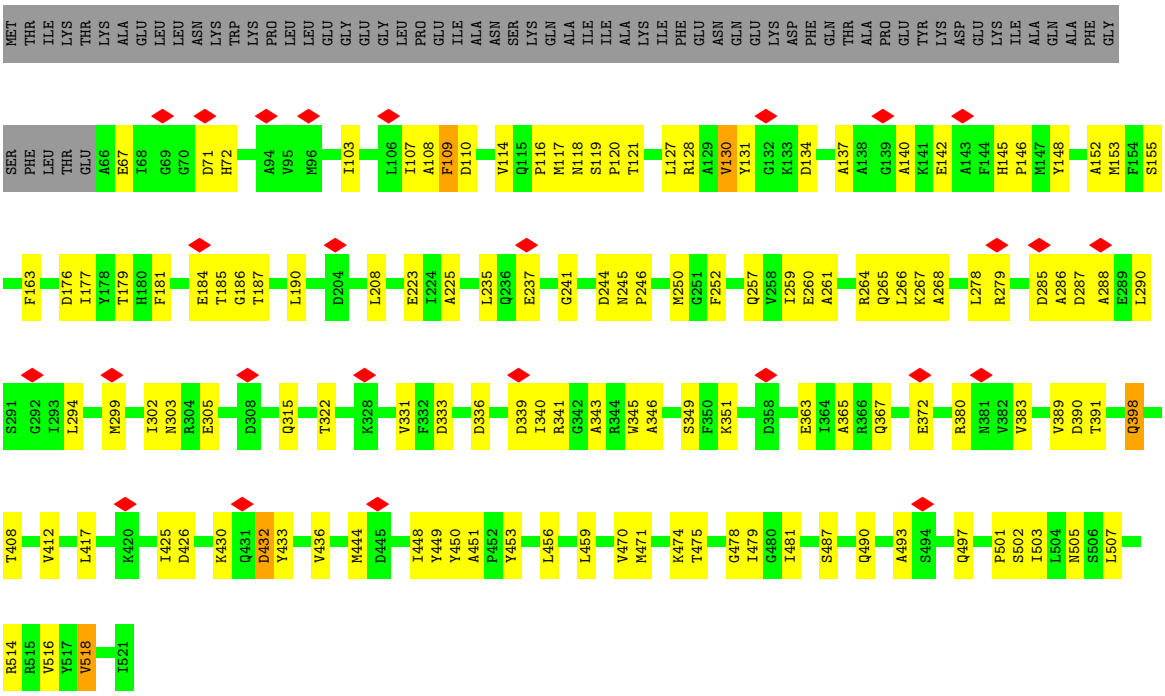




• Molecule 6: gp23, major capsid protein

Chain Ac:

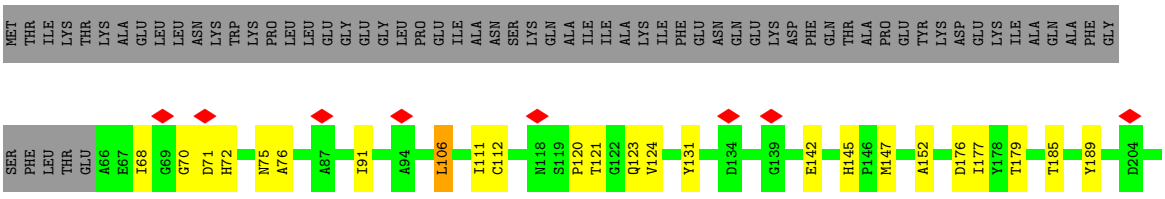


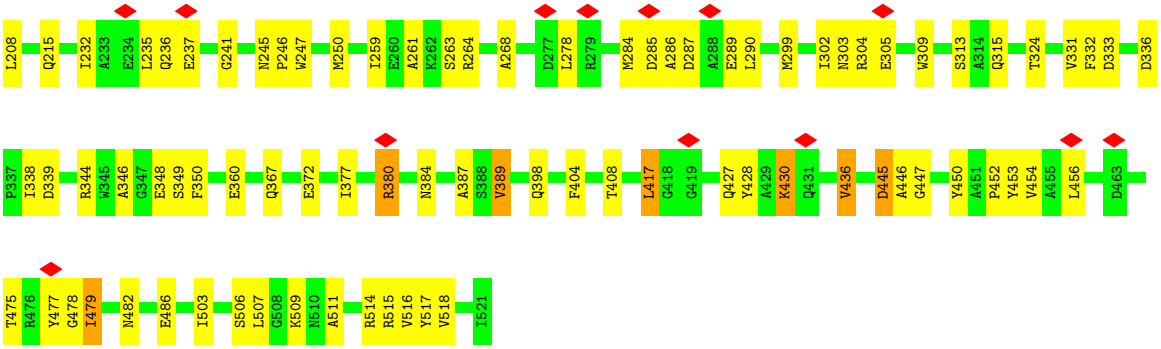



• Molecule 6: gp23, major capsid protein

Chain Ad:



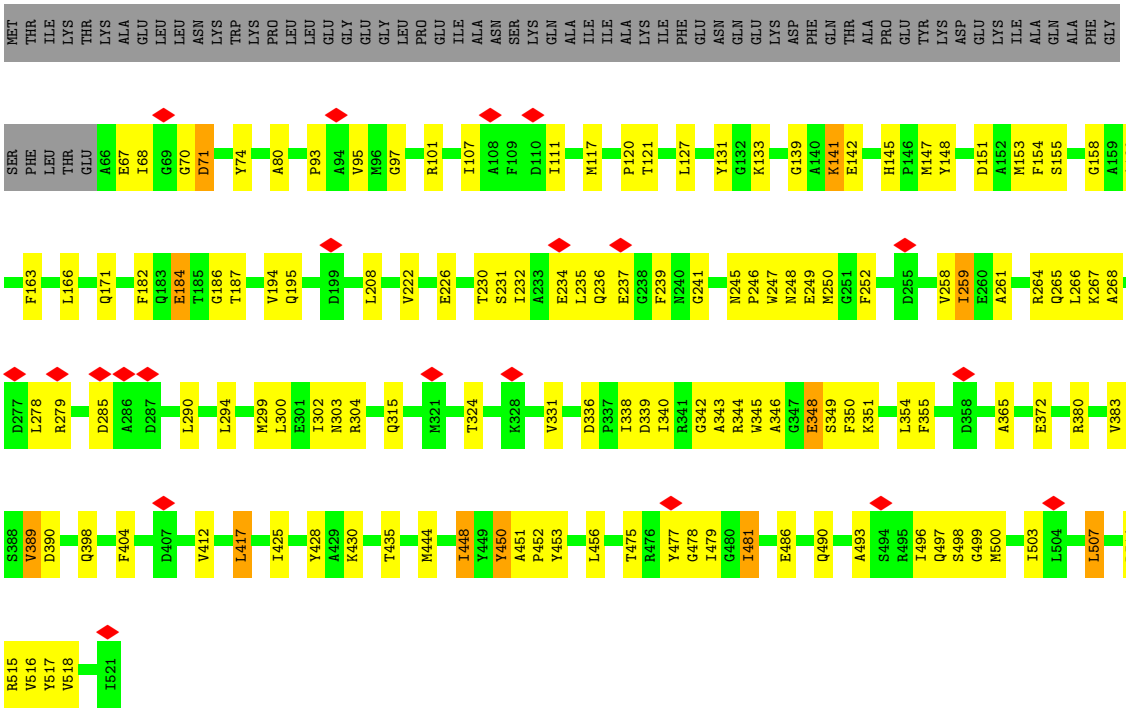






• Molecule 6: gp23, major capsid protein

Chain Ae:

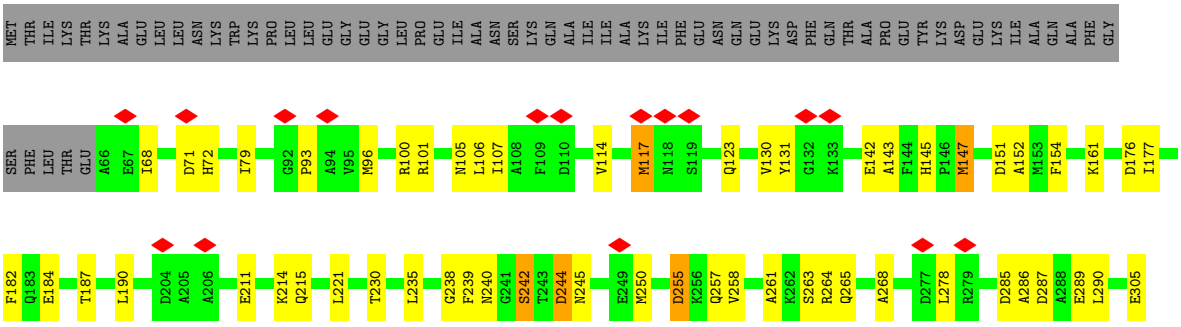


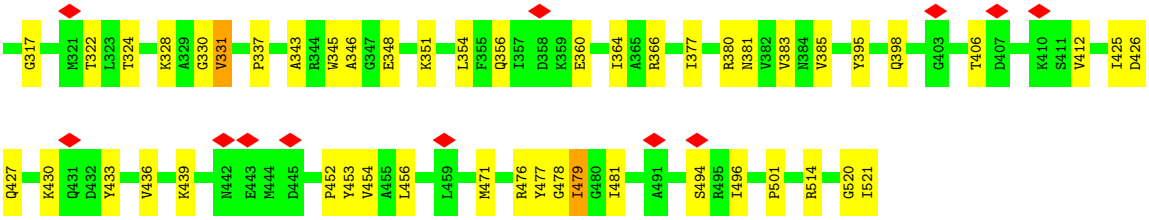




• Molecule 6: gp23, major capsid protein

Chain Af:



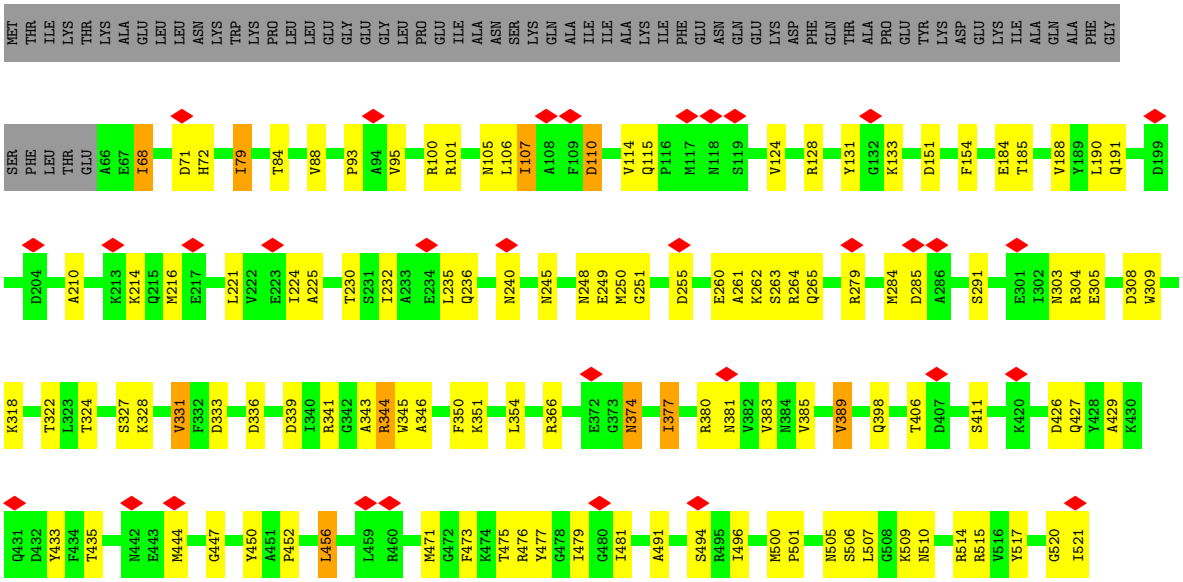






• Molecule 6: gp23, major capsid protein

Chain Ag:

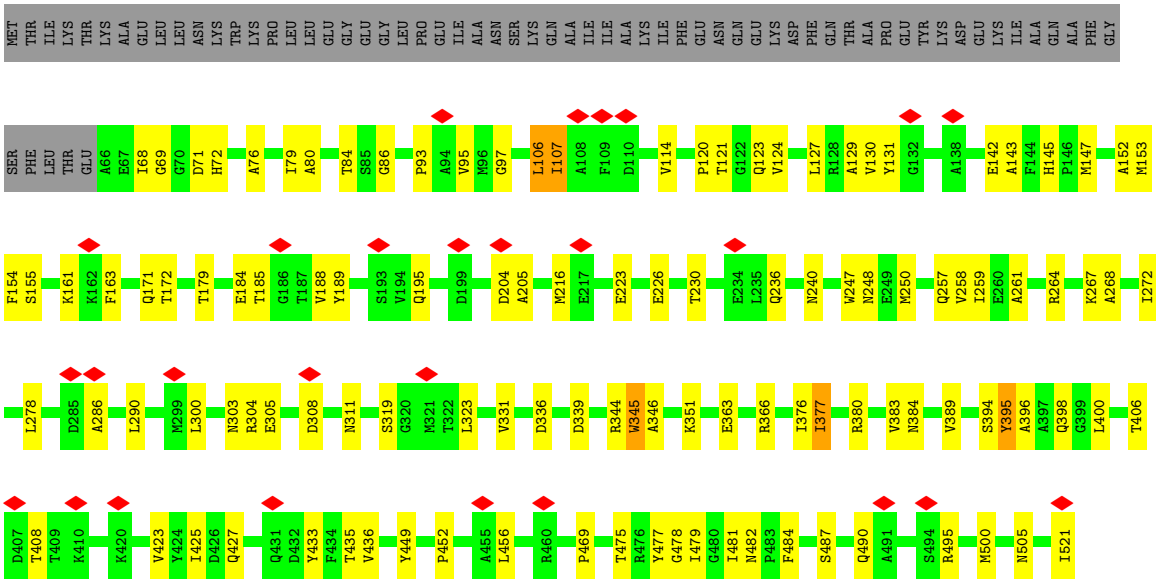



• Molecule 6: gp23, major capsid protein

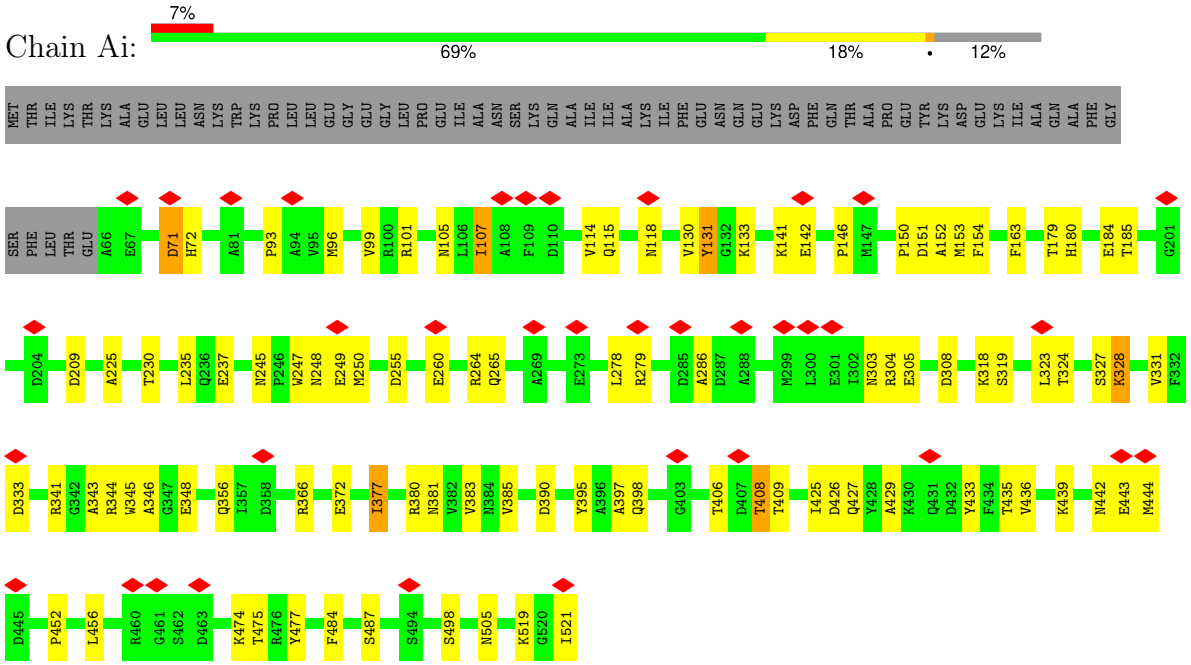
Chain Ah:



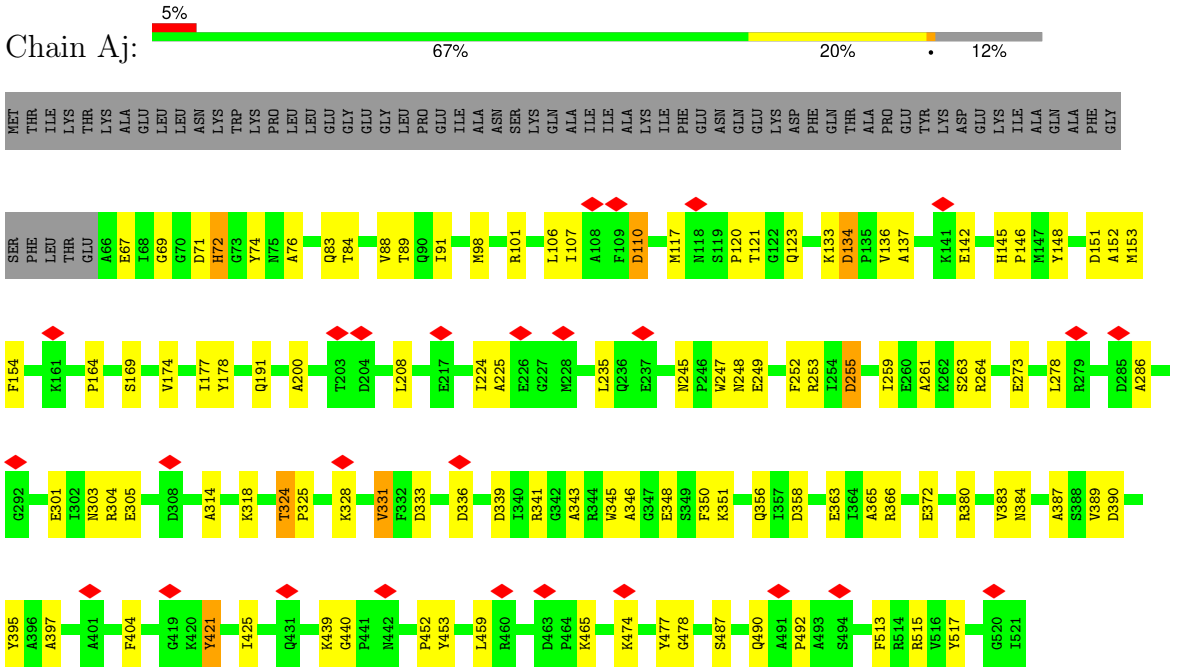

• Molecule 6: gp23, major capsid protein

Chain Ai:



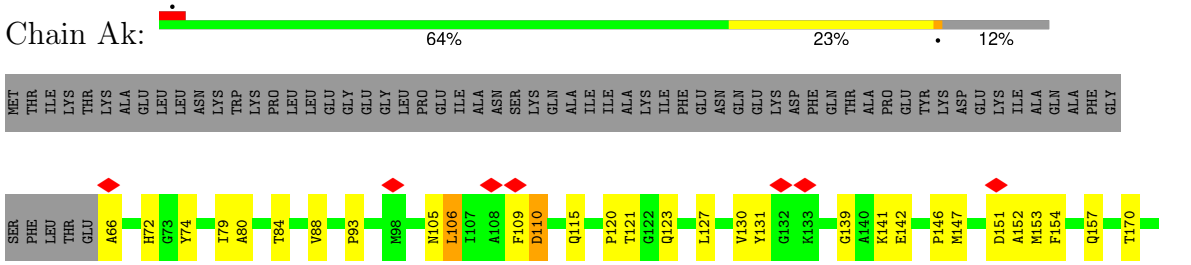

• Molecule 6: gp23, major capsid protein

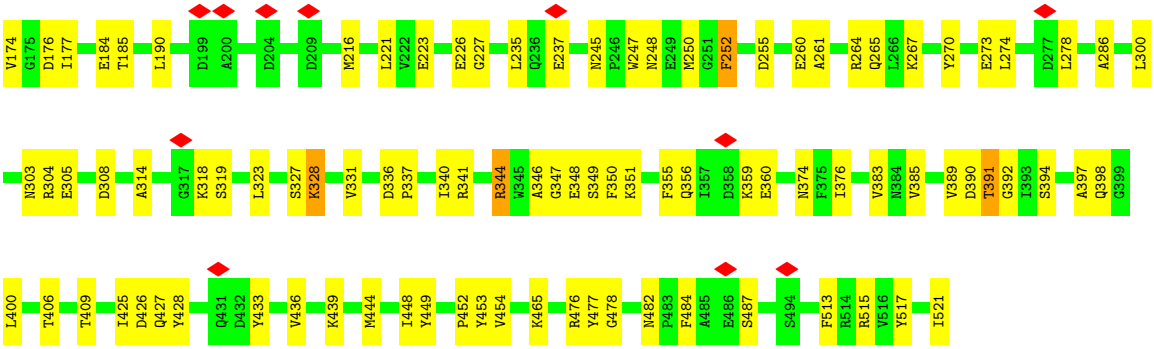
Chain Aj:




• Molecule 6: gp23, major capsid protein

Chain Ak:







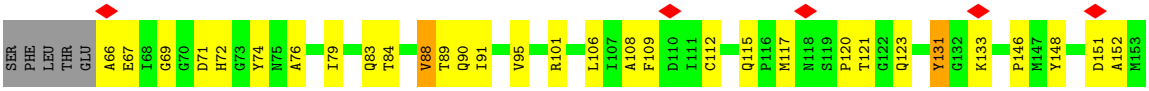


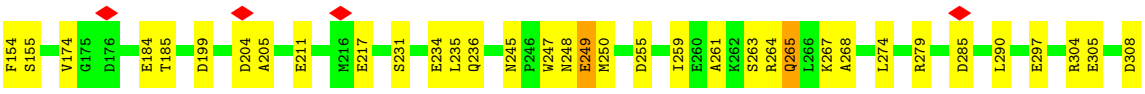
• Molecule 6: gp23, major capsid protein

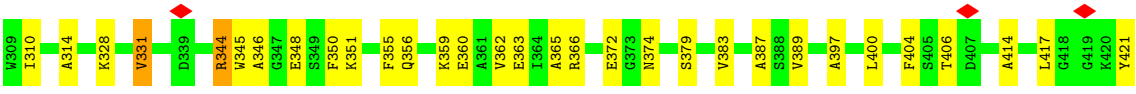
Chain Am:

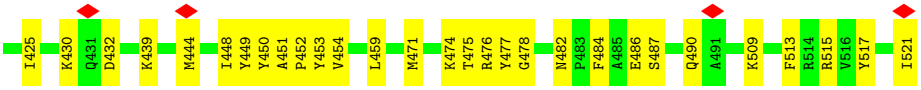








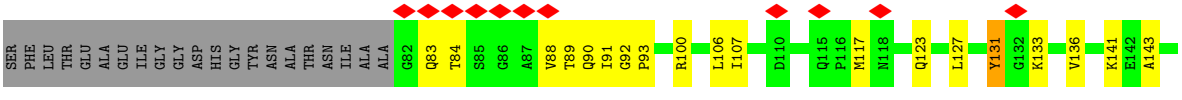


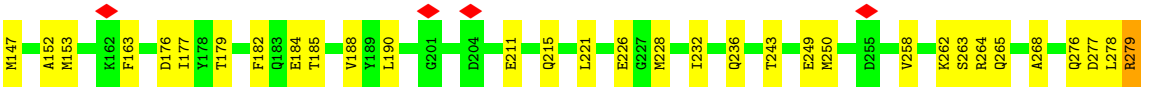
• Molecule 6: gp23, major capsid protein

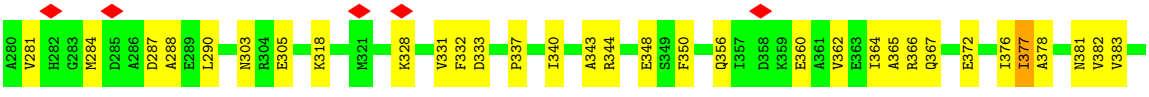
Chain An:

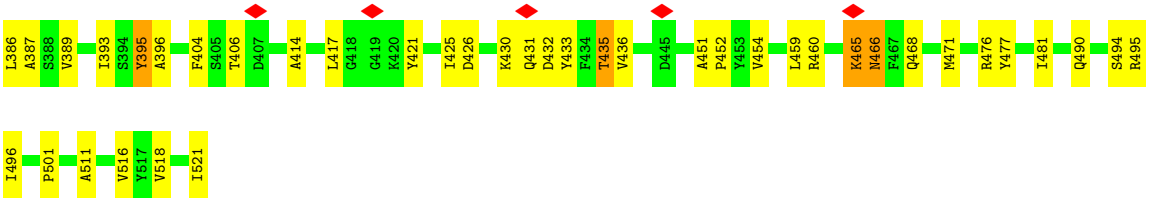






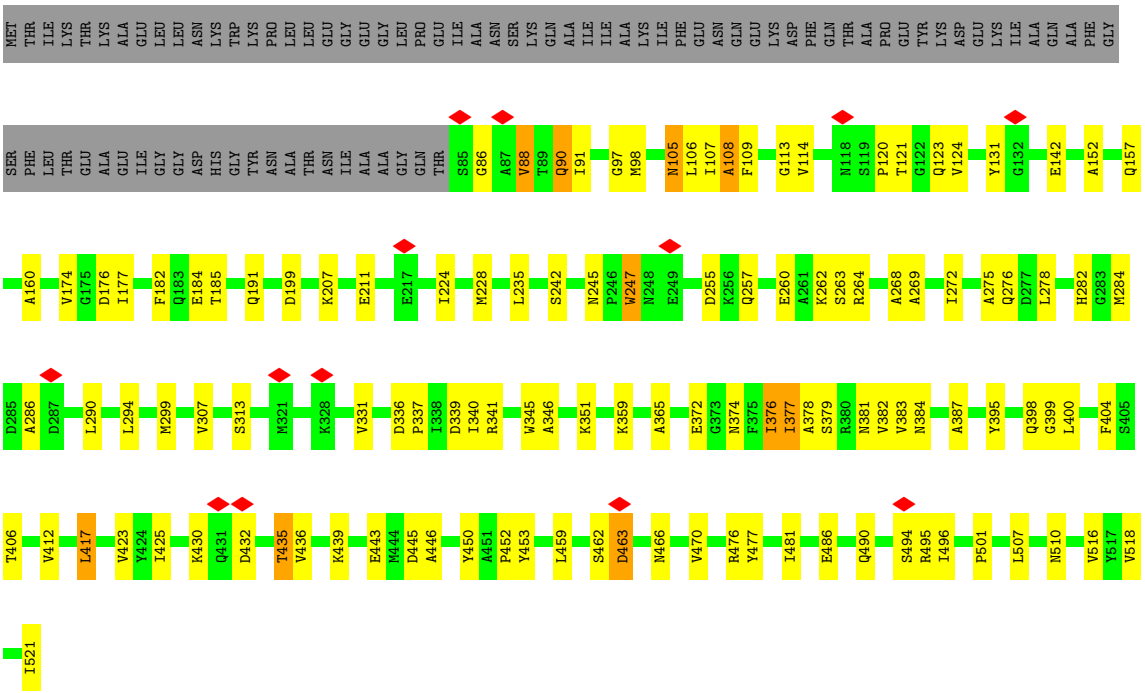




• Molecule 6: gp23, major capsid protein

Chain Ao:

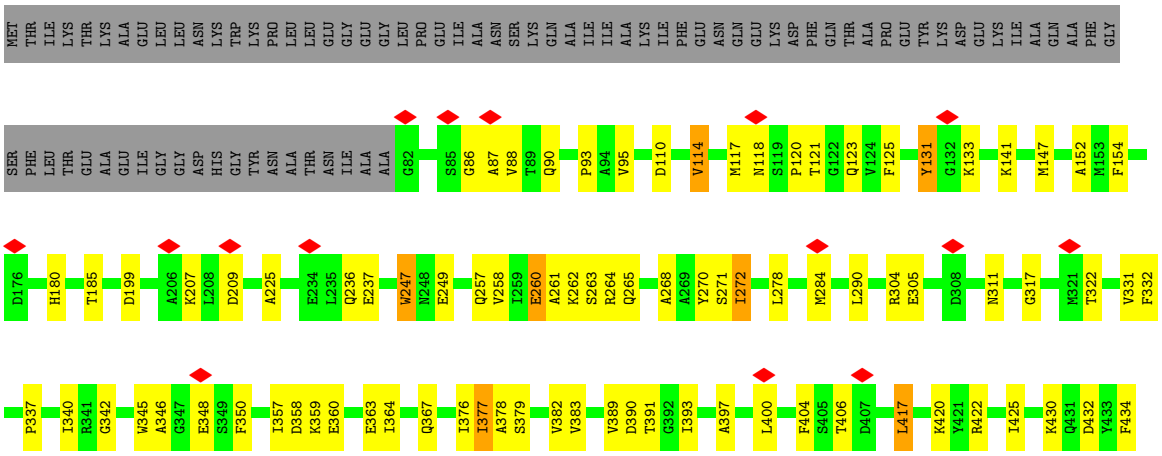


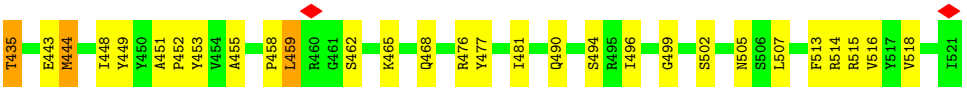



• Molecule 6: gp23, major capsid protein

Chain Ap:



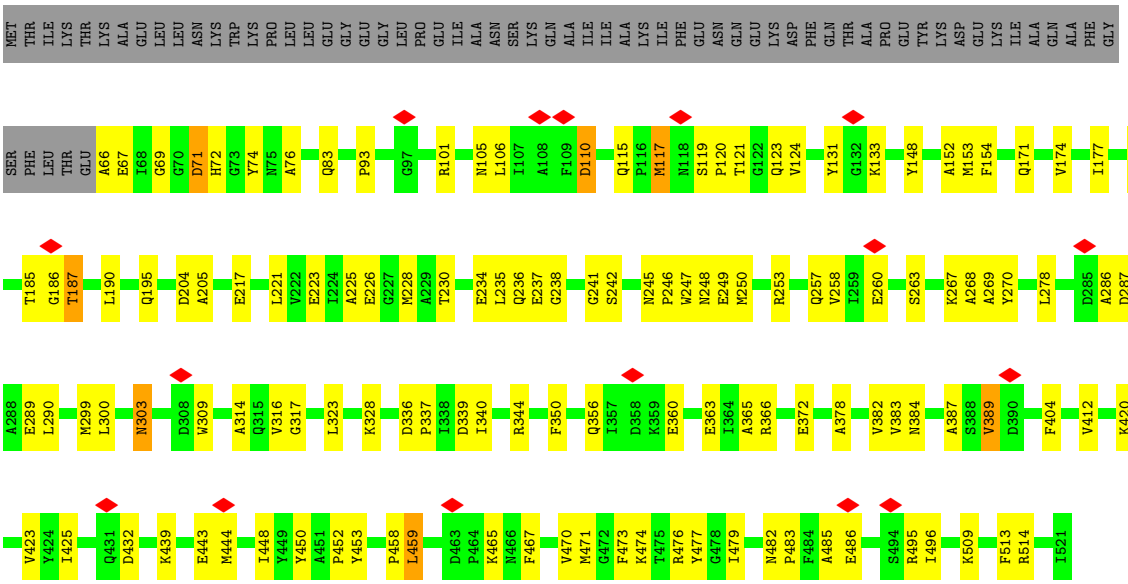






• Molecule 6: gp23, major capsid protein

Chain Au:

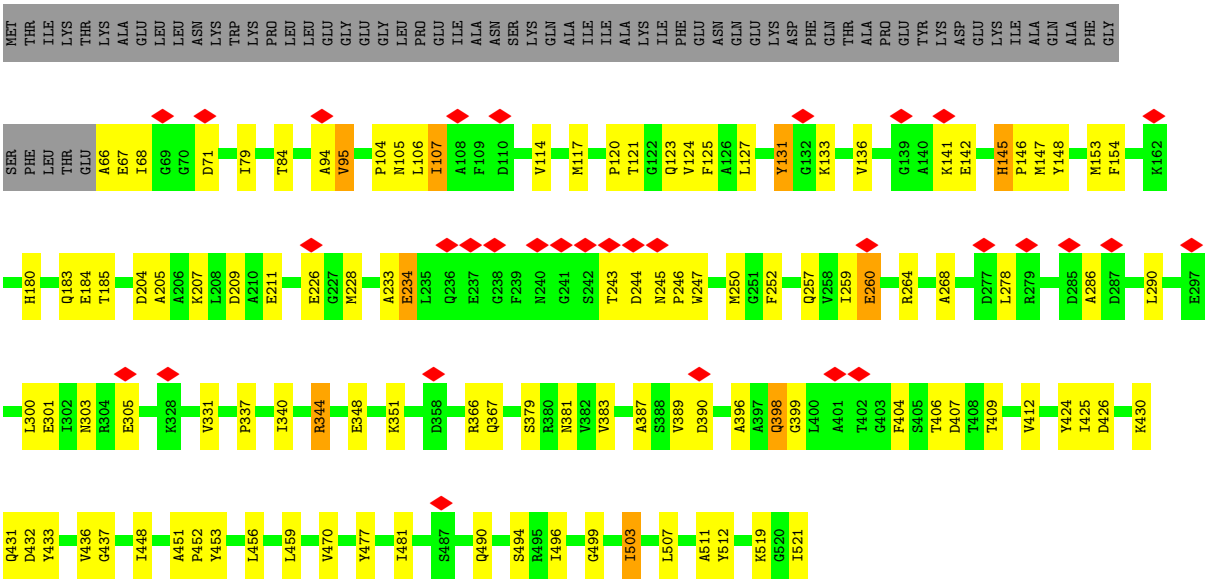



• Molecule 6: gp23, major capsid protein

Chain Aw:

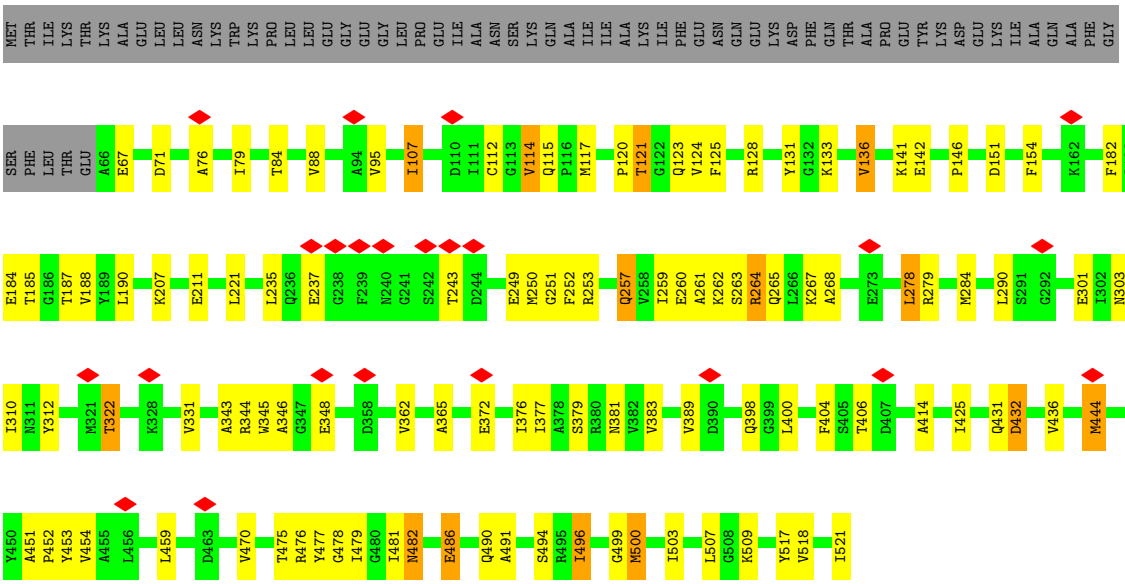



• Molecule 6: gp23, major capsid protein

Chain Ay:

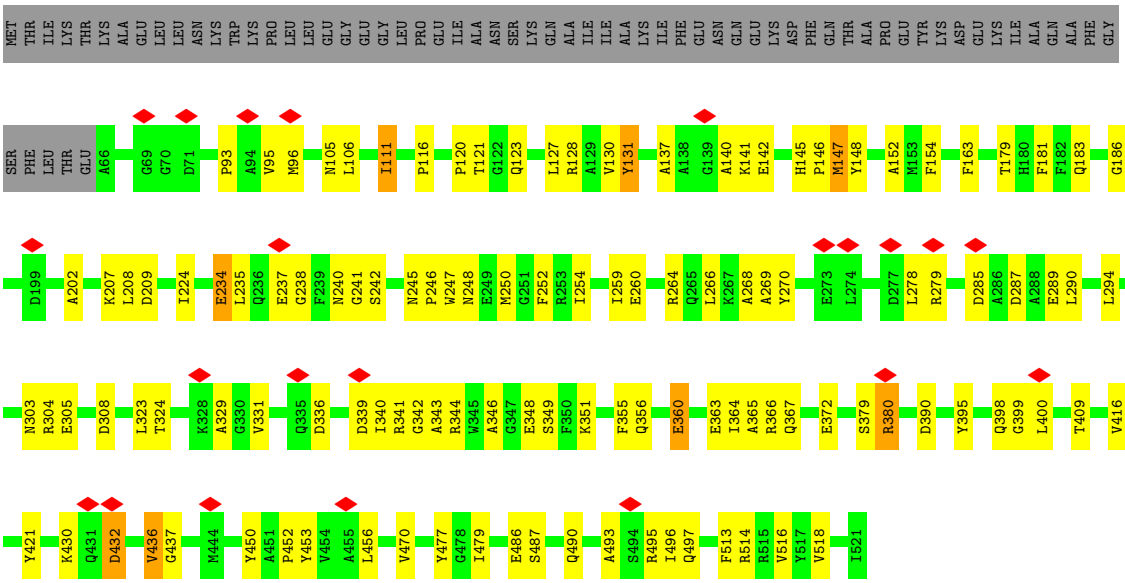




• Molecule 6: gp23, major capsid protein

Chain Az:

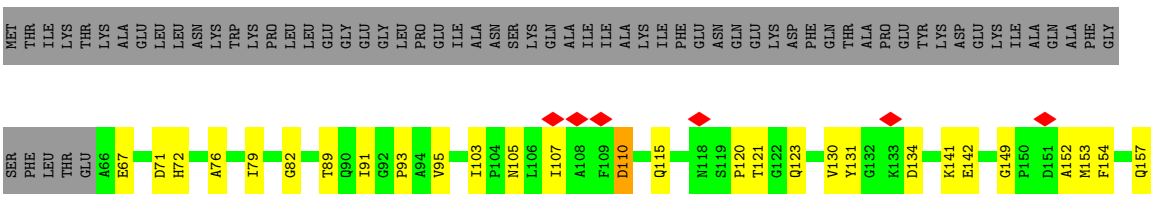


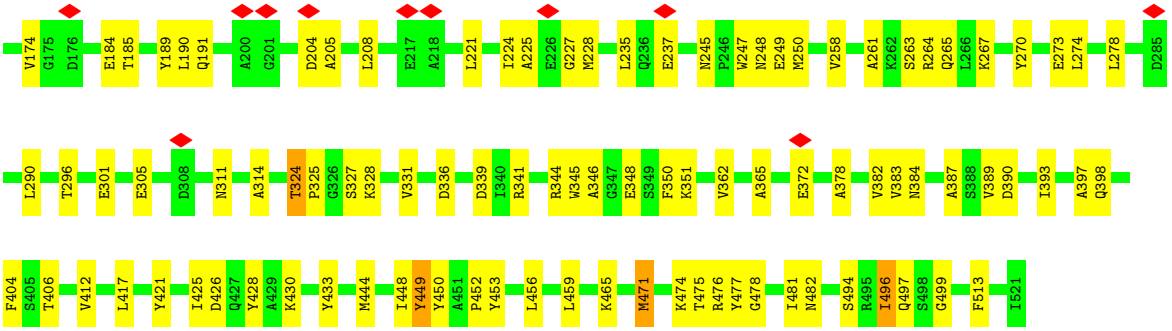



• Molecule 6: gp23, major capsid protein

Chain BI:



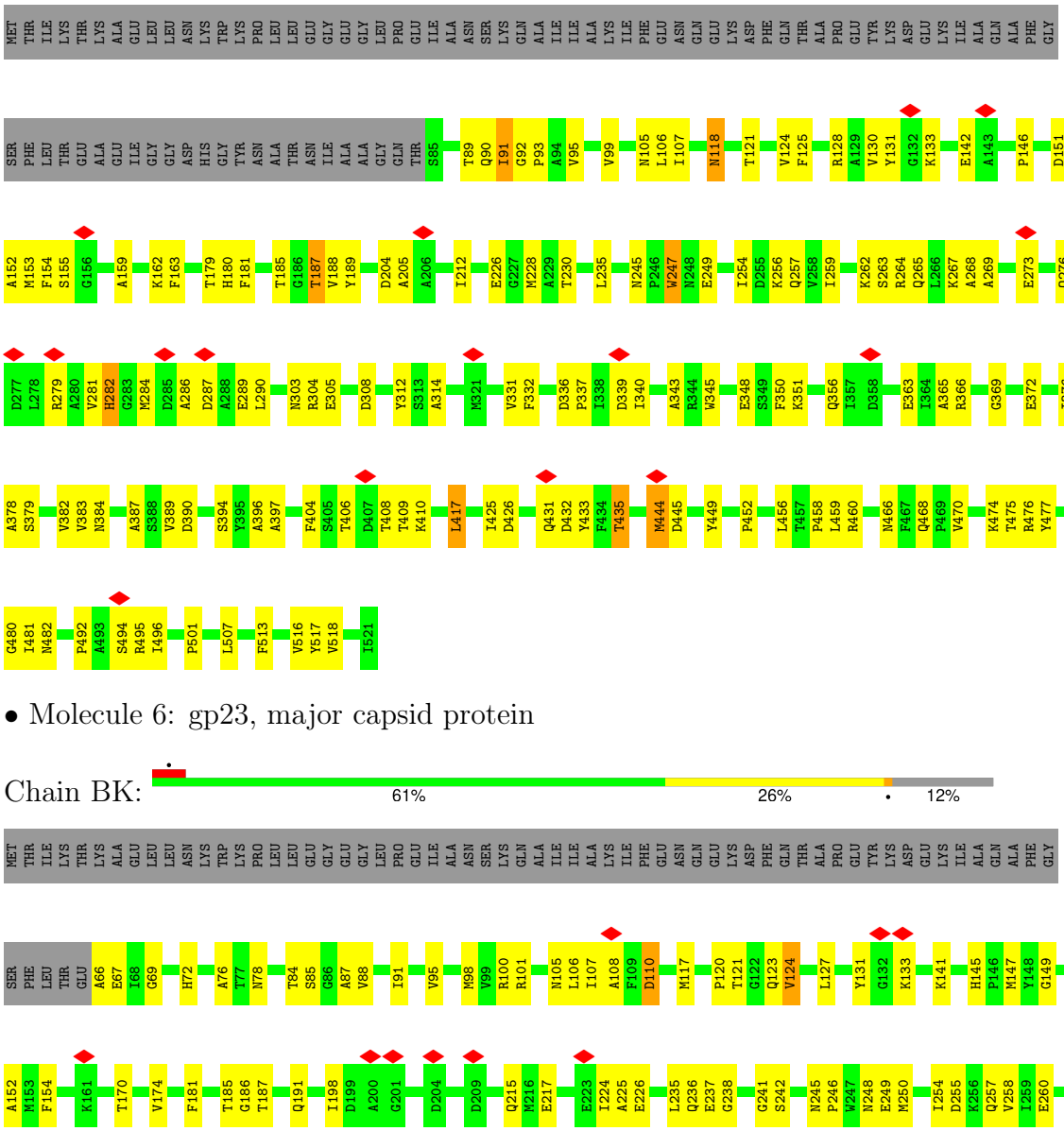






• Molecule 6: gp23, major capsid protein

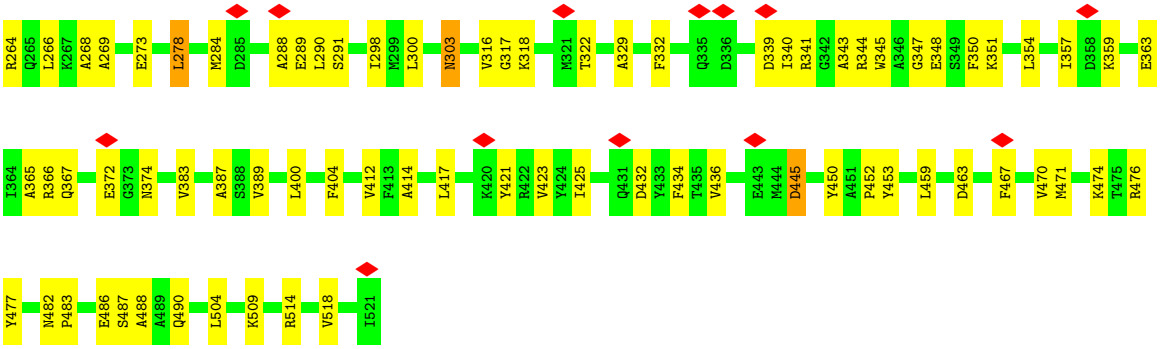
Chain BJ:




• Molecule 6: gp23, major capsid protein

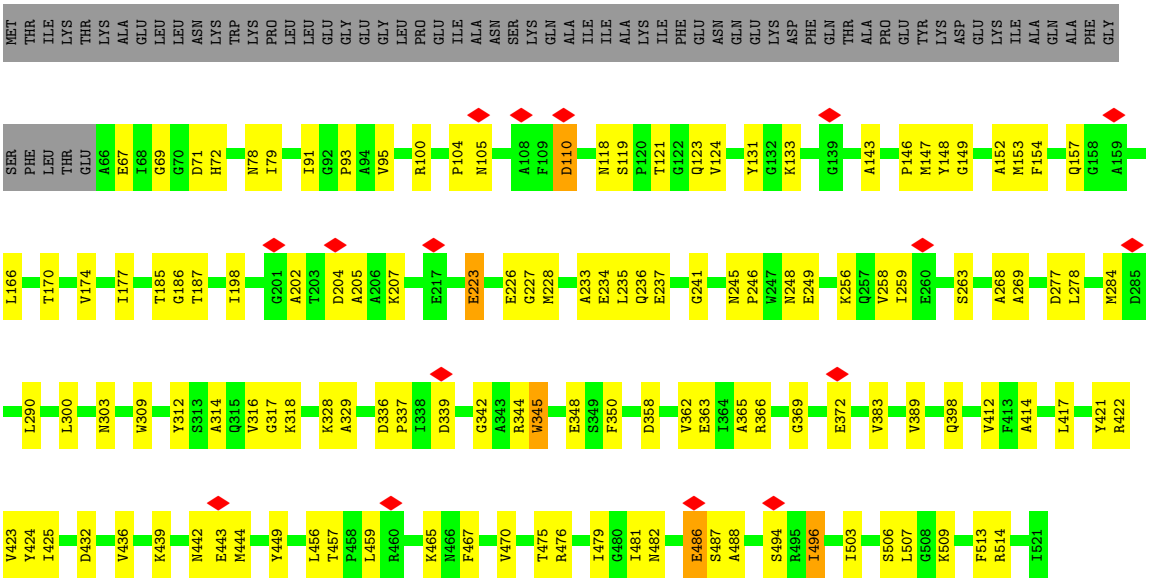
Chain BK:




• Molecule 6: gp23, major capsid protein

Chain BM:

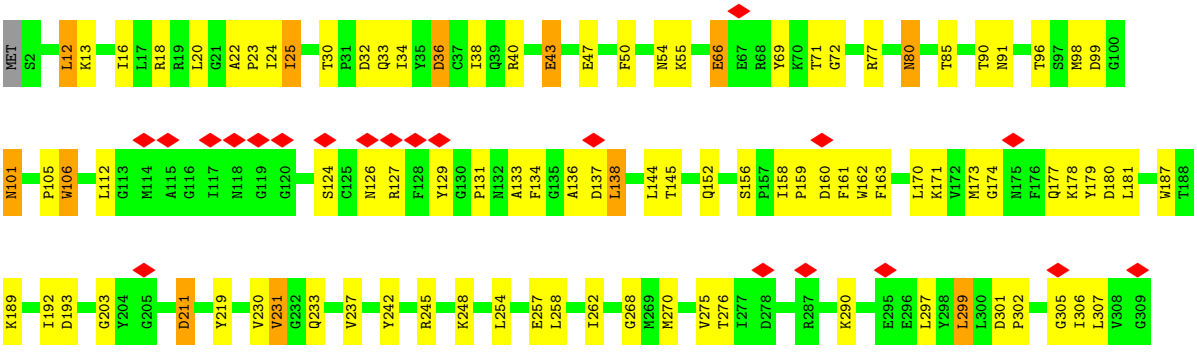



• Molecule 7: gp13, neck protein

Chain A6:

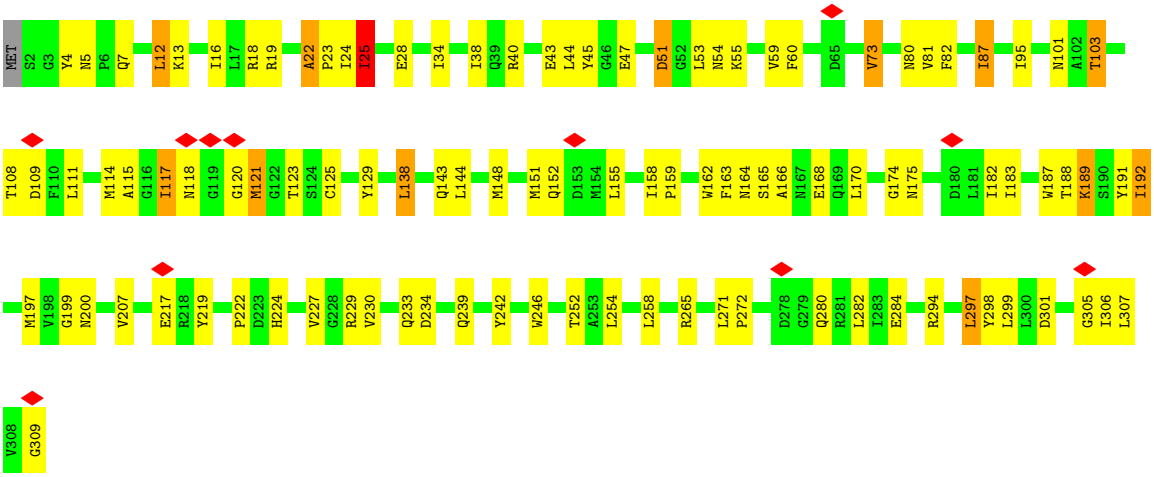



• Molecule 7: gp13, neck protein

Chain AY:

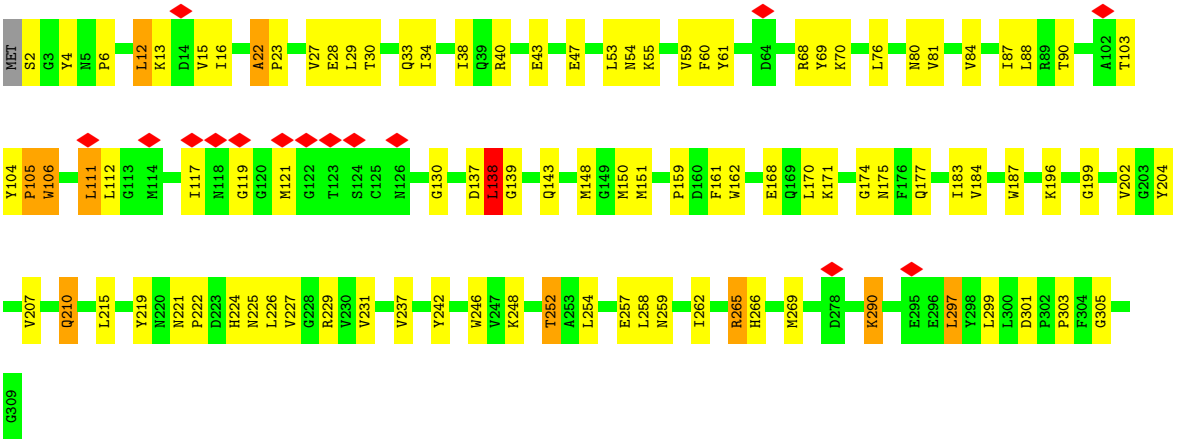





• Molecule 7: gp13, neck protein

Chain Aa:

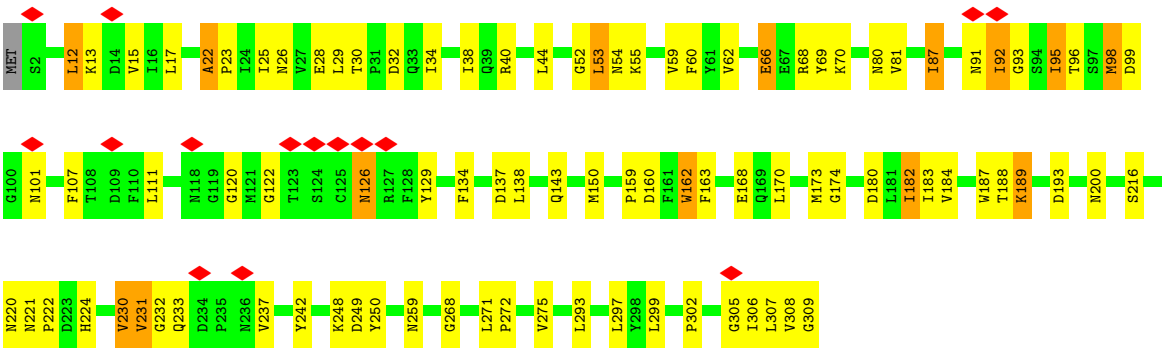



• Molecule 7: gp13, neck protein

Chain Ab:

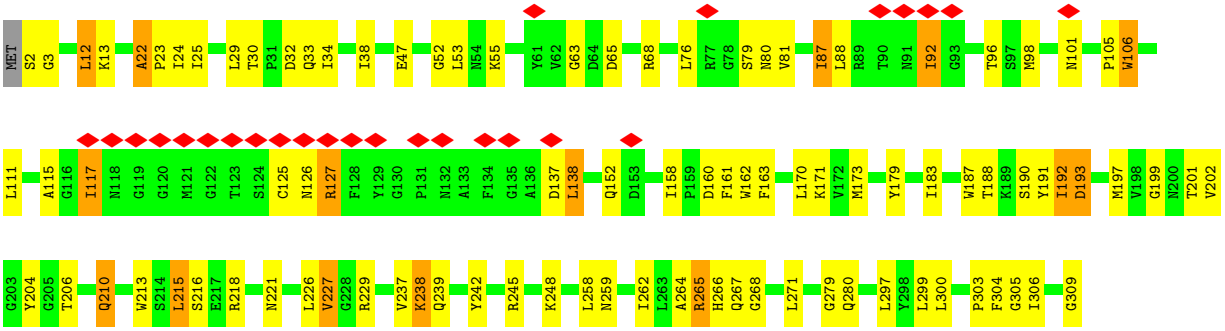



• Molecule 7: gp13, neck protein

Chain Al:

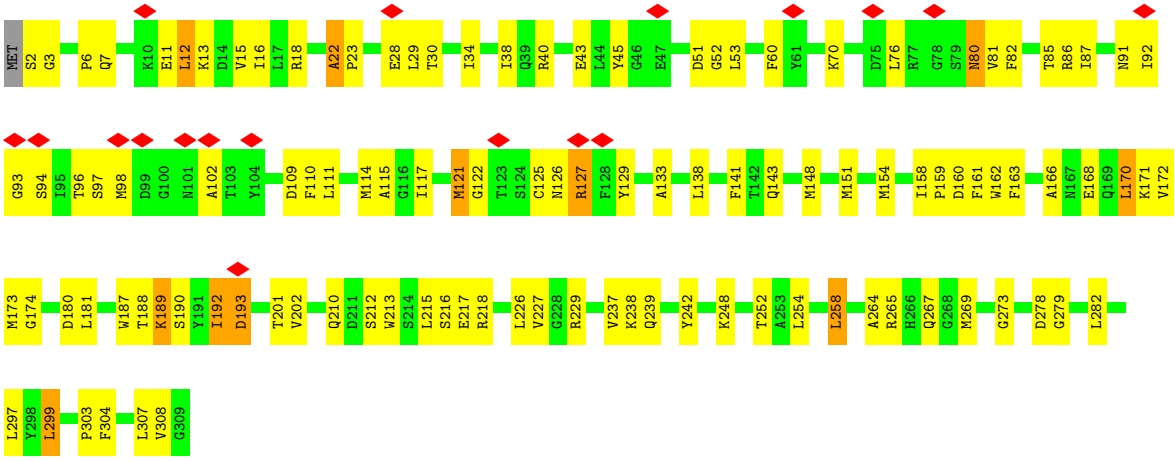




• Molecule 7: gp13, neck protein

Chain Aq:

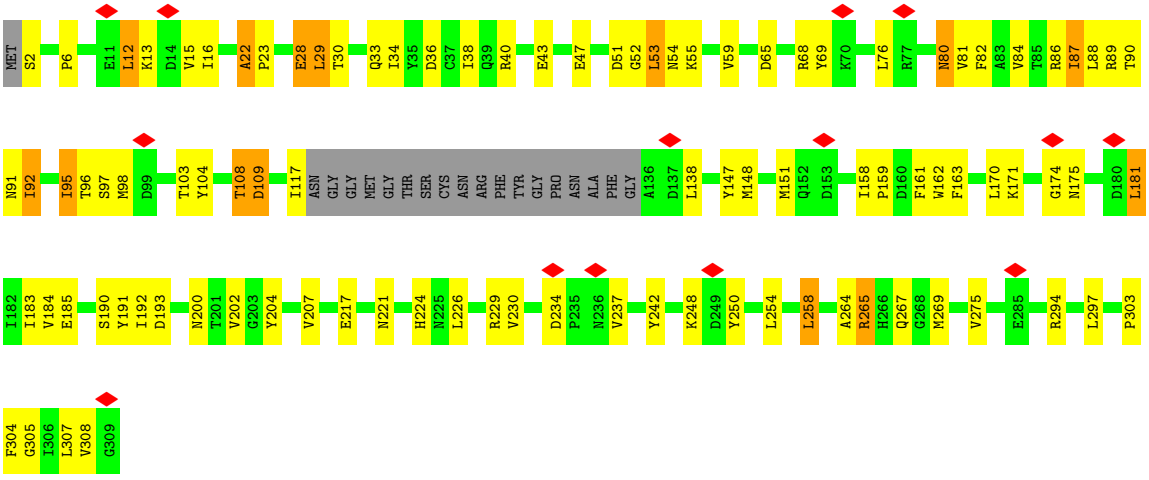


• Molecule 7: gp13, neck protein

Chain Ar:

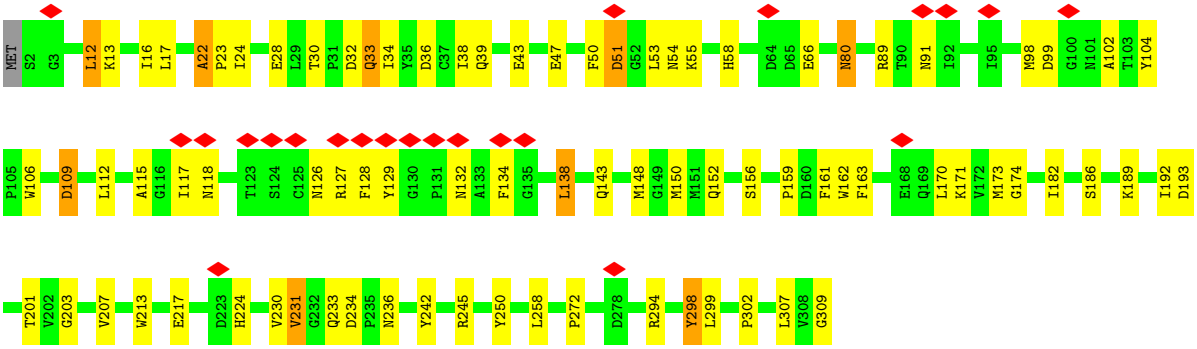


• Molecule 7: gp13, neck protein

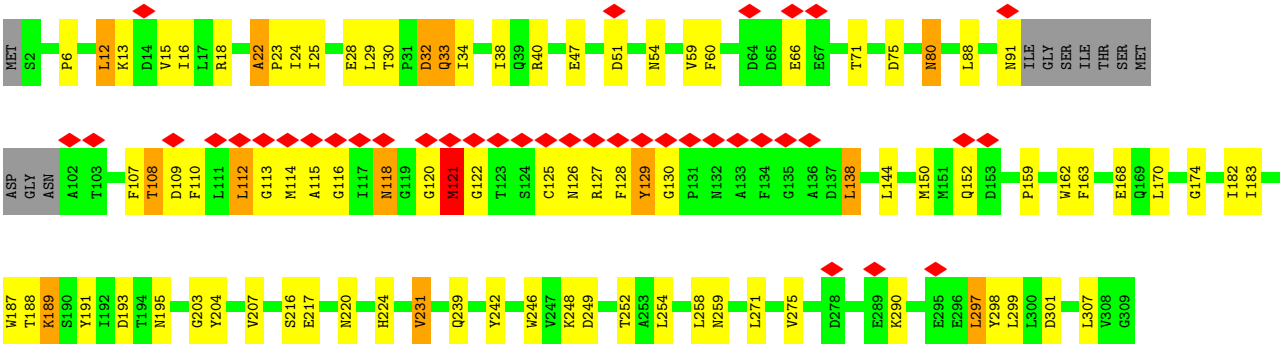
Chain As:





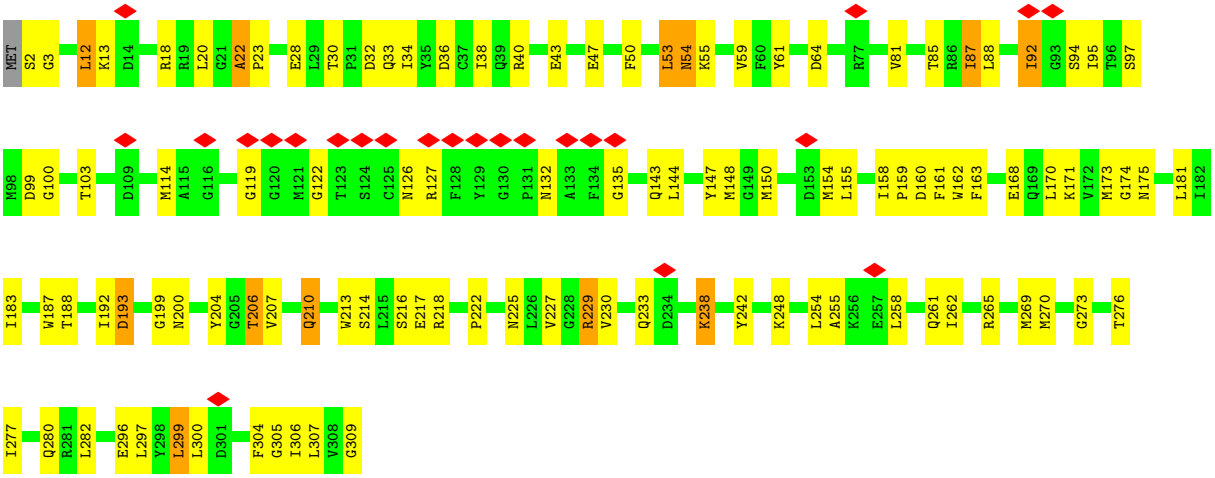

• Molecule 7: gp13, neck protein




• Molecule 7: gp13, neck protein




• Molecule 7: gp13, neck protein

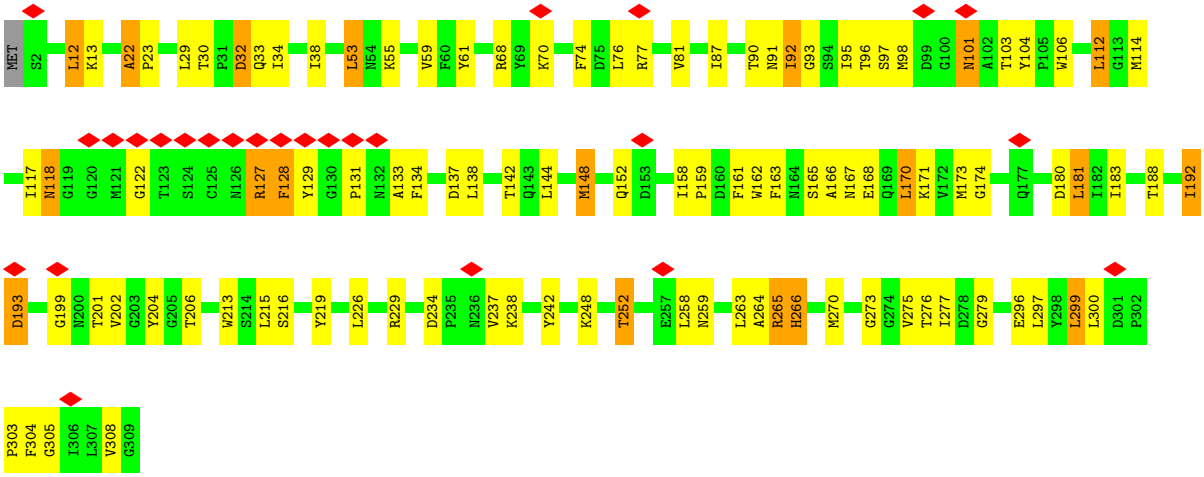





• Molecule 7: gp13, neck protein

Chain BL:

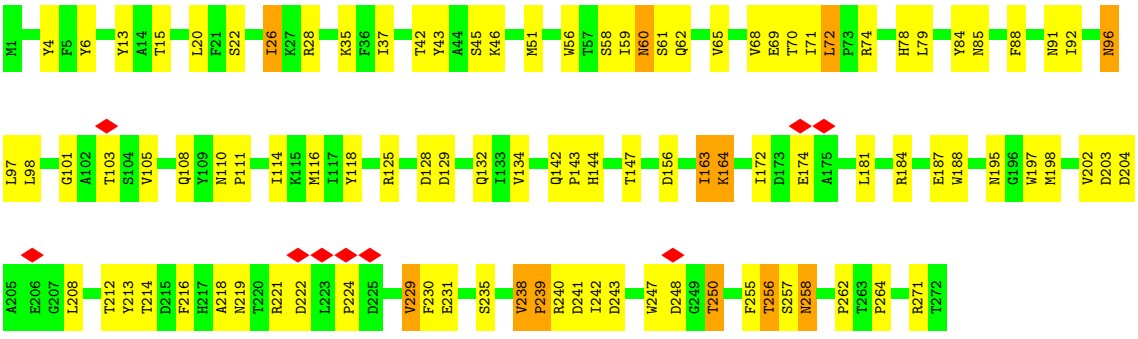



• Molecule 8: gp15, tail terminator protein

Chain AB:

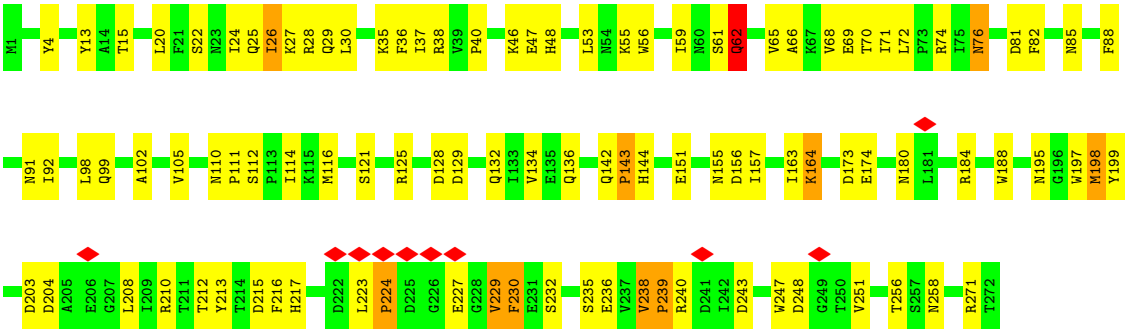



• Molecule 8: gp15, tail terminator protein

Chain q:

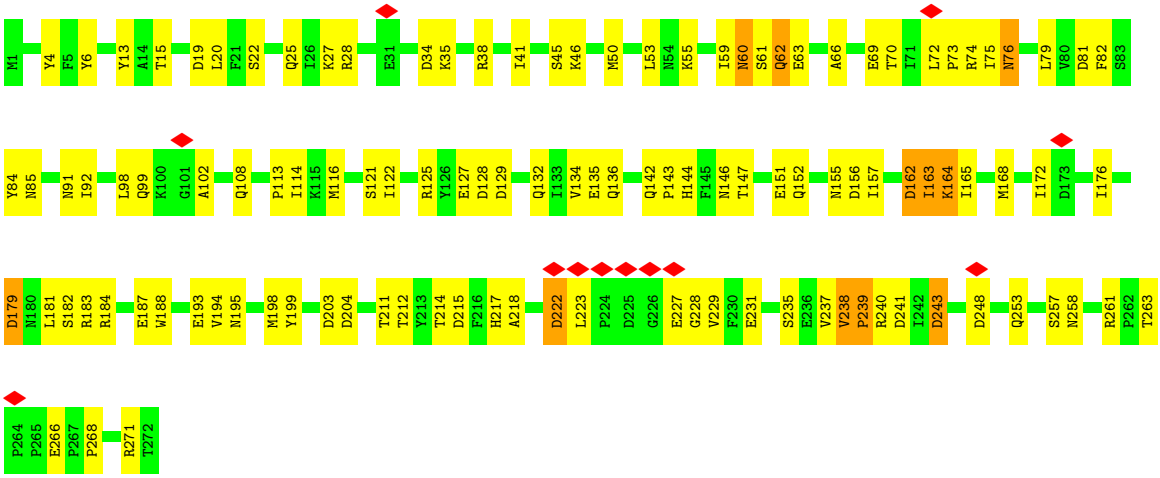




• Molecule 8: gp15, tail terminator protein

Chain r:

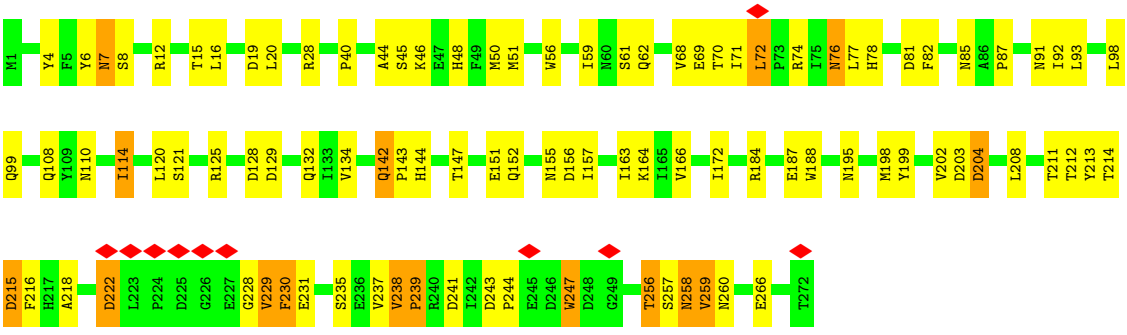


• Molecule 8: gp15, tail terminator protein

Chain s:

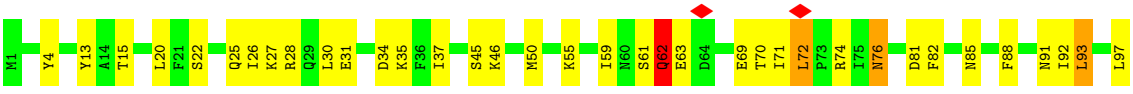


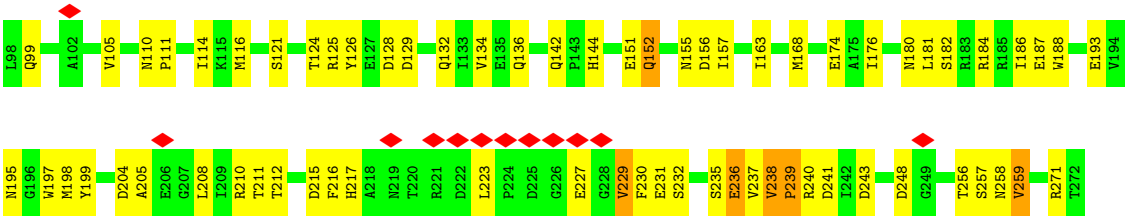



• Molecule 8: gp15, tail terminator protein

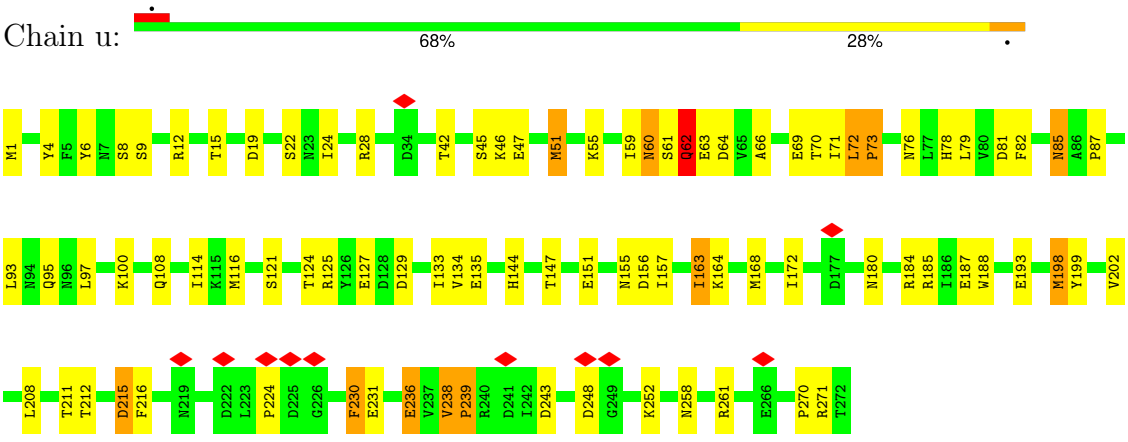
Chain t:



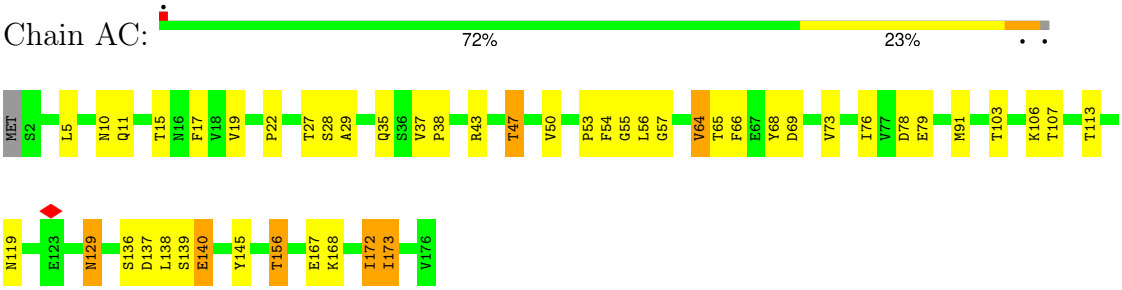





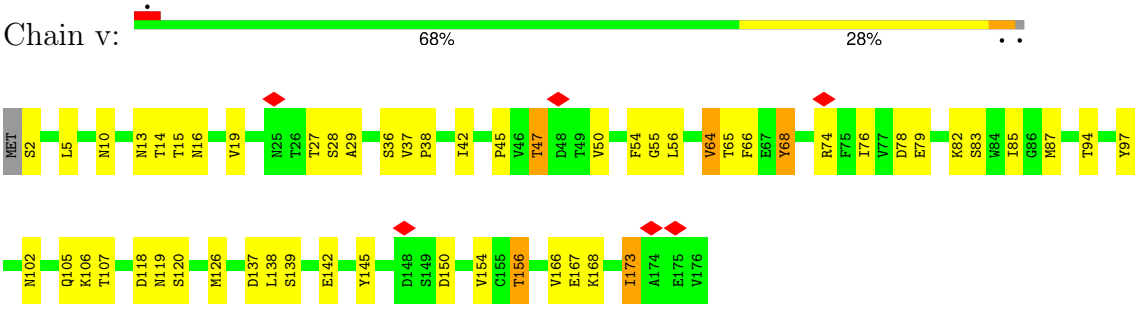

• Molecule 8: gp15, tail terminator protein



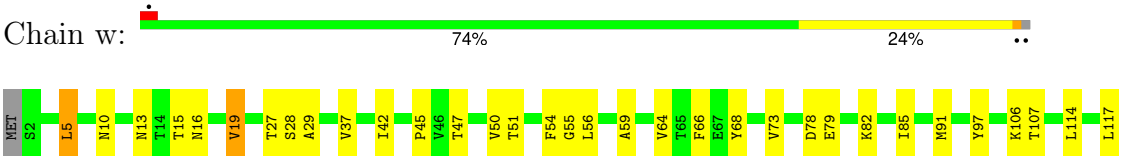

• Molecule 9: gp3, tube terminator protein

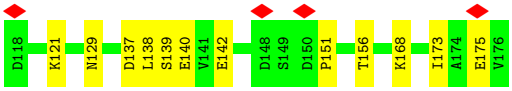



• Molecule 9: gp3, tube terminator protein




• Molecule 9: gp3, tube terminator protein





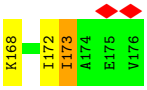

• Molecule 9: gp3, tube terminator protein

Chain x:










• Molecule 9: gp3, tube terminator protein

Chain y:





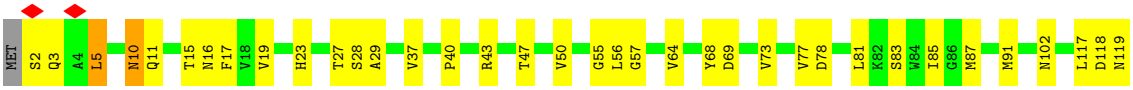


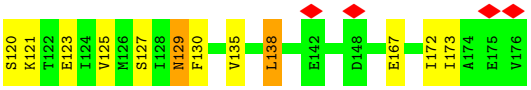



• Molecule 9: gp3, tube terminator protein

Chain z:



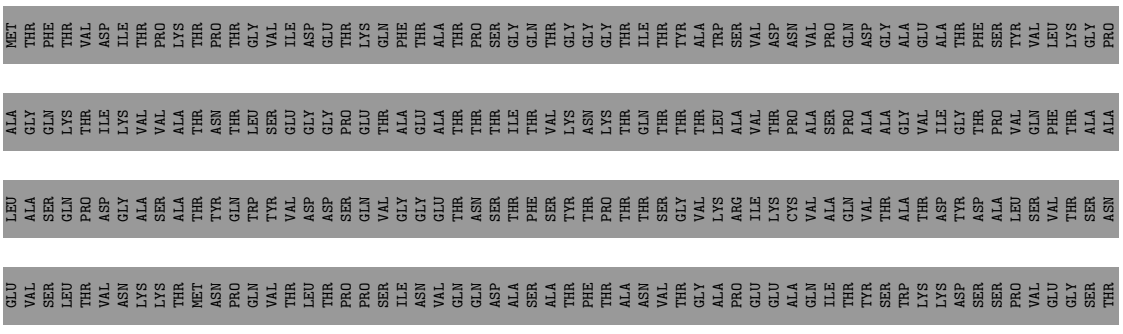



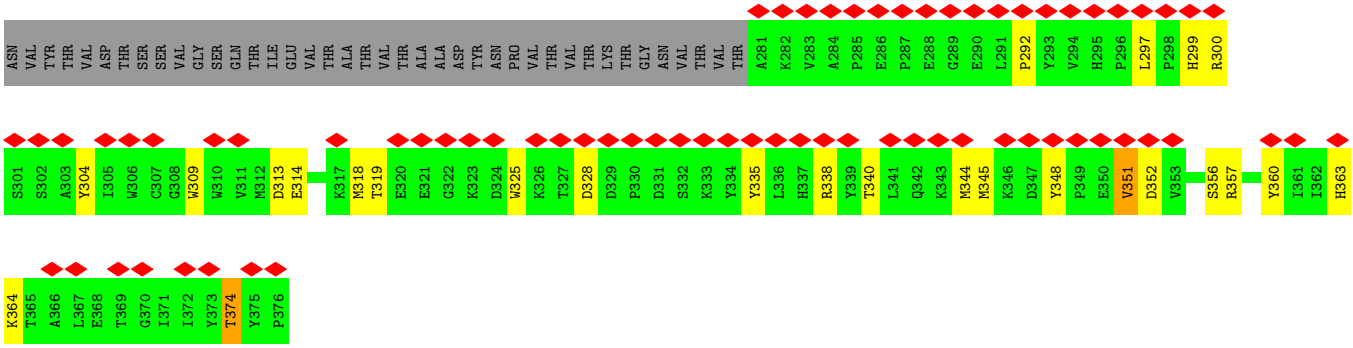




• Molecule 10: Hoc, highly immunogenic outer capsid protein

Chain AQ:



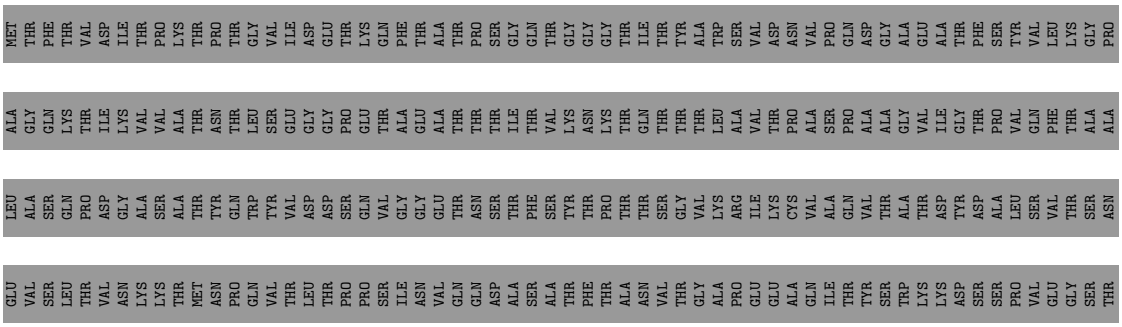



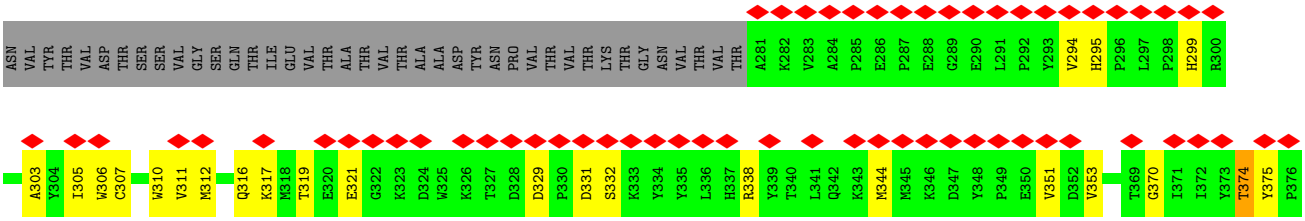



• Molecule 10: Hoc, highly immunogenic outer capsid protein

Chain AR:



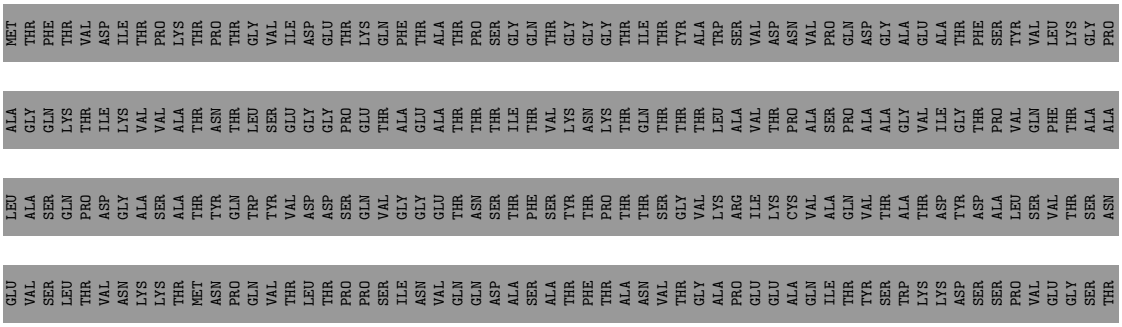



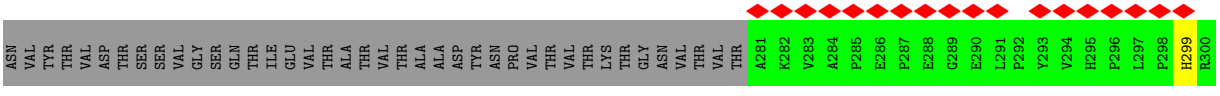



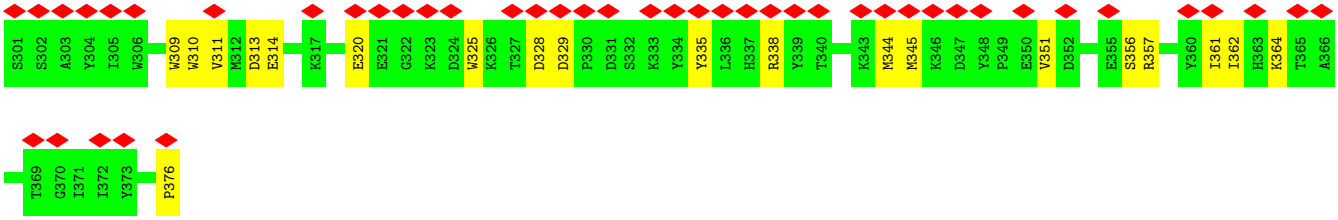

• Molecule 10: Hoc, highly immunogenic outer capsid protein

Chain AS:



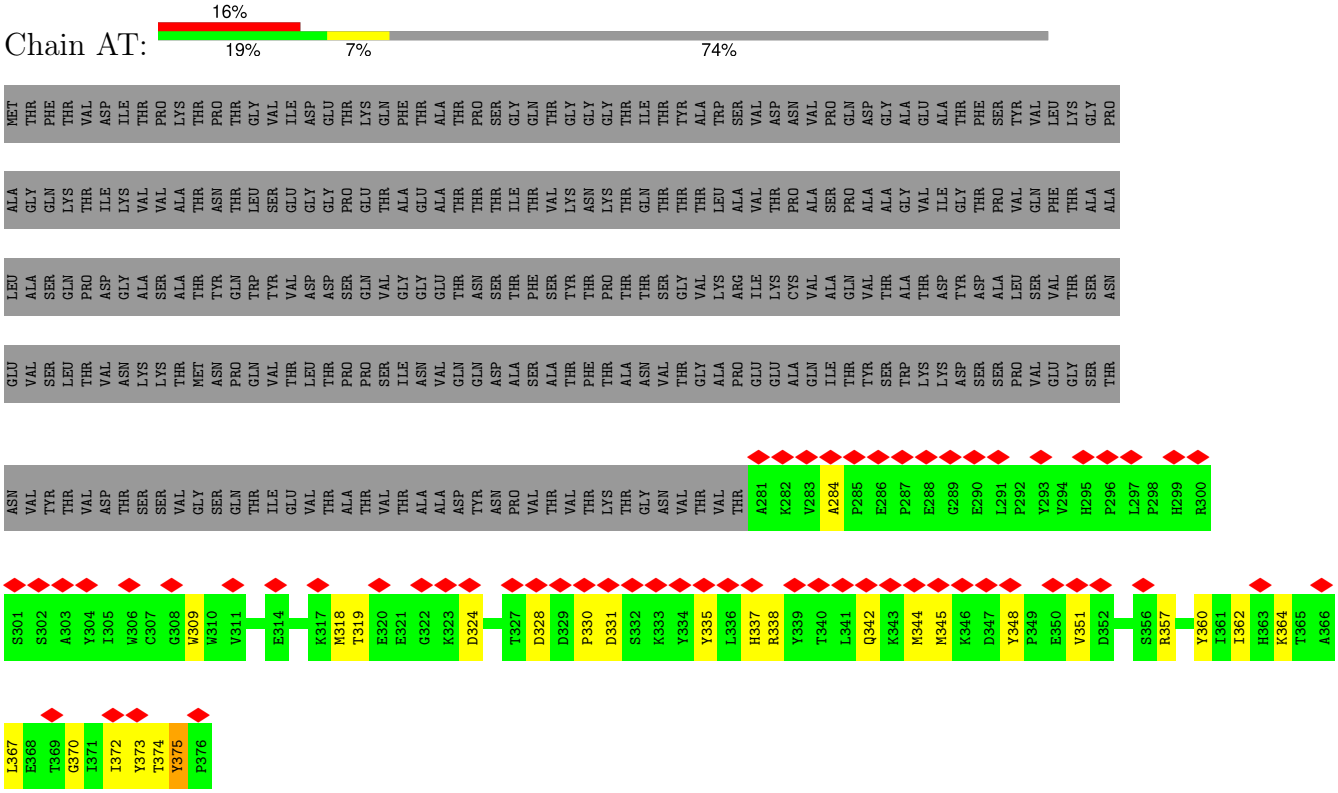





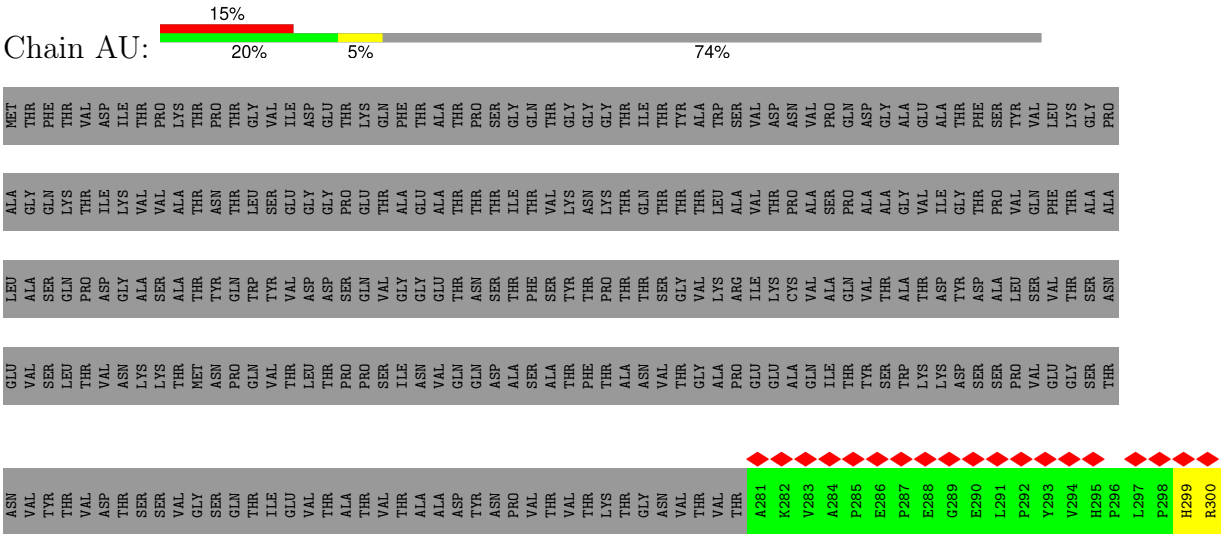

• Molecule 10: Hoc, highly immunogenic outer capsid protein

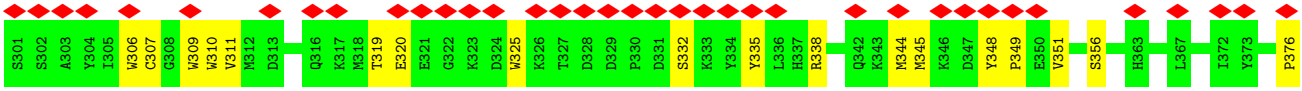
Chain AT:




• Molecule 10: Hoc, highly immunogenic outer capsid protein

Chain AU:

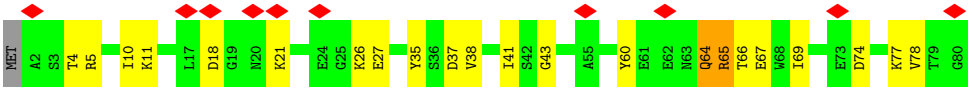





• Molecule 11: Soc, small outer capsid protein

Chain BN:

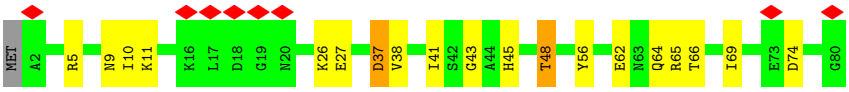



• Molecule 11: Soc, small outer capsid protein

Chain BO:

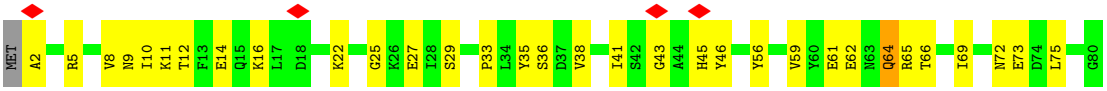



• Molecule 11: Soc, small outer capsid protein

Chain BP:

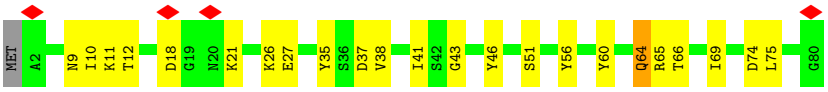



• Molecule 11: Soc, small outer capsid protein

Chain BQ:

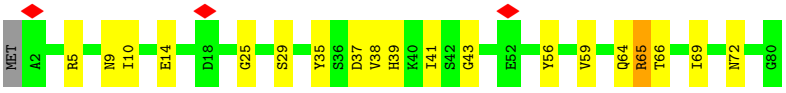



• Molecule 11: Soc, small outer capsid protein

Chain BR:

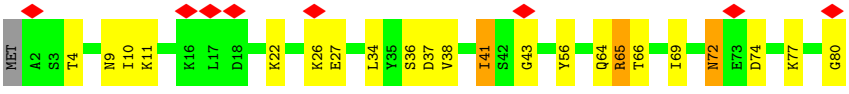



• Molecule 11: Soc, small outer capsid protein

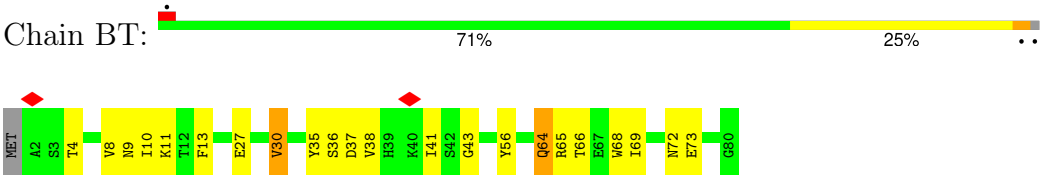
Chain BS:



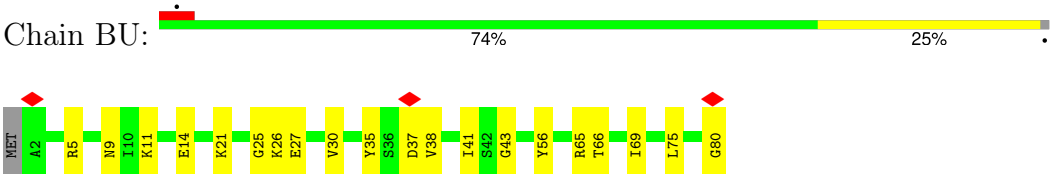

• Molecule 11: Soc, small outer capsid protein

Chain BT:



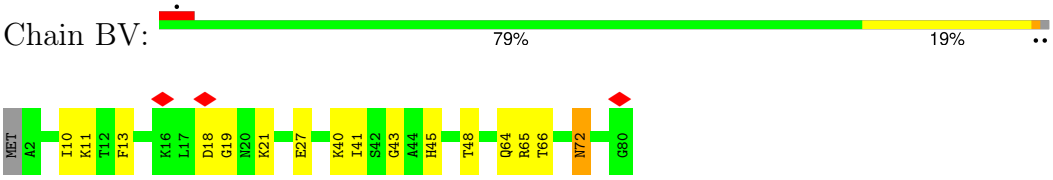

• Molecule 11: Soc, small outer capsid protein

Chain BU:



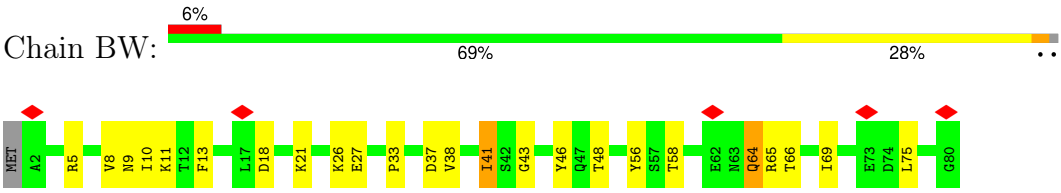

• Molecule 11: Soc, small outer capsid protein

Chain BV:




• Molecule 11: Soc, small outer capsid protein

Chain BW:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 69000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 38 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.090 | Depositor |
| Minimum map value | -0.059 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.006 | Depositor |
| Recommended contour level | 0.015 | Depositor |
| Map size (Å) | 646.4, 646.4, 646.4 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.616, 1.616, 1.616 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | 0 | 0.12 | 0/2042 | 0.40 | 0/2768 |
| 1 | k | 0.13 | 0/2042 | 0.40 | 0/2768 |
| 1 | l | 0.13 | 0/2042 | 0.41 | 0/2768 |
| 1 | m | 0.12 | 0/2042 | 0.38 | 0/2768 |
| 1 | n | 0.13 | 0/2042 | 0.38 | 0/2768 |
| 1 | p | 0.13 | 0/2042 | 0.39 | 0/2768 |
| 2 | 1 | 0.11 | 0/5077 | 0.31 | 1/6907 (0.0%) |
| 2 | 2 | 0.11 | 0/5077 | 0.31 | 0/6907 |
| 2 | 3 | 0.11 | 0/5077 | 0.32 | 1/6907 (0.0%) |
| 2 | 4 | 0.11 | 0/5077 | 0.31 | 0/6907 |
| 2 | 5 | 0.11 | 0/5077 | 0.31 | 0/6907 |
| 2 | AD | 0.11 | 0/5077 | 0.30 | 0/6907 |
| 2 | AK | 0.10 | 0/5092 | 0.30 | 0/6928 |
| 2 | AL | 0.11 | 0/5092 | 0.31 | 0/6928 |
| 2 | AM | 0.10 | 0/5092 | 0.29 | 0/6928 |
| 2 | AN | 0.10 | 0/5092 | 0.31 | 0/6928 |
| 2 | AO | 0.11 | 0/5092 | 0.32 | 0/6928 |
| 2 | AP | 0.11 | 0/5092 | 0.30 | 0/6928 |
| 2 | B1 | 0.10 | 0/5092 | 0.32 | 0/6928 |
| 2 | B2 | 0.11 | 0/5092 | 0.30 | 0/6928 |
| 2 | B3 | 0.10 | 0/5092 | 0.31 | 0/6928 |
| 2 | B4 | 0.10 | 0/5092 | 0.32 | 1/6928 (0.0%) |
| 2 | B5 | 0.10 | 0/5092 | 0.30 | 0/6928 |
| 2 | B6 | 0.10 | 0/5092 | 0.29 | 0/6928 |
| 2 | B7 | 0.10 | 0/5092 | 0.30 | 0/6928 |
| 2 | Bp | 0.11 | 0/5092 | 0.31 | 0/6928 |
| 2 | Bq | 0.10 | 0/5092 | 0.30 | 0/6928 |
| 2 | Br | 0.10 | 0/5092 | 0.30 | 0/6928 |
| 2 | Bs | 0.10 | 0/5092 | 0.31 | 0/6928 |
| 2 | Bt | 0.10 | 0/5092 | 0.29 | 0/6928 |
| 2 | Bu | 0.10 | 0/5092 | 0.31 | 0/6928 |
| 2 | Bv | 0.10 | 0/5092 | 0.31 | 0/6928 |
| 2 | Bw | 0.10 | 0/5092 | 0.32 | 1/6928 (0.0%) |
| 2 | Bx | 0.10 | 0/5092 | 0.32 | 0/6928 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | By | 0.11 | 0/5092 | 0.32 | 0/6928 |
| 2 | Bz | 0.10 | 0/5092 | 0.32 | 1/6928 (0.0%) |
| 3 | 6 | 0.12 | 0/1325 | 0.37 | 0/1797 |
| 3 | 7 | 0.12 | 0/1325 | 0.35 | 0/1797 |
| 3 | 8 | 0.12 | 0/1325 | 0.36 | 0/1797 |
| 3 | 9 | 0.13 | 0/1325 | 0.37 | 0/1797 |
| 3 | AA | 0.12 | 0/1325 | 0.38 | 1/1797 (0.1%) |
| 3 | AE | 0.15 | 0/1333 | 0.39 | 0/1807 |
| 3 | AF | 0.12 | 0/1333 | 0.32 | 0/1807 |
| 3 | AG | 0.13 | 0/1333 | 0.31 | 0/1807 |
| 3 | AH | 0.12 | 0/1333 | 0.31 | 0/1807 |
| 3 | AI | 0.11 | 0/1333 | 0.34 | 0/1807 |
| 3 | AJ | 0.11 | 0/1333 | 0.33 | 0/1807 |
| 3 | BX | 0.11 | 0/1333 | 0.33 | 0/1807 |
| 3 | BY | 0.11 | 0/1333 | 0.32 | 0/1807 |
| 3 | BZ | 0.10 | 0/1333 | 0.32 | 0/1807 |
| 3 | Ba | 0.11 | 0/1333 | 0.34 | 0/1807 |
| 3 | Bb | 0.10 | 0/1333 | 0.33 | 0/1807 |
| 3 | Bc | 0.10 | 0/1333 | 0.32 | 0/1807 |
| 3 | Bd | 0.11 | 0/1333 | 0.32 | 0/1807 |
| 3 | Be | 0.11 | 0/1333 | 0.33 | 0/1807 |
| 3 | Bf | 0.10 | 0/1333 | 0.29 | 0/1807 |
| 3 | Bg | 0.11 | 0/1333 | 0.34 | 0/1807 |
| 3 | Bh | 0.11 | 0/1333 | 0.34 | 0/1807 |
| 3 | Bi | 0.11 | 0/1333 | 0.32 | 0/1807 |
| 3 | Bj | 0.11 | 0/1333 | 0.33 | 0/1807 |
| 3 | Bk | 0.11 | 0/1333 | 0.32 | 0/1807 |
| 3 | Bl | 0.12 | 0/1333 | 0.33 | 0/1807 |
| 3 | Bm | 0.15 | 0/1333 | 0.38 | 1/1807 (0.1%) |
| 3 | Bn | 0.17 | 0/1333 | 0.38 | 0/1807 |
| 3 | Bo | 0.10 | 0/1333 | 0.31 | 0/1807 |
| 3 | o | 0.13 | 0/1325 | 0.36 | 0/1797 |
| 4 | A | 0.11 | 0/608 | 0.20 | 0/825 |
| 4 | B | 0.10 | 0/608 | 0.19 | 0/825 |
| 4 | C | 0.10 | 0/608 | 0.21 | 0/825 |
| 4 | D | 0.09 | 0/608 | 0.20 | 0/825 |
| 4 | E | 0.09 | 0/608 | 0.20 | 0/825 |
| 4 | F | 0.09 | 0/608 | 0.19 | 0/825 |
| 4 | G | 0.09 | 0/608 | 0.18 | 0/825 |
| 4 | H | 0.11 | 0/608 | 0.22 | 0/825 |
| 4 | I | 0.09 | 0/608 | 0.21 | 0/825 |
| 4 | J | 0.09 | 0/608 | 0.20 | 0/825 |
| 4 | K | 0.10 | 0/608 | 0.20 | 0/825 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 4 | L | 0.09 | 0/608 | 0.19 | 0/825 |
| 4 | M | 0.09 | 0/608 | 0.19 | 0/825 |
| 4 | N | 0.08 | 0/608 | 0.17 | 0/825 |
| 4 | O | 0.10 | 0/608 | 0.20 | 0/825 |
| 4 | P | 0.10 | 0/608 | 0.19 | 0/825 |
| 4 | Q | 0.09 | 0/608 | 0.18 | 0/825 |
| 4 | R | 0.10 | 0/608 | 0.22 | 0/825 |
| 4 | S | 0.09 | 0/608 | 0.20 | 0/825 |
| 4 | T | 0.10 | 0/608 | 0.20 | 0/825 |
| 4 | U | 0.10 | 0/608 | 0.19 | 0/825 |
| 4 | V | 0.09 | 0/608 | 0.20 | 0/825 |
| 4 | W | 0.09 | 0/608 | 0.20 | 0/825 |
| 4 | X | 0.09 | 0/608 | 0.21 | 0/825 |
| 4 | Y | 0.09 | 0/608 | 0.19 | 0/825 |
| 4 | Z | 0.09 | 0/608 | 0.20 | 0/825 |
| 4 | a | 0.09 | 0/608 | 0.18 | 0/825 |
| 4 | b | 0.09 | 0/608 | 0.19 | 0/825 |
| 4 | c | 0.10 | 0/608 | 0.21 | 0/825 |
| 4 | d | 0.09 | 0/608 | 0.18 | 0/825 |
| 4 | e | 0.09 | 0/608 | 0.19 | 0/825 |
| 4 | f | 0.10 | 0/608 | 0.20 | 0/825 |
| 4 | g | 0.10 | 0/608 | 0.20 | 0/825 |
| 4 | h | 0.09 | 0/608 | 0.19 | 0/825 |
| 4 | i | 0.09 | 0/608 | 0.20 | 0/825 |
| 4 | j | 0.10 | 0/608 | 0.21 | 0/825 |
| 5 | A0 | 0.12 | 0/4222 | 0.33 | 0/5693 |
| 5 | A1 | 0.12 | 0/4222 | 0.31 | 0/5693 |
| 5 | A2 | 0.11 | 0/4214 | 0.33 | 0/5682 |
| 5 | A3 | 0.12 | 0/4214 | 0.33 | 0/5682 |
| 5 | Av | 0.11 | 0/4214 | 0.31 | 0/5682 |
| 5 | Ax | 0.11 | 0/4214 | 0.29 | 0/5682 |
| 5 | BA | 0.11 | 0/4153 | 0.31 | 0/5600 |
| 5 | BB | 0.11 | 0/4070 | 0.30 | 0/5482 |
| 5 | BD | 0.13 | 0/4214 | 0.33 | 1/5682 (0.0%) |
| 5 | BF | 0.11 | 0/4214 | 0.30 | 0/5682 |
| 5 | BG | 0.11 | 0/4116 | 0.32 | 0/5548 |
| 5 | BH | 0.11 | 0/4170 | 0.29 | 0/5626 |
| 6 | A4 | 0.12 | 0/3493 | 0.34 | 0/4731 |
| 6 | A5 | 0.10 | 0/3493 | 0.31 | 0/4731 |
| 6 | A7 | 0.11 | 0/3493 | 0.31 | 0/4731 |
| 6 | A8 | 0.11 | 0/3377 | 0.31 | 0/4573 |
| 6 | A9 | 0.11 | 0/3493 | 0.32 | 0/4731 |
| 6 | AV | 0.12 | 0/3493 | 0.32 | 0/4731 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 6 | AW | 0.11 | 0/3493 | 0.31 | 0/4731 |
| 6 | AX | 0.11 | 0/3493 | 0.30 | 0/4731 |
| 6 | AZ | 0.12 | 0/3493 | 0.34 | 2/4731 (0.0%) |
| 6 | Ac | 0.11 | 0/3493 | 0.32 | 0/4731 |
| 6 | Ad | 0.11 | 0/3493 | 0.31 | 0/4731 |
| 6 | Ae | 0.11 | 0/3493 | 0.31 | 0/4731 |
| 6 | Af | 0.11 | 0/3493 | 0.31 | 0/4731 |
| 6 | Ag | 0.12 | 0/3493 | 0.31 | 0/4731 |
| 6 | Ah | 0.11 | 0/3493 | 0.29 | 0/4731 |
| 6 | Ai | 0.10 | 0/3493 | 0.31 | 1/4731 (0.0%) |
| 6 | Aj | 0.11 | 0/3493 | 0.32 | 0/4731 |
| 6 | Ak | 0.12 | 0/3493 | 0.29 | 0/4731 |
| 6 | Am | 0.12 | 0/3493 | 0.33 | 0/4731 |
| 6 | An | 0.12 | 0/3377 | 0.31 | 0/4573 |
| 6 | Ao | 0.11 | 0/3357 | 0.31 | 0/4546 |
| 6 | Ap | 0.12 | 0/3377 | 0.31 | 0/4573 |
| 6 | Au | 0.11 | 0/3493 | 0.31 | 0/4731 |
| 6 | Aw | 0.12 | 0/3493 | 0.32 | 0/4731 |
| 6 | Ay | 0.11 | 0/3493 | 0.30 | 0/4731 |
| 6 | Az | 0.11 | 0/3493 | 0.31 | 0/4731 |
| 6 | BI | 0.11 | 0/3493 | 0.29 | 0/4731 |
| 6 | BJ | 0.12 | 0/3357 | 0.32 | 0/4546 |
| 6 | BK | 0.11 | 0/3493 | 0.31 | 0/4731 |
| 6 | BM | 0.12 | 0/3493 | 0.34 | 0/4731 |
| 7 | A6 | 0.11 | 0/2496 | 0.29 | 0/3383 |
| 7 | AY | 0.12 | 0/2493 | 0.32 | 0/3379 |
| 7 | Aa | 0.12 | 0/2496 | 0.33 | 0/3383 |
| 7 | Ab | 0.11 | 0/2496 | 0.31 | 0/3383 |
| 7 | Al | 0.13 | 0/2493 | 0.34 | 1/3379 (0.0%) |
| 7 | Aq | 0.12 | 0/2496 | 0.32 | 0/3383 |
| 7 | Ar | 0.12 | 0/2363 | 0.30 | 0/3203 |
| 7 | As | 0.11 | 0/2496 | 0.31 | 0/3383 |
| 7 | At | 0.12 | 0/2428 | 0.31 | 0/3290 |
| 7 | BC | 0.12 | 0/2496 | 0.30 | 0/3383 |
| 7 | BE | 0.12 | 0/2496 | 0.31 | 0/3383 |
| 7 | BL | 0.12 | 0/2496 | 0.32 | 0/3383 |
| 8 | AB | 0.15 | 0/2287 | 0.37 | 0/3109 |
| 8 | q | 0.16 | 0/2287 | 0.38 | 0/3109 |
| 8 | r | 0.15 | 0/2287 | 0.37 | 0/3109 |
| 8 | s | 0.15 | 0/2287 | 0.37 | 0/3109 |
| 8 | t | 0.14 | 0/2287 | 0.37 | 0/3109 |
| 8 | u | 0.15 | 0/2287 | 0.38 | 0/3109 |
| 9 | AC | 0.13 | 0/1418 | 0.33 | 0/1939 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 9 | v | 0.13 | 0/1418 | 0.32 | 0/1939 |
| 9 | w | 0.13 | 0/1418 | 0.32 | 0/1939 |
| 9 | x | 0.13 | 0/1418 | 0.34 | 0/1939 |
| 9 | y | 0.12 | 0/1418 | 0.31 | 0/1939 |
| 9 | z | 0.12 | 0/1418 | 0.31 | 0/1939 |
| 10 | AQ | 0.09 | 0/833 | 0.27 | 0/1133 |
| 10 | AR | 0.10 | 0/833 | 0.29 | 0/1133 |
| 10 | AS | 0.09 | 0/833 | 0.27 | 0/1133 |
| 10 | AT | 0.10 | 0/833 | 0.31 | 0/1133 |
| 10 | AU | 0.10 | 0/833 | 0.28 | 0/1133 |
| 11 | BN | 0.10 | 0/651 | 0.28 | 0/880 |
| 11 | BO | 0.10 | 0/651 | 0.27 | 0/880 |
| 11 | BP | 0.11 | 0/651 | 0.32 | 0/880 |
| 11 | BQ | 0.10 | 0/651 | 0.31 | 0/880 |
| 11 | BR | 0.10 | 0/651 | 0.32 | 0/880 |
| 11 | BS | 0.10 | 0/651 | 0.29 | 0/880 |
| 11 | BT | 0.11 | 0/651 | 0.30 | 0/880 |
| 11 | BU | 0.11 | 0/651 | 0.30 | 0/880 |
| 11 | BV | 0.11 | 0/651 | 0.29 | 0/880 |
| 11 | BW | 0.10 | 0/651 | 0.30 | 0/880 |
| All | All | 0.11 | 0/443809 | 0.31 | 12/602060 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 6 | A4 | 0 | 1 |
| 8 | s | 0 | 1 |
| 8 | u | 0 | 1 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | AZ | 118 | ASN | CA-C-N | 6.56 | 133.51 | 121.70 |
| 6 | AZ | 118 | ASN | C-N-CA | 6.56 | 133.51 | 121.70 |
| 2 | Bw | 482 | ASP | N-CA-C | -6.35 | 107.39 | 114.62 |
| 2 | 3 | 482 | ASP | N-CA-C | -5.92 | 107.05 | 114.56 |
| 3 | Bm | 125 | LYS | N-CA-C | -5.51 | 103.63 | 111.24 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | Al | 227 | VAL | N-CA-C | -5.36 | 108.28 | 113.53 |
| 2 | 1 | 309 | ILE | N-CA-C | -5.30 | 107.55 | 112.43 |
| 6 | Ai | 118 | ASN | N-CA-C | -5.28 | 106.78 | 113.43 |
| 2 | Bz | 482 | ASP | N-CA-C | -5.27 | 108.10 | 114.75 |
| 3 | AA | 25 | ILE | N-CA-C | -5.23 | 107.73 | 112.96 |
| 5 | BD | 317 | SER | N-CA-C | -5.20 | 108.69 | 114.62 |
| 2 | B4 | 136 | ALA | CB-CA-C | -5.04 | 110.38 | 117.23 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 6 | A4 | 254 | ILE | Peptide |
| 8 | s | 142 | GLN | Peptide |
| 8 | u | 72 | LEU | Peptide |

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 0 | 1993 | 0 | 1903 | 59 | 0 |
| 1 | k | 1993 | 0 | 1903 | 59 | 0 |
| 1 | l | 1993 | 0 | 1903 | 60 | 0 |
| 1 | m | 1993 | 0 | 1903 | 79 | 0 |
| 1 | n | 1993 | 0 | 1903 | 61 | 0 |
| 1 | p | 1993 | 0 | 1903 | 73 | 0 |
| 2 | 1 | 4985 | 0 | 4900 | 127 | 0 |
| 2 | 2 | 4985 | 0 | 4900 | 117 | 0 |
| 2 | 3 | 4985 | 0 | 4900 | 120 | 0 |
| 2 | 4 | 4985 | 0 | 4900 | 125 | 0 |
| 2 | 5 | 4985 | 0 | 4900 | 118 | 0 |
| 2 | AD | 4985 | 0 | 4900 | 117 | 0 |
| 2 | AK | 5000 | 0 | 4918 | 125 | 0 |
| 2 | AL | 5000 | 0 | 4918 | 126 | 0 |
| 2 | AM | 5000 | 0 | 4918 | 114 | 0 |
| 2 | AN | 5000 | 0 | 4918 | 118 | 0 |
| 2 | AO | 5000 | 0 | 4918 | 124 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | AP | 5000 | 0 | 4918 | 129 | 0 |
| 2 | B1 | 5000 | 0 | 4918 | 142 | 0 |
| 2 | B2 | 5000 | 0 | 4918 | 128 | 0 |
| 2 | B3 | 5000 | 0 | 4918 | 134 | 0 |
| 2 | B4 | 5000 | 0 | 4918 | 131 | 0 |
| 2 | B5 | 5000 | 0 | 4918 | 121 | 0 |
| 2 | B6 | 5000 | 0 | 4918 | 143 | 0 |
| 2 | B7 | 5000 | 0 | 4918 | 113 | 0 |
| 2 | Bp | 5000 | 0 | 4918 | 125 | 0 |
| 2 | Bq | 5000 | 0 | 4918 | 121 | 0 |
| 2 | Br | 5000 | 0 | 4918 | 117 | 0 |
| 2 | Bs | 5000 | 0 | 4918 | 126 | 0 |
| 2 | Bt | 5000 | 0 | 4918 | 136 | 0 |
| 2 | Bu | 5000 | 0 | 4918 | 136 | 0 |
| 2 | Bv | 5000 | 0 | 4918 | 133 | 0 |
| 2 | Bw | 5000 | 0 | 4918 | 119 | 0 |
| 2 | Bx | 5000 | 0 | 4918 | 115 | 0 |
| 2 | By | 5000 | 0 | 4918 | 114 | 0 |
| 2 | Bz | 5000 | 0 | 4918 | 142 | 0 |
| 3 | 6 | 1296 | 0 | 1243 | 42 | 0 |
| 3 | 7 | 1296 | 0 | 1243 | 41 | 0 |
| 3 | 8 | 1296 | 0 | 1243 | 51 | 0 |
| 3 | 9 | 1296 | 0 | 1243 | 48 | 0 |
| 3 | AA | 1296 | 0 | 1243 | 55 | 0 |
| 3 | AE | 1304 | 0 | 1255 | 44 | 0 |
| 3 | AF | 1304 | 0 | 1255 | 50 | 0 |
| 3 | AG | 1304 | 0 | 1255 | 49 | 0 |
| 3 | AH | 1304 | 0 | 1255 | 46 | 0 |
| 3 | AI | 1304 | 0 | 1255 | 45 | 0 |
| 3 | AJ | 1304 | 0 | 1255 | 45 | 0 |
| 3 | BX | 1304 | 0 | 1255 | 51 | 0 |
| 3 | BY | 1304 | 0 | 1255 | 46 | 0 |
| 3 | BZ | 1304 | 0 | 1255 | 39 | 0 |
| 3 | Ba | 1304 | 0 | 1255 | 40 | 0 |
| 3 | Bb | 1304 | 0 | 1255 | 47 | 0 |
| 3 | Bc | 1304 | 0 | 1255 | 39 | 0 |
| 3 | Bd | 1304 | 0 | 1255 | 50 | 0 |
| 3 | Be | 1304 | 0 | 1255 | 44 | 0 |
| 3 | Bf | 1304 | 0 | 1255 | 44 | 0 |
| 3 | Bg | 1304 | 0 | 1255 | 52 | 0 |
| 3 | Bh | 1304 | 0 | 1255 | 55 | 0 |
| 3 | Bi | 1304 | 0 | 1255 | 49 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | Bj | 1304 | 0 | 1255 | 48 | 0 |
| 3 | Bk | 1304 | 0 | 1255 | 51 | 0 |
| 3 | Bl | 1304 | 0 | 1255 | 40 | 0 |
| 3 | Bm | 1304 | 0 | 1255 | 37 | 0 |
| 3 | Bn | 1304 | 0 | 1255 | 55 | 0 |
| 3 | Bo | 1304 | 0 | 1255 | 44 | 0 |
| 3 | o | 1296 | 0 | 1243 | 50 | 0 |
| 4 | A | 601 | 0 | 600 | 14 | 0 |
| 4 | B | 601 | 0 | 600 | 7 | 0 |
| 4 | C | 601 | 0 | 600 | 8 | 0 |
| 4 | D | 601 | 0 | 600 | 7 | 0 |
| 4 | E | 601 | 0 | 600 | 5 | 0 |
| 4 | F | 601 | 0 | 600 | 10 | 0 |
| 4 | G | 601 | 0 | 600 | 12 | 0 |
| 4 | H | 601 | 0 | 600 | 15 | 0 |
| 4 | I | 601 | 0 | 600 | 9 | 0 |
| 4 | J | 601 | 0 | 600 | 8 | 0 |
| 4 | K | 601 | 0 | 600 | 15 | 0 |
| 4 | L | 601 | 0 | 600 | 16 | 0 |
| 4 | M | 601 | 0 | 600 | 16 | 0 |
| 4 | N | 601 | 0 | 600 | 7 | 0 |
| 4 | O | 601 | 0 | 600 | 12 | 0 |
| 4 | P | 601 | 0 | 600 | 10 | 0 |
| 4 | Q | 601 | 0 | 600 | 10 | 0 |
| 4 | R | 601 | 0 | 600 | 11 | 0 |
| 4 | S | 601 | 0 | 600 | 8 | 0 |
| 4 | T | 601 | 0 | 600 | 8 | 0 |
| 4 | U | 601 | 0 | 600 | 13 | 0 |
| 4 | V | 601 | 0 | 600 | 11 | 0 |
| 4 | W | 601 | 0 | 600 | 13 | 0 |
| 4 | X | 601 | 0 | 600 | 10 | 0 |
| 4 | Y | 601 | 0 | 600 | 8 | 0 |
| 4 | Z | 601 | 0 | 600 | 10 | 0 |
| 4 | a | 601 | 0 | 600 | 11 | 0 |
| 4 | b | 601 | 0 | 600 | 10 | 0 |
| 4 | c | 601 | 0 | 600 | 9 | 0 |
| 4 | d | 601 | 0 | 600 | 9 | 0 |
| 4 | e | 601 | 0 | 600 | 8 | 0 |
| 4 | f | 601 | 0 | 600 | 12 | 0 |
| 4 | g | 601 | 0 | 600 | 12 | 0 |
| 4 | h | 601 | 0 | 600 | 14 | 0 |
| 4 | i | 601 | 0 | 600 | 15 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | j | 601 | 0 | 600 | 11 | 0 |
| 5 | A0 | 4140 | 0 | 4075 | 101 | 0 |
| 5 | A1 | 4140 | 0 | 4076 | 101 | 0 |
| 5 | A2 | 4132 | 0 | 4070 | 92 | 0 |
| 5 | A3 | 4132 | 0 | 4070 | 130 | 0 |
| 5 | Av | 4132 | 0 | 4070 | 106 | 0 |
| 5 | Ax | 4132 | 0 | 4070 | 91 | 0 |
| 5 | BA | 4074 | 0 | 4013 | 103 | 0 |
| 5 | BB | 3995 | 0 | 3948 | 119 | 0 |
| 5 | BD | 4132 | 0 | 4071 | 81 | 0 |
| 5 | BF | 4132 | 0 | 4070 | 110 | 0 |
| 5 | BG | 4039 | 0 | 3976 | 108 | 0 |
| 5 | BH | 4091 | 0 | 4018 | 91 | 0 |
| 6 | A4 | 3425 | 0 | 3371 | 78 | 0 |
| 6 | A5 | 3425 | 0 | 3371 | 93 | 0 |
| 6 | A7 | 3425 | 0 | 3371 | 78 | 0 |
| 6 | A8 | 3311 | 0 | 3271 | 94 | 0 |
| 6 | A9 | 3425 | 0 | 3371 | 98 | 0 |
| 6 | AV | 3425 | 0 | 3371 | 105 | 0 |
| 6 | AW | 3425 | 0 | 3371 | 76 | 0 |
| 6 | AX | 3425 | 0 | 3371 | 80 | 0 |
| 6 | AZ | 3425 | 0 | 3371 | 87 | 0 |
| 6 | Ac | 3425 | 0 | 3371 | 79 | 0 |
| 6 | Ad | 3425 | 0 | 3371 | 68 | 0 |
| 6 | Ae | 3425 | 0 | 3371 | 87 | 0 |
| 6 | Af | 3425 | 0 | 3371 | 76 | 0 |
| 6 | Ag | 3425 | 0 | 3371 | 88 | 0 |
| 6 | Ah | 3425 | 0 | 3371 | 81 | 0 |
| 6 | Ai | 3425 | 0 | 3371 | 72 | 0 |
| 6 | Aj | 3425 | 0 | 3371 | 77 | 0 |
| 6 | Ak | 3425 | 0 | 3371 | 91 | 0 |
| 6 | Am | 3425 | 0 | 3371 | 93 | 0 |
| 6 | An | 3311 | 0 | 3271 | 85 | 0 |
| 6 | Ao | 3291 | 0 | 3253 | 90 | 0 |
| 6 | Ap | 3311 | 0 | 3271 | 84 | 0 |
| 6 | Au | 3425 | 0 | 3371 | 97 | 0 |
| 6 | Aw | 3425 | 0 | 3371 | 72 | 0 |
| 6 | Ay | 3425 | 0 | 3371 | 79 | 0 |
| 6 | Az | 3425 | 0 | 3371 | 79 | 0 |
| 6 | BI | 3425 | 0 | 3371 | 89 | 0 |
| 6 | BJ | 3291 | 0 | 3253 | 95 | 0 |
| 6 | BK | 3425 | 0 | 3371 | 102 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 6 | BM | 3425 | 0 | 3371 | 89 | 0 |
| 7 | A6 | 2438 | 0 | 2356 | 79 | 0 |
| 7 | AY | 2435 | 0 | 2352 | 79 | 0 |
| 7 | Aa | 2438 | 0 | 2356 | 67 | 0 |
| 7 | Ab | 2438 | 0 | 2356 | 70 | 0 |
| 7 | Al | 2435 | 0 | 2352 | 85 | 0 |
| 7 | Aq | 2438 | 0 | 2356 | 89 | 0 |
| 7 | Ar | 2310 | 0 | 2245 | 78 | 0 |
| 7 | As | 2438 | 0 | 2356 | 65 | 0 |
| 7 | At | 2371 | 0 | 2291 | 65 | 0 |
| 7 | BC | 2438 | 0 | 2356 | 85 | 0 |
| 7 | BE | 2438 | 0 | 2356 | 85 | 0 |
| 7 | BL | 2438 | 0 | 2357 | 78 | 0 |
| 8 | AB | 2227 | 0 | 2152 | 70 | 0 |
| 8 | q | 2227 | 0 | 2152 | 75 | 0 |
| 8 | r | 2227 | 0 | 2152 | 86 | 0 |
| 8 | s | 2227 | 0 | 2152 | 75 | 0 |
| 8 | t | 2227 | 0 | 2152 | 76 | 0 |
| 8 | u | 2227 | 0 | 2152 | 62 | 0 |
| 9 | AC | 1383 | 0 | 1344 | 35 | 0 |
| 9 | v | 1383 | 0 | 1344 | 40 | 0 |
| 9 | w | 1383 | 0 | 1344 | 31 | 0 |
| 9 | x | 1383 | 0 | 1344 | 21 | 0 |
| 9 | y | 1383 | 0 | 1344 | 38 | 0 |
| 9 | z | 1383 | 0 | 1344 | 32 | 0 |
| 10 | AQ | 805 | 0 | 763 | 18 | 0 |
| 10 | AR | 805 | 0 | 763 | 14 | 0 |
| 10 | AS | 805 | 0 | 763 | 11 | 0 |
| 10 | AT | 805 | 0 | 763 | 15 | 0 |
| 10 | AU | 805 | 0 | 763 | 16 | 0 |
| 11 | BN | 636 | 0 | 612 | 14 | 0 |
| 11 | BO | 636 | 0 | 612 | 10 | 0 |
| 11 | BP | 636 | 0 | 612 | 19 | 0 |
| 11 | BQ | 636 | 0 | 612 | 12 | 0 |
| 11 | BR | 636 | 0 | 612 | 12 | 0 |
| 11 | BS | 636 | 0 | 612 | 14 | 0 |
| 11 | BT | 636 | 0 | 612 | 13 | 0 |
| 11 | BU | 636 | 0 | 612 | 13 | 0 |
| 11 | BV | 636 | 0 | 612 | 8 | 0 |
| 11 | BW | 636 | 0 | 612 | 16 | 0 |
| All | All | 435087 | 0 | 426149 | 9490 | 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 11.

All (9490) 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:l:25:GLU:HG2 | 1:l:29:PRO:HD3 | 1.54 | 0.90 |
| 3:Bk:104:PRO:O | 3:Bk:108:LYS:HB2 | 1.72 | 0.90 |
| 1:m:25:GLU:HG2 | 1:m:29:PRO:HD3 | 1.53 | 0.89 |
| 1:n:25:GLU:HG2 | 1:n:29:PRO:HD3 | 1.55 | 0.87 |
| 1:k:68:PRO:HA | 1:k:75:ASP:HB2 | 1.57 | 0.86 |
| 1:m:68:PRO:HA | 1:m:75:ASP:HB2 | 1.59 | 0.84 |
| 2:AM:400:ARG:NH1 | 2:AM:403:CYS:SG | 2.50 | 0.84 |
| 2:3:252:LEU:HB3 | 2:3:336:GLY:HA2 | 1.58 | 0.83 |
| 2:B4:57:PRO:HB3 | 2:B4:62:ALA:HA | 1.61 | 0.83 |
| 1:n:68:PRO:HA | 1:n:75:ASP:HB2 | 1.58 | 0.82 |
| 6:Ag:101:ARG:HD3 | 6:Ak:146:PRO:HD3 | 1.61 | 0.82 |
| 7:Aa:87:ILE:HD13 | 7:Aa:159:PRO:HG2 | 1.61 | 0.82 |
| 3:o:5:ASP:O | 3:o:7:THR:N | 2.13 | 0.82 |
| 1:0:25:GLU:HG2 | 1:0:29:PRO:HD3 | 1.62 | 0.81 |
| 2:Bp:256:PRO:HG2 | 2:Bp:339:THR:H | 1.46 | 0.81 |
| 1:k:25:GLU:HG2 | 1:k:29:PRO:HD3 | 1.62 | 0.81 |
| 2:AK:400:ARG:NH1 | 2:AK:403:CYS:SG | 2.54 | 0.80 |
| 2:AN:228:GLY:HA2 | 2:AN:345:SER:HB3 | 1.62 | 0.80 |
| 3:9:5:ASP:O | 3:9:7:THR:N | 2.15 | 0.80 |
| 6:A7:110:ASP:OD1 | 6:A7:110:ASP:N | 2.14 | 0.80 |
| 2:Bx:135:ASP:HB3 | 2:Bx:139:LYS:HB2 | 1.64 | 0.79 |
| 7:BC:95:ILE:HD11 | 7:BE:107:PHE:HB3 | 1.64 | 0.79 |
| 3:BY:64:ARG:HH12 | 3:Bb:95:GLN:HG2 | 1.48 | 0.79 |
| 2:Bw:400:ARG:NH1 | 2:Bw:403:CYS:SG | 2.56 | 0.79 |
| 3:AA:5:ASP:O | 3:AA:7:THR:N | 2.15 | 0.79 |
| 2:AP:400:ARG:NH1 | 2:AP:403:CYS:SG | 2.55 | 0.79 |
| 4:d:48:THR:HG21 | 4:i:47:PRO:HB2 | 1.64 | 0.79 |
| 7:AY:138:LEU:HB3 | 5:BD:273:ILE:HD11 | 1.65 | 0.79 |
| 6:A8:96:MET:HG2 | 6:A9:117:MET:HE3 | 1.64 | 0.79 |
| 2:Bx:400:ARG:NH1 | 2:Bx:403:CYS:SG | 2.56 | 0.79 |
| 5:A1:102:TYR:O | 5:BB:408:ARG:NH1 | 2.16 | 0.78 |
| 6:A9:237:GLU:HB3 | 6:Au:465:LYS:HB3 | 1.63 | 0.78 |
| 2:Bq:456:TYR:HB3 | 2:Bq:504:LYS:HB3 | 1.65 | 0.78 |
| 4:V:47:PRO:HB2 | 4:f:48:THR:HG21 | 1.66 | 0.78 |
| 3:8:5:ASP:O | 3:8:7:THR:N | 2.16 | 0.78 |
| 1:p:25:GLU:HG2 | 1:p:29:PRO:HD3 | 1.66 | 0.78 |
| 2:Bq:256:PRO:HG2 | 2:Bq:339:THR:H | 1.49 | 0.77 |
| 2:Bx:256:PRO:HG2 | 2:Bx:339:THR:H | 1.49 | 0.77 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:q:210:ARG:HD3 | 8:q:240:ARG:HG2 | 1.65 | 0.77 |
| 2:B7:481:THR:HB | 2:B7:555:ARG:HH12 | 1.49 | 0.77 |
| 6:BJ:383:VAL:HG21 | 6:BJ:425:ILE:HG12 | 1.66 | 0.77 |
| 6:Au:383:VAL:HG21 | 6:Au:425:ILE:HG12 | 1.66 | 0.77 |
| 2:Bp:400:ARG:NH1 | 2:Bp:403:CYS:SG | 2.56 | 0.77 |
| 6:Ak:264:ARG:NH2 | 6:Ao:152:ALA:O | 2.18 | 0.77 |
| 6:A9:241:GLY:HA3 | 11:BO:43:GLY:HA2 | 1.65 | 0.77 |
| 7:Al:12:LEU:HD13 | 7:Al:38:ILE:HD12 | 1.66 | 0.77 |
| 2:B2:57:PRO:HB3 | 2:B2:62:ALA:HA | 1.66 | 0.77 |
| 6:BM:110:ASP:N | 6:BM:110:ASP:OD1 | 2.17 | 0.77 |
| 3:6:5:ASP:O | 3:6:7:THR:N | 2.18 | 0.77 |
| 2:Bw:228:GLY:HA2 | 2:Bw:345:SER:HB3 | 1.66 | 0.77 |
| 3:AA:17:ARG:HH22 | 9:y:47:THR:HG21 | 1.50 | 0.77 |
| 3:Bk:37:LYS:HZ1 | 3:Bk:74:MET:HG2 | 1.49 | 0.77 |
| 2:Bq:400:ARG:NH1 | 2:Bq:403:CYS:SG | 2.58 | 0.77 |
| 2:Bs:400:ARG:NH1 | 2:Bs:403:CYS:SG | 2.59 | 0.77 |
| 2:AL:121:VAL:HG22 | 2:AL:166:ASN:HB3 | 1.67 | 0.76 |
| 2:B5:400:ARG:NH1 | 2:B5:403:CYS:SG | 2.58 | 0.76 |
| 2:B6:400:ARG:NH1 | 2:B6:403:CYS:SG | 2.56 | 0.76 |
| 3:8:114:ARG:HB3 | 3:8:126:GLU:HG3 | 1.67 | 0.76 |
| 5:A1:282:ARG:HA | 5:BB:278:ARG:HH22 | 1.50 | 0.76 |
| 6:A4:131:TYR:HB3 | 6:A4:250:MET:HG2 | 1.67 | 0.76 |
| 6:AZ:383:VAL:HG21 | 6:AZ:425:ILE:HG12 | 1.67 | 0.76 |
| 2:B1:400:ARG:NH1 | 2:B1:403:CYS:SG | 2.59 | 0.76 |
| 6:A9:114:VAL:HG11 | 5:Ax:67:PRO:HG3 | 1.68 | 0.76 |
| 2:B1:44:VAL:HG11 | 2:B1:50:LEU:HB3 | 1.66 | 0.76 |
| 1:p:68:PRO:HA | 1:p:75:ASP:HB2 | 1.65 | 0.76 |
| 2:AO:560:LEU:HD21 | 2:AO:601:ILE:HD11 | 1.67 | 0.76 |
| 3:o:114:ARG:HG2 | 3:o:126:GLU:HG3 | 1.67 | 0.76 |
| 3:Bn:82:ARG:HH12 | 3:Bn:138:GLY:HA2 | 1.50 | 0.76 |
| 2:1:617:VAL:HG13 | 2:1:622:GLU:HB2 | 1.68 | 0.76 |
| 7:Al:55:LYS:HE3 | 7:BE:173:MET:HE1 | 1.68 | 0.76 |
| 5:A1:303:HIS:NE2 | 7:Aq:161:PHE:O | 2.19 | 0.76 |
| 2:AK:228:GLY:HA2 | 2:AK:345:SER:HB3 | 1.68 | 0.76 |
| 6:Aj:264:ARG:NH2 | 6:An:152:ALA:O | 2.18 | 0.76 |
| 2:Bp:560:LEU:HD21 | 2:Bp:601:ILE:HD11 | 1.67 | 0.76 |
| 6:AV:110:ASP:N | 6:AV:110:ASP:OD1 | 2.19 | 0.75 |
| 6:A7:76:ALA:HB1 | 6:A8:496:ILE:HG22 | 1.68 | 0.75 |
| 6:Au:105:ASN:HB2 | 6:Au:412:VAL:HG23 | 1.68 | 0.75 |
| 2:Bq:135:ASP:HB3 | 2:Bq:139:LYS:HB2 | 1.67 | 0.75 |
| 6:A5:344:ARG:HD2 | 6:AW:344:ARG:HH21 | 1.51 | 0.75 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BD:158:PHE:HB2 | 5:BD:236:VAL:HB | 1.67 | 0.75 |
| 6:AV:237:GLU:HG2 | 6:AV:246:PRO:HA | 1.69 | 0.75 |
| 5:Av:72:THR:HG23 | 5:Av:155:ARG:HH21 | 1.51 | 0.75 |
| 2:AP:493:GLY:HA2 | 2:Bp:572:LEU:HD23 | 1.68 | 0.75 |
| 6:BK:322:THR:HG22 | 6:BK:359:LYS:HG2 | 1.67 | 0.75 |
| 2:Bx:209:ASP:N | 2:Bx:209:ASP:OD1 | 2.19 | 0.75 |
| 2:AO:378:CYS:HB2 | 2:AO:410:PRO:HA | 1.68 | 0.75 |
| 7:Al:201:THR:O | 7:Al:229:ARG:NH2 | 2.19 | 0.75 |
| 6:Az:241:GLY:HA3 | 11:BU:43:GLY:HA2 | 1.68 | 0.75 |
| 1:k:216:ASP:HB3 | 1:k:219:ALA:HB2 | 1.69 | 0.74 |
| 2:B3:617:VAL:HG13 | 2:B3:622:GLU:HB2 | 1.70 | 0.74 |
| 4:Z:48:THR:HG21 | 4:e:47:PRO:HB2 | 1.69 | 0.74 |
| 3:6:114:ARG:HG2 | 3:6:126:GLU:HG3 | 1.69 | 0.74 |
| 5:A0:232:LYS:O | 5:A0:234:ALA:N | 2.20 | 0.74 |
| 5:Ax:214:SER:HB3 | 5:Ax:217:CYS:HB2 | 1.69 | 0.74 |
| 6:AX:383:VAL:HG21 | 6:AX:425:ILE:HG12 | 1.70 | 0.74 |
| 2:B1:57:PRO:HB3 | 2:B1:62:ALA:HA | 1.69 | 0.74 |
| 2:B3:400:ARG:NH1 | 2:B3:403:CYS:SG | 2.59 | 0.74 |
| 6:A7:131:TYR:HB3 | 6:A7:250:MET:HG2 | 1.70 | 0.74 |
| 2:AD:453:ASN:HD21 | 2:AD:505:LEU:HG | 1.53 | 0.74 |
| 2:B2:256:PRO:HG2 | 2:B2:339:THR:H | 1.53 | 0.74 |
| 5:A0:255:HIS:NE2 | 7:At:130:GLY:O | 2.21 | 0.74 |
| 5:A3:232:LYS:O | 5:A3:234:ALA:N | 2.20 | 0.74 |
| 6:A9:383:VAL:HG21 | 6:A9:425:ILE:HG12 | 1.70 | 0.74 |
| 6:An:88:VAL:HG11 | 6:An:278:LEU:HD21 | 1.68 | 0.74 |
| 2:B2:32:LYS:HG2 | 2:B2:350:VAL:HG21 | 1.70 | 0.74 |
| 2:B7:559:MET:SD | 2:B7:563:ASN:ND2 | 2.61 | 0.74 |
| 5:BA:72:THR:HG23 | 5:BA:155:ARG:HH21 | 1.52 | 0.74 |
| 6:BM:383:VAL:HG21 | 6:BM:425:ILE:HG12 | 1.69 | 0.74 |
| 5:A0:60:THR:HA | 5:A0:64:SER:HB3 | 1.68 | 0.74 |
| 6:Ac:383:VAL:HG21 | 6:Ac:425:ILE:HG12 | 1.68 | 0.74 |
| 6:Ak:110:ASP:OD1 | 6:Ak:110:ASP:N | 2.21 | 0.74 |
| 1:p:216:ASP:HB3 | 1:p:219:ALA:HB2 | 1.68 | 0.74 |
| 2:1:488:TRP:O | 2:1:552:ASN:ND2 | 2.21 | 0.73 |
| 2:Br:110:TYR:H | 2:Br:138:GLY:HA3 | 1.52 | 0.73 |
| 7:BL:12:LEU:HD13 | 7:BL:38:ILE:HD12 | 1.69 | 0.73 |
| 7:BL:201:THR:O | 7:BL:229:ARG:NH2 | 2.21 | 0.73 |
| 6:Af:452:PRO:HA | 6:Af:477:TYR:HA | 1.68 | 0.73 |
| 6:AV:76:ALA:HB1 | 6:AZ:496:ILE:HG12 | 1.68 | 0.73 |
| 6:Ak:465:LYS:HB3 | 6:Az:237:GLU:HB3 | 1.69 | 0.73 |
| 6:Aw:121:THR:HG23 | 6:BM:79:ILE:HG23 | 1.69 | 0.73 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AP:92:SER:HB3 | 2:AP:340:LEU:HB3 | 1.69 | 0.73 |
| 6:Af:93:PRO:HB2 | 6:Aj:123:GLN:HB3 | 1.70 | 0.73 |
| 5:A1:204:GLU:HB2 | 5:A1:232:LYS:HB2 | 1.71 | 0.73 |
| 6:A9:237:GLU:HG2 | 6:A9:246:PRO:HA | 1.71 | 0.73 |
| 6:Ak:115:GLN:NE2 | 6:Ak:444:MET:SD | 2.62 | 0.73 |
| 5:BB:161:ILE:HB | 5:BB:173:GLU:HB3 | 1.70 | 0.73 |
| 6:BI:383:VAL:HG21 | 6:BI:425:ILE:HG12 | 1.70 | 0.73 |
| 6:A9:154:PHE:O | 6:A9:248:ASN:ND2 | 2.20 | 0.73 |
| 2:AL:453:ASN:HB2 | 2:AL:506:ALA:HB3 | 1.71 | 0.73 |
| 8:s:212:THR:HG1 | 8:s:235:SER:HG | 1.32 | 0.73 |
| 7:Aa:117:ILE:HG23 | 7:Aa:119:GLY:H | 1.54 | 0.73 |
| 6:Ac:237:GLU:HB3 | 6:BI:465:LYS:HB3 | 1.68 | 0.73 |
| 6:Ai:101:ARG:HD3 | 6:Am:146:PRO:HD3 | 1.71 | 0.73 |
| 2:B6:256:PRO:HG2 | 2:B6:339:THR:H | 1.53 | 0.73 |
| 3:Be:28:LEU:HD22 | 3:Be:84:LYS:HB3 | 1.69 | 0.73 |
| 6:AX:146:PRO:HD3 | 6:BK:101:ARG:HD3 | 1.71 | 0.72 |
| 6:Af:255:ASP:N | 6:Af:255:ASP:OD1 | 2.22 | 0.72 |
| 6:Aj:264:ARG:NH1 | 6:Aj:477:TYR:OH | 2.21 | 0.72 |
| 2:B5:256:PRO:HG2 | 2:B5:339:THR:H | 1.53 | 0.72 |
| 1:l:68:PRO:HA | 1:l:75:ASP:HB2 | 1.70 | 0.72 |
| 2:AN:400:ARG:NH1 | 2:AN:403:CYS:SG | 2.61 | 0.72 |
| 6:Ag:264:ARG:NH2 | 6:Ak:152:ALA:O | 2.21 | 0.72 |
| 6:BM:422:ARG:NH1 | 6:BM:424:TYR:OH | 2.23 | 0.72 |
| 1:p:155:TYR:HB2 | 1:p:158:PHE:HA | 1.70 | 0.72 |
| 6:Ap:358:ASP:OD2 | 6:BI:384:ASN:ND2 | 2.22 | 0.72 |
| 3:Bi:19:ASN:OD1 | 3:Bi:19:ASN:N | 2.22 | 0.72 |
| 2:Bt:228:GLY:HA2 | 2:Bt:345:SER:HB3 | 1.70 | 0.72 |
| 2:2:368:VAL:HG23 | 2:2:400:ARG:HH21 | 1.54 | 0.72 |
| 2:4:488:TRP:O | 2:4:552:ASN:ND2 | 2.22 | 0.72 |
| 6:Ad:299:MET:HA | 6:Ad:302:ILE:HD12 | 1.70 | 0.72 |
| 2:B6:32:LYS:HG2 | 2:B6:350:VAL:HG21 | 1.72 | 0.72 |
| 11:BW:5:ARG:HH21 | 11:BW:33:PRO:HB3 | 1.54 | 0.72 |
| 2:Bz:566:ARG:HA | 2:Bz:569:LYS:HD2 | 1.71 | 0.72 |
| 6:Aj:383:VAL:HG21 | 6:Aj:425:ILE:HG12 | 1.71 | 0.72 |
| 6:An:163:PHE:HB2 | 6:An:179:THR:HG23 | 1.72 | 0.72 |
| 7:BL:81:VAL:HG12 | 7:BL:188:THR:HG22 | 1.70 | 0.72 |
| 6:BK:106:LEU:HD21 | 6:BK:300:LEU:HD23 | 1.69 | 0.72 |
| 6:A7:264:ARG:NH2 | 6:A8:152:ALA:O | 2.23 | 0.72 |
| 5:BA:328:MET:SD | 5:BH:282:ARG:NH1 | 2.62 | 0.72 |
| 3:6:54:MET:O | 3:6:55:ASN:ND2 | 2.22 | 0.72 |
| 7:BE:117:ILE:HG21 | 7:BE:141:PHE:HB2 | 1.70 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A0:79:TYR:OH | 5:A0:255:HIS:ND1 | 2.23 | 0.72 |
| 5:A2:458:LYS:NZ | 5:BF:451:ASP:O | 2.22 | 0.72 |
| 7:BC:127:ARG:HG2 | 6:BJ:458:PRO:HG2 | 1.70 | 0.72 |
| 2:Bt:256:PRO:HG2 | 2:Bt:339:THR:H | 1.55 | 0.72 |
| 2:Bv:379:ALA:HA | 2:Bv:411:ARG:HB2 | 1.72 | 0.72 |
| 6:AW:255:ASP:OD1 | 6:AW:255:ASP:N | 2.20 | 0.72 |
| 2:B4:456:TYR:HB3 | 2:B4:503:ILE:HG23 | 1.71 | 0.72 |
| 5:BH:474:GLU:HG3 | 5:BH:475:PRO:HD3 | 1.72 | 0.72 |
| 2:Bt:493:GLY:HA2 | 2:Bu:572:LEU:HD23 | 1.71 | 0.72 |
| 2:Bz:560:LEU:HD21 | 2:Bz:601:ILE:HD11 | 1.72 | 0.72 |
| 6:AX:107:ILE:O | 6:AX:303:ASN:ND2 | 2.22 | 0.71 |
| 7:Aa:104:TYR:O | 7:Aa:106:TRP:N | 2.22 | 0.71 |
| 6:Aw:383:VAL:HG21 | 6:Aw:425:ILE:HG12 | 1.71 | 0.71 |
| 2:AO:135:ASP:HB3 | 2:AO:139:LYS:HB2 | 1.72 | 0.71 |
| 2:B7:57:PRO:HB3 | 2:B7:62:ALA:HA | 1.71 | 0.71 |
| 4:X:48:THR:HG21 | 4:c:47:PRO:HB2 | 1.71 | 0.71 |
| 4:Y:48:THR:HG21 | 4:d:47:PRO:HB2 | 1.73 | 0.71 |
| 6:AZ:79:ILE:HG23 | 6:Ad:121:THR:HG23 | 1.71 | 0.71 |
| 6:Au:152:ALA:O | 6:BJ:264:ARG:NH2 | 2.23 | 0.71 |
| 6:BM:241:GLY:HA3 | 11:BQ:43:GLY:HA2 | 1.72 | 0.71 |
| 8:t:28:ARG:NH2 | 8:t:129:ASP:OD2 | 2.22 | 0.71 |
| 7:Ab:308:VAL:HG12 | 5:Av:332:GLU:HG2 | 1.72 | 0.71 |
| 6:Ap:377:ILE:HG23 | 6:Ap:435:THR:HG23 | 1.73 | 0.71 |
| 1:k:155:TYR:HB2 | 1:k:158:PHE:HA | 1.73 | 0.71 |
| 8:u:46:LYS:HB3 | 8:u:51:MET:HG3 | 1.73 | 0.71 |
| 2:5:488:TRP:O | 2:5:552:ASN:ND2 | 2.23 | 0.71 |
| 6:Ae:496:ILE:HG12 | 6:Ay:76:ALA:HB1 | 1.73 | 0.71 |
| 6:BK:237:GLU:HG2 | 6:BK:246:PRO:HA | 1.71 | 0.71 |
| 2:3:471:ALA:HA | 2:3:474:ILE:HG12 | 1.72 | 0.71 |
| 3:9:17:ARG:HH22 | 9:x:47:THR:HG21 | 1.56 | 0.71 |
| 2:AO:273:PRO:HB3 | 2:AO:278:GLN:HB3 | 1.73 | 0.71 |
| 6:Aj:110:ASP:N | 6:Aj:110:ASP:OD1 | 2.24 | 0.71 |
| 7:BC:199:GLY:O | 7:BC:204:TYR:OH | 2.08 | 0.71 |
| 3:Bn:113:VAL:HG13 | 3:Bn:127:ILE:HG23 | 1.73 | 0.71 |
| 4:M:48:THR:HG21 | 4:N:47:PRO:HB2 | 1.71 | 0.71 |
| 6:A8:367:GLN:HB3 | 6:A8:511:ALA:HB1 | 1.73 | 0.71 |
| 6:A8:377:ILE:HG23 | 6:A8:435:THR:HG23 | 1.72 | 0.71 |
| 6:A9:340:ILE:HG13 | 6:A9:343:ALA:H | 1.56 | 0.71 |
| 2:AM:383:LEU:HD11 | 2:AM:436:TYR:HD1 | 1.54 | 0.71 |
| 7:BE:12:LEU:HD13 | 7:BE:38:ILE:HD12 | 1.73 | 0.71 |
| 6:AX:79:ILE:HG23 | 6:Az:121:THR:HB | 1.72 | 0.70 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Ab:70:LYS:NZ | 5:Ax:318:THR:O | 2.21 | 0.70 |
| 6:AX:131:TYR:HB3 | 6:AX:250:MET:HG2 | 1.74 | 0.70 |
| 6:Ac:268:ALA:HB1 | 6:Ac:290:LEU:HD13 | 1.72 | 0.70 |
| 6:Au:268:ALA:HB1 | 6:Au:290:LEU:HD13 | 1.73 | 0.70 |
| 2:Bu:256:PRO:HG2 | 2:Bu:339:THR:H | 1.56 | 0.70 |
| 1:0:199:LEU:O | 1:0:202:ASN:ND2 | 2.23 | 0.70 |
| 2:Br:166:ASN:N | 2:Br:166:ASN:OD1 | 2.24 | 0.70 |
| 4:E:47:PRO:HB2 | 4:U:48:THR:HG21 | 1.72 | 0.70 |
| 5:A0:267:LEU:HD12 | 5:A0:365:PHE:HD2 | 1.55 | 0.70 |
| 5:BB:277:THR:HG23 | 5:BB:278:ARG:HG3 | 1.73 | 0.70 |
| 3:Bh:113:VAL:HG13 | 3:Bh:127:ILE:HG23 | 1.74 | 0.70 |
| 6:Am:131:TYR:HB3 | 6:Am:250:MET:HG2 | 1.74 | 0.70 |
| 7:Aq:122:GLY:HA2 | 7:Aq:126:ASN:HB3 | 1.72 | 0.70 |
| 2:B3:104:SER:HG | 2:B3:183:THR:HG1 | 1.34 | 0.70 |
| 2:B3:423:VAL:HG11 | 2:B3:513:GLN:HB3 | 1.72 | 0.70 |
| 3:Bi:113:VAL:HG13 | 3:Bi:127:ILE:HG23 | 1.72 | 0.70 |
| 5:A0:64:SER:HB2 | 6:BJ:410:LYS:HG2 | 1.74 | 0.70 |
| 6:A7:268:ALA:HB1 | 6:A7:290:LEU:HD23 | 1.72 | 0.70 |
| 2:AK:470:LEU:HD23 | 2:AK:525:VAL:HG21 | 1.74 | 0.70 |
| 7:Aq:201:THR:O | 7:Aq:229:ARG:NH2 | 2.24 | 0.70 |
| 7:Aq:264:ALA:HA | 7:Aq:267:GLN:HB2 | 1.73 | 0.70 |
| 5:BH:469:MET:HE3 | 5:BH:490:ILE:HG23 | 1.73 | 0.70 |
| 3:BZ:137:VAL:HB | 3:BZ:155:VAL:HG13 | 1.73 | 0.70 |
| 2:Bw:66:MET:HB3 | 2:Bw:468:VAL:HG11 | 1.73 | 0.70 |
| 8:r:99:GLN:HE21 | 8:r:102:ALA:HA | 1.57 | 0.70 |
| 6:A4:105:ASN:ND2 | 6:A4:409:THR:O | 2.25 | 0.70 |
| 6:AW:278:LEU:HD12 | 6:AW:286:ALA:HB2 | 1.73 | 0.70 |
| 5:Av:6:LEU:O | 5:Av:8:LEU:N | 2.25 | 0.70 |
| 3:Bj:28:LEU:HD22 | 3:Bj:84:LYS:HB3 | 1.74 | 0.70 |
| 2:3:617:VAL:HG13 | 2:3:622:GLU:HB2 | 1.73 | 0.70 |
| 6:A9:235:LEU:O | 6:A9:245:ASN:ND2 | 2.24 | 0.70 |
| 6:Af:345:TRP:CG | 6:Af:346:ALA:H | 2.09 | 0.70 |
| 6:Ao:377:ILE:HG23 | 6:Ao:435:THR:HG23 | 1.72 | 0.70 |
| 2:B4:116:ILE:HG12 | 2:B4:171:ILE:HG12 | 1.74 | 0.70 |
| 3:Bk:63:ASP:HB3 | 3:Bo:147:ASN:HB3 | 1.74 | 0.70 |
| 3:7:54:MET:O | 3:7:55:ASN:ND2 | 2.23 | 0.70 |
| 2:AM:47:GLU:OE2 | 2:AM:73:GLN:NE2 | 2.25 | 0.70 |
| 6:Am:115:GLN:NE2 | 6:Am:444:MET:SD | 2.65 | 0.70 |
| 2:B3:256:PRO:HG2 | 2:B3:339:THR:H | 1.57 | 0.70 |
| 11:BW:11:LYS:HG3 | 11:BW:27:GLU:HG2 | 1.73 | 0.70 |
| 2:Bp:454:TYR:HB3 | 2:Bp:467:TRP:HD1 | 1.57 | 0.70 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bw:118:VAL:HB | 2:Bw:126:GLU:HB3 | 1.74 | 0.70 |
| 1:m:216:ASP:HB3 | 1:m:219:ALA:HB2 | 1.72 | 0.70 |
| 6:A4:503:ILE:HG13 | 6:A4:507:LEU:HD12 | 1.73 | 0.70 |
| 7:At:88:LEU:HD23 | 7:At:183:ILE:HG22 | 1.73 | 0.70 |
| 2:Bw:193:ILE:HG12 | 2:Bw:205:MET:HE3 | 1.74 | 0.70 |
| 2:Bw:488:TRP:O | 2:Bw:552:ASN:ND2 | 2.25 | 0.70 |
| 6:Af:479:ILE:HD11 | 6:Af:501:PRO:HG3 | 1.72 | 0.69 |
| 4:G:48:THR:HG21 | 4:R:47:PRO:HB2 | 1.74 | 0.69 |
| 3:7:5:ASP:O | 3:7:7:THR:N | 2.24 | 0.69 |
| 3:8:7:THR:HG23 | 3:8:14:ASP:H | 1.57 | 0.69 |
| 2:B5:490:SER:O | 2:B5:496:ARG:NH1 | 2.25 | 0.69 |
| 2:Bz:400:ARG:NH1 | 2:Bz:403:CYS:SG | 2.63 | 0.69 |
| 2:AL:256:PRO:HG2 | 2:AL:339:THR:H | 1.56 | 0.69 |
| 6:AV:482:ASN:ND2 | 6:AV:483:PRO:O | 2.24 | 0.69 |
| 6:Ak:264:ARG:NH1 | 6:Ak:477:TYR:OH | 2.25 | 0.69 |
| 2:B1:128:GLU:HB2 | 2:B1:146:PRO:HG2 | 1.75 | 0.69 |
| 2:B3:493:GLY:HA2 | 2:B4:572:LEU:HD23 | 1.73 | 0.69 |
| 2:Bt:400:ARG:NH1 | 2:Bt:403:CYS:SG | 2.65 | 0.69 |
| 3:9:7:THR:HG23 | 3:9:14:ASP:H | 1.57 | 0.69 |
| 2:AN:118:VAL:HB | 2:AN:126:GLU:HB3 | 1.72 | 0.69 |
| 6:AZ:131:TYR:HB3 | 6:AZ:250:MET:HG2 | 1.73 | 0.69 |
| 7:Al:81:VAL:HG12 | 7:Al:188:THR:HG22 | 1.73 | 0.69 |
| 3:Bn:28:LEU:HD22 | 3:Bn:84:LYS:HB3 | 1.73 | 0.69 |
| 2:Bq:40:GLN:H | 2:Bq:81:VAL:HG23 | 1.58 | 0.69 |
| 3:9:52:GLY:HA2 | 3:9:57:LYS:HA | 1.75 | 0.69 |
| 3:AJ:113:VAL:HG13 | 3:AJ:127:ILE:HG23 | 1.73 | 0.69 |
| 7:AY:309:GLY:O | 5:BD:309:LYS:NZ | 2.25 | 0.69 |
| 6:Ag:79:ILE:HG23 | 6:Ak:121:THR:HG23 | 1.74 | 0.69 |
| 6:Ag:110:ASP:N | 6:Ag:110:ASP:OD1 | 2.26 | 0.69 |
| 7:Ar:87:ILE:HG21 | 7:Ar:159:PRO:HG2 | 1.74 | 0.69 |
| 5:Av:66:GLU:O | 5:Av:70:LYS:NZ | 2.25 | 0.69 |
| 5:Ax:52:SER:HB3 | 5:Ax:55:ASN:HB3 | 1.72 | 0.69 |
| 7:BL:163:PHE:HB2 | 7:BL:170:LEU:HD12 | 1.74 | 0.69 |
| 2:Bp:57:PRO:HB3 | 2:Bp:62:ALA:HA | 1.73 | 0.69 |
| 2:Bz:28:ALA:HB2 | 2:Bz:370:VAL:HG21 | 1.75 | 0.69 |
| 3:6:7:THR:HG23 | 3:6:14:ASP:H | 1.58 | 0.69 |
| 5:A3:485:THR:OG1 | 5:BG:501:GLU:OE1 | 2.11 | 0.69 |
| 7:BC:12:LEU:HD13 | 7:BC:38:ILE:HD12 | 1.73 | 0.69 |
| 6:BK:263:SER:HB3 | 6:BK:476:ARG:HG2 | 1.74 | 0.69 |
| 3:Bf:113:VAL:HG13 | 3:Bf:127:ILE:HG23 | 1.74 | 0.69 |
| 8:s:230:PHE:HB3 | 8:s:258:ASN:HA | 1.75 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A8:417:LEU:HB2 | 6:A8:421:TYR:HB2 | 1.73 | 0.69 |
| 2:AO:455:LYS:HD2 | 2:AO:457:GLN:HB2 | 1.73 | 0.69 |
| 10:AT:348:TYR:HB2 | 10:AT:351:VAL:HG12 | 1.74 | 0.69 |
| 6:Ag:318:LYS:NZ | 6:Ag:327:SER:OG | 2.23 | 0.69 |
| 6:Ay:343:ALA:HB1 | 6:Ay:348:GLU:HG3 | 1.75 | 0.69 |
| 2:B2:582:SER:O | 2:B2:586:THR:OG1 | 2.10 | 0.69 |
| 2:B6:57:PRO:HA | 2:B6:61:THR:HB | 1.75 | 0.69 |
| 3:Bd:113:VAL:HG13 | 3:Bd:127:ILE:HG23 | 1.75 | 0.69 |
| 3:Bk:113:VAL:HG13 | 3:Bk:127:ILE:HG23 | 1.74 | 0.69 |
| 2:Br:135:ASP:HB3 | 2:Br:139:LYS:HB2 | 1.75 | 0.69 |
| 2:Br:379:ALA:HA | 2:Br:411:ARG:HB2 | 1.73 | 0.69 |
| 4:d:10:PHE:O | 4:d:54:ASN:ND2 | 2.23 | 0.69 |
| 1:k:224:ILE:HG13 | 1:l:71:ILE:HD12 | 1.73 | 0.69 |
| 2:4:617:VAL:HG13 | 2:4:622:GLU:HB2 | 1.73 | 0.69 |
| 6:Ak:383:VAL:HG21 | 6:Ak:425:ILE:HG12 | 1.74 | 0.69 |
| 6:Ap:87:ALA:H | 7:BE:93:GLY:HA2 | 1.58 | 0.69 |
| 2:Bv:125:ILE:HD12 | 2:Bv:153:LYS:HG2 | 1.74 | 0.69 |
| 8:u:211:THR:HG22 | 8:u:236:GLU:HB2 | 1.75 | 0.69 |
| 1:0:68:PRO:HA | 1:0:75:ASP:HB2 | 1.75 | 0.69 |
| 6:Ac:340:ILE:HG13 | 6:Ac:343:ALA:H | 1.57 | 0.69 |
| 6:Ad:336:ASP:HB3 | 6:Ad:339:ASP:HB2 | 1.73 | 0.69 |
| 2:B4:256:PRO:HG2 | 2:B4:339:THR:H | 1.58 | 0.69 |
| 5:BG:290:GLY:O | 5:BG:291:ASN:ND2 | 2.23 | 0.69 |
| 2:By:456:TYR:HB3 | 2:By:504:LYS:HB3 | 1.72 | 0.69 |
| 5:A3:137:LEU:HG | 5:A3:174:LEU:HD12 | 1.75 | 0.68 |
| 2:AM:256:PRO:HG2 | 2:AM:339:THR:H | 1.57 | 0.68 |
| 6:AX:109:PHE:HE1 | 6:AX:306:VAL:HG21 | 1.58 | 0.68 |
| 7:Aa:12:LEU:HD13 | 7:Aa:38:ILE:HD12 | 1.74 | 0.68 |
| 6:Af:383:VAL:HG21 | 6:Af:425:ILE:HG12 | 1.73 | 0.68 |
| 7:Ar:12:LEU:HD13 | 7:Ar:38:ILE:HD12 | 1.73 | 0.68 |
| 3:BX:55:ASN:OD1 | 3:Bb:19:ASN:ND2 | 2.26 | 0.68 |
| 2:Bt:617:VAL:HG22 | 2:Bt:622:GLU:HB2 | 1.74 | 0.68 |
| 8:s:28:ARG:NH2 | 8:s:129:ASP:OD2 | 2.26 | 0.68 |
| 2:5:538:ASP:HB2 | 2:5:551:ILE:HB | 1.75 | 0.68 |
| 6:Af:278:LEU:HD12 | 6:Af:286:ALA:HB2 | 1.75 | 0.68 |
| 5:BA:392:SER:OG | 5:BH:458:LYS:NZ | 2.26 | 0.68 |
| 5:BF:72:THR:OG1 | 5:BF:155:ARG:NH2 | 2.26 | 0.68 |
| 1:l:63:ARG:H | 1:l:136:ASP:HB3 | 1.58 | 0.68 |
| 2:AM:331:PRO:HB2 | 2:AM:334:PHE:HB2 | 1.74 | 0.68 |
| 6:Ag:381:ASN:HB3 | 6:Ag:521:ILE:HG21 | 1.74 | 0.68 |
| 2:B4:220:PRO:HG2 | 2:B4:338:LEU:HD11 | 1.74 | 0.68 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:BJ:387:ALA:HB2 | 6:BJ:404:PHE:HB2 | 1.76 | 0.68 |
| 3:Bk:54:MET:HE2 | 3:Bl:1:MET:HE1 | 1.74 | 0.68 |
| 1:m:243:LYS:HB3 | 8:s:4:TYR:HB3 | 1.74 | 0.68 |
| 6:AV:452:PRO:HA | 6:AV:477:TYR:HA | 1.75 | 0.68 |
| 5:Ax:379:ARG:NH1 | 5:Ax:400:GLU:OE2 | 2.27 | 0.68 |
| 6:BJ:481:ILE:HD11 | 6:BJ:501:PRO:HB3 | 1.74 | 0.68 |
| 6:BK:149:GLY:H | 6:BK:186:GLY:HA2 | 1.57 | 0.68 |
| 6:Ai:452:PRO:HA | 6:Ai:477:TYR:HA | 1.74 | 0.68 |
| 3:BY:113:VAL:HG13 | 3:BY:127:ILE:HG23 | 1.75 | 0.68 |
| 2:Bz:455:LYS:HE3 | 2:Bz:502:VAL:HG22 | 1.75 | 0.68 |
| 4:P:48:THR:HG21 | 4:U:47:PRO:HB2 | 1.74 | 0.68 |
| 6:A4:260:GLU:OE2 | 6:A9:72:HIS:ND1 | 2.27 | 0.68 |
| 6:Ap:383:VAL:HG21 | 6:Ap:425:ILE:HG12 | 1.76 | 0.68 |
| 5:Av:232:LYS:O | 5:Av:234:ALA:N | 2.26 | 0.68 |
| 6:Az:237:GLU:HG2 | 6:Az:246:PRO:HA | 1.74 | 0.68 |
| 2:B7:211:GLN:O | 2:B7:329:ASN:ND2 | 2.27 | 0.68 |
| 2:B7:239:VAL:HG23 | 2:B7:280:ALA:HB3 | 1.76 | 0.68 |
| 2:Bw:645:THR:OG1 | 2:Bx:629:ILE:O | 2.12 | 0.68 |
| 4:X:27:ASN:ND2 | 4:h:35:ASP:OD1 | 2.27 | 0.68 |
| 2:2:647:THR:OG1 | 2:AP:633:ARG:NH1 | 2.26 | 0.68 |
| 6:A4:254:ILE:HG12 | 6:Aj:89:THR:H | 1.58 | 0.68 |
| 6:Ay:383:VAL:HG21 | 6:Ay:425:ILE:HG12 | 1.74 | 0.68 |
| 2:B6:206:THR:HA | 2:B6:211:GLN:HE21 | 1.59 | 0.68 |
| 2:Bt:254:ILE:HD11 | 2:Bt:261:ARG:HB2 | 1.76 | 0.68 |
| 5:A3:183:GLN:HB3 | 5:A3:207:ILE:HG23 | 1.76 | 0.68 |
| 5:A3:232:LYS:HE2 | 5:A3:233:ALA:H | 1.59 | 0.68 |
| 6:A7:152:ALA:O | 6:AW:264:ARG:NH2 | 2.27 | 0.68 |
| 7:Al:2:SER:N | 4:R:30:GLU:OE2 | 2.26 | 0.68 |
| 7:Ar:69:TYR:O | 5:BA:320:LYS:NZ | 2.26 | 0.68 |
| 2:Br:455:LYS:NZ | 2:Br:473:ASP:OD2 | 2.27 | 0.68 |
| 8:t:230:PHE:HB3 | 8:t:258:ASN:HA | 1.76 | 0.68 |
| 6:AV:336:ASP:HB3 | 6:AV:339:ASP:HB2 | 1.75 | 0.68 |
| 2:B1:118:VAL:HB | 2:B1:126:GLU:HB3 | 1.76 | 0.68 |
| 7:BC:269:MET:SD | 1:p:50:SER:OG | 2.51 | 0.68 |
| 6:BI:336:ASP:HB3 | 6:BI:339:ASP:HB2 | 1.76 | 0.68 |
| 2:Bw:256:PRO:HG2 | 2:Bw:339:THR:H | 1.59 | 0.68 |
| 2:Bx:490:SER:O | 2:Bx:496:ARG:NH1 | 2.26 | 0.68 |
| 2:3:310:TYR:O | 2:3:314:PHE:HB2 | 1.93 | 0.68 |
| 2:3:488:TRP:O | 2:3:552:ASN:ND2 | 2.26 | 0.68 |
| 6:A7:79:ILE:HG23 | 6:A8:121:THR:HB | 1.76 | 0.68 |
| 8:AB:212:THR:HG1 | 8:AB:235:SER:HG | 1.36 | 0.68 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AW:381:ASN:HB3 | 6:AW:521:ILE:HG21 | 1.74 | 0.68 |
| 7:Ab:12:LEU:HD21 | 7:Ab:248:LYS:HG2 | 1.75 | 0.68 |
| 6:Ak:452:PRO:HA | 6:Ak:477:TYR:HA | 1.75 | 0.68 |
| 2:B7:110:TYR:HE2 | 2:B7:171:ILE:HG21 | 1.59 | 0.68 |
| 5:BA:158:PHE:HB2 | 5:BA:236:VAL:HB | 1.76 | 0.68 |
| 3:Bo:72:THR:HG22 | 3:Bo:154:GLU:HG3 | 1.75 | 0.68 |
| 2:3:490:SER:O | 2:3:496:ARG:NH1 | 2.26 | 0.67 |
| 2:4:490:SER:O | 2:4:496:ARG:NH1 | 2.27 | 0.67 |
| 6:AV:268:ALA:HB1 | 6:AV:290:LEU:HD13 | 1.74 | 0.67 |
| 6:An:91:ILE:HG22 | 6:An:92:GLY:H | 1.58 | 0.67 |
| 6:An:264:ARG:NH2 | 6:BK:152:ALA:O | 2.28 | 0.67 |
| 6:An:383:VAL:HG21 | 6:An:425:ILE:HG12 | 1.76 | 0.67 |
| 3:Bh:40:ALA:H | 3:Bh:69:TRP:HE1 | 1.41 | 0.67 |
| 2:Bs:490:SER:O | 2:Bs:496:ARG:NH1 | 2.26 | 0.67 |
| 2:Bw:135:ASP:HB3 | 2:Bw:139:LYS:HB2 | 1.76 | 0.67 |
| 4:e:48:THR:HG21 | 4:j:47:PRO:HB2 | 1.74 | 0.67 |
| 2:1:639:THR:HB | 2:AO:624:VAL:HG12 | 1.75 | 0.67 |
| 6:A5:279:ARG:NH2 | 6:A5:285:ASP:OD1 | 2.27 | 0.67 |
| 2:AL:559:MET:SD | 2:AL:563:ASN:ND2 | 2.66 | 0.67 |
| 2:AN:488:TRP:O | 2:AN:552:ASN:ND2 | 2.28 | 0.67 |
| 6:AX:66:ALA:N | 6:Af:240:ASN:OD1 | 2.28 | 0.67 |
| 5:Av:376:PRO:HB3 | 5:Av:399:ASP:HB2 | 1.75 | 0.67 |
| 2:B3:220:PRO:HG2 | 2:B3:338:LEU:HD11 | 1.75 | 0.67 |
| 2:Bu:312:ASP:OD1 | 2:Bu:312:ASP:N | 2.26 | 0.67 |
| 2:Bx:521:ALA:HA | 2:Bx:539:LYS:HE3 | 1.75 | 0.67 |
| 2:Bx:617:VAL:HG22 | 2:Bx:622:GLU:HB2 | 1.76 | 0.67 |
| 2:AN:135:ASP:HB3 | 2:AN:139:LYS:HB2 | 1.76 | 0.67 |
| 6:AZ:131:TYR:HE1 | 6:AZ:141:LYS:HB2 | 1.57 | 0.67 |
| 6:Ai:383:VAL:HG21 | 6:Ai:425:ILE:HG12 | 1.76 | 0.67 |
| 6:Aj:151:ASP:HB3 | 6:Aj:154:PHE:HB2 | 1.77 | 0.67 |
| 6:Au:235:LEU:O | 6:Au:245:ASN:ND2 | 2.27 | 0.67 |
| 11:BO:64:GLN:O | 11:BO:66:THR:N | 2.27 | 0.67 |
| 2:Bu:40:GLN:H | 2:Bu:81:VAL:HG23 | 1.58 | 0.67 |
| 1:m:155:TYR:HB2 | 1:m:158:PHE:HA | 1.75 | 0.67 |
| 5:A2:64:SER:HB3 | 5:A2:67:PRO:HG2 | 1.77 | 0.67 |
| 6:A7:264:ARG:NH1 | 6:A7:477:TYR:OH | 2.28 | 0.67 |
| 2:AP:490:SER:O | 2:AP:496:ARG:NH1 | 2.25 | 0.67 |
| 7:AY:18:ARG:HA | 7:AY:22:ALA:HA | 1.75 | 0.67 |
| 6:Af:101:ARG:HD3 | 6:Aj:146:PRO:HD3 | 1.75 | 0.67 |
| 6:BK:198:ILE:HA | 6:BK:215:GLN:HE22 | 1.59 | 0.67 |
| 2:Bt:57:PRO:HB2 | 2:Bt:62:ALA:HA | 1.76 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:s:215:ASP:N | 8:s:215:ASP:OD1 | 2.28 | 0.67 |
| 6:Ap:432:ASP:HB3 | 6:Ap:518:VAL:HG23 | 1.76 | 0.67 |
| 2:B6:51:VAL:HG22 | 2:B6:65:PHE:HZ | 1.57 | 0.67 |
| 2:B6:642:PHE:HB2 | 2:Bq:12:GLU:HA | 1.75 | 0.67 |
| 1:l:155:TYR:HB2 | 1:l:158:PHE:HA | 1.76 | 0.67 |
| 2:2:563:ASN:ND2 | 2:2:591:TYR:OH | 2.27 | 0.67 |
| 5:A1:315:ASP:OD1 | 7:As:91:ASN:ND2 | 2.26 | 0.67 |
| 6:A5:278:LEU:HD12 | 6:A5:286:ALA:HB2 | 1.76 | 0.67 |
| 6:A5:432:ASP:HB3 | 6:A5:518:VAL:HG23 | 1.76 | 0.67 |
| 2:AK:110:TYR:H | 2:AK:138:GLY:HA3 | 1.59 | 0.67 |
| 6:AV:459:LEU:HD11 | 6:AV:474:LYS:HG2 | 1.76 | 0.67 |
| 7:Ab:120:GLY:HA3 | 5:BA:259:LYS:HB2 | 1.76 | 0.67 |
| 5:BA:283:ARG:NH1 | 5:BA:334:TYR:OH | 2.28 | 0.67 |
| 3:Bn:114:ARG:HG2 | 3:Bn:126:GLU:HG3 | 1.76 | 0.67 |
| 3:7:96:GLY:O | 3:o:56:ARG:NH2 | 2.27 | 0.67 |
| 5:A1:458:LYS:NZ | 5:BD:451:ASP:O | 2.25 | 0.67 |
| 2:AN:66:MET:HG2 | 2:AN:468:VAL:HG21 | 1.76 | 0.67 |
| 6:AV:235:LEU:O | 6:AV:245:ASN:ND2 | 2.28 | 0.67 |
| 6:Ai:131:TYR:HD2 | 6:Ai:250:MET:HE3 | 1.60 | 0.67 |
| 3:o:17:ARG:HH22 | 9:z:47:THR:HG21 | 1.58 | 0.67 |
| 2:AK:331:PRO:HB2 | 2:AK:334:PHE:HB2 | 1.77 | 0.67 |
| 6:Ae:346:ALA:HB2 | 6:Ai:341:ARG:HD3 | 1.77 | 0.67 |
| 5:BB:129:GLU:OE1 | 5:BB:425:ASN:ND2 | 2.28 | 0.67 |
| 2:Bs:455:LYS:HD2 | 2:Bs:457:GLN:HB2 | 1.77 | 0.67 |
| 3:9:16:ALA:HB2 | 3:AA:77:GLU:HA | 1.77 | 0.67 |
| 5:A3:216:ALA:O | 5:BF:248:LYS:NZ | 2.28 | 0.67 |
| 6:Ae:380:ARG:HH21 | 6:Ai:366:ARG:HD2 | 1.60 | 0.67 |
| 6:Ao:383:VAL:HG21 | 6:Ao:425:ILE:HG12 | 1.76 | 0.67 |
| 2:B2:645:THR:OG1 | 2:B3:629:ILE:O | 2.13 | 0.67 |
| 5:BF:184:TYR:OH | 5:BF:204:GLU:OE1 | 2.13 | 0.67 |
| 5:BF:366:ARG:HE | 5:BF:380:ILE:HD11 | 1.58 | 0.67 |
| 11:BW:38:VAL:HG11 | 11:BW:69:ILE:HG12 | 1.76 | 0.67 |
| 3:Ba:54:MET:HE3 | 3:Be:20:LEU:HA | 1.76 | 0.67 |
| 3:Bn:137:VAL:HB | 3:Bn:155:VAL:HG13 | 1.77 | 0.67 |
| 2:Bx:140:ILE:O | 2:Bx:141:LYS:NZ | 2.27 | 0.67 |
| 4:F:23:SER:HB3 | 4:F:46:ARG:HE | 1.60 | 0.67 |
| 3:AG:64:ARG:HH12 | 3:AH:95:GLN:HG2 | 1.60 | 0.67 |
| 6:Ac:278:LEU:HD12 | 6:Ac:286:ALA:HB2 | 1.76 | 0.67 |
| 6:Af:264:ARG:NH2 | 6:Aj:152:ALA:O | 2.28 | 0.67 |
| 6:Am:383:VAL:HG21 | 6:Am:425:ILE:HG12 | 1.77 | 0.67 |
| 6:Am:515:ARG:NH2 | 6:Am:517:TYR:OH | 2.27 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B7:96:ALA:HB2 | 2:B7:191:SER:HA | 1.77 | 0.67 |
| 7:BE:90:THR:O | 7:BE:94:SER:OG | 2.11 | 0.67 |
| 5:A3:309:LYS:NZ | 7:Al:309:GLY:O | 2.27 | 0.66 |
| 5:A3:397:THR:HG23 | 5:A3:400:GLU:HB2 | 1.76 | 0.66 |
| 2:AD:413:THR:HG23 | 2:AD:414:VAL:HG23 | 1.77 | 0.66 |
| 3:AF:113:VAL:HG13 | 3:AF:127:ILE:HG23 | 1.76 | 0.66 |
| 5:Ax:94:GLU:HG3 | 5:Ax:379:ARG:HH21 | 1.60 | 0.66 |
| 3:Bd:82:ARG:HH12 | 3:Bd:138:GLY:HA2 | 1.60 | 0.66 |
| 2:Bv:235:GLU:OE2 | 2:Bv:261:ARG:NH2 | 2.27 | 0.66 |
| 4:W:27:ASN:ND2 | 4:g:35:ASP:OD1 | 2.29 | 0.66 |
| 2:3:605:ARG:HG2 | 2:3:607:VAL:HG23 | 1.78 | 0.66 |
| 2:AN:131:ILE:HG12 | 2:AN:143:ILE:HG22 | 1.76 | 0.66 |
| 6:Ao:90:GLN:OE1 | 6:BM:256:LYS:NZ | 2.28 | 0.66 |
| 7:At:138:LEU:HB3 | 5:BH:273:ILE:HD11 | 1.77 | 0.66 |
| 5:BH:290:GLY:O | 5:BH:291:ASN:ND2 | 2.28 | 0.66 |
| 2:2:237:GLU:OE1 | 2:2:284:ARG:NH1 | 2.28 | 0.66 |
| 2:AD:488:TRP:O | 2:AD:552:ASN:ND2 | 2.28 | 0.66 |
| 2:AP:456:TYR:HB3 | 2:AP:504:LYS:HB3 | 1.77 | 0.66 |
| 7:Aq:91:ASN:HB2 | 7:Aq:94:SER:HB3 | 1.77 | 0.66 |
| 7:At:12:LEU:HD13 | 7:At:38:ILE:HD12 | 1.78 | 0.66 |
| 5:Av:483:HIS:HB3 | 5:BB:508:GLU:HG2 | 1.77 | 0.66 |
| 2:Bu:560:LEU:HD21 | 2:Bu:601:ILE:HD11 | 1.78 | 0.66 |
| 8:r:212:THR:OG1 | 8:r:235:SER:OG | 2.13 | 0.66 |
| 2:3:66:MET:HG2 | 2:3:468:VAL:HG21 | 1.76 | 0.66 |
| 5:A0:376:PRO:HB3 | 5:A0:399:ASP:HB2 | 1.77 | 0.66 |
| 7:AY:111:LEU:HB2 | 6:Ao:272:ILE:HD11 | 1.77 | 0.66 |
| 6:Af:100:ARG:NH1 | 6:Af:289:GLU:OE2 | 2.28 | 0.66 |
| 2:B6:32:LYS:HD2 | 2:B6:355:LEU:HD21 | 1.77 | 0.66 |
| 5:A0:72:THR:HG23 | 5:A0:155:ARG:HH21 | 1.60 | 0.66 |
| 2:AL:116:ILE:HD11 | 2:AL:131:ILE:HG13 | 1.77 | 0.66 |
| 6:Ad:380:ARG:NH2 | 6:Ah:363:GLU:OE1 | 2.28 | 0.66 |
| 5:BG:72:THR:OG1 | 5:BG:155:ARG:NH2 | 2.28 | 0.66 |
| 3:BX:41:LEU:HG | 3:BX:127:ILE:HD13 | 1.78 | 0.66 |
| 3:BZ:113:VAL:HG13 | 3:BZ:127:ILE:HG23 | 1.77 | 0.66 |
| 2:Bq:488:TRP:O | 2:Bq:552:ASN:ND2 | 2.29 | 0.66 |
| 9:y:19:VAL:HG21 | 9:y:37:VAL:HG21 | 1.75 | 0.66 |
| 5:A0:35:LYS:O | 5:BH:176:ARG:NH2 | 2.29 | 0.66 |
| 2:AO:35:TRP:HB2 | 2:AO:230:LEU:HD12 | 1.75 | 0.66 |
| 7:Aa:143:GLN:OE1 | 5:Ax:263:GLN:NE2 | 2.29 | 0.66 |
| 5:Av:377:LEU:HD23 | 5:BB:381:PRO:HB2 | 1.76 | 0.66 |
| 6:BK:154:PHE:O | 6:BK:248:ASN:ND2 | 2.26 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bt:166:ASN:OD1 | 2:Bt:166:ASN:N | 2.22 | 0.66 |
| 2:By:490:SER:O | 2:By:496:ARG:NH1 | 2.27 | 0.66 |
| 5:A0:160:LYS:NZ | 5:A0:233:ALA:O | 2.28 | 0.66 |
| 8:AB:238:VAL:HG22 | 8:AB:239:PRO:HD2 | 1.76 | 0.66 |
| 8:AB:240:ARG:NH2 | 2:AD:620:ARG:O | 2.29 | 0.66 |
| 2:AP:126:GLU:HA | 2:AP:149:LYS:HD2 | 1.77 | 0.66 |
| 7:Aa:265:ARG:NH1 | 1:k:49:GLU:OE2 | 2.29 | 0.66 |
| 6:An:90:GLN:HG2 | 6:An:281:VAL:HG21 | 1.78 | 0.66 |
| 6:Au:110:ASP:N | 6:Au:110:ASP:OD1 | 2.29 | 0.66 |
| 6:BI:387:ALA:HB2 | 6:BI:404:PHE:HB2 | 1.76 | 0.66 |
| 3:Bm:40:ALA:O | 3:Bm:69:TRP:NE1 | 2.28 | 0.66 |
| 2:Bq:34:GLN:NE2 | 2:Bq:58:THR:OG1 | 2.29 | 0.66 |
| 8:u:28:ARG:NH2 | 8:u:129:ASP:OD2 | 2.28 | 0.66 |
| 8:AB:46:LYS:HB3 | 8:AB:51:MET:HG3 | 1.75 | 0.66 |
| 3:AE:22:GLN:NE2 | 3:AJ:1:MET:SD | 2.68 | 0.66 |
| 2:AM:135:ASP:HB3 | 2:AM:139:LYS:HB2 | 1.77 | 0.66 |
| 6:Ah:131:TYR:HD2 | 6:Ah:250:MET:HE3 | 1.61 | 0.66 |
| 6:Au:117:MET:HB2 | 6:Au:453:TYR:HB2 | 1.77 | 0.66 |
| 6:Au:237:GLU:HG2 | 6:Au:246:PRO:HA | 1.78 | 0.66 |
| 3:Bc:113:VAL:HG13 | 3:Bc:127:ILE:HG23 | 1.77 | 0.66 |
| 2:Br:90:LYS:NZ | 2:Br:190:ASP:OD1 | 2.29 | 0.66 |
| 2:Bu:518:TYR:OH | 2:Bu:550:ARG:NH1 | 2.29 | 0.66 |
| 4:T:7:ASP:N | 4:T:7:ASP:OD1 | 2.29 | 0.66 |
| 1:l:231:TYR:OH | 8:s:15:THR:OG1 | 2.14 | 0.66 |
| 1:0:155:TYR:HB2 | 1:0:158:PHE:HA | 1.77 | 0.66 |
| 6:A5:456:LEU:H | 6:A5:475:THR:HG22 | 1.61 | 0.66 |
| 6:AV:152:ALA:O | 6:Ap:264:ARG:NH2 | 2.29 | 0.66 |
| 6:Ac:279:ARG:NH2 | 6:Ac:285:ASP:OD1 | 2.26 | 0.66 |
| 6:Af:235:LEU:O | 6:Af:245:ASN:ND2 | 2.29 | 0.66 |
| 6:Ag:115:GLN:NE2 | 6:Ag:444:MET:SD | 2.69 | 0.66 |
| 6:Ap:264:ARG:NH1 | 6:Ap:477:TYR:OH | 2.29 | 0.66 |
| 3:Bo:137:VAL:HB | 3:Bo:155:VAL:HG13 | 1.77 | 0.66 |
| 5:A3:448:PHE:O | 5:A3:450:ARG:NH1 | 2.29 | 0.66 |
| 6:A9:465:LYS:HB3 | 6:BK:237:GLU:HB3 | 1.78 | 0.66 |
| 8:AB:144:HIS:HB2 | 8:AB:164:LYS:HB3 | 1.78 | 0.66 |
| 7:AY:175:ASN:ND2 | 5:BD:323:ASN:O | 2.29 | 0.66 |
| 7:Aa:161:PHE:HA | 7:Aa:171:LYS:O | 1.96 | 0.66 |
| 7:Aq:303:PRO:HG3 | 5:BD:289:THR:HG22 | 1.78 | 0.66 |
| 6:BM:237:GLU:HG2 | 6:BM:246:PRO:HA | 1.78 | 0.66 |
| 2:Bt:66:MET:O | 2:Bt:70:ASN:ND2 | 2.28 | 0.66 |
| 4:Y:27:ASN:ND2 | 4:i:35:ASP:OD1 | 2.28 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:l:216:ASP:HB3 | 1:l:219:ALA:HB2 | 1.78 | 0.66 |
| 8:r:155:ASN:O | 8:r:157:ILE:N | 2.28 | 0.66 |
| 2:5:498:GLN:HG2 | 2:5:534:VAL:HG12 | 1.78 | 0.65 |
| 5:A3:281:ASP:O | 5:BF:278:ARG:NH2 | 2.28 | 0.65 |
| 6:A9:270:TYR:HA | 6:Aj:67:GLU:HB2 | 1.78 | 0.65 |
| 2:AK:117:THR:HG23 | 2:AK:127:THR:HG22 | 1.76 | 0.65 |
| 2:AL:237:GLU:OE1 | 2:AL:284:ARG:NH1 | 2.30 | 0.65 |
| 2:AN:57:PRO:HB3 | 2:AN:62:ALA:HA | 1.78 | 0.65 |
| 6:Ag:452:PRO:HA | 6:Ag:477:TYR:HA | 1.76 | 0.65 |
| 2:B7:117:THR:HG23 | 2:B7:127:THR:HG22 | 1.78 | 0.65 |
| 2:B7:129:GLY:HA3 | 2:B7:145:ILE:HD13 | 1.77 | 0.65 |
| 4:Y:47:PRO:HB2 | 4:i:48:THR:HG21 | 1.77 | 0.65 |
| 2:3:191:SER:HB3 | 2:3:342:GLY:HA3 | 1.78 | 0.65 |
| 2:4:571:ARG:NH2 | 2:4:587:GLU:OE1 | 2.29 | 0.65 |
| 2:B1:592:LEU:HD23 | 2:B1:604:TYR:HB2 | 1.77 | 0.65 |
| 2:B2:453:ASN:HB2 | 2:B2:506:ALA:HB3 | 1.77 | 0.65 |
| 2:Bt:481:THR:HG23 | 2:Bt:496:ARG:HD2 | 1.78 | 0.65 |
| 2:Bt:488:TRP:O | 2:Bt:552:ASN:ND2 | 2.29 | 0.65 |
| 2:Bv:566:ARG:HA | 2:Bv:569:LYS:HD2 | 1.77 | 0.65 |
| 4:K:9:PRO:HD3 | 4:K:57:VAL:HG21 | 1.78 | 0.65 |
| 3:o:54:MET:O | 3:o:55:ASN:ND2 | 2.29 | 0.65 |
| 1:0:127:VAL:O | 1:0:128:ASN:ND2 | 2.29 | 0.65 |
| 2:3:455:LYS:NZ | 2:3:473:ASP:OD2 | 2.29 | 0.65 |
| 7:A6:138:LEU:HB3 | 5:BF:273:ILE:HD11 | 1.78 | 0.65 |
| 3:AE:72:THR:HG22 | 3:AE:154:GLU:HG3 | 1.78 | 0.65 |
| 6:Af:264:ARG:NH1 | 6:Af:305:GLU:OE1 | 2.29 | 0.65 |
| 6:Ah:264:ARG:NH2 | 6:BI:152:ALA:O | 2.29 | 0.65 |
| 7:At:125:CYS:SG | 7:At:126:ASN:N | 2.69 | 0.65 |
| 6:Ay:131:TYR:HB3 | 6:Ay:250:MET:HG2 | 1.78 | 0.65 |
| 2:B7:642:PHE:HB2 | 2:Br:12:GLU:HG2 | 1.77 | 0.65 |
| 8:s:108:GLN:HB2 | 8:s:202:VAL:HG12 | 1.78 | 0.65 |
| 6:A7:71:ASP:OD1 | 6:A7:72:HIS:N | 2.30 | 0.65 |
| 6:Am:235:LEU:O | 6:Am:245:ASN:ND2 | 2.30 | 0.65 |
| 6:Ap:268:ALA:HB1 | 6:Ap:290:LEU:HD13 | 1.77 | 0.65 |
| 2:B1:220:PRO:HG2 | 2:B1:338:LEU:HD11 | 1.77 | 0.65 |
| 5:BD:290:GLY:O | 5:BD:291:ASN:ND2 | 2.28 | 0.65 |
| 11:BQ:11:LYS:HG3 | 11:BQ:27:GLU:HG2 | 1.77 | 0.65 |
| 2:Bv:375:ALA:HB3 | 2:Bv:407:CYS:HA | 1.79 | 0.65 |
| 4:H:10:PHE:HB3 | 4:H:22:ILE:HG12 | 1.78 | 0.65 |
| 1:m:231:TYR:HH | 8:t:15:THR:HG1 | 1.42 | 0.65 |
| 3:o:52:GLY:HA2 | 3:o:57:LYS:HA | 1.76 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:q:85:ASN:ND2 | 8:q:195:ASN:OD1 | 2.29 | 0.65 |
| 9:v:19:VAL:HG21 | 9:v:37:VAL:HG21 | 1.78 | 0.65 |
| 2:3:252:LEU:HG | 2:3:263:SER:HB2 | 1.78 | 0.65 |
| 5:A1:263:GLN:NE2 | 7:AY:143:GLN:OE1 | 2.29 | 0.65 |
| 3:AE:31:ASN:OD1 | 3:AE:31:ASN:N | 2.29 | 0.65 |
| 2:Bz:521:ALA:HB1 | 2:Bz:541:ALA:HA | 1.78 | 0.65 |
| 8:q:212:THR:HG1 | 8:q:235:SER:HG | 1.40 | 0.65 |
| 2:2:228:GLY:HA2 | 2:2:345:SER:HB3 | 1.79 | 0.65 |
| 2:3:430:ARG:HG3 | 2:3:522:ILE:HD11 | 1.78 | 0.65 |
| 6:A9:181:PHE:HD1 | 6:A9:187:THR:HB | 1.62 | 0.65 |
| 10:AS:345:MET:HE3 | 10:AS:364:LYS:HG3 | 1.79 | 0.65 |
| 6:AX:493:ALA:O | 6:AX:497:GLN:NE2 | 2.30 | 0.65 |
| 6:Ag:264:ARG:NH1 | 6:Ag:477:TYR:OH | 2.30 | 0.65 |
| 6:Ak:449:TYR:OH | 6:Ak:482:ASN:ND2 | 2.25 | 0.65 |
| 7:As:12:LEU:HD13 | 7:As:38:ILE:HD12 | 1.77 | 0.65 |
| 4:B:47:PRO:HB2 | 4:R:48:THR:HG21 | 1.76 | 0.65 |
| 7:BE:309:GLY:O | 5:BG:309:LYS:NZ | 2.29 | 0.65 |
| 3:Bj:19:ASN:OD1 | 3:Bj:19:ASN:N | 2.27 | 0.65 |
| 2:Bt:110:TYR:H | 2:Bt:138:GLY:HA3 | 1.61 | 0.65 |
| 2:Bv:645:THR:OG1 | 2:Bw:629:ILE:O | 2.14 | 0.65 |
| 9:x:15:THR:OG1 | 9:x:16:ASN:N | 2.29 | 0.65 |
| 2:4:563:ASN:ND2 | 2:4:591:TYR:OH | 2.30 | 0.65 |
| 7:AY:192:ILE:HG12 | 7:AY:222:PRO:HB2 | 1.79 | 0.65 |
| 6:Ah:264:ARG:NH1 | 6:Ah:477:TYR:OH | 2.30 | 0.65 |
| 5:BD:455:ALA:HA | 5:BD:458:LYS:HD3 | 1.77 | 0.65 |
| 6:BK:452:PRO:HA | 6:BK:477:TYR:HA | 1.79 | 0.65 |
| 2:Br:264:THR:O | 2:Br:266:LYS:N | 2.30 | 0.65 |
| 8:q:142:GLN:O | 8:q:144:HIS:N | 2.30 | 0.65 |
| 2:5:202:GLU:HA | 2:5:205:MET:HG2 | 1.79 | 0.65 |
| 5:A2:158:PHE:HB2 | 5:A2:236:VAL:HB | 1.79 | 0.65 |
| 2:AL:135:ASP:HB3 | 2:AL:139:LYS:HB2 | 1.79 | 0.65 |
| 6:AV:226:GLU:OE2 | 6:Ap:262:LYS:NZ | 2.29 | 0.65 |
| 7:Ab:200:ASN:ND2 | 7:Ab:231:VAL:O | 2.28 | 0.65 |
| 6:Ad:456:LEU:H | 6:Ad:475:THR:HG22 | 1.62 | 0.65 |
| 7:BC:261:GLN:NE2 | 7:BE:285:GLU:OE1 | 2.30 | 0.65 |
| 3:BX:25:ILE:HG22 | 3:BX:27:TYR:H | 1.61 | 0.65 |
| 1:n:243:LYS:H | 8:t:4:TYR:H | 1.45 | 0.65 |
| 8:s:7:ASN:OD1 | 8:s:7:ASN:N | 2.29 | 0.65 |
| 3:7:52:GLY:HA2 | 3:7:57:LYS:HA | 1.79 | 0.65 |
| 3:AI:106:GLU:O | 3:AI:109:LYS:NZ | 2.30 | 0.65 |
| 7:AY:12:LEU:HD13 | 7:AY:38:ILE:HD12 | 1.79 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AY:123:THR:HG22 | 7:AY:125:CYS:H | 1.60 | 0.65 |
| 7:Al:199:GLY:O | 7:Al:204:TYR:OH | 2.15 | 0.65 |
| 3:Bh:17:ARG:HG3 | 3:Bh:20:LEU:HD12 | 1.78 | 0.65 |
| 5:A2:440:GLU:HA | 5:A2:443:ASN:HD22 | 1.61 | 0.65 |
| 2:AO:488:TRP:O | 2:AO:552:ASN:ND2 | 2.29 | 0.65 |
| 6:AZ:118:ASN:HB2 | 6:AZ:119:SER:HB2 | 1.77 | 0.65 |
| 6:AZ:235:LEU:HD23 | 7:BC:92:ILE:HG22 | 1.78 | 0.65 |
| 6:Ag:336:ASP:HB3 | 6:Ag:339:ASP:HB2 | 1.78 | 0.65 |
| 6:Ai:230:THR:HB | 6:Ay:71:ASP:HB3 | 1.79 | 0.65 |
| 2:B2:488:TRP:HB3 | 2:B2:556:LEU:HD12 | 1.79 | 0.65 |
| 2:B6:560:LEU:HD21 | 2:B6:601:ILE:HD11 | 1.78 | 0.65 |
| 2:Bt:453:ASN:HB2 | 2:Bt:506:ALA:HB3 | 1.77 | 0.65 |
| 8:r:25:GLN:O | 8:r:136:GLN:NE2 | 2.30 | 0.65 |
| 2:3:211:GLN:NE2 | 2:3:329:ASN:OD1 | 2.29 | 0.64 |
| 2:3:571:ARG:NH2 | 2:3:587:GLU:OE1 | 2.30 | 0.64 |
| 6:AX:249:GLU:OE2 | 6:Ak:66:ALA:N | 2.29 | 0.64 |
| 7:Aq:269:MET:SD | 1:l:50:SER:OG | 2.54 | 0.64 |
| 7:Ar:264:ALA:HA | 7:Ar:267:GLN:HB2 | 1.78 | 0.64 |
| 6:Au:115:GLN:NE2 | 6:Au:444:MET:SD | 2.70 | 0.64 |
| 5:Av:33:ALA:HB2 | 5:Av:188:ILE:HD13 | 1.79 | 0.64 |
| 2:B4:368:VAL:O | 2:B4:400:ARG:NH2 | 2.30 | 0.64 |
| 2:Bs:264:THR:O | 2:Bs:266:LYS:N | 2.30 | 0.64 |
| 2:Bu:490:SER:O | 2:Bu:496:ARG:NH1 | 2.30 | 0.64 |
| 2:Bv:635:ILE:HD11 | 2:Bw:576:ASN:HD22 | 1.60 | 0.64 |
| 1:k:185:LEU:HD22 | 1:k:197:SER:HB2 | 1.79 | 0.64 |
| 2:1:32:LYS:HE2 | 2:1:350:VAL:HB | 1.79 | 0.64 |
| 5:A0:504:GLN:NE2 | 5:A0:508:GLU:OE2 | 2.30 | 0.64 |
| 6:Af:190:LEU:HB3 | 6:Af:221:LEU:HB3 | 1.80 | 0.64 |
| 7:Aq:143:GLN:OE1 | 5:BB:263:GLN:NE2 | 2.29 | 0.64 |
| 2:Bq:654:LEU:HD13 | 2:Br:605:ARG:HD3 | 1.78 | 0.64 |
| 2:1:423:VAL:HG21 | 2:1:513:GLN:HB3 | 1.80 | 0.64 |
| 6:Af:264:ARG:NH1 | 6:Af:477:TYR:OH | 2.30 | 0.64 |
| 6:Ah:521:ILE:HA | 6:BI:341:ARG:HH22 | 1.62 | 0.64 |
| 6:Au:154:PHE:O | 6:Au:248:ASN:ND2 | 2.30 | 0.64 |
| 5:Ax:290:GLY:O | 5:Ax:291:ASN:ND2 | 2.26 | 0.64 |
| 2:B2:638:ILE:HG12 | 2:B3:623:PHE:HB3 | 1.80 | 0.64 |
| 2:B3:100:GLU:HB3 | 2:B3:188:ILE:HD11 | 1.79 | 0.64 |
| 6:BK:383:VAL:HG21 | 6:BK:425:ILE:HG12 | 1.78 | 0.64 |
| 2:Bt:239:VAL:HG22 | 2:Bt:280:ALA:HB3 | 1.79 | 0.64 |
| 4:b:44:MET:HE1 | 4:g:44:MET:HG2 | 1.78 | 0.64 |
| 2:1:455:LYS:HB2 | 2:1:470:LEU:HD13 | 1.79 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:AE:125:LYS:HG2 | 3:AF:79:HIS:HB2 | 1.79 | 0.64 |
| 3:AH:114:ARG:HG2 | 3:AH:126:GLU:HG3 | 1.78 | 0.64 |
| 2:AM:654:LEU:HD13 | 2:By:605:ARG:HD3 | 1.80 | 0.64 |
| 7:Al:65:ASP:HB3 | 7:Al:68:ARG:HB2 | 1.77 | 0.64 |
| 7:As:22:ALA:HB1 | 7:As:23:PRO:HD2 | 1.80 | 0.64 |
| 6:Au:153:MET:HE1 | 6:Au:177:ILE:HD13 | 1.79 | 0.64 |
| 6:BK:123:GLN:HG2 | 6:BK:258:VAL:HG12 | 1.80 | 0.64 |
| 4:K:48:THR:HG21 | 4:L:47:PRO:HB2 | 1.78 | 0.64 |
| 5:A0:451:ASP:O | 5:BG:458:LYS:NZ | 2.26 | 0.64 |
| 7:A6:230:VAL:HG21 | 7:A6:233:GLN:HE21 | 1.62 | 0.64 |
| 6:A7:98:MET:HE2 | 6:A8:127:LEU:HB2 | 1.79 | 0.64 |
| 2:AD:563:ASN:ND2 | 2:AD:591:TYR:OH | 2.31 | 0.64 |
| 7:As:12:LEU:HD12 | 7:As:242:TYR:HD2 | 1.62 | 0.64 |
| 2:B3:166:ASN:OD1 | 2:B3:166:ASN:N | 2.27 | 0.64 |
| 5:BG:178:ASP:HB3 | 5:BG:181:GLN:HB2 | 1.78 | 0.64 |
| 6:BK:235:LEU:O | 6:BK:245:ASN:ND2 | 2.30 | 0.64 |
| 6:BK:318:LYS:NZ | 6:BK:339:ASP:OD1 | 2.30 | 0.64 |
| 3:Bc:40:ALA:O | 3:Bc:69:TRP:NE1 | 2.27 | 0.64 |
| 3:Bh:114:ARG:HG2 | 3:Bh:126:GLU:HG3 | 1.80 | 0.64 |
| 3:Bo:43:ALA:O | 3:Bo:162:TRP:NE1 | 2.31 | 0.64 |
| 2:Bs:375:ALA:HB3 | 2:Bs:407:CYS:HA | 1.80 | 0.64 |
| 2:3:538:ASP:HB2 | 2:3:551:ILE:HB | 1.79 | 0.64 |
| 5:A1:198:ILE:HG21 | 5:BD:8:LEU:HD21 | 1.80 | 0.64 |
| 7:Aa:40:ARG:HH21 | 7:Aa:254:LEU:HD22 | 1.63 | 0.64 |
| 6:Az:131:TYR:HB3 | 6:Az:250:MET:HG2 | 1.79 | 0.64 |
| 2:B4:139:LYS:HB3 | 2:B4:141:LYS:HZ3 | 1.62 | 0.64 |
| 6:BI:428:TYR:O | 6:BI:430:LYS:NZ | 2.31 | 0.64 |
| 6:BK:268:ALA:HB1 | 6:BK:290:LEU:HD13 | 1.79 | 0.64 |
| 2:By:35:TRP:HB2 | 2:By:230:LEU:HD12 | 1.78 | 0.64 |
| 4:W:35:ASP:OD1 | 4:b:27:ASN:ND2 | 2.31 | 0.64 |
| 4:a:48:THR:HG21 | 4:f:47:PRO:HB2 | 1.79 | 0.64 |
| 1:0:216:ASP:HB3 | 1:0:219:ALA:HB2 | 1.80 | 0.64 |
| 2:3:545:PRO:HG3 | 2:4:271:TYR:HB3 | 1.78 | 0.64 |
| 3:7:56:ARG:HG3 | 3:9:99:ILE:HG22 | 1.78 | 0.64 |
| 6:A7:151:ASP:HB3 | 6:A7:154:PHE:HB2 | 1.79 | 0.64 |
| 9:AC:19:VAL:HG21 | 9:AC:37:VAL:HG21 | 1.78 | 0.64 |
| 2:AK:490:SER:O | 2:AK:496:ARG:NH1 | 2.31 | 0.64 |
| 6:Ah:79:ILE:HG23 | 6:BI:121:THR:HG23 | 1.80 | 0.64 |
| 6:Ah:131:TYR:HB3 | 6:Ah:250:MET:HG2 | 1.80 | 0.64 |
| 6:An:131:TYR:HE1 | 6:An:141:LYS:HB2 | 1.62 | 0.64 |
| 5:Ax:467:ILE:HD13 | 5:BA:473:ALA:HB2 | 1.79 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Az:147:MET:HG3 | 6:Az:367:GLN:HA | 1.80 | 0.64 |
| 7:BE:193:ASP:O | 7:BE:242:TYR:OH | 2.16 | 0.64 |
| 5:BF:278:ARG:NH1 | 5:BG:330:MET:O | 2.30 | 0.64 |
| 5:BF:289:THR:HG22 | 7:BL:303:PRO:HG3 | 1.78 | 0.64 |
| 3:BX:113:VAL:HG13 | 3:BX:127:ILE:HG23 | 1.79 | 0.64 |
| 3:Bb:106:GLU:O | 3:Bb:109:LYS:NZ | 2.29 | 0.64 |
| 3:Bi:117:ALA:HB3 | 3:Bi:122:THR:HB | 1.79 | 0.64 |
| 3:Bk:63:ASP:OD2 | 3:Bo:147:ASN:ND2 | 2.31 | 0.64 |
| 2:Bs:135:ASP:HB3 | 2:Bs:139:LYS:HB2 | 1.78 | 0.64 |
| 1:0:173:LYS:HB3 | 8:q:69:GLU:HB2 | 1.79 | 0.64 |
| 3:6:52:GLY:HA2 | 3:6:57:LYS:HA | 1.80 | 0.64 |
| 5:A2:214:SER:HB3 | 5:A2:221:MET:HB2 | 1.80 | 0.64 |
| 6:A5:459:LEU:HD21 | 6:A5:474:LYS:HE2 | 1.80 | 0.64 |
| 6:A7:383:VAL:HG21 | 6:A7:425:ILE:HG12 | 1.80 | 0.64 |
| 6:A9:279:ARG:NH1 | 5:Av:62:PHE:O | 2.31 | 0.64 |
| 8:AB:256:THR:OG1 | 8:AB:257:SER:N | 2.29 | 0.64 |
| 6:AW:263:SER:HB3 | 6:AW:476:ARG:HG2 | 1.78 | 0.64 |
| 6:AW:268:ALA:HB1 | 6:AW:290:LEU:HD13 | 1.79 | 0.64 |
| 6:Ae:456:LEU:H | 6:Ae:475:THR:HG22 | 1.63 | 0.64 |
| 6:Ag:481:ILE:HD11 | 6:Ag:501:PRO:HA | 1.80 | 0.64 |
| 6:Ai:93:PRO:O | 6:Am:123:GLN:NE2 | 2.31 | 0.64 |
| 6:Am:76:ALA:HB1 | 6:BJ:496:ILE:HG22 | 1.80 | 0.64 |
| 6:Aw:131:TYR:HD2 | 6:Aw:250:MET:HE3 | 1.63 | 0.64 |
| 3:BY:85:PHE:HB3 | 3:BY:137:VAL:HG21 | 1.80 | 0.64 |
| 3:Be:162:TRP:O | 3:Bh:95:GLN:NE2 | 2.30 | 0.64 |
| 2:1:38:ALA:HA | 2:1:82:ARG:HB3 | 1.78 | 0.64 |
| 2:5:490:SER:O | 2:5:496:ARG:NH1 | 2.31 | 0.64 |
| 6:A8:383:VAL:HG21 | 6:A8:425:ILE:HG12 | 1.79 | 0.64 |
| 8:AB:125:ARG:NH1 | 8:u:47:GLU:OE2 | 2.31 | 0.64 |
| 3:AG:8:ARG:O | 3:AH:31:ASN:ND2 | 2.30 | 0.64 |
| 10:AU:325:TRP:HA | 10:AU:338:ARG:HH21 | 1.62 | 0.64 |
| 6:Au:121:THR:OG1 | 6:BJ:90:GLN:O | 2.14 | 0.64 |
| 2:B5:521:ALA:HA | 2:B5:539:LYS:HE3 | 1.80 | 0.64 |
| 2:B6:645:THR:OG1 | 2:B7:629:ILE:O | 2.15 | 0.64 |
| 6:BK:105:ASN:HB2 | 6:BK:412:VAL:HG23 | 1.79 | 0.64 |
| 2:Bp:239:VAL:HG22 | 2:Bp:280:ALA:HB3 | 1.80 | 0.64 |
| 2:2:620:ARG:NH1 | 2:2:622:GLU:OE2 | 2.31 | 0.64 |
| 5:A0:473:ALA:HB2 | 5:BH:467:ILE:HD13 | 1.80 | 0.64 |
| 2:AM:154:ALA:HA | 2:AM:157:VAL:HG22 | 1.80 | 0.64 |
| 6:Ac:152:ALA:O | 6:Aw:264:ARG:NH2 | 2.31 | 0.64 |
| 6:Ac:456:LEU:H | 6:Ac:475:THR:HG22 | 1.63 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ah:278:LEU:HD12 | 6:Ah:286:ALA:HB2 | 1.79 | 0.64 |
| 2:B1:617:VAL:HG13 | 2:B1:622:GLU:HB2 | 1.80 | 0.64 |
| 6:BM:417:LEU:HB3 | 6:BM:421:TYR:HB2 | 1.79 | 0.64 |
| 3:BY:104:PRO:O | 3:BY:108:LYS:HB2 | 1.97 | 0.64 |
| 8:u:155:ASN:O | 8:u:157:ILE:N | 2.31 | 0.64 |
| 3:8:54:MET:O | 3:8:55:ASN:ND2 | 2.31 | 0.63 |
| 3:AF:19:ASN:OD1 | 3:AF:19:ASN:N | 2.26 | 0.63 |
| 3:AH:17:ARG:HG3 | 3:AH:20:LEU:HD12 | 1.80 | 0.63 |
| 2:AK:237:GLU:OE1 | 2:AK:284:ARG:NH2 | 2.28 | 0.63 |
| 7:Ar:151:MET:HE2 | 7:At:110:PHE:HB2 | 1.81 | 0.63 |
| 7:At:121:MET:SD | 7:At:122:GLY:N | 2.68 | 0.63 |
| 5:BA:282:ARG:HA | 5:BH:278:ARG:HH22 | 1.63 | 0.63 |
| 5:BH:379:ARG:NH1 | 5:BH:400:GLU:OE2 | 2.30 | 0.63 |
| 2:Bt:459:ASP:OD2 | 2:Bt:466:ARG:NH1 | 2.31 | 0.63 |
| 2:Bu:110:TYR:HE1 | 2:Bu:171:ILE:HG21 | 1.63 | 0.63 |
| 2:Bx:477:LEU:HD21 | 2:Bx:497:GLY:HA2 | 1.81 | 0.63 |
| 4:b:48:THR:HG21 | 4:g:47:PRO:HB2 | 1.80 | 0.63 |
| 1:n:41:ILE:HD13 | 1:p:5:ASP:HB2 | 1.80 | 0.63 |
| 6:A5:241:GLY:HA3 | 11:BT:43:GLY:HA2 | 1.80 | 0.63 |
| 3:AF:1:MET:SD | 3:AG:22:GLN:NE2 | 2.72 | 0.63 |
| 6:AV:142:GLU:H | 6:AV:490:GLN:HG2 | 1.63 | 0.63 |
| 7:Ab:62:VAL:HG13 | 7:Ab:68:ARG:HB2 | 1.78 | 0.63 |
| 6:Ae:383:VAL:HG21 | 6:Ae:425:ILE:HG12 | 1.79 | 0.63 |
| 6:Au:299:MET:HE1 | 5:BH:65:TYR:HB2 | 1.80 | 0.63 |
| 2:B4:91:ASN:ND2 | 2:B4:195:LEU:O | 2.30 | 0.63 |
| 2:Bu:561:LYS:HD2 | 2:Bw:10:LEU:HD13 | 1.80 | 0.63 |
| 4:f:36:THR:OG1 | 4:f:37:GLN:N | 2.32 | 0.63 |
| 1:l:213:ILE:HG21 | 8:s:70:THR:HA | 1.79 | 0.63 |
| 8:q:28:ARG:NH2 | 8:q:129:ASP:OD2 | 2.32 | 0.63 |
| 2:2:110:TYR:HE1 | 2:2:171:ILE:HG21 | 1.64 | 0.63 |
| 5:A1:89:ASP:OD2 | 5:BB:256:ARG:NH1 | 2.32 | 0.63 |
| 10:AQ:374:THR:HG21 | 6:AX:337:PRO:HG2 | 1.79 | 0.63 |
| 6:An:262:LYS:NZ | 6:BK:226:GLU:OE2 | 2.31 | 0.63 |
| 6:Au:363:GLU:OE2 | 6:Au:366:ARG:NH1 | 2.30 | 0.63 |
| 2:B1:364:ASP:OD1 | 2:Bz:514:ARG:NH1 | 2.29 | 0.63 |
| 5:BB:72:THR:OG1 | 5:BB:155:ARG:NH2 | 2.30 | 0.63 |
| 2:4:94:PRO:HB2 | 2:4:219:ILE:HD12 | 1.80 | 0.63 |
| 2:AO:645:THR:OG1 | 2:B5:629:ILE:O | 2.15 | 0.63 |
| 7:Aa:269:MET:SD | 1:k:50:SER:OG | 2.57 | 0.63 |
| 6:Ac:459:LEU:HD21 | 6:Ac:474:LYS:HE2 | 1.80 | 0.63 |
| 7:Aq:192:ILE:HD11 | 7:Aq:226:LEU:HD11 | 1.79 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B7:378:CYS:HB2 | 2:B7:410:PRO:HA | 1.79 | 0.63 |
| 2:B7:538:ASP:N | 2:B7:538:ASP:OD1 | 2.29 | 0.63 |
| 5:BG:379:ARG:NH1 | 5:BG:400:GLU:OE2 | 2.31 | 0.63 |
| 2:Bp:550:ARG:HB3 | 2:Bp:553:VAL:HG12 | 1.79 | 0.63 |
| 2:Bs:560:LEU:HD21 | 2:Bs:601:ILE:HD11 | 1.80 | 0.63 |
| 2:Bu:70:ASN:OD1 | 2:Bu:457:GLN:NE2 | 2.28 | 0.63 |
| 4:g:10:PHE:HB3 | 4:g:22:ILE:HG12 | 1.81 | 0.63 |
| 1:n:154:PRO:HA | 1:n:167:ARG:HD3 | 1.80 | 0.63 |
| 2:2:654:LEU:HD13 | 2:AP:605:ARG:HH11 | 1.62 | 0.63 |
| 5:A3:495:ASP:HA | 5:A3:498:ILE:HB | 1.81 | 0.63 |
| 8:AB:128:ASP:HB3 | 1:p:76:LEU:HD21 | 1.80 | 0.63 |
| 2:AO:206:THR:HA | 2:AO:211:GLN:HE21 | 1.64 | 0.63 |
| 6:Ae:279:ARG:NH2 | 6:Ae:285:ASP:OD1 | 2.31 | 0.63 |
| 6:Af:268:ALA:HB1 | 6:Af:290:LEU:HD13 | 1.80 | 0.63 |
| 6:Ag:154:PHE:O | 6:Ag:248:ASN:ND2 | 2.31 | 0.63 |
| 6:Ag:380:ARG:NH1 | 6:Ag:427:GLN:O | 2.32 | 0.63 |
| 6:Ap:271:SER:HA | 6:Ap:468:GLN:HB3 | 1.81 | 0.63 |
| 7:Aq:161:PHE:HA | 7:Aq:171:LYS:O | 1.98 | 0.63 |
| 2:B5:510:ARG:H | 2:B5:513:GLN:HE21 | 1.46 | 0.63 |
| 5:BB:310:ASN:HB3 | 5:BB:325:GLN:HA | 1.80 | 0.63 |
| 5:BD:397:THR:O | 5:BD:399:ASP:N | 2.31 | 0.63 |
| 5:BG:245:CYS:SG | 5:BG:246:CYS:N | 2.71 | 0.63 |
| 3:Bo:113:VAL:HG13 | 3:Bo:127:ILE:HG23 | 1.80 | 0.63 |
| 2:Bt:391:LYS:NZ | 2:Bt:440:ASN:O | 2.32 | 0.63 |
| 4:W:10:PHE:HB3 | 4:W:22:ILE:HG12 | 1.80 | 0.63 |
| 2:2:252:LEU:HB3 | 2:2:336:GLY:HA2 | 1.79 | 0.63 |
| 2:4:605:ARG:HB3 | 2:4:628:TYR:HD1 | 1.63 | 0.63 |
| 6:A5:237:GLU:HB3 | 6:Aj:465:LYS:HB3 | 1.79 | 0.63 |
| 6:A5:266:LEU:HB3 | 6:A5:294:LEU:HD22 | 1.81 | 0.63 |
| 3:AA:114:ARG:HG2 | 3:AA:126:GLU:HG3 | 1.80 | 0.63 |
| 7:Aa:61:TYR:O | 7:Aa:68:ARG:NH1 | 2.31 | 0.63 |
| 5:BA:7:SER:O | 5:BA:9:PHE:N | 2.31 | 0.63 |
| 3:Bm:17:ARG:HG3 | 3:Bm:20:LEU:HD12 | 1.81 | 0.63 |
| 4:W:48:THR:HG21 | 4:b:47:PRO:HB2 | 1.80 | 0.63 |
| 2:2:38:ALA:HA | 2:2:82:ARG:HB3 | 1.79 | 0.63 |
| 2:5:161:PRO:HB2 | 2:5:187:ILE:HB | 1.79 | 0.63 |
| 5:A1:281:ASP:O | 5:BB:278:ARG:NH2 | 2.32 | 0.63 |
| 5:A2:432:ILE:HG23 | 5:A2:436:GLU:HB2 | 1.80 | 0.63 |
| 6:A4:107:ILE:O | 6:A4:303:ASN:ND2 | 2.31 | 0.63 |
| 6:A5:430:LYS:HG2 | 6:AW:216:MET:HE1 | 1.81 | 0.63 |
| 3:AE:11:GLU:OE2 | 3:AF:31:ASN:ND2 | 2.32 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AK:455:LYS:NZ | 2:AK:473:ASP:OD2 | 2.30 | 0.63 |
| 6:Ag:350:PHE:HB2 | 6:Ag:389:VAL:HG11 | 1.80 | 0.63 |
| 6:Ah:344:ARG:HH21 | 6:BI:344:ARG:HH12 | 1.46 | 0.63 |
| 2:B1:488:TRP:HB3 | 2:B1:556:LEU:HD12 | 1.81 | 0.63 |
| 5:BD:73:ARG:NH2 | 5:BD:181:GLN:OE1 | 2.31 | 0.63 |
| 11:BP:11:LYS:HG3 | 11:BP:27:GLU:HG2 | 1.81 | 0.63 |
| 3:Bk:41:LEU:HD12 | 3:Bk:127:ILE:HD13 | 1.79 | 0.63 |
| 2:Bs:202:GLU:OE1 | 2:Bs:203:ALA:N | 2.32 | 0.63 |
| 2:Bw:453:ASN:HB2 | 2:Bw:506:ALA:HB3 | 1.81 | 0.63 |
| 2:Bw:538:ASP:N | 2:Bw:538:ASP:OD1 | 2.31 | 0.63 |
| 8:u:85:ASN:HD22 | 8:u:87:PRO:HD2 | 1.63 | 0.63 |
| 8:u:215:ASP:OD1 | 8:u:215:ASP:N | 2.32 | 0.63 |
| 6:A4:136:VAL:HG13 | 6:A4:253:ARG:HD2 | 1.81 | 0.63 |
| 3:AE:47:GLU:OE1 | 3:Ba:148:ASN:ND2 | 2.32 | 0.63 |
| 3:AI:28:LEU:HB3 | 3:AI:84:LYS:HE3 | 1.79 | 0.63 |
| 6:AZ:279:ARG:NH2 | 6:AZ:285:ASP:OD1 | 2.31 | 0.63 |
| 2:B3:561:LYS:HD2 | 2:B5:10:LEU:HD13 | 1.80 | 0.63 |
| 6:BK:363:GLU:OE2 | 6:BK:366:ARG:NH1 | 2.32 | 0.63 |
| 2:Bw:561:LYS:HD2 | 2:By:10:LEU:HD13 | 1.79 | 0.63 |
| 3:o:39:THR:OG1 | 3:o:69:TRP:NE1 | 2.32 | 0.63 |
| 8:q:230:PHE:HB3 | 8:q:258:ASN:HA | 1.81 | 0.63 |
| 2:1:637:TYR:HB2 | 2:AO:622:GLU:HG2 | 1.80 | 0.63 |
| 3:7:74:MET:HA | 3:7:152:THR:HG22 | 1.81 | 0.63 |
| 3:8:56:ARG:NH2 | 3:AA:96:GLY:O | 2.32 | 0.63 |
| 5:A3:72:THR:HG23 | 5:A3:155:ARG:HH21 | 1.64 | 0.63 |
| 8:AB:28:ARG:NH2 | 8:AB:129:ASP:OD2 | 2.32 | 0.63 |
| 2:AM:490:SER:O | 2:AM:496:ARG:NH1 | 2.29 | 0.63 |
| 7:Aq:12:LEU:HD13 | 7:Aq:38:ILE:HD12 | 1.81 | 0.63 |
| 6:Aw:398:GLN:OE1 | 6:Aw:399:GLY:N | 2.32 | 0.63 |
| 5:Ax:283:ARG:HH21 | 5:BA:278:ARG:HD2 | 1.62 | 0.63 |
| 2:B5:228:GLY:HA2 | 2:B5:345:SER:HB3 | 1.80 | 0.63 |
| 2:Bu:538:ASP:OD1 | 2:Bu:538:ASP:N | 2.31 | 0.63 |
| 2:Bz:20:VAL:HG21 | 2:Bz:46:ASN:HD21 | 1.64 | 0.63 |
| 4:K:34:ALA:H | 4:L:26:LYS:HA | 1.62 | 0.63 |
| 1:n:155:TYR:HB2 | 1:n:158:PHE:HA | 1.80 | 0.63 |
| 2:3:368:VAL:HG23 | 2:3:400:ARG:HH21 | 1.63 | 0.62 |
| 6:A5:261:ALA:HA | 6:A5:478:GLY:HA3 | 1.80 | 0.62 |
| 6:A5:515:ARG:NH2 | 6:A5:517:TYR:OH | 2.32 | 0.62 |
| 2:AD:605:ARG:HG2 | 2:AD:607:VAL:HG23 | 1.80 | 0.62 |
| 2:AL:28:ALA:HB2 | 2:AL:370:VAL:HG21 | 1.80 | 0.62 |
| 2:AP:645:THR:OG1 | 2:Bp:629:ILE:O | 2.16 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Aa:210:GLN:HG2 | 7:Aa:227:VAL:HG13 | 1.81 | 0.62 |
| 6:Ac:257:GLN:NE2 | 6:Ac:481:ILE:O | 2.32 | 0.62 |
| 2:B6:220:PRO:HD2 | 2:B6:338:LEU:HD11 | 1.80 | 0.62 |
| 5:BA:310:ASN:HA | 5:BA:326:HIS:H | 1.62 | 0.62 |
| 3:Bo:85:PHE:HB3 | 3:Bo:137:VAL:HG21 | 1.81 | 0.62 |
| 2:Bx:34:GLN:NE2 | 2:Bx:56:GLN:O | 2.32 | 0.62 |
| 2:By:24:THR:O | 2:By:483:ASN:ND2 | 2.32 | 0.62 |
| 2:Bz:550:ARG:HB3 | 2:Bz:553:VAL:HG12 | 1.81 | 0.62 |
| 1:l:78:ASN:ND2 | 1:l:179:GLU:OE1 | 2.32 | 0.62 |
| 1:m:177:SER:HB2 | 1:m:207:LEU:HB3 | 1.78 | 0.62 |
| 8:t:155:ASN:O | 8:t:157:ILE:N | 2.32 | 0.62 |
| 2:AL:131:ILE:HG12 | 2:AL:143:ILE:HG22 | 1.80 | 0.62 |
| 7:Ab:173:MET:HE1 | 7:Ar:55:LYS:HD3 | 1.82 | 0.62 |
| 7:Ab:193:ASP:O | 7:Ab:242:TYR:OH | 2.18 | 0.62 |
| 6:Ad:452:PRO:HB3 | 6:Ad:477:TYR:HD1 | 1.64 | 0.62 |
| 6:Af:152:ALA:O | 6:Az:264:ARG:NH2 | 2.32 | 0.62 |
| 6:An:377:ILE:HG23 | 6:An:435:THR:HG23 | 1.81 | 0.62 |
| 5:BF:245:CYS:SG | 5:BF:246:CYS:N | 2.72 | 0.62 |
| 3:Bl:85:PHE:HB3 | 3:Bl:137:VAL:HG21 | 1.79 | 0.62 |
| 2:Bp:645:THR:OG1 | 2:Bq:629:ILE:O | 2.16 | 0.62 |
| 2:Bx:559:MET:SD | 2:Bx:563:ASN:ND2 | 2.71 | 0.62 |
| 1:k:204:VAL:HA | 8:r:66:ALA:HB2 | 1.79 | 0.62 |
| 2:4:34:GLN:HE21 | 2:4:230:LEU:HD11 | 1.63 | 0.62 |
| 2:4:36:GLY:O | 2:4:82:ARG:NH1 | 2.31 | 0.62 |
| 2:4:547:PRO:HG2 | 8:t:229:VAL:HG13 | 1.81 | 0.62 |
| 6:A5:299:MET:HA | 6:A5:302:ILE:HD12 | 1.80 | 0.62 |
| 10:AS:344:MET:HE2 | 10:AS:351:VAL:HB | 1.80 | 0.62 |
| 7:Ab:143:GLN:NE2 | 5:BA:263:GLN:OE1 | 2.32 | 0.62 |
| 6:Af:79:ILE:HG23 | 6:Aj:121:THR:HG23 | 1.81 | 0.62 |
| 2:B4:239:VAL:HG22 | 2:B4:280:ALA:HB3 | 1.81 | 0.62 |
| 2:B5:98:ASN:HB2 | 2:B5:188:ILE:HD12 | 1.82 | 0.62 |
| 3:Bg:23:VAL:HG11 | 3:Bg:39:THR:HG21 | 1.81 | 0.62 |
| 3:Bg:113:VAL:HG13 | 3:Bg:127:ILE:HG23 | 1.80 | 0.62 |
| 2:Br:375:ALA:HB3 | 2:Br:407:CYS:HA | 1.82 | 0.62 |
| 2:Bx:414:VAL:HB | 2:Bx:426:LEU:HD21 | 1.80 | 0.62 |
| 4:E:48:THR:HG21 | 4:P:47:PRO:HB2 | 1.80 | 0.62 |
| 4:H:5:LEU:HD13 | 4:H:61:ASN:HB3 | 1.81 | 0.62 |
| 8:q:238:VAL:HG22 | 8:q:239:PRO:HD2 | 1.80 | 0.62 |
| 2:1:271:TYR:HB3 | 2:AD:545:PRO:HG3 | 1.79 | 0.62 |
| 2:3:511:GLN:OE1 | 2:3:514:ARG:NH2 | 2.31 | 0.62 |
| 6:A9:147:MET:HB3 | 6:A9:185:THR:HG22 | 1.81 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AK:220:PRO:HG2 | 2:AK:338:LEU:HD11 | 1.81 | 0.62 |
| 2:AN:121:VAL:HG13 | 2:AN:166:ASN:HA | 1.81 | 0.62 |
| 6:Ad:268:ALA:HB1 | 6:Ad:290:LEU:HD13 | 1.80 | 0.62 |
| 6:Ae:450:TYR:HB2 | 6:Ae:479:ILE:HG22 | 1.80 | 0.62 |
| 6:Ap:131:TYR:HE1 | 6:Ap:141:LYS:HB2 | 1.64 | 0.62 |
| 2:B4:450:ILE:O | 2:B4:523:ASN:ND2 | 2.32 | 0.62 |
| 5:BB:355:ASN:ND2 | 5:BB:359:MET:SD | 2.72 | 0.62 |
| 6:BJ:377:ILE:HG12 | 6:BJ:435:THR:HG23 | 1.81 | 0.62 |
| 3:BX:19:ASN:OD1 | 3:BX:19:ASN:N | 2.32 | 0.62 |
| 3:Bd:72:THR:HG22 | 3:Bd:154:GLU:HG3 | 1.80 | 0.62 |
| 2:Bx:517:LEU:HD23 | 2:Bx:524:PRO:HB3 | 1.80 | 0.62 |
| 1:0:176:TYR:HD1 | 8:q:71:ILE:HG23 | 1.64 | 0.62 |
| 6:A4:76:ALA:HB1 | 6:A5:496:ILE:HG12 | 1.82 | 0.62 |
| 6:A8:249:GLU:OE1 | 6:Au:66:ALA:N | 2.32 | 0.62 |
| 3:AF:31:ASN:OD1 | 3:AF:31:ASN:N | 2.30 | 0.62 |
| 2:AO:379:ALA:HB2 | 2:AO:454:TYR:HE2 | 1.65 | 0.62 |
| 6:AX:131:TYR:HD2 | 6:AX:250:MET:HE3 | 1.64 | 0.62 |
| 6:Ac:235:LEU:O | 6:Ac:245:ASN:ND2 | 2.33 | 0.62 |
| 6:Ai:381:ASN:HB3 | 6:Ai:521:ILE:HG21 | 1.79 | 0.62 |
| 4:B:66:LYS:NZ | 4:G:3:ILE:O | 2.31 | 0.62 |
| 2:B2:110:TYR:H | 2:B2:138:GLY:HA3 | 1.64 | 0.62 |
| 6:BJ:257:GLN:NE2 | 6:BJ:481:ILE:O | 2.31 | 0.62 |
| 3:BZ:4:ASP:OD2 | 2:Bu:593:GLN:NE2 | 2.32 | 0.62 |
| 3:Bd:43:ALA:O | 3:Bd:162:TRP:NE1 | 2.32 | 0.62 |
| 2:Bu:455:LYS:NZ | 2:Bu:473:ASP:OD1 | 2.32 | 0.62 |
| 2:By:269:PHE:HE2 | 2:By:282:ILE:HG12 | 1.63 | 0.62 |
| 4:b:62:ILE:HD12 | 4:g:58:LEU:HD22 | 1.81 | 0.62 |
| 2:2:66:MET:HG2 | 2:2:468:VAL:HG21 | 1.81 | 0.62 |
| 2:2:90:LYS:HD3 | 2:2:194:LEU:HB2 | 1.81 | 0.62 |
| 7:A6:161:PHE:O | 5:BF:303:HIS:NE2 | 2.32 | 0.62 |
| 2:AL:225:LEU:HD12 | 2:AL:324:PHE:HB2 | 1.81 | 0.62 |
| 6:Ac:432:ASP:HB3 | 6:Ac:518:VAL:HG22 | 1.81 | 0.62 |
| 6:Ao:262:LYS:NZ | 6:BM:226:GLU:OE2 | 2.33 | 0.62 |
| 5:BF:474:GLU:HG3 | 5:BF:475:PRO:HD3 | 1.82 | 0.62 |
| 3:BZ:23:VAL:HG12 | 3:BZ:113:VAL:HB | 1.81 | 0.62 |
| 3:Bf:1:MET:SD | 3:Bi:22:GLN:NE2 | 2.72 | 0.62 |
| 3:Bg:28:LEU:HD22 | 3:Bg:84:LYS:HB3 | 1.79 | 0.62 |
| 2:Bp:379:ALA:HA | 2:Bp:411:ARG:HB2 | 1.81 | 0.62 |
| 2:Bs:453:ASN:HB2 | 2:Bs:506:ALA:HB3 | 1.82 | 0.62 |
| 2:Bu:400:ARG:NH1 | 2:Bu:403:CYS:SG | 2.73 | 0.62 |
| 2:Bv:119:LYS:HE3 | 2:Bv:122:SER:HA | 1.80 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:l:127:VAL:O | 1:l:128:ASN:ND2 | 2.27 | 0.62 |
| 2:1:240:SER:OG | 2:1:334:PHE:O | 2.17 | 0.62 |
| 2:AD:32:LYS:HE2 | 2:AD:350:VAL:HB | 1.82 | 0.62 |
| 2:AD:51:VAL:HG22 | 2:AD:65:PHE:HZ | 1.63 | 0.62 |
| 2:AN:430:ARG:HG3 | 2:AN:522:ILE:HD11 | 1.79 | 0.62 |
| 7:Aa:28:GLU:HG2 | 1:l:31:VAL:HG12 | 1.80 | 0.62 |
| 6:Ap:322:THR:HG22 | 6:Ap:359:LYS:HG2 | 1.80 | 0.62 |
| 5:Ax:373:LEU:O | 5:Ax:374:ARG:HB2 | 1.97 | 0.62 |
| 3:Bm:82:ARG:HH12 | 3:Bm:138:GLY:HA2 | 1.64 | 0.62 |
| 2:Bp:227:PRO:HB2 | 2:Bp:345:SER:HB3 | 1.82 | 0.62 |
| 2:Br:92:SER:HB3 | 2:Br:340:LEU:HB3 | 1.81 | 0.62 |
| 2:Bv:98:ASN:HB2 | 2:Bv:188:ILE:HD12 | 1.82 | 0.62 |
| 4:E:27:ASN:ND2 | 4:U:35:ASP:OD1 | 2.33 | 0.62 |
| 1:n:87:ALA:HB2 | 1:p:26:ILE:HG23 | 1.80 | 0.62 |
| 6:A7:465:LYS:HB3 | 6:Ae:237:GLU:HB3 | 1.80 | 0.62 |
| 6:A8:462:SER:HB2 | 7:Ab:111:LEU:HD21 | 1.80 | 0.62 |
| 3:AF:104:PRO:O | 3:AF:108:LYS:HB2 | 1.99 | 0.62 |
| 3:AI:72:THR:HG22 | 3:AI:154:GLU:HG3 | 1.81 | 0.62 |
| 2:AL:488:TRP:O | 2:AL:552:ASN:ND2 | 2.32 | 0.62 |
| 7:AY:163:PHE:HB2 | 7:AY:170:LEU:HD13 | 1.80 | 0.62 |
| 6:Aj:76:ALA:HB1 | 6:An:496:ILE:HG22 | 1.80 | 0.62 |
| 6:Ao:157:GLN:HA | 6:Ao:228:MET:HE2 | 1.81 | 0.62 |
| 5:Av:166:ARG:NH2 | 5:Ax:26:GLU:OE1 | 2.33 | 0.62 |
| 2:B5:16:GLN:NE2 | 2:B5:460:LYS:O | 2.31 | 0.62 |
| 3:Bk:8:ARG:O | 3:Bn:31:ASN:ND2 | 2.33 | 0.62 |
| 2:Bw:378:CYS:HB2 | 2:Bw:410:PRO:HA | 1.80 | 0.62 |
| 9:x:168:LYS:HD2 | 9:y:85:ILE:HG21 | 1.81 | 0.62 |
| 2:2:620:ARG:O | 8:r:240:ARG:NH2 | 2.32 | 0.62 |
| 3:6:96:GLY:O | 3:AA:56:ARG:NH2 | 2.33 | 0.62 |
| 5:A2:374:ARG:NH2 | 5:BF:93:SER:OG | 2.32 | 0.62 |
| 5:A3:355:ASN:ND2 | 5:A3:359:MET:SD | 2.73 | 0.62 |
| 2:AK:11:LYS:HG2 | 2:AK:13:THR:HG23 | 1.81 | 0.62 |
| 2:AP:102:THR:HB | 2:AP:183:THR:HB | 1.82 | 0.62 |
| 6:Ae:237:GLU:HG2 | 6:Ae:246:PRO:HA | 1.81 | 0.62 |
| 7:At:108:THR:HB | 6:BJ:281:VAL:HG13 | 1.82 | 0.62 |
| 7:At:193:ASP:O | 7:At:242:TYR:OH | 2.18 | 0.62 |
| 5:Ax:397:THR:HG23 | 5:Ax:400:GLU:HB2 | 1.82 | 0.62 |
| 6:Ay:268:ALA:HB1 | 6:Ay:290:LEU:HD13 | 1.82 | 0.62 |
| 2:B7:264:THR:O | 2:B7:266:LYS:N | 2.33 | 0.62 |
| 11:BR:64:GLN:O | 11:BR:66:THR:N | 2.33 | 0.62 |
| 3:BY:137:VAL:HB | 3:BY:155:VAL:HG13 | 1.80 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A9:422:ARG:NH2 | 6:A9:424:TYR:OH | 2.33 | 0.62 |
| 2:AL:378:CYS:HB2 | 2:AL:410:PRO:HA | 1.82 | 0.62 |
| 6:Ad:131:TYR:HB3 | 6:Ad:250:MET:HG2 | 1.82 | 0.62 |
| 6:Aj:255:ASP:OD1 | 6:Aj:255:ASP:N | 2.33 | 0.62 |
| 6:Ap:332:PHE:HB3 | 6:Ap:518:VAL:HG12 | 1.81 | 0.62 |
| 5:Ax:89:ASP:OD2 | 5:BA:256:ARG:NH1 | 2.33 | 0.62 |
| 2:B3:401:GLN:O | 2:B3:561:LYS:NZ | 2.33 | 0.62 |
| 4:P:23:SER:OG | 4:P:26:LYS:NZ | 2.31 | 0.62 |
| 1:k:243:LYS:H | 8:q:4:TYR:H | 1.48 | 0.62 |
| 5:A1:72:THR:HG23 | 5:A1:155:ARG:HH21 | 1.65 | 0.61 |
| 6:A4:482:ASN:ND2 | 6:A4:483:PRO:O | 2.33 | 0.61 |
| 6:AW:383:VAL:HG21 | 6:AW:425:ILE:HG12 | 1.82 | 0.61 |
| 7:Ar:76:LEU:HD13 | 7:Ar:81:VAL:HG21 | 1.82 | 0.61 |
| 5:Ax:497:GLU:OE1 | 5:Ax:500:GLN:NE2 | 2.27 | 0.61 |
| 2:B1:100:GLU:HB3 | 2:B1:188:ILE:HD11 | 1.80 | 0.61 |
| 2:B2:36:GLY:O | 2:B2:82:ARG:NH1 | 2.32 | 0.61 |
| 5:BF:390:PHE:HZ | 5:BF:452:SER:HB2 | 1.65 | 0.61 |
| 6:BK:387:ALA:HB2 | 6:BK:404:PHE:HB2 | 1.82 | 0.61 |
| 11:BO:26:LYS:NZ | 11:BO:74:ASP:OD2 | 2.32 | 0.61 |
| 2:Bt:202:GLU:OE1 | 2:Bt:203:ALA:N | 2.31 | 0.61 |
| 2:Bz:470:LEU:HD11 | 2:Bz:499:ILE:HG21 | 1.80 | 0.61 |
| 4:X:9:PRO:HD3 | 4:X:57:VAL:HG21 | 1.81 | 0.61 |
| 8:q:213:TYR:HB3 | 8:q:271:ARG:HH21 | 1.65 | 0.61 |
| 8:t:25:GLN:O | 8:t:136:GLN:NE2 | 2.33 | 0.61 |
| 5:A2:72:THR:HG23 | 5:A2:155:ARG:HH21 | 1.64 | 0.61 |
| 2:AL:550:ARG:HB3 | 2:AL:553:VAL:HG12 | 1.82 | 0.61 |
| 2:AM:235:GLU:OE2 | 2:AM:261:ARG:NH2 | 2.33 | 0.61 |
| 2:AP:438:ASP:OD1 | 2:AP:438:ASP:N | 2.30 | 0.61 |
| 10:AR:316:GLN:NE2 | 10:AR:374:THR:O | 2.33 | 0.61 |
| 6:AX:105:ASN:ND2 | 6:AX:409:THR:O | 2.33 | 0.61 |
| 6:Ag:230:THR:HB | 6:Aw:71:ASP:HB3 | 1.80 | 0.61 |
| 6:Ak:106:LEU:HB3 | 6:Ak:303:ASN:HD22 | 1.64 | 0.61 |
| 6:An:417:LEU:HB2 | 6:An:421:TYR:HB2 | 1.83 | 0.61 |
| 5:Av:434:GLU:O | 5:Av:438:ASN:ND2 | 2.33 | 0.61 |
| 6:BK:278:LEU:HD22 | 6:BK:284:MET:HB2 | 1.81 | 0.61 |
| 3:Bi:90:SER:HA | 3:Bi:94:GLY:H | 1.65 | 0.61 |
| 3:Bn:40:ALA:O | 3:Bn:69:TRP:NE1 | 2.33 | 0.61 |
| 3:Bn:80:ASP:OD2 | 3:Bn:84:LYS:NZ | 2.33 | 0.61 |
| 2:Bq:110:TYR:H | 2:Bq:138:GLY:HA3 | 1.65 | 0.61 |
| 2:Bt:521:ALA:HA | 2:Bt:539:LYS:HD3 | 1.81 | 0.61 |
| 2:Bv:133:GLU:HB3 | 2:Bv:142:LYS:HB3 | 1.82 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bz:511:GLN:OE1 | 2:Bz:514:ARG:NH2 | 2.33 | 0.61 |
| 8:r:72:LEU:O | 8:r:74:ARG:N | 2.33 | 0.61 |
| 2:3:639:THR:HB | 2:AK:624:VAL:HG12 | 1.83 | 0.61 |
| 7:A6:36:ASP:OD1 | 7:A6:40:ARG:NH1 | 2.33 | 0.61 |
| 3:AA:22:GLN:OE1 | 3:AA:114:ARG:NH2 | 2.33 | 0.61 |
| 8:AB:70:THR:HG22 | 1:p:213:ILE:HD13 | 1.82 | 0.61 |
| 8:AB:184:ARG:NH1 | 8:u:45:SER:OG | 2.33 | 0.61 |
| 3:AE:63:ASP:HB3 | 3:Ba:147:ASN:HB3 | 1.83 | 0.61 |
| 2:AO:264:THR:O | 2:AO:266:LYS:N | 2.33 | 0.61 |
| 7:Al:76:LEU:HB3 | 7:Al:79:SER:HB3 | 1.81 | 0.61 |
| 5:Ax:275:ARG:NH1 | 5:Ax:353:ALA:O | 2.31 | 0.61 |
| 2:B1:120:TYR:HE1 | 2:B1:166:ASN:HD22 | 1.47 | 0.61 |
| 2:B2:49:ASP:OD1 | 2:B2:49:ASP:N | 2.33 | 0.61 |
| 2:Bu:135:ASP:HB3 | 2:Bu:139:LYS:HB2 | 1.81 | 0.61 |
| 2:Bx:383:LEU:HD23 | 2:Bx:410:PRO:HG2 | 1.81 | 0.61 |
| 2:Bz:93:SER:HB3 | 2:Bz:191:SER:HB2 | 1.82 | 0.61 |
| 4:F:9:PRO:HD3 | 4:F:57:VAL:HG21 | 1.82 | 0.61 |
| 3:o:7:THR:HG23 | 3:o:14:ASP:H | 1.65 | 0.61 |
| 6:A5:324:THR:HB | 6:A5:327:SER:HB2 | 1.83 | 0.61 |
| 6:Ai:385:VAL:HG21 | 6:Ai:521:ILE:HD12 | 1.81 | 0.61 |
| 6:Ao:235:LEU:O | 6:Ao:245:ASN:ND2 | 2.33 | 0.61 |
| 2:B4:24:THR:O | 2:B4:483:ASN:ND2 | 2.29 | 0.61 |
| 2:B5:135:ASP:HB3 | 2:B5:139:LYS:HB2 | 1.81 | 0.61 |
| 2:B7:49:ASP:OD1 | 2:B7:49:ASP:N | 2.33 | 0.61 |
| 6:BJ:282:HIS:HB3 | 6:BJ:284:MET:HG2 | 1.80 | 0.61 |
| 6:BK:340:ILE:HG13 | 6:BK:343:ALA:H | 1.65 | 0.61 |
| 3:Bc:85:PHE:HB3 | 3:Bc:137:VAL:HG21 | 1.83 | 0.61 |
| 3:Bj:113:VAL:HG13 | 3:Bj:127:ILE:HG23 | 1.82 | 0.61 |
| 2:Bs:596:LYS:NZ | 2:Bs:602:TYR:O | 2.33 | 0.61 |
| 2:Bu:238:ILE:HG12 | 2:Bu:281:ILE:HG23 | 1.81 | 0.61 |
| 3:7:39:THR:OG1 | 3:7:69:TRP:NE1 | 2.30 | 0.61 |
| 5:A0:38:ASP:OD2 | 5:A0:186:ARG:NH2 | 2.33 | 0.61 |
| 5:A3:66:GLU:H | 5:A3:69:MET:HE3 | 1.65 | 0.61 |
| 3:AF:80:ASP:OD1 | 3:AF:84:LYS:NZ | 2.34 | 0.61 |
| 2:AK:129:GLY:HA3 | 2:AK:145:ILE:HD13 | 1.81 | 0.61 |
| 2:AK:239:VAL:HG22 | 2:AK:280:ALA:HB3 | 1.83 | 0.61 |
| 2:AO:28:ALA:HB2 | 2:AO:370:VAL:HG21 | 1.82 | 0.61 |
| 2:AP:41:ILE:HD11 | 2:AP:361:PHE:HB3 | 1.81 | 0.61 |
| 6:Ag:235:LEU:O | 6:Ag:245:ASN:ND2 | 2.33 | 0.61 |
| 6:Ao:406:THR:OG1 | 6:BM:372:GLU:OE2 | 2.18 | 0.61 |
| 2:B3:571:ARG:NH2 | 2:B3:587:GLU:OE1 | 2.32 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bp:66:MET:HG2 | 2:Bp:468:VAL:HG21 | 1.82 | 0.61 |
| 4:A:62:ILE:HD12 | 4:F:58:LEU:HD22 | 1.81 | 0.61 |
| 5:A1:467:ILE:HD13 | 5:BB:473:ALA:HB2 | 1.82 | 0.61 |
| 2:AD:94:PRO:HB2 | 2:AD:219:ILE:HD12 | 1.83 | 0.61 |
| 2:AL:57:PRO:HB3 | 2:AL:62:ALA:HA | 1.82 | 0.61 |
| 6:Ae:171:GLN:OE1 | 6:Ae:195:GLN:NE2 | 2.33 | 0.61 |
| 6:Ao:264:ARG:NH2 | 6:BM:152:ALA:O | 2.32 | 0.61 |
| 7:As:250:TYR:OH | 7:As:294:ARG:NH2 | 2.33 | 0.61 |
| 6:Ay:253:ARG:HH22 | 6:Ay:491:ALA:HB1 | 1.65 | 0.61 |
| 6:Ay:278:LEU:HD12 | 6:Ay:284:MET:HB2 | 1.83 | 0.61 |
| 7:BC:150:MET:HE3 | 5:BH:329:SER:HB2 | 1.82 | 0.61 |
| 6:BI:235:LEU:O | 6:BI:245:ASN:ND2 | 2.32 | 0.61 |
| 6:BJ:449:TYR:OH | 6:BJ:482:ASN:ND2 | 2.34 | 0.61 |
| 3:Be:137:VAL:HB | 3:Be:155:VAL:HG13 | 1.83 | 0.61 |
| 2:Bv:198:ILE:HD11 | 2:Bv:225:LEU:HD11 | 1.83 | 0.61 |
| 2:Bw:446:THR:OG1 | 2:Bw:554:ARG:NH2 | 2.30 | 0.61 |
| 2:Bw:473:ASP:HB3 | 2:Bw:499:ILE:HD12 | 1.83 | 0.61 |
| 2:Bx:455:LYS:NZ | 2:Bx:473:ASP:OD2 | 2.33 | 0.61 |
| 2:By:90:LYS:NZ | 2:By:190:ASP:OD1 | 2.32 | 0.61 |
| 2:4:383:LEU:HD22 | 2:4:439:ASN:HB2 | 1.83 | 0.61 |
| 2:4:590:GLN:HE22 | 3:9:8:ARG:HH12 | 1.48 | 0.61 |
| 2:5:413:THR:HG23 | 2:5:414:VAL:HG23 | 1.82 | 0.61 |
| 3:AE:63:ASP:OD2 | 3:Ba:147:ASN:ND2 | 2.34 | 0.61 |
| 3:AG:128:GLU:H | 3:AG:163:GLU:HB2 | 1.65 | 0.61 |
| 2:AP:239:VAL:HG22 | 2:AP:280:ALA:HB3 | 1.82 | 0.61 |
| 10:AQ:357:ARG:HA | 6:An:344:ARG:HD2 | 1.81 | 0.61 |
| 10:AS:313:ASP:OD2 | 10:AS:357:ARG:NH2 | 2.34 | 0.61 |
| 5:Av:379:ARG:NH2 | 5:Av:400:GLU:OE1 | 2.32 | 0.61 |
| 2:B6:521:ALA:HB1 | 2:B6:541:ALA:HA | 1.83 | 0.61 |
| 5:BB:379:ARG:NH1 | 5:BB:400:GLU:OE2 | 2.31 | 0.61 |
| 4:N:48:THR:HG21 | 4:O:47:PRO:HB2 | 1.82 | 0.61 |
| 8:u:69:GLU:HG2 | 8:u:70:THR:H | 1.66 | 0.61 |
| 2:1:34:GLN:NE2 | 2:1:56:GLN:O | 2.33 | 0.61 |
| 2:1:563:ASN:ND2 | 2:1:591:TYR:OH | 2.34 | 0.61 |
| 3:AH:25:ILE:HG23 | 3:AH:111:ALA:HB2 | 1.81 | 0.61 |
| 2:AL:264:THR:O | 2:AL:266:LYS:N | 2.34 | 0.61 |
| 2:AP:647:THR:O | 2:Bp:630:GLN:NE2 | 2.34 | 0.61 |
| 6:Ad:503:ILE:HG23 | 6:Ad:507:LEU:HD13 | 1.82 | 0.61 |
| 6:An:90:GLN:OE1 | 7:Aq:94:SER:OG | 2.19 | 0.61 |
| 2:B1:308:ASN:ND2 | 2:B1:313:ASP:OD2 | 2.33 | 0.61 |
| 6:BM:363:GLU:OE2 | 6:BM:366:ARG:NH1 | 2.33 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Be:85:PHE:HB3 | 3:Be:137:VAL:HG21 | 1.81 | 0.61 |
| 3:Bh:46:VAL:HG22 | 3:Bh:64:ARG:HE | 1.65 | 0.61 |
| 2:Bs:104:SER:OG | 2:Bs:183:THR:OG1 | 2.19 | 0.61 |
| 4:W:47:PRO:HB2 | 4:g:48:THR:HG21 | 1.82 | 0.61 |
| 1:k:213:ILE:HD13 | 8:r:70:THR:HG22 | 1.82 | 0.61 |
| 2:3:390:GLN:NE2 | 2:3:408:SER:O | 2.28 | 0.61 |
| 3:7:72:THR:HG22 | 3:7:154:GLU:HG2 | 1.83 | 0.61 |
| 5:A0:487:MET:HG3 | 5:A0:491:LEU:HD12 | 1.82 | 0.61 |
| 6:A5:264:ARG:NH1 | 6:A5:305:GLU:OE1 | 2.32 | 0.61 |
| 8:AB:45:SER:OG | 8:q:184:ARG:NH1 | 2.33 | 0.61 |
| 2:AD:246:LYS:H | 2:AD:246:LYS:HD3 | 1.66 | 0.61 |
| 3:AI:114:ARG:HG2 | 3:AI:126:GLU:HG3 | 1.82 | 0.61 |
| 3:AJ:23:VAL:HG11 | 3:AJ:39:THR:HG21 | 1.83 | 0.61 |
| 2:AK:368:VAL:HG23 | 2:AK:400:ARG:HH21 | 1.65 | 0.61 |
| 10:AR:319:THR:HG21 | 10:AR:370:GLY:HA3 | 1.82 | 0.61 |
| 6:Ah:95:VAL:HG22 | 6:Ah:97:GLY:H | 1.65 | 0.61 |
| 2:B4:453:ASN:HD21 | 2:B4:505:LEU:HG | 1.66 | 0.61 |
| 3:Bh:85:PHE:HB3 | 3:Bh:137:VAL:HG21 | 1.83 | 0.61 |
| 2:Bq:556:LEU:HD21 | 2:Bq:601:ILE:HG12 | 1.82 | 0.61 |
| 2:Br:237:GLU:OE1 | 2:Br:284:ARG:NH1 | 2.34 | 0.61 |
| 2:Bz:159:GLU:OE1 | 2:Bz:167:TRP:NE1 | 2.34 | 0.61 |
| 4:c:9:PRO:HD3 | 4:c:57:VAL:HG21 | 1.81 | 0.61 |
| 1:k:78:ASN:ND2 | 1:k:179:GLU:OE1 | 2.34 | 0.61 |
| 8:r:45:SER:OG | 8:s:184:ARG:NH1 | 2.33 | 0.61 |
| 2:1:33:PHE:O | 2:1:82:ARG:NH2 | 2.34 | 0.61 |
| 2:1:590:GLN:HE22 | 3:6:8:ARG:HH22 | 1.49 | 0.61 |
| 3:AF:114:ARG:HG2 | 3:AF:126:GLU:HG2 | 1.81 | 0.61 |
| 2:AM:239:VAL:HG22 | 2:AM:280:ALA:HB3 | 1.83 | 0.61 |
| 2:AP:481:THR:HG23 | 2:AP:496:ARG:HD2 | 1.82 | 0.61 |
| 7:Ab:22:ALA:HB1 | 7:Ab:23:PRO:HD2 | 1.83 | 0.61 |
| 7:Al:111:LEU:HD12 | 6:Ap:462:SER:HB2 | 1.83 | 0.61 |
| 2:B1:366:GLU:OE2 | 2:Bz:514:ARG:NH1 | 2.34 | 0.61 |
| 2:B6:131:ILE:HA | 2:B6:143:ILE:HG22 | 1.83 | 0.61 |
| 7:BE:22:ALA:HB1 | 7:BE:23:PRO:HD2 | 1.82 | 0.61 |
| 5:BF:291:ASN:HD21 | 7:BL:299:LEU:HD13 | 1.66 | 0.61 |
| 5:BG:373:LEU:O | 5:BG:374:ARG:HB2 | 2.00 | 0.61 |
| 3:BX:101:GLY:HA3 | 3:Bn:118:ARG:HG3 | 1.83 | 0.61 |
| 3:Bh:54:MET:HB2 | 3:Bl:20:LEU:HD23 | 1.83 | 0.61 |
| 2:Bq:538:ASP:N | 2:Bq:538:ASP:OD1 | 2.32 | 0.61 |
| 4:a:44:MET:HE2 | 4:f:25:ILE:HD13 | 1.83 | 0.61 |
| 1:m:53:MET:HE3 | 1:n:31:VAL:HG11 | 1.83 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:n:177:SER:OG | 1:n:210:ILE:O | 2.19 | 0.61 |
| 2:1:598:LEU:HD21 | 3:6:8:ARG:HG2 | 1.83 | 0.60 |
| 5:A2:485:THR:OG1 | 5:BF:501:GLU:OE1 | 2.17 | 0.60 |
| 5:A3:18:ARG:HD2 | 5:A3:21:LYS:HE3 | 1.83 | 0.60 |
| 5:A3:495:ASP:N | 5:A3:495:ASP:OD1 | 2.30 | 0.60 |
| 8:AB:213:TYR:HB3 | 8:AB:271:ARG:HH21 | 1.65 | 0.60 |
| 2:AP:450:ILE:O | 2:AP:523:ASN:ND2 | 2.34 | 0.60 |
| 7:AY:22:ALA:HB1 | 7:AY:23:PRO:HD2 | 1.81 | 0.60 |
| 6:Ae:241:GLY:HA3 | 11:BS:43:GLY:HA2 | 1.82 | 0.60 |
| 6:Ae:261:ALA:HA | 6:Ae:478:GLY:HA3 | 1.82 | 0.60 |
| 7:Al:29:LEU:HD21 | 7:Al:259:ASN:HB2 | 1.83 | 0.60 |
| 5:Av:467:ILE:HD13 | 5:Ax:473:ALA:HB2 | 1.82 | 0.60 |
| 2:B1:110:TYR:HE1 | 2:B1:171:ILE:HG21 | 1.66 | 0.60 |
| 2:B2:560:LEU:HD21 | 2:B2:601:ILE:HD11 | 1.83 | 0.60 |
| 3:BX:11:GLU:OE1 | 2:Bs:486:GLN:NE2 | 2.34 | 0.60 |
| 2:Bp:517:LEU:HG | 2:Bp:522:ILE:HB | 1.81 | 0.60 |
| 1:k:175:ILE:HG22 | 8:r:125:ARG:HD2 | 1.82 | 0.60 |
| 8:r:218:ALA:H | 8:r:229:VAL:HB | 1.66 | 0.60 |
| 1:0:64:GLU:HB2 | 1:0:79:LYS:HG2 | 1.83 | 0.60 |
| 2:1:511:GLN:NE2 | 2:2:5:SER:OG | 2.34 | 0.60 |
| 5:A1:55:ASN:O | 5:A1:59:GLN:NE2 | 2.34 | 0.60 |
| 2:AK:125:ILE:HG22 | 2:AK:149:LYS:HB2 | 1.83 | 0.60 |
| 2:AK:378:CYS:HB2 | 2:AK:410:PRO:HA | 1.82 | 0.60 |
| 2:AM:220:PRO:HG2 | 2:AM:338:LEU:HD11 | 1.83 | 0.60 |
| 2:AO:239:VAL:HG22 | 2:AO:280:ALA:HB3 | 1.82 | 0.60 |
| 6:Aw:264:ARG:NH1 | 6:Aw:305:GLU:OE1 | 2.34 | 0.60 |
| 6:Az:360:GLU:HB3 | 6:Az:436:VAL:HG11 | 1.83 | 0.60 |
| 5:BA:178:ASP:HB3 | 5:BA:181:GLN:HG2 | 1.83 | 0.60 |
| 7:BC:127:ARG:NH2 | 5:BG:246:CYS:SG | 2.74 | 0.60 |
| 5:BF:160:LYS:HE3 | 5:BF:236:VAL:HG22 | 1.83 | 0.60 |
| 6:BJ:345:TRP:HB2 | 6:BJ:348:GLU:HG2 | 1.82 | 0.60 |
| 11:BO:10:ILE:HG12 | 11:BO:48:THR:HB | 1.83 | 0.60 |
| 3:Be:132:LEU:HD13 | 3:Be:159:LEU:HB3 | 1.83 | 0.60 |
| 2:Bq:118:VAL:HB | 2:Bq:126:GLU:HB3 | 1.83 | 0.60 |
| 2:Bv:276:ASP:N | 2:Bv:276:ASP:OD1 | 2.34 | 0.60 |
| 2:Bz:455:LYS:NZ | 2:Bz:473:ASP:OD1 | 2.35 | 0.60 |
| 8:q:25:GLN:O | 8:q:136:GLN:NE2 | 2.26 | 0.60 |
| 8:s:85:ASN:ND2 | 8:s:195:ASN:OD1 | 2.34 | 0.60 |
| 9:x:47:THR:HG23 | 9:x:61:ARG:HB2 | 1.83 | 0.60 |
| 2:1:571:ARG:NH2 | 2:1:587:GLU:OE1 | 2.34 | 0.60 |
| 2:2:423:VAL:HG21 | 2:2:513:GLN:HB3 | 1.84 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A3:458:LYS:NZ | 5:BG:451:ASP:O | 2.24 | 0.60 |
| 3:AF:56:ARG:NH2 | 3:AH:96:GLY:O | 2.34 | 0.60 |
| 3:AG:47:GLU:OE1 | 3:Bg:148:ASN:ND2 | 2.34 | 0.60 |
| 6:AX:123:GLN:HE21 | 6:BK:95:VAL:HB | 1.66 | 0.60 |
| 6:Af:184:GLU:HB2 | 6:Af:366:ARG:HH22 | 1.65 | 0.60 |
| 6:Ak:235:LEU:O | 6:Ak:245:ASN:ND2 | 2.34 | 0.60 |
| 6:Ay:107:ILE:O | 6:Ay:303:ASN:ND2 | 2.26 | 0.60 |
| 6:Ay:263:SER:HB3 | 6:Ay:476:ARG:HG2 | 1.83 | 0.60 |
| 6:Az:367:GLN:O | 6:Az:487:SER:OG | 2.18 | 0.60 |
| 2:B2:24:THR:O | 2:B2:483:ASN:ND2 | 2.32 | 0.60 |
| 2:B6:90:LYS:NZ | 2:B6:190:ASP:OD1 | 2.34 | 0.60 |
| 7:BE:109:ASP:HA | 7:BE:112:LEU:HD12 | 1.84 | 0.60 |
| 11:BW:26:LYS:HD2 | 11:BW:75:LEU:HD23 | 1.82 | 0.60 |
| 3:BZ:106:GLU:O | 3:BZ:109:LYS:NZ | 2.33 | 0.60 |
| 2:Bp:455:LYS:HB2 | 2:Bp:470:LEU:HD13 | 1.84 | 0.60 |
| 2:Bu:209:ASP:N | 2:Bu:209:ASP:OD1 | 2.34 | 0.60 |
| 2:By:264:THR:O | 2:By:266:LYS:N | 2.34 | 0.60 |
| 2:Bz:490:SER:O | 2:Bz:496:ARG:NH1 | 2.26 | 0.60 |
| 4:G:62:ILE:HD12 | 4:R:58:LEU:HD22 | 1.83 | 0.60 |
| 1:n:231:TYR:OH | 8:u:15:THR:OG1 | 2.18 | 0.60 |
| 1:0:87:ALA:HB1 | 1:k:27:LEU:HD23 | 1.82 | 0.60 |
| 5:A3:335:TRP:HB2 | 7:A6:307:LEU:HB2 | 1.82 | 0.60 |
| 6:AV:395:TYR:HD1 | 6:AV:396:ALA:H | 1.50 | 0.60 |
| 7:AY:95:ILE:HD13 | 7:Aq:111:LEU:HD13 | 1.83 | 0.60 |
| 7:AY:121:MET:SD | 7:AY:121:MET:N | 2.74 | 0.60 |
| 5:Ax:93:SER:OG | 5:BA:374:ARG:NH2 | 2.34 | 0.60 |
| 2:B3:455:LYS:HD2 | 2:B3:502:VAL:HG22 | 1.81 | 0.60 |
| 2:Bt:525:VAL:HG22 | 2:Bt:535:LEU:HD23 | 1.83 | 0.60 |
| 2:Bw:526:THR:OG1 | 2:Bx:366:GLU:OE2 | 2.16 | 0.60 |
| 2:By:29:LEU:O | 2:By:80:VAL:HA | 2.01 | 0.60 |
| 4:J:62:ILE:HD12 | 4:K:58:LEU:HD22 | 1.84 | 0.60 |
| 1:k:127:VAL:O | 1:k:128:ASN:ND2 | 2.26 | 0.60 |
| 8:t:45:SER:OG | 8:u:184:ARG:NH1 | 2.34 | 0.60 |
| 4:A:31:ILE:HG22 | 7:A6:231:VAL:HG23 | 1.83 | 0.60 |
| 5:A1:41:ARG:HH12 | 5:A1:64:SER:HA | 1.67 | 0.60 |
| 6:A4:216:MET:HE1 | 6:A9:430:LYS:HG3 | 1.82 | 0.60 |
| 6:A9:365:ALA:HB2 | 6:A9:372:GLU:HA | 1.83 | 0.60 |
| 2:AL:391:LYS:HG2 | 2:AL:443:ILE:HD13 | 1.83 | 0.60 |
| 6:AX:234:GLU:OE2 | 6:BK:476:ARG:NH2 | 2.34 | 0.60 |
| 6:Ah:268:ALA:HB1 | 6:Ah:290:LEU:HD13 | 1.84 | 0.60 |
| 6:Ak:131:TYR:HB3 | 6:Ak:250:MET:HG2 | 1.82 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Al:239:GLN:O | 7:BE:167:ASN:ND2 | 2.35 | 0.60 |
| 6:Am:400:LEU:HD11 | 6:BJ:417:LEU:HD22 | 1.84 | 0.60 |
| 7:At:32:ASP:OD1 | 7:At:204:TYR:OH | 2.20 | 0.60 |
| 7:At:216:SER:O | 7:At:220:ASN:ND2 | 2.31 | 0.60 |
| 2:B2:596:LYS:NZ | 2:B2:602:TYR:O | 2.32 | 0.60 |
| 2:B5:18:THR:HG22 | 2:B5:460:LYS:HZ2 | 1.66 | 0.60 |
| 5:BA:55:ASN:H | 5:BA:58:PHE:HB3 | 1.66 | 0.60 |
| 6:BK:181:PHE:HD1 | 6:BK:187:THR:HB | 1.66 | 0.60 |
| 11:BS:64:GLN:O | 11:BS:66:THR:N | 2.35 | 0.60 |
| 2:Bt:42:LYS:NZ | 2:Bt:43:GLN:O | 2.34 | 0.60 |
| 2:Bu:131:ILE:HG12 | 2:Bu:143:ILE:HG22 | 1.83 | 0.60 |
| 2:By:256:PRO:HG2 | 2:By:339:THR:H | 1.65 | 0.60 |
| 8:r:222:ASP:N | 8:r:222:ASP:OD1 | 2.33 | 0.60 |
| 8:t:93:LEU:HD21 | 9:y:121:LYS:HB3 | 1.83 | 0.60 |
| 2:4:331:PRO:HB2 | 2:4:334:PHE:HB2 | 1.82 | 0.60 |
| 5:A0:354:ASP:OD1 | 5:A0:354:ASP:N | 2.32 | 0.60 |
| 7:A6:163:PHE:HB2 | 7:A6:170:LEU:HD13 | 1.83 | 0.60 |
| 9:AC:66:PHE:H | 9:z:57:GLY:HA2 | 1.67 | 0.60 |
| 2:AL:22:ASN:ND2 | 2:AL:76:ASN:OD1 | 2.34 | 0.60 |
| 6:Ae:299:MET:HA | 6:Ae:302:ILE:HD12 | 1.83 | 0.60 |
| 6:Ai:107:ILE:O | 6:Ai:303:ASN:ND2 | 2.28 | 0.60 |
| 6:Am:417:LEU:HB3 | 6:Am:421:TYR:HB2 | 1.82 | 0.60 |
| 7:Ar:163:PHE:HB2 | 7:Ar:170:LEU:HD13 | 1.83 | 0.60 |
| 2:B3:427:VAL:O | 2:B3:431:THR:OG1 | 2.19 | 0.60 |
| 2:B5:206:THR:HA | 2:B5:211:GLN:HE21 | 1.66 | 0.60 |
| 6:BJ:350:PHE:HB2 | 6:BJ:389:VAL:HG11 | 1.84 | 0.60 |
| 3:Bi:40:ALA:O | 3:Bi:69:TRP:NE1 | 2.35 | 0.60 |
| 2:Bs:571:ARG:NH2 | 2:Bs:587:GLU:OE1 | 2.35 | 0.60 |
| 1:m:147:PHE:HB3 | 1:m:171:ALA:HB1 | 1.83 | 0.60 |
| 8:r:179:ASP:N | 8:r:179:ASP:OD1 | 2.35 | 0.60 |
| 9:w:27:THR:O | 9:w:29:ALA:N | 2.34 | 0.60 |
| 2:1:528:THR:HB | 2:AO:366:GLU:HB2 | 1.84 | 0.60 |
| 2:3:241:LYS:HB2 | 2:3:273:PRO:HB2 | 1.84 | 0.60 |
| 2:5:391:LYS:HG2 | 2:5:443:ILE:HD11 | 1.84 | 0.60 |
| 3:6:141:GLN:HG3 | 3:o:40:ALA:HB2 | 1.84 | 0.60 |
| 6:A4:146:PRO:HD3 | 6:A9:101:ARG:HD3 | 1.84 | 0.60 |
| 6:A5:287:ASP:OD1 | 6:A5:288:ALA:N | 2.34 | 0.60 |
| 3:AA:54:MET:O | 3:AA:55:ASN:ND2 | 2.34 | 0.60 |
| 2:AD:490:SER:O | 2:AD:496:ARG:NH1 | 2.34 | 0.60 |
| 7:Ab:98:MET:HG3 | 6:Au:459:LEU:HD13 | 1.83 | 0.60 |
| 7:Al:12:LEU:HD12 | 7:Al:242:TYR:HD2 | 1.66 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Al:303:PRO:HG3 | 5:BG:289:THR:HG22 | 1.83 | 0.60 |
| 6:Am:459:LEU:HD11 | 6:Am:474:LYS:HE2 | 1.84 | 0.60 |
| 6:Ao:105:ASN:N | 6:Ao:105:ASN:OD1 | 2.34 | 0.60 |
| 6:Ap:110:ASP:OD2 | 6:Ap:422:ARG:NH1 | 2.34 | 0.60 |
| 7:As:143:GLN:OE1 | 5:Av:263:GLN:NE2 | 2.35 | 0.60 |
| 5:Av:175:ARG:NH1 | 5:Ax:30:SER:OG | 2.34 | 0.60 |
| 6:Az:279:ARG:NH2 | 6:Az:285:ASP:OD1 | 2.33 | 0.60 |
| 2:B5:272:GLY:O | 2:B5:274:GLN:NE2 | 2.35 | 0.60 |
| 2:B7:134:VAL:HG12 | 2:B7:140:ILE:HG22 | 1.83 | 0.60 |
| 7:BE:214:SER:OG | 7:BE:217:GLU:OE1 | 2.18 | 0.60 |
| 5:BF:373:LEU:O | 5:BF:374:ARG:HB2 | 2.02 | 0.60 |
| 1:k:147:PHE:HB3 | 1:k:171:ALA:HB1 | 1.84 | 0.60 |
| 3:o:148:ASN:HB3 | 9:y:45:PRO:HB2 | 1.83 | 0.60 |
| 4:A:9:PRO:HD3 | 4:A:57:VAL:HG21 | 1.83 | 0.60 |
| 5:A3:67:PRO:HA | 6:AV:114:VAL:HB | 1.83 | 0.60 |
| 6:A5:131:TYR:HB3 | 6:A5:250:MET:HG2 | 1.84 | 0.60 |
| 3:AF:85:PHE:HB3 | 3:AF:137:VAL:HG21 | 1.83 | 0.60 |
| 7:AY:54:ASN:HA | 7:BL:162:TRP:HE1 | 1.67 | 0.60 |
| 6:Ad:264:ARG:NH1 | 6:Ad:305:GLU:OE1 | 2.35 | 0.60 |
| 6:Ad:452:PRO:HA | 6:Ad:477:TYR:HA | 1.83 | 0.60 |
| 7:As:126:ASN:HD22 | 7:As:128:PHE:H | 1.50 | 0.60 |
| 2:B1:272:GLY:O | 2:B1:274:GLN:NE2 | 2.35 | 0.60 |
| 2:B6:57:PRO:HB3 | 2:B6:62:ALA:HA | 1.84 | 0.60 |
| 6:BJ:365:ALA:HB2 | 6:BJ:372:GLU:HA | 1.84 | 0.60 |
| 2:Bs:41:ILE:HD11 | 2:Bs:361:PHE:HB3 | 1.83 | 0.60 |
| 2:Bw:430:ARG:HH21 | 2:Bw:541:ALA:HB1 | 1.65 | 0.60 |
| 8:r:243:ASP:N | 8:r:243:ASP:OD1 | 2.32 | 0.60 |
| 2:2:202:GLU:O | 2:2:206:THR:OG1 | 2.19 | 0.60 |
| 2:3:496:ARG:NH2 | 2:AK:573:PHE:O | 2.34 | 0.60 |
| 5:A1:59:GLN:OE1 | 6:BK:100:ARG:NH2 | 2.35 | 0.60 |
| 6:A5:309:TRP:NE1 | 6:AW:225:ALA:O | 2.35 | 0.60 |
| 6:A9:110:ASP:OD1 | 6:A9:110:ASP:N | 2.27 | 0.60 |
| 2:AK:40:GLN:H | 2:AK:81:VAL:HG23 | 1.66 | 0.60 |
| 2:AL:617:VAL:HG22 | 2:AL:622:GLU:HB2 | 1.83 | 0.60 |
| 2:AM:498:GLN:HA | 2:AM:534:VAL:HG12 | 1.84 | 0.60 |
| 2:AN:23:SER:OG | 2:AN:74:TYR:O | 2.20 | 0.60 |
| 6:AX:482:ASN:OD1 | 6:AX:483:PRO:O | 2.19 | 0.60 |
| 6:Ac:479:ILE:HD11 | 6:Ac:501:PRO:HG3 | 1.83 | 0.60 |
| 6:Ah:336:ASP:HB3 | 6:Ah:339:ASP:HB2 | 1.84 | 0.60 |
| 6:BJ:263:SER:HB3 | 6:BJ:476:ARG:HG2 | 1.82 | 0.60 |
| 2:Bq:254:ILE:HG13 | 2:Bq:337:ILE:HB | 1.84 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:X:58:LEU:HD22 | 4:h:62:ILE:HD12 | 1.84 | 0.60 |
| 1:0:61:VAL:HB | 1:0:137:LEU:HB2 | 1.83 | 0.60 |
| 7:A6:25:ILE:HD12 | 7:Al:265:ARG:HG3 | 1.83 | 0.60 |
| 6:AV:278:LEU:HD22 | 6:AV:284:MET:HB2 | 1.83 | 0.60 |
| 7:Aa:222:PRO:O | 7:Aa:225:ASN:ND2 | 2.34 | 0.60 |
| 7:At:112:LEU:HD21 | 7:At:129:TYR:HE2 | 1.66 | 0.60 |
| 2:B1:230:LEU:HD21 | 2:B1:285:ARG:HD2 | 1.84 | 0.60 |
| 5:BD:366:ARG:NH1 | 5:BD:382:GLN:OE1 | 2.34 | 0.60 |
| 11:BP:64:GLN:O | 11:BP:66:THR:N | 2.34 | 0.60 |
| 2:Bx:220:PRO:HG2 | 2:Bx:338:LEU:HD11 | 1.83 | 0.60 |
| 2:Bz:394:VAL:HG11 | 2:Bz:443:ILE:HD12 | 1.84 | 0.60 |
| 1:n:182:ASN:HA | 1:n:205:ARG:HG3 | 1.83 | 0.60 |
| 5:A2:467:ILE:HD13 | 5:BD:473:ALA:HB2 | 1.84 | 0.59 |
| 6:A8:383:VAL:HG12 | 6:A8:406:THR:HG22 | 1.84 | 0.59 |
| 8:AB:71:ILE:HA | 1:p:176:TYR:HA | 1.83 | 0.59 |
| 2:AL:478:CYS:O | 2:AL:555:ARG:NH1 | 2.35 | 0.59 |
| 10:AQ:344:MET:HE2 | 10:AQ:351:VAL:HB | 1.82 | 0.59 |
| 10:AQ:348:TYR:HB2 | 10:AQ:351:VAL:HG12 | 1.82 | 0.59 |
| 6:AV:181:PHE:HD1 | 6:AV:187:THR:HB | 1.67 | 0.59 |
| 6:Ai:115:GLN:NE2 | 6:Ai:444:MET:SD | 2.74 | 0.59 |
| 6:Aj:459:LEU:HD11 | 6:Aj:474:LYS:HE2 | 1.84 | 0.59 |
| 2:B3:57:PRO:HG3 | 2:B3:65:PHE:HB3 | 1.84 | 0.59 |
| 2:B5:639:THR:HB | 2:B6:624:VAL:HG12 | 1.84 | 0.59 |
| 6:BI:131:TYR:HB3 | 6:BI:250:MET:HG2 | 1.83 | 0.59 |
| 11:BS:69:ILE:O | 11:BS:72:ASN:ND2 | 2.35 | 0.59 |
| 11:BV:11:LYS:HG3 | 11:BV:27:GLU:HG2 | 1.83 | 0.59 |
| 3:BZ:42:PRO:HG2 | 3:BZ:127:ILE:HD11 | 1.83 | 0.59 |
| 3:Bc:24:GLU:OE1 | 3:Bc:33:THR:OG1 | 2.18 | 0.59 |
| 3:Bj:24:GLU:OE1 | 3:Bj:33:THR:OG1 | 2.20 | 0.59 |
| 2:Bu:33:PHE:HA | 2:Bu:61:THR:HG23 | 1.84 | 0.59 |
| 4:M:62:ILE:HD12 | 4:N:58:LEU:HD22 | 1.84 | 0.59 |
| 4:Z:47:PRO:HB2 | 4:j:48:THR:HG21 | 1.83 | 0.59 |
| 1:k:231:TYR:OH | 8:r:15:THR:OG1 | 2.15 | 0.59 |
| 8:s:72:LEU:O | 8:s:74:ARG:N | 2.35 | 0.59 |
| 5:A1:76:ILE:HD12 | 5:A1:180:ARG:HB3 | 1.84 | 0.59 |
| 7:A6:193:ASP:O | 7:A6:242:TYR:OH | 2.19 | 0.59 |
| 2:AN:36:GLY:O | 2:AN:82:ARG:NH1 | 2.35 | 0.59 |
| 2:AO:465:ASN:HB2 | 2:B5:317:LYS:HZ2 | 1.66 | 0.59 |
| 2:AP:585:ARG:NH2 | 2:AP:608:CYS:O | 2.35 | 0.59 |
| 6:Ai:519:LYS:NZ | 6:Am:217:GLU:OE1 | 2.30 | 0.59 |
| 6:Ak:400:LEU:HD11 | 6:Ao:417:LEU:HD22 | 1.82 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:An:100:ARG:HH21 | 6:An:284:MET:HE1 | 1.66 | 0.59 |
| 6:An:452:PRO:HA | 6:An:477:TYR:HA | 1.85 | 0.59 |
| 2:B2:538:ASP:O | 2:B2:551:ILE:N | 2.27 | 0.59 |
| 2:B5:394:VAL:HG11 | 2:B5:443:ILE:HD12 | 1.84 | 0.59 |
| 2:B5:563:ASN:ND2 | 2:B5:591:TYR:OH | 2.33 | 0.59 |
| 5:BA:281:ASP:O | 5:BH:278:ARG:NH2 | 2.35 | 0.59 |
| 7:BC:30:THR:HG23 | 7:BE:24:ILE:HD11 | 1.84 | 0.59 |
| 7:BL:159:PRO:HB3 | 7:BL:174:GLY:O | 2.02 | 0.59 |
| 6:BM:235:LEU:O | 6:BM:245:ASN:ND2 | 2.36 | 0.59 |
| 2:Bp:98:ASN:HB2 | 2:Bp:188:ILE:HD11 | 1.82 | 0.59 |
| 2:Bu:450:ILE:O | 2:Bu:523:ASN:ND2 | 2.35 | 0.59 |
| 2:Bx:375:ALA:HB3 | 2:Bx:407:CYS:HA | 1.84 | 0.59 |
| 4:a:62:ILE:HD12 | 4:f:58:LEU:HD22 | 1.84 | 0.59 |
| 8:u:230:PHE:HB3 | 8:u:258:ASN:HA | 1.83 | 0.59 |
| 9:w:51:THR:HG22 | 9:w:59:ALA:HB2 | 1.83 | 0.59 |
| 2:3:514:ARG:NH1 | 2:AK:366:GLU:OE2 | 2.35 | 0.59 |
| 2:5:623:PHE:HB3 | 8:u:212:THR:HG22 | 1.84 | 0.59 |
| 9:AC:168:LYS:HB3 | 9:AC:173:ILE:HD11 | 1.83 | 0.59 |
| 3:AF:106:GLU:O | 3:AF:109:LYS:NZ | 2.36 | 0.59 |
| 3:AH:23:VAL:HG11 | 3:AH:39:THR:HG21 | 1.84 | 0.59 |
| 10:AT:360:TYR:OH | 6:Ae:342:GLY:O | 2.18 | 0.59 |
| 6:AZ:72:HIS:ND1 | 6:AZ:83:GLN:O | 2.33 | 0.59 |
| 6:Ac:121:THR:HG22 | 6:Ac:260:GLU:HG3 | 1.84 | 0.59 |
| 6:Ae:268:ALA:HB1 | 6:Ae:290:LEU:HD13 | 1.83 | 0.59 |
| 6:Af:71:ASP:OD1 | 6:Af:72:HIS:ND1 | 2.35 | 0.59 |
| 6:Ai:264:ARG:NH2 | 6:Am:152:ALA:O | 2.34 | 0.59 |
| 6:Aj:153:MET:HE1 | 6:Aj:177:ILE:HD13 | 1.84 | 0.59 |
| 6:Am:121:THR:HA | 6:Am:259:ILE:O | 2.03 | 0.59 |
| 6:An:328:LYS:NZ | 6:An:333:ASP:OD2 | 2.33 | 0.59 |
| 2:B6:617:VAL:HG22 | 2:B6:622:GLU:HB2 | 1.84 | 0.59 |
| 5:BD:70:LYS:NZ | 5:BD:215:TYR:OH | 2.35 | 0.59 |
| 5:BG:37:ASP:N | 5:BG:37:ASP:OD1 | 2.35 | 0.59 |
| 11:BV:64:GLN:O | 11:BV:66:THR:N | 2.35 | 0.59 |
| 3:Bi:85:PHE:HB3 | 3:Bi:137:VAL:HG21 | 1.84 | 0.59 |
| 3:Bj:72:THR:HG22 | 3:Bj:154:GLU:HG3 | 1.83 | 0.59 |
| 2:Bs:308:ASN:ND2 | 2:Bs:313:ASP:OD2 | 2.36 | 0.59 |
| 2:Bz:453:ASN:HB2 | 2:Bz:506:ALA:HB3 | 1.83 | 0.59 |
| 1:0:137:LEU:HB3 | 1:0:146:LEU:HD21 | 1.84 | 0.59 |
| 2:3:620:ARG:NH1 | 2:3:622:GLU:OE2 | 2.35 | 0.59 |
| 5:A0:467:ILE:HD13 | 5:BG:473:ALA:HB2 | 1.82 | 0.59 |
| 8:AB:15:THR:OG1 | 1:p:231:TYR:OH | 2.21 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:18:THR:HG21 | 2:AD:47:GLU:HB3 | 1.84 | 0.59 |
| 2:AK:57:PRO:HA | 2:AK:61:THR:HB | 1.85 | 0.59 |
| 2:AN:98:ASN:HA | 2:AN:147:THR:HG21 | 1.84 | 0.59 |
| 2:AN:545:PRO:HD3 | 2:AO:271:TYR:HB3 | 1.84 | 0.59 |
| 6:AW:452:PRO:HA | 6:AW:477:TYR:HA | 1.84 | 0.59 |
| 6:Ai:93:PRO:HB2 | 6:Am:123:GLN:HB3 | 1.84 | 0.59 |
| 6:Aj:154:PHE:O | 6:Aj:248:ASN:ND2 | 2.35 | 0.59 |
| 6:Au:253:ARG:HH21 | 6:Au:495:ARG:HG2 | 1.67 | 0.59 |
| 5:Ax:111:LEU:HD11 | 5:Ax:444:ILE:HD11 | 1.85 | 0.59 |
| 2:B6:375:ALA:HB3 | 2:B6:407:CYS:HA | 1.83 | 0.59 |
| 2:B6:593:GLN:NE2 | 3:Bk:4:ASP:OD2 | 2.35 | 0.59 |
| 2:B7:556:LEU:HD11 | 2:B7:601:ILE:HG23 | 1.83 | 0.59 |
| 5:BB:244:ASP:O | 5:BB:247:GLY:N | 2.35 | 0.59 |
| 3:BX:114:ARG:HG2 | 3:BX:126:GLU:HG3 | 1.85 | 0.59 |
| 3:Bb:43:ALA:HA | 3:Be:138:GLY:HA3 | 1.85 | 0.59 |
| 3:Bb:125:LYS:NZ | 3:Be:83:GLN:OE1 | 2.35 | 0.59 |
| 2:Bq:375:ALA:HB3 | 2:Bq:407:CYS:HA | 1.84 | 0.59 |
| 2:Bq:514:ARG:NH1 | 2:Br:366:GLU:OE2 | 2.35 | 0.59 |
| 2:Bw:36:GLY:O | 2:Bw:82:ARG:NH1 | 2.33 | 0.59 |
| 4:M:58:LEU:HD22 | 4:O:62:ILE:HD12 | 1.85 | 0.59 |
| 8:r:76:ASN:HD21 | 8:r:121:SER:HB2 | 1.66 | 0.59 |
| 6:A4:383:VAL:HG12 | 6:A4:406:THR:HG22 | 1.84 | 0.59 |
| 6:A9:268:ALA:HB1 | 6:A9:290:LEU:HD13 | 1.83 | 0.59 |
| 2:AD:285:ARG:HG2 | 2:AD:286:ASN:HD22 | 1.66 | 0.59 |
| 3:AE:56:ARG:NH2 | 3:AG:96:GLY:O | 2.35 | 0.59 |
| 2:AM:163:LEU:HD11 | 2:AM:187:ILE:HG12 | 1.84 | 0.59 |
| 7:AY:25:ILE:HD12 | 7:BL:265:ARG:HG3 | 1.83 | 0.59 |
| 6:AZ:503:ILE:HG13 | 6:AZ:507:LEU:HD13 | 1.84 | 0.59 |
| 6:Ah:172:THR:O | 6:Ah:195:GLN:NE2 | 2.36 | 0.59 |
| 2:B7:550:ARG:HB3 | 2:B7:553:VAL:HG12 | 1.83 | 0.59 |
| 5:BG:495:ASP:OD1 | 5:BG:495:ASP:N | 2.34 | 0.59 |
| 2:Bs:33:PHE:HB2 | 2:Bs:82:ARG:HG3 | 1.84 | 0.59 |
| 2:Bw:617:VAL:HG22 | 2:Bw:622:GLU:HB2 | 1.84 | 0.59 |
| 2:By:211:GLN:OE1 | 2:By:329:ASN:ND2 | 2.36 | 0.59 |
| 2:Bz:109:ASN:HB2 | 2:Bz:177:GLY:HA2 | 1.84 | 0.59 |
| 2:4:18:THR:HG21 | 2:4:47:GLU:HB3 | 1.85 | 0.59 |
| 2:4:645:THR:OG1 | 2:AL:629:ILE:O | 2.20 | 0.59 |
| 2:5:571:ARG:NH2 | 2:5:587:GLU:OE1 | 2.34 | 0.59 |
| 3:9:40:ALA:O | 3:9:69:TRP:NE1 | 2.35 | 0.59 |
| 6:A4:254:ILE:HB | 6:Aj:88:VAL:HA | 1.84 | 0.59 |
| 3:AJ:114:ARG:HG2 | 3:AJ:126:GLU:HG2 | 1.84 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AN:197:GLU:HG3 | 2:AN:199:GLU:HG2 | 1.85 | 0.59 |
| 2:AO:104:SER:OG | 2:AO:183:THR:OG1 | 2.20 | 0.59 |
| 6:AX:459:LEU:HD11 | 6:AX:474:LYS:HE2 | 1.84 | 0.59 |
| 2:B2:26:THR:HA | 2:B2:77:ASP:O | 2.01 | 0.59 |
| 2:B3:135:ASP:HB3 | 2:B3:139:LYS:HB2 | 1.85 | 0.59 |
| 2:B6:394:VAL:HG11 | 2:B6:443:ILE:HD12 | 1.84 | 0.59 |
| 5:A2:41:ARG:HG3 | 5:A2:183:GLN:HE21 | 1.68 | 0.59 |
| 2:AK:225:LEU:HD22 | 2:AK:321:GLU:HA | 1.85 | 0.59 |
| 2:AL:455:LYS:HG3 | 2:AL:502:VAL:HG13 | 1.85 | 0.59 |
| 2:AN:205:MET:O | 2:AN:211:GLN:NE2 | 2.35 | 0.59 |
| 6:Ac:267:LYS:HE2 | 6:Ac:470:VAL:HG11 | 1.84 | 0.59 |
| 6:Aj:145:HIS:HB3 | 6:Aj:148:TYR:HB2 | 1.84 | 0.59 |
| 6:Ak:390:ASP:HB2 | 6:Ak:397:ALA:HB3 | 1.84 | 0.59 |
| 2:B4:33:PHE:HB2 | 2:B4:82:ARG:HG3 | 1.84 | 0.59 |
| 5:BB:178:ASP:HB3 | 5:BB:181:GLN:HB2 | 1.84 | 0.59 |
| 6:BI:265:GLN:HB3 | 6:BI:474:LYS:HB3 | 1.84 | 0.59 |
| 6:BJ:133:LYS:HG2 | 6:BJ:249:GLU:HB2 | 1.83 | 0.59 |
| 11:BQ:60:TYR:HD1 | 11:BQ:64:GLN:HG2 | 1.68 | 0.59 |
| 3:Ba:39:THR:HG22 | 3:Ba:71:VAL:HG22 | 1.84 | 0.59 |
| 2:Bp:368:VAL:O | 2:Bp:400:ARG:NH2 | 2.36 | 0.59 |
| 2:Bp:378:CYS:HB2 | 2:Bp:410:PRO:HA | 1.83 | 0.59 |
| 2:Bq:571:ARG:NH2 | 2:Bq:587:GLU:OE1 | 2.35 | 0.59 |
| 2:Bt:645:THR:OG1 | 2:Bu:629:ILE:O | 2.21 | 0.59 |
| 2:By:430:ARG:HG3 | 2:By:522:ILE:HD11 | 1.85 | 0.59 |
| 3:9:72:THR:HG22 | 3:9:154:GLU:HG2 | 1.84 | 0.59 |
| 3:AH:24:GLU:OE1 | 3:AH:33:THR:OG1 | 2.21 | 0.59 |
| 6:Ae:107:ILE:HA | 6:Ae:412:VAL:HG21 | 1.83 | 0.59 |
| 7:As:109:ASP:OD1 | 7:As:132:ASN:ND2 | 2.31 | 0.59 |
| 7:As:193:ASP:O | 7:As:242:TYR:OH | 2.21 | 0.59 |
| 6:Au:121:THR:HG22 | 6:Au:260:GLU:HA | 1.85 | 0.59 |
| 2:B2:308:ASN:ND2 | 2:B2:313:ASP:OD2 | 2.36 | 0.59 |
| 6:BM:78:ASN:ND2 | 11:BW:5:ARG:O | 2.33 | 0.59 |
| 3:BY:56:ARG:NH2 | 3:Be:96:GLY:O | 2.35 | 0.59 |
| 8:s:256:THR:OG1 | 8:s:257:SER:N | 2.36 | 0.59 |
| 2:4:256:PRO:HG2 | 2:4:339:THR:H | 1.68 | 0.59 |
| 5:A1:80:ARG:NH2 | 5:A1:153:ASP:OD2 | 2.35 | 0.59 |
| 3:AA:101:GLY:N | 3:AF:119:ASP:O | 2.36 | 0.59 |
| 2:AD:237:GLU:HB3 | 2:AD:282:ILE:HG13 | 1.85 | 0.59 |
| 2:AN:20:VAL:HG21 | 2:By:611:THR:HG21 | 1.85 | 0.59 |
| 2:AO:222:VAL:HG11 | 2:AO:236:ILE:HG21 | 1.85 | 0.59 |
| 2:AP:350:VAL:HG13 | 2:AP:354:ASP:HB2 | 1.85 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AY:87:ILE:HD13 | 7:AY:158:ILE:HB | 1.83 | 0.59 |
| 6:Ae:417:LEU:HD22 | 6:Ay:400:LEU:HD11 | 1.83 | 0.59 |
| 2:B3:526:THR:OG1 | 2:B4:366:GLU:OE1 | 2.19 | 0.59 |
| 2:B6:39:PHE:HE1 | 2:B6:83:ALA:HA | 1.67 | 0.59 |
| 5:BA:366:ARG:HE | 5:BA:380:ILE:HD11 | 1.68 | 0.59 |
| 5:BA:467:ILE:HD13 | 5:BH:473:ALA:HB2 | 1.84 | 0.59 |
| 6:BJ:268:ALA:HB1 | 6:BJ:290:LEU:HD13 | 1.84 | 0.59 |
| 3:BY:106:GLU:O | 3:BY:109:LYS:NZ | 2.36 | 0.59 |
| 3:Bk:114:ARG:HG2 | 3:Bk:126:GLU:HG3 | 1.84 | 0.59 |
| 2:Bq:459:ASP:OD2 | 2:Bq:466:ARG:NH1 | 2.34 | 0.59 |
| 2:Br:159:GLU:O | 2:Br:162:THR:N | 2.36 | 0.59 |
| 2:Br:521:ALA:HB1 | 2:Br:541:ALA:HA | 1.83 | 0.59 |
| 2:Bz:230:LEU:HD21 | 2:Bz:285:ARG:HD2 | 1.85 | 0.59 |
| 4:X:53:ARG:NH2 | 4:c:12:ASP:OD2 | 2.36 | 0.59 |
| 1:k:87:ALA:HB2 | 1:l:26:ILE:HG23 | 1.84 | 0.59 |
| 9:x:119:ASN:HD22 | 9:y:79:GLU:HB2 | 1.66 | 0.59 |
| 2:2:605:ARG:HB3 | 2:2:628:TYR:HD1 | 1.67 | 0.59 |
| 6:A5:117:MET:HG3 | 6:A5:451:ALA:HB1 | 1.85 | 0.59 |
| 8:AB:72:LEU:O | 8:AB:74:ARG:N | 2.36 | 0.59 |
| 3:AG:25:ILE:HD12 | 3:AG:28:LEU:HD12 | 1.85 | 0.59 |
| 2:AO:511:GLN:OE1 | 2:AO:514:ARG:NH2 | 2.36 | 0.59 |
| 10:AR:344:MET:HE2 | 10:AR:351:VAL:HB | 1.85 | 0.59 |
| 6:Ao:481:ILE:HD11 | 6:Ao:501:PRO:HB3 | 1.83 | 0.59 |
| 5:Av:46:SER:HB3 | 5:Av:49:GLU:HB2 | 1.85 | 0.59 |
| 5:Av:97:SER:HB2 | 5:Ax:405:LYS:HD2 | 1.84 | 0.59 |
| 6:Az:365:ALA:HB2 | 6:Az:372:GLU:HA | 1.84 | 0.59 |
| 2:B4:29:LEU:HB2 | 2:B4:78:LEU:HD11 | 1.85 | 0.59 |
| 6:BI:263:SER:HB3 | 6:BI:476:ARG:HG2 | 1.83 | 0.59 |
| 6:BJ:269:ALA:HA | 6:BJ:470:VAL:HA | 1.84 | 0.59 |
| 3:Bj:85:PHE:HB3 | 3:Bj:137:VAL:HG21 | 1.84 | 0.59 |
| 2:Bu:66:MET:HB3 | 2:Bu:468:VAL:HG11 | 1.85 | 0.59 |
| 4:c:44:MET:HE1 | 4:h:44:MET:HG2 | 1.83 | 0.59 |
| 2:1:368:VAL:HG23 | 2:1:400:ARG:HH21 | 1.67 | 0.58 |
| 5:A0:77:ASP:O | 5:A0:81:ASN:ND2 | 2.36 | 0.58 |
| 6:A9:151:ASP:HB3 | 6:A9:154:PHE:HB2 | 1.85 | 0.58 |
| 3:AE:37:LYS:HZ1 | 3:AE:74:MET:HG2 | 1.67 | 0.58 |
| 3:AG:114:ARG:HG2 | 3:AG:126:GLU:HG3 | 1.84 | 0.58 |
| 2:AN:119:LYS:O | 2:AN:167:TRP:HA | 2.03 | 0.58 |
| 2:AO:368:VAL:O | 2:AO:400:ARG:NH2 | 2.36 | 0.58 |
| 6:Au:115:GLN:NE2 | 6:Au:443:GLU:O | 2.36 | 0.58 |
| 6:Aw:125:PHE:HZ | 6:BI:91:ILE:HA | 1.66 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B5:246:LYS:HB2 | 2:B5:250:ALA:HB2 | 1.84 | 0.58 |
| 5:BB:390:PHE:HZ | 5:BB:452:SER:HB2 | 1.68 | 0.58 |
| 3:Bl:114:ARG:NH2 | 3:Bl:116:TYR:OH | 2.30 | 0.58 |
| 2:Bt:235:GLU:OE2 | 2:Bt:261:ARG:NH2 | 2.36 | 0.58 |
| 2:Bx:202:GLU:OE1 | 2:Bx:203:ALA:N | 2.31 | 0.58 |
| 4:W:9:PRO:HD3 | 4:W:57:VAL:HG21 | 1.83 | 0.58 |
| 3:7:140:LEU:HD11 | 3:7:151:GLN:HB2 | 1.85 | 0.58 |
| 5:A1:127:LEU:HD11 | 5:BB:496:GLU:HG3 | 1.85 | 0.58 |
| 6:A5:315:GLN:OE1 | 6:A5:514:ARG:NH1 | 2.36 | 0.58 |
| 2:AD:617:VAL:HG13 | 2:AD:622:GLU:HB2 | 1.84 | 0.58 |
| 2:AK:159:GLU:HB3 | 2:AK:163:LEU:HA | 1.85 | 0.58 |
| 6:AV:95:VAL:HA | 6:AZ:123:GLN:HG2 | 1.85 | 0.58 |
| 6:Ah:264:ARG:NH1 | 6:Ah:305:GLU:OE1 | 2.36 | 0.58 |
| 6:Ap:114:VAL:HG21 | 5:BF:59:GLN:HG3 | 1.85 | 0.58 |
| 7:Aq:91:ASN:O | 7:Aq:93:GLY:N | 2.37 | 0.58 |
| 7:At:29:LEU:HD21 | 7:At:259:ASN:HB2 | 1.83 | 0.58 |
| 2:B4:538:ASP:N | 2:B4:538:ASP:OD1 | 2.34 | 0.58 |
| 2:B6:498:GLN:NE2 | 2:B6:531:ASP:OD1 | 2.36 | 0.58 |
| 2:Bs:576:ASN:O | 2:Bs:576:ASN:ND2 | 2.35 | 0.58 |
| 4:M:10:PHE:HB3 | 4:M:22:ILE:HG12 | 1.84 | 0.58 |
| 4:R:9:PRO:HD3 | 4:R:57:VAL:HG21 | 1.85 | 0.58 |
| 8:t:99:GLN:OE1 | 8:t:210:ARG:NH2 | 2.36 | 0.58 |
| 2:5:617:VAL:HG13 | 2:5:622:GLU:HB2 | 1.85 | 0.58 |
| 3:6:86:VAL:HG12 | 3:6:137:VAL:HG21 | 1.84 | 0.58 |
| 3:8:89:GLN:NE2 | 3:8:135:THR:O | 2.36 | 0.58 |
| 6:A5:235:LEU:O | 6:A5:245:ASN:ND2 | 2.37 | 0.58 |
| 6:A5:346:ALA:HA | 6:A5:349:SER:HB3 | 1.86 | 0.58 |
| 6:A9:272:ILE:HG12 | 5:Av:66:GLU:HG3 | 1.85 | 0.58 |
| 8:AB:91:ASN:OD1 | 8:AB:92:ILE:N | 2.37 | 0.58 |
| 2:AL:134:VAL:HG12 | 2:AL:140:ILE:HG22 | 1.85 | 0.58 |
| 2:AM:134:VAL:HG12 | 2:AM:140:ILE:HG22 | 1.84 | 0.58 |
| 2:AP:256:PRO:HG2 | 2:AP:339:THR:H | 1.68 | 0.58 |
| 6:AZ:345:TRP:CD1 | 6:AZ:346:ALA:H | 2.21 | 0.58 |
| 6:Af:182:PHE:HB2 | 6:Af:184:GLU:O | 2.04 | 0.58 |
| 7:Aq:114:MET:HE1 | 6:BK:474:LYS:HE3 | 1.84 | 0.58 |
| 6:Au:106:LEU:HD12 | 5:BH:224:ALA:HB3 | 1.85 | 0.58 |
| 6:Aw:426:ASP:OD2 | 6:Aw:433:TYR:OH | 2.19 | 0.58 |
| 2:B1:22:ASN:ND2 | 2:B1:76:ASN:OD1 | 2.36 | 0.58 |
| 2:B4:430:ARG:HG3 | 2:B4:522:ILE:HD11 | 1.85 | 0.58 |
| 2:Bp:414:VAL:HG23 | 2:Bp:422:ALA:HB1 | 1.85 | 0.58 |
| 2:Bq:163:LEU:HD11 | 2:Bq:187:ILE:HG12 | 1.84 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bu:378:CYS:HB2 | 2:Bu:410:PRO:HA | 1.85 | 0.58 |
| 2:Bx:57:PRO:HA | 2:Bx:61:THR:HB | 1.85 | 0.58 |
| 4:i:9:PRO:HD3 | 4:i:57:VAL:HG21 | 1.85 | 0.58 |
| 1:m:175:ILE:HG13 | 8:t:125:ARG:HD2 | 1.85 | 0.58 |
| 8:s:72:LEU:HD12 | 8:s:125:ARG:HB2 | 1.86 | 0.58 |
| 9:v:118:ASP:O | 9:v:120:SER:N | 2.35 | 0.58 |
| 2:5:18:THR:HG21 | 2:5:47:GLU:HB3 | 1.85 | 0.58 |
| 5:A0:208:TYR:HB3 | 5:A0:228:ILE:HB | 1.86 | 0.58 |
| 5:A2:256:ARG:HH21 | 5:A2:372:ALA:HA | 1.67 | 0.58 |
| 6:A4:278:LEU:HD12 | 6:A4:284:MET:HB2 | 1.85 | 0.58 |
| 7:A6:180:ASP:OD1 | 7:A6:181:LEU:N | 2.35 | 0.58 |
| 3:AH:56:ARG:NH2 | 3:AJ:96:GLY:O | 2.34 | 0.58 |
| 2:AL:118:VAL:HB | 2:AL:126:GLU:HB3 | 1.84 | 0.58 |
| 2:AL:482:ASP:OD2 | 2:AL:483:ASN:ND2 | 2.36 | 0.58 |
| 2:AM:521:ALA:HB1 | 2:AM:541:ALA:HA | 1.83 | 0.58 |
| 6:AW:190:LEU:HB3 | 6:AW:221:LEU:HB3 | 1.86 | 0.58 |
| 6:Aj:328:LYS:HB3 | 6:Aj:331:VAL:HG13 | 1.84 | 0.58 |
| 6:Ak:131:TYR:HD2 | 6:Ak:250:MET:HE3 | 1.67 | 0.58 |
| 6:Am:374:ASN:ND2 | 6:Am:439:LYS:O | 2.34 | 0.58 |
| 5:Ax:158:PHE:HB2 | 5:Ax:236:VAL:HB | 1.85 | 0.58 |
| 2:B3:414:VAL:HG23 | 2:B3:422:ALA:HB1 | 1.84 | 0.58 |
| 2:B6:498:GLN:HA | 2:B6:534:VAL:HG12 | 1.84 | 0.58 |
| 5:BA:209:ASP:N | 5:BA:209:ASP:OD1 | 2.36 | 0.58 |
| 11:BV:18:ASP:HB3 | 11:BV:21:LYS:HD3 | 1.86 | 0.58 |
| 2:Bt:378:CYS:HG | 2:Bt:454:TYR:HH | 1.46 | 0.58 |
| 2:Bt:417:ILE:HB | 2:Bt:421:ARG:HB3 | 1.86 | 0.58 |
| 2:Bu:104:SER:OG | 2:Bu:183:THR:OG1 | 2.21 | 0.58 |
| 2:Bw:653:GLU:HB2 | 2:Bz:16:GLN:HG3 | 1.84 | 0.58 |
| 2:4:281:ILE:HD12 | 2:4:295:LEU:HD12 | 1.86 | 0.58 |
| 2:5:585:ARG:NH1 | 9:z:167:GLU:OE2 | 2.36 | 0.58 |
| 7:A6:203:GLY:H | 4:Q:31:ILE:HG22 | 1.67 | 0.58 |
| 6:A8:235:LEU:O | 6:A8:245:ASN:ND2 | 2.35 | 0.58 |
| 6:Ac:131:TYR:HB3 | 6:Ac:250:MET:HG2 | 1.86 | 0.58 |
| 6:Ac:241:GLY:HA3 | 11:BW:43:GLY:HA2 | 1.85 | 0.58 |
| 2:B3:19:VAL:HG21 | 2:Bz:655:THR:HB | 1.84 | 0.58 |
| 2:B3:653:GLU:HB2 | 2:B6:16:GLN:HG3 | 1.86 | 0.58 |
| 5:BB:160:LYS:HB3 | 5:BB:171:ILE:HG13 | 1.84 | 0.58 |
| 7:BC:12:LEU:HD21 | 7:BC:248:LYS:HG2 | 1.84 | 0.58 |
| 5:BG:61:ILE:HG12 | 5:BG:207:ILE:HD13 | 1.84 | 0.58 |
| 3:BZ:78:ALA:HA | 3:Bo:124:THR:HB | 1.84 | 0.58 |
| 3:Bd:19:ASN:OD1 | 3:Bd:19:ASN:N | 2.31 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bi:125:LYS:NZ | 3:Bl:83:GLN:OE1 | 2.36 | 0.58 |
| 2:By:135:ASP:HB3 | 2:By:139:LYS:HB2 | 1.85 | 0.58 |
| 1:l:154:PRO:HA | 1:l:167:ARG:HD3 | 1.84 | 0.58 |
| 2:2:528:THR:HA | 2:AP:367:SER:HA | 1.86 | 0.58 |
| 2:3:563:ASN:ND2 | 2:3:591:TYR:OH | 2.37 | 0.58 |
| 2:AO:379:ALA:HA | 2:AO:411:ARG:HB2 | 1.86 | 0.58 |
| 6:Af:130:VAL:HG12 | 6:Af:142:GLU:HA | 1.84 | 0.58 |
| 6:Ah:106:LEU:HD23 | 6:Ah:300:LEU:HD23 | 1.85 | 0.58 |
| 5:Av:278:ARG:HD2 | 5:BB:283:ARG:HH21 | 1.69 | 0.58 |
| 6:Az:142:GLU:HG3 | 6:Az:145:HIS:HB2 | 1.86 | 0.58 |
| 2:B5:455:LYS:HD3 | 2:B5:502:VAL:HG22 | 1.86 | 0.58 |
| 2:B6:454:TYR:HB3 | 2:B6:467:TRP:HD1 | 1.69 | 0.58 |
| 6:BM:202:ALA:HB1 | 6:BM:207:LYS:HB3 | 1.86 | 0.58 |
| 2:Bw:362:PHE:HA | 2:Bw:368:VAL:HG21 | 1.84 | 0.58 |
| 2:Bx:455:LYS:HD2 | 2:Bx:502:VAL:HG22 | 1.85 | 0.58 |
| 4:N:9:PRO:HD3 | 4:N:57:VAL:HG21 | 1.84 | 0.58 |
| 8:t:26:ILE:HG13 | 8:t:37:ILE:HG13 | 1.85 | 0.58 |
| 7:A6:55:LYS:HD2 | 7:Al:173:MET:HE1 | 1.84 | 0.58 |
| 7:A6:112:LEU:HD22 | 6:BM:457:THR:HG21 | 1.85 | 0.58 |
| 2:AD:33:PHE:HA | 2:AD:61:THR:HG23 | 1.84 | 0.58 |
| 3:AF:24:GLU:OE1 | 3:AF:33:THR:OG1 | 2.20 | 0.58 |
| 3:AH:17:ARG:HH21 | 3:AI:150:ILE:HG22 | 1.68 | 0.58 |
| 10:AU:344:MET:HE2 | 10:AU:351:VAL:HB | 1.85 | 0.58 |
| 2:B5:95:ILE:HG22 | 2:B5:188:ILE:HG21 | 1.85 | 0.58 |
| 2:B6:470:LEU:HD23 | 2:B6:525:VAL:HG21 | 1.84 | 0.58 |
| 7:BE:207:VAL:HG22 | 4:R:31:ILE:HG12 | 1.86 | 0.58 |
| 5:BH:99:ALA:O | 5:BH:411:GLN:NE2 | 2.36 | 0.58 |
| 11:BU:38:VAL:HG11 | 11:BU:69:ILE:HG12 | 1.85 | 0.58 |
| 2:Bq:585:ARG:NH2 | 2:Bq:608:CYS:O | 2.36 | 0.58 |
| 2:Bv:82:ARG:NH2 | 2:Bv:227:PRO:O | 2.35 | 0.58 |
| 2:Bz:135:ASP:HB3 | 2:Bz:139:LYS:HB2 | 1.85 | 0.58 |
| 4:G:9:PRO:HD3 | 4:G:57:VAL:HG21 | 1.85 | 0.58 |
| 4:H:23:SER:OG | 4:H:26:LYS:NZ | 2.33 | 0.58 |
| 4:M:12:ASP:HB2 | 4:O:52:LEU:HD21 | 1.86 | 0.58 |
| 1:l:239:ASN:OD1 | 1:l:239:ASN:N | 2.36 | 0.58 |
| 3:o:22:GLN:HB2 | 3:o:116:TYR:HE1 | 1.68 | 0.58 |
| 8:u:8:SER:OG | 8:u:12:ARG:NH1 | 2.36 | 0.58 |
| 2:1:229:GLU:N | 2:1:345:SER:OG | 2.35 | 0.58 |
| 2:2:605:ARG:HG2 | 2:2:607:VAL:HG23 | 1.85 | 0.58 |
| 5:A1:154:SER:OG | 5:A1:155:ARG:NH1 | 2.37 | 0.58 |
| 5:A2:367:GLN:HA | 5:A2:377:LEU:HD11 | 1.85 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A7:235:LEU:O | 6:A7:245:ASN:ND2 | 2.37 | 0.58 |
| 6:Au:482:ASN:ND2 | 6:Au:483:PRO:O | 2.36 | 0.58 |
| 6:Az:235:LEU:O | 6:Az:245:ASN:ND2 | 2.37 | 0.58 |
| 2:B1:19:VAL:HG21 | 2:Bx:655:THR:HB | 1.86 | 0.58 |
| 2:B4:571:ARG:NH1 | 2:B4:583:SER:OG | 2.36 | 0.58 |
| 2:Bv:518:TYR:OH | 2:Bv:550:ARG:NH1 | 2.36 | 0.58 |
| 2:Bz:571:ARG:NH2 | 2:Bz:587:GLU:OE1 | 2.36 | 0.58 |
| 5:A2:277:THR:O | 5:A2:282:ARG:NH1 | 2.37 | 0.58 |
| 2:AL:470:LEU:HD23 | 2:AL:525:VAL:HG21 | 1.84 | 0.58 |
| 2:AO:90:LYS:HB3 | 2:AO:191:SER:HB3 | 1.85 | 0.58 |
| 10:AT:344:MET:HE2 | 10:AT:351:VAL:HB | 1.84 | 0.58 |
| 10:AT:345:MET:HE3 | 10:AT:364:LYS:HG3 | 1.86 | 0.58 |
| 7:Aq:12:LEU:HD21 | 7:Aq:248:LYS:HG2 | 1.86 | 0.58 |
| 2:B1:264:THR:O | 2:B1:266:LYS:N | 2.37 | 0.58 |
| 2:B2:41:ILE:HD11 | 2:B2:361:PHE:HB3 | 1.86 | 0.58 |
| 7:BC:206:THR:HB | 7:BC:227:VAL:HG23 | 1.86 | 0.58 |
| 3:Ba:64:ARG:HB2 | 3:Bd:93:ALA:HB1 | 1.86 | 0.58 |
| 3:Bk:46:VAL:HG22 | 3:Bk:64:ARG:HB3 | 1.84 | 0.58 |
| 2:Bq:89:ALA:HA | 2:Bq:345:SER:HA | 1.84 | 0.58 |
| 2:Bq:550:ARG:HB3 | 2:Bq:553:VAL:HG12 | 1.86 | 0.58 |
| 2:Bx:455:LYS:HG3 | 2:Bx:502:VAL:HG13 | 1.85 | 0.58 |
| 2:Bz:365:ARG:HA | 2:Bz:400:ARG:HE | 1.68 | 0.58 |
| 2:Bz:596:LYS:NZ | 2:Bz:602:TYR:O | 2.37 | 0.58 |
| 8:r:27:LYS:NZ | 8:r:34:ASP:OD2 | 2.36 | 0.58 |
| 8:r:152:GLN:HE21 | 8:r:199:TYR:HB2 | 1.67 | 0.58 |
| 8:u:261:ARG:HA | 8:u:271:ARG:HD3 | 1.86 | 0.58 |
| 2:1:61:THR:O | 2:1:63:ASP:N | 2.37 | 0.58 |
| 6:A4:387:ALA:HB2 | 6:A4:404:PHE:HB2 | 1.86 | 0.58 |
| 6:A5:265:GLN:HG2 | 6:A5:474:LYS:HB3 | 1.85 | 0.58 |
| 6:A5:268:ALA:HB1 | 6:A5:290:LEU:HD13 | 1.86 | 0.58 |
| 2:AD:92:SER:HB3 | 2:AD:340:LEU:HB3 | 1.86 | 0.58 |
| 2:AD:571:ARG:NH2 | 2:AD:587:GLU:OE1 | 2.34 | 0.58 |
| 3:AE:25:ILE:O | 3:AE:27:TYR:N | 2.37 | 0.58 |
| 3:AH:69:TRP:HB2 | 3:AH:159:LEU:HD23 | 1.86 | 0.58 |
| 2:AM:202:GLU:OE1 | 2:AM:203:ALA:N | 2.36 | 0.58 |
| 6:Aj:106:LEU:HB3 | 6:Aj:303:ASN:HD22 | 1.68 | 0.58 |
| 6:Am:328:LYS:HB3 | 6:Am:331:VAL:HG13 | 1.86 | 0.58 |
| 6:Au:269:ALA:HA | 6:Au:470:VAL:HA | 1.86 | 0.58 |
| 2:B3:638:ILE:HD13 | 2:B4:568:SER:HB2 | 1.86 | 0.58 |
| 2:B7:509:THR:O | 2:B7:514:ARG:NH1 | 2.37 | 0.58 |
| 5:BF:54:TYR:O | 5:BF:59:GLN:NE2 | 2.37 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BF:190:THR:HG22 | 5:BF:199:VAL:HG12 | 1.84 | 0.58 |
| 2:Bt:550:ARG:HB3 | 2:Bt:553:VAL:HG12 | 1.86 | 0.58 |
| 2:Bu:98:ASN:HB2 | 2:Bu:188:ILE:HD12 | 1.85 | 0.58 |
| 2:Bv:36:GLY:O | 2:Bv:82:ARG:NH1 | 2.37 | 0.58 |
| 4:V:26:LYS:HA | 4:f:34:ALA:H | 1.69 | 0.58 |
| 5:A3:80:ARG:NH2 | 5:A3:153:ASP:OD2 | 2.37 | 0.57 |
| 6:A9:336:ASP:HB3 | 6:A9:339:ASP:HB2 | 1.85 | 0.57 |
| 8:AB:181:LEU:HD22 | 1:p:170:THR:HG21 | 1.86 | 0.57 |
| 2:AD:451:ASP:OD1 | 2:AD:452:GLY:N | 2.37 | 0.57 |
| 3:AE:125:LYS:NZ | 3:AF:83:GLN:OE1 | 2.28 | 0.57 |
| 3:AF:23:VAL:HG11 | 3:AF:39:THR:HG21 | 1.86 | 0.57 |
| 2:AL:639:THR:HB | 2:Bv:624:VAL:HG12 | 1.85 | 0.57 |
| 6:Ad:264:ARG:NH2 | 6:Ah:152:ALA:O | 2.36 | 0.57 |
| 6:Ae:95:VAL:HG22 | 6:Ae:97:GLY:H | 1.69 | 0.57 |
| 7:At:59:VAL:HG12 | 7:At:183:ILE:HG13 | 1.86 | 0.57 |
| 2:B2:378:CYS:HG | 2:B2:454:TYR:HH | 1.36 | 0.57 |
| 2:B3:490:SER:O | 2:B3:496:ARG:NH1 | 2.35 | 0.57 |
| 3:Bb:72:THR:HG22 | 3:Bb:154:GLU:HG3 | 1.85 | 0.57 |
| 2:Br:272:GLY:O | 2:Br:274:GLN:NE2 | 2.34 | 0.57 |
| 2:Bu:254:ILE:HG22 | 2:Bu:257:GLY:H | 1.68 | 0.57 |
| 2:Bw:211:GLN:OE1 | 2:Bw:329:ASN:ND2 | 2.36 | 0.57 |
| 2:Bx:97:GLY:N | 2:Bx:188:ILE:O | 2.37 | 0.57 |
| 8:r:151:GLU:OE1 | 8:r:199:TYR:OH | 2.21 | 0.57 |
| 8:r:238:VAL:HG22 | 8:r:239:PRO:HD2 | 1.86 | 0.57 |
| 2:1:456:TYR:HD2 | 2:1:504:LYS:HB3 | 1.67 | 0.57 |
| 3:6:39:THR:OG1 | 3:6:69:TRP:NE1 | 2.36 | 0.57 |
| 5:A0:477:ILE:HA | 5:A0:481:ILE:HG23 | 1.84 | 0.57 |
| 5:A2:426:LEU:HD13 | 5:A2:432:ILE:HD12 | 1.86 | 0.57 |
| 2:AD:220:PRO:HG2 | 2:AD:338:LEU:HD11 | 1.85 | 0.57 |
| 3:AH:55:ASN:OD1 | 3:Bj:19:ASN:ND2 | 2.38 | 0.57 |
| 2:AK:521:ALA:HA | 2:AK:539:LYS:HG2 | 1.86 | 0.57 |
| 2:AP:366:GLU:OE1 | 2:AP:367:SER:N | 2.37 | 0.57 |
| 2:AP:654:LEU:HD22 | 2:Bp:605:ARG:HD3 | 1.86 | 0.57 |
| 6:AW:377:ILE:HG23 | 6:AW:435:THR:HB | 1.85 | 0.57 |
| 6:AZ:278:LEU:HD12 | 6:AZ:284:MET:HB2 | 1.85 | 0.57 |
| 7:Aa:210:GLN:O | 7:Aa:210:GLN:NE2 | 2.32 | 0.57 |
| 6:Ad:408:THR:HG21 | 6:Ad:427:GLN:HB3 | 1.86 | 0.57 |
| 6:Ae:131:TYR:HB3 | 6:Ae:250:MET:HG2 | 1.85 | 0.57 |
| 6:Ag:263:SER:HB3 | 6:Ag:476:ARG:HG3 | 1.85 | 0.57 |
| 6:Ai:131:TYR:HB3 | 6:Ai:250:MET:HG2 | 1.85 | 0.57 |
| 6:Ak:385:VAL:O | 6:Ak:389:VAL:HG13 | 2.04 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Aq:6:PRO:HG3 | 7:Aq:15:VAL:HG21 | 1.86 | 0.57 |
| 7:Ar:12:LEU:HD12 | 7:Ar:242:TYR:HD2 | 1.68 | 0.57 |
| 7:Ar:162:TRP:NE1 | 7:At:54:ASN:HA | 2.19 | 0.57 |
| 6:Az:105:ASN:ND2 | 6:Az:409:THR:O | 2.37 | 0.57 |
| 6:Az:340:ILE:HG13 | 6:Az:343:ALA:H | 1.67 | 0.57 |
| 2:B1:365:ARG:NH2 | 2:B1:400:ARG:O | 2.33 | 0.57 |
| 2:B3:378:CYS:SG | 2:B3:454:TYR:OH | 2.59 | 0.57 |
| 2:B4:43:GLN:NE2 | 2:B4:77:ASP:OD2 | 2.36 | 0.57 |
| 7:BC:87:ILE:HD13 | 7:BC:158:ILE:HB | 1.85 | 0.57 |
| 6:BI:417:LEU:HB3 | 6:BI:421:TYR:HB2 | 1.85 | 0.57 |
| 6:BM:337:PRO:O | 6:BM:342:GLY:N | 2.25 | 0.57 |
| 3:Bb:113:VAL:HG13 | 3:Bb:127:ILE:HG23 | 1.85 | 0.57 |
| 3:Bd:140:LEU:HD13 | 3:Bd:153:PHE:HB3 | 1.85 | 0.57 |
| 3:Bh:132:LEU:HD21 | 3:Bh:157:LEU:HD13 | 1.86 | 0.57 |
| 3:Bo:19:ASN:OD1 | 3:Bo:19:ASN:N | 2.28 | 0.57 |
| 2:Bp:235:GLU:HB3 | 2:Bp:284:ARG:HB2 | 1.85 | 0.57 |
| 2:Bs:521:ALA:HB1 | 2:Bs:541:ALA:HA | 1.86 | 0.57 |
| 2:Bw:159:GLU:HB3 | 2:Bw:163:LEU:HA | 1.85 | 0.57 |
| 2:By:645:THR:HG21 | 2:Bz:628:TYR:HD2 | 1.69 | 0.57 |
| 8:t:237:VAL:HG13 | 8:t:240:ARG:HA | 1.87 | 0.57 |
| 2:2:394:VAL:HG11 | 2:2:443:ILE:HD12 | 1.86 | 0.57 |
| 2:5:654:LEU:HD23 | 2:AD:16:GLN:HG3 | 1.86 | 0.57 |
| 3:6:95:GLN:NE2 | 3:o:162:TRP:O | 2.36 | 0.57 |
| 7:A6:245:ARG:NH2 | 7:Al:47:GLU:OE1 | 2.37 | 0.57 |
| 6:A7:351:LYS:NZ | 6:A7:390:ASP:O | 2.37 | 0.57 |
| 3:AJ:94:GLY:HA3 | 3:AJ:100:THR:HG23 | 1.85 | 0.57 |
| 7:Aa:2:SER:N | 4:U:30:GLU:OE2 | 2.37 | 0.57 |
| 6:Ac:137:ALA:HB3 | 6:Ac:140:ALA:HB2 | 1.87 | 0.57 |
| 6:Ac:148:TYR:HD1 | 6:Ac:186:GLY:HA2 | 1.69 | 0.57 |
| 7:As:112:LEU:HD12 | 7:As:117:ILE:HG13 | 1.85 | 0.57 |
| 5:Ax:161:ILE:HD11 | 5:BA:30:SER:HB2 | 1.86 | 0.57 |
| 2:B6:414:VAL:HG23 | 2:B6:422:ALA:HB1 | 1.85 | 0.57 |
| 11:BR:39:HIS:ND1 | 11:BR:39:HIS:O | 2.37 | 0.57 |
| 3:Ba:56:ARG:NH2 | 3:Bg:96:GLY:O | 2.37 | 0.57 |
| 3:Bl:37:LYS:HZ1 | 3:Bl:74:MET:HG2 | 1.69 | 0.57 |
| 3:Bm:114:ARG:HG2 | 3:Bm:126:GLU:HG3 | 1.87 | 0.57 |
| 4:e:62:ILE:HD12 | 4:j:58:LEU:HD22 | 1.85 | 0.57 |
| 8:t:61:SER:OG | 8:t:62:GLN:N | 2.37 | 0.57 |
| 9:v:27:THR:O | 9:v:29:ALA:N | 2.37 | 0.57 |
| 2:1:454:TYR:HD2 | 2:1:467:TRP:HD1 | 1.51 | 0.57 |
| 6:A8:431:GLN:NE2 | 6:A9:217:GLU:OE2 | 2.37 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:254:ILE:N | 2:AD:259:GLY:O | 2.36 | 0.57 |
| 2:AD:383:LEU:HD23 | 2:AD:410:PRO:HG2 | 1.86 | 0.57 |
| 2:AD:450:ILE:O | 2:AD:523:ASN:ND2 | 2.38 | 0.57 |
| 2:B6:41:ILE:HD11 | 2:B6:361:PHE:HB3 | 1.86 | 0.57 |
| 2:B6:521:ALA:HA | 2:B6:539:LYS:HE3 | 1.84 | 0.57 |
| 3:Bd:24:GLU:OE1 | 3:Bd:33:THR:OG1 | 2.19 | 0.57 |
| 2:Bu:159:GLU:OE1 | 2:Bu:167:TRP:NE1 | 2.37 | 0.57 |
| 2:Bx:596:LYS:NZ | 2:Bx:602:TYR:O | 2.37 | 0.57 |
| 2:By:57:PRO:HB2 | 2:By:62:ALA:HA | 1.87 | 0.57 |
| 2:By:57:PRO:HA | 2:By:61:THR:HB | 1.86 | 0.57 |
| 4:j:10:PHE:O | 4:j:54:ASN:ND2 | 2.33 | 0.57 |
| 8:u:24:ILE:HG21 | 8:u:133:ILE:HG23 | 1.86 | 0.57 |
| 2:3:92:SER:HB3 | 2:3:340:LEU:HB3 | 1.87 | 0.57 |
| 3:6:56:ARG:HG3 | 3:8:99:ILE:HG22 | 1.85 | 0.57 |
| 5:A2:132:ASP:O | 5:A2:136:HIS:ND1 | 2.37 | 0.57 |
| 5:A3:115:LYS:NZ | 5:A3:443:ASN:OD1 | 2.36 | 0.57 |
| 6:A8:231:SER:HB3 | 6:AW:71:ASP:HB3 | 1.86 | 0.57 |
| 3:AE:55:ASN:OD1 | 3:Ba:19:ASN:ND2 | 2.37 | 0.57 |
| 3:AG:25:ILE:O | 3:AG:27:TYR:N | 2.37 | 0.57 |
| 2:AK:655:THR:HB | 2:AL:19:VAL:HG21 | 1.86 | 0.57 |
| 2:AN:470:LEU:HD23 | 2:AN:525:VAL:HG21 | 1.86 | 0.57 |
| 6:AX:260:GLU:OE1 | 6:AX:261:ALA:N | 2.36 | 0.57 |
| 7:Ab:12:LEU:HD12 | 7:Ab:242:TYR:HD2 | 1.70 | 0.57 |
| 7:Aq:308:VAL:HG12 | 5:BD:332:GLU:HG2 | 1.86 | 0.57 |
| 6:Az:336:ASP:HB3 | 6:Az:339:ASP:HB2 | 1.85 | 0.57 |
| 2:B1:16:GLN:HE22 | 2:B1:460:LYS:HB2 | 1.69 | 0.57 |
| 2:B3:331:PRO:HB2 | 2:B3:334:PHE:HB2 | 1.85 | 0.57 |
| 5:BB:376:PRO:HG2 | 5:BB:379:ARG:HG3 | 1.85 | 0.57 |
| 5:BD:111:LEU:HD11 | 5:BD:444:ILE:HD11 | 1.87 | 0.57 |
| 7:BE:12:LEU:HD12 | 7:BE:242:TYR:HD2 | 1.69 | 0.57 |
| 6:BM:318:LYS:NZ | 6:BM:339:ASP:OD1 | 2.37 | 0.57 |
| 11:BP:72:ASN:HA | 11:BP:75:LEU:HG | 1.85 | 0.57 |
| 3:Bf:72:THR:HG22 | 3:Bf:154:GLU:HG3 | 1.87 | 0.57 |
| 3:Bh:56:ARG:NH2 | 3:Bn:96:GLY:O | 2.36 | 0.57 |
| 2:Bv:378:CYS:HB2 | 2:Bv:410:PRO:HA | 1.86 | 0.57 |
| 1:m:223:GLN:NE2 | 1:n:69:ASP:OD1 | 2.38 | 0.57 |
| 9:z:117:LEU:HD12 | 9:z:121:LYS:HD2 | 1.85 | 0.57 |
| 1:0:26:ILE:HG23 | 1:p:87:ALA:HB2 | 1.86 | 0.57 |
| 5:A0:7:SER:O | 5:A0:9:PHE:N | 2.37 | 0.57 |
| 6:Ag:131:TYR:HD2 | 6:Ag:250:MET:HE3 | 1.69 | 0.57 |
| 6:Ak:304:ARG:NH2 | 6:Ak:308:ASP:OD1 | 2.38 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ak:346:ALA:HA | 6:Ak:349:SER:HB3 | 1.87 | 0.57 |
| 7:BC:210:GLN:HA | 7:BC:227:VAL:HG13 | 1.86 | 0.57 |
| 6:BJ:235:LEU:O | 6:BJ:245:ASN:ND2 | 2.37 | 0.57 |
| 3:BY:96:GLY:O | 3:Bk:56:ARG:NH2 | 2.37 | 0.57 |
| 3:Bb:25:ILE:HD12 | 3:Bb:28:LEU:HD12 | 1.86 | 0.57 |
| 2:Bq:526:THR:OG1 | 2:Bq:527:GLY:N | 2.36 | 0.57 |
| 2:Bt:118:VAL:HB | 2:Bt:126:GLU:HB3 | 1.86 | 0.57 |
| 2:Bu:373:PHE:HB2 | 2:Bu:405:VAL:HG22 | 1.86 | 0.57 |
| 2:Bx:406:LEU:HD13 | 2:Bx:475:ALA:HB2 | 1.87 | 0.57 |
| 2:By:417:ILE:HD13 | 2:By:417:ILE:H | 1.69 | 0.57 |
| 4:K:62:ILE:HD12 | 4:L:58:LEU:HD22 | 1.86 | 0.57 |
| 1:p:101:SER:O | 8:q:180:ASN:ND2 | 2.37 | 0.57 |
| 3:8:70:THR:HG22 | 3:8:156:THR:HG22 | 1.86 | 0.57 |
| 4:A:48:THR:HG21 | 4:F:47:PRO:HB2 | 1.86 | 0.57 |
| 5:A2:34:PRO:HG3 | 5:BF:175:ARG:HE | 1.69 | 0.57 |
| 5:A3:111:LEU:HD11 | 5:A3:444:ILE:HD11 | 1.87 | 0.57 |
| 9:AC:91:MET:HE1 | 9:AC:138:LEU:HB2 | 1.87 | 0.57 |
| 2:AD:272:GLY:O | 2:AD:274:GLN:NE2 | 2.38 | 0.57 |
| 2:AD:511:GLN:OE1 | 2:AD:514:ARG:NH2 | 2.38 | 0.57 |
| 3:AJ:14:ASP:OD1 | 3:AJ:17:ARG:NH2 | 2.38 | 0.57 |
| 6:AW:356:GLN:NE2 | 6:AW:360:GLU:OE2 | 2.38 | 0.57 |
| 7:Aa:22:ALA:HB1 | 7:Aa:23:PRO:HD2 | 1.86 | 0.57 |
| 7:Ab:99:ASP:OD2 | 6:Au:267:LYS:NZ | 2.38 | 0.57 |
| 6:Ad:333:ASP:HB3 | 6:Ad:336:ASP:HB2 | 1.87 | 0.57 |
| 6:Ai:318:LYS:NZ | 6:Ai:356:GLN:OE1 | 2.37 | 0.57 |
| 6:Ak:265:GLN:HG3 | 6:Ao:247:TRP:HE1 | 1.69 | 0.57 |
| 7:At:60:PHE:HB2 | 7:At:182:ILE:HG13 | 1.86 | 0.57 |
| 2:B1:629:ILE:O | 2:Bz:645:THR:OG1 | 2.22 | 0.57 |
| 2:B3:154:ALA:HA | 2:B3:157:VAL:HG22 | 1.86 | 0.57 |
| 6:BM:153:MET:HE1 | 6:BM:177:ILE:HD13 | 1.87 | 0.57 |
| 2:Bq:166:ASN:OD1 | 2:Bq:166:ASN:N | 2.37 | 0.57 |
| 2:Bt:135:ASP:HB3 | 2:Bt:139:LYS:HB2 | 1.86 | 0.57 |
| 2:Bw:154:ALA:HA | 2:Bw:157:VAL:HG22 | 1.86 | 0.57 |
| 1:m:233:GLU:HG3 | 1:m:234:PRO:HD2 | 1.85 | 0.57 |
| 8:s:48:HIS:ND1 | 8:t:182:SER:O | 2.37 | 0.57 |
| 1:0:77:LYS:HE2 | 8:q:29:GLN:HB3 | 1.85 | 0.57 |
| 2:4:102:THR:HB | 2:4:183:THR:HB | 1.86 | 0.57 |
| 5:A0:211:ALA:HA | 5:A0:224:ALA:H | 1.70 | 0.57 |
| 2:AD:32:LYS:NZ | 2:AD:60:GLU:OE2 | 2.34 | 0.57 |
| 2:AD:595:ILE:HG22 | 2:AD:600:GLY:HA3 | 1.86 | 0.57 |
| 2:AL:607:VAL:HB | 2:AL:626:THR:HG23 | 1.87 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:AU:332:SER:OG | 10:AU:338:ARG:NH1 | 2.37 | 0.57 |
| 6:AV:465:LYS:HB3 | 6:Au:237:GLU:HB3 | 1.87 | 0.57 |
| 6:Am:117:MET:HE1 | 6:Am:261:ALA:HB2 | 1.85 | 0.57 |
| 2:B3:232:ASP:OD2 | 2:B3:342:GLY:N | 2.36 | 0.57 |
| 2:B6:102:THR:HB | 2:B6:183:THR:HB | 1.86 | 0.57 |
| 5:BB:497:GLU:O | 5:BB:501:GLU:HG2 | 2.04 | 0.57 |
| 11:BW:64:GLN:O | 11:BW:66:THR:N | 2.37 | 0.57 |
| 3:Ba:85:PHE:HB3 | 3:Ba:137:VAL:HG21 | 1.86 | 0.57 |
| 3:Ba:114:ARG:HG2 | 3:Ba:126:GLU:HG3 | 1.86 | 0.57 |
| 2:Bs:33:PHE:HA | 2:Bs:61:THR:HG23 | 1.85 | 0.57 |
| 2:Bt:378:CYS:SG | 2:Bt:454:TYR:OH | 2.58 | 0.57 |
| 2:Bv:454:TYR:HB3 | 2:Bv:467:TRP:HD1 | 1.68 | 0.57 |
| 2:Bx:33:PHE:HA | 2:Bx:61:THR:HG23 | 1.86 | 0.57 |
| 8:t:91:ASN:OD1 | 8:t:92:ILE:N | 2.37 | 0.57 |
| 9:x:25:ASN:OD1 | 9:x:25:ASN:N | 2.37 | 0.57 |
| 9:z:50:VAL:HG13 | 9:z:55:GLY:HA2 | 1.87 | 0.57 |
| 2:3:59:ALA:HB2 | 2:AK:299:ARG:HH22 | 1.70 | 0.57 |
| 3:7:138:GLY:HA3 | 3:7:153:PHE:HB2 | 1.87 | 0.57 |
| 5:A0:496:GLU:OE1 | 5:BH:124:ASN:ND2 | 2.38 | 0.57 |
| 2:AD:459:ASP:OD2 | 2:AD:462:ASN:N | 2.36 | 0.57 |
| 2:AO:612:ASN:HB3 | 2:AO:624:VAL:HG23 | 1.87 | 0.57 |
| 2:AP:454:TYR:HB3 | 2:AP:467:TRP:HD1 | 1.69 | 0.57 |
| 7:AY:4:TYR:HE2 | 7:AY:19:ARG:HD2 | 1.70 | 0.57 |
| 7:AY:51:ASP:OD2 | 7:BL:166:ALA:N | 2.38 | 0.57 |
| 6:Ae:230:THR:HB | 6:Au:71:ASP:HB2 | 1.86 | 0.57 |
| 7:Al:265:ARG:NH1 | 1:n:49:GLU:OE2 | 2.37 | 0.57 |
| 6:An:481:ILE:HD11 | 6:An:501:PRO:HB3 | 1.86 | 0.57 |
| 6:Ap:247:TRP:HE3 | 6:BI:267:LYS:HD3 | 1.70 | 0.57 |
| 6:Ap:383:VAL:HG12 | 6:Ap:406:THR:HG22 | 1.86 | 0.57 |
| 7:Ar:22:ALA:HB1 | 7:Ar:23:PRO:HD2 | 1.87 | 0.57 |
| 5:Av:256:ARG:NH1 | 5:BB:89:ASP:OD2 | 2.36 | 0.57 |
| 5:Av:495:ASP:OD1 | 5:Av:495:ASP:N | 2.23 | 0.57 |
| 6:Aw:245:ASN:O | 6:Aw:247:TRP:N | 2.38 | 0.57 |
| 2:B1:34:GLN:OE1 | 2:B1:58:THR:OG1 | 2.23 | 0.57 |
| 2:B4:254:ILE:HG22 | 2:B4:257:GLY:H | 1.68 | 0.57 |
| 2:B4:593:GLN:NE2 | 3:Bi:4:ASP:OD2 | 2.37 | 0.57 |
| 6:BI:459:LEU:HD11 | 6:BI:474:LYS:HE2 | 1.86 | 0.57 |
| 6:BJ:181:PHE:HD1 | 6:BJ:187:THR:HG23 | 1.69 | 0.57 |
| 6:BK:459:LEU:HD11 | 6:BK:474:LYS:HE2 | 1.86 | 0.57 |
| 3:BX:28:LEU:HD22 | 3:BX:84:LYS:HB3 | 1.86 | 0.57 |
| 2:Bu:596:LYS:NZ | 2:Bu:602:TYR:O | 2.31 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:Z:27:ASN:ND2 | 4:j:35:ASP:OD1 | 2.37 | 0.57 |
| 9:w:42:ILE:HB | 9:w:66:PHE:HE1 | 1.68 | 0.57 |
| 2:1:131:ILE:HD13 | 2:1:140:ILE:HG21 | 1.87 | 0.57 |
| 6:A8:252:PHE:N | 6:Au:67:GLU:OE2 | 2.29 | 0.57 |
| 3:AF:39:THR:HG22 | 3:AF:71:VAL:HG22 | 1.86 | 0.57 |
| 3:AH:113:VAL:HG13 | 3:AH:127:ILE:HG23 | 1.87 | 0.57 |
| 2:AL:490:SER:O | 2:AL:496:ARG:NH1 | 2.38 | 0.57 |
| 2:AM:109:ASN:H | 2:AM:137:ASP:HB2 | 1.68 | 0.57 |
| 2:AM:264:THR:O | 2:AM:266:LYS:N | 2.38 | 0.57 |
| 2:AM:494:TYR:CZ | 2:By:569:LYS:HD3 | 2.40 | 0.57 |
| 2:AN:478:CYS:O | 2:AN:555:ARG:NH1 | 2.38 | 0.57 |
| 2:AP:119:LYS:HG2 | 2:AP:124:ASP:HA | 1.85 | 0.57 |
| 2:AP:571:ARG:NH2 | 2:AP:587:GLU:OE1 | 2.37 | 0.57 |
| 6:AV:105:ASN:HB2 | 6:AV:412:VAL:HG23 | 1.86 | 0.57 |
| 7:Aa:13:LYS:HG3 | 7:Aa:34:ILE:HG21 | 1.86 | 0.57 |
| 6:Af:381:ASN:HB3 | 6:Af:521:ILE:HG21 | 1.87 | 0.57 |
| 6:Aj:452:PRO:HA | 6:Aj:477:TYR:HA | 1.86 | 0.57 |
| 6:Am:79:ILE:HG23 | 6:BJ:121:THR:HB | 1.87 | 0.57 |
| 6:Ao:107:ILE:O | 6:Ao:109:PHE:N | 2.38 | 0.57 |
| 6:Au:171:GLN:OE1 | 6:Au:195:GLN:NE2 | 2.38 | 0.57 |
| 5:Av:293:PRO:O | 5:Av:295:ARG:N | 2.37 | 0.57 |
| 6:Az:351:LYS:NZ | 6:Az:390:ASP:O | 2.37 | 0.57 |
| 2:B2:131:ILE:HG12 | 2:B2:143:ILE:HG22 | 1.86 | 0.57 |
| 2:B4:121:VAL:HG22 | 2:B4:166:ASN:HB3 | 1.86 | 0.57 |
| 2:B4:378:CYS:SG | 2:B4:454:TYR:OH | 2.62 | 0.57 |
| 2:B6:217:TYR:HB2 | 2:B6:219:ILE:HD12 | 1.87 | 0.57 |
| 7:BC:132:ASN:ND2 | 5:BG:245:CYS:SG | 2.70 | 0.57 |
| 7:BE:163:PHE:HB2 | 7:BE:170:LEU:HD13 | 1.87 | 0.57 |
| 5:BG:181:GLN:HG3 | 5:BG:209:ASP:HB2 | 1.87 | 0.57 |
| 5:BG:244:ASP:HB2 | 5:BG:251:ILE:HD13 | 1.87 | 0.57 |
| 3:Bf:25:ILE:HG23 | 3:Bf:111:ALA:HB2 | 1.86 | 0.57 |
| 2:Bp:244:TYR:O | 2:Bp:266:LYS:NZ | 2.28 | 0.57 |
| 2:Bx:90:LYS:NZ | 2:Bx:190:ASP:OD1 | 2.32 | 0.57 |
| 1:m:176:TYR:HE2 | 1:m:179:GLU:HG3 | 1.70 | 0.57 |
| 1:m:198:GLU:O | 1:m:205:ARG:NH2 | 2.38 | 0.57 |
| 8:s:45:SER:OG | 8:t:184:ARG:NH1 | 2.37 | 0.57 |
| 1:0:57:GLU:HA | 1:0:87:ALA:HA | 1.87 | 0.56 |
| 5:A1:175:ARG:NH1 | 5:BB:32:THR:O | 2.37 | 0.56 |
| 6:A5:95:VAL:HG22 | 6:A5:97:GLY:H | 1.70 | 0.56 |
| 6:A9:278:LEU:HD22 | 6:A9:284:MET:HB2 | 1.87 | 0.56 |
| 3:AF:72:THR:HG22 | 3:AF:154:GLU:HG3 | 1.86 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:AJ:72:THR:HG22 | 3:AJ:154:GLU:HG3 | 1.86 | 0.56 |
| 6:Ae:142:GLU:HG3 | 6:Ae:145:HIS:HB2 | 1.86 | 0.56 |
| 3:BX:56:ARG:NH2 | 3:Bd:96:GLY:O | 2.38 | 0.56 |
| 3:BY:23:VAL:HG11 | 3:BY:39:THR:HG21 | 1.87 | 0.56 |
| 3:BZ:22:GLN:NE2 | 3:Bo:1:MET:SD | 2.77 | 0.56 |
| 3:Ba:19:ASN:OD1 | 3:Ba:19:ASN:N | 2.36 | 0.56 |
| 3:Bb:57:LYS:HE2 | 3:Bi:147:ASN:HD21 | 1.70 | 0.56 |
| 3:Bb:114:ARG:HG2 | 3:Bb:126:GLU:HG3 | 1.87 | 0.56 |
| 3:Bl:113:VAL:HG13 | 3:Bl:127:ILE:HG23 | 1.87 | 0.56 |
| 2:Br:557:PHE:HB3 | 2:Br:561:LYS:HZ3 | 1.70 | 0.56 |
| 2:Bx:417:ILE:H | 2:Bx:417:ILE:HD13 | 1.70 | 0.56 |
| 4:J:9:PRO:HD3 | 4:J:57:VAL:HG21 | 1.86 | 0.56 |
| 4:V:12:ASP:OD2 | 4:f:53:ARG:NH2 | 2.38 | 0.56 |
| 1:n:87:ALA:HB1 | 1:p:27:LEU:HD23 | 1.86 | 0.56 |
| 2:2:133:GLU:HB2 | 2:2:142:LYS:HB2 | 1.87 | 0.56 |
| 2:4:455:LYS:NZ | 2:4:473:ASP:OD2 | 2.30 | 0.56 |
| 6:A5:127:LEU:HD11 | 6:A5:252:PHE:HB2 | 1.87 | 0.56 |
| 6:A9:147:MET:SD | 6:A9:487:SER:OG | 2.60 | 0.56 |
| 2:AK:643:VAL:HG13 | 2:AL:14:THR:HG22 | 1.86 | 0.56 |
| 2:AO:202:GLU:OE1 | 2:AO:203:ALA:N | 2.37 | 0.56 |
| 2:AP:163:LEU:HD11 | 2:AP:187:ILE:HG12 | 1.87 | 0.56 |
| 6:AX:68:ILE:HD12 | 6:Af:235:LEU:HD21 | 1.87 | 0.56 |
| 6:AX:154:PHE:O | 6:AX:248:ASN:ND2 | 2.28 | 0.56 |
| 7:AY:13:LYS:HG3 | 7:AY:34:ILE:HG21 | 1.86 | 0.56 |
| 7:Ab:91:ASN:ND2 | 7:Ab:180:ASP:OD2 | 2.39 | 0.56 |
| 7:Ab:163:PHE:HB2 | 7:Ab:170:LEU:HD13 | 1.87 | 0.56 |
| 6:Ac:340:ILE:HB | 6:Ac:343:ALA:HB3 | 1.87 | 0.56 |
| 6:Ap:459:LEU:HB3 | 6:BM:467:PHE:CG | 2.40 | 0.56 |
| 6:Au:372:GLU:OE1 | 6:Au:420:LYS:NZ | 2.38 | 0.56 |
| 2:B2:206:THR:HA | 2:B2:211:GLN:HE21 | 1.70 | 0.56 |
| 2:B4:159:GLU:HB3 | 2:B4:163:LEU:HA | 1.87 | 0.56 |
| 2:B5:514:ARG:NH1 | 2:B6:366:GLU:OE2 | 2.38 | 0.56 |
| 2:B7:23:SER:OG | 2:B7:74:TYR:O | 2.22 | 0.56 |
| 5:BA:97:SER:HB2 | 5:BH:405:LYS:HD2 | 1.86 | 0.56 |
| 3:BX:140:LEU:HD23 | 3:Bm:41:LEU:HD23 | 1.87 | 0.56 |
| 3:BY:61:ALA:HB3 | 3:BZ:118:ARG:HH12 | 1.70 | 0.56 |
| 3:Bg:8:ARG:HD2 | 3:Bj:34:PHE:HE2 | 1.70 | 0.56 |
| 3:Bh:58:ILE:HD11 | 3:Bi:6:VAL:HG21 | 1.87 | 0.56 |
| 2:Bu:571:ARG:NH1 | 2:Bu:583:SER:OG | 2.34 | 0.56 |
| 2:Bz:494:TYR:HH | 2:Bz:536:TYR:HH | 1.40 | 0.56 |
| 1:k:11:LYS:HG3 | 1:k:15:ARG:HH12 | 1.69 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:l:164:ASN:ND2 | 1:l:164:ASN:O | 2.35 | 0.56 |
| 1:m:87:ALA:HB1 | 1:n:27:LEU:HD23 | 1.88 | 0.56 |
| 8:t:238:VAL:HG22 | 8:t:239:PRO:HD2 | 1.87 | 0.56 |
| 2:3:44:VAL:HG11 | 2:3:50:LEU:HB2 | 1.86 | 0.56 |
| 2:3:498:GLN:HB3 | 2:3:534:VAL:HG12 | 1.86 | 0.56 |
| 2:5:567:SER:O | 2:5:571:ARG:HG2 | 2.05 | 0.56 |
| 3:9:148:ASN:HB3 | 9:w:45:PRO:HB2 | 1.87 | 0.56 |
| 5:A0:236:VAL:HG21 | 5:A0:421:PRO:HG3 | 1.87 | 0.56 |
| 5:A2:282:ARG:NH2 | 5:BF:328:MET:O | 2.38 | 0.56 |
| 5:A2:451:ASP:O | 5:BD:458:LYS:NZ | 2.26 | 0.56 |
| 5:A3:198:ILE:HG21 | 5:BG:8:LEU:HD11 | 1.85 | 0.56 |
| 5:A3:432:ILE:HG23 | 5:A3:436:GLU:HB2 | 1.87 | 0.56 |
| 6:A4:247:TRP:HH2 | 7:As:98:MET:HG2 | 1.70 | 0.56 |
| 6:A4:442:ASN:OD1 | 6:A4:443:GLU:N | 2.39 | 0.56 |
| 6:A9:105:ASN:HB2 | 6:A9:412:VAL:HG23 | 1.87 | 0.56 |
| 6:A9:279:ARG:HH21 | 5:Av:227:LYS:HG3 | 1.70 | 0.56 |
| 3:AA:21:PHE:HZ | 3:AA:38:ALA:HA | 1.69 | 0.56 |
| 3:AF:54:MET:HE3 | 3:Bd:20:LEU:HA | 1.87 | 0.56 |
| 2:AN:498:GLN:HA | 2:AN:534:VAL:HG12 | 1.87 | 0.56 |
| 10:AR:329:ASP:O | 10:AR:338:ARG:NH2 | 2.39 | 0.56 |
| 6:AW:131:TYR:HB3 | 6:AW:250:MET:HG2 | 1.88 | 0.56 |
| 6:AX:119:SER:OG | 6:AX:121:THR:O | 2.24 | 0.56 |
| 7:AY:111:LEU:HD21 | 6:Ao:462:SER:HB2 | 1.87 | 0.56 |
| 7:Aa:111:LEU:HD22 | 7:Aa:137:ASP:HB3 | 1.88 | 0.56 |
| 7:Aa:248:LYS:O | 7:Aa:252:THR:OG1 | 2.23 | 0.56 |
| 7:Ab:13:LYS:HG3 | 7:Ab:34:ILE:HG21 | 1.87 | 0.56 |
| 6:Ac:145:HIS:ND1 | 6:Ac:146:PRO:O | 2.34 | 0.56 |
| 6:Ad:430:LYS:HE2 | 6:Ah:188:VAL:HG22 | 1.87 | 0.56 |
| 6:Aj:235:LEU:O | 6:Aj:245:ASN:ND2 | 2.39 | 0.56 |
| 6:Ak:350:PHE:HB3 | 6:Ak:389:VAL:HG12 | 1.87 | 0.56 |
| 6:An:83:GLN:NE2 | 6:An:84:THR:O | 2.37 | 0.56 |
| 6:Ao:387:ALA:HB2 | 6:Ao:404:PHE:HB2 | 1.87 | 0.56 |
| 6:Au:356:GLN:NE2 | 6:Au:360:GLU:OE2 | 2.38 | 0.56 |
| 5:Ax:267:LEU:HD12 | 5:Ax:365:PHE:HD2 | 1.71 | 0.56 |
| 2:B2:20:VAL:HG21 | 2:B2:46:ASN:HD21 | 1.70 | 0.56 |
| 2:B4:312:ASP:N | 2:B4:312:ASP:OD1 | 2.37 | 0.56 |
| 2:B6:117:THR:HG23 | 2:B6:127:THR:HG22 | 1.87 | 0.56 |
| 2:B6:147:THR:HG22 | 2:B6:150:ILE:HD12 | 1.86 | 0.56 |
| 7:BC:33:GLN:HE22 | 7:BC:262:ILE:HD11 | 1.70 | 0.56 |
| 7:BC:163:PHE:HA | 7:BC:170:LEU:HA | 1.88 | 0.56 |
| 5:BF:150:TRP:HD1 | 5:BF:156:ILE:HG22 | 1.70 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:BK:482:ASN:ND2 | 6:BK:483:PRO:O | 2.38 | 0.56 |
| 11:BO:38:VAL:HG11 | 11:BO:69:ILE:HG12 | 1.86 | 0.56 |
| 3:BZ:147:ASN:ND2 | 3:Bn:63:ASP:OD2 | 2.38 | 0.56 |
| 3:Bg:40:ALA:O | 3:Bg:69:TRP:NE1 | 2.33 | 0.56 |
| 2:Br:118:VAL:HB | 2:Br:126:GLU:HB3 | 1.86 | 0.56 |
| 2:Bt:592:LEU:HD23 | 2:Bt:604:TYR:HB2 | 1.86 | 0.56 |
| 2:Bu:33:PHE:HB2 | 2:Bu:82:ARG:HG3 | 1.87 | 0.56 |
| 2:Bv:92:SER:HB3 | 2:Bv:340:LEU:HB3 | 1.88 | 0.56 |
| 2:Bv:609:ASP:OD1 | 2:Bv:609:ASP:N | 2.38 | 0.56 |
| 2:Bw:90:LYS:NZ | 2:Bw:190:ASP:OD1 | 2.38 | 0.56 |
| 2:By:383:LEU:HD22 | 2:By:439:ASN:HD22 | 1.71 | 0.56 |
| 4:I:52:LEU:HD21 | 4:T:12:ASP:HB2 | 1.86 | 0.56 |
| 1:l:63:ARG:HH22 | 8:s:125:ARG:HH22 | 1.53 | 0.56 |
| 1:p:151:TRP:HZ2 | 8:u:59:ILE:HD12 | 1.70 | 0.56 |
| 8:q:216:PHE:O | 8:q:217:HIS:ND1 | 2.38 | 0.56 |
| 8:u:238:VAL:HG22 | 8:u:239:PRO:HD2 | 1.86 | 0.56 |
| 8:u:248:ASP:N | 8:u:248:ASP:OD1 | 2.38 | 0.56 |
| 2:5:531:ASP:OD1 | 2:5:532:GLY:N | 2.39 | 0.56 |
| 2:AD:241:LYS:HB2 | 2:AD:273:PRO:HB2 | 1.86 | 0.56 |
| 2:AD:453:ASN:ND2 | 2:AD:454:TYR:O | 2.38 | 0.56 |
| 2:AL:638:ILE:HG12 | 2:Bv:623:PHE:HB3 | 1.86 | 0.56 |
| 2:AP:368:VAL:O | 2:AP:400:ARG:NH2 | 2.39 | 0.56 |
| 6:AX:343:ALA:HB1 | 6:AX:348:GLU:HG3 | 1.88 | 0.56 |
| 6:Ao:257:GLN:NE2 | 6:Ao:481:ILE:O | 2.38 | 0.56 |
| 6:Ap:260:GLU:OE1 | 6:Ap:261:ALA:N | 2.38 | 0.56 |
| 7:Aq:162:TRP:HE1 | 7:As:54:ASN:HA | 1.71 | 0.56 |
| 6:Au:452:PRO:HA | 6:Au:477:TYR:HA | 1.88 | 0.56 |
| 6:Aw:351:LYS:NZ | 6:Aw:390:ASP:O | 2.38 | 0.56 |
| 6:Ay:131:TYR:HD2 | 6:Ay:250:MET:HE3 | 1.71 | 0.56 |
| 2:B1:28:ALA:HB2 | 2:B1:370:VAL:HG21 | 1.85 | 0.56 |
| 2:B2:454:TYR:HB3 | 2:B2:467:TRP:HD1 | 1.70 | 0.56 |
| 2:B5:119:LYS:NZ | 2:B5:124:ASP:OD1 | 2.36 | 0.56 |
| 2:B5:159:GLU:HB3 | 2:B5:163:LEU:HA | 1.87 | 0.56 |
| 2:B6:351:THR:HG23 | 2:B6:354:ASP:H | 1.70 | 0.56 |
| 6:BM:154:PHE:O | 6:BM:248:ASN:ND2 | 2.37 | 0.56 |
| 3:Bd:41:LEU:H | 3:Bd:41:LEU:HD12 | 1.70 | 0.56 |
| 3:Bf:37:LYS:HZ2 | 3:Bf:74:MET:HG2 | 1.70 | 0.56 |
| 3:Bg:59:ASN:ND2 | 3:Bj:159:LEU:O | 2.38 | 0.56 |
| 2:Br:42:LYS:NZ | 2:Br:43:GLN:O | 2.32 | 0.56 |
| 2:Bt:637:TYR:HB2 | 2:Bu:622:GLU:HG2 | 1.88 | 0.56 |
| 1:m:62:PRO:HG3 | 1:m:84:TRP:HZ3 | 1.69 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:383:LEU:HD13 | 2:2:439:ASN:HB2 | 1.86 | 0.56 |
| 5:A0:129:GLU:OE1 | 5:A0:425:ASN:ND2 | 2.38 | 0.56 |
| 5:A2:473:ALA:HB2 | 5:BF:467:ILE:HD13 | 1.88 | 0.56 |
| 6:A8:267:LYS:HD3 | 6:A9:247:TRP:CD2 | 2.40 | 0.56 |
| 2:AD:455:LYS:HE3 | 2:AD:457:GLN:HB2 | 1.88 | 0.56 |
| 2:AK:585:ARG:HH21 | 2:AK:609:ASP:HB3 | 1.70 | 0.56 |
| 6:Ac:336:ASP:HB3 | 6:Ac:339:ASP:HB2 | 1.87 | 0.56 |
| 7:Ar:304:PHE:HZ | 5:BA:301:MET:HE2 | 1.70 | 0.56 |
| 7:At:12:LEU:HD21 | 7:At:248:LYS:HG2 | 1.86 | 0.56 |
| 6:Au:123:GLN:HG3 | 6:BJ:93:PRO:HB2 | 1.86 | 0.56 |
| 2:B1:571:ARG:NH2 | 2:B1:587:GLU:OE1 | 2.39 | 0.56 |
| 2:B3:130:LYS:HZ3 | 2:B3:132:THR:HG22 | 1.70 | 0.56 |
| 7:BE:138:LEU:HB3 | 5:BG:273:ILE:HD11 | 1.87 | 0.56 |
| 2:Bt:514:ARG:NH1 | 2:Bu:366:GLU:OE2 | 2.39 | 0.56 |
| 5:A1:464:GLU:HG3 | 5:BB:469:MET:HE2 | 1.87 | 0.56 |
| 5:A2:45:VAL:HG12 | 5:A2:46:SER:H | 1.71 | 0.56 |
| 6:A8:130:VAL:HG12 | 6:A8:142:GLU:HA | 1.88 | 0.56 |
| 3:AG:4:ASP:OD2 | 2:AM:593:GLN:NE2 | 2.38 | 0.56 |
| 3:AH:137:VAL:HB | 3:AH:155:VAL:HG13 | 1.88 | 0.56 |
| 2:AP:236:ILE:HD11 | 2:AP:323:ILE:HG21 | 1.86 | 0.56 |
| 7:AY:114:MET:HB3 | 7:BL:148:MET:HE1 | 1.88 | 0.56 |
| 6:Ag:322:THR:OG1 | 6:Ag:514:ARG:NH2 | 2.38 | 0.56 |
| 6:Ah:71:ASP:OD1 | 6:Ah:72:HIS:N | 2.39 | 0.56 |
| 7:At:13:LYS:HG3 | 7:At:34:ILE:HG21 | 1.86 | 0.56 |
| 6:Az:268:ALA:HB1 | 6:Az:290:LEU:HD13 | 1.87 | 0.56 |
| 2:B1:455:LYS:NZ | 2:B1:457:GLN:OE1 | 2.38 | 0.56 |
| 2:B1:455:LYS:HG3 | 2:B1:502:VAL:HG13 | 1.88 | 0.56 |
| 2:B2:639:THR:HB | 2:B3:624:VAL:HG12 | 1.87 | 0.56 |
| 5:BA:176:ARG:O | 5:BH:35:LYS:NZ | 2.37 | 0.56 |
| 7:BE:20:LEU:HD21 | 7:BE:256:LYS:HB2 | 1.88 | 0.56 |
| 5:BF:111:LEU:HD11 | 5:BF:444:ILE:HD11 | 1.87 | 0.56 |
| 5:BG:466:ARG:HD2 | 5:BG:490:ILE:O | 2.06 | 0.56 |
| 6:BI:456:LEU:H | 6:BI:475:THR:HB | 1.69 | 0.56 |
| 3:Bc:72:THR:HG22 | 3:Bc:154:GLU:HG3 | 1.87 | 0.56 |
| 3:Bj:125:LYS:NZ | 3:Bm:83:GLN:OE1 | 2.39 | 0.56 |
| 2:Bp:198:ILE:HG23 | 2:Bp:324:PHE:HE2 | 1.70 | 0.56 |
| 2:Br:22:ASN:ND2 | 2:Br:76:ASN:OD1 | 2.38 | 0.56 |
| 2:Bw:463:ASP:OD1 | 2:Bx:317:LYS:NZ | 2.39 | 0.56 |
| 2:1:296:SER:N | 2:1:309:ILE:O | 2.35 | 0.56 |
| 2:4:510:ARG:HG2 | 2:4:511:GLN:H | 1.70 | 0.56 |
| 6:A4:279:ARG:NH2 | 6:A4:285:ASP:OD1 | 2.38 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A5:383:VAL:HG21 | 6:A5:425:ILE:HG12 | 1.86 | 0.56 |
| 6:A9:204:ASP:OD1 | 6:A9:205:ALA:N | 2.39 | 0.56 |
| 3:AA:74:MET:HA | 3:AA:152:THR:HG22 | 1.88 | 0.56 |
| 2:AD:211:GLN:OE1 | 2:AD:329:ASN:ND2 | 2.39 | 0.56 |
| 2:AK:526:THR:OG1 | 2:Bs:366:GLU:OE2 | 2.24 | 0.56 |
| 6:AV:414:ALA:HB3 | 6:AV:423:VAL:HG13 | 1.87 | 0.56 |
| 6:Ak:454:VAL:HG22 | 6:Ak:476:ARG:HB3 | 1.86 | 0.56 |
| 6:Ak:484:PHE:O | 6:Ak:487:SER:OG | 2.24 | 0.56 |
| 2:B6:102:THR:N | 2:B6:183:THR:O | 2.38 | 0.56 |
| 2:B6:135:ASP:HB3 | 2:B6:139:LYS:HB2 | 1.88 | 0.56 |
| 11:BN:60:TYR:HD1 | 11:BN:64:GLN:HG2 | 1.70 | 0.56 |
| 3:Bi:114:ARG:HG2 | 3:Bi:126:GLU:HG3 | 1.88 | 0.56 |
| 2:Bs:617:VAL:HG22 | 2:Bs:622:GLU:HB2 | 1.87 | 0.56 |
| 9:y:27:THR:O | 9:y:29:ALA:N | 2.38 | 0.56 |
| 6:A4:125:PHE:HZ | 6:Aj:91:ILE:HA | 1.70 | 0.56 |
| 6:A8:110:ASP:OD2 | 6:A8:422:ARG:NH1 | 2.39 | 0.56 |
| 3:AG:1:MET:SD | 3:AH:22:GLN:NE2 | 2.78 | 0.56 |
| 7:AY:54:ASN:HA | 7:BL:162:TRP:NE1 | 2.21 | 0.56 |
| 7:Aa:6:PRO:HG3 | 7:Aa:15:VAL:HG21 | 1.87 | 0.56 |
| 6:Am:345:TRP:HH2 | 6:BJ:351:LYS:HD2 | 1.69 | 0.56 |
| 6:An:343:ALA:HB1 | 6:An:348:GLU:HG3 | 1.87 | 0.56 |
| 7:Aq:210:GLN:OE1 | 7:Aq:218:ARG:NH2 | 2.35 | 0.56 |
| 2:B2:32:LYS:HD2 | 2:B2:355:LEU:HD21 | 1.88 | 0.56 |
| 2:B4:247:GLY:O | 2:B4:263:SER:OG | 2.24 | 0.56 |
| 2:B4:417:ILE:HG22 | 2:B4:418:PRO:HD2 | 1.87 | 0.56 |
| 2:B6:11:LYS:HG2 | 2:B6:13:THR:HG23 | 1.88 | 0.56 |
| 3:Bg:56:ARG:NH2 | 3:Bm:96:GLY:O | 2.39 | 0.56 |
| 3:Bh:19:ASN:OD1 | 3:Bh:19:ASN:N | 2.35 | 0.56 |
| 3:Bi:39:THR:HG22 | 3:Bi:71:VAL:HG13 | 1.88 | 0.56 |
| 3:Bj:83:GLN:HA | 3:Bj:86:VAL:HG22 | 1.87 | 0.56 |
| 3:Bo:90:SER:OG | 3:Bo:95:GLN:NE2 | 2.27 | 0.56 |
| 2:Bv:560:LEU:HD21 | 2:Bv:601:ILE:HD11 | 1.88 | 0.56 |
| 2:Bw:467:TRP:HH2 | 2:Bx:199:GLU:HB2 | 1.70 | 0.56 |
| 4:N:62:ILE:HD12 | 4:O:58:LEU:HD22 | 1.88 | 0.56 |
| 1:p:177:SER:OG | 1:p:210:ILE:O | 2.24 | 0.56 |
| 2:2:87:ASP:N | 2:2:87:ASP:OD1 | 2.38 | 0.56 |
| 2:3:91:ASN:N | 2:3:91:ASN:OD1 | 2.39 | 0.56 |
| 2:3:417:ILE:H | 2:3:417:ILE:HD13 | 1.70 | 0.56 |
| 2:4:473:ASP:OD1 | 2:4:473:ASP:N | 2.39 | 0.56 |
| 5:A0:434:GLU:O | 5:A0:438:ASN:ND2 | 2.30 | 0.56 |
| 5:A1:422:LEU:O | 5:A1:426:LEU:HG | 2.06 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A2:273:ILE:HD11 | 7:BL:138:LEU:HB3 | 1.87 | 0.56 |
| 2:AL:2:THR:OG1 | 2:AL:3:LEU:N | 2.31 | 0.56 |
| 2:AO:209:ASP:O | 2:AO:213:ASN:ND2 | 2.34 | 0.56 |
| 10:AR:294:VAL:HG12 | 10:AR:305:ILE:HB | 1.88 | 0.56 |
| 10:AT:319:THR:HG21 | 10:AT:370:GLY:HA3 | 1.87 | 0.56 |
| 6:AV:103:ILE:HD12 | 6:AV:296:THR:HG21 | 1.86 | 0.56 |
| 6:AX:172:THR:HG1 | 6:AX:196:VAL:H | 1.53 | 0.56 |
| 6:Ai:319:SER:HA | 6:Ai:323:LEU:HB2 | 1.88 | 0.56 |
| 6:Am:84:THR:OG1 | 6:Am:88:VAL:O | 2.23 | 0.56 |
| 6:An:495:ARG:NH1 | 11:BT:36:SER:O | 2.38 | 0.56 |
| 7:As:13:LYS:HG3 | 7:As:34:ILE:HG21 | 1.87 | 0.56 |
| 6:Ay:444:MET:O | 6:Ay:449:TYR:OH | 2.24 | 0.56 |
| 2:B2:118:VAL:HB | 2:B2:126:GLU:HB3 | 1.88 | 0.56 |
| 5:BA:161:ILE:HB | 5:BA:173:GLU:HB3 | 1.87 | 0.56 |
| 3:BX:39:THR:HG22 | 3:BX:71:VAL:HG22 | 1.87 | 0.56 |
| 3:Bf:64:ARG:HG2 | 3:Bi:93:ALA:HB1 | 1.86 | 0.56 |
| 3:Bk:137:VAL:HB | 3:Bk:155:VAL:HG13 | 1.88 | 0.56 |
| 2:Bp:487:THR:HG21 | 2:Bp:559:MET:HE3 | 1.88 | 0.56 |
| 2:Bu:379:ALA:HA | 2:Bu:411:ARG:HB2 | 1.87 | 0.56 |
| 2:Bv:521:ALA:HB1 | 2:Bv:541:ALA:HA | 1.87 | 0.56 |
| 2:Bw:11:LYS:HG2 | 2:Bw:13:THR:HG23 | 1.87 | 0.56 |
| 5:A2:97:SER:HB2 | 5:BD:405:LYS:HD2 | 1.87 | 0.56 |
| 2:AP:617:VAL:HG22 | 2:AP:622:GLU:HB2 | 1.87 | 0.56 |
| 6:Ah:130:VAL:HG12 | 6:Ah:142:GLU:HA | 1.88 | 0.56 |
| 6:Am:264:ARG:NH2 | 6:BJ:152:ALA:O | 2.37 | 0.56 |
| 6:Ay:365:ALA:HB2 | 6:Ay:372:GLU:HA | 1.87 | 0.56 |
| 2:B1:70:ASN:ND2 | 2:B1:457:GLN:OE1 | 2.38 | 0.56 |
| 2:B5:514:ARG:NH1 | 2:B6:364:ASP:OD1 | 2.31 | 0.56 |
| 6:BJ:456:LEU:H | 6:BJ:475:THR:HB | 1.70 | 0.56 |
| 11:BS:38:VAL:HG11 | 11:BS:69:ILE:HG12 | 1.87 | 0.56 |
| 3:Be:4:ASP:OD2 | 2:Bz:593:GLN:NE2 | 2.39 | 0.56 |
| 3:Bl:125:LYS:NZ | 3:Bo:83:GLN:OE1 | 2.28 | 0.56 |
| 2:Bp:117:THR:HG23 | 2:Bp:127:THR:HG22 | 1.87 | 0.56 |
| 2:Bp:653:GLU:HB2 | 2:Bs:16:GLN:HG3 | 1.86 | 0.56 |
| 2:Bt:536:TYR:HE1 | 2:Bu:572:LEU:HD21 | 1.71 | 0.56 |
| 2:Bv:430:ARG:NH2 | 2:Bv:443:ILE:O | 2.38 | 0.56 |
| 2:By:635:ILE:HD11 | 2:Bz:576:ASN:HD22 | 1.71 | 0.56 |
| 2:Bz:26:THR:HA | 2:Bz:77:ASP:O | 2.06 | 0.56 |
| 4:K:34:ALA:HB3 | 4:L:26:LYS:HG2 | 1.87 | 0.56 |
| 2:3:101:TYR:CZ | 2:3:143:ILE:HG12 | 2.40 | 0.55 |
| 5:A0:98:ASP:OD2 | 5:A0:379:ARG:NH2 | 2.39 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A5:237:GLU:HG2 | 6:A5:246:PRO:HA | 1.89 | 0.55 |
| 2:AD:28:ALA:HB2 | 2:AD:370:VAL:HG21 | 1.87 | 0.55 |
| 6:AV:79:ILE:HG23 | 6:AZ:121:THR:HG22 | 1.88 | 0.55 |
| 6:AW:345:TRP:CD1 | 6:AW:347:GLY:H | 2.24 | 0.55 |
| 6:AX:398:GLN:HE22 | 6:Az:355:PHE:HB2 | 1.71 | 0.55 |
| 6:Ao:345:TRP:CD1 | 6:Ao:346:ALA:H | 2.24 | 0.55 |
| 6:Ap:257:GLN:NE2 | 6:Ap:481:ILE:O | 2.39 | 0.55 |
| 5:Ax:97:SER:HB2 | 5:BA:405:LYS:HD2 | 1.89 | 0.55 |
| 2:B2:209:ASP:OD1 | 2:B2:209:ASP:N | 2.32 | 0.55 |
| 2:B2:498:GLN:HA | 2:B2:534:VAL:HG12 | 1.88 | 0.55 |
| 2:B7:61:THR:HG22 | 2:B7:65:PHE:HB2 | 1.88 | 0.55 |
| 3:Bc:39:THR:HG22 | 3:Bc:71:VAL:HG13 | 1.88 | 0.55 |
| 3:Bn:62:GLY:O | 3:Bo:118:ARG:NH2 | 2.40 | 0.55 |
| 2:Bs:40:GLN:H | 2:Bs:81:VAL:HG23 | 1.70 | 0.55 |
| 2:Bu:401:GLN:O | 2:Bu:561:LYS:NZ | 2.38 | 0.55 |
| 2:Bx:563:ASN:ND2 | 2:Bx:591:TYR:OH | 2.31 | 0.55 |
| 4:P:44:MET:HE1 | 4:U:44:MET:HG2 | 1.87 | 0.55 |
| 1:k:64:GLU:HB2 | 1:k:79:LYS:HG3 | 1.88 | 0.55 |
| 8:q:256:THR:HG21 | 8:q:271:ARG:HB3 | 1.88 | 0.55 |
| 9:y:80:GLU:OE1 | 9:y:82:LYS:NZ | 2.39 | 0.55 |
| 1:0:154:PRO:HA | 1:0:167:ARG:HD3 | 1.87 | 0.55 |
| 2:5:398:ASP:O | 2:5:401:GLN:NE2 | 2.36 | 0.55 |
| 2:5:424:ASP:OD1 | 2:5:516:ARG:NH2 | 2.39 | 0.55 |
| 2:5:605:ARG:HG2 | 2:5:607:VAL:HG23 | 1.86 | 0.55 |
| 5:A0:405:LYS:NZ | 5:BH:451:ASP:OD2 | 2.38 | 0.55 |
| 6:A7:372:GLU:OE2 | 6:AW:406:THR:OG1 | 2.22 | 0.55 |
| 6:A9:380:ARG:HH21 | 6:A9:408:THR:HG21 | 1.71 | 0.55 |
| 9:AC:79:GLU:OE1 | 9:z:119:ASN:ND2 | 2.39 | 0.55 |
| 3:AF:41:LEU:HD23 | 3:AG:82:ARG:HH21 | 1.71 | 0.55 |
| 2:AK:350:VAL:HG13 | 2:AK:354:ASP:HB2 | 1.87 | 0.55 |
| 2:AL:220:PRO:HG2 | 2:AL:338:LEU:HD11 | 1.88 | 0.55 |
| 6:Ak:347:GLY:HA2 | 6:Ak:398:GLN:HB2 | 1.88 | 0.55 |
| 6:An:279:ARG:NH1 | 7:As:115:ALA:O | 2.39 | 0.55 |
| 5:Ax:211:ALA:H | 5:Ax:225:GLY:HA3 | 1.71 | 0.55 |
| 2:B1:70:ASN:OD1 | 2:B1:457:GLN:NE2 | 2.32 | 0.55 |
| 2:B1:391:LYS:HG3 | 2:B1:443:ILE:HD13 | 1.88 | 0.55 |
| 2:B5:128:GLU:HB2 | 2:B5:146:PRO:HG2 | 1.88 | 0.55 |
| 2:B5:237:GLU:OE1 | 2:B5:284:ARG:NH1 | 2.32 | 0.55 |
| 5:BH:112:ASN:HB3 | 5:BH:445:LYS:HB2 | 1.88 | 0.55 |
| 6:BM:148:TYR:HA | 6:BM:186:GLY:H | 1.70 | 0.55 |
| 3:BX:96:GLY:O | 3:Bj:56:ARG:NH2 | 2.39 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bn:83:GLN:HA | 3:Bn:86:VAL:HG22 | 1.88 | 0.55 |
| 2:Bt:131:ILE:HG23 | 2:Bt:143:ILE:HG22 | 1.88 | 0.55 |
| 2:Bw:131:ILE:HG23 | 2:Bw:143:ILE:HG22 | 1.88 | 0.55 |
| 1:l:83:ALA:HB3 | 1:l:201:LEU:HD21 | 1.88 | 0.55 |
| 1:p:176:TYR:HE2 | 1:p:179:GLU:HG3 | 1.70 | 0.55 |
| 9:v:139:SER:HB3 | 9:v:156:THR:H | 1.71 | 0.55 |
| 9:z:27:THR:O | 9:z:29:ALA:N | 2.38 | 0.55 |
| 2:1:310:TYR:O | 2:1:314:PHE:HB2 | 2.06 | 0.55 |
| 2:1:490:SER:O | 2:1:496:ARG:NH1 | 2.38 | 0.55 |
| 2:AD:379:ALA:HB2 | 2:AD:411:ARG:HB2 | 1.88 | 0.55 |
| 3:AG:56:ARG:NH2 | 3:AI:96:GLY:O | 2.38 | 0.55 |
| 3:AI:59:ASN:ND2 | 3:AJ:159:LEU:O | 2.39 | 0.55 |
| 7:Aa:162:TRP:HE1 | 7:Ab:54:ASN:HA | 1.71 | 0.55 |
| 6:Af:145:HIS:CE1 | 6:Af:147:MET:HB2 | 2.41 | 0.55 |
| 6:An:147:MET:HE2 | 6:An:367:GLN:HG2 | 1.89 | 0.55 |
| 7:Ar:36:ASP:OD2 | 7:At:18:ARG:NH1 | 2.39 | 0.55 |
| 2:B2:211:GLN:OE1 | 2:B2:329:ASN:ND2 | 2.40 | 0.55 |
| 2:B4:409:PRO:O | 2:B4:454:TYR:OH | 2.24 | 0.55 |
| 2:B6:235:GLU:OE2 | 2:B6:261:ARG:NH1 | 2.39 | 0.55 |
| 5:BG:310:ASN:HB3 | 5:BG:325:GLN:HA | 1.88 | 0.55 |
| 7:BL:22:ALA:HB1 | 7:BL:23:PRO:HD2 | 1.89 | 0.55 |
| 11:BR:14:GLU:HB3 | 11:BR:25:GLY:H | 1.72 | 0.55 |
| 3:BZ:24:GLU:OE1 | 3:BZ:33:THR:OG1 | 2.24 | 0.55 |
| 3:Bk:5:ASP:OD2 | 3:Bk:8:ARG:NH2 | 2.40 | 0.55 |
| 2:Br:240:SER:OG | 2:Br:243:ASP:OD1 | 2.24 | 0.55 |
| 2:Bv:412:GLU:HA | 2:Bv:415:VAL:HG12 | 1.88 | 0.55 |
| 4:G:53:ARG:NH2 | 4:R:12:ASP:OD2 | 2.39 | 0.55 |
| 8:t:85:ASN:ND2 | 8:t:195:ASN:OD1 | 2.39 | 0.55 |
| 2:1:406:LEU:HD11 | 2:1:475:ALA:HB2 | 1.87 | 0.55 |
| 2:3:561:LYS:NZ | 8:s:231:GLU:OE2 | 2.34 | 0.55 |
| 5:A1:8:LEU:HD21 | 5:BB:29:VAL:HG22 | 1.88 | 0.55 |
| 5:A1:66:GLU:HA | 5:A1:70:LYS:HD3 | 1.88 | 0.55 |
| 5:A1:140:GLN:O | 5:A1:141:ARG:NE | 2.39 | 0.55 |
| 8:AB:85:ASN:ND2 | 8:AB:195:ASN:OD1 | 2.38 | 0.55 |
| 3:AE:17:ARG:HH21 | 3:AF:150:ILE:HG22 | 1.70 | 0.55 |
| 6:Ah:449:TYR:OH | 6:Ah:482:ASN:OD1 | 2.23 | 0.55 |
| 6:Aj:324:THR:HG22 | 6:Aj:325:PRO:HD2 | 1.89 | 0.55 |
| 6:Ao:463:ASP:OD1 | 6:Ao:463:ASP:N | 2.39 | 0.55 |
| 7:At:80:ASN:OD1 | 7:At:80:ASN:N | 2.38 | 0.55 |
| 5:Av:190:THR:OG1 | 5:Av:191:GLU:N | 2.38 | 0.55 |
| 2:B2:202:GLU:OE1 | 2:B2:203:ALA:N | 2.40 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BE:159:PRO:HB3 | 7:BE:174:GLY:O | 2.07 | 0.55 |
| 11:BP:10:ILE:HD11 | 11:BP:35:TYR:HE1 | 1.72 | 0.55 |
| 1:m:177:SER:OG | 1:m:210:ILE:O | 2.21 | 0.55 |
| 2:1:47:GLU:OE2 | 2:1:461:TYR:OH | 2.24 | 0.55 |
| 3:8:17:ARG:HH22 | 9:w:47:THR:HG21 | 1.71 | 0.55 |
| 6:A8:268:ALA:HB1 | 6:A8:290:LEU:HD22 | 1.89 | 0.55 |
| 2:AD:647:THR:OG1 | 2:AN:633:ARG:NH1 | 2.39 | 0.55 |
| 2:AK:135:ASP:HB3 | 2:AK:139:LYS:HB2 | 1.87 | 0.55 |
| 2:AK:264:THR:O | 2:AK:266:LYS:N | 2.40 | 0.55 |
| 2:AK:453:ASN:HB2 | 2:AK:506:ALA:HB3 | 1.89 | 0.55 |
| 7:Ab:60:PHE:HB2 | 7:Ab:182:ILE:HG13 | 1.88 | 0.55 |
| 5:Av:223:GLU:OE1 | 5:Av:224:ALA:N | 2.37 | 0.55 |
| 5:Ax:474:GLU:HG3 | 5:Ax:475:PRO:HD3 | 1.89 | 0.55 |
| 2:B4:135:ASP:HB3 | 2:B4:139:LYS:HB2 | 1.89 | 0.55 |
| 2:B5:373:PHE:HB2 | 2:B5:405:VAL:HG22 | 1.88 | 0.55 |
| 2:B7:40:GLN:H | 2:B7:81:VAL:HG23 | 1.71 | 0.55 |
| 5:BD:454:PHE:CZ | 5:BD:458:LYS:HD2 | 2.41 | 0.55 |
| 5:BH:275:ARG:NH1 | 5:BH:353:ALA:O | 2.38 | 0.55 |
| 6:BI:264:ARG:NH1 | 6:BI:477:TYR:OH | 2.40 | 0.55 |
| 11:BN:77:LYS:NZ | 11:BN:78:VAL:O | 2.39 | 0.55 |
| 3:BY:4:ASP:OD1 | 3:BY:4:ASP:N | 2.38 | 0.55 |
| 3:Ba:97:ASN:O | 3:Bn:3:VAL:N | 2.34 | 0.55 |
| 3:Bc:106:GLU:O | 3:Bc:109:LYS:NZ | 2.33 | 0.55 |
| 3:Bg:47:GLU:OE1 | 3:Bk:148:ASN:ND2 | 2.39 | 0.55 |
| 2:Br:202:GLU:OE1 | 2:Br:203:ALA:N | 2.35 | 0.55 |
| 2:Bv:576:ASN:ND2 | 2:Bv:622:GLU:O | 2.40 | 0.55 |
| 2:Bx:206:THR:HA | 2:Bx:211:GLN:HE21 | 1.71 | 0.55 |
| 4:H:9:PRO:HD3 | 4:H:57:VAL:HG21 | 1.87 | 0.55 |
| 1:n:127:VAL:O | 1:n:128:ASN:ND2 | 2.31 | 0.55 |
| 8:t:27:LYS:NZ | 8:t:34:ASP:OD2 | 2.32 | 0.55 |
| 2:2:98:ASN:HB2 | 2:2:188:ILE:HD12 | 1.89 | 0.55 |
| 2:3:193:ILE:HD11 | 2:3:204:ALA:HB1 | 1.87 | 0.55 |
| 3:7:132:LEU:HD21 | 3:7:157:LEU:HD13 | 1.87 | 0.55 |
| 5:A2:109:VAL:HG23 | 5:A2:134:LEU:HD21 | 1.89 | 0.55 |
| 5:A3:156:ILE:HG22 | 5:A3:238:ALA:HB3 | 1.87 | 0.55 |
| 7:A6:12:LEU:HD13 | 7:A6:38:ILE:HD12 | 1.89 | 0.55 |
| 3:AG:58:ILE:HD12 | 3:Bd:6:VAL:HG21 | 1.89 | 0.55 |
| 6:Am:452:PRO:HA | 6:Am:477:TYR:HA | 1.87 | 0.55 |
| 6:An:431:GLN:NE2 | 6:BK:217:GLU:OE2 | 2.40 | 0.55 |
| 2:B6:391:LYS:NZ | 2:B6:440:ASN:O | 2.40 | 0.55 |
| 5:BG:39:GLY:H | 5:BG:250:ILE:HD11 | 1.71 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BH:477:ILE:HA | 5:BH:481:ILE:HG23 | 1.88 | 0.55 |
| 6:BM:105:ASN:HB2 | 6:BM:412:VAL:HG23 | 1.87 | 0.55 |
| 3:BX:1:MET:SD | 3:Ba:22:GLN:NE2 | 2.80 | 0.55 |
| 3:Be:56:ARG:NH2 | 3:Bk:96:GLY:O | 2.40 | 0.55 |
| 2:Bq:428:ASN:HA | 2:Bq:433:ALA:HB3 | 1.89 | 0.55 |
| 2:Bq:478:CYS:O | 2:Bq:555:ARG:NH1 | 2.37 | 0.55 |
| 2:Bu:365:ARG:NH2 | 2:Bu:400:ARG:O | 2.37 | 0.55 |
| 2:Bu:592:LEU:HD23 | 2:Bu:604:TYR:HB2 | 1.88 | 0.55 |
| 2:Bx:521:ALA:HB1 | 2:Bx:541:ALA:HA | 1.88 | 0.55 |
| 4:C:10:PHE:O | 4:C:54:ASN:ND2 | 2.33 | 0.55 |
| 4:W:62:ILE:HD12 | 4:b:58:LEU:HD22 | 1.88 | 0.55 |
| 4:d:9:PRO:O | 4:d:20:SER:N | 2.33 | 0.55 |
| 5:A1:41:ARG:HH11 | 5:A1:67:PRO:HG2 | 1.71 | 0.55 |
| 5:A2:115:LYS:NZ | 5:A2:443:ASN:OD1 | 2.39 | 0.55 |
| 5:A2:183:GLN:HB3 | 5:A2:207:ILE:HG13 | 1.87 | 0.55 |
| 6:A7:120:PRO:HD3 | 6:A7:453:TYR:CZ | 2.42 | 0.55 |
| 3:AH:120:ALA:HB3 | 3:AH:121:LYS:HE2 | 1.89 | 0.55 |
| 2:AM:41:ILE:HD11 | 2:AM:361:PHE:HB3 | 1.89 | 0.55 |
| 2:AM:645:THR:OG1 | 2:By:629:ILE:O | 2.24 | 0.55 |
| 7:Aa:76:LEU:HD13 | 7:Aa:81:VAL:HG21 | 1.88 | 0.55 |
| 7:Ab:12:LEU:HD13 | 7:Ab:38:ILE:HD12 | 1.88 | 0.55 |
| 6:Ac:260:GLU:HG2 | 6:Ac:261:ALA:H | 1.72 | 0.55 |
| 6:Ae:131:TYR:HD2 | 6:Ae:250:MET:HE3 | 1.72 | 0.55 |
| 6:Ai:96:MET:N | 6:Am:123:GLN:O | 2.40 | 0.55 |
| 7:Ar:12:LEU:HD21 | 7:Ar:248:LYS:HG2 | 1.88 | 0.55 |
| 7:Ar:59:VAL:HG12 | 7:Ar:183:ILE:HG13 | 1.87 | 0.55 |
| 7:Ar:162:TRP:HE1 | 7:At:54:ASN:HA | 1.72 | 0.55 |
| 7:At:12:LEU:HD12 | 7:At:242:TYR:HD2 | 1.72 | 0.55 |
| 6:Aw:387:ALA:HB2 | 6:Aw:404:PHE:HB2 | 1.89 | 0.55 |
| 2:B2:364:ASP:O | 2:B2:367:SER:N | 2.40 | 0.55 |
| 5:BD:178:ASP:HB3 | 5:BD:181:GLN:HB2 | 1.88 | 0.55 |
| 6:BK:350:PHE:HB2 | 6:BK:389:VAL:HG11 | 1.88 | 0.55 |
| 11:BT:64:GLN:O | 11:BT:66:THR:N | 2.39 | 0.55 |
| 3:Bh:63:ASP:OD1 | 3:Bh:64:ARG:N | 2.39 | 0.55 |
| 2:Bw:311:ILE:HB | 2:Bw:327:ALA:HB2 | 1.89 | 0.55 |
| 4:V:58:LEU:HD22 | 4:f:62:ILE:HD12 | 1.88 | 0.55 |
| 8:q:203:ASP:OD1 | 8:q:204:ASP:N | 2.39 | 0.55 |
| 2:2:70:ASN:OD1 | 2:2:457:GLN:NE2 | 2.38 | 0.55 |
| 3:8:20:LEU:HD23 | 9:v:54:PHE:HB3 | 1.89 | 0.55 |
| 5:A1:374:ARG:NH2 | 5:BD:93:SER:OG | 2.39 | 0.55 |
| 7:A6:90:THR:OG1 | 7:A6:91:ASN:N | 2.39 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A7:121:THR:HG23 | 6:AW:79:ILE:HG23 | 1.87 | 0.55 |
| 6:A9:269:ALA:HA | 6:A9:470:VAL:HA | 1.88 | 0.55 |
| 2:AD:528:THR:HG21 | 2:AN:569:LYS:HZ1 | 1.72 | 0.55 |
| 3:AH:25:ILE:O | 3:AH:27:TYR:N | 2.35 | 0.55 |
| 2:AM:57:PRO:HB2 | 2:AM:62:ALA:HA | 1.87 | 0.55 |
| 2:AO:430:ARG:HG3 | 2:AO:522:ILE:HD11 | 1.88 | 0.55 |
| 6:AW:479:ILE:HD11 | 6:AW:501:PRO:HG3 | 1.88 | 0.55 |
| 7:AY:192:ILE:HB | 7:AY:197:MET:HE2 | 1.88 | 0.55 |
| 6:Ao:379:SER:OG | 6:Ao:432:ASP:OD1 | 2.25 | 0.55 |
| 5:Av:367:GLN:OE1 | 5:BB:382:GLN:NE2 | 2.40 | 0.55 |
| 4:B:44:MET:HG2 | 4:R:44:MET:HE1 | 1.89 | 0.55 |
| 2:B5:432:ALA:HB2 | 2:B5:440:ASN:HD22 | 1.71 | 0.55 |
| 2:B7:655:THR:HB | 2:Br:19:VAL:HG21 | 1.89 | 0.55 |
| 5:BD:6:LEU:HD22 | 5:BD:6:LEU:H | 1.70 | 0.55 |
| 6:BI:274:LEU:HD13 | 6:BM:69:GLY:HA2 | 1.88 | 0.55 |
| 3:Bb:25:ILE:O | 3:Bb:27:TYR:N | 2.39 | 0.55 |
| 3:Bk:43:ALA:O | 3:Bk:162:TRP:NE1 | 2.40 | 0.55 |
| 2:Bs:16:GLN:NE2 | 2:Bs:460:LYS:O | 2.39 | 0.55 |
| 2:Bu:368:VAL:HB | 2:Bu:400:ARG:HH21 | 1.70 | 0.55 |
| 2:Bw:116:ILE:HD11 | 2:Bw:131:ILE:HD11 | 1.88 | 0.55 |
| 2:Bz:33:PHE:HA | 2:Bz:61:THR:HG23 | 1.89 | 0.55 |
| 2:Bz:70:ASN:OD1 | 2:Bz:457:GLN:NE2 | 2.29 | 0.55 |
| 1:l:6:LYS:NZ | 1:l:23:GLU:OE2 | 2.40 | 0.55 |
| 1:l:213:ILE:HD13 | 8:s:70:THR:HG22 | 1.88 | 0.55 |
| 8:q:134:VAL:HG21 | 8:q:188:TRP:CE3 | 2.42 | 0.55 |
| 8:s:155:ASN:O | 8:s:157:ILE:N | 2.40 | 0.55 |
| 9:w:50:VAL:HG13 | 9:w:55:GLY:HA2 | 1.88 | 0.55 |
| 5:A1:220:ARG:HD2 | 5:A1:222:TYR:H | 1.72 | 0.55 |
| 6:A7:278:LEU:HD23 | 6:A7:286:ALA:HB2 | 1.89 | 0.55 |
| 6:A9:118:ASN:HB3 | 7:Aa:130:GLY:HA3 | 1.88 | 0.55 |
| 6:A9:317:GLY:HA2 | 6:A9:514:ARG:HE | 1.70 | 0.55 |
| 3:AE:23:VAL:HG11 | 3:AE:39:THR:HG21 | 1.89 | 0.55 |
| 2:AO:51:VAL:HG22 | 2:AO:65:PHE:HZ | 1.70 | 0.55 |
| 6:Ac:380:ARG:HE | 6:Ag:366:ARG:HB2 | 1.72 | 0.55 |
| 6:BK:133:LYS:HG2 | 6:BK:249:GLU:HB3 | 1.89 | 0.55 |
| 11:BR:38:VAL:HG11 | 11:BR:69:ILE:HG12 | 1.89 | 0.55 |
| 3:BX:23:VAL:HG11 | 3:BX:39:THR:HG21 | 1.88 | 0.55 |
| 3:Be:54:MET:HB2 | 3:Bi:20:LEU:HD23 | 1.89 | 0.55 |
| 3:Bo:114:ARG:HG2 | 3:Bo:126:GLU:HG3 | 1.88 | 0.55 |
| 2:Bs:526:THR:OG1 | 2:Bt:366:GLU:OE1 | 2.24 | 0.55 |
| 2:Bt:459:ASP:OD2 | 2:Bt:462:ASN:ND2 | 2.38 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:By:157:VAL:HG23 | 2:By:159:GLU:H | 1.71 | 0.55 |
| 2:Bz:455:LYS:HD2 | 2:Bz:468:VAL:HB | 1.88 | 0.55 |
| 1:n:57:GLU:HA | 1:n:87:ALA:HA | 1.89 | 0.55 |
| 1:n:177:SER:HB2 | 1:n:207:LEU:HB3 | 1.88 | 0.55 |
| 8:r:146:ASN:ND2 | 9:v:119:ASN:OD1 | 2.40 | 0.55 |
| 8:t:174:GLU:HG2 | 8:t:186:ILE:HG23 | 1.89 | 0.55 |
| 2:1:18:THR:OG1 | 2:1:19:VAL:N | 2.39 | 0.55 |
| 2:1:654:LEU:HD22 | 2:2:17:SER:HB3 | 1.89 | 0.55 |
| 2:3:70:ASN:OD1 | 2:3:457:GLN:NE2 | 2.40 | 0.55 |
| 5:A1:215:TYR:HA | 5:BB:248:LYS:HE2 | 1.89 | 0.55 |
| 6:A8:397:ALA:HB1 | 6:A9:393:ILE:HG22 | 1.88 | 0.55 |
| 6:A9:452:PRO:HA | 6:A9:477:TYR:HA | 1.89 | 0.55 |
| 9:AC:106:LYS:HG3 | 9:AC:107:THR:HG23 | 1.88 | 0.55 |
| 3:AF:58:ILE:HD12 | 3:Ba:6:VAL:HG21 | 1.89 | 0.55 |
| 3:AG:72:THR:HG22 | 3:AG:154:GLU:HG3 | 1.89 | 0.55 |
| 3:AI:41:LEU:HB3 | 3:AJ:140:LEU:HB3 | 1.88 | 0.55 |
| 6:AW:456:LEU:H | 6:AW:475:THR:HG22 | 1.70 | 0.55 |
| 7:Ab:305:GLY:HA2 | 5:Av:304:VAL:HG13 | 1.87 | 0.55 |
| 7:At:15:VAL:HG11 | 7:At:248:LYS:HD2 | 1.89 | 0.55 |
| 6:Aw:278:LEU:HD23 | 6:Aw:286:ALA:HB2 | 1.89 | 0.55 |
| 2:B4:254:ILE:HG13 | 2:B4:337:ILE:HB | 1.89 | 0.55 |
| 5:BF:306:ASN:O | 5:BF:310:ASN:ND2 | 2.40 | 0.55 |
| 5:BF:394:THR:HG23 | 5:BF:457:LEU:HB3 | 1.89 | 0.55 |
| 5:BH:161:ILE:HD12 | 5:BH:173:GLU:HB3 | 1.88 | 0.55 |
| 3:Bc:4:ASP:OD1 | 3:Bc:4:ASP:N | 2.38 | 0.55 |
| 3:Bf:73:VAL:HG21 | 3:Bf:85:PHE:HE2 | 1.71 | 0.55 |
| 3:Bf:85:PHE:HB3 | 3:Bf:137:VAL:HG21 | 1.87 | 0.55 |
| 2:Bp:89:ALA:HA | 2:Bp:345:SER:HA | 1.88 | 0.55 |
| 2:Bw:24:THR:O | 2:Bw:483:ASN:ND2 | 2.31 | 0.55 |
| 2:Bx:51:VAL:HG22 | 2:Bx:65:PHE:HZ | 1.71 | 0.55 |
| 4:H:10:PHE:O | 4:H:54:ASN:ND2 | 2.35 | 0.55 |
| 2:2:94:PRO:HB2 | 2:2:219:ILE:HD12 | 1.88 | 0.54 |
| 2:3:281:ILE:HD12 | 2:3:295:LEU:HD12 | 1.89 | 0.54 |
| 2:4:451:ASP:OD1 | 2:4:452:GLY:N | 2.40 | 0.54 |
| 5:A0:111:LEU:HD11 | 5:A0:444:ILE:HD11 | 1.89 | 0.54 |
| 6:A5:300:LEU:HG | 6:AW:150:PRO:HG3 | 1.88 | 0.54 |
| 7:A6:144:LEU:HB3 | 7:BL:117:ILE:HG22 | 1.90 | 0.54 |
| 6:A7:100:ARG:NH2 | 6:A7:289:GLU:OE2 | 2.40 | 0.54 |
| 2:AK:46:ASN:OD1 | 2:AK:47:GLU:N | 2.40 | 0.54 |
| 6:AZ:66:ALA:N | 6:Ah:240:ASN:OD1 | 2.39 | 0.54 |
| 6:Ah:484:PHE:O | 6:Ah:487:SER:OG | 2.19 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Aj:84:THR:OG1 | 6:Aj:88:VAL:O | 2.24 | 0.54 |
| 6:Ak:154:PHE:O | 6:Ak:248:ASN:ND2 | 2.38 | 0.54 |
| 6:Am:117:MET:HG3 | 6:Am:451:ALA:HB1 | 1.89 | 0.54 |
| 6:Au:336:ASP:HB3 | 6:Au:339:ASP:HB2 | 1.89 | 0.54 |
| 6:Az:154:PHE:O | 6:Az:248:ASN:ND2 | 2.40 | 0.54 |
| 2:B2:33:PHE:HA | 2:B2:61:THR:HG23 | 1.88 | 0.54 |
| 2:B2:411:ARG:O | 2:B2:415:VAL:HB | 2.07 | 0.54 |
| 2:B7:119:LYS:HE3 | 2:B7:122:SER:HA | 1.89 | 0.54 |
| 5:BG:489:ASP:O | 5:BG:492:GLN:NE2 | 2.40 | 0.54 |
| 7:BL:59:VAL:HG12 | 7:BL:183:ILE:HG13 | 1.89 | 0.54 |
| 3:Bl:100:THR:OG1 | 3:Bl:101:GLY:N | 2.39 | 0.54 |
| 3:Bn:28:LEU:HB3 | 3:Bn:84:LYS:HD3 | 1.89 | 0.54 |
| 2:Bt:264:THR:HB | 2:Bt:267:ALA:HB3 | 1.89 | 0.54 |
| 8:u:185:ARG:NH1 | 8:u:187:GLU:OE1 | 2.38 | 0.54 |
| 2:3:423:VAL:HG21 | 2:3:513:GLN:HB3 | 1.89 | 0.54 |
| 5:A2:477:ILE:HG22 | 5:A2:481:ILE:HB | 1.90 | 0.54 |
| 5:A3:256:ARG:HH11 | 5:BG:86:TYR:HB2 | 1.71 | 0.54 |
| 8:AB:218:ALA:HB3 | 8:AB:229:VAL:HG11 | 1.89 | 0.54 |
| 3:AH:97:ASN:HA | 3:Ba:3:VAL:HG12 | 1.89 | 0.54 |
| 3:AI:23:VAL:HG11 | 3:AI:39:THR:HG21 | 1.88 | 0.54 |
| 2:AK:256:PRO:HG2 | 2:AK:339:THR:H | 1.71 | 0.54 |
| 7:AY:294:ARG:NH1 | 7:AY:298:TYR:OH | 2.39 | 0.54 |
| 6:Af:117:MET:HB2 | 6:Af:453:TYR:HD1 | 1.72 | 0.54 |
| 6:Aj:264:ARG:NH1 | 6:Aj:305:GLU:OE1 | 2.40 | 0.54 |
| 7:Al:238:LYS:H | 7:Al:238:LYS:HD3 | 1.72 | 0.54 |
| 6:An:383:VAL:HG12 | 6:An:406:THR:HG22 | 1.88 | 0.54 |
| 6:Ao:160:ALA:HB3 | 6:Ao:228:MET:HE3 | 1.89 | 0.54 |
| 2:B1:166:ASN:OD1 | 2:B1:166:ASN:N | 2.32 | 0.54 |
| 2:B2:57:PRO:HA | 2:B2:61:THR:HB | 1.90 | 0.54 |
| 2:B3:455:LYS:HG3 | 2:B3:502:VAL:HG13 | 1.89 | 0.54 |
| 3:Be:113:VAL:HG13 | 3:Be:127:ILE:HG12 | 1.90 | 0.54 |
| 2:Bp:453:ASN:HB2 | 2:Bp:506:ALA:HB3 | 1.90 | 0.54 |
| 2:Bq:521:ALA:HB1 | 2:Bq:541:ALA:HA | 1.89 | 0.54 |
| 2:Bs:239:VAL:HG22 | 2:Bs:280:ALA:HB3 | 1.89 | 0.54 |
| 2:Bt:159:GLU:HB3 | 2:Bt:163:LEU:HA | 1.89 | 0.54 |
| 2:Bx:95:ILE:HD11 | 2:Bx:214:LEU:HG | 1.90 | 0.54 |
| 2:Bz:256:PRO:HG2 | 2:Bz:339:THR:H | 1.72 | 0.54 |
| 4:K:35:ASP:OD1 | 4:L:27:ASN:ND2 | 2.39 | 0.54 |
| 4:P:52:LEU:HD21 | 4:U:12:ASP:HB2 | 1.89 | 0.54 |
| 2:1:12:GLU:HG2 | 2:AD:642:PHE:HB2 | 1.90 | 0.54 |
| 2:1:225:LEU:HB3 | 2:1:324:PHE:HB2 | 1.88 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:401:GLN:O | 2:2:561:LYS:NZ | 2.39 | 0.54 |
| 2:4:455:LYS:HE3 | 2:4:502:VAL:HG22 | 1.89 | 0.54 |
| 5:A2:381:PRO:HB3 | 5:BD:377:LEU:HD23 | 1.90 | 0.54 |
| 5:A3:180:ARG:NH2 | 5:BF:246:CYS:SG | 2.77 | 0.54 |
| 6:A5:264:ARG:NH2 | 6:AW:152:ALA:O | 2.38 | 0.54 |
| 2:AP:488:TRP:HB3 | 2:AP:556:LEU:HD13 | 1.88 | 0.54 |
| 6:Ad:360:GLU:HB3 | 6:Ad:436:VAL:HG11 | 1.89 | 0.54 |
| 6:Aj:387:ALA:HB2 | 6:Aj:404:PHE:HB2 | 1.89 | 0.54 |
| 7:Al:206:THR:HG21 | 7:Al:213:TRP:HE1 | 1.72 | 0.54 |
| 6:Am:486:GLU:HG3 | 6:Am:509:LYS:HB3 | 1.88 | 0.54 |
| 2:B1:16:GLN:HG3 | 2:Bx:653:GLU:HA | 1.89 | 0.54 |
| 2:B1:284:ARG:HG2 | 2:B1:289:ILE:HD13 | 1.89 | 0.54 |
| 2:B5:299:ARG:H | 2:B5:299:ARG:HD2 | 1.72 | 0.54 |
| 2:B6:227:PRO:HB2 | 2:B6:345:SER:HB3 | 1.90 | 0.54 |
| 5:BB:396:ILE:HG23 | 5:BB:400:GLU:HB3 | 1.89 | 0.54 |
| 7:BC:95:ILE:HG23 | 7:BE:111:LEU:HD11 | 1.90 | 0.54 |
| 6:BJ:390:ASP:HB2 | 6:BJ:397:ALA:HB3 | 1.90 | 0.54 |
| 7:BL:273:GLY:O | 1:n:160:GLN:NE2 | 2.40 | 0.54 |
| 3:Bf:100:THR:OG1 | 3:Bf:101:GLY:N | 2.40 | 0.54 |
| 3:Bg:55:ASN:HA | 3:Bk:19:ASN:HD22 | 1.73 | 0.54 |
| 1:p:127:VAL:O | 1:p:128:ASN:ND2 | 2.33 | 0.54 |
| 2:4:57:PRO:HG3 | 2:4:65:PHE:CD1 | 2.42 | 0.54 |
| 2:4:360:ASP:OD1 | 2:4:392:HIS:NE2 | 2.28 | 0.54 |
| 2:5:586:THR:HG21 | 9:z:129:ASN:HD22 | 1.72 | 0.54 |
| 5:A3:273:ILE:HD11 | 7:Al:138:LEU:HB3 | 1.88 | 0.54 |
| 2:AD:592:LEU:HD23 | 2:AD:604:TYR:HB2 | 1.89 | 0.54 |
| 3:AI:17:ARG:HG3 | 3:AI:20:LEU:HD12 | 1.90 | 0.54 |
| 2:AO:473:ASP:HB3 | 2:AO:499:ILE:HD12 | 1.88 | 0.54 |
| 7:AY:101:ASN:ND2 | 6:BK:463:ASP:OD2 | 2.40 | 0.54 |
| 7:Aa:27:VAL:HG12 | 7:Aa:29:LEU:HD23 | 1.90 | 0.54 |
| 7:Aa:43:GLU:O | 7:Aa:47:GLU:HG2 | 2.08 | 0.54 |
| 6:Ag:190:LEU:HB3 | 6:Ag:221:LEU:HB3 | 1.90 | 0.54 |
| 6:Ai:264:ARG:NH1 | 6:Ai:477:TYR:HH | 2.05 | 0.54 |
| 6:Ai:426:ASP:OD2 | 6:Ai:433:TYR:OH | 2.25 | 0.54 |
| 6:Ap:93:PRO:HD3 | 7:BE:98:MET:HG2 | 1.90 | 0.54 |
| 6:Ap:502:SER:OG | 6:Ap:505:ASN:OD1 | 2.22 | 0.54 |
| 5:Av:423:LYS:HG3 | 5:Av:437:TRP:CD1 | 2.42 | 0.54 |
| 2:B1:36:GLY:O | 2:B1:82:ARG:NH1 | 2.38 | 0.54 |
| 2:B1:66:MET:HG2 | 2:B1:468:VAL:HG21 | 1.90 | 0.54 |
| 2:B1:417:ILE:HB | 2:B1:421:ARG:HH11 | 1.73 | 0.54 |
| 2:B6:360:ASP:OD1 | 2:B6:392:HIS:NE2 | 2.30 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BE:106:TRP:HE1 | 7:BE:116:GLY:HA3 | 1.73 | 0.54 |
| 5:BG:188:ILE:HG22 | 5:BG:190:THR:HG22 | 1.89 | 0.54 |
| 3:Bg:19:ASN:OD1 | 3:Bg:19:ASN:N | 2.29 | 0.54 |
| 2:Bv:163:LEU:HD11 | 2:Bv:187:ILE:HG12 | 1.88 | 0.54 |
| 2:Bx:41:ILE:HD11 | 2:Bx:361:PHE:HB3 | 1.88 | 0.54 |
| 4:F:80:GLN:HB2 | 4:Q:79:ILE:HD11 | 1.90 | 0.54 |
| 1:l:41:ILE:HD13 | 1:m:5:ASP:HB2 | 1.88 | 0.54 |
| 1:l:112:ASP:HB2 | 1:l:173:LYS:HD3 | 1.89 | 0.54 |
| 8:q:112:SER:HB2 | 8:r:142:GLN:HE22 | 1.73 | 0.54 |
| 9:z:19:VAL:HG21 | 9:z:37:VAL:HG21 | 1.88 | 0.54 |
| 5:A3:88:VAL:HG23 | 5:A3:373:LEU:HD11 | 1.89 | 0.54 |
| 5:A3:304:VAL:HG13 | 7:A6:305:GLY:HA2 | 1.89 | 0.54 |
| 6:A5:365:ALA:HB2 | 6:A5:372:GLU:HA | 1.88 | 0.54 |
| 3:AA:114:ARG:NH2 | 3:AA:116:TYR:OH | 2.27 | 0.54 |
| 9:AC:50:VAL:HG13 | 9:AC:55:GLY:HA2 | 1.90 | 0.54 |
| 2:AP:302:LYS:HB3 | 2:AP:306:ASP:HA | 1.89 | 0.54 |
| 2:AP:641:ASN:HB2 | 2:Bp:626:THR:HG22 | 1.90 | 0.54 |
| 6:Ad:241:GLY:HA3 | 11:BR:43:GLY:HA2 | 1.88 | 0.54 |
| 6:Af:239:PHE:O | 6:Af:242:SER:OG | 2.25 | 0.54 |
| 6:Ah:171:GLN:HE21 | 6:Ah:195:GLN:HE21 | 1.55 | 0.54 |
| 6:Ap:448:ILE:HG22 | 6:Ap:481:ILE:HD13 | 1.89 | 0.54 |
| 2:B2:479:ALA:O | 2:B2:483:ASN:ND2 | 2.36 | 0.54 |
| 5:BA:453:TYR:OH | 5:BH:459:GLU:OE2 | 2.23 | 0.54 |
| 7:BL:265:ARG:NH1 | 1:m:49:GLU:OE2 | 2.39 | 0.54 |
| 3:BX:9:ALA:O | 3:Ba:35:GLN:NE2 | 2.36 | 0.54 |
| 3:BY:54:MET:O | 3:BY:56:ARG:N | 2.41 | 0.54 |
| 3:Ba:11:GLU:OE1 | 2:Bv:486:GLN:NE2 | 2.39 | 0.54 |
| 3:Bl:64:ARG:NH2 | 3:Bo:95:GLN:OE1 | 2.40 | 0.54 |
| 2:Bq:23:SER:OG | 2:Bq:74:TYR:O | 2.26 | 0.54 |
| 2:Br:490:SER:O | 2:Br:496:ARG:NH1 | 2.33 | 0.54 |
| 2:Bv:612:ASN:HB3 | 2:Bv:624:VAL:HG23 | 1.90 | 0.54 |
| 2:Bx:23:SER:OG | 2:Bx:74:TYR:O | 2.26 | 0.54 |
| 2:Bx:84:VAL:HG13 | 2:Bx:346:SER:HB3 | 1.90 | 0.54 |
| 1:l:25:GLU:HG3 | 1:l:26:ILE:H | 1.73 | 0.54 |
| 1:n:151:TRP:HZ2 | 8:t:59:ILE:HD12 | 1.73 | 0.54 |
| 5:A0:381:PRO:HB2 | 5:BG:377:LEU:HD23 | 1.90 | 0.54 |
| 5:A2:303:HIS:NE2 | 7:BL:161:PHE:O | 2.41 | 0.54 |
| 5:A3:57:ALA:O | 5:A3:60:THR:OG1 | 2.22 | 0.54 |
| 6:A7:217:GLU:OE1 | 6:AW:519:LYS:NZ | 2.36 | 0.54 |
| 2:AP:654:LEU:HD22 | 2:Bp:605:ARG:HH11 | 1.72 | 0.54 |
| 10:AT:328:ASP:O | 10:AT:338:ARG:NH2 | 2.41 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AV:430:LYS:HG3 | 6:AZ:216:MET:HE1 | 1.88 | 0.54 |
| 7:Ab:87:ILE:HG23 | 7:Ab:184:VAL:HG12 | 1.90 | 0.54 |
| 6:Ai:345:TRP:HB2 | 6:Am:344:ARG:HH21 | 1.72 | 0.54 |
| 6:Ak:270:TYR:HA | 6:BK:67:GLU:HB2 | 1.89 | 0.54 |
| 2:B1:495:ASN:OD1 | 2:B1:495:ASN:N | 2.35 | 0.54 |
| 2:B4:378:CYS:HG | 2:B4:454:TYR:HH | 1.55 | 0.54 |
| 2:B5:351:THR:OG1 | 2:B5:352:ALA:N | 2.41 | 0.54 |
| 2:B6:33:PHE:O | 2:B6:82:ARG:NH2 | 2.41 | 0.54 |
| 2:B6:368:VAL:O | 2:B6:400:ARG:NH2 | 2.41 | 0.54 |
| 5:BB:37:ASP:OD2 | 5:BB:413:LYS:NZ | 2.39 | 0.54 |
| 7:BE:163:PHE:HD1 | 7:BE:170:LEU:HB2 | 1.72 | 0.54 |
| 6:BJ:130:VAL:HG12 | 6:BJ:142:GLU:HA | 1.90 | 0.54 |
| 7:BL:98:MET:N | 7:BL:152:GLN:OE1 | 2.40 | 0.54 |
| 11:BQ:64:GLN:O | 11:BQ:66:THR:N | 2.40 | 0.54 |
| 3:BX:138:GLY:HA3 | 3:Bm:43:ALA:HA | 1.90 | 0.54 |
| 3:BY:1:MET:SD | 3:Bb:22:GLN:NE2 | 2.81 | 0.54 |
| 2:Bv:426:LEU:HD22 | 2:Bv:522:ILE:HD13 | 1.89 | 0.54 |
| 2:Bw:110:TYR:HB2 | 2:Bw:138:GLY:HA2 | 1.88 | 0.54 |
| 4:E:58:LEU:HD22 | 4:U:62:ILE:HD12 | 1.89 | 0.54 |
| 9:x:36:SER:OG | 9:x:74:ARG:NH2 | 2.41 | 0.54 |
| 9:x:74:ARG:HH11 | 9:x:154:VAL:HG11 | 1.72 | 0.54 |
| 5:A0:180:ARG:NH1 | 7:BC:122:GLY:O | 2.41 | 0.54 |
| 6:A7:344:ARG:HH11 | 6:A7:344:ARG:H | 1.54 | 0.54 |
| 9:AC:137:ASP:OD1 | 9:AC:138:LEU:N | 2.41 | 0.54 |
| 3:AF:63:ASP:OD2 | 3:Bd:147:ASN:ND2 | 2.40 | 0.54 |
| 3:AI:39:THR:HG22 | 3:AI:71:VAL:HG13 | 1.89 | 0.54 |
| 2:AM:639:THR:HB | 2:By:624:VAL:HG12 | 1.90 | 0.54 |
| 6:AX:387:ALA:HB2 | 6:AX:404:PHE:HB2 | 1.89 | 0.54 |
| 6:Af:105:ASN:HB2 | 6:Af:412:VAL:HG13 | 1.89 | 0.54 |
| 6:Ag:304:ARG:NH2 | 6:Ag:308:ASP:OD1 | 2.41 | 0.54 |
| 6:Ak:264:ARG:NH1 | 6:Ak:305:GLU:OE1 | 2.41 | 0.54 |
| 6:Az:356:GLN:NE2 | 6:Az:360:GLU:OE1 | 2.33 | 0.54 |
| 2:B2:154:ALA:HA | 2:B2:157:VAL:HG22 | 1.90 | 0.54 |
| 3:BX:114:ARG:HB3 | 3:BX:123:VAL:HG13 | 1.89 | 0.54 |
| 3:Bo:83:GLN:NE2 | 3:Bo:87:ASP:OD1 | 2.41 | 0.54 |
| 1:l:147:PHE:HB3 | 1:l:171:ALA:HB1 | 1.88 | 0.54 |
| 2:1:413:THR:HG23 | 2:1:414:VAL:HG23 | 1.89 | 0.54 |
| 2:1:463:ASP:HB3 | 2:AO:308:ASN:HB2 | 1.89 | 0.54 |
| 5:A2:335:TRP:HB2 | 7:AY:307:LEU:HB2 | 1.90 | 0.54 |
| 7:A6:152:GLN:NE2 | 7:A6:156:SER:OG | 2.41 | 0.54 |
| 9:AC:27:THR:O | 9:AC:29:ALA:N | 2.39 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:37:PRO:HB2 | 2:AD:40:GLN:HB3 | 1.90 | 0.54 |
| 2:AK:617:VAL:HA | 2:AK:620:ARG:HG2 | 1.90 | 0.54 |
| 2:AK:638:ILE:HG12 | 2:Bs:623:PHE:HB3 | 1.89 | 0.54 |
| 2:AN:126:GLU:OE2 | 2:AN:129:GLY:N | 2.41 | 0.54 |
| 6:AV:118:ASN:OD1 | 6:AV:118:ASN:N | 2.41 | 0.54 |
| 7:Aa:162:TRP:NE1 | 7:Ab:54:ASN:HA | 2.23 | 0.54 |
| 7:Ab:15:VAL:HG11 | 7:Ab:248:LYS:HD2 | 1.88 | 0.54 |
| 6:Ai:105:ASN:ND2 | 6:Ai:409:THR:O | 2.40 | 0.54 |
| 7:As:30:THR:HA | 1:m:8:LEU:O | 2.08 | 0.54 |
| 5:Av:461:GLU:HG2 | 5:Ax:465:ARG:HH22 | 1.72 | 0.54 |
| 6:Aw:127:LEU:HD23 | 6:BM:100:ARG:HG2 | 1.90 | 0.54 |
| 2:B3:373:PHE:HB2 | 2:B3:405:VAL:HG22 | 1.89 | 0.54 |
| 2:B5:195:LEU:HD22 | 2:B5:201:ALA:HB1 | 1.88 | 0.54 |
| 5:BD:160:LYS:NZ | 5:BD:233:ALA:O | 2.39 | 0.54 |
| 5:BF:99:ALA:O | 5:BF:411:GLN:NE2 | 2.41 | 0.54 |
| 3:Bb:56:ARG:HG3 | 3:Bc:3:VAL:HG23 | 1.90 | 0.54 |
| 3:Bk:55:ASN:OD1 | 3:Bo:19:ASN:ND2 | 2.40 | 0.54 |
| 2:Br:83:ALA:HB2 | 2:Br:358:ALA:HB2 | 1.89 | 0.54 |
| 2:Bu:89:ALA:HA | 2:Bu:345:SER:HA | 1.89 | 0.54 |
| 2:Bv:28:ALA:HB2 | 2:Bv:370:VAL:HG21 | 1.90 | 0.54 |
| 2:Bv:455:LYS:NZ | 2:Bv:473:ASP:OD1 | 2.37 | 0.54 |
| 2:Bx:509:THR:O | 2:Bx:514:ARG:NH1 | 2.41 | 0.54 |
| 2:By:33:PHE:HA | 2:By:61:THR:HG23 | 1.88 | 0.54 |
| 8:s:40:PRO:HG2 | 8:s:74:ARG:HG2 | 1.89 | 0.54 |
| 2:1:202:GLU:O | 2:1:206:THR:OG1 | 2.20 | 0.54 |
| 6:A5:133:LYS:HG2 | 6:A5:249:GLU:HB2 | 1.88 | 0.54 |
| 2:AM:511:GLN:NE2 | 2:AN:5:SER:OG | 2.41 | 0.54 |
| 2:AO:131:ILE:HD13 | 2:AO:140:ILE:HG21 | 1.88 | 0.54 |
| 7:AY:80:ASN:HB2 | 7:AY:189:LYS:HD3 | 1.89 | 0.54 |
| 6:AZ:264:ARG:NH2 | 6:Ad:152:ALA:O | 2.40 | 0.54 |
| 6:AZ:406:THR:OG1 | 6:Ad:372:GLU:OE2 | 2.23 | 0.54 |
| 6:Ad:506:SER:HA | 6:Ad:509:LYS:HB2 | 1.90 | 0.54 |
| 6:Ae:493:ALA:O | 6:Ae:497:GLN:NE2 | 2.40 | 0.54 |
| 6:Ae:515:ARG:NH2 | 6:Ae:517:TYR:OH | 2.39 | 0.54 |
| 6:Ai:345:TRP:CG | 6:Ai:346:ALA:H | 2.25 | 0.54 |
| 6:Aj:249:GLU:OE1 | 6:Aj:249:GLU:N | 2.41 | 0.54 |
| 7:Al:192:ILE:HD11 | 7:Al:226:LEU:HD11 | 1.90 | 0.54 |
| 6:Am:345:TRP:CG | 6:Am:346:ALA:H | 2.26 | 0.54 |
| 6:Ay:260:GLU:H | 6:Ay:500:MET:HE3 | 1.73 | 0.54 |
| 2:B2:119:LYS:HE3 | 2:B2:122:SER:HA | 1.90 | 0.54 |
| 2:B5:643:VAL:HG13 | 2:Bp:14:THR:HG22 | 1.89 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B6:291:GLN:HE22 | 2:B6:320:SER:HB2 | 1.72 | 0.54 |
| 2:B7:571:ARG:NH2 | 2:B7:587:GLU:OE1 | 2.39 | 0.54 |
| 7:BE:80:ASN:HD21 | 7:BE:222:PRO:HG2 | 1.72 | 0.54 |
| 7:BL:77:ARG:NH1 | 7:BL:167:ASN:O | 2.41 | 0.54 |
| 3:Bc:1:MET:HE3 | 3:Bh:99:ILE:HD12 | 1.90 | 0.54 |
| 3:Bj:114:ARG:HB3 | 3:Bj:123:VAL:HG13 | 1.90 | 0.54 |
| 2:Bq:100:GLU:HB3 | 2:Bq:188:ILE:HD11 | 1.89 | 0.54 |
| 3:o:148:ASN:HA | 9:y:47:THR:HG22 | 1.88 | 0.54 |
| 8:q:48:HIS:ND1 | 8:r:182:SER:O | 2.41 | 0.54 |
| 2:2:566:ARG:HA | 2:2:569:LYS:HE2 | 1.88 | 0.54 |
| 2:3:331:PRO:HB2 | 2:3:334:PHE:HB2 | 1.90 | 0.54 |
| 5:A3:383:ASP:O | 5:A3:385:GLN:N | 2.41 | 0.54 |
| 3:AA:161:TYR:CZ | 3:o:97:ASN:HB2 | 2.43 | 0.54 |
| 9:AC:168:LYS:HD2 | 9:v:85:ILE:HG21 | 1.90 | 0.54 |
| 3:AE:96:GLY:O | 3:AI:56:ARG:NH2 | 2.34 | 0.54 |
| 6:AW:166:LEU:HD11 | 6:AW:198:ILE:HG13 | 1.90 | 0.54 |
| 6:Ak:190:LEU:HD21 | 6:Ak:216:MET:HE2 | 1.89 | 0.54 |
| 6:Ao:199:ASP:OD2 | 6:Ao:207:LYS:NZ | 2.33 | 0.54 |
| 7:As:163:PHE:HB2 | 7:As:170:LEU:HD13 | 1.89 | 0.54 |
| 6:Au:101:ARG:NE | 6:Ay:142:GLU:OE2 | 2.41 | 0.54 |
| 6:Au:344:ARG:HE | 6:BJ:345:TRP:HE1 | 1.55 | 0.54 |
| 6:Aw:268:ALA:HB1 | 6:Aw:290:LEU:HD13 | 1.89 | 0.54 |
| 5:Ax:173:GLU:HG2 | 5:Ax:175:ARG:HE | 1.71 | 0.54 |
| 7:BC:154:MET:HE1 | 5:BG:273:ILE:HD13 | 1.90 | 0.54 |
| 5:BH:373:LEU:O | 5:BH:374:ARG:HB2 | 2.08 | 0.54 |
| 6:BI:110:ASP:N | 6:BI:110:ASP:OD1 | 2.41 | 0.54 |
| 6:BI:228:MET:HE1 | 6:BI:247:TRP:HZ3 | 1.72 | 0.54 |
| 2:Bu:628:TYR:OH | 2:Bw:15:VAL:O | 2.24 | 0.54 |
| 2:Bx:550:ARG:HB3 | 2:Bx:553:VAL:HG12 | 1.89 | 0.54 |
| 4:Q:6:ASN:ND2 | 4:Q:61:ASN:OD1 | 2.38 | 0.54 |
| 2:3:51:VAL:HG22 | 2:3:65:PHE:HZ | 1.73 | 0.53 |
| 2:4:108:SER:HB3 | 2:4:178:LEU:HD11 | 1.89 | 0.53 |
| 6:A7:453:TYR:HD2 | 6:A7:476:ARG:HD2 | 1.73 | 0.53 |
| 6:A8:305:GLU:HA | 6:A9:225:ALA:HB3 | 1.89 | 0.53 |
| 3:AG:64:ARG:NH1 | 3:AH:95:GLN:HG2 | 2.22 | 0.53 |
| 2:AM:302:LYS:O | 2:AM:307:SER:N | 2.39 | 0.53 |
| 2:AM:455:LYS:HE2 | 2:AM:502:VAL:HG22 | 1.90 | 0.53 |
| 2:AO:26:THR:HA | 2:AO:77:ASP:O | 2.08 | 0.53 |
| 6:AV:123:GLN:HE21 | 6:Ap:93:PRO:HB2 | 1.72 | 0.53 |
| 6:Ad:380:ARG:HH21 | 6:Ah:363:GLU:HA | 1.73 | 0.53 |
| 6:Af:238:GLY:HA2 | 6:Af:242:SER:HB2 | 1.90 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ai:484:PHE:O | 6:Ai:487:SER:OG | 2.24 | 0.53 |
| 6:Ak:157:GLN:NE2 | 6:Ak:227:GLY:O | 2.41 | 0.53 |
| 6:Am:444:MET:O | 6:Am:449:TYR:OH | 2.26 | 0.53 |
| 7:Ar:305:GLY:HA2 | 5:Ax:304:VAL:HG22 | 1.89 | 0.53 |
| 6:Au:486:GLU:HB2 | 6:Au:509:LYS:HB3 | 1.88 | 0.53 |
| 5:Ax:190:THR:HG22 | 5:Ax:199:VAL:HG12 | 1.90 | 0.53 |
| 2:B1:41:ILE:HD11 | 2:B1:361:PHE:HB3 | 1.90 | 0.53 |
| 2:B2:617:VAL:HG13 | 2:B2:622:GLU:HB2 | 1.91 | 0.53 |
| 2:B6:384:GLU:HG2 | 2:B6:439:ASN:HD21 | 1.72 | 0.53 |
| 2:B7:100:GLU:HB3 | 2:B7:188:ILE:HD11 | 1.90 | 0.53 |
| 7:BL:192:ILE:HD11 | 7:BL:226:LEU:HD11 | 1.89 | 0.53 |
| 11:BP:38:VAL:HG11 | 11:BP:69:ILE:HG12 | 1.89 | 0.53 |
| 3:Bh:64:ARG:HH12 | 3:Bk:95:GLN:HG2 | 1.74 | 0.53 |
| 2:Bs:100:GLU:OE2 | 2:Bs:186:LYS:NZ | 2.36 | 0.53 |
| 2:Bu:509:THR:HB | 2:Bu:513:GLN:HB2 | 1.90 | 0.53 |
| 2:Bv:368:VAL:HG12 | 2:Bv:370:VAL:HG22 | 1.90 | 0.53 |
| 2:Bv:373:PHE:HB2 | 2:Bv:405:VAL:HG22 | 1.89 | 0.53 |
| 2:Bz:90:LYS:NZ | 2:Bz:190:ASP:OD1 | 2.41 | 0.53 |
| 9:v:36:SER:OG | 9:v:74:ARG:NH2 | 2.41 | 0.53 |
| 2:1:166:ASN:N | 2:1:166:ASN:OD1 | 2.41 | 0.53 |
| 2:1:281:ILE:HD12 | 2:1:295:LEU:HD12 | 1.90 | 0.53 |
| 2:1:511:GLN:OE1 | 2:1:514:ARG:NH2 | 2.39 | 0.53 |
| 2:4:508:GLU:N | 2:4:508:GLU:OE1 | 2.41 | 0.53 |
| 2:4:550:ARG:HB3 | 2:4:553:VAL:HG12 | 1.89 | 0.53 |
| 3:6:17:ARG:HH22 | 9:AC:47:THR:HG21 | 1.73 | 0.53 |
| 5:A3:382:GLN:NE2 | 5:BF:371:MET:SD | 2.71 | 0.53 |
| 6:A7:365:ALA:HB2 | 6:A7:372:GLU:HA | 1.90 | 0.53 |
| 6:A8:154:PHE:O | 6:A8:248:ASN:ND2 | 2.40 | 0.53 |
| 6:AV:318:LYS:NZ | 6:AV:339:ASP:OD1 | 2.40 | 0.53 |
| 6:AX:265:GLN:HB3 | 6:AX:474:LYS:HB3 | 1.90 | 0.53 |
| 7:Ab:307:LEU:HB2 | 5:Av:335:TRP:HB2 | 1.90 | 0.53 |
| 6:Ad:237:GLU:HG2 | 6:Ad:246:PRO:HA | 1.89 | 0.53 |
| 6:Ae:346:ALA:HA | 6:Ae:349:SER:HB3 | 1.90 | 0.53 |
| 6:Ai:105:ASN:O | 6:Ai:427:GLN:NE2 | 2.40 | 0.53 |
| 5:Av:398:ARG:HE | 5:BB:379:ARG:NH1 | 2.06 | 0.53 |
| 2:B1:596:LYS:NZ | 2:B1:602:TYR:O | 2.42 | 0.53 |
| 2:B3:222:VAL:HG13 | 2:B3:325:ALA:HB2 | 1.89 | 0.53 |
| 2:B7:592:LEU:HD23 | 2:B7:604:TYR:HB2 | 1.89 | 0.53 |
| 5:BB:44:GLU:OE2 | 5:BB:197:LYS:NZ | 2.40 | 0.53 |
| 7:BE:257:GLU:OE1 | 7:BE:290:LYS:NZ | 2.30 | 0.53 |
| 6:BM:268:ALA:HB1 | 6:BM:290:LEU:HD13 | 1.89 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bk:46:VAL:N | 3:Bn:135:THR:O | 2.33 | 0.53 |
| 2:Bp:37:PRO:HG2 | 2:Bp:42:LYS:HD2 | 1.90 | 0.53 |
| 2:Br:380:GLY:H | 2:Br:411:ARG:HD2 | 1.72 | 0.53 |
| 2:Br:400:ARG:NH1 | 2:Br:403:CYS:SG | 2.82 | 0.53 |
| 2:Bs:291:GLN:HE22 | 2:Bs:320:SER:HB2 | 1.72 | 0.53 |
| 2:Bu:368:VAL:O | 2:Bu:400:ARG:NH2 | 2.36 | 0.53 |
| 2:By:33:PHE:O | 2:By:82:ARG:NH2 | 2.42 | 0.53 |
| 2:By:41:ILE:HD11 | 2:By:361:PHE:HB3 | 1.90 | 0.53 |
| 2:By:453:ASN:HB2 | 2:By:506:ALA:HB3 | 1.89 | 0.53 |
| 8:q:155:ASN:O | 8:q:157:ILE:N | 2.39 | 0.53 |
| 8:s:78:HIS:NE2 | 8:t:174:GLU:OE1 | 2.41 | 0.53 |
| 2:1:514:ARG:NH1 | 2:AO:366:GLU:OE2 | 2.42 | 0.53 |
| 2:4:647:THR:OG1 | 2:AL:633:ARG:NH1 | 2.42 | 0.53 |
| 2:5:209:ASP:O | 2:5:213:ASN:ND2 | 2.29 | 0.53 |
| 2:5:261:ARG:HH21 | 2:5:337:ILE:HD13 | 1.72 | 0.53 |
| 5:A2:366:ARG:NH1 | 5:A2:382:GLN:OE1 | 2.41 | 0.53 |
| 5:A3:405:LYS:HD2 | 5:BG:97:SER:HB2 | 1.90 | 0.53 |
| 3:AI:28:LEU:HD22 | 3:AI:84:LYS:HB3 | 1.90 | 0.53 |
| 2:AM:585:ARG:NH2 | 2:AM:608:CYS:O | 2.41 | 0.53 |
| 2:AN:509:THR:HB | 2:AN:513:GLN:HB2 | 1.91 | 0.53 |
| 10:AS:335:TYR:HA | 10:AS:338:ARG:HD3 | 1.90 | 0.53 |
| 6:AZ:252:PHE:N | 6:Am:67:GLU:OE2 | 2.29 | 0.53 |
| 6:AZ:400:LEU:HD11 | 6:Ad:417:LEU:HD22 | 1.90 | 0.53 |
| 6:Ad:447:GLY:HA2 | 6:Ad:482:ASN:HB2 | 1.91 | 0.53 |
| 6:Ag:131:TYR:HB3 | 6:Ag:250:MET:HG2 | 1.90 | 0.53 |
| 6:Ag:374:ASN:N | 6:Ag:374:ASN:OD1 | 2.40 | 0.53 |
| 6:Au:181:PHE:HD1 | 6:Au:187:THR:HB | 1.73 | 0.53 |
| 4:B:62:ILE:HD12 | 4:G:58:LEU:HD22 | 1.91 | 0.53 |
| 2:B3:375:ALA:HB3 | 2:B3:407:CYS:HA | 1.90 | 0.53 |
| 2:B3:547:PRO:HD3 | 2:B6:304:ILE:HB | 1.90 | 0.53 |
| 2:B3:654:LEU:HD13 | 2:B4:605:ARG:HD3 | 1.89 | 0.53 |
| 2:B5:116:ILE:HD12 | 2:B5:171:ILE:HG12 | 1.90 | 0.53 |
| 2:B6:79:ARG:HE | 2:B6:370:VAL:HG13 | 1.73 | 0.53 |
| 2:B7:41:ILE:HD11 | 2:B7:361:PHE:HB3 | 1.91 | 0.53 |
| 7:BE:161:PHE:O | 5:BG:303:HIS:NE2 | 2.41 | 0.53 |
| 5:BG:236:VAL:HG13 | 5:BG:420:ASP:HB3 | 1.91 | 0.53 |
| 3:Bb:37:LYS:NZ | 3:Bb:152:THR:OG1 | 2.41 | 0.53 |
| 3:Be:114:ARG:HG2 | 3:Be:126:GLU:HG3 | 1.89 | 0.53 |
| 3:Bh:44:GLY:O | 3:Bk:89:GLN:NE2 | 2.40 | 0.53 |
| 3:Bl:43:ALA:O | 3:Bl:162:TRP:NE1 | 2.39 | 0.53 |
| 2:Bp:118:VAL:HB | 2:Bp:126:GLU:HB3 | 1.90 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bx:170:GLU:HA | 2:Bx:182:ILE:HD11 | 1.90 | 0.53 |
| 2:Bx:411:ARG:O | 2:Bx:415:VAL:HB | 2.08 | 0.53 |
| 1:m:76:LEU:HD21 | 8:t:128:ASP:HB3 | 1.89 | 0.53 |
| 1:m:101:SER:O | 8:u:180:ASN:ND2 | 2.41 | 0.53 |
| 8:r:85:ASN:HB3 | 8:r:113:PRO:HB2 | 1.90 | 0.53 |
| 8:r:164:LYS:NZ | 9:v:119:ASN:OD1 | 2.41 | 0.53 |
| 8:r:240:ARG:HH12 | 8:r:268:PRO:HG2 | 1.72 | 0.53 |
| 2:2:110:TYR:CZ | 2:2:177:GLY:HA3 | 2.43 | 0.53 |
| 2:3:304:ILE:HG13 | 2:3:305:TYR:H | 1.74 | 0.53 |
| 3:AI:70:THR:HG22 | 3:AI:156:THR:HG22 | 1.89 | 0.53 |
| 2:AM:130:LYS:HZ3 | 2:AM:132:THR:HA | 1.73 | 0.53 |
| 2:AM:470:LEU:HD23 | 2:AM:525:VAL:HG21 | 1.90 | 0.53 |
| 2:AN:639:THR:HB | 2:B2:624:VAL:HG12 | 1.90 | 0.53 |
| 2:AN:643:VAL:HG13 | 2:AO:14:THR:HG22 | 1.90 | 0.53 |
| 2:AO:135:ASP:N | 2:AO:139:LYS:O | 2.34 | 0.53 |
| 6:AV:495:ARG:NH1 | 6:Ap:86:GLY:H | 2.05 | 0.53 |
| 6:Ae:131:TYR:HA | 6:Ae:250:MET:HA | 1.91 | 0.53 |
| 6:Ae:304:ARG:HD3 | 6:Ae:428:TYR:HD2 | 1.73 | 0.53 |
| 6:Aj:351:LYS:NZ | 6:Aj:390:ASP:O | 2.42 | 0.53 |
| 6:Aw:245:ASN:C | 6:Aw:247:TRP:H | 2.17 | 0.53 |
| 2:B1:538:ASP:HB2 | 2:B1:551:ILE:HB | 1.90 | 0.53 |
| 2:B3:379:ALA:HB2 | 2:B3:454:TYR:HE2 | 1.73 | 0.53 |
| 5:BH:209:ASP:HB3 | 5:BH:227:LYS:HE3 | 1.90 | 0.53 |
| 6:BI:452:PRO:HA | 6:BI:477:TYR:HA | 1.91 | 0.53 |
| 3:Ba:23:VAL:HG11 | 3:Ba:39:THR:HG21 | 1.91 | 0.53 |
| 3:Ba:58:ILE:HD12 | 3:Bb:6:VAL:HG21 | 1.89 | 0.53 |
| 3:Bf:104:PRO:HA | 3:Bf:107:TYR:CZ | 2.43 | 0.53 |
| 3:Bk:70:THR:HG22 | 3:Bk:156:THR:HG22 | 1.91 | 0.53 |
| 3:Bl:39:THR:HG22 | 3:Bl:71:VAL:HG13 | 1.90 | 0.53 |
| 2:Bw:423:VAL:HG21 | 2:Bw:513:GLN:HB3 | 1.90 | 0.53 |
| 2:Bz:488:TRP:HB3 | 2:Bz:556:LEU:HD12 | 1.91 | 0.53 |
| 3:o:74:MET:HA | 3:o:152:THR:HG22 | 1.91 | 0.53 |
| 1:0:245:PHE:HE1 | 8:q:38:ARG:HD3 | 1.74 | 0.53 |
| 2:1:642:PHE:HB2 | 2:2:12:GLU:HG3 | 1.90 | 0.53 |
| 2:2:573:PHE:HE2 | 8:r:237:VAL:HG21 | 1.72 | 0.53 |
| 2:4:401:GLN:NE2 | 8:t:257:SER:OG | 2.41 | 0.53 |
| 2:5:59:ALA:HB2 | 2:AM:299:ARG:HH22 | 1.72 | 0.53 |
| 2:5:116:ILE:N | 2:5:129:GLY:O | 2.42 | 0.53 |
| 3:9:64:ARG:NH2 | 3:AA:95:GLN:OE1 | 2.42 | 0.53 |
| 5:A1:379:ARG:NH2 | 5:A1:400:GLU:OE1 | 2.42 | 0.53 |
| 3:AA:98:GLU:HA | 3:AE:2:PHE:HA | 1.89 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:AG:119:ASP:HA | 3:o:101:GLY:HA3 | 1.90 | 0.53 |
| 2:AO:147:THR:OG1 | 2:AO:256:PRO:O | 2.25 | 0.53 |
| 6:Am:268:ALA:HB3 | 6:Am:471:MET:HG2 | 1.89 | 0.53 |
| 7:At:195:ASN:HA | 7:At:204:TYR:HD2 | 1.73 | 0.53 |
| 2:B7:3:LEU:HD11 | 2:B7:9:GLU:HB2 | 1.90 | 0.53 |
| 5:BD:38:ASP:HA | 5:BD:250:ILE:HD11 | 1.90 | 0.53 |
| 5:BD:290:GLY:C | 5:BD:291:ASN:HD22 | 2.17 | 0.53 |
| 3:BX:97:ASN:HA | 3:Bk:3:VAL:HG12 | 1.91 | 0.53 |
| 3:Bb:76:ASP:OD1 | 3:Bb:80:ASP:N | 2.37 | 0.53 |
| 3:Bm:23:VAL:HG11 | 3:Bm:39:THR:HG21 | 1.91 | 0.53 |
| 3:Bn:129:ILE:HG21 | 3:Bn:159:LEU:HD22 | 1.91 | 0.53 |
| 3:Bo:82:ARG:HH12 | 3:Bo:138:GLY:HA2 | 1.74 | 0.53 |
| 2:Bq:110:TYR:N | 2:Bq:138:GLY:HA3 | 2.24 | 0.53 |
| 2:Bq:526:THR:OG1 | 2:Br:366:GLU:OE1 | 2.25 | 0.53 |
| 2:Br:538:ASP:N | 2:Br:538:ASP:OD1 | 2.40 | 0.53 |
| 2:Bt:2:THR:OG1 | 2:Bt:3:LEU:N | 2.42 | 0.53 |
| 2:Bu:29:LEU:HB3 | 2:Bu:80:VAL:HG23 | 1.90 | 0.53 |
| 2:Bw:126:GLU:HA | 2:Bw:149:LYS:HD2 | 1.90 | 0.53 |
| 2:By:391:LYS:HG2 | 2:By:443:ILE:HD13 | 1.90 | 0.53 |
| 2:Bz:414:VAL:HG23 | 2:Bz:422:ALA:HB1 | 1.89 | 0.53 |
| 2:4:46:ASN:OD1 | 2:4:46:ASN:N | 2.41 | 0.53 |
| 2:5:295:LEU:HA | 2:5:309:ILE:HB | 1.91 | 0.53 |
| 3:6:56:ARG:NH2 | 3:8:96:GLY:O | 2.37 | 0.53 |
| 5:A1:116:SER:HB3 | 5:A1:123:LYS:HE2 | 1.90 | 0.53 |
| 6:A8:182:PHE:HB2 | 6:A8:184:GLU:O | 2.09 | 0.53 |
| 3:AH:19:ASN:OD1 | 3:AH:19:ASN:N | 2.33 | 0.53 |
| 6:AV:148:TYR:HD1 | 6:AV:186:GLY:H | 1.56 | 0.53 |
| 6:AV:384:ASN:HD21 | 6:AZ:362:VAL:HG21 | 1.73 | 0.53 |
| 6:AW:336:ASP:HB3 | 6:AW:339:ASP:HB2 | 1.90 | 0.53 |
| 7:AY:12:LEU:HD12 | 7:AY:242:TYR:HD2 | 1.73 | 0.53 |
| 6:AZ:153:MET:HE1 | 6:AZ:226:GLU:HB2 | 1.90 | 0.53 |
| 6:Ad:450:TYR:HA | 6:Ad:479:ILE:HG22 | 1.90 | 0.53 |
| 6:Af:426:ASP:OD2 | 6:Af:433:TYR:OH | 2.27 | 0.53 |
| 6:Ao:278:LEU:HD23 | 6:Ao:286:ALA:HB2 | 1.90 | 0.53 |
| 7:Ar:90:THR:OG1 | 7:Ar:91:ASN:N | 2.42 | 0.53 |
| 7:As:161:PHE:HA | 7:As:171:LYS:O | 2.08 | 0.53 |
| 5:Av:55:ASN:OD1 | 5:Av:55:ASN:N | 2.39 | 0.53 |
| 2:B7:70:ASN:OD1 | 2:B7:457:GLN:NE2 | 2.37 | 0.53 |
| 2:B7:151:ILE:O | 2:B7:155:LYS:HG2 | 2.09 | 0.53 |
| 7:BC:13:LYS:HG3 | 7:BC:34:ILE:HG21 | 1.91 | 0.53 |
| 3:Bf:3:VAL:HG12 | 3:Bk:97:ASN:HA | 1.89 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bn:85:PHE:HB3 | 3:Bn:137:VAL:HG21 | 1.91 | 0.53 |
| 2:Br:298:LYS:NZ | 2:Br:299:ARG:O | 2.40 | 0.53 |
| 4:X:47:PRO:HB2 | 4:h:48:THR:HG21 | 1.91 | 0.53 |
| 1:m:175:ILE:HB | 8:t:72:LEU:HD23 | 1.89 | 0.53 |
| 2:5:417:ILE:H | 2:5:417:ILE:HD13 | 1.73 | 0.53 |
| 5:A1:45:VAL:HG12 | 5:A1:46:SER:H | 1.73 | 0.53 |
| 5:A3:312:VAL:HG13 | 5:A3:321:ILE:HG23 | 1.90 | 0.53 |
| 5:A3:423:LYS:HG3 | 5:A3:437:TRP:CD1 | 2.44 | 0.53 |
| 6:A7:247:TRP:CH2 | 6:AW:265:GLN:HB3 | 2.44 | 0.53 |
| 3:AH:11:GLU:OE1 | 2:AN:486:GLN:NE2 | 2.41 | 0.53 |
| 3:AJ:97:ASN:HA | 3:Bg:3:VAL:HG12 | 1.90 | 0.53 |
| 2:AM:101:TYR:O | 2:AM:216:LYS:NZ | 2.38 | 0.53 |
| 2:AO:159:GLU:HB3 | 2:AO:163:LEU:HA | 1.89 | 0.53 |
| 2:AP:23:SER:OG | 2:AP:74:TYR:O | 2.27 | 0.53 |
| 6:AZ:459:LEU:HD11 | 6:AZ:474:LYS:HG2 | 1.91 | 0.53 |
| 6:Af:356:GLN:NE2 | 6:Af:360:GLU:OE2 | 2.41 | 0.53 |
| 6:Ai:264:ARG:NH1 | 6:Ai:477:TYR:OH | 2.42 | 0.53 |
| 6:Au:270:TYR:HB3 | 6:Au:290:LEU:HD12 | 1.90 | 0.53 |
| 2:B1:45:THR:OG1 | 2:B1:49:ASP:OD2 | 2.25 | 0.53 |
| 2:B4:246:LYS:HB2 | 2:B4:250:ALA:HB2 | 1.91 | 0.53 |
| 2:B5:163:LEU:HG | 2:B5:187:ILE:HG12 | 1.90 | 0.53 |
| 2:B5:375:ALA:HB3 | 2:B5:407:CYS:HA | 1.91 | 0.53 |
| 2:B6:205:MET:O | 2:B6:211:GLN:NE2 | 2.42 | 0.53 |
| 2:B7:490:SER:O | 2:B7:496:ARG:NH1 | 2.41 | 0.53 |
| 5:BA:454:PHE:CE2 | 5:BA:458:LYS:HD2 | 2.44 | 0.53 |
| 7:BC:40:ARG:HH21 | 7:BC:254:LEU:HD22 | 1.73 | 0.53 |
| 7:BC:88:LEU:HD13 | 7:BC:183:ILE:HG22 | 1.90 | 0.53 |
| 5:BF:210:THR:O | 5:BF:213:GLU:HB2 | 2.08 | 0.53 |
| 5:BH:249:ASN:OD1 | 5:BH:250:ILE:N | 2.42 | 0.53 |
| 6:BI:365:ALA:HB2 | 6:BI:372:GLU:HA | 1.91 | 0.53 |
| 3:BY:97:ASN:O | 3:Bl:3:VAL:N | 2.37 | 0.53 |
| 3:Bd:55:ASN:HB2 | 3:Bh:20:LEU:HD21 | 1.90 | 0.53 |
| 3:Bg:85:PHE:HB3 | 3:Bg:137:VAL:HG21 | 1.89 | 0.53 |
| 3:Bl:24:GLU:OE1 | 3:Bl:33:THR:OG1 | 2.26 | 0.53 |
| 2:Br:70:ASN:ND2 | 2:Br:457:GLN:OE1 | 2.41 | 0.53 |
| 2:Bt:474:ILE:HG22 | 2:Bt:535:LEU:HD11 | 1.90 | 0.53 |
| 2:Bu:273:PRO:HB3 | 2:Bu:278:GLN:HB2 | 1.89 | 0.53 |
| 2:Bx:99:ILE:HD12 | 2:Bx:150:ILE:HD13 | 1.90 | 0.53 |
| 2:Bz:198:ILE:HD11 | 2:Bz:225:LEU:HD11 | 1.91 | 0.53 |
| 4:c:48:THR:HG21 | 4:h:47:PRO:HB2 | 1.90 | 0.53 |
| 1:m:11:LYS:HG3 | 1:m:15:ARG:HH21 | 1.73 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:p:6:LYS:NZ | 1:p:23:GLU:OE2 | 2.41 | 0.53 |
| 2:3:514:ARG:NH1 | 2:AK:364:ASP:OD1 | 2.27 | 0.53 |
| 6:AW:498:SER:O | 6:AW:505:ASN:ND2 | 2.42 | 0.53 |
| 7:AY:163:PHE:HA | 7:AY:170:LEU:HA | 1.90 | 0.53 |
| 6:Ac:341:ARG:NH1 | 6:Aw:521:ILE:O | 2.41 | 0.53 |
| 6:Ae:139:GLY:O | 6:Ae:141:LYS:NZ | 2.40 | 0.53 |
| 6:Af:322:THR:OG1 | 6:Af:514:ARG:NH2 | 2.41 | 0.53 |
| 6:Ag:93:PRO:O | 6:Ak:123:GLN:NE2 | 2.42 | 0.53 |
| 6:Ag:260:GLU:OE1 | 6:Ag:261:ALA:N | 2.42 | 0.53 |
| 6:Ai:343:ALA:HB1 | 6:Ai:348:GLU:HB2 | 1.90 | 0.53 |
| 2:B1:590:GLN:NE2 | 3:Bh:108:LYS:O | 2.40 | 0.53 |
| 2:B2:82:ARG:NH1 | 2:B2:227:PRO:O | 2.40 | 0.53 |
| 5:BF:401:LEU:HD22 | 5:BF:405:LYS:HE3 | 1.91 | 0.53 |
| 5:BH:376:PRO:HG2 | 5:BH:379:ARG:HG3 | 1.90 | 0.53 |
| 6:BK:351:LYS:HA | 6:BK:354:LEU:HD12 | 1.91 | 0.53 |
| 3:Bb:54:MET:HE1 | 3:Bf:22:GLN:HG3 | 1.90 | 0.53 |
| 2:Bs:20:VAL:HG21 | 2:Bs:46:ASN:HD21 | 1.74 | 0.53 |
| 2:Bs:26:THR:HA | 2:Bs:77:ASP:O | 2.08 | 0.53 |
| 2:By:116:ILE:N | 2:By:129:GLY:O | 2.42 | 0.53 |
| 2:By:521:ALA:HB1 | 2:By:541:ALA:HA | 1.90 | 0.53 |
| 2:Bz:117:THR:HG23 | 2:Bz:127:THR:HG22 | 1.91 | 0.53 |
| 4:J:44:MET:HG2 | 4:L:44:MET:HE1 | 1.91 | 0.53 |
| 1:k:172:GLY:HA3 | 8:r:183:ARG:HH12 | 1.72 | 0.53 |
| 1:n:11:LYS:HG3 | 1:n:15:ARG:HH21 | 1.73 | 0.53 |
| 9:y:129:ASN:OD1 | 9:y:129:ASN:N | 2.41 | 0.53 |
| 2:1:592:LEU:HD23 | 2:1:604:TYR:HB2 | 1.89 | 0.53 |
| 2:2:23:SER:OG | 2:2:483:ASN:OD1 | 2.27 | 0.53 |
| 5:A1:158:PHE:HB2 | 5:A1:236:VAL:HB | 1.91 | 0.53 |
| 5:A1:459:GLU:OE2 | 5:BD:453:TYR:OH | 2.20 | 0.53 |
| 5:A2:319:GLY:O | 7:BL:70:LYS:NZ | 2.42 | 0.53 |
| 6:A4:301:GLU:OE1 | 6:A5:155:SER:OG | 2.25 | 0.53 |
| 3:AE:114:ARG:HG2 | 3:AE:126:GLU:HG3 | 1.90 | 0.53 |
| 2:AN:490:SER:O | 2:AN:496:ARG:NH1 | 2.41 | 0.53 |
| 6:AV:74:TYR:HD2 | 6:AZ:500:MET:HE1 | 1.73 | 0.53 |
| 6:AZ:452:PRO:HA | 6:AZ:477:TYR:HA | 1.89 | 0.53 |
| 7:Aa:29:LEU:HD21 | 7:Aa:259:ASN:HB2 | 1.90 | 0.53 |
| 6:Ac:290:LEU:HD21 | 6:Ag:251:GLY:HA2 | 1.91 | 0.53 |
| 6:Ac:315:GLN:OE1 | 6:Ac:514:ARG:NH1 | 2.41 | 0.53 |
| 6:Ai:442:ASN:OD1 | 6:Ai:443:GLU:N | 2.42 | 0.53 |
| 7:Ar:303:PRO:HG3 | 5:Ax:289:THR:HG22 | 1.91 | 0.53 |
| 7:As:152:GLN:NE2 | 7:As:156:SER:OG | 2.41 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:Av:183:GLN:HE21 | 5:Av:207:ILE:HD11 | 1.74 | 0.53 |
| 6:Az:148:TYR:HD1 | 6:Az:186:GLY:HA2 | 1.73 | 0.53 |
| 2:B2:455:LYS:NZ | 2:B2:457:GLN:OE1 | 2.42 | 0.53 |
| 2:B3:510:ARG:HE | 2:B4:363:ALA:HB3 | 1.74 | 0.53 |
| 2:B5:36:GLY:O | 2:B5:82:ARG:NH1 | 2.42 | 0.53 |
| 5:BG:355:ASN:ND2 | 5:BG:359:MET:SD | 2.82 | 0.53 |
| 5:BH:8:LEU:H | 5:BH:8:LEU:HD12 | 1.73 | 0.53 |
| 3:BZ:82:ARG:HH12 | 3:BZ:138:GLY:HA2 | 1.74 | 0.53 |
| 3:Be:115:GLN:OE1 | 3:Bh:79:HIS:NE2 | 2.42 | 0.53 |
| 3:Bf:25:ILE:O | 3:Bf:27:TYR:N | 2.42 | 0.53 |
| 3:Bh:54:MET:HE1 | 3:Bl:22:GLN:HG3 | 1.90 | 0.53 |
| 2:Br:391:LYS:HG2 | 2:Br:443:ILE:HD13 | 1.90 | 0.53 |
| 2:Bs:205:MET:HE1 | 2:Bs:221:GLY:HA3 | 1.91 | 0.53 |
| 2:Bs:440:ASN:OD1 | 2:Bs:440:ASN:N | 2.41 | 0.53 |
| 2:Bt:119:LYS:HE3 | 2:Bt:122:SER:HA | 1.91 | 0.53 |
| 2:Bt:487:THR:HG21 | 2:Bt:559:MET:HE3 | 1.91 | 0.53 |
| 4:C:76:ILE:HB | 4:S:76:ILE:HD11 | 1.91 | 0.53 |
| 9:y:118:ASP:HB3 | 9:y:123:GLU:HG3 | 1.91 | 0.53 |
| 2:2:620:ARG:NH2 | 8:r:266:GLU:O | 2.42 | 0.53 |
| 3:6:72:THR:HG22 | 3:6:154:GLU:HG2 | 1.89 | 0.53 |
| 5:A3:367:GLN:OE1 | 5:BG:382:GLN:NE2 | 2.41 | 0.53 |
| 6:A5:318:LYS:HG3 | 6:A5:516:VAL:HG11 | 1.91 | 0.53 |
| 6:A8:228:MET:HE3 | 6:A8:233:ALA:HB2 | 1.90 | 0.53 |
| 3:AI:83:GLN:HA | 3:AI:86:VAL:HG22 | 1.91 | 0.53 |
| 2:AM:454:TYR:HB3 | 2:AM:467:TRP:HD1 | 1.74 | 0.53 |
| 2:AM:550:ARG:HB3 | 2:AM:553:VAL:HG12 | 1.91 | 0.53 |
| 2:AN:412:GLU:HA | 2:AN:415:VAL:HG12 | 1.90 | 0.53 |
| 2:AO:459:ASP:OD2 | 2:AO:466:ARG:NH1 | 2.42 | 0.53 |
| 10:AQ:345:MET:HE3 | 10:AQ:364:LYS:HG3 | 1.90 | 0.53 |
| 6:Ad:278:LEU:HD12 | 6:Ad:286:ALA:HB2 | 1.90 | 0.53 |
| 6:Ah:257:GLN:NE2 | 6:Ah:481:ILE:O | 2.42 | 0.53 |
| 6:Ak:120:PRO:HD3 | 6:Ak:453:TYR:CZ | 2.44 | 0.53 |
| 6:An:182:PHE:HB2 | 6:An:184:GLU:O | 2.09 | 0.53 |
| 6:Ao:113:GLY:H | 6:Ao:446:ALA:HB3 | 1.73 | 0.53 |
| 6:Ao:365:ALA:HB2 | 6:Ao:372:GLU:HA | 1.91 | 0.53 |
| 6:Ao:495:ARG:NH2 | 6:BK:87:ALA:O | 2.43 | 0.53 |
| 5:Av:188:ILE:HG22 | 5:Av:202:TYR:HB3 | 1.90 | 0.53 |
| 6:Aw:117:MET:HG3 | 6:Aw:451:ALA:HB1 | 1.91 | 0.53 |
| 6:Aw:379:SER:OG | 6:Aw:432:ASP:OD1 | 2.25 | 0.53 |
| 5:Ax:454:PHE:CZ | 5:Ax:458:LYS:HD2 | 2.44 | 0.53 |
| 6:Ay:190:LEU:HB3 | 6:Ay:221:LEU:HB3 | 1.90 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Az:269:ALA:HA | 6:Az:470:VAL:HA | 1.91 | 0.53 |
| 2:B2:490:SER:O | 2:B2:496:ARG:NH1 | 2.35 | 0.53 |
| 2:B6:642:PHE:CZ | 2:B7:561:LYS:HG2 | 2.43 | 0.53 |
| 2:B7:378:CYS:SG | 2:B7:454:TYR:OH | 2.56 | 0.53 |
| 2:B7:568:SER:HA | 2:B7:571:ARG:HG2 | 1.89 | 0.53 |
| 6:BK:344:ARG:NH2 | 6:BK:348:GLU:OE2 | 2.42 | 0.53 |
| 7:BL:12:LEU:HD12 | 7:BL:242:TYR:HD2 | 1.74 | 0.53 |
| 3:Bd:54:MET:HB2 | 3:Bh:20:LEU:HD23 | 1.91 | 0.53 |
| 3:Be:39:THR:HG22 | 3:Be:71:VAL:HG13 | 1.91 | 0.53 |
| 2:Bp:272:GLY:O | 2:Bp:274:GLN:NE2 | 2.42 | 0.53 |
| 2:Bq:234:ILE:HB | 2:Bq:340:LEU:HD12 | 1.89 | 0.53 |
| 2:By:446:THR:OG1 | 2:By:554:ARG:NH2 | 2.41 | 0.53 |
| 1:n:61:VAL:HB | 1:n:137:LEU:HB2 | 1.91 | 0.53 |
| 1:p:154:PRO:HA | 1:p:167:ARG:HD3 | 1.91 | 0.53 |
| 2:2:240:SER:OG | 2:2:334:PHE:O | 2.27 | 0.52 |
| 2:5:22:ASN:ND2 | 2:5:76:ASN:OD1 | 2.42 | 0.52 |
| 5:A0:236:VAL:HG13 | 5:A0:420:ASP:HB3 | 1.89 | 0.52 |
| 5:A3:282:ARG:HA | 5:BF:278:ARG:HH22 | 1.74 | 0.52 |
| 7:A6:268:GLY:HA3 | 7:BL:275:VAL:HA | 1.90 | 0.52 |
| 7:A6:270:MET:HE2 | 1:n:157:PRO:HB3 | 1.90 | 0.52 |
| 6:A7:314:ALA:HA | 6:A7:513:PHE:HB2 | 1.92 | 0.52 |
| 2:AM:655:THR:HB | 2:AN:19:VAL:HG21 | 1.91 | 0.52 |
| 7:AY:159:PRO:HB3 | 7:AY:174:GLY:O | 2.08 | 0.52 |
| 6:AZ:125:PHE:HZ | 6:Am:91:ILE:HA | 1.74 | 0.52 |
| 6:Ak:521:ILE:O | 6:Ao:359:LYS:NZ | 2.32 | 0.52 |
| 6:An:263:SER:HB3 | 6:An:476:ARG:HG2 | 1.91 | 0.52 |
| 7:Aq:162:TRP:NE1 | 7:As:54:ASN:HA | 2.23 | 0.52 |
| 2:B1:54:PHE:HE2 | 2:B1:82:ARG:HB2 | 1.74 | 0.52 |
| 2:B1:102:THR:HB | 2:B1:183:THR:HB | 1.91 | 0.52 |
| 2:B3:417:ILE:HD13 | 2:B3:417:ILE:H | 1.72 | 0.52 |
| 2:B4:70:ASN:ND2 | 2:B4:457:GLN:OE1 | 2.39 | 0.52 |
| 2:B7:284:ARG:HG2 | 2:B7:289:ILE:HD13 | 1.90 | 0.52 |
| 7:BE:12:LEU:O | 7:BE:16:ILE:HG12 | 2.08 | 0.52 |
| 6:BJ:452:PRO:HA | 6:BJ:477:TYR:HA | 1.90 | 0.52 |
| 3:Bh:55:ASN:OD1 | 3:Bl:19:ASN:ND2 | 2.42 | 0.52 |
| 2:Bs:639:THR:HB | 2:Bt:624:VAL:HG12 | 1.90 | 0.52 |
| 2:Bt:261:ARG:HH12 | 2:Bt:337:ILE:HG21 | 1.72 | 0.52 |
| 2:Bu:32:LYS:HD2 | 2:Bu:350:VAL:HG11 | 1.92 | 0.52 |
| 2:Bu:110:TYR:CE1 | 2:Bu:171:ILE:HG21 | 2.44 | 0.52 |
| 2:By:273:PRO:HB3 | 2:By:278:GLN:HB2 | 1.90 | 0.52 |
| 1:k:152:VAL:HG22 | 1:k:169:ILE:HG23 | 1.91 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1:467:TRP:CZ3 | 2:AO:199:GLU:HB2 | 2.45 | 0.52 |
| 2:4:496:ARG:NH2 | 2:AL:573:PHE:O | 2.35 | 0.52 |
| 3:6:97:ASN:HB2 | 3:o:161:TYR:CZ | 2.44 | 0.52 |
| 3:7:14:ASP:OD1 | 3:7:15:PHE:N | 2.42 | 0.52 |
| 5:A0:289:THR:HB | 5:A0:292:MET:HE3 | 1.91 | 0.52 |
| 5:A3:289:THR:HB | 5:A3:292:MET:HE3 | 1.91 | 0.52 |
| 6:A4:142:GLU:OE2 | 6:A9:101:ARG:NE | 2.38 | 0.52 |
| 2:AL:117:THR:HG23 | 2:AL:127:THR:HG22 | 1.91 | 0.52 |
| 2:AM:432:ALA:HB2 | 2:AM:440:ASN:HD22 | 1.75 | 0.52 |
| 2:AO:550:ARG:HB3 | 2:AO:553:VAL:HG12 | 1.91 | 0.52 |
| 2:AP:209:ASP:OD1 | 2:AP:209:ASP:N | 2.37 | 0.52 |
| 6:Ae:120:PRO:HD3 | 6:Ae:453:TYR:CZ | 2.44 | 0.52 |
| 6:Ae:344:ARG:HH21 | 6:Ay:344:ARG:HD3 | 1.74 | 0.52 |
| 6:Ae:351:LYS:NZ | 6:Ae:390:ASP:O | 2.42 | 0.52 |
| 6:Ae:435:THR:HG23 | 6:Ae:515:ARG:HB3 | 1.91 | 0.52 |
| 6:Ai:130:VAL:HG12 | 6:Ai:142:GLU:HA | 1.91 | 0.52 |
| 6:Au:384:ASN:HD21 | 6:Ay:362:VAL:HG21 | 1.74 | 0.52 |
| 5:Av:69:MET:N | 5:Av:69:MET:SD | 2.81 | 0.52 |
| 6:Az:131:TYR:HE1 | 6:Az:141:LYS:HG3 | 1.74 | 0.52 |
| 6:Az:270:TYR:HB3 | 6:Az:290:LEU:HD12 | 1.91 | 0.52 |
| 2:B1:373:PHE:HB2 | 2:B1:405:VAL:HG22 | 1.91 | 0.52 |
| 2:B6:240:SER:OG | 2:B6:243:ASP:OD1 | 2.27 | 0.52 |
| 6:BJ:107:ILE:O | 6:BJ:303:ASN:ND2 | 2.40 | 0.52 |
| 6:BJ:343:ALA:HB1 | 6:BJ:348:GLU:HG3 | 1.91 | 0.52 |
| 7:BL:76:LEU:HB2 | 7:BL:168:GLU:HG3 | 1.91 | 0.52 |
| 6:BM:336:ASP:HB3 | 6:BM:339:ASP:HB2 | 1.90 | 0.52 |
| 6:BM:449:TYR:OH | 6:BM:482:ASN:OD1 | 2.24 | 0.52 |
| 2:Bw:456:TYR:HB3 | 2:Bw:503:ILE:HG12 | 1.91 | 0.52 |
| 2:Bw:505:LEU:HD21 | 2:Bw:525:VAL:HG12 | 1.92 | 0.52 |
| 2:By:462:ASN:HB2 | 2:By:464:VAL:HG22 | 1.90 | 0.52 |
| 4:c:62:ILE:HD12 | 4:h:58:LEU:HD22 | 1.90 | 0.52 |
| 8:s:228:GLY:O | 8:s:258:ASN:ND2 | 2.42 | 0.52 |
| 1:0:78:ASN:ND2 | 1:0:179:GLU:OE1 | 2.42 | 0.52 |
| 1:0:243:LYS:H | 8:AB:4:TYR:H | 1.57 | 0.52 |
| 2:2:57:PRO:HG3 | 2:2:65:PHE:CD1 | 2.44 | 0.52 |
| 2:2:97:GLY:O | 2:2:147:THR:OG1 | 2.25 | 0.52 |
| 2:3:126:GLU:HG2 | 2:3:146:PRO:HD2 | 1.91 | 0.52 |
| 2:5:278:GLN:HG2 | 2:5:296:SER:HB3 | 1.92 | 0.52 |
| 2:5:430:ARG:HG3 | 2:5:522:ILE:HD11 | 1.90 | 0.52 |
| 5:A3:82:LEU:HD23 | 5:A3:254:LEU:HD22 | 1.90 | 0.52 |
| 6:A9:322:THR:OG1 | 6:A9:514:ARG:NH2 | 2.42 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A9:443:GLU:HG3 | 5:Ax:70:LYS:HD3 | 1.90 | 0.52 |
| 6:AW:105:ASN:HB2 | 6:AW:412:VAL:HG13 | 1.91 | 0.52 |
| 7:Ab:160:ASP:OD1 | 7:Ab:160:ASP:N | 2.36 | 0.52 |
| 6:Ac:299:MET:HA | 6:Ac:302:ILE:HD12 | 1.89 | 0.52 |
| 6:Ae:226:GLU:O | 6:Ay:264:ARG:NH1 | 2.42 | 0.52 |
| 6:Ag:500:MET:O | 6:Ag:505:ASN:ND2 | 2.41 | 0.52 |
| 6:Ai:474:LYS:NZ | 6:Am:234:GLU:OE2 | 2.42 | 0.52 |
| 6:Aj:318:LYS:NZ | 6:Aj:356:GLN:OE1 | 2.36 | 0.52 |
| 7:Aq:159:PRO:HB3 | 7:Aq:174:GLY:O | 2.09 | 0.52 |
| 6:Au:350:PHE:HB2 | 6:Au:389:VAL:HG11 | 1.91 | 0.52 |
| 2:B1:152:ALA:O | 2:B1:156:GLU:HG2 | 2.10 | 0.52 |
| 2:B3:162:THR:HA | 2:B3:186:LYS:HB2 | 1.91 | 0.52 |
| 2:B3:261:ARG:HH12 | 2:B3:337:ILE:HG13 | 1.74 | 0.52 |
| 5:BA:136:HIS:NE2 | 5:BA:171:ILE:O | 2.42 | 0.52 |
| 5:BA:209:ASP:HB3 | 5:BA:227:LYS:HE2 | 1.90 | 0.52 |
| 7:BC:159:PRO:HB3 | 7:BC:174:GLY:O | 2.10 | 0.52 |
| 7:BC:270:MET:HA | 7:BC:276:THR:HG22 | 1.92 | 0.52 |
| 6:BM:233:ALA:HA | 6:BM:236:GLN:HG3 | 1.92 | 0.52 |
| 3:Bf:90:SER:HA | 3:Bf:94:GLY:H | 1.74 | 0.52 |
| 3:Bo:25:ILE:O | 3:Bo:27:TYR:N | 2.42 | 0.52 |
| 2:Bq:269:PHE:HE1 | 2:Bq:282:ILE:HG12 | 1.73 | 0.52 |
| 2:Bv:152:ALA:O | 2:Bv:156:GLU:HG2 | 2.10 | 0.52 |
| 2:Bw:110:TYR:HE1 | 2:Bw:171:ILE:HG21 | 1.73 | 0.52 |
| 2:Bw:232:ASP:OD2 | 2:Bw:342:GLY:N | 2.43 | 0.52 |
| 1:k:52:GLN:NE2 | 1:l:21:THR:O | 2.43 | 0.52 |
| 1:n:152:VAL:HG22 | 1:n:169:ILE:HG23 | 1.91 | 0.52 |
| 9:z:91:MET:HG3 | 9:z:135:VAL:HB | 1.90 | 0.52 |
| 2:1:253:PRO:HA | 2:1:260:THR:HG22 | 1.90 | 0.52 |
| 5:A2:244:ASP:OD1 | 5:A2:245:CYS:N | 2.37 | 0.52 |
| 6:A8:466:ASN:OD1 | 6:A8:466:ASN:N | 2.39 | 0.52 |
| 6:A9:290:LEU:HD11 | 6:Aj:67:GLU:HG3 | 1.91 | 0.52 |
| 2:AD:424:ASP:OD1 | 2:AD:516:ARG:NH2 | 2.42 | 0.52 |
| 3:AE:37:LYS:NZ | 3:AE:152:THR:OG1 | 2.41 | 0.52 |
| 2:AL:43:GLN:NE2 | 2:AL:77:ASP:OD2 | 2.43 | 0.52 |
| 2:AN:66:MET:O | 2:AN:70:ASN:ND2 | 2.29 | 0.52 |
| 2:AO:378:CYS:SG | 2:AO:454:TYR:OH | 2.65 | 0.52 |
| 2:AO:498:GLN:HA | 2:AO:534:VAL:HG12 | 1.92 | 0.52 |
| 2:AP:302:LYS:O | 2:AP:307:SER:N | 2.43 | 0.52 |
| 6:AW:404:PHE:HB3 | 6:AW:414:ALA:HB1 | 1.92 | 0.52 |
| 6:AX:336:ASP:HB3 | 6:AX:339:ASP:HB2 | 1.91 | 0.52 |
| 6:Aj:145:HIS:CD2 | 6:Aj:146:PRO:HD2 | 2.45 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Al:22:ALA:HB1 | 7:Al:23:PRO:HD2 | 1.91 | 0.52 |
| 6:Au:226:GLU:OE2 | 6:BJ:262:LYS:NZ | 2.43 | 0.52 |
| 2:B1:42:LYS:NZ | 2:B1:43:GLN:O | 2.33 | 0.52 |
| 5:BD:126:MET:HG2 | 5:BD:426:LEU:HD11 | 1.91 | 0.52 |
| 6:BJ:466:ASN:ND2 | 6:BJ:468:GLN:OE1 | 2.42 | 0.52 |
| 6:BM:365:ALA:HB2 | 6:BM:372:GLU:HA | 1.90 | 0.52 |
| 3:Bb:25:ILE:HG23 | 3:Bb:111:ALA:HB2 | 1.91 | 0.52 |
| 2:Bq:451:ASP:OD1 | 2:Bq:452:GLY:N | 2.38 | 0.52 |
| 1:n:25:GLU:HG3 | 1:n:26:ILE:H | 1.74 | 0.52 |
| 8:q:105:VAL:HG21 | 8:q:208:LEU:HD12 | 1.91 | 0.52 |
| 9:v:15:THR:OG1 | 9:v:16:ASN:N | 2.42 | 0.52 |
| 9:z:118:ASP:O | 9:z:120:SER:N | 2.39 | 0.52 |
| 2:1:450:ILE:HD13 | 2:1:522:ILE:HG12 | 1.92 | 0.52 |
| 2:2:642:PHE:HB2 | 2:3:12:GLU:HG3 | 1.91 | 0.52 |
| 2:5:195:LEU:HD23 | 2:5:225:LEU:HA | 1.91 | 0.52 |
| 5:A2:210:THR:HA | 5:A2:213:GLU:HB2 | 1.91 | 0.52 |
| 6:A5:145:HIS:ND1 | 6:A5:146:PRO:O | 2.43 | 0.52 |
| 2:AD:57:PRO:HG3 | 2:AD:65:PHE:CD1 | 2.44 | 0.52 |
| 2:AN:346:SER:O | 2:AN:348:ALA:N | 2.43 | 0.52 |
| 6:Ac:264:ARG:NH1 | 6:Ac:305:GLU:OE1 | 2.38 | 0.52 |
| 6:Ay:379:SER:OG | 6:Ay:432:ASP:OD1 | 2.23 | 0.52 |
| 2:B2:10:LEU:HD13 | 2:Bz:561:LYS:HD2 | 1.92 | 0.52 |
| 2:B3:84:VAL:HG13 | 2:B3:346:SER:HB3 | 1.92 | 0.52 |
| 2:B7:285:ARG:HG2 | 2:B7:286:ASN:HD22 | 1.75 | 0.52 |
| 6:BK:317:GLY:HA2 | 6:BK:514:ARG:HE | 1.74 | 0.52 |
| 11:BW:10:ILE:HG12 | 11:BW:48:THR:HB | 1.92 | 0.52 |
| 3:Bj:94:GLY:HA3 | 3:Bj:100:THR:HG23 | 1.92 | 0.52 |
| 2:Bp:401:GLN:O | 2:Bp:561:LYS:NZ | 2.42 | 0.52 |
| 2:Bw:373:PHE:HB2 | 2:Bw:405:VAL:HG22 | 1.92 | 0.52 |
| 4:O:23:SER:OG | 4:O:26:LYS:NZ | 2.42 | 0.52 |
| 1:k:57:GLU:HG3 | 1:l:27:LEU:HD12 | 1.91 | 0.52 |
| 1:l:152:VAL:HG22 | 1:l:169:ILE:HG23 | 1.90 | 0.52 |
| 1:m:154:PRO:HG3 | 8:s:59:ILE:HG22 | 1.91 | 0.52 |
| 1:m:188:ASN:OD1 | 1:m:189:GLU:N | 2.39 | 0.52 |
| 8:q:72:LEU:O | 8:q:74:ARG:N | 2.42 | 0.52 |
| 8:q:76:ASN:ND2 | 8:q:121:SER:HB2 | 2.25 | 0.52 |
| 2:1:35:TRP:HB2 | 2:1:230:LEU:HD12 | 1.92 | 0.52 |
| 3:7:56:ARG:NH2 | 3:9:96:GLY:O | 2.36 | 0.52 |
| 5:A0:293:PRO:O | 5:A0:295:ARG:N | 2.42 | 0.52 |
| 5:A1:256:ARG:NH1 | 5:BD:89:ASP:OD2 | 2.43 | 0.52 |
| 5:A2:39:GLY:HA3 | 5:A2:250:ILE:HG12 | 1.92 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A4:456:LEU:HA | 6:A4:475:THR:HG22 | 1.90 | 0.52 |
| 7:A6:12:LEU:HD12 | 7:A6:242:TYR:HD2 | 1.75 | 0.52 |
| 7:A6:54:ASN:HA | 7:Al:162:TRP:NE1 | 2.25 | 0.52 |
| 3:AI:97:ASN:HA | 3:Bd:3:VAL:HG12 | 1.91 | 0.52 |
| 2:AM:494:TYR:O | 2:AM:498:GLN:NE2 | 2.42 | 0.52 |
| 10:AS:344:MET:HG2 | 10:AS:351:VAL:HG11 | 1.91 | 0.52 |
| 7:Al:34:ILE:O | 7:Al:38:ILE:HG12 | 2.09 | 0.52 |
| 6:An:305:GLU:HA | 6:BK:225:ALA:HB3 | 1.91 | 0.52 |
| 7:Ar:202:VAL:HG13 | 4:h:31:ILE:HG22 | 1.92 | 0.52 |
| 7:As:104:TYR:HB2 | 7:As:106:TRP:HD1 | 1.74 | 0.52 |
| 6:Au:217:GLU:OE2 | 6:BJ:431:GLN:NE2 | 2.43 | 0.52 |
| 5:Av:348:ASP:OD1 | 5:Av:349:THR:N | 2.40 | 0.52 |
| 2:B3:391:LYS:NZ | 2:B3:440:ASN:O | 2.42 | 0.52 |
| 5:BA:63:GLY:HA2 | 5:BA:65:TYR:CZ | 2.44 | 0.52 |
| 5:BB:455:ALA:O | 5:BB:459:GLU:HG2 | 2.09 | 0.52 |
| 5:BD:244:ASP:OD1 | 5:BD:245:CYS:N | 2.42 | 0.52 |
| 5:BF:39:GLY:H | 5:BF:250:ILE:HD11 | 1.74 | 0.52 |
| 5:BF:113:LEU:O | 5:BF:123:LYS:NZ | 2.37 | 0.52 |
| 6:BI:264:ARG:NH1 | 6:BI:477:TYR:HH | 2.07 | 0.52 |
| 6:BI:426:ASP:OD2 | 6:BI:433:TYR:OH | 2.24 | 0.52 |
| 6:BK:266:LEU:HD12 | 6:BK:298:ILE:HG13 | 1.90 | 0.52 |
| 2:Br:66:MET:HG2 | 2:Br:468:VAL:HG21 | 1.92 | 0.52 |
| 2:Br:383:LEU:HD22 | 2:Br:439:ASN:HB3 | 1.92 | 0.52 |
| 2:Bs:131:ILE:HD11 | 2:Bs:171:ILE:HD13 | 1.89 | 0.52 |
| 2:Bv:254:ILE:HG22 | 2:Bv:257:GLY:H | 1.74 | 0.52 |
| 2:Bw:332:GLU:OE1 | 2:Bw:332:GLU:N | 2.42 | 0.52 |
| 2:Bz:118:VAL:HB | 2:Bz:126:GLU:HB3 | 1.91 | 0.52 |
| 2:Bz:451:ASP:OD2 | 2:Bz:470:LEU:HB3 | 2.10 | 0.52 |
| 4:K:52:LEU:HD21 | 4:L:12:ASP:HB2 | 1.90 | 0.52 |
| 3:o:23:VAL:HG13 | 3:o:36:CYS:SG | 2.49 | 0.52 |
| 9:z:129:ASN:OD1 | 9:z:129:ASN:N | 2.42 | 0.52 |
| 2:2:273:PRO:HB3 | 2:2:278:GLN:HB2 | 1.91 | 0.52 |
| 2:3:116:ILE:HG21 | 2:3:143:ILE:HD12 | 1.91 | 0.52 |
| 2:3:278:GLN:HG2 | 2:3:296:SER:HB3 | 1.92 | 0.52 |
| 2:3:310:TYR:O | 2:3:314:PHE:CB | 2.57 | 0.52 |
| 3:6:14:ASP:OD1 | 3:6:15:PHE:N | 2.42 | 0.52 |
| 5:A2:91:ALA:HB1 | 5:A2:375:VAL:HG21 | 1.92 | 0.52 |
| 5:A2:423:LYS:HG3 | 5:A2:437:TRP:CD1 | 2.45 | 0.52 |
| 5:A3:62:PHE:HB2 | 6:AV:422:ARG:HH11 | 1.75 | 0.52 |
| 8:AB:22:SER:HB2 | 1:p:221:VAL:HG13 | 1.92 | 0.52 |
| 3:AF:4:ASP:OD2 | 2:AL:593:GLN:NE2 | 2.42 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AK:97:GLY:O | 2:AK:147:THR:OG1 | 2.23 | 0.52 |
| 2:AK:118:VAL:HB | 2:AK:126:GLU:HB3 | 1.91 | 0.52 |
| 2:AL:154:ALA:HA | 2:AL:157:VAL:HG22 | 1.92 | 0.52 |
| 7:Ab:81:VAL:HG22 | 7:Ab:188:THR:HG22 | 1.91 | 0.52 |
| 6:Ac:351:LYS:NZ | 6:Ac:390:ASP:O | 2.41 | 0.52 |
| 6:Af:520:GLY:O | 6:Aj:341:ARG:NH2 | 2.39 | 0.52 |
| 6:Ah:383:VAL:HG21 | 6:Ah:425:ILE:HG12 | 1.91 | 0.52 |
| 6:Ai:154:PHE:O | 6:Ai:248:ASN:ND2 | 2.35 | 0.52 |
| 6:Ak:344:ARG:H | 6:Ak:344:ARG:HE | 1.56 | 0.52 |
| 7:Al:125:CYS:SG | 7:Al:126:ASN:N | 2.82 | 0.52 |
| 6:Am:268:ALA:HB1 | 6:Am:290:LEU:HD22 | 1.91 | 0.52 |
| 7:As:104:TYR:HB2 | 7:As:106:TRP:CD1 | 2.43 | 0.52 |
| 7:At:163:PHE:HA | 7:At:170:LEU:HA | 1.91 | 0.52 |
| 6:Aw:127:LEU:HD11 | 6:Aw:252:PHE:HB2 | 1.92 | 0.52 |
| 2:B2:527:GLY:HA2 | 2:B2:533:TYR:HD2 | 1.73 | 0.52 |
| 2:B4:91:ASN:N | 2:B4:193:ILE:O | 2.42 | 0.52 |
| 7:BC:213:TRP:O | 7:BC:218:ARG:NH2 | 2.42 | 0.52 |
| 6:BJ:494:SER:C | 6:BJ:496:ILE:H | 2.18 | 0.52 |
| 3:Bd:8:ARG:HG2 | 3:Bg:31:ASN:HB3 | 1.91 | 0.52 |
| 3:Bh:39:THR:HG22 | 3:Bh:71:VAL:HG13 | 1.92 | 0.52 |
| 3:Bl:129:ILE:HG23 | 3:Bl:162:TRP:HB3 | 1.90 | 0.52 |
| 3:Bo:25:ILE:HD12 | 3:Bo:28:LEU:HD12 | 1.92 | 0.52 |
| 2:Bp:454:TYR:HB3 | 2:Bp:467:TRP:CD1 | 2.41 | 0.52 |
| 2:Bx:453:ASN:HD21 | 2:Bx:525:VAL:H | 1.57 | 0.52 |
| 4:g:9:PRO:HD3 | 4:g:57:VAL:HG21 | 1.90 | 0.52 |
| 1:n:164:ASN:ND2 | 1:n:164:ASN:O | 2.42 | 0.52 |
| 1:p:25:GLU:HG3 | 1:p:26:ILE:H | 1.74 | 0.52 |
| 2:4:408:SER:HB2 | 2:4:471:ALA:HB3 | 1.92 | 0.52 |
| 5:A0:31:ILE:H | 5:A0:31:ILE:HD13 | 1.74 | 0.52 |
| 5:A1:454:PHE:CZ | 5:A1:458:LYS:HD2 | 2.45 | 0.52 |
| 5:A3:209:ASP:N | 5:A3:209:ASP:OD1 | 2.40 | 0.52 |
| 7:A6:66:GLU:HA | 7:A6:69:TYR:HB3 | 1.91 | 0.52 |
| 8:AB:203:ASP:OD1 | 8:AB:204:ASP:N | 2.43 | 0.52 |
| 3:AJ:19:ASN:OD1 | 3:AJ:19:ASN:N | 2.31 | 0.52 |
| 2:AL:51:VAL:HG22 | 2:AL:65:PHE:HZ | 1.75 | 0.52 |
| 6:Am:345:TRP:CE3 | 6:BJ:348:GLU:HB2 | 2.44 | 0.52 |
| 6:Am:365:ALA:HB2 | 6:Am:372:GLU:HA | 1.92 | 0.52 |
| 6:An:350:PHE:HB2 | 6:An:389:VAL:HG11 | 1.92 | 0.52 |
| 6:An:426:ASP:OD2 | 6:An:433:TYR:OH | 2.23 | 0.52 |
| 6:Aw:120:PRO:HD3 | 6:Aw:453:TYR:CZ | 2.45 | 0.52 |
| 2:B3:284:ARG:HG2 | 2:B3:289:ILE:HD13 | 1.90 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B3:455:LYS:HB2 | 2:B3:470:LEU:HD13 | 1.92 | 0.52 |
| 2:B4:36:GLY:O | 2:B4:82:ARG:NH1 | 2.43 | 0.52 |
| 5:BB:463:LEU:HD13 | 5:BB:466:ARG:HH21 | 1.74 | 0.52 |
| 5:BD:423:LYS:HG3 | 5:BD:437:TRP:CD1 | 2.45 | 0.52 |
| 7:BE:13:LYS:HG3 | 7:BE:34:ILE:HG21 | 1.91 | 0.52 |
| 6:BM:71:ASP:OD1 | 6:BM:72:HIS:N | 2.42 | 0.52 |
| 3:Be:80:ASP:OD1 | 3:Be:84:LYS:NZ | 2.42 | 0.52 |
| 3:Bg:72:THR:HG22 | 3:Bg:154:GLU:HG3 | 1.92 | 0.52 |
| 3:Bj:17:ARG:HG3 | 3:Bj:20:LEU:HD12 | 1.91 | 0.52 |
| 2:Bq:391:LYS:NZ | 2:Bq:440:ASN:O | 2.43 | 0.52 |
| 2:Bs:28:ALA:HB2 | 2:Bs:370:VAL:HG21 | 1.90 | 0.52 |
| 2:Bv:70:ASN:OD1 | 2:Bv:457:GLN:NE2 | 2.43 | 0.52 |
| 1:p:97:GLU:OE1 | 1:p:97:GLU:N | 2.43 | 0.52 |
| 9:w:56:LEU:O | 9:y:97:TYR:HB3 | 2.10 | 0.52 |
| 3:7:114:ARG:HG2 | 3:7:126:GLU:HG3 | 1.91 | 0.52 |
| 3:9:83:GLN:HA | 3:9:86:VAL:HG22 | 1.92 | 0.52 |
| 3:9:94:GLY:HA3 | 3:9:100:THR:HB | 1.91 | 0.52 |
| 6:A5:107:ILE:HA | 6:A5:412:VAL:HG21 | 1.91 | 0.52 |
| 7:A6:124:SER:HA | 5:BF:77:ASP:HB3 | 1.92 | 0.52 |
| 6:A8:387:ALA:HB2 | 6:A8:404:PHE:HB2 | 1.92 | 0.52 |
| 8:AB:248:ASP:OD1 | 8:AB:248:ASP:N | 2.42 | 0.52 |
| 2:AD:353:GLY:HA2 | 2:AD:356:MET:HG2 | 1.92 | 0.52 |
| 2:AM:35:TRP:HH2 | 2:AM:224:ALA:HB1 | 1.75 | 0.52 |
| 2:AP:44:VAL:HG11 | 2:AP:50:LEU:HB2 | 1.92 | 0.52 |
| 2:AP:455:LYS:HD3 | 2:AP:502:VAL:HG13 | 1.92 | 0.52 |
| 10:AT:309:TRP:HB2 | 10:AT:357:ARG:HG3 | 1.91 | 0.52 |
| 7:Ab:138:LEU:HB3 | 5:Ax:273:ILE:HD11 | 1.91 | 0.52 |
| 6:Ac:261:ALA:HA | 6:Ac:478:GLY:HA3 | 1.92 | 0.52 |
| 6:Ag:264:ARG:NH1 | 6:Ag:477:TYR:HH | 2.08 | 0.52 |
| 6:Ag:351:LYS:HG3 | 6:Ag:354:LEU:HD12 | 1.91 | 0.52 |
| 6:Ao:269:ALA:HA | 6:Ao:470:VAL:HA | 1.91 | 0.52 |
| 7:Ar:90:THR:HB | 7:Ar:183:ILE:HD13 | 1.91 | 0.52 |
| 5:Ax:206:PHE:HE2 | 5:Ax:232:LYS:HG2 | 1.75 | 0.52 |
| 2:B5:34:GLN:NE2 | 2:B5:58:THR:OG1 | 2.43 | 0.52 |
| 5:BA:292:MET:HE3 | 5:BA:297:ALA:HA | 1.91 | 0.52 |
| 5:BA:474:GLU:O | 5:BA:477:ILE:HG13 | 2.09 | 0.52 |
| 5:BB:258:VAL:O | 5:BB:262:ASN:ND2 | 2.43 | 0.52 |
| 7:BL:248:LYS:O | 7:BL:252:THR:OG1 | 2.26 | 0.52 |
| 3:BY:97:ASN:HA | 3:Bl:3:VAL:HG12 | 1.92 | 0.52 |
| 2:Bq:455:LYS:NZ | 2:Bq:473:ASP:OD2 | 2.43 | 0.52 |
| 2:Bu:159:GLU:HB3 | 2:Bu:163:LEU:HA | 1.92 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bv:451:ASP:OD1 | 2:Bv:452:GLY:N | 2.37 | 0.52 |
| 2:Bx:163:LEU:HD11 | 2:Bx:187:ILE:HG12 | 1.92 | 0.52 |
| 2:By:454:TYR:HB3 | 2:By:467:TRP:HD1 | 1.74 | 0.52 |
| 2:Bz:365:ARG:HB2 | 2:Bz:400:ARG:HG3 | 1.90 | 0.52 |
| 4:W:34:ALA:HA | 4:W:41:GLU:HG2 | 1.91 | 0.52 |
| 4:Z:35:ASP:OD1 | 4:e:27:ASN:ND2 | 2.43 | 0.52 |
| 1:m:166:ILE:O | 1:m:167:ARG:NH1 | 2.42 | 0.52 |
| 8:r:168:MET:HG3 | 8:r:193:GLU:HB2 | 1.91 | 0.52 |
| 2:1:394:VAL:HG11 | 2:1:443:ILE:HG21 | 1.91 | 0.52 |
| 2:3:63:ASP:OD2 | 2:3:379:ALA:HB3 | 2.10 | 0.52 |
| 2:4:17:SER:O | 2:4:460:LYS:NZ | 2.43 | 0.52 |
| 5:A0:156:ILE:HG22 | 5:A0:238:ALA:HB3 | 1.92 | 0.52 |
| 5:A0:364:TRP:HD1 | 5:BH:359:MET:HE1 | 1.75 | 0.52 |
| 6:A8:344:ARG:NH1 | 6:A8:348:GLU:OE2 | 2.42 | 0.52 |
| 3:AH:28:LEU:HD22 | 3:AH:84:LYS:HB3 | 1.92 | 0.52 |
| 2:AK:444:SER:OG | 2:AK:543:SER:OG | 2.27 | 0.52 |
| 2:AO:617:VAL:HG22 | 2:AO:622:GLU:HB2 | 1.90 | 0.52 |
| 2:AO:654:LEU:HD13 | 2:B5:605:ARG:HD3 | 1.91 | 0.52 |
| 10:AU:345:MET:HG2 | 10:AU:351:VAL:HG21 | 1.92 | 0.52 |
| 7:Aa:202:VAL:HG23 | 4:Y:31:ILE:HG12 | 1.92 | 0.52 |
| 6:Ac:502:SER:OG | 6:Ac:505:ASN:OD1 | 2.25 | 0.52 |
| 7:Al:115:ALA:HB2 | 6:Ap:272:ILE:HG12 | 1.91 | 0.52 |
| 6:Ao:120:PRO:HD3 | 6:Ao:453:TYR:CZ | 2.45 | 0.52 |
| 6:Ao:182:PHE:HB2 | 6:Ao:184:GLU:O | 2.10 | 0.52 |
| 2:B1:251:LEU:HB3 | 2:B1:260:THR:HB | 1.91 | 0.52 |
| 2:B1:545:PRO:HB2 | 2:B4:304:ILE:HD13 | 1.92 | 0.52 |
| 2:B1:549:ASP:OD2 | 2:B4:271:TYR:OH | 2.20 | 0.52 |
| 2:B2:444:SER:OG | 2:B2:543:SER:OG | 2.22 | 0.52 |
| 2:B6:20:VAL:HG21 | 2:B6:46:ASN:HD21 | 1.75 | 0.52 |
| 2:B6:431:THR:HA | 2:B6:442:ASN:HD21 | 1.75 | 0.52 |
| 7:BC:161:PHE:HA | 7:BC:171:LYS:O | 2.10 | 0.52 |
| 3:BY:101:GLY:HA3 | 3:Bo:118:ARG:HG3 | 1.91 | 0.52 |
| 3:BZ:4:ASP:OD1 | 3:BZ:4:ASP:N | 2.39 | 0.52 |
| 3:Ba:25:ILE:HD12 | 3:Ba:28:LEU:HD12 | 1.92 | 0.52 |
| 2:Bq:373:PHE:HB2 | 2:Bq:405:VAL:HG22 | 1.91 | 0.52 |
| 2:Br:561:LYS:HD2 | 2:Bt:10:LEU:HD13 | 1.90 | 0.52 |
| 2:Bs:91:ASN:OD1 | 2:Bs:91:ASN:N | 2.42 | 0.52 |
| 2:Bs:222:VAL:HG21 | 2:Bs:238:ILE:HD11 | 1.91 | 0.52 |
| 2:Bt:379:ALA:HA | 2:Bt:411:ARG:HB2 | 1.91 | 0.52 |
| 2:Bv:444:SER:HB3 | 2:Bv:544:VAL:HG22 | 1.92 | 0.52 |
| 2:Bv:454:TYR:HB3 | 2:Bv:467:TRP:CD1 | 2.45 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:44:MET:HE3 | 4:I:44:MET:HE3 | 1.92 | 0.52 |
| 1:m:176:TYR:HA | 8:t:71:ILE:HA | 1.91 | 0.52 |
| 1:p:118:ILE:HD12 | 1:p:167:ARG:HB3 | 1.91 | 0.52 |
| 8:u:95:GLN:N | 9:y:7:GLN:OE1 | 2.43 | 0.52 |
| 2:3:427:VAL:O | 2:3:431:THR:OG1 | 2.24 | 0.51 |
| 2:5:31:GLY:HA2 | 2:5:355:LEU:HD21 | 1.92 | 0.51 |
| 2:5:451:ASP:OD1 | 2:5:452:GLY:N | 2.42 | 0.51 |
| 2:5:455:LYS:HB2 | 2:5:470:LEU:HD13 | 1.92 | 0.51 |
| 5:A1:150:TRP:HD1 | 5:A1:156:ILE:HG22 | 1.74 | 0.51 |
| 5:A3:103:GLU:OE1 | 5:A3:449:HIS:NE2 | 2.42 | 0.51 |
| 6:A4:261:ALA:HA | 6:A4:478:GLY:HA3 | 1.93 | 0.51 |
| 6:A4:264:ARG:NH2 | 6:A5:152:ALA:O | 2.43 | 0.51 |
| 7:A6:179:TYR:HB3 | 6:Ao:86:GLY:HA3 | 1.91 | 0.51 |
| 6:A7:123:GLN:NE2 | 6:AW:93:PRO:O | 2.43 | 0.51 |
| 6:A9:387:ALA:HB2 | 6:A9:404:PHE:HB2 | 1.92 | 0.51 |
| 9:AC:38:PRO:HB3 | 9:v:142:GLU:HA | 1.92 | 0.51 |
| 2:AM:209:ASP:OD1 | 2:AM:209:ASP:N | 2.43 | 0.51 |
| 6:Ag:68:ILE:HD12 | 6:Ao:235:LEU:HD21 | 1.92 | 0.51 |
| 6:Ah:398:GLN:HB3 | 6:BI:351:LYS:HD3 | 1.92 | 0.51 |
| 6:Ak:391:THR:OG1 | 6:Ak:392:GLY:N | 2.41 | 0.51 |
| 6:Ao:106:LEU:HD11 | 6:Ao:299:MET:HE3 | 1.92 | 0.51 |
| 6:Ap:494:SER:C | 6:Ap:496:ILE:H | 2.18 | 0.51 |
| 7:Aq:166:ALA:N | 7:As:51:ASP:OD2 | 2.38 | 0.51 |
| 7:Ar:40:ARG:HH21 | 7:Ar:254:LEU:HD22 | 1.76 | 0.51 |
| 7:Ar:89:ARG:HG2 | 7:Ar:95:ILE:HG22 | 1.91 | 0.51 |
| 6:Ay:117:MET:HG3 | 6:Ay:451:ALA:HB1 | 1.92 | 0.51 |
| 6:Ay:267:LYS:HE3 | 6:Ay:470:VAL:HG21 | 1.92 | 0.51 |
| 4:B:10:PHE:O | 4:B:54:ASN:ND2 | 2.39 | 0.51 |
| 2:B1:366:GLU:OE1 | 2:Bz:526:THR:OG1 | 2.28 | 0.51 |
| 2:B3:133:GLU:HB3 | 2:B3:142:LYS:HB3 | 1.92 | 0.51 |
| 2:B4:408:SER:HB3 | 2:B4:454:TYR:HE1 | 1.75 | 0.51 |
| 6:BJ:153:MET:HB2 | 6:BJ:189:TYR:CZ | 2.45 | 0.51 |
| 6:BK:417:LEU:HB3 | 6:BK:421:TYR:HB2 | 1.92 | 0.51 |
| 7:BL:104:TYR:O | 7:BL:106:TRP:N | 2.39 | 0.51 |
| 6:BM:100:ARG:HH21 | 6:BM:284:MET:HE3 | 1.74 | 0.51 |
| 6:BM:185:THR:HG23 | 6:BM:366:ARG:HH21 | 1.75 | 0.51 |
| 3:Bb:19:ASN:OD1 | 3:Bb:19:ASN:N | 2.42 | 0.51 |
| 3:Bd:56:ARG:NH2 | 3:Bj:96:GLY:O | 2.42 | 0.51 |
| 3:Bk:24:GLU:OE1 | 3:Bk:33:THR:OG1 | 2.26 | 0.51 |
| 2:Bs:470:LEU:HD23 | 2:Bs:525:VAL:HG21 | 1.92 | 0.51 |
| 2:Bx:269:PHE:CZ | 2:Bx:282:ILE:HG13 | 2.45 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:b:10:PHE:O | 4:b:54:ASN:ND2 | 2.35 | 0.51 |
| 9:w:5:LEU:H | 9:w:5:LEU:HD12 | 1.75 | 0.51 |
| 1:0:213:ILE:HD13 | 8:q:70:THR:HG22 | 1.92 | 0.51 |
| 1:0:231:TYR:OH | 8:q:15:THR:OG1 | 2.18 | 0.51 |
| 8:AB:69:GLU:HG2 | 8:AB:70:THR:H | 1.75 | 0.51 |
| 3:AE:97:ASN:HB3 | 3:Bj:2:PHE:HB3 | 1.91 | 0.51 |
| 2:AP:34:GLN:OE1 | 2:AP:58:THR:OG1 | 2.28 | 0.51 |
| 2:AP:135:ASP:OD1 | 2:AP:136:ALA:N | 2.42 | 0.51 |
| 6:AV:413:PHE:HE1 | 6:AV:422:ARG:HB3 | 1.75 | 0.51 |
| 6:Ae:231:SER:HB3 | 6:Au:71:ASP:HB3 | 1.92 | 0.51 |
| 6:Ag:305:GLU:HG3 | 6:Ag:309:TRP:CD1 | 2.45 | 0.51 |
| 6:Ai:328:LYS:HE3 | 6:Ai:333:ASP:HB3 | 1.92 | 0.51 |
| 6:Aj:358:ASP:OD1 | 6:Aj:421:TYR:OH | 2.28 | 0.51 |
| 7:Al:193:ASP:O | 7:Al:242:TYR:OH | 2.29 | 0.51 |
| 7:Ar:12:LEU:O | 7:Ar:16:ILE:HG12 | 2.09 | 0.51 |
| 7:As:203:GLY:HA2 | 4:U:32:LEU:HD23 | 1.91 | 0.51 |
| 6:Aw:337:PRO:HA | 6:Aw:340:ILE:HG12 | 1.92 | 0.51 |
| 2:B3:30:ALA:HB3 | 2:B3:359:TRP:CE2 | 2.45 | 0.51 |
| 2:B5:632:ALA:HB1 | 2:B6:575:LEU:HD11 | 1.91 | 0.51 |
| 2:B6:571:ARG:NH2 | 2:B6:587:GLU:OE1 | 2.43 | 0.51 |
| 5:BB:470:LEU:HD12 | 5:BB:491:LEU:HD21 | 1.92 | 0.51 |
| 3:BY:35:GLN:NE2 | 3:BY:76:ASP:OD2 | 2.43 | 0.51 |
| 3:BZ:37:LYS:HZ1 | 3:BZ:74:MET:HG2 | 1.75 | 0.51 |
| 2:Bu:362:PHE:HA | 2:Bu:368:VAL:HG21 | 1.92 | 0.51 |
| 2:Bu:617:VAL:HG22 | 2:Bu:622:GLU:HB2 | 1.91 | 0.51 |
| 2:Bv:311:ILE:HB | 2:Bv:327:ALA:HB2 | 1.92 | 0.51 |
| 2:By:526:THR:OG1 | 2:Bz:366:GLU:OE1 | 2.27 | 0.51 |
| 2:4:378:CYS:SG | 2:4:454:TYR:OH | 2.55 | 0.51 |
| 2:4:592:LEU:HD23 | 2:4:604:TYR:HB2 | 1.91 | 0.51 |
| 5:A3:94:GLU:OE2 | 5:A3:379:ARG:NH1 | 2.35 | 0.51 |
| 5:A3:162:ILE:HD11 | 5:A3:167:PRO:HA | 1.93 | 0.51 |
| 7:A6:161:PHE:HA | 7:A6:171:LYS:O | 2.11 | 0.51 |
| 7:A6:173:MET:HE3 | 7:BL:55:LYS:HE2 | 1.91 | 0.51 |
| 6:A8:395:TYR:HD1 | 6:A8:396:ALA:H | 1.58 | 0.51 |
| 6:A9:269:ALA:HB2 | 6:A9:470:VAL:HG13 | 1.93 | 0.51 |
| 2:AD:494:TYR:OH | 2:AD:531:ASP:OD1 | 2.28 | 0.51 |
| 10:AQ:335:TYR:HA | 10:AQ:338:ARG:HD3 | 1.91 | 0.51 |
| 6:AV:78:ASN:ND2 | 11:BR:5:ARG:O | 2.43 | 0.51 |
| 6:Aj:363:GLU:OE2 | 6:Aj:366:ARG:NH2 | 2.38 | 0.51 |
| 6:Ak:273:GLU:HB2 | 6:Az:234:GLU:HG2 | 1.93 | 0.51 |
| 6:Am:69:GLY:N | 6:Au:234:GLU:OE2 | 2.40 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Ar:92:ILE:HD11 | 7:Ar:181:LEU:HD13 | 1.92 | 0.51 |
| 6:Au:263:SER:HB3 | 6:Au:476:ARG:HG2 | 1.92 | 0.51 |
| 5:Ax:355:ASN:ND2 | 5:Ax:359:MET:SD | 2.84 | 0.51 |
| 6:Az:486:GLU:N | 6:Az:486:GLU:OE1 | 2.39 | 0.51 |
| 2:B3:473:ASP:HB3 | 2:B3:499:ILE:HD12 | 1.90 | 0.51 |
| 2:B5:11:LYS:HG2 | 2:B5:13:THR:HG23 | 1.93 | 0.51 |
| 6:BM:119:SER:OG | 6:BM:121:THR:O | 2.29 | 0.51 |
| 3:Bc:69:TRP:HB2 | 3:Bc:159:LEU:HD23 | 1.91 | 0.51 |
| 3:Bk:106:GLU:O | 3:Bk:109:LYS:NZ | 2.43 | 0.51 |
| 2:Br:100:GLU:HB3 | 2:Br:188:ILE:HD11 | 1.92 | 0.51 |
| 4:F:23:SER:OG | 4:F:26:LYS:NZ | 2.44 | 0.51 |
| 4:Z:26:LYS:HA | 4:j:34:ALA:H | 1.75 | 0.51 |
| 1:m:164:ASN:O | 1:m:164:ASN:ND2 | 2.43 | 0.51 |
| 2:1:5:SER:OG | 2:AD:515:ASP:OD1 | 2.28 | 0.51 |
| 2:2:450:ILE:O | 2:2:523:ASN:ND2 | 2.44 | 0.51 |
| 5:A2:182:VAL:HG22 | 5:A2:208:TYR:HD1 | 1.75 | 0.51 |
| 6:A5:336:ASP:HB3 | 6:A5:339:ASP:HB2 | 1.92 | 0.51 |
| 3:AA:76:ASP:OD1 | 3:AA:77:GLU:N | 2.43 | 0.51 |
| 3:AH:41:LEU:H | 3:AH:41:LEU:HD12 | 1.76 | 0.51 |
| 3:AJ:24:GLU:OE1 | 3:AJ:33:THR:OG1 | 2.27 | 0.51 |
| 6:Ad:120:PRO:HD3 | 6:Ad:453:TYR:CZ | 2.46 | 0.51 |
| 6:Aj:83:GLN:OE1 | 11:BP:36:SER:OG | 2.21 | 0.51 |
| 6:Ap:152:ALA:O | 6:BI:264:ARG:NH2 | 2.44 | 0.51 |
| 7:Ar:151:MET:HE1 | 7:At:113:GLY:HA2 | 1.92 | 0.51 |
| 7:At:54:ASN:OD1 | 7:At:188:THR:OG1 | 2.22 | 0.51 |
| 6:Aw:131:TYR:HB3 | 6:Aw:250:MET:HG2 | 1.91 | 0.51 |
| 2:B3:82:ARG:NH2 | 2:B3:227:PRO:O | 2.42 | 0.51 |
| 2:B4:601:ILE:HG23 | 2:B4:629:ILE:HG13 | 1.93 | 0.51 |
| 5:BB:188:ILE:HG22 | 5:BB:202:TYR:HB3 | 1.91 | 0.51 |
| 5:BF:208:TYR:OH | 5:BF:213:GLU:OE2 | 2.24 | 0.51 |
| 11:BV:18:ASP:OD1 | 11:BV:19:GLY:N | 2.36 | 0.51 |
| 3:BX:124:THR:OG1 | 3:Ba:77:GLU:O | 2.24 | 0.51 |
| 3:Bh:40:ALA:O | 3:Bh:69:TRP:NE1 | 2.43 | 0.51 |
| 2:Br:119:LYS:NZ | 2:Br:124:ASP:OD1 | 2.44 | 0.51 |
| 2:Bv:101:TYR:OH | 2:Bv:216:LYS:O | 2.25 | 0.51 |
| 2:By:616:SER:O | 2:By:620:ARG:NE | 2.40 | 0.51 |
| 2:Bz:617:VAL:HG23 | 2:Bz:620:ARG:HE | 1.76 | 0.51 |
| 4:H:44:MET:HE1 | 4:S:44:MET:HG2 | 1.91 | 0.51 |
| 4:W:27:ASN:HD22 | 4:g:35:ASP:HA | 1.75 | 0.51 |
| 1:p:159:TYR:HB3 | 1:p:162:GLY:HA2 | 1.92 | 0.51 |
| 8:r:22:SER:O | 8:r:38:ARG:NH1 | 2.44 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:r:69:GLU:HG2 | 8:r:70:THR:H | 1.75 | 0.51 |
| 2:1:498:GLN:HB3 | 2:1:534:VAL:HG12 | 1.93 | 0.51 |
| 2:5:30:ALA:HB3 | 2:5:359:TRP:CE2 | 2.46 | 0.51 |
| 6:A4:383:VAL:HG21 | 6:A4:425:ILE:HG12 | 1.90 | 0.51 |
| 6:A9:285:ASP:HA | 5:Av:65:TYR:HE2 | 1.74 | 0.51 |
| 3:AH:63:ASP:OD2 | 3:Bj:147:ASN:ND2 | 2.38 | 0.51 |
| 6:Ac:493:ALA:O | 6:Ac:497:GLN:NE2 | 2.35 | 0.51 |
| 6:An:287:ASP:OD2 | 6:An:460:ARG:NH2 | 2.44 | 0.51 |
| 6:Aw:481:ILE:N | 6:Aw:499:GLY:O | 2.38 | 0.51 |
| 4:B:58:LEU:HD22 | 4:R:62:ILE:HD12 | 1.91 | 0.51 |
| 2:B2:378:CYS:SG | 2:B2:454:TYR:OH | 2.55 | 0.51 |
| 2:B7:575:LEU:HB3 | 2:B7:577:ASN:HD22 | 1.76 | 0.51 |
| 5:BA:39:GLY:HA3 | 5:BA:250:ILE:HG12 | 1.93 | 0.51 |
| 7:BC:265:ARG:NH1 | 1:p:49:GLU:OE2 | 2.43 | 0.51 |
| 6:BJ:332:PHE:HB3 | 6:BJ:518:VAL:HG12 | 1.92 | 0.51 |
| 3:Bc:125:LYS:NZ | 3:Bf:83:GLN:OE1 | 2.37 | 0.51 |
| 3:Bg:82:ARG:HH12 | 3:Bg:138:GLY:HA2 | 1.74 | 0.51 |
| 3:Bn:39:THR:HG22 | 3:Bn:71:VAL:HG13 | 1.93 | 0.51 |
| 2:Br:641:ASN:N | 2:Br:641:ASN:OD1 | 2.43 | 0.51 |
| 4:E:62:ILE:HD12 | 4:P:58:LEU:HD22 | 1.92 | 0.51 |
| 1:m:170:THR:HG21 | 8:t:181:LEU:HD22 | 1.93 | 0.51 |
| 1:n:198:GLU:OE1 | 1:n:198:GLU:N | 2.42 | 0.51 |
| 8:s:238:VAL:HG22 | 8:s:239:PRO:HD2 | 1.91 | 0.51 |
| 2:2:152:ALA:O | 2:2:156:GLU:HG2 | 2.10 | 0.51 |
| 2:2:406:LEU:HD11 | 2:2:475:ALA:HB2 | 1.92 | 0.51 |
| 7:A6:54:ASN:HA | 7:Al:162:TRP:CD1 | 2.46 | 0.51 |
| 2:AN:98:ASN:HB2 | 2:AN:188:ILE:HD11 | 1.91 | 0.51 |
| 2:AN:653:GLU:O | 2:AO:17:SER:OG | 2.19 | 0.51 |
| 6:AV:77:THR:OG1 | 11:BN:5:ARG:NH2 | 2.44 | 0.51 |
| 6:AW:351:LYS:NZ | 6:AW:395:TYR:O | 2.43 | 0.51 |
| 6:Ad:380:ARG:CZ | 6:Ah:366:ARG:HD2 | 2.41 | 0.51 |
| 6:Af:257:GLN:NE2 | 6:Af:481:ILE:O | 2.43 | 0.51 |
| 6:Ah:264:ARG:NH1 | 6:Ah:477:TYR:HH | 2.07 | 0.51 |
| 6:Ai:71:ASP:HB2 | 6:BJ:230:THR:HB | 1.91 | 0.51 |
| 6:Am:83:GLN:OE1 | 11:BN:5:ARG:NH1 | 2.43 | 0.51 |
| 5:Av:398:ARG:NH2 | 5:BB:400:GLU:OE2 | 2.43 | 0.51 |
| 2:B3:11:LYS:HG2 | 2:B3:13:THR:HG23 | 1.92 | 0.51 |
| 2:B3:36:GLY:O | 2:B3:82:ARG:NH1 | 2.42 | 0.51 |
| 2:B5:455:LYS:HZ2 | 2:B5:457:GLN:HB2 | 1.75 | 0.51 |
| 2:B6:225:LEU:HD13 | 2:B6:324:PHE:HB2 | 1.93 | 0.51 |
| 7:BC:214:SER:OG | 7:BC:217:GLU:OE1 | 2.27 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BD:94:GLU:OE2 | 5:BD:379:ARG:NE | 2.41 | 0.51 |
| 5:BD:477:ILE:HA | 5:BD:481:ILE:HG23 | 1.92 | 0.51 |
| 7:BE:15:VAL:HG11 | 7:BE:248:LYS:HD2 | 1.92 | 0.51 |
| 5:BF:328:MET:HE3 | 7:BL:308:VAL:HG13 | 1.92 | 0.51 |
| 2:Bq:528:THR:HA | 2:Br:367:SER:HA | 1.93 | 0.51 |
| 2:Br:97:GLY:O | 2:Br:147:THR:OG1 | 2.27 | 0.51 |
| 2:By:46:ASN:OD1 | 2:By:47:GLU:N | 2.43 | 0.51 |
| 2:By:457:GLN:HA | 2:By:503:ILE:HG23 | 1.92 | 0.51 |
| 2:Bz:112:VAL:HG13 | 2:Bz:134:VAL:HG13 | 1.92 | 0.51 |
| 2:Bz:480:ARG:O | 2:Bz:484:VAL:HG12 | 2.10 | 0.51 |
| 4:V:52:LEU:HD21 | 4:a:12:ASP:HB2 | 1.92 | 0.51 |
| 4:Z:58:LEU:HD22 | 4:j:62:ILE:HD12 | 1.93 | 0.51 |
| 8:u:61:SER:OG | 8:u:62:GLN:N | 2.37 | 0.51 |
| 9:v:137:ASP:OD1 | 9:v:138:LEU:N | 2.43 | 0.51 |
| 1:0:41:ILE:HD13 | 1:k:5:ASP:HB2 | 1.93 | 0.51 |
| 2:4:455:LYS:HB2 | 2:4:470:LEU:HD13 | 1.92 | 0.51 |
| 3:8:86:VAL:HG12 | 3:8:137:VAL:HG21 | 1.92 | 0.51 |
| 3:9:132:LEU:HD21 | 3:9:157:LEU:HD13 | 1.92 | 0.51 |
| 7:A6:211:ASP:OD1 | 7:A6:211:ASP:N | 2.43 | 0.51 |
| 3:AA:52:GLY:HA2 | 3:AA:57:LYS:HA | 1.91 | 0.51 |
| 9:AC:43:ARG:NH1 | 9:AC:69:ASP:OD1 | 2.43 | 0.51 |
| 2:AD:202:GLU:O | 2:AD:206:THR:OG1 | 2.16 | 0.51 |
| 3:AE:85:PHE:HB3 | 3:AE:137:VAL:HG21 | 1.92 | 0.51 |
| 2:AL:240:SER:OG | 2:AL:243:ASP:OD1 | 2.29 | 0.51 |
| 2:AO:310:TYR:HE2 | 2:AO:312:ASP:HB2 | 1.76 | 0.51 |
| 6:AX:131:TYR:HA | 6:AX:250:MET:HA | 1.93 | 0.51 |
| 6:AX:496:ILE:HG12 | 6:BK:76:ALA:HB1 | 1.92 | 0.51 |
| 6:AZ:237:GLU:OE1 | 6:AZ:243:THR:OG1 | 2.29 | 0.51 |
| 6:Ad:235:LEU:O | 6:Ad:245:ASN:ND2 | 2.44 | 0.51 |
| 7:Aq:40:ARG:HE | 7:Aq:254:LEU:HD13 | 1.76 | 0.51 |
| 7:Ar:30:THR:HG23 | 7:Ar:33:GLN:HE22 | 1.75 | 0.51 |
| 7:At:112:LEU:HD13 | 7:At:115:ALA:H | 1.75 | 0.51 |
| 5:Av:230:ILE:HG21 | 5:Av:235:VAL:HG23 | 1.93 | 0.51 |
| 6:Aw:207:LYS:O | 6:Aw:211:GLU:HG2 | 2.11 | 0.51 |
| 5:BA:360:GLU:OE1 | 5:BA:363:ARG:NH1 | 2.44 | 0.51 |
| 6:BI:130:VAL:HG12 | 6:BI:142:GLU:HA | 1.93 | 0.51 |
| 3:Bb:8:ARG:HD2 | 3:Be:34:PHE:HE2 | 1.76 | 0.51 |
| 3:Bb:56:ARG:HD3 | 3:Bh:99:ILE:HG12 | 1.92 | 0.51 |
| 3:Be:4:ASP:OD1 | 3:Be:4:ASP:N | 2.40 | 0.51 |
| 3:Bi:40:ALA:H | 3:Bi:69:TRP:HE1 | 1.57 | 0.51 |
| 2:Bs:498:GLN:HA | 2:Bs:534:VAL:HG12 | 1.93 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:I:9:PRO:HD3 | 4:I:57:VAL:HG21 | 1.92 | 0.51 |
| 1:m:118:ILE:HD11 | 1:m:169:ILE:HD11 | 1.93 | 0.51 |
| 9:w:137:ASP:OD1 | 9:w:138:LEU:N | 2.43 | 0.51 |
| 2:2:279:TYR:OH | 2:2:332:GLU:O | 2.29 | 0.51 |
| 2:4:605:ARG:HG2 | 2:4:607:VAL:HG23 | 1.93 | 0.51 |
| 3:7:70:THR:HG22 | 3:7:156:THR:HG22 | 1.92 | 0.51 |
| 5:A1:276:ILE:HD13 | 7:Aq:143:GLN:HB2 | 1.93 | 0.51 |
| 6:A9:71:ASP:OD1 | 6:A9:72:HIS:N | 2.44 | 0.51 |
| 2:AL:205:MET:O | 2:AL:211:GLN:NE2 | 2.39 | 0.51 |
| 2:AL:454:TYR:HB3 | 2:AL:467:TRP:HD1 | 1.76 | 0.51 |
| 2:AO:47:GLU:OE1 | 2:AO:461:TYR:OH | 2.28 | 0.51 |
| 2:AP:110:TYR:HE1 | 2:AP:171:ILE:HG21 | 1.76 | 0.51 |
| 6:AV:241:GLY:HA3 | 11:BV:43:GLY:HA2 | 1.93 | 0.51 |
| 6:AV:350:PHE:HB2 | 6:AV:389:VAL:HG11 | 1.93 | 0.51 |
| 6:AW:350:PHE:HB2 | 6:AW:389:VAL:HG11 | 1.93 | 0.51 |
| 6:AX:142:GLU:OE2 | 6:BK:101:ARG:NE | 2.38 | 0.51 |
| 7:AY:34:ILE:O | 7:AY:38:ILE:HG12 | 2.10 | 0.51 |
| 6:Ak:93:PRO:HB2 | 6:Ao:123:GLN:HB3 | 1.93 | 0.51 |
| 7:Aq:265:ARG:NH1 | 1:l:49:GLU:OE2 | 2.44 | 0.51 |
| 7:Ar:30:THR:OG1 | 7:Ar:33:GLN:OE1 | 2.28 | 0.51 |
| 6:Au:185:THR:HG23 | 6:Au:366:ARG:HH21 | 1.76 | 0.51 |
| 5:Ax:442:ASN:O | 5:Ax:442:ASN:ND2 | 2.43 | 0.51 |
| 4:B:48:THR:HG21 | 4:G:47:PRO:HB2 | 1.91 | 0.51 |
| 2:B3:159:GLU:HG3 | 2:B3:167:TRP:HE1 | 1.76 | 0.51 |
| 5:BB:110:ALA:HB3 | 5:BB:447:GLU:HG3 | 1.92 | 0.51 |
| 5:BB:348:ASP:OD1 | 5:BB:349:THR:N | 2.42 | 0.51 |
| 2:Bs:24:THR:O | 2:Bs:483:ASN:ND2 | 2.35 | 0.51 |
| 2:Bt:209:ASP:O | 2:Bt:213:ASN:ND2 | 2.32 | 0.51 |
| 2:Bu:252:LEU:HG | 2:Bu:263:SER:HB3 | 1.92 | 0.51 |
| 2:Bv:66:MET:HG2 | 2:Bv:468:VAL:HG21 | 1.92 | 0.51 |
| 2:Bz:480:ARG:C | 2:Bz:482:ASP:H | 2.18 | 0.51 |
| 4:K:29:GLU:OE2 | 4:K:46:ARG:NH1 | 2.43 | 0.51 |
| 1:m:127:VAL:O | 1:m:128:ASN:ND2 | 2.30 | 0.51 |
| 1:n:143:ASP:OD1 | 1:p:159:TYR:OH | 2.27 | 0.51 |
| 8:r:85:ASN:ND2 | 8:r:195:ASN:OD1 | 2.43 | 0.51 |
| 5:A0:31:ILE:HG22 | 5:A0:198:ILE:HG22 | 1.93 | 0.51 |
| 2:AD:252:LEU:HG | 2:AD:263:SER:HB2 | 1.93 | 0.51 |
| 3:AJ:58:ILE:HD11 | 3:Bm:6:VAL:HG21 | 1.93 | 0.51 |
| 2:AM:526:THR:OG1 | 2:AM:527:GLY:N | 2.44 | 0.51 |
| 2:AM:642:PHE:HB3 | 2:By:557:PHE:HE1 | 1.76 | 0.51 |
| 2:AN:655:THR:HB | 2:AO:19:VAL:HG21 | 1.93 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AP:33:PHE:HA | 2:AP:61:THR:HG23 | 1.93 | 0.51 |
| 2:AP:228:GLY:HA2 | 2:AP:345:SER:HB2 | 1.92 | 0.51 |
| 10:AU:345:MET:HA | 10:AU:351:VAL:HG11 | 1.93 | 0.51 |
| 6:AZ:171:GLN:NE2 | 6:AZ:195:GLN:OE1 | 2.43 | 0.51 |
| 6:Ac:153:MET:HE2 | 6:Ac:225:ALA:HA | 1.93 | 0.51 |
| 6:Ac:287:ASP:OD1 | 6:Ac:288:ALA:N | 2.43 | 0.51 |
| 6:Ac:346:ALA:HA | 6:Ac:349:SER:HB3 | 1.93 | 0.51 |
| 6:Ah:406:THR:OG1 | 6:BI:372:GLU:OE2 | 2.29 | 0.51 |
| 6:Ai:264:ARG:NH1 | 6:Ai:305:GLU:OE1 | 2.44 | 0.51 |
| 6:An:268:ALA:HB1 | 6:An:290:LEU:HD13 | 1.93 | 0.51 |
| 6:Ao:263:SER:HB3 | 6:Ao:476:ARG:HG2 | 1.92 | 0.51 |
| 7:Aq:22:ALA:HB1 | 7:Aq:23:PRO:HD2 | 1.91 | 0.51 |
| 7:At:307:LEU:HB2 | 5:BA:335:TRP:HB2 | 1.91 | 0.51 |
| 6:Au:76:ALA:HB1 | 6:Ay:496:ILE:HG12 | 1.92 | 0.51 |
| 6:Aw:123:GLN:HG2 | 6:BM:95:VAL:HA | 1.93 | 0.51 |
| 2:B1:148:ALA:O | 2:B1:151:ILE:HG13 | 2.11 | 0.51 |
| 7:BC:238:LYS:HD3 | 7:BC:238:LYS:H | 1.76 | 0.51 |
| 7:BE:34:ILE:O | 7:BE:38:ILE:HG12 | 2.11 | 0.51 |
| 3:Bc:108:LYS:HB3 | 3:Bc:131:GLY:HA2 | 1.92 | 0.51 |
| 3:Bk:124:THR:HB | 3:Bn:78:ALA:HA | 1.93 | 0.51 |
| 2:Bp:617:VAL:HG22 | 2:Bp:622:GLU:HB2 | 1.92 | 0.51 |
| 2:Br:511:GLN:OE1 | 2:Br:514:ARG:NH2 | 2.44 | 0.51 |
| 2:Bt:66:MET:HB3 | 2:Bt:468:VAL:HG11 | 1.93 | 0.51 |
| 2:Bv:446:THR:OG1 | 2:Bv:554:ARG:NH2 | 2.43 | 0.51 |
| 1:n:204:VAL:HA | 8:u:66:ALA:HB2 | 1.91 | 0.51 |
| 2:2:488:TRP:O | 2:2:552:ASN:ND2 | 2.41 | 0.51 |
| 2:4:515:ASP:OD1 | 2:5:5:SER:OG | 2.23 | 0.51 |
| 5:A1:249:ASN:OD1 | 5:A1:250:ILE:N | 2.43 | 0.51 |
| 5:A2:284:VAL:HG22 | 5:BF:334:TYR:HB2 | 1.93 | 0.51 |
| 5:A3:211:ALA:HB2 | 5:A3:225:GLY:HA2 | 1.92 | 0.51 |
| 6:A8:490:GLN:N | 6:A8:490:GLN:OE1 | 2.44 | 0.51 |
| 8:AB:91:ASN:O | 8:AB:110:ASN:ND2 | 2.39 | 0.51 |
| 9:AC:56:LEU:O | 9:w:97:TYR:HB3 | 2.11 | 0.51 |
| 3:AF:75:ASN:HD21 | 3:AF:79:HIS:CG | 2.28 | 0.51 |
| 3:AG:57:LYS:HE2 | 3:Bj:147:ASN:HD21 | 1.74 | 0.51 |
| 2:AO:510:ARG:HA | 2:B5:364:ASP:HB2 | 1.93 | 0.51 |
| 2:AP:91:ASN:OD1 | 2:AP:91:ASN:N | 2.42 | 0.51 |
| 7:Aa:12:LEU:O | 7:Aa:16:ILE:HG12 | 2.11 | 0.51 |
| 6:Ac:130:VAL:HA | 6:Ac:142:GLU:HA | 1.93 | 0.51 |
| 7:BC:175:ASN:HD21 | 7:BE:99:ASP:HB2 | 1.76 | 0.51 |
| 5:BD:432:ILE:HG13 | 5:BD:436:GLU:HB2 | 1.93 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:BP:5:ARG:HH21 | 11:BP:33:PRO:HB3 | 1.75 | 0.51 |
| 11:BU:26:LYS:HD2 | 11:BU:75:LEU:HD23 | 1.93 | 0.51 |
| 3:Bd:63:ASP:OD2 | 3:Bh:147:ASN:ND2 | 2.44 | 0.51 |
| 3:Bj:8:ARG:HD2 | 3:Bm:34:PHE:HE2 | 1.75 | 0.51 |
| 2:Bw:635:ILE:HD13 | 2:Bx:623:PHE:HB2 | 1.93 | 0.51 |
| 2:Bx:432:ALA:HB2 | 2:Bx:440:ASN:HD22 | 1.74 | 0.51 |
| 1:k:86:PHE:CE2 | 1:k:88:ALA:HB2 | 2.46 | 0.51 |
| 1:0:164:ASN:O | 1:0:164:ASN:ND2 | 2.44 | 0.50 |
| 1:0:214:ASN:OD1 | 8:q:55:LYS:NZ | 2.34 | 0.50 |
| 2:3:102:THR:HB | 2:3:183:THR:HB | 1.93 | 0.50 |
| 2:5:240:SER:OG | 2:5:334:PHE:O | 2.28 | 0.50 |
| 5:A0:106:THR:OG1 | 5:A0:107:GLU:N | 2.43 | 0.50 |
| 5:A1:282:ARG:NH2 | 5:BD:328:MET:O | 2.44 | 0.50 |
| 6:A4:109:PHE:HE1 | 6:A4:306:VAL:HG21 | 1.75 | 0.50 |
| 3:AG:90:SER:HA | 3:AG:94:GLY:HA2 | 1.93 | 0.50 |
| 6:AW:100:ARG:NH1 | 6:AW:289:GLU:OE2 | 2.40 | 0.50 |
| 7:Aa:4:TYR:HB3 | 7:As:39:GLN:HG2 | 1.92 | 0.50 |
| 6:Ad:68:ILE:HG22 | 6:Ad:70:GLY:H | 1.75 | 0.50 |
| 6:Ag:265:GLN:HB3 | 6:Ak:247:TRP:CH2 | 2.47 | 0.50 |
| 7:Ar:308:VAL:HB | 5:Ax:311:ARG:HH22 | 1.76 | 0.50 |
| 7:At:120:GLY:O | 7:At:122:GLY:N | 2.44 | 0.50 |
| 2:B3:254:ILE:HG13 | 2:B3:337:ILE:HB | 1.92 | 0.50 |
| 2:B4:521:ALA:HB1 | 2:B4:541:ALA:HA | 1.93 | 0.50 |
| 2:B6:135:ASP:OD1 | 2:B6:136:ALA:N | 2.45 | 0.50 |
| 5:BA:293:PRO:O | 5:BA:295:ARG:N | 2.43 | 0.50 |
| 7:BC:12:LEU:HD12 | 7:BC:242:TYR:HD2 | 1.76 | 0.50 |
| 6:BM:123:GLN:HG2 | 6:BM:258:VAL:HG12 | 1.93 | 0.50 |
| 3:Bk:23:VAL:HG11 | 3:Bk:39:THR:HG21 | 1.93 | 0.50 |
| 2:Bp:427:VAL:HG22 | 2:Bp:520:GLU:HG3 | 1.92 | 0.50 |
| 2:Bq:394:VAL:HG11 | 2:Bq:443:ILE:HD12 | 1.92 | 0.50 |
| 2:Bw:26:THR:HA | 2:Bw:77:ASP:O | 2.11 | 0.50 |
| 2:Bz:239:VAL:HG22 | 2:Bz:280:ALA:HB3 | 1.92 | 0.50 |
| 1:l:176:TYR:HA | 8:s:71:ILE:HA | 1.93 | 0.50 |
| 1:n:6:LYS:NZ | 1:n:23:GLU:OE2 | 2.43 | 0.50 |
| 1:n:173:LYS:HB3 | 8:u:69:GLU:HB2 | 1.93 | 0.50 |
| 8:q:243:ASP:OD1 | 8:q:243:ASP:N | 2.42 | 0.50 |
| 8:s:222:ASP:OD1 | 8:s:222:ASP:N | 2.43 | 0.50 |
| 2:3:505:LEU:HD21 | 2:3:525:VAL:HG12 | 1.92 | 0.50 |
| 2:4:20:VAL:HG21 | 2:AK:611:THR:HG21 | 1.92 | 0.50 |
| 3:6:76:ASP:OD1 | 3:6:80:ASP:N | 2.35 | 0.50 |
| 5:A3:190:THR:OG1 | 5:A3:191:GLU:N | 2.44 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:A6:96:THR:O | 7:A6:152:GLN:NE2 | 2.45 | 0.50 |
| 6:A7:476:ARG:HH21 | 6:A8:230:THR:HG21 | 1.77 | 0.50 |
| 6:A9:350:PHE:HB2 | 6:A9:389:VAL:HG11 | 1.94 | 0.50 |
| 2:AK:254:ILE:HD11 | 2:AK:261:ARG:HB2 | 1.93 | 0.50 |
| 2:AN:159:GLU:OE2 | 2:AN:166:ASN:ND2 | 2.44 | 0.50 |
| 2:AN:217:TYR:HB2 | 2:AN:219:ILE:HD12 | 1.93 | 0.50 |
| 2:AN:362:PHE:O | 2:AN:400:ARG:NE | 2.44 | 0.50 |
| 2:AP:272:GLY:O | 2:AP:274:GLN:NE2 | 2.44 | 0.50 |
| 10:AS:310:TRP:CD1 | 10:AS:311:VAL:HG23 | 2.45 | 0.50 |
| 6:AX:173:THR:HB | 6:AX:176:ASP:HB2 | 1.94 | 0.50 |
| 6:Af:263:SER:HB3 | 6:Af:476:ARG:HG2 | 1.92 | 0.50 |
| 7:Al:55:LYS:HE2 | 7:BE:162:TRP:HD1 | 1.76 | 0.50 |
| 7:Al:163:PHE:HA | 7:Al:170:LEU:HA | 1.92 | 0.50 |
| 7:Al:210:GLN:HA | 7:Al:227:VAL:HG13 | 1.94 | 0.50 |
| 6:Am:350:PHE:HB2 | 6:Am:389:VAL:HG11 | 1.93 | 0.50 |
| 6:An:90:GLN:NE2 | 6:An:277:ASP:OD2 | 2.45 | 0.50 |
| 6:Ao:107:ILE:HG12 | 6:Ao:412:VAL:HG21 | 1.93 | 0.50 |
| 6:Au:106:LEU:HD21 | 6:Au:300:LEU:HD23 | 1.93 | 0.50 |
| 5:BH:66:GLU:H | 5:BH:67:PRO:HD2 | 1.76 | 0.50 |
| 6:BJ:379:SER:OG | 6:BJ:432:ASP:OD1 | 2.26 | 0.50 |
| 3:BX:63:ASP:OD1 | 3:BX:64:ARG:N | 2.42 | 0.50 |
| 3:BZ:23:VAL:HG11 | 3:BZ:39:THR:HG21 | 1.93 | 0.50 |
| 3:Bb:3:VAL:HG12 | 3:Bg:97:ASN:HA | 1.92 | 0.50 |
| 3:Bc:17:ARG:HG3 | 3:Bc:20:LEU:HD12 | 1.92 | 0.50 |
| 3:Bl:21:PHE:HZ | 3:Bl:38:ALA:HA | 1.76 | 0.50 |
| 2:Bq:84:VAL:HG13 | 2:Bq:346:SER:HB3 | 1.93 | 0.50 |
| 2:Bq:308:ASN:ND2 | 2:Bq:313:ASP:OD2 | 2.43 | 0.50 |
| 2:Bw:206:THR:HA | 2:Bw:211:GLN:HE21 | 1.76 | 0.50 |
| 8:s:143:PRO:O | 8:s:166:VAL:HA | 2.11 | 0.50 |
| 8:u:81:ASP:OD1 | 8:u:82:PHE:N | 2.43 | 0.50 |
| 1:0:62:PRO:HG3 | 1:0:84:TRP:HZ3 | 1.74 | 0.50 |
| 2:3:470:LEU:HD11 | 2:3:499:ILE:HG21 | 1.93 | 0.50 |
| 2:4:237:GLU:OE1 | 2:4:284:ARG:NH1 | 2.44 | 0.50 |
| 5:A0:303:HIS:NE2 | 7:BC:161:PHE:O | 2.44 | 0.50 |
| 5:A3:381:PRO:HB2 | 5:BF:377:LEU:HD23 | 1.93 | 0.50 |
| 3:AJ:63:ASP:HB3 | 3:BX:147:ASN:HB3 | 1.93 | 0.50 |
| 2:AL:137:ASP:OD1 | 2:AL:137:ASP:N | 2.37 | 0.50 |
| 2:AM:298:LYS:NZ | 2:AM:299:ARG:O | 2.41 | 0.50 |
| 2:AN:550:ARG:HB3 | 2:AN:553:VAL:HG12 | 1.91 | 0.50 |
| 2:AO:30:ALA:HB3 | 2:AO:359:TRP:CE2 | 2.47 | 0.50 |
| 10:AU:310:TRP:CD1 | 10:AU:311:VAL:HG23 | 2.46 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AV:237:GLU:HB3 | 6:BM:465:LYS:HB3 | 1.92 | 0.50 |
| 6:AZ:93:PRO:HA | 6:Ad:121:THR:O | 2.12 | 0.50 |
| 6:Af:211:GLU:HA | 6:Af:214:LYS:HD2 | 1.92 | 0.50 |
| 6:Ai:163:PHE:HB2 | 6:Ai:179:THR:HG23 | 1.92 | 0.50 |
| 7:Al:202:VAL:HG13 | 4:f:31:ILE:HG22 | 1.92 | 0.50 |
| 6:An:395:TYR:HD1 | 6:An:396:ALA:H | 1.59 | 0.50 |
| 6:Ao:268:ALA:HB1 | 6:Ao:290:LEU:HD13 | 1.92 | 0.50 |
| 6:Ao:376:ILE:HG23 | 6:Ao:423:VAL:HG22 | 1.93 | 0.50 |
| 7:Aq:170:LEU:HD11 | 7:Aq:172:VAL:HG23 | 1.93 | 0.50 |
| 5:Av:382:GLN:NE2 | 5:Ax:367:GLN:OE1 | 2.45 | 0.50 |
| 6:Ay:264:ARG:HH21 | 6:Ay:301:GLU:HB3 | 1.76 | 0.50 |
| 2:B1:135:ASP:OD1 | 2:B1:136:ALA:N | 2.44 | 0.50 |
| 2:B1:578:ALA:HA | 2:B1:581:ARG:HE | 1.75 | 0.50 |
| 2:B3:239:VAL:HG13 | 2:B3:280:ALA:HB3 | 1.92 | 0.50 |
| 2:B4:494:TYR:O | 2:B4:498:GLN:NE2 | 2.43 | 0.50 |
| 2:B4:521:ALA:HA | 2:B4:539:LYS:HG2 | 1.93 | 0.50 |
| 2:B5:151:ILE:O | 2:B5:155:LYS:HG3 | 2.11 | 0.50 |
| 5:BA:228:ILE:HG12 | 5:BH:196:THR:HG21 | 1.93 | 0.50 |
| 7:BE:191:TYR:HD1 | 7:BE:193:ASP:H | 1.58 | 0.50 |
| 5:BH:72:THR:OG1 | 5:BH:155:ARG:NH2 | 2.32 | 0.50 |
| 5:BH:209:ASP:HA | 5:BH:227:LYS:HA | 1.93 | 0.50 |
| 6:BI:290:LEU:HD21 | 6:BM:67:GLU:HG3 | 1.92 | 0.50 |
| 6:BI:449:TYR:OH | 6:BI:482:ASN:OD1 | 2.28 | 0.50 |
| 6:BK:110:ASP:OD1 | 6:BK:110:ASP:N | 2.36 | 0.50 |
| 6:BK:365:ALA:HB2 | 6:BK:372:GLU:HA | 1.93 | 0.50 |
| 3:BX:22:GLN:OE1 | 3:BX:114:ARG:NH2 | 2.38 | 0.50 |
| 3:BY:3:VAL:HG12 | 3:Bd:97:ASN:HA | 1.93 | 0.50 |
| 3:Bc:42:PRO:HD3 | 3:Bc:69:TRP:CD1 | 2.47 | 0.50 |
| 3:Bl:37:LYS:HB2 | 3:Bl:74:MET:HG3 | 1.94 | 0.50 |
| 2:Bq:510:ARG:HH12 | 2:Bq:513:GLN:HE22 | 1.60 | 0.50 |
| 2:Br:556:LEU:HD11 | 2:Br:601:ILE:HG23 | 1.94 | 0.50 |
| 2:Bt:585:ARG:NH2 | 2:Bt:608:CYS:O | 2.44 | 0.50 |
| 2:Bu:57:PRO:HA | 2:Bu:61:THR:HB | 1.93 | 0.50 |
| 2:Bv:453:ASN:HB2 | 2:Bv:506:ALA:HB3 | 1.93 | 0.50 |
| 1:l:86:PHE:CE2 | 1:l:88:ALA:HB2 | 2.46 | 0.50 |
| 1:p:86:PHE:CE2 | 1:p:88:ALA:HB2 | 2.47 | 0.50 |
| 8:t:215:ASP:OD1 | 8:t:215:ASP:N | 2.44 | 0.50 |
| 1:0:177:SER:HB2 | 1:0:207:LEU:HB3 | 1.94 | 0.50 |
| 2:3:113:GLY:HA3 | 2:3:131:ILE:HB | 1.92 | 0.50 |
| 2:3:241:LYS:O | 2:3:244:TYR:HB2 | 2.10 | 0.50 |
| 2:3:406:LEU:HD11 | 2:3:475:ALA:HB2 | 1.93 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:5:44:VAL:HG11 | 2:5:50:LEU:HB2 | 1.92 | 0.50 |
| 3:7:83:GLN:HA | 3:7:86:VAL:HG22 | 1.93 | 0.50 |
| 7:A6:12:LEU:O | 7:A6:16:ILE:HG12 | 2.12 | 0.50 |
| 3:AA:147:ASN:OD1 | 9:x:65:THR:OG1 | 2.28 | 0.50 |
| 3:AG:31:ASN:OD1 | 3:AG:31:ASN:N | 2.40 | 0.50 |
| 6:AW:345:TRP:HD1 | 6:AW:346:ALA:N | 2.09 | 0.50 |
| 6:Ae:71:ASP:HB3 | 6:Am:231:SER:HB3 | 1.93 | 0.50 |
| 6:Ai:304:ARG:NH2 | 6:Ai:308:ASP:OD1 | 2.45 | 0.50 |
| 6:Aj:136:VAL:HG22 | 6:Aj:253:ARG:HH11 | 1.77 | 0.50 |
| 7:Al:191:TYR:HA | 7:Al:239:GLN:HE21 | 1.76 | 0.50 |
| 6:An:288:ALA:HB2 | 7:As:126:ASN:HB3 | 1.94 | 0.50 |
| 7:Aq:267:GLN:HG3 | 7:Aq:279:GLY:H | 1.76 | 0.50 |
| 7:Aq:299:LEU:HD12 | 5:BD:291:ASN:ND2 | 2.27 | 0.50 |
| 7:At:108:THR:OG1 | 7:At:109:ASP:N | 2.40 | 0.50 |
| 7:At:163:PHE:HB2 | 7:At:170:LEU:HD13 | 1.93 | 0.50 |
| 2:B4:538:ASP:O | 2:B4:550:ARG:NE | 2.45 | 0.50 |
| 2:B5:39:PHE:HE2 | 2:B5:86:ARG:HD2 | 1.76 | 0.50 |
| 5:BB:94:GLU:HG3 | 5:BB:379:ARG:HH21 | 1.76 | 0.50 |
| 5:BD:208:TYR:HB3 | 5:BD:228:ILE:HG23 | 1.94 | 0.50 |
| 5:BG:399:ASP:OD1 | 5:BG:399:ASP:N | 2.44 | 0.50 |
| 6:BI:351:LYS:NZ | 6:BI:390:ASP:O | 2.44 | 0.50 |
| 11:BS:10:ILE:HD13 | 11:BS:41:ILE:HG21 | 1.91 | 0.50 |
| 3:BX:51:VAL:HG12 | 3:Bb:150:ILE:HD12 | 1.93 | 0.50 |
| 3:Bd:58:ILE:HD12 | 3:Be:6:VAL:HG21 | 1.92 | 0.50 |
| 3:Be:114:ARG:NH2 | 3:Be:116:TYR:OH | 2.41 | 0.50 |
| 3:Bf:119:ASP:OD1 | 3:Bh:101:GLY:N | 2.44 | 0.50 |
| 3:Bj:58:ILE:HD12 | 3:Bk:6:VAL:HG21 | 1.93 | 0.50 |
| 3:Bk:72:THR:HG22 | 3:Bk:154:GLU:HG3 | 1.92 | 0.50 |
| 2:Bq:170:GLU:OE1 | 2:Bq:171:ILE:N | 2.43 | 0.50 |
| 2:Bq:490:SER:O | 2:Bq:496:ARG:NH1 | 2.44 | 0.50 |
| 2:Bs:114:ASP:OD1 | 2:Bs:114:ASP:N | 2.43 | 0.50 |
| 2:Bv:525:VAL:HG22 | 2:Bv:535:LEU:HD23 | 1.94 | 0.50 |
| 2:By:457:GLN:HG2 | 2:By:458:TYR:H | 1.76 | 0.50 |
| 2:Bz:601:ILE:HD13 | 2:Bz:629:ILE:HB | 1.93 | 0.50 |
| 1:n:101:SER:HA | 1:n:110:VAL:HA | 1.93 | 0.50 |
| 8:s:142:GLN:O | 8:s:144:HIS:N | 2.44 | 0.50 |
| 9:x:13:ASN:H | 9:x:16:ASN:ND2 | 2.09 | 0.50 |
| 2:5:559:MET:SD | 2:5:563:ASN:ND2 | 2.84 | 0.50 |
| 6:A4:258:VAL:HG21 | 6:A9:76:ALA:HA | 1.94 | 0.50 |
| 6:A7:373:GLY:HA2 | 6:A7:438:TYR:HB2 | 1.92 | 0.50 |
| 6:A9:279:ARG:CZ | 5:Av:62:PHE:HA | 2.42 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:AB:108:GLN:HE21 | 8:AB:202:VAL:HG12 | 1.76 | 0.50 |
| 8:AB:163:ILE:HD13 | 8:AB:163:ILE:H | 1.75 | 0.50 |
| 2:AM:417:ILE:HD13 | 2:AM:417:ILE:H | 1.75 | 0.50 |
| 7:AY:24:ILE:O | 7:AY:25:ILE:HG12 | 2.11 | 0.50 |
| 6:Ae:266:LEU:HB3 | 6:Ae:294:LEU:HD22 | 1.94 | 0.50 |
| 6:Ah:145:HIS:CE1 | 6:Ah:147:MET:HB2 | 2.47 | 0.50 |
| 6:Aj:350:PHE:HB2 | 6:Aj:389:VAL:HG11 | 1.93 | 0.50 |
| 5:Ax:497:GLU:O | 5:Ax:501:GLU:HG2 | 2.12 | 0.50 |
| 2:B3:90:LYS:NZ | 2:B3:190:ASP:OD1 | 2.44 | 0.50 |
| 2:B3:202:GLU:OE1 | 2:B3:203:ALA:N | 2.45 | 0.50 |
| 2:B4:32:LYS:HG3 | 2:B4:350:VAL:HG21 | 1.92 | 0.50 |
| 2:B4:542:THR:OG1 | 2:B4:544:VAL:O | 2.29 | 0.50 |
| 7:BC:22:ALA:HB1 | 7:BC:23:PRO:HD2 | 1.93 | 0.50 |
| 6:BI:115:GLN:NE2 | 6:BI:444:MET:SD | 2.85 | 0.50 |
| 6:BJ:118:ASN:OD1 | 6:BJ:118:ASN:N | 2.35 | 0.50 |
| 6:BK:85:SER:HB2 | 11:BU:35:TYR:HE2 | 1.77 | 0.50 |
| 3:BZ:120:ALA:HB1 | 3:Bo:1:MET:HE2 | 1.92 | 0.50 |
| 2:Bp:44:VAL:HG11 | 2:Bp:50:LEU:HB2 | 1.92 | 0.50 |
| 2:Bp:264:THR:HB | 2:Bp:267:ALA:HB3 | 1.92 | 0.50 |
| 2:Bt:633:ARG:NH1 | 2:Bu:619:ASP:O | 2.45 | 0.50 |
| 2:By:163:LEU:HD12 | 2:By:187:ILE:H | 1.77 | 0.50 |
| 2:Bz:473:ASP:HB3 | 2:Bz:499:ILE:HD12 | 1.94 | 0.50 |
| 4:J:47:PRO:HB2 | 4:L:48:THR:HG21 | 1.93 | 0.50 |
| 3:o:86:VAL:HG12 | 3:o:137:VAL:HG21 | 1.93 | 0.50 |
| 1:p:5:ASP:OD2 | 1:p:8:LEU:N | 2.45 | 0.50 |
| 8:q:81:ASP:OD1 | 8:q:82:PHE:N | 2.45 | 0.50 |
| 9:y:137:ASP:OD1 | 9:y:138:LEU:N | 2.45 | 0.50 |
| 2:1:645:THR:OG1 | 2:AO:629:ILE:O | 2.29 | 0.50 |
| 2:2:545:PRO:HG3 | 2:3:271:TYR:HB2 | 1.94 | 0.50 |
| 2:4:538:ASP:OD1 | 2:4:538:ASP:N | 2.45 | 0.50 |
| 2:4:645:THR:HG21 | 2:4:651:PHE:HB3 | 1.92 | 0.50 |
| 5:A2:111:LEU:HD11 | 5:A2:444:ILE:HD11 | 1.93 | 0.50 |
| 5:A3:132:ASP:O | 5:A3:136:HIS:ND1 | 2.45 | 0.50 |
| 6:A4:398:GLN:HE22 | 6:A5:355:PHE:HB2 | 1.76 | 0.50 |
| 6:A7:387:ALA:HB2 | 6:A7:404:PHE:HB2 | 1.93 | 0.50 |
| 3:AA:114:ARG:HH21 | 3:AA:116:TYR:HH | 1.54 | 0.50 |
| 2:AD:44:VAL:HG11 | 2:AD:50:LEU:HB2 | 1.93 | 0.50 |
| 10:AU:348:TYR:HB2 | 10:AU:351:VAL:HG12 | 1.93 | 0.50 |
| 6:AW:494:SER:C | 6:AW:496:ILE:H | 2.20 | 0.50 |
| 6:Ae:154:PHE:O | 6:Ae:248:ASN:ND2 | 2.39 | 0.50 |
| 6:Aj:261:ALA:HA | 6:Aj:478:GLY:HA3 | 1.93 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Al:245:ARG:HB2 | 7:BE:43:GLU:HG2 | 1.94 | 0.50 |
| 7:Aq:94:SER:HB2 | 7:Aq:96:THR:HG23 | 1.94 | 0.50 |
| 7:At:150:MET:HE3 | 5:BA:329:SER:HB2 | 1.93 | 0.50 |
| 2:B1:99:ILE:HD12 | 2:B1:150:ILE:HD13 | 1.92 | 0.50 |
| 2:B1:401:GLN:NE2 | 2:B3:10:LEU:O | 2.37 | 0.50 |
| 2:B2:417:ILE:H | 2:B2:417:ILE:HD13 | 1.76 | 0.50 |
| 2:B2:453:ASN:HD21 | 2:B2:505:LEU:HG | 1.75 | 0.50 |
| 7:BC:18:ARG:HA | 7:BC:22:ALA:HA | 1.93 | 0.50 |
| 6:BI:324:THR:HG22 | 6:BI:325:PRO:HD2 | 1.93 | 0.50 |
| 6:BK:273:GLU:OE1 | 6:BK:273:GLU:N | 2.44 | 0.50 |
| 11:BN:26:LYS:NZ | 11:BN:74:ASP:O | 2.44 | 0.50 |
| 11:BW:9:ASN:HB3 | 11:BW:56:TYR:HE2 | 1.75 | 0.50 |
| 2:Bv:527:GLY:HA2 | 2:Bv:533:TYR:HD1 | 1.76 | 0.50 |
| 4:D:25:ILE:H | 4:T:45:ASN:HD21 | 1.60 | 0.50 |
| 4:O:9:PRO:O | 4:O:20:SER:N | 2.44 | 0.50 |
| 4:X:52:LEU:HD21 | 4:c:12:ASP:HB2 | 1.94 | 0.50 |
| 1:n:148:GLU:HB2 | 1:n:174:PHE:HD1 | 1.77 | 0.50 |
| 3:o:147:ASN:OD1 | 9:y:65:THR:OG1 | 2.27 | 0.50 |
| 1:p:201:LEU:HB3 | 1:p:205:ARG:HH21 | 1.77 | 0.50 |
| 8:r:248:ASP:OD1 | 8:r:248:ASP:N | 2.42 | 0.50 |
| 1:0:147:PHE:HB3 | 1:0:171:ALA:HB1 | 1.94 | 0.50 |
| 2:3:163:LEU:HD22 | 2:3:167:TRP:CE2 | 2.47 | 0.50 |
| 2:4:406:LEU:HD11 | 2:4:475:ALA:HB2 | 1.94 | 0.50 |
| 2:4:586:THR:HG21 | 9:y:129:ASN:HD22 | 1.77 | 0.50 |
| 5:A2:256:ARG:NH1 | 5:BF:89:ASP:OD2 | 2.45 | 0.50 |
| 6:A4:365:ALA:HB2 | 6:A4:372:GLU:HA | 1.92 | 0.50 |
| 6:A5:287:ASP:HB2 | 6:A5:471:MET:HE1 | 1.93 | 0.50 |
| 2:AN:43:GLN:NE2 | 2:AN:77:ASP:OD2 | 2.45 | 0.50 |
| 2:AP:220:PRO:HG2 | 2:AP:338:LEU:HD11 | 1.94 | 0.50 |
| 10:AQ:309:TRP:HB3 | 10:AQ:356:SER:HB3 | 1.92 | 0.50 |
| 6:AW:345:TRP:HD1 | 6:AW:347:GLY:H | 1.59 | 0.50 |
| 6:AX:264:ARG:NH2 | 6:Az:152:ALA:O | 2.44 | 0.50 |
| 7:AY:60:PHE:HB2 | 7:AY:182:ILE:HG13 | 1.94 | 0.50 |
| 7:AY:230:VAL:HB | 7:AY:233:GLN:HG2 | 1.93 | 0.50 |
| 7:Aa:199:GLY:O | 7:Aa:204:TYR:OH | 2.29 | 0.50 |
| 6:Ac:266:LEU:HB3 | 6:Ac:294:LEU:HD22 | 1.92 | 0.50 |
| 5:Av:487:MET:HG3 | 5:Ax:480:TYR:HD1 | 1.76 | 0.50 |
| 2:B1:564:ILE:HD11 | 2:Bz:642:PHE:CZ | 2.47 | 0.50 |
| 2:B1:614:THR:O | 2:B1:616:SER:N | 2.39 | 0.50 |
| 2:B5:22:ASN:OD1 | 2:B5:22:ASN:N | 2.45 | 0.50 |
| 2:B7:116:ILE:HD11 | 2:B7:131:ILE:HG12 | 1.92 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B7:264:THR:OG1 | 2:B7:284:ARG:NH2 | 2.44 | 0.50 |
| 5:BH:156:ILE:HG22 | 5:BH:238:ALA:HB3 | 1.94 | 0.50 |
| 6:BI:82:GLY:O | 6:BI:89:THR:OG1 | 2.22 | 0.50 |
| 7:BL:131:PRO:O | 7:BL:133:ALA:N | 2.45 | 0.50 |
| 7:BL:266:HIS:O | 1:m:54:ARG:NH2 | 2.39 | 0.50 |
| 11:BP:16:LYS:HD3 | 11:BP:22:LYS:HG2 | 1.93 | 0.50 |
| 3:Ba:49:ILE:HG12 | 3:Ba:60:VAL:HG12 | 1.94 | 0.50 |
| 3:Bj:43:ALA:HA | 3:Bm:138:GLY:HA3 | 1.93 | 0.50 |
| 2:Bt:455:LYS:HD2 | 2:Bt:457:GLN:HB2 | 1.93 | 0.50 |
| 1:p:183:PRO:HD2 | 1:p:205:ARG:HG3 | 1.92 | 0.50 |
| 9:z:43:ARG:NH1 | 9:z:69:ASP:OD1 | 2.38 | 0.50 |
| 2:2:304:ILE:HG13 | 2:2:305:TYR:H | 1.76 | 0.50 |
| 2:4:304:ILE:HG13 | 2:4:305:TYR:H | 1.76 | 0.50 |
| 2:5:108:SER:HB3 | 2:5:178:LEU:HD11 | 1.93 | 0.50 |
| 3:7:101:GLY:HA3 | 3:AI:119:ASP:HA | 1.93 | 0.50 |
| 5:A3:45:VAL:HG12 | 5:A3:46:SER:H | 1.76 | 0.50 |
| 5:A3:182:VAL:HG22 | 5:A3:208:TYR:HD1 | 1.77 | 0.50 |
| 6:A8:292:GLY:HA2 | 5:BA:67:PRO:HD3 | 1.92 | 0.50 |
| 6:A8:459:LEU:HB3 | 6:Au:467:PHE:CD2 | 2.46 | 0.50 |
| 2:AM:550:ARG:NH1 | 2:AM:636:ASN:OD1 | 2.45 | 0.50 |
| 2:AN:453:ASN:HB3 | 2:AN:507:ILE:HG12 | 1.94 | 0.50 |
| 2:AN:455:LYS:NZ | 2:AN:457:GLN:OE1 | 2.41 | 0.50 |
| 2:AO:131:ILE:HG12 | 2:AO:143:ILE:HG22 | 1.94 | 0.50 |
| 2:AO:214:LEU:HB2 | 2:AO:329:ASN:HD22 | 1.77 | 0.50 |
| 6:AV:278:LEU:HD23 | 6:AV:282:HIS:HB2 | 1.94 | 0.50 |
| 7:AY:151:MET:HG3 | 7:Aq:138:LEU:HD11 | 1.94 | 0.50 |
| 7:Al:161:PHE:HA | 7:Al:171:LYS:O | 2.12 | 0.50 |
| 7:Ar:265:ARG:HG3 | 7:At:25:ILE:HD12 | 1.93 | 0.50 |
| 7:As:30:THR:OG1 | 7:As:33:GLN:OE1 | 2.19 | 0.50 |
| 7:As:80:ASN:N | 7:As:80:ASN:OD1 | 2.44 | 0.50 |
| 7:At:34:ILE:O | 7:At:38:ILE:HG12 | 2.12 | 0.50 |
| 6:Au:101:ARG:HD3 | 6:Ay:146:PRO:HD3 | 1.94 | 0.50 |
| 2:B1:302:LYS:O | 2:B1:307:SER:N | 2.41 | 0.50 |
| 2:B4:411:ARG:HG2 | 2:B4:415:VAL:HB | 1.94 | 0.50 |
| 2:B5:211:GLN:OE1 | 2:B5:329:ASN:ND2 | 2.40 | 0.50 |
| 5:BA:495:ASP:OD1 | 5:BA:495:ASP:N | 2.44 | 0.50 |
| 5:BG:99:ALA:O | 5:BG:411:GLN:NE2 | 2.45 | 0.50 |
| 11:BP:9:ASN:HB3 | 11:BP:56:TYR:HE2 | 1.76 | 0.50 |
| 3:BY:17:ARG:HG3 | 3:BY:20:LEU:HD12 | 1.94 | 0.50 |
| 3:Bg:5:ASP:OD2 | 3:Bg:8:ARG:NH2 | 2.45 | 0.50 |
| 3:Bj:16:ALA:HB3 | 3:Bm:75:ASN:HB3 | 1.94 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bp:601:ILE:HG23 | 2:Bp:630:GLN:H | 1.76 | 0.50 |
| 2:Br:653:GLU:O | 2:Bu:17:SER:OG | 2.26 | 0.50 |
| 2:Bv:134:VAL:HG12 | 2:Bv:140:ILE:HA | 1.94 | 0.50 |
| 2:Bw:379:ALA:HB2 | 2:Bw:454:TYR:HE2 | 1.77 | 0.50 |
| 2:By:638:ILE:HG23 | 2:Bz:623:PHE:HD2 | 1.77 | 0.50 |
| 2:Bz:41:ILE:HD11 | 2:Bz:361:PHE:HB3 | 1.94 | 0.50 |
| 4:C:9:PRO:HD3 | 4:C:57:VAL:HG21 | 1.94 | 0.50 |
| 4:C:44:MET:HE2 | 4:H:25:ILE:HD13 | 1.93 | 0.50 |
| 1:k:60:TYR:OH | 1:k:136:ASP:OD2 | 2.28 | 0.50 |
| 8:r:102:ALA:HB1 | 8:r:241:ASP:HB3 | 1.94 | 0.50 |
| 8:s:6:TYR:CD1 | 8:t:132:GLN:HG2 | 2.47 | 0.50 |
| 8:s:134:VAL:HG21 | 8:s:188:TRP:CE3 | 2.47 | 0.50 |
| 8:s:238:VAL:HG13 | 8:s:239:PRO:HD2 | 1.94 | 0.50 |
| 9:v:78:ASP:OD2 | 9:v:82:LYS:NZ | 2.41 | 0.50 |
| 9:w:168:LYS:HB3 | 9:w:173:ILE:HD11 | 1.94 | 0.50 |
| 2:2:310:TYR:O | 2:2:314:PHE:CB | 2.60 | 0.50 |
| 2:3:157:VAL:HG23 | 2:3:159:GLU:H | 1.76 | 0.50 |
| 2:5:582:SER:OG | 9:z:167:GLU:OE1 | 2.29 | 0.50 |
| 5:A0:171:ILE:HD11 | 5:A0:424:THR:HG22 | 1.94 | 0.50 |
| 5:A2:217:CYS:HA | 6:BM:442:ASN:HA | 1.94 | 0.50 |
| 6:A5:340:ILE:HG13 | 6:A5:343:ALA:H | 1.77 | 0.50 |
| 6:A7:72:HIS:CE1 | 6:A8:121:THR:HG21 | 2.46 | 0.50 |
| 2:AK:222:VAL:HG21 | 2:AK:238:ILE:HD11 | 1.94 | 0.50 |
| 2:AK:394:VAL:HG11 | 2:AK:443:ILE:HD12 | 1.93 | 0.50 |
| 2:AK:505:LEU:HD21 | 2:AK:525:VAL:HG12 | 1.93 | 0.50 |
| 2:AL:457:GLN:HA | 2:AL:503:ILE:HG23 | 1.94 | 0.50 |
| 2:AM:455:LYS:HD3 | 2:AM:457:GLN:HB2 | 1.94 | 0.50 |
| 10:AU:332:SER:HB2 | 10:AU:335:TYR:HB2 | 1.94 | 0.50 |
| 6:Ac:176:ASP:OD1 | 6:Ac:177:ILE:N | 2.45 | 0.50 |
| 6:Ag:450:TYR:HA | 6:Ag:479:ILE:HG22 | 1.92 | 0.50 |
| 7:Al:127:ARG:NH1 | 6:Ap:284:MET:SD | 2.85 | 0.50 |
| 2:B5:31:GLY:O | 2:B5:82:ARG:HA | 2.12 | 0.50 |
| 2:B6:159:GLU:HB3 | 2:B6:163:LEU:HA | 1.92 | 0.50 |
| 6:BJ:494:SER:HA | 11:BR:37:ASP:CG | 2.37 | 0.50 |
| 3:BY:24:GLU:OE1 | 3:BY:33:THR:OG1 | 2.27 | 0.50 |
| 3:Bb:31:ASN:OD1 | 3:Bb:35:GLN:NE2 | 2.44 | 0.50 |
| 3:Bc:114:ARG:HG2 | 3:Bc:126:GLU:HG3 | 1.94 | 0.50 |
| 3:Bh:76:ASP:OD1 | 3:Bh:80:ASP:N | 2.42 | 0.50 |
| 2:Bq:239:VAL:HA | 2:Bq:335:SER:HA | 1.94 | 0.50 |
| 2:Bq:561:LYS:HG2 | 2:Bs:10:LEU:HD22 | 1.94 | 0.50 |
| 2:Bt:20:VAL:HG21 | 2:Bt:46:ASN:HD21 | 1.77 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bt:107:GLY:HA3 | 2:Bt:110:TYR:HE1 | 1.77 | 0.50 |
| 2:Bv:379:ALA:HB2 | 2:Bv:454:TYR:HE2 | 1.76 | 0.50 |
| 2:By:222:VAL:HG21 | 2:By:238:ILE:HD11 | 1.93 | 0.50 |
| 8:q:91:ASN:OD1 | 8:q:92:ILE:N | 2.45 | 0.50 |
| 9:y:118:ASP:O | 9:y:120:SER:N | 2.45 | 0.50 |
| 2:1:295:LEU:HA | 2:1:309:ILE:HB | 1.95 | 0.49 |
| 3:8:75:ASN:HB3 | 3:8:151:GLN:HG3 | 1.94 | 0.49 |
| 8:AB:97:LEU:HB2 | 9:z:5:LEU:HD23 | 1.94 | 0.49 |
| 2:AM:244:TYR:HD1 | 2:AM:265:ALA:HB1 | 1.77 | 0.49 |
| 2:AM:510:ARG:HG2 | 2:AM:511:GLN:H | 1.77 | 0.49 |
| 6:An:521:ILE:HA | 6:BK:341:ARG:HH22 | 1.77 | 0.49 |
| 7:At:30:THR:C | 7:At:32:ASP:H | 2.20 | 0.49 |
| 6:Au:268:ALA:HB3 | 6:Au:471:MET:HG2 | 1.94 | 0.49 |
| 5:Av:31:ILE:H | 5:Av:31:ILE:HD13 | 1.76 | 0.49 |
| 6:Aw:104:PRO:HD2 | 6:Aw:300:LEU:HD21 | 1.93 | 0.49 |
| 2:B1:157:VAL:HG23 | 2:B1:159:GLU:H | 1.77 | 0.49 |
| 2:B3:15:VAL:H | 2:Bz:643:VAL:HG22 | 1.77 | 0.49 |
| 2:B4:66:MET:HG2 | 2:B4:468:VAL:HG21 | 1.94 | 0.49 |
| 2:B4:561:LYS:HD2 | 2:B6:10:LEU:HD13 | 1.92 | 0.49 |
| 2:B5:134:VAL:HG12 | 2:B5:140:ILE:HG22 | 1.94 | 0.49 |
| 2:B5:205:MET:O | 2:B5:211:GLN:NE2 | 2.45 | 0.49 |
| 2:B6:37:PRO:HG3 | 2:B6:226:TYR:CZ | 2.45 | 0.49 |
| 5:BA:188:ILE:HG22 | 5:BA:202:TYR:HB3 | 1.94 | 0.49 |
| 6:BK:124:VAL:HG13 | 6:BK:257:GLN:HB2 | 1.94 | 0.49 |
| 3:BX:24:GLU:HB3 | 3:BX:112:ILE:HG23 | 1.93 | 0.49 |
| 3:BY:47:GLU:OE1 | 3:Bc:148:ASN:ND2 | 2.44 | 0.49 |
| 2:Bs:494:TYR:CZ | 2:Bt:569:LYS:HD3 | 2.47 | 0.49 |
| 2:Bu:585:ARG:NH2 | 2:Bu:608:CYS:O | 2.40 | 0.49 |
| 4:a:66:LYS:NZ | 4:a:70:GLU:OE2 | 2.44 | 0.49 |
| 1:n:207:LEU:HD11 | 8:u:66:ALA:HB3 | 1.94 | 0.49 |
| 1:n:235:TYR:OH | 8:u:19:ASP:OD2 | 2.27 | 0.49 |
| 2:2:365:ARG:NH1 | 8:r:253:GLN:OE1 | 2.45 | 0.49 |
| 2:2:398:ASP:O | 2:2:401:GLN:HG2 | 2.13 | 0.49 |
| 2:2:634:SER:HB2 | 2:AP:574:GLU:H | 1.76 | 0.49 |
| 2:3:107:GLY:HA3 | 2:3:110:TYR:HE2 | 1.76 | 0.49 |
| 2:3:240:SER:OG | 2:3:334:PHE:O | 2.23 | 0.49 |
| 2:4:117:THR:HA | 2:4:127:THR:HA | 1.94 | 0.49 |
| 2:5:61:THR:O | 2:5:63:ASP:N | 2.44 | 0.49 |
| 2:5:268:VAL:HG21 | 2:5:282:ILE:HD11 | 1.94 | 0.49 |
| 5:A0:495:ASP:OD1 | 5:A0:495:ASP:N | 2.38 | 0.49 |
| 5:A2:223:GLU:HG3 | 5:BD:197:LYS:HG3 | 1.94 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A8:317:GLY:HA3 | 6:A8:516:VAL:HG12 | 1.94 | 0.49 |
| 8:AB:255:PHE:O | 2:AD:401:GLN:NE2 | 2.45 | 0.49 |
| 2:AD:637:TYR:HB2 | 2:AN:622:GLU:HG2 | 1.94 | 0.49 |
| 3:AH:39:THR:HG22 | 3:AH:71:VAL:HG22 | 1.93 | 0.49 |
| 3:AH:54:MET:HE3 | 3:Bj:20:LEU:HA | 1.93 | 0.49 |
| 10:AQ:360:TYR:OH | 6:Az:342:GLY:O | 2.30 | 0.49 |
| 6:AV:88:VAL:HG12 | 6:BJ:254:ILE:HD12 | 1.93 | 0.49 |
| 6:AW:344:ARG:O | 6:AW:345:TRP:HB3 | 2.13 | 0.49 |
| 7:Ab:216:SER:O | 7:Ab:220:ASN:ND2 | 2.34 | 0.49 |
| 6:Ak:267:LYS:HD3 | 6:Ao:247:TRP:HE3 | 1.77 | 0.49 |
| 6:Am:264:ARG:NE | 6:BJ:155:SER:OG | 2.43 | 0.49 |
| 6:Ap:121:THR:HB | 6:BI:79:ILE:HG23 | 1.93 | 0.49 |
| 7:Aq:34:ILE:O | 7:Aq:38:ILE:HG12 | 2.11 | 0.49 |
| 7:Aq:76:LEU:HD13 | 7:Aq:81:VAL:HG21 | 1.94 | 0.49 |
| 6:Au:83:GLN:NE2 | 11:BS:36:SER:OG | 2.38 | 0.49 |
| 6:Au:119:SER:OG | 6:BJ:92:GLY:O | 2.20 | 0.49 |
| 2:B2:264:THR:O | 2:B2:266:LYS:N | 2.46 | 0.49 |
| 2:B3:40:GLN:H | 2:B3:81:VAL:HG23 | 1.77 | 0.49 |
| 2:B6:641:ASN:HB2 | 2:B7:626:THR:HG22 | 1.94 | 0.49 |
| 5:BA:423:LYS:HG3 | 5:BA:437:TRP:CD1 | 2.47 | 0.49 |
| 7:BC:162:TRP:CD1 | 7:BE:55:LYS:H | 2.29 | 0.49 |
| 6:BI:103:ILE:HD12 | 6:BI:296:THR:HG21 | 1.94 | 0.49 |
| 6:BM:344:ARG:NH2 | 6:BM:348:GLU:OE2 | 2.45 | 0.49 |
| 3:Bj:100:THR:OG1 | 3:Bj:101:GLY:N | 2.46 | 0.49 |
| 3:Bo:23:VAL:HG11 | 3:Bo:39:THR:HG21 | 1.95 | 0.49 |
| 3:Bo:136:ASN:O | 3:Bo:136:ASN:ND2 | 2.43 | 0.49 |
| 2:Bs:125:ILE:HG22 | 2:Bs:149:LYS:HD3 | 1.94 | 0.49 |
| 2:Bu:576:ASN:HD21 | 2:Bu:623:PHE:HD1 | 1.59 | 0.49 |
| 2:Bv:116:ILE:HD12 | 2:Bv:171:ILE:HG12 | 1.94 | 0.49 |
| 2:Bx:26:THR:HB | 2:Bx:77:ASP:HB3 | 1.95 | 0.49 |
| 2:By:101:TYR:CZ | 2:By:143:ILE:HG12 | 2.47 | 0.49 |
| 2:Bz:57:PRO:HB3 | 2:Bz:62:ALA:HA | 1.93 | 0.49 |
| 2:Bz:236:ILE:HD11 | 2:Bz:323:ILE:HG21 | 1.94 | 0.49 |
| 1:n:109:GLN:HG2 | 8:u:70:THR:HG21 | 1.94 | 0.49 |
| 8:s:44:ALA:HB3 | 8:s:78:HIS:HB2 | 1.94 | 0.49 |
| 8:s:91:ASN:OD1 | 8:s:92:ILE:N | 2.44 | 0.49 |
| 2:1:23:SER:HB3 | 2:1:74:TYR:O | 2.12 | 0.49 |
| 2:4:220:PRO:HG2 | 2:4:338:LEU:HD11 | 1.93 | 0.49 |
| 5:A1:473:ALA:HB2 | 5:BD:467:ILE:HD13 | 1.95 | 0.49 |
| 5:A3:178:ASP:HB3 | 5:A3:181:GLN:HG2 | 1.94 | 0.49 |
| 6:A5:331:VAL:HG21 | 6:A5:519:LYS:HE2 | 1.94 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A5:350:PHE:HB2 | 6:A5:389:VAL:HG11 | 1.94 | 0.49 |
| 3:AI:17:ARG:HH21 | 3:AJ:150:ILE:HG22 | 1.77 | 0.49 |
| 3:AJ:100:THR:OG1 | 3:AJ:101:GLY:N | 2.45 | 0.49 |
| 2:AK:91:ASN:HA | 2:AK:227:PRO:HA | 1.94 | 0.49 |
| 2:AM:453:ASN:HD21 | 2:AM:525:VAL:HB | 1.76 | 0.49 |
| 2:AN:209:ASP:OD1 | 2:AN:209:ASP:N | 2.45 | 0.49 |
| 2:AN:332:GLU:N | 2:AN:332:GLU:OE1 | 2.43 | 0.49 |
| 2:AP:406:LEU:HD13 | 2:AP:475:ALA:HB2 | 1.94 | 0.49 |
| 2:AP:521:ALA:HB1 | 2:AP:541:ALA:HA | 1.94 | 0.49 |
| 6:Ac:237:GLU:HG2 | 6:Ac:246:PRO:HA | 1.94 | 0.49 |
| 6:Ac:380:ARG:NH2 | 6:Ag:366:ARG:HH11 | 2.10 | 0.49 |
| 6:Ad:142:GLU:HG3 | 6:Ad:145:HIS:HB2 | 1.94 | 0.49 |
| 6:Ae:503:ILE:HG23 | 6:Ae:507:LEU:HD12 | 1.93 | 0.49 |
| 6:Ah:305:GLU:HA | 6:BI:225:ALA:HB3 | 1.93 | 0.49 |
| 6:Ah:400:LEU:HD11 | 6:BI:417:LEU:HG | 1.93 | 0.49 |
| 6:Ai:264:ARG:NE | 6:Am:155:SER:OG | 2.37 | 0.49 |
| 6:Ao:255:ASP:OD1 | 6:Ao:495:ARG:NE | 2.43 | 0.49 |
| 7:Aq:2:SER:OG | 7:Aq:3:GLY:N | 2.44 | 0.49 |
| 6:Aw:131:TYR:HE1 | 6:Aw:141:LYS:HB2 | 1.77 | 0.49 |
| 2:B2:101:TYR:CZ | 2:B2:143:ILE:HG12 | 2.47 | 0.49 |
| 6:BM:149:GLY:H | 6:BM:186:GLY:HA2 | 1.77 | 0.49 |
| 11:BP:29:SER:HB2 | 11:BP:59:VAL:HG22 | 1.94 | 0.49 |
| 11:BP:62:GLU:HG2 | 11:BT:4:THR:HG21 | 1.92 | 0.49 |
| 3:Bh:28:LEU:HD22 | 3:Bh:84:LYS:HB3 | 1.93 | 0.49 |
| 3:Bm:140:LEU:HD13 | 3:Bm:153:PHE:HB3 | 1.93 | 0.49 |
| 2:Bp:157:VAL:HG23 | 2:Bp:159:GLU:H | 1.77 | 0.49 |
| 2:Bp:246:LYS:HB2 | 2:Bp:250:ALA:HB2 | 1.94 | 0.49 |
| 2:Bq:222:VAL:HG21 | 2:Bq:238:ILE:HD11 | 1.93 | 0.49 |
| 2:Bs:550:ARG:HB3 | 2:Bs:553:VAL:HG12 | 1.94 | 0.49 |
| 2:Bs:653:GLU:HB2 | 2:Bv:16:GLN:HA | 1.94 | 0.49 |
| 2:Bv:470:LEU:HD23 | 2:Bv:525:VAL:HG21 | 1.93 | 0.49 |
| 2:Bw:202:GLU:OE1 | 2:Bw:203:ALA:N | 2.46 | 0.49 |
| 4:M:44:MET:HE2 | 4:N:25:ILE:HD13 | 1.93 | 0.49 |
| 1:n:147:PHE:HB3 | 1:n:171:ALA:HB1 | 1.93 | 0.49 |
| 2:1:411:ARG:HG3 | 2:1:415:VAL:HG21 | 1.94 | 0.49 |
| 2:4:235:GLU:HG3 | 2:4:284:ARG:HB2 | 1.93 | 0.49 |
| 6:A4:229:ALA:HB3 | 6:A4:232:ILE:HG12 | 1.94 | 0.49 |
| 6:A7:67:GLU:OE2 | 6:Ay:252:PHE:N | 2.42 | 0.49 |
| 2:AN:91:ASN:N | 2:AN:91:ASN:OD1 | 2.45 | 0.49 |
| 2:AP:148:ALA:O | 2:AP:151:ILE:HG13 | 2.12 | 0.49 |
| 7:Aa:265:ARG:HG3 | 7:Ab:25:ILE:HD12 | 1.94 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ae:80:ALA:HA | 6:Ae:93:PRO:HG3 | 1.95 | 0.49 |
| 6:Af:328:LYS:HB3 | 6:Af:331:VAL:HG13 | 1.95 | 0.49 |
| 6:Ai:151:ASP:HB3 | 6:Ai:154:PHE:HB2 | 1.94 | 0.49 |
| 6:Ap:360:GLU:OE1 | 6:Ap:514:ARG:NH1 | 2.45 | 0.49 |
| 7:Aq:30:THR:HG22 | 7:As:24:ILE:HD11 | 1.94 | 0.49 |
| 5:Ax:115:LYS:HD3 | 5:Ax:445:LYS:HE3 | 1.92 | 0.49 |
| 6:Az:240:ASN:HD22 | 6:BK:66:ALA:HB3 | 1.77 | 0.49 |
| 6:Az:493:ALA:O | 6:Az:497:GLN:NE2 | 2.45 | 0.49 |
| 2:B1:29:LEU:HB2 | 2:B1:78:LEU:HD11 | 1.94 | 0.49 |
| 2:B1:225:LEU:HD23 | 2:B1:226:TYR:CZ | 2.47 | 0.49 |
| 2:B2:446:THR:OG1 | 2:B2:554:ARG:NH2 | 2.45 | 0.49 |
| 5:BF:477:ILE:HA | 5:BF:481:ILE:HG23 | 1.92 | 0.49 |
| 5:BG:244:ASP:O | 5:BG:246:CYS:N | 2.45 | 0.49 |
| 3:BY:28:LEU:HD22 | 3:BY:84:LYS:HB3 | 1.95 | 0.49 |
| 3:Bf:134:PRO:HA | 3:Bf:157:LEU:HA | 1.94 | 0.49 |
| 2:Bp:351:THR:HG23 | 2:Bp:354:ASP:H | 1.77 | 0.49 |
| 2:Bp:455:LYS:HD2 | 2:Bp:502:VAL:HG22 | 1.94 | 0.49 |
| 2:Bt:91:ASN:N | 2:Bt:91:ASN:OD1 | 2.45 | 0.49 |
| 2:Bu:611:THR:HG21 | 2:Bw:20:VAL:HG21 | 1.94 | 0.49 |
| 2:Bv:455:LYS:HD3 | 2:Bv:502:VAL:HG22 | 1.94 | 0.49 |
| 2:Bw:498:GLN:HA | 2:Bw:534:VAL:HG12 | 1.93 | 0.49 |
| 8:q:26:ILE:HG12 | 8:q:37:ILE:HG12 | 1.94 | 0.49 |
| 8:r:228:GLY:O | 8:r:258:ASN:ND2 | 2.40 | 0.49 |
| 8:u:108:GLN:HB2 | 8:u:202:VAL:HG12 | 1.92 | 0.49 |
| 2:2:561:LYS:HD3 | 8:r:231:GLU:HG2 | 1.93 | 0.49 |
| 2:4:157:VAL:HG23 | 2:4:159:GLU:H | 1.76 | 0.49 |
| 2:5:57:PRO:HG3 | 2:5:65:PHE:CD1 | 2.48 | 0.49 |
| 2:5:132:THR:HB | 2:5:142:LYS:HB2 | 1.93 | 0.49 |
| 2:5:609:ASP:HB2 | 2:5:611:THR:HG22 | 1.94 | 0.49 |
| 3:7:134:PRO:HA | 3:7:157:LEU:HA | 1.95 | 0.49 |
| 6:A5:142:GLU:H | 6:A5:490:GLN:HG2 | 1.76 | 0.49 |
| 7:A6:50:PHE:HB3 | 7:A6:302:PRO:HD3 | 1.94 | 0.49 |
| 8:AB:243:ASP:OD1 | 8:AB:243:ASP:N | 2.43 | 0.49 |
| 9:AC:103:THR:O | 9:AC:107:THR:OG1 | 2.30 | 0.49 |
| 2:AD:37:PRO:O | 2:AD:82:ARG:HB3 | 2.12 | 0.49 |
| 2:AD:401:GLN:O | 2:AD:561:LYS:NZ | 2.45 | 0.49 |
| 2:AK:70:ASN:ND2 | 2:AK:457:GLN:OE1 | 2.41 | 0.49 |
| 2:AN:311:ILE:HB | 2:AN:327:ALA:HB2 | 1.95 | 0.49 |
| 2:AO:222:VAL:HG21 | 2:AO:238:ILE:HD11 | 1.95 | 0.49 |
| 2:AP:455:LYS:HG2 | 2:AP:457:GLN:HB2 | 1.93 | 0.49 |
| 6:AW:171:GLN:NE2 | 6:AW:172:THR:O | 2.45 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AZ:121:THR:HG23 | 6:AZ:260:GLU:HG2 | 1.94 | 0.49 |
| 6:Ap:345:TRP:O | 6:Ap:348:GLU:N | 2.31 | 0.49 |
| 5:Av:259:LYS:NZ | 5:Av:263:GLN:OE1 | 2.41 | 0.49 |
| 5:Ax:55:ASN:O | 5:Ax:59:GLN:HG2 | 2.13 | 0.49 |
| 6:Ay:184:GLU:O | 6:Ay:185:THR:OG1 | 2.29 | 0.49 |
| 2:B1:440:ASN:N | 2:B1:440:ASN:OD1 | 2.44 | 0.49 |
| 2:B4:451:ASP:OD1 | 2:B4:452:GLY:N | 2.45 | 0.49 |
| 2:B6:247:GLY:O | 2:B6:263:SER:OG | 2.31 | 0.49 |
| 2:B7:35:TRP:HH2 | 2:B7:224:ALA:HB1 | 1.77 | 0.49 |
| 5:BF:39:GLY:HA3 | 5:BF:250:ILE:HG12 | 1.95 | 0.49 |
| 5:BF:91:ALA:HB1 | 5:BF:375:VAL:HG21 | 1.93 | 0.49 |
| 7:BL:137:ASP:OD1 | 7:BL:137:ASP:N | 2.46 | 0.49 |
| 11:BN:18:ASP:HB3 | 11:BN:21:LYS:HD3 | 1.93 | 0.49 |
| 11:BU:21:LYS:HA | 11:BU:80:GLY:HA2 | 1.95 | 0.49 |
| 3:BX:54:MET:O | 3:BX:56:ARG:N | 2.46 | 0.49 |
| 3:Bb:58:ILE:H | 3:Bb:58:ILE:HD13 | 1.76 | 0.49 |
| 3:Bc:37:LYS:HB2 | 3:Bc:74:MET:HE3 | 1.94 | 0.49 |
| 3:Bk:83:GLN:HA | 3:Bk:86:VAL:HG22 | 1.93 | 0.49 |
| 2:Bq:423:VAL:HG21 | 2:Bq:513:GLN:HB3 | 1.94 | 0.49 |
| 2:Bs:538:ASP:HB2 | 2:Bs:551:ILE:HB | 1.95 | 0.49 |
| 2:Bu:30:ALA:HB3 | 2:Bu:359:TRP:CE2 | 2.48 | 0.49 |
| 2:Bu:95:ILE:HD13 | 2:Bu:213:ASN:HB2 | 1.93 | 0.49 |
| 2:Bv:202:GLU:OE1 | 2:Bv:203:ALA:N | 2.36 | 0.49 |
| 2:Bx:116:ILE:HD13 | 2:Bx:171:ILE:HG23 | 1.94 | 0.49 |
| 8:t:256:THR:HG21 | 8:t:271:ARG:HB2 | 1.94 | 0.49 |
| 8:u:9:SER:HB3 | 8:u:198:MET:HE2 | 1.95 | 0.49 |
| 1:0:180:GLU:HB2 | 8:q:30:LEU:HD21 | 1.94 | 0.49 |
| 1:0:223:GLN:NE2 | 1:k:69:ASP:OD1 | 2.45 | 0.49 |
| 2:1:102:THR:HB | 2:1:183:THR:HB | 1.94 | 0.49 |
| 2:1:205:MET:O | 2:1:211:GLN:NE2 | 2.45 | 0.49 |
| 2:3:467:TRP:HH2 | 2:AK:199:GLU:HB2 | 1.78 | 0.49 |
| 2:4:278:GLN:HG2 | 2:4:296:SER:HB3 | 1.94 | 0.49 |
| 2:4:514:ARG:NH1 | 2:AL:366:GLU:OE2 | 2.46 | 0.49 |
| 3:8:18:PRO:HB2 | 3:9:146:SER:HB2 | 1.94 | 0.49 |
| 3:9:46:VAL:HG22 | 3:9:64:ARG:HD2 | 1.94 | 0.49 |
| 3:9:114:ARG:HG2 | 3:9:126:GLU:HG2 | 1.95 | 0.49 |
| 5:A2:81:ASN:HD22 | 7:BL:122:GLY:HA2 | 1.77 | 0.49 |
| 6:A4:117:MET:HG2 | 6:A4:118:ASN:H | 1.78 | 0.49 |
| 7:A6:13:LYS:HG3 | 7:A6:34:ILE:HG21 | 1.95 | 0.49 |
| 3:AG:54:MET:HE3 | 3:Bg:20:LEU:HA | 1.94 | 0.49 |
| 2:AK:106:PRO:HB2 | 2:AK:139:LYS:HD2 | 1.94 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AL:488:TRP:HB3 | 2:AL:556:LEU:HD13 | 1.93 | 0.49 |
| 2:AM:518:TYR:HE1 | 2:AM:537:GLY:HA3 | 1.78 | 0.49 |
| 2:AO:514:ARG:NH1 | 2:B5:364:ASP:OD1 | 2.45 | 0.49 |
| 2:AP:454:TYR:HB3 | 2:AP:467:TRP:CD1 | 2.47 | 0.49 |
| 6:AV:85:SER:HB2 | 11:BR:35:TYR:HE2 | 1.78 | 0.49 |
| 6:AW:340:ILE:HG13 | 6:AW:343:ALA:H | 1.77 | 0.49 |
| 6:AZ:254:ILE:HD12 | 6:Am:88:VAL:HB | 1.95 | 0.49 |
| 6:Af:151:ASP:HB3 | 6:Af:154:PHE:HB2 | 1.94 | 0.49 |
| 6:Ag:240:ASN:OD1 | 6:Aw:66:ALA:N | 2.45 | 0.49 |
| 6:Ak:151:ASP:HB3 | 6:Ak:154:PHE:HB2 | 1.93 | 0.49 |
| 6:Am:404:PHE:HB3 | 6:Am:414:ALA:HB1 | 1.93 | 0.49 |
| 7:As:159:PRO:HB3 | 7:As:174:GLY:O | 2.12 | 0.49 |
| 5:Av:45:VAL:HG22 | 5:Av:57:ALA:HB2 | 1.93 | 0.49 |
| 2:B1:225:LEU:HD12 | 2:B1:324:PHE:HB2 | 1.95 | 0.49 |
| 2:B1:364:ASP:O | 2:B1:367:SER:N | 2.44 | 0.49 |
| 2:B2:346:SER:O | 2:B2:350:VAL:HG23 | 2.12 | 0.49 |
| 2:B3:593:GLN:NE2 | 3:Bh:4:ASP:OD2 | 2.42 | 0.49 |
| 5:BD:469:MET:HG2 | 5:BD:490:ILE:HG23 | 1.94 | 0.49 |
| 7:BL:180:ASP:OD1 | 7:BL:181:LEU:N | 2.42 | 0.49 |
| 3:Bb:69:TRP:HB2 | 3:Bb:159:LEU:HD23 | 1.93 | 0.49 |
| 2:Bq:239:VAL:HG22 | 2:Bq:280:ALA:HB3 | 1.95 | 0.49 |
| 2:Br:91:ASN:HB2 | 2:Br:193:ILE:HG23 | 1.95 | 0.49 |
| 2:Br:331:PRO:HB2 | 2:Br:334:PHE:HB2 | 1.94 | 0.49 |
| 2:Br:430:ARG:HG3 | 2:Br:522:ILE:HD11 | 1.95 | 0.49 |
| 2:Bs:133:GLU:HB3 | 2:Bs:141:LYS:HB2 | 1.94 | 0.49 |
| 2:Bu:251:LEU:HD22 | 2:Bu:262:ALA:HA | 1.94 | 0.49 |
| 2:Bv:46:ASN:OD1 | 2:Bv:47:GLU:N | 2.46 | 0.49 |
| 2:Bv:488:TRP:HB3 | 2:Bv:556:LEU:HD12 | 1.95 | 0.49 |
| 2:Bw:455:LYS:HD3 | 2:Bw:502:VAL:HG13 | 1.94 | 0.49 |
| 1:k:76:LEU:HD21 | 8:r:128:ASP:HB3 | 1.94 | 0.49 |
| 1:m:176:TYR:CE2 | 1:m:179:GLU:HG3 | 2.47 | 0.49 |
| 8:r:261:ARG:HA | 8:r:271:ARG:HD3 | 1.95 | 0.49 |
| 2:1:510:ARG:HG3 | 2:AO:364:ASP:HB2 | 1.94 | 0.49 |
| 2:1:569:LYS:HD2 | 8:q:251:VAL:HG11 | 1.94 | 0.49 |
| 2:2:351:THR:OG1 | 2:2:352:ALA:N | 2.46 | 0.49 |
| 2:4:597:ALA:HB1 | 3:9:3:VAL:HA | 1.94 | 0.49 |
| 2:5:575:LEU:HD11 | 8:u:97:LEU:HD21 | 1.93 | 0.49 |
| 3:8:98:GLU:HA | 3:AI:2:PHE:HA | 1.93 | 0.49 |
| 3:8:103:LYS:NZ | 3:AJ:13:GLY:O | 2.40 | 0.49 |
| 2:AK:26:THR:HA | 2:AK:77:ASP:O | 2.13 | 0.49 |
| 2:AK:41:ILE:HD13 | 2:AK:81:VAL:HB | 1.95 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AO:10:LEU:HD13 | 2:B2:561:LYS:HD2 | 1.94 | 0.49 |
| 2:AO:417:ILE:H | 2:AO:417:ILE:HD13 | 1.76 | 0.49 |
| 2:AO:521:ALA:HB1 | 2:AO:541:ALA:HA | 1.95 | 0.49 |
| 10:AR:303:ALA:HB3 | 10:AR:344:MET:HE3 | 1.95 | 0.49 |
| 6:AV:467:PHE:CD2 | 6:BJ:459:LEU:HB3 | 2.47 | 0.49 |
| 7:AY:18:ARG:HD3 | 7:BL:32:ASP:HB3 | 1.95 | 0.49 |
| 6:AZ:432:ASP:HB3 | 6:AZ:518:VAL:HG22 | 1.94 | 0.49 |
| 6:Ac:120:PRO:HD3 | 6:Ac:453:TYR:CZ | 2.48 | 0.49 |
| 6:Ad:515:ARG:NH1 | 6:Ad:517:TYR:OH | 2.46 | 0.49 |
| 6:Ae:145:HIS:HB3 | 6:Ae:148:TYR:HB2 | 1.93 | 0.49 |
| 6:Ae:336:ASP:HB3 | 6:Ae:339:ASP:HB2 | 1.94 | 0.49 |
| 6:Af:123:GLN:HB3 | 6:Az:93:PRO:HB2 | 1.93 | 0.49 |
| 6:Ai:131:TYR:CD2 | 6:Ai:250:MET:HE3 | 2.45 | 0.49 |
| 6:Am:184:GLU:O | 6:Am:185:THR:OG1 | 2.28 | 0.49 |
| 6:An:190:LEU:HB3 | 6:An:221:LEU:HB3 | 1.95 | 0.49 |
| 6:Ap:199:ASP:OD2 | 6:Ap:207:LYS:NZ | 2.32 | 0.49 |
| 6:Au:241:GLY:HA3 | 11:BN:43:GLY:HA2 | 1.95 | 0.49 |
| 6:Aw:107:ILE:HD13 | 6:Aw:424:TYR:CD1 | 2.48 | 0.49 |
| 2:B4:488:TRP:O | 2:B4:552:ASN:ND2 | 2.42 | 0.49 |
| 2:B6:28:ALA:HB2 | 2:B6:370:VAL:HG11 | 1.95 | 0.49 |
| 2:B6:99:ILE:O | 2:B6:100:GLU:HG3 | 2.13 | 0.49 |
| 2:B6:446:THR:OG1 | 2:B6:554:ARG:NH2 | 2.46 | 0.49 |
| 5:BA:38:ASP:OD2 | 5:BA:186:ARG:NH2 | 2.45 | 0.49 |
| 5:BA:184:TYR:OH | 5:BA:204:GLU:OE1 | 2.31 | 0.49 |
| 5:BG:455:ALA:HA | 5:BG:458:LYS:HD3 | 1.94 | 0.49 |
| 3:Bm:42:PRO:HG3 | 3:Bm:69:TRP:CD1 | 2.48 | 0.49 |
| 3:Bn:51:VAL:N | 3:Bn:58:ILE:O | 2.42 | 0.49 |
| 2:Br:571:ARG:NH1 | 2:Br:583:SER:OG | 2.46 | 0.49 |
| 2:Bs:379:ALA:HB2 | 2:Bs:454:TYR:HE2 | 1.78 | 0.49 |
| 2:Bu:36:GLY:O | 2:Bu:82:ARG:NH1 | 2.41 | 0.49 |
| 2:Bv:642:PHE:CZ | 2:Bw:561:LYS:HG2 | 2.47 | 0.49 |
| 2:Bw:159:GLU:OE2 | 2:Bw:166:ASN:ND2 | 2.46 | 0.49 |
| 4:F:44:MET:HE2 | 4:Q:25:ILE:HD13 | 1.95 | 0.49 |
| 4:V:62:ILE:HD12 | 4:a:58:LEU:HD22 | 1.94 | 0.49 |
| 1:m:175:ILE:HD11 | 8:t:125:ARG:HH11 | 1.78 | 0.49 |
| 2:5:351:THR:OG1 | 2:5:352:ALA:N | 2.46 | 0.49 |
| 5:A0:162:ILE:HD11 | 5:A0:167:PRO:HA | 1.93 | 0.49 |
| 5:A3:348:ASP:OD1 | 5:A3:349:THR:N | 2.46 | 0.49 |
| 7:A6:40:ARG:HH21 | 7:A6:254:LEU:HD22 | 1.77 | 0.49 |
| 6:A8:287:ASP:HA | 6:A8:290:LEU:HD12 | 1.95 | 0.49 |
| 3:AJ:70:THR:HG23 | 3:AJ:156:THR:HG22 | 1.94 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AL:119:LYS:HE3 | 2:AL:122:SER:HA | 1.95 | 0.49 |
| 2:AM:110:TYR:CE1 | 2:AM:177:GLY:HA3 | 2.48 | 0.49 |
| 2:AN:82:ARG:NH2 | 2:AN:227:PRO:O | 2.42 | 0.49 |
| 10:AT:331:ASP:OD1 | 10:AT:331:ASP:N | 2.46 | 0.49 |
| 6:AW:426:ASP:OD2 | 6:AW:433:TYR:OH | 2.30 | 0.49 |
| 6:AX:76:ALA:HB1 | 6:Az:496:ILE:HG12 | 1.95 | 0.49 |
| 6:AZ:131:TYR:CD2 | 6:AZ:250:MET:HE3 | 2.48 | 0.49 |
| 7:Aa:34:ILE:O | 7:Aa:38:ILE:HG12 | 2.12 | 0.49 |
| 7:Aa:159:PRO:HB3 | 7:Aa:174:GLY:O | 2.13 | 0.49 |
| 6:Ai:408:THR:HG21 | 6:Ai:427:GLN:HB3 | 1.95 | 0.49 |
| 6:Ak:390:ASP:OD2 | 6:Ak:394:SER:OG | 2.30 | 0.49 |
| 6:Ap:496:ILE:HG22 | 6:BI:76:ALA:HB1 | 1.95 | 0.49 |
| 7:Ar:13:LYS:HG3 | 7:Ar:34:ILE:HG21 | 1.94 | 0.49 |
| 7:Ar:191:TYR:HD2 | 7:Ar:193:ASP:H | 1.60 | 0.49 |
| 7:As:43:GLU:O | 7:As:47:GLU:HG2 | 2.12 | 0.49 |
| 6:Ay:124:VAL:HG21 | 6:Ay:444:MET:HE1 | 1.95 | 0.49 |
| 6:Az:111:ILE:H | 6:Az:111:ILE:HD13 | 1.77 | 0.49 |
| 2:B1:42:LYS:HE2 | 2:B1:53:THR:HG21 | 1.93 | 0.49 |
| 2:B1:206:THR:HA | 2:B1:211:GLN:HE21 | 1.78 | 0.49 |
| 2:B5:264:THR:O | 2:B5:266:LYS:N | 2.46 | 0.49 |
| 2:B6:61:THR:HG22 | 2:B6:65:PHE:HB2 | 1.94 | 0.49 |
| 2:B7:29:LEU:O | 2:B7:80:VAL:HA | 2.13 | 0.49 |
| 5:BA:476:PHE:HB3 | 5:BA:480:TYR:HB2 | 1.95 | 0.49 |
| 6:BK:414:ALA:HB3 | 6:BK:423:VAL:HG13 | 1.95 | 0.49 |
| 7:BL:81:VAL:HA | 7:BL:188:THR:HA | 1.94 | 0.49 |
| 11:BP:9:ASN:HB3 | 11:BP:56:TYR:CE2 | 2.47 | 0.49 |
| 3:Bj:48:LYS:HG3 | 3:Bj:59:ASN:HB3 | 1.94 | 0.49 |
| 3:Bn:23:VAL:HG11 | 3:Bn:39:THR:HG21 | 1.94 | 0.49 |
| 3:Bn:51:VAL:HB | 3:Bn:58:ILE:HG12 | 1.95 | 0.49 |
| 2:Bp:545:PRO:HD3 | 2:Bs:271:TYR:HB3 | 1.93 | 0.49 |
| 2:Bu:302:LYS:O | 2:Bu:307:SER:N | 2.46 | 0.49 |
| 4:G:44:MET:HE2 | 4:R:25:ILE:HD13 | 1.94 | 0.49 |
| 4:M:47:PRO:HB2 | 4:O:48:THR:HG21 | 1.93 | 0.49 |
| 9:v:50:VAL:HG13 | 9:v:55:GLY:HA2 | 1.95 | 0.49 |
| 2:2:256:PRO:HG2 | 2:2:339:THR:H | 1.78 | 0.49 |
| 2:4:374:ILE:HG12 | 2:4:406:LEU:HD11 | 1.93 | 0.49 |
| 3:7:113:VAL:HG13 | 3:7:127:ILE:HG23 | 1.93 | 0.49 |
| 5:A0:276:ILE:HD13 | 7:BC:143:GLN:HB2 | 1.95 | 0.49 |
| 7:A6:134:PHE:HB2 | 7:Al:106:TRP:CD1 | 2.48 | 0.49 |
| 2:AD:600:GLY:O | 2:AD:632:ALA:HB2 | 2.13 | 0.49 |
| 2:AP:100:GLU:OE2 | 2:AP:186:LYS:NZ | 2.33 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AW:151:ASP:HB3 | 6:AW:154:PHE:HB2 | 1.95 | 0.49 |
| 6:AW:311:ASN:OD1 | 6:AW:515:ARG:NE | 2.46 | 0.49 |
| 6:AZ:267:LYS:HG3 | 6:Ad:247:TRP:CE3 | 2.48 | 0.49 |
| 6:AZ:416:VAL:HG12 | 6:AZ:419:GLY:H | 1.78 | 0.49 |
| 6:Aj:333:ASP:HB3 | 6:Aj:336:ASP:HB2 | 1.95 | 0.49 |
| 6:An:494:SER:C | 6:An:496:ILE:H | 2.20 | 0.49 |
| 6:Ap:337:PRO:O | 6:Ap:342:GLY:N | 2.43 | 0.49 |
| 6:Ap:458:PRO:HG2 | 5:BF:70:LYS:HD2 | 1.94 | 0.49 |
| 5:Av:27:ASP:HB2 | 5:BB:164:PRO:HG2 | 1.95 | 0.49 |
| 6:Ay:120:PRO:O | 6:Ay:121:THR:OG1 | 2.25 | 0.49 |
| 6:Ay:452:PRO:HA | 6:Ay:477:TYR:HA | 1.94 | 0.49 |
| 2:B2:272:GLY:O | 2:B2:274:GLN:NE2 | 2.46 | 0.49 |
| 2:B2:510:ARG:HG2 | 2:B2:511:GLN:H | 1.78 | 0.49 |
| 2:B3:581:ARG:HG2 | 2:B3:623:PHE:HE1 | 1.78 | 0.49 |
| 2:B6:79:ARG:NH2 | 2:B6:369:ASP:OD1 | 2.46 | 0.49 |
| 2:B6:511:GLN:OE1 | 2:Bq:5:SER:OG | 2.31 | 0.49 |
| 2:B7:26:THR:HA | 2:B7:77:ASP:O | 2.12 | 0.49 |
| 2:B7:409:PRO:HD3 | 2:B7:451:ASP:HB3 | 1.94 | 0.49 |
| 5:BB:82:LEU:HD22 | 5:BB:258:VAL:HG22 | 1.93 | 0.49 |
| 7:BC:97:SER:HB3 | 7:BC:103:THR:HA | 1.95 | 0.49 |
| 7:BC:135:GLY:O | 5:BG:259:LYS:NZ | 2.33 | 0.49 |
| 6:BI:71:ASP:OD1 | 6:BI:72:HIS:N | 2.45 | 0.49 |
| 7:BL:30:THR:OG1 | 7:BL:33:GLN:OE1 | 2.17 | 0.49 |
| 6:BM:350:PHE:HB2 | 6:BM:389:VAL:HG11 | 1.93 | 0.49 |
| 11:BN:11:LYS:HG3 | 11:BN:27:GLU:HG2 | 1.94 | 0.49 |
| 3:BY:25:ILE:HD13 | 3:BY:88:TRP:HZ3 | 1.78 | 0.49 |
| 3:BY:128:GLU:HB3 | 3:BY:130:LYS:HE2 | 1.95 | 0.49 |
| 3:Bl:41:LEU:HD12 | 3:Bl:42:PRO:HD2 | 1.93 | 0.49 |
| 2:Bp:23:SER:OG | 2:Bp:74:TYR:O | 2.29 | 0.49 |
| 2:Bt:362:PHE:O | 2:Bt:400:ARG:NE | 2.46 | 0.49 |
| 2:Bx:556:LEU:HD11 | 2:Bx:601:ILE:HG12 | 1.95 | 0.49 |
| 2:By:110:TYR:CE1 | 2:By:177:GLY:HA3 | 2.48 | 0.49 |
| 1:k:214:ASN:OD1 | 8:r:55:LYS:NZ | 2.37 | 0.49 |
| 8:t:151:GLU:OE1 | 8:t:199:TYR:OH | 2.27 | 0.49 |
| 9:w:91:MET:HE1 | 9:w:138:LEU:HB2 | 1.94 | 0.49 |
| 2:1:304:ILE:HG13 | 2:1:305:TYR:H | 1.78 | 0.49 |
| 2:2:278:GLN:HG2 | 2:2:296:SER:HB3 | 1.94 | 0.49 |
| 5:A0:39:GLY:H | 5:A0:250:ILE:HD11 | 1.78 | 0.49 |
| 5:A1:245:CYS:HB2 | 7:AY:125:CYS:HA | 1.95 | 0.49 |
| 6:A8:275:ALA:HA | 6:A8:286:ALA:HB1 | 1.95 | 0.49 |
| 6:A8:336:ASP:HB3 | 6:A8:339:ASP:HB2 | 1.95 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A9:317:GLY:HA3 | 6:A9:516:VAL:HG22 | 1.94 | 0.49 |
| 3:AE:24:GLU:OE1 | 3:AE:33:THR:OG1 | 2.27 | 0.49 |
| 3:AE:49:ILE:HD11 | 3:Ba:150:ILE:HB | 1.94 | 0.49 |
| 3:AG:137:VAL:HB | 3:AG:155:VAL:HG13 | 1.95 | 0.49 |
| 3:AG:140:LEU:HD13 | 3:AG:153:PHE:HB3 | 1.95 | 0.49 |
| 2:AO:521:ALA:HA | 2:AO:539:LYS:HE3 | 1.95 | 0.49 |
| 6:Ac:367:GLN:O | 6:Ac:487:SER:OG | 2.30 | 0.49 |
| 6:Ad:315:GLN:HB2 | 6:Ad:514:ARG:HG2 | 1.95 | 0.49 |
| 6:Am:236:GLN:HB2 | 6:Am:247:TRP:CZ2 | 2.48 | 0.49 |
| 7:Aq:13:LYS:HG3 | 7:Aq:34:ILE:HG21 | 1.94 | 0.49 |
| 2:B3:642:PHE:CE2 | 2:B4:564:ILE:HD11 | 2.48 | 0.49 |
| 2:B5:378:CYS:HB2 | 2:B5:410:PRO:HA | 1.95 | 0.49 |
| 5:BA:271:VAL:HG21 | 5:BA:362:ILE:HD11 | 1.95 | 0.49 |
| 5:BB:157:PHE:HB2 | 5:BB:177:LEU:HB2 | 1.94 | 0.49 |
| 7:BC:307:LEU:HB2 | 5:BH:335:TRP:HB2 | 1.95 | 0.49 |
| 5:BF:497:GLU:HA | 5:BF:500:GLN:HG2 | 1.95 | 0.49 |
| 6:BI:350:PHE:HB3 | 6:BI:389:VAL:HG11 | 1.95 | 0.49 |
| 3:BY:39:THR:HG22 | 3:BY:71:VAL:HG22 | 1.94 | 0.49 |
| 3:Bc:64:ARG:NH1 | 3:Bf:95:GLN:HG3 | 2.28 | 0.49 |
| 3:Bd:64:ARG:HB2 | 3:Bg:93:ALA:HB1 | 1.95 | 0.49 |
| 3:Bl:23:VAL:HG11 | 3:Bl:39:THR:HG21 | 1.95 | 0.49 |
| 2:Bu:151:ILE:O | 2:Bu:155:LYS:HG2 | 2.12 | 0.49 |
| 2:Bu:202:GLU:OE1 | 2:Bu:203:ALA:N | 2.45 | 0.49 |
| 2:Bw:641:ASN:HB2 | 2:Bx:626:THR:HA | 1.95 | 0.49 |
| 2:Bz:444:SER:HG | 2:Bz:543:SER:HG | 1.58 | 0.49 |
| 4:L:9:PRO:HD3 | 4:L:57:VAL:HG21 | 1.94 | 0.49 |
| 4:L:32:LEU:HB2 | 4:L:43:SER:H | 1.78 | 0.49 |
| 1:p:152:VAL:HG22 | 1:p:169:ILE:HG23 | 1.94 | 0.49 |
| 2:1:413:THR:OG1 | 2:1:425:ASN:HB3 | 2.13 | 0.48 |
| 2:3:554:ARG:NH1 | 8:s:231:GLU:OE2 | 2.40 | 0.48 |
| 3:6:79:HIS:CD2 | 3:o:125:LYS:HG2 | 2.48 | 0.48 |
| 5:A0:84:ASN:ND2 | 7:BC:119:GLY:O | 2.42 | 0.48 |
| 7:A6:80:ASN:N | 7:A6:80:ASN:OD1 | 2.45 | 0.48 |
| 7:A6:159:PRO:HB3 | 7:A6:174:GLY:O | 2.13 | 0.48 |
| 7:A6:171:LYS:HD2 | 7:BL:219:TYR:CE2 | 2.47 | 0.48 |
| 9:AC:22:PRO:HB2 | 2:AD:571:ARG:HH12 | 1.78 | 0.48 |
| 2:AD:33:PHE:HB2 | 2:AD:82:ARG:HG3 | 1.95 | 0.48 |
| 2:AD:616:SER:O | 2:AD:620:ARG:HG2 | 2.13 | 0.48 |
| 3:AE:142:LEU:HD22 | 3:AJ:41:LEU:HD13 | 1.95 | 0.48 |
| 2:AL:116:ILE:HB | 2:AL:129:GLY:HA3 | 1.95 | 0.48 |
| 2:AN:119:LYS:HA | 2:AN:124:ASP:HA | 1.93 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AP:159:GLU:O | 2:AP:162:THR:N | 2.46 | 0.48 |
| 2:AP:430:ARG:HG3 | 2:AP:522:ILE:HD11 | 1.95 | 0.48 |
| 6:AV:79:ILE:HG21 | 6:AZ:258:VAL:HB | 1.94 | 0.48 |
| 6:AW:265:GLN:HB2 | 6:AW:474:LYS:HG3 | 1.95 | 0.48 |
| 6:AX:123:GLN:HG2 | 6:BK:95:VAL:HA | 1.95 | 0.48 |
| 6:AX:344:ARG:NE | 6:AX:348:GLU:OE2 | 2.46 | 0.48 |
| 7:AY:5:ASN:OD1 | 7:AY:7:GLN:NE2 | 2.46 | 0.48 |
| 7:AY:12:LEU:O | 7:AY:16:ILE:HG12 | 2.13 | 0.48 |
| 7:AY:219:TYR:CE1 | 7:BL:171:LYS:HD2 | 2.48 | 0.48 |
| 6:AZ:264:ARG:NH1 | 6:AZ:305:GLU:OE1 | 2.46 | 0.48 |
| 6:Ae:365:ALA:HB2 | 6:Ae:372:GLU:HA | 1.95 | 0.48 |
| 6:Ai:237:GLU:HB2 | 6:Ai:247:TRP:HE1 | 1.77 | 0.48 |
| 7:As:34:ILE:O | 7:As:38:ILE:HG12 | 2.13 | 0.48 |
| 6:Ay:494:SER:C | 6:Ay:496:ILE:H | 2.21 | 0.48 |
| 2:B4:70:ASN:ND2 | 2:B4:473:ASP:OD2 | 2.46 | 0.48 |
| 2:B4:264:THR:HB | 2:B4:267:ALA:HB3 | 1.94 | 0.48 |
| 5:BA:91:ALA:HB1 | 5:BA:375:VAL:HG21 | 1.93 | 0.48 |
| 5:BD:277:THR:HG23 | 5:BD:278:ARG:HG3 | 1.94 | 0.48 |
| 5:BF:488:LYS:HD2 | 5:BF:493:MET:O | 2.12 | 0.48 |
| 2:Bq:514:ARG:HH22 | 2:Br:366:GLU:HG2 | 1.78 | 0.48 |
| 2:Bs:418:PRO:HG2 | 2:Bs:421:ARG:HB2 | 1.95 | 0.48 |
| 2:Bt:252:LEU:HG | 2:Bt:263:SER:HB3 | 1.94 | 0.48 |
| 2:Bu:446:THR:HG21 | 2:Bu:548:PHE:HB2 | 1.95 | 0.48 |
| 2:Bu:521:ALA:HB1 | 2:Bu:541:ALA:HA | 1.94 | 0.48 |
| 2:Bv:137:ASP:OD1 | 2:Bv:137:ASP:N | 2.44 | 0.48 |
| 1:k:127:VAL:C | 1:k:128:ASN:HD22 | 2.19 | 0.48 |
| 2:1:44:VAL:HG13 | 2:1:49:ASP:HB2 | 1.95 | 0.48 |
| 5:A1:54:TYR:OH | 6:BK:100:ARG:NH1 | 2.45 | 0.48 |
| 6:A5:96:MET:N | 6:AW:123:GLN:O | 2.46 | 0.48 |
| 2:AD:256:PRO:HG2 | 2:AD:339:THR:H | 1.77 | 0.48 |
| 2:AL:652:ASP:HB3 | 2:AM:458:TYR:CE2 | 2.48 | 0.48 |
| 2:AM:312:ASP:OD1 | 2:AM:327:ALA:N | 2.36 | 0.48 |
| 2:AP:70:ASN:OD1 | 2:AP:457:GLN:NE2 | 2.44 | 0.48 |
| 7:AY:109:ASP:OD2 | 7:AY:129:TYR:OH | 2.27 | 0.48 |
| 6:Ac:268:ALA:HB3 | 6:Ac:471:MET:HG2 | 1.93 | 0.48 |
| 6:Ag:133:LYS:HG2 | 6:Ag:249:GLU:HB2 | 1.96 | 0.48 |
| 6:Ag:520:GLY:O | 6:Ak:341:ARG:NH2 | 2.41 | 0.48 |
| 6:Ak:252:PHE:HD1 | 6:Ak:252:PHE:H | 1.59 | 0.48 |
| 5:Av:29:VAL:HG21 | 5:Av:198:ILE:HD13 | 1.94 | 0.48 |
| 5:Av:56:ALA:HA | 5:Av:59:GLN:HE21 | 1.78 | 0.48 |
| 6:Ay:312:TYR:CZ | 6:Ay:507:LEU:HG | 2.48 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B4:32:LYS:HD2 | 2:B4:350:VAL:HG11 | 1.94 | 0.48 |
| 2:B4:373:PHE:HB2 | 2:B4:405:VAL:HG22 | 1.95 | 0.48 |
| 2:B5:116:ILE:HD11 | 2:B5:131:ILE:HG13 | 1.96 | 0.48 |
| 2:B5:126:GLU:HB2 | 2:B5:150:ILE:HD11 | 1.95 | 0.48 |
| 2:B7:42:LYS:NZ | 2:B7:43:GLN:O | 2.36 | 0.48 |
| 5:BD:494:THR:HG23 | 5:BD:497:GLU:H | 1.78 | 0.48 |
| 5:BH:125:MET:O | 5:BH:129:GLU:HG2 | 2.13 | 0.48 |
| 6:BK:78:ASN:ND2 | 11:BU:5:ARG:O | 2.44 | 0.48 |
| 11:BT:10:ILE:HD11 | 11:BT:35:TYR:CE1 | 2.48 | 0.48 |
| 11:BT:11:LYS:HG3 | 11:BT:27:GLU:HG2 | 1.94 | 0.48 |
| 3:BX:83:GLN:HA | 3:BX:86:VAL:HG22 | 1.95 | 0.48 |
| 3:Bb:74:MET:HE3 | 3:Bb:150:ILE:HD11 | 1.95 | 0.48 |
| 2:Bs:560:LEU:O | 2:Bs:564:ILE:HG12 | 2.14 | 0.48 |
| 2:Bt:110:TYR:N | 2:Bt:138:GLY:HA3 | 2.27 | 0.48 |
| 2:Bt:406:LEU:HD13 | 2:Bt:475:ALA:HB2 | 1.95 | 0.48 |
| 2:Bu:352:ALA:HB2 | 2:Bu:385:THR:HA | 1.95 | 0.48 |
| 2:Bw:418:PRO:HG2 | 2:Bw:421:ARG:HE | 1.78 | 0.48 |
| 1:k:56:VAL:HG11 | 1:k:140:PHE:HE1 | 1.78 | 0.48 |
| 1:p:137:LEU:HB3 | 1:p:146:LEU:HD21 | 1.95 | 0.48 |
| 8:t:204:ASP:OD1 | 8:t:205:ALA:N | 2.46 | 0.48 |
| 9:w:139:SER:HB3 | 9:w:156:THR:H | 1.77 | 0.48 |
| 1:0:76:LEU:HD21 | 8:q:128:ASP:HB3 | 1.93 | 0.48 |
| 2:2:571:ARG:NH2 | 2:2:587:GLU:OE1 | 2.38 | 0.48 |
| 2:3:464:VAL:HG12 | 2:AK:313:ASP:HB3 | 1.95 | 0.48 |
| 3:6:97:ASN:O | 3:6:97:ASN:ND2 | 2.41 | 0.48 |
| 3:8:148:ASN:HA | 9:v:47:THR:HG22 | 1.96 | 0.48 |
| 3:9:58:ILE:HG12 | 3:AF:6:VAL:HG21 | 1.96 | 0.48 |
| 4:A:44:MET:HE1 | 4:F:44:MET:HG2 | 1.94 | 0.48 |
| 5:A2:175:ARG:NH1 | 5:BD:32:THR:O | 2.46 | 0.48 |
| 6:A7:284:MET:HE1 | 6:A8:127:LEU:HD13 | 1.95 | 0.48 |
| 6:A8:345:TRP:O | 6:A8:348:GLU:HG2 | 2.13 | 0.48 |
| 6:A9:108:ALA:HB2 | 6:A9:303:ASN:HB2 | 1.95 | 0.48 |
| 6:A9:315:GLN:HE21 | 6:A9:514:ARG:HD3 | 1.78 | 0.48 |
| 8:AB:71:ILE:HG21 | 1:p:211:HIS:HA | 1.94 | 0.48 |
| 3:AH:22:GLN:HB2 | 3:AH:116:TYR:HE1 | 1.78 | 0.48 |
| 3:AH:58:ILE:HD13 | 3:AH:58:ILE:H | 1.78 | 0.48 |
| 2:AL:247:GLY:O | 2:AL:263:SER:OG | 2.31 | 0.48 |
| 2:AL:526:THR:OG1 | 2:AL:527:GLY:N | 2.44 | 0.48 |
| 7:Aa:301:ASP:N | 7:Aa:301:ASP:OD1 | 2.45 | 0.48 |
| 6:Ad:332:PHE:HB3 | 6:Ad:518:VAL:HG12 | 1.95 | 0.48 |
| 6:Ae:300:LEU:HG | 6:Ai:150:PRO:HG3 | 1.95 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ai:235:LEU:O | 6:Ai:245:ASN:ND2 | 2.46 | 0.48 |
| 6:Ai:265:GLN:HB3 | 6:Am:247:TRP:CZ3 | 2.47 | 0.48 |
| 6:Ai:278:LEU:HD12 | 6:Ai:286:ALA:HB2 | 1.94 | 0.48 |
| 6:Ao:494:SER:C | 6:Ao:496:ILE:H | 2.20 | 0.48 |
| 6:Ao:494:SER:HA | 11:BU:37:ASP:CG | 2.37 | 0.48 |
| 7:Aq:212:SER:HB2 | 7:Aq:227:VAL:HG21 | 1.95 | 0.48 |
| 7:At:118:ASN:OD1 | 7:At:118:ASN:N | 2.44 | 0.48 |
| 2:B2:110:TYR:CE1 | 2:B2:177:GLY:HA3 | 2.49 | 0.48 |
| 2:B3:488:TRP:HB3 | 2:B3:556:LEU:HD12 | 1.96 | 0.48 |
| 2:B4:66:MET:HE1 | 2:B4:459:ASP:HB2 | 1.95 | 0.48 |
| 2:B4:106:PRO:HB3 | 2:B4:139:LYS:HA | 1.95 | 0.48 |
| 2:B4:518:TYR:OH | 2:B4:538:ASP:OD1 | 2.32 | 0.48 |
| 2:B6:34:GLN:NE2 | 2:B6:56:GLN:O | 2.46 | 0.48 |
| 2:B6:272:GLY:O | 2:B6:274:GLN:NE2 | 2.47 | 0.48 |
| 7:BE:70:LYS:NZ | 5:BG:318:THR:O | 2.46 | 0.48 |
| 5:BF:44:GLU:HB3 | 5:BF:188:ILE:HB | 1.95 | 0.48 |
| 5:BG:94:GLU:HG3 | 5:BG:379:ARG:HH21 | 1.78 | 0.48 |
| 5:BG:209:ASP:O | 5:BG:211:ALA:N | 2.46 | 0.48 |
| 5:BG:474:GLU:HG3 | 5:BG:475:PRO:HD3 | 1.95 | 0.48 |
| 3:BX:82:ARG:HH12 | 3:BX:138:GLY:HA2 | 1.78 | 0.48 |
| 3:Bk:75:ASN:ND2 | 3:Bk:151:GLN:OE1 | 2.42 | 0.48 |
| 2:Bp:378:CYS:SG | 2:Bp:454:TYR:OH | 2.61 | 0.48 |
| 2:Br:230:LEU:HD23 | 2:Br:233:LYS:HB2 | 1.95 | 0.48 |
| 2:Br:302:LYS:O | 2:Br:307:SER:N | 2.45 | 0.48 |
| 2:Bt:90:LYS:NZ | 2:Bt:190:ASP:OD1 | 2.33 | 0.48 |
| 2:Bt:455:LYS:HG3 | 2:Bt:468:VAL:HG23 | 1.94 | 0.48 |
| 2:Bt:455:LYS:NZ | 2:Bt:473:ASP:OD1 | 2.45 | 0.48 |
| 2:Bw:133:GLU:HB3 | 2:Bw:142:LYS:HB3 | 1.95 | 0.48 |
| 2:Bw:427:VAL:HG22 | 2:Bw:520:GLU:HG3 | 1.96 | 0.48 |
| 2:Bx:195:LEU:HD12 | 2:Bx:198:ILE:HD12 | 1.95 | 0.48 |
| 8:s:241:ASP:OD1 | 8:s:241:ASP:N | 2.46 | 0.48 |
| 8:s:258:ASN:OD1 | 8:s:258:ASN:N | 2.45 | 0.48 |
| 9:y:91:MET:HE1 | 9:y:138:LEU:HB2 | 1.95 | 0.48 |
| 2:1:457:GLN:HG2 | 2:1:458:TYR:H | 1.78 | 0.48 |
| 2:4:521:ALA:HB1 | 2:4:541:ALA:HA | 1.94 | 0.48 |
| 2:5:128:GLU:HB2 | 2:5:146:PRO:HG2 | 1.94 | 0.48 |
| 3:8:97:ASN:O | 3:8:97:ASN:ND2 | 2.46 | 0.48 |
| 5:A1:397:THR:OG1 | 5:A1:399:ASP:OD1 | 2.24 | 0.48 |
| 5:A2:293:PRO:O | 5:A2:295:ARG:N | 2.46 | 0.48 |
| 5:A3:381:PRO:HA | 5:A3:384:GLN:HG2 | 1.94 | 0.48 |
| 6:A7:131:TYR:HA | 6:A7:250:MET:HA | 1.96 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:AB:61:SER:OG | 8:AB:62:GLN:N | 2.43 | 0.48 |
| 2:AK:131:ILE:HD13 | 2:AK:140:ILE:HG21 | 1.94 | 0.48 |
| 2:AK:464:VAL:HG12 | 2:Bs:313:ASP:HB3 | 1.95 | 0.48 |
| 2:AL:455:LYS:HD2 | 2:AL:502:VAL:HG22 | 1.96 | 0.48 |
| 2:AM:157:VAL:HG23 | 2:AM:159:GLU:H | 1.78 | 0.48 |
| 2:AN:107:GLY:HA3 | 2:AN:110:TYR:HE1 | 1.79 | 0.48 |
| 2:AN:115:LYS:HB3 | 2:AN:172:SER:HB3 | 1.96 | 0.48 |
| 2:AN:148:ALA:O | 2:AN:151:ILE:HG13 | 2.14 | 0.48 |
| 2:AP:135:ASP:N | 2:AP:139:LYS:O | 2.40 | 0.48 |
| 6:AV:365:ALA:HB2 | 6:AV:372:GLU:HG2 | 1.96 | 0.48 |
| 6:AZ:374:ASN:OD1 | 6:AZ:374:ASN:N | 2.45 | 0.48 |
| 6:An:460:ARG:HH21 | 7:As:112:LEU:HD11 | 1.77 | 0.48 |
| 2:B1:4:LEU:HD11 | 2:B1:267:ALA:HA | 1.95 | 0.48 |
| 2:B1:417:ILE:HD13 | 2:B1:417:ILE:H | 1.79 | 0.48 |
| 2:B2:3:LEU:HD11 | 2:B2:9:GLU:HB2 | 1.96 | 0.48 |
| 2:B2:66:MET:HE1 | 2:B2:459:ASP:HB2 | 1.94 | 0.48 |
| 5:BH:190:THR:HG22 | 5:BH:199:VAL:HG12 | 1.94 | 0.48 |
| 3:Bj:43:ALA:O | 3:Bj:162:TRP:NE1 | 2.46 | 0.48 |
| 2:Bp:455:LYS:HG3 | 2:Bp:502:VAL:HG13 | 1.94 | 0.48 |
| 2:Bq:645:THR:OG1 | 2:Br:629:ILE:O | 2.30 | 0.48 |
| 2:Br:596:LYS:NZ | 2:Br:602:TYR:O | 2.41 | 0.48 |
| 2:Bt:451:ASP:OD1 | 2:Bt:452:GLY:N | 2.40 | 0.48 |
| 2:Bu:364:ASP:O | 2:Bu:367:SER:N | 2.43 | 0.48 |
| 2:Bu:617:VAL:HA | 2:Bu:620:ARG:HD2 | 1.95 | 0.48 |
| 2:Bx:235:GLU:OE2 | 2:Bx:261:ARG:NH1 | 2.46 | 0.48 |
| 2:Bx:427:VAL:HG13 | 2:Bx:520:GLU:HG3 | 1.95 | 0.48 |
| 2:By:240:SER:OG | 2:By:243:ASP:OD1 | 2.31 | 0.48 |
| 2:Bz:163:LEU:HD11 | 2:Bz:187:ILE:HG12 | 1.94 | 0.48 |
| 2:Bz:527:GLY:HA2 | 2:Bz:533:TYR:CD2 | 2.48 | 0.48 |
| 4:H:62:ILE:HD12 | 4:S:58:LEU:HD22 | 1.95 | 0.48 |
| 4:M:36:THR:OG1 | 4:M:37:GLN:N | 2.45 | 0.48 |
| 1:k:74:GLU:OE1 | 8:r:127:GLU:N | 2.46 | 0.48 |
| 9:w:168:LYS:HD2 | 9:x:85:ILE:HG21 | 1.94 | 0.48 |
| 2:3:467:TRP:CH2 | 2:AK:199:GLU:HB2 | 2.48 | 0.48 |
| 2:3:569:LYS:O | 2:3:572:LEU:HB2 | 2.13 | 0.48 |
| 2:5:569:LYS:O | 2:5:572:LEU:HB2 | 2.13 | 0.48 |
| 5:A0:216:ALA:O | 5:A0:218:ASP:N | 2.46 | 0.48 |
| 5:A3:184:TYR:OH | 5:A3:204:GLU:OE1 | 2.31 | 0.48 |
| 2:AK:148:ALA:O | 2:AK:151:ILE:HG13 | 2.13 | 0.48 |
| 2:AO:193:ILE:HG21 | 2:AO:223:VAL:HG11 | 1.94 | 0.48 |
| 6:AV:426:ASP:OD2 | 6:AV:433:TYR:OH | 2.27 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:Av:190:THR:HA | 5:Av:199:VAL:HA | 1.95 | 0.48 |
| 6:Az:304:ARG:NH2 | 6:Az:308:ASP:OD1 | 2.46 | 0.48 |
| 2:B1:69:MET:O | 2:B1:73:GLN:HG2 | 2.14 | 0.48 |
| 2:B5:225:LEU:HD22 | 2:B5:321:GLU:HA | 1.94 | 0.48 |
| 7:BL:264:ALA:HB2 | 7:BL:279:GLY:HA3 | 1.94 | 0.48 |
| 3:BZ:95:GLN:HG2 | 3:Bo:64:ARG:NH1 | 2.28 | 0.48 |
| 3:Bd:114:ARG:HB3 | 3:Bd:123:VAL:HG13 | 1.95 | 0.48 |
| 3:Bi:2:PHE:HD2 | 3:Bn:97:ASN:HB3 | 1.79 | 0.48 |
| 3:Bl:103:LYS:O | 3:Bl:106:GLU:HG2 | 2.13 | 0.48 |
| 2:Bp:368:VAL:HG12 | 2:Bp:370:VAL:HG22 | 1.94 | 0.48 |
| 2:Bs:360:ASP:OD1 | 2:Bs:392:HIS:NE2 | 2.39 | 0.48 |
| 2:Bs:495:ASN:OD1 | 2:Bs:495:ASN:N | 2.44 | 0.48 |
| 2:Bv:247:GLY:O | 2:Bv:263:SER:OG | 2.32 | 0.48 |
| 2:Bx:43:GLN:NE2 | 2:Bx:77:ASP:OD2 | 2.46 | 0.48 |
| 4:X:44:MET:HE3 | 4:h:44:MET:HE3 | 1.95 | 0.48 |
| 9:v:106:LYS:HG3 | 9:v:107:THR:HG23 | 1.94 | 0.48 |
| 2:5:94:PRO:HB2 | 2:5:219:ILE:HD12 | 1.95 | 0.48 |
| 2:5:590:GLN:OE1 | 3:AA:8:ARG:NH2 | 2.47 | 0.48 |
| 5:A1:64:SER:O | 5:A1:183:GLN:NE2 | 2.31 | 0.48 |
| 5:A3:392:SER:HB2 | 5:BF:394:THR:HB | 1.94 | 0.48 |
| 6:A4:151:ASP:HB3 | 6:A4:154:PHE:HB2 | 1.94 | 0.48 |
| 2:AD:514:ARG:NH1 | 2:AN:366:GLU:OE2 | 2.46 | 0.48 |
| 2:AD:609:ASP:HB2 | 2:AD:611:THR:HG22 | 1.94 | 0.48 |
| 2:AN:642:PHE:CE2 | 2:B2:564:ILE:HD11 | 2.48 | 0.48 |
| 2:AO:100:GLU:HB3 | 2:AO:188:ILE:HD11 | 1.96 | 0.48 |
| 2:AO:285:ARG:HE | 2:AO:322:TYR:HE2 | 1.61 | 0.48 |
| 2:AO:351:THR:HG23 | 2:AO:354:ASP:H | 1.79 | 0.48 |
| 2:AO:549:ASP:OD2 | 2:AP:271:TYR:OH | 2.26 | 0.48 |
| 10:AU:309:TRP:HB3 | 10:AU:356:SER:HB3 | 1.96 | 0.48 |
| 6:Ae:235:LEU:O | 6:Ae:245:ASN:ND2 | 2.46 | 0.48 |
| 6:Ae:340:ILE:HG13 | 6:Ae:343:ALA:H | 1.78 | 0.48 |
| 6:Aj:305:GLU:OE1 | 6:Aj:477:TYR:OH | 2.17 | 0.48 |
| 6:Ap:452:PRO:HA | 6:Ap:477:TYR:HA | 1.95 | 0.48 |
| 7:Aq:12:LEU:O | 7:Aq:16:ILE:HG12 | 2.13 | 0.48 |
| 7:Aq:180:ASP:OD1 | 7:Aq:181:LEU:N | 2.46 | 0.48 |
| 6:Aw:503:ILE:HA | 6:Aw:507:LEU:HB2 | 1.96 | 0.48 |
| 2:B1:57:PRO:HG3 | 2:B1:65:PHE:HB3 | 1.95 | 0.48 |
| 2:B1:135:ASP:HB3 | 2:B1:139:LYS:HB2 | 1.94 | 0.48 |
| 2:B2:368:VAL:HG12 | 2:B2:370:VAL:HG22 | 1.96 | 0.48 |
| 2:B6:120:TYR:HE1 | 2:B6:166:ASN:HD22 | 1.60 | 0.48 |
| 2:B6:157:VAL:HG23 | 2:B6:159:GLU:H | 1.78 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B6:222:VAL:HG11 | 2:B6:236:ILE:HG21 | 1.95 | 0.48 |
| 2:B6:549:ASP:OD2 | 2:Bq:271:TYR:OH | 2.27 | 0.48 |
| 5:BB:99:ALA:HB2 | 5:BB:407:ILE:HD12 | 1.96 | 0.48 |
| 7:BC:162:TRP:CD1 | 7:BE:54:ASN:HA | 2.49 | 0.48 |
| 5:BF:304:VAL:HG13 | 7:BL:305:GLY:HA2 | 1.95 | 0.48 |
| 5:BF:383:ASP:OD1 | 5:BF:383:ASP:N | 2.46 | 0.48 |
| 5:BG:73:ARG:HG3 | 5:BG:180:ARG:HD2 | 1.94 | 0.48 |
| 5:BH:129:GLU:OE1 | 5:BH:429:LYS:NZ | 2.37 | 0.48 |
| 7:BL:202:VAL:HG22 | 4:M:31:ILE:HG12 | 1.96 | 0.48 |
| 7:BL:204:TYR:CD1 | 7:BL:226:LEU:HD13 | 2.48 | 0.48 |
| 3:BY:64:ARG:NH1 | 3:Bb:95:GLN:HG2 | 2.24 | 0.48 |
| 3:Be:3:VAL:N | 3:Bj:97:ASN:O | 2.44 | 0.48 |
| 3:Bf:137:VAL:HB | 3:Bf:155:VAL:HG13 | 1.95 | 0.48 |
| 3:Bh:8:ARG:HA | 3:Bh:11:GLU:HG2 | 1.95 | 0.48 |
| 3:Bh:137:VAL:HB | 3:Bh:155:VAL:HG13 | 1.96 | 0.48 |
| 3:Bm:54:MET:HE2 | 3:Bn:1:MET:HE2 | 1.95 | 0.48 |
| 2:Bz:188:ILE:HG22 | 2:Bz:190:ASP:H | 1.78 | 0.48 |
| 4:V:9:PRO:HD3 | 4:V:57:VAL:HG21 | 1.96 | 0.48 |
| 4:e:23:SER:OG | 4:e:26:LYS:NZ | 2.37 | 0.48 |
| 3:o:20:LEU:HA | 9:y:54:PHE:HD1 | 1.77 | 0.48 |
| 8:r:61:SER:OG | 8:r:62:GLN:N | 2.44 | 0.48 |
| 8:t:62:GLN:HB3 | 8:t:63:GLU:H | 1.48 | 0.48 |
| 9:v:10:ASN:O | 9:w:79:GLU:N | 2.47 | 0.48 |
| 3:6:161:TYR:CZ | 3:7:97:ASN:HB2 | 2.49 | 0.48 |
| 5:A1:339:ARG:O | 5:BB:290:GLY:HA2 | 2.14 | 0.48 |
| 6:A4:119:SER:O | 6:A4:121:THR:N | 2.47 | 0.48 |
| 6:A4:400:LEU:HD11 | 6:A5:417:LEU:HD22 | 1.95 | 0.48 |
| 7:A6:219:TYR:CE2 | 7:Al:171:LYS:HD2 | 2.49 | 0.48 |
| 6:A8:263:SER:HB3 | 6:A8:476:ARG:HG2 | 1.95 | 0.48 |
| 6:A8:282:HIS:O | 6:A8:282:HIS:ND1 | 2.45 | 0.48 |
| 8:AB:238:VAL:HB | 8:AB:250:THR:HB | 1.95 | 0.48 |
| 3:AG:23:VAL:HG11 | 3:AG:39:THR:HG21 | 1.95 | 0.48 |
| 2:AK:49:ASP:N | 2:AK:49:ASP:OD1 | 2.47 | 0.48 |
| 6:AX:182:PHE:HB2 | 6:AX:184:GLU:O | 2.14 | 0.48 |
| 6:AX:263:SER:HB3 | 6:AX:476:ARG:HG2 | 1.95 | 0.48 |
| 7:AY:59:VAL:HG12 | 7:AY:183:ILE:HG13 | 1.96 | 0.48 |
| 6:Af:364:ILE:HD11 | 6:Af:436:VAL:HG13 | 1.95 | 0.48 |
| 6:Ah:319:SER:HA | 6:Ah:323:LEU:HB2 | 1.95 | 0.48 |
| 6:Aj:397:ALA:HB1 | 6:An:393:ILE:HB | 1.96 | 0.48 |
| 7:Al:87:ILE:HD13 | 7:Al:158:ILE:HB | 1.94 | 0.48 |
| 6:An:211:GLU:OE2 | 6:An:215:GLN:NE2 | 2.44 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:An:386:LEU:HD13 | 6:An:417:LEU:HD11 | 1.95 | 0.48 |
| 6:Ao:242:SER:OG | 6:Ao:245:ASN:ND2 | 2.42 | 0.48 |
| 7:Ar:28:GLU:HB3 | 1:k:31:VAL:HG12 | 1.96 | 0.48 |
| 5:Av:389:MET:HE3 | 5:Ax:395:SER:HB2 | 1.95 | 0.48 |
| 2:B1:99:ILE:HD13 | 2:B1:184:LEU:HD22 | 1.96 | 0.48 |
| 2:B6:166:ASN:OD1 | 2:B6:166:ASN:N | 2.31 | 0.48 |
| 2:B6:278:GLN:HG2 | 2:B6:296:SER:HB3 | 1.95 | 0.48 |
| 2:B7:116:ILE:HG21 | 2:B7:143:ILE:HD12 | 1.96 | 0.48 |
| 5:BA:317:SER:O | 5:BA:319:GLY:N | 2.46 | 0.48 |
| 5:BF:220:ARG:HG2 | 5:BF:221:MET:H | 1.78 | 0.48 |
| 5:BF:301:MET:HE2 | 5:BF:301:MET:HB3 | 1.81 | 0.48 |
| 5:BF:499:GLU:HG3 | 5:BF:503:LYS:HE2 | 1.94 | 0.48 |
| 11:BP:72:ASN:OD1 | 11:BP:73:GLU:N | 2.46 | 0.48 |
| 3:BZ:19:ASN:OD1 | 3:BZ:19:ASN:N | 2.38 | 0.48 |
| 3:Bl:37:LYS:NZ | 3:Bl:152:THR:OG1 | 2.38 | 0.48 |
| 3:Bo:51:VAL:HG23 | 3:Bo:58:ILE:HG12 | 1.95 | 0.48 |
| 2:Bp:364:ASP:O | 2:Bp:367:SER:N | 2.44 | 0.48 |
| 2:Br:31:GLY:O | 2:Br:82:ARG:HA | 2.14 | 0.48 |
| 2:Bu:453:ASN:HD21 | 2:Bu:470:LEU:HD22 | 1.78 | 0.48 |
| 2:Bu:572:LEU:HD12 | 2:Bu:572:LEU:HA | 1.75 | 0.48 |
| 2:Bv:346:SER:O | 2:Bv:350:VAL:HG23 | 2.14 | 0.48 |
| 2:Bw:355:LEU:HD12 | 2:Bw:389:VAL:HG21 | 1.96 | 0.48 |
| 1:k:164:ASN:O | 1:k:164:ASN:ND2 | 2.47 | 0.48 |
| 1:m:243:LYS:H | 8:s:4:TYR:H | 1.60 | 0.48 |
| 1:p:66:VAL:HB | 1:p:77:LYS:HB3 | 1.95 | 0.48 |
| 8:s:203:ASP:OD1 | 8:s:204:ASP:N | 2.47 | 0.48 |
| 9:y:5:LEU:HD23 | 9:y:5:LEU:H | 1.79 | 0.48 |
| 9:z:15:THR:OG1 | 9:z:16:ASN:N | 2.47 | 0.48 |
| 2:1:50:LEU:O | 2:1:54:PHE:HB2 | 2.14 | 0.48 |
| 2:3:638:ILE:HG23 | 2:AK:623:PHE:HD2 | 1.78 | 0.48 |
| 5:A1:63:GLY:HA2 | 6:BK:288:ALA:HB3 | 1.96 | 0.48 |
| 6:A4:362:VAL:HG21 | 6:A9:384:ASN:HD21 | 1.78 | 0.48 |
| 6:A4:494:SER:C | 6:A4:496:ILE:H | 2.21 | 0.48 |
| 6:A4:521:ILE:O | 6:A5:359:LYS:NZ | 2.46 | 0.48 |
| 6:A5:137:ALA:HB3 | 6:A5:140:ALA:HB2 | 1.95 | 0.48 |
| 3:AA:83:GLN:HA | 3:AA:86:VAL:HG22 | 1.95 | 0.48 |
| 2:AK:33:PHE:O | 2:AK:82:ARG:NH2 | 2.47 | 0.48 |
| 2:AL:211:GLN:O | 2:AL:329:ASN:ND2 | 2.47 | 0.48 |
| 2:AN:247:GLY:HA2 | 2:AN:266:LYS:HE2 | 1.94 | 0.48 |
| 2:AN:601:ILE:HG21 | 2:AN:629:ILE:HB | 1.96 | 0.48 |
| 2:AP:424:ASP:OD1 | 2:AP:516:ARG:NH2 | 2.46 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:AT:362:ILE:HD12 | 10:AT:367:LEU:HD13 | 1.94 | 0.48 |
| 6:AX:494:SER:C | 6:AX:496:ILE:H | 2.22 | 0.48 |
| 6:Ae:148:TYR:HD1 | 6:Ae:186:GLY:HA2 | 1.78 | 0.48 |
| 6:Ah:120:PRO:O | 6:Ah:121:THR:OG1 | 2.28 | 0.48 |
| 6:Ah:452:PRO:HA | 6:Ah:477:TYR:HA | 1.96 | 0.48 |
| 6:Ao:336:ASP:HB3 | 6:Ao:339:ASP:HB2 | 1.95 | 0.48 |
| 7:Aq:159:PRO:HB2 | 7:Aq:172:VAL:HG13 | 1.96 | 0.48 |
| 7:Aq:267:GLN:NE2 | 7:Aq:278:ASP:OD1 | 2.45 | 0.48 |
| 7:Ar:6:PRO:HG3 | 7:Ar:15:VAL:HG21 | 1.96 | 0.48 |
| 6:Au:225:ALA:HB3 | 6:BJ:305:GLU:HA | 1.94 | 0.48 |
| 6:Aw:252:PHE:N | 6:BI:67:GLU:OE2 | 2.47 | 0.48 |
| 2:B4:23:SER:O | 2:B4:76:ASN:HB2 | 2.14 | 0.48 |
| 2:B7:273:PRO:HD3 | 2:B7:280:ALA:HB2 | 1.95 | 0.48 |
| 5:BA:320:LYS:HD3 | 5:BA:321:ILE:H | 1.79 | 0.48 |
| 7:BC:173:MET:HE1 | 7:BE:55:LYS:HD2 | 1.94 | 0.48 |
| 7:BC:305:GLY:HA2 | 5:BH:304:VAL:HG13 | 1.96 | 0.48 |
| 5:BF:459:GLU:OE1 | 5:BF:459:GLU:N | 2.44 | 0.48 |
| 6:BM:263:SER:HB3 | 6:BM:476:ARG:HB3 | 1.95 | 0.48 |
| 3:Ba:40:ALA:H | 3:Ba:69:TRP:HE1 | 1.60 | 0.48 |
| 3:Bf:146:SER:HB2 | 3:Bf:149:GLU:HB2 | 1.96 | 0.48 |
| 3:Bn:90:SER:OG | 3:Bn:95:GLN:OE1 | 2.28 | 0.48 |
| 2:Bp:240:SER:OG | 2:Bp:243:ASP:OD1 | 2.32 | 0.48 |
| 2:Bp:464:VAL:HG12 | 2:Bq:313:ASP:HB3 | 1.95 | 0.48 |
| 2:Bq:653:GLU:HB2 | 2:Bt:16:GLN:HG3 | 1.95 | 0.48 |
| 2:Br:566:ARG:HA | 2:Br:569:LYS:HE2 | 1.96 | 0.48 |
| 2:Bt:252:LEU:HB3 | 2:Bt:336:GLY:HA2 | 1.96 | 0.48 |
| 2:Bu:102:THR:N | 2:Bu:183:THR:O | 2.47 | 0.48 |
| 2:Bu:195:LEU:H | 2:Bu:195:LEU:HD23 | 1.78 | 0.48 |
| 2:Bw:33:PHE:O | 2:Bw:82:ARG:NE | 2.47 | 0.48 |
| 2:Bx:106:PRO:HB2 | 2:Bx:139:LYS:HZ2 | 1.78 | 0.48 |
| 2:Bz:39:PHE:HE1 | 2:Bz:84:VAL:H | 1.62 | 0.48 |
| 2:1:455:LYS:HE3 | 2:1:502:VAL:HG22 | 1.96 | 0.48 |
| 2:1:633:ARG:HD3 | 2:AO:619:ASP:HA | 1.95 | 0.48 |
| 2:3:398:ASP:O | 2:3:401:GLN:HG3 | 2.14 | 0.48 |
| 2:4:41:ILE:HD11 | 2:4:361:PHE:HB3 | 1.96 | 0.48 |
| 2:4:117:THR:HG23 | 2:4:127:THR:HG22 | 1.94 | 0.48 |
| 2:5:92:SER:HB3 | 2:5:340:LEU:HB3 | 1.96 | 0.48 |
| 3:7:17:ARG:HH22 | 9:v:47:THR:HG21 | 1.78 | 0.48 |
| 5:A1:469:MET:HE1 | 5:BD:460:ALA:HB1 | 1.95 | 0.48 |
| 5:A2:82:LEU:HD11 | 5:A2:261:ALA:HB3 | 1.96 | 0.48 |
| 3:AJ:54:MET:H | 3:AJ:54:MET:HG2 | 1.40 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AP:40:GLN:H | 2:AP:81:VAL:HG23 | 1.79 | 0.48 |
| 7:AY:43:GLU:O | 7:AY:47:GLU:HG2 | 2.13 | 0.48 |
| 7:AY:144:LEU:O | 7:AY:148:MET:HG2 | 2.14 | 0.48 |
| 6:Ad:264:ARG:NE | 6:Ah:155:SER:OG | 2.45 | 0.48 |
| 6:Ae:265:GLN:HB3 | 6:Ai:247:TRP:CZ3 | 2.49 | 0.48 |
| 6:Af:343:ALA:HB1 | 6:Af:348:GLU:HB2 | 1.95 | 0.48 |
| 6:Ak:184:GLU:O | 6:Ak:185:THR:OG1 | 2.28 | 0.48 |
| 6:Au:72:HIS:C | 6:Au:74:TYR:H | 2.22 | 0.48 |
| 6:Aw:204:ASP:OD1 | 6:Aw:205:ALA:N | 2.47 | 0.48 |
| 2:B1:29:LEU:O | 2:B1:80:VAL:HA | 2.13 | 0.48 |
| 2:B2:163:LEU:HD11 | 2:B2:187:ILE:HG12 | 1.95 | 0.48 |
| 2:B4:33:PHE:HA | 2:B4:61:THR:HG23 | 1.96 | 0.48 |
| 2:B4:46:ASN:OD1 | 2:B4:47:GLU:N | 2.47 | 0.48 |
| 2:B5:495:ASN:OD1 | 2:B5:495:ASN:N | 2.46 | 0.48 |
| 5:BB:190:THR:HG22 | 5:BB:199:VAL:HG12 | 1.95 | 0.48 |
| 7:BC:94:SER:OG | 7:BC:97:SER:O | 2.24 | 0.48 |
| 7:BC:148:MET:HB3 | 7:BE:107:PHE:CE1 | 2.49 | 0.48 |
| 5:BF:82:LEU:HD11 | 5:BF:261:ALA:HB3 | 1.96 | 0.48 |
| 5:BF:129:GLU:OE1 | 5:BF:425:ASN:ND2 | 2.47 | 0.48 |
| 2:Br:159:GLU:HB3 | 2:Br:163:LEU:HA | 1.96 | 0.48 |
| 2:Br:419:VAL:HG13 | 2:Br:507:ILE:HB | 1.96 | 0.48 |
| 2:Bt:32:LYS:NZ | 2:Bt:60:GLU:OE2 | 2.35 | 0.48 |
| 2:Bu:99:ILE:O | 2:Bu:100:GLU:HG3 | 2.13 | 0.48 |
| 2:Bv:641:ASN:HB2 | 2:Bw:626:THR:HG22 | 1.95 | 0.48 |
| 2:By:645:THR:OG1 | 2:Bz:629:ILE:O | 2.23 | 0.48 |
| 4:L:53:ARG:NH2 | 4:L:56:GLU:OE1 | 2.44 | 0.48 |
| 4:d:41:GLU:N | 4:d:41:GLU:OE1 | 2.47 | 0.48 |
| 1:l:156:ASP:HB3 | 1:l:157:PRO:HD3 | 1.96 | 0.48 |
| 8:r:203:ASP:OD1 | 8:r:204:ASP:N | 2.45 | 0.48 |
| 2:5:514:ARG:NH1 | 2:AM:366:GLU:OE2 | 2.46 | 0.48 |
| 2:5:592:LEU:HD23 | 2:5:604:TYR:HB2 | 1.95 | 0.48 |
| 3:7:75:ASN:HB3 | 3:7:151:GLN:HG3 | 1.95 | 0.48 |
| 4:A:44:MET:HE3 | 4:Q:44:MET:HE3 | 1.96 | 0.48 |
| 6:A4:108:ALA:HB1 | 6:A4:109:PHE:CD2 | 2.49 | 0.48 |
| 6:A5:127:LEU:HD13 | 6:A5:254:ILE:HG12 | 1.96 | 0.48 |
| 9:AC:57:GLY:HA2 | 9:v:66:PHE:H | 1.79 | 0.48 |
| 3:AF:75:ASN:OD1 | 3:AF:79:HIS:HA | 2.14 | 0.48 |
| 3:AI:58:ILE:HD13 | 3:AI:58:ILE:H | 1.79 | 0.48 |
| 3:AI:132:LEU:HD12 | 3:AI:159:LEU:HB3 | 1.96 | 0.48 |
| 2:AK:29:LEU:O | 2:AK:80:VAL:HA | 2.14 | 0.48 |
| 2:AK:153:LYS:O | 2:AK:157:VAL:HG22 | 2.14 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AL:299:ARG:H | 2:AL:299:ARG:HD2 | 1.78 | 0.48 |
| 2:AO:406:LEU:HD13 | 2:AO:475:ALA:HB2 | 1.94 | 0.48 |
| 6:AZ:136:VAL:HG13 | 6:AZ:253:ARG:HH11 | 1.78 | 0.48 |
| 7:Ab:232:GLY:O | 4:i:37:GLN:NE2 | 2.46 | 0.48 |
| 6:Ac:128:ARG:NH1 | 6:Ac:490:GLN:O | 2.47 | 0.48 |
| 6:Af:383:VAL:HG12 | 6:Af:406:THR:HG22 | 1.96 | 0.48 |
| 6:Ag:345:TRP:NE1 | 6:Ak:348:GLU:HB2 | 2.29 | 0.48 |
| 6:Ao:345:TRP:NE1 | 6:BM:348:GLU:HB3 | 2.29 | 0.48 |
| 6:Ap:490:GLN:OE1 | 6:Ap:490:GLN:N | 2.47 | 0.48 |
| 7:Aq:86:ARG:HH22 | 5:BD:312:VAL:HG23 | 1.79 | 0.48 |
| 7:At:18:ARG:HA | 7:At:22:ALA:HA | 1.95 | 0.48 |
| 6:Au:278:LEU:HD12 | 6:Au:286:ALA:HB2 | 1.96 | 0.48 |
| 6:Aw:367:GLN:HB3 | 6:Aw:511:ALA:HB1 | 1.96 | 0.48 |
| 6:Az:285:ASP:HB3 | 6:Az:287:ASP:OD1 | 2.14 | 0.48 |
| 6:BI:105:ASN:HB2 | 6:BI:412:VAL:HG13 | 1.95 | 0.48 |
| 3:Be:89:GLN:NE2 | 3:Be:135:THR:O | 2.47 | 0.48 |
| 3:Bf:48:LYS:NZ | 3:Bi:68:ASP:OD1 | 2.45 | 0.48 |
| 3:Bo:106:GLU:O | 3:Bo:109:LYS:NZ | 2.47 | 0.48 |
| 2:Bp:110:TYR:CD1 | 2:Bp:177:GLY:HA3 | 2.49 | 0.48 |
| 2:Bq:655:THR:HB | 2:Bt:19:VAL:HG21 | 1.96 | 0.48 |
| 2:Bs:206:THR:HA | 2:Bs:211:GLN:HE21 | 1.79 | 0.48 |
| 2:Bx:332:GLU:OE1 | 2:Bx:332:GLU:N | 2.35 | 0.48 |
| 9:y:11:GLN:HA | 9:z:78:ASP:HA | 1.96 | 0.48 |
| 2:1:590:GLN:NE2 | 3:6:8:ARG:HH22 | 2.12 | 0.47 |
| 5:A1:41:ARG:NH1 | 5:A1:67:PRO:HG2 | 2.28 | 0.47 |
| 5:A3:291:ASN:OD1 | 7:A6:299:LEU:HD13 | 2.14 | 0.47 |
| 6:A4:131:TYR:HD2 | 6:A4:250:MET:HE3 | 1.79 | 0.47 |
| 7:A6:30:THR:C | 7:A6:32:ASP:H | 2.22 | 0.47 |
| 6:A7:131:TYR:HE1 | 6:A7:141:LYS:HB2 | 1.78 | 0.47 |
| 6:A7:232:ILE:O | 6:A7:236:GLN:HG2 | 2.14 | 0.47 |
| 8:AB:6:TYR:CD1 | 8:q:132:GLN:HG2 | 2.48 | 0.47 |
| 8:AB:13:TYR:CG | 8:AB:116:MET:HE1 | 2.48 | 0.47 |
| 8:AB:78:HIS:NE2 | 8:q:174:GLU:OE1 | 2.38 | 0.47 |
| 3:AJ:54:MET:HE3 | 3:BX:20:LEU:HA | 1.96 | 0.47 |
| 3:AJ:97:ASN:HB3 | 3:Bg:2:PHE:HB3 | 1.96 | 0.47 |
| 2:AP:101:TYR:O | 2:AP:216:LYS:NZ | 2.40 | 0.47 |
| 2:AP:514:ARG:NH2 | 2:Bp:364:ASP:OD1 | 2.41 | 0.47 |
| 10:AT:374:THR:OG1 | 10:AT:375:TYR:N | 2.47 | 0.47 |
| 6:AX:176:ASP:OD1 | 6:AX:177:ILE:N | 2.45 | 0.47 |
| 6:Ag:385:VAL:O | 6:Ag:389:VAL:HG22 | 2.14 | 0.47 |
| 6:Ap:390:ASP:H | 6:Ap:397:ALA:HB3 | 1.79 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Au:270:TYR:CZ | 6:Au:287:ASP:HB3 | 2.49 | 0.47 |
| 5:Av:312:VAL:HG13 | 5:Av:321:ILE:HG23 | 1.96 | 0.47 |
| 6:Aw:180:HIS:NE2 | 6:Aw:209:ASP:OD1 | 2.41 | 0.47 |
| 6:Az:254:ILE:O | 6:Az:495:ARG:NH2 | 2.47 | 0.47 |
| 2:B1:41:ILE:HD13 | 2:B1:81:VAL:HB | 1.96 | 0.47 |
| 2:B5:242:ALA:O | 2:B5:246:LYS:NZ | 2.46 | 0.47 |
| 2:B5:642:PHE:CZ | 2:B6:564:ILE:HD11 | 2.49 | 0.47 |
| 2:B6:430:ARG:HH21 | 2:B6:541:ALA:HB1 | 1.78 | 0.47 |
| 5:BA:132:ASP:O | 5:BA:136:HIS:ND1 | 2.43 | 0.47 |
| 7:BE:12:LEU:HD21 | 7:BE:248:LYS:HG2 | 1.96 | 0.47 |
| 5:BH:350:LEU:HD12 | 5:BH:351:PRO:HD2 | 1.96 | 0.47 |
| 7:BL:161:PHE:HA | 7:BL:171:LYS:O | 2.14 | 0.47 |
| 3:BZ:47:GLU:N | 3:BZ:63:ASP:O | 2.45 | 0.47 |
| 3:Bl:41:LEU:HD11 | 3:Bl:127:ILE:HG21 | 1.96 | 0.47 |
| 2:Bq:252:LEU:HB3 | 2:Bq:335:SER:O | 2.14 | 0.47 |
| 2:Bq:409:PRO:O | 2:Bq:454:TYR:OH | 2.25 | 0.47 |
| 2:Br:118:VAL:HG22 | 2:Br:169:ALA:HB2 | 1.95 | 0.47 |
| 2:Br:135:ASP:OD1 | 2:Br:136:ALA:N | 2.47 | 0.47 |
| 2:Bu:355:LEU:HD12 | 2:Bu:389:VAL:HG21 | 1.95 | 0.47 |
| 2:Bu:488:TRP:HE1 | 2:Bu:489:MET:HE2 | 1.78 | 0.47 |
| 2:Bv:224:ALA:HB2 | 2:Bv:340:LEU:HD13 | 1.95 | 0.47 |
| 2:By:66:MET:HG2 | 2:By:468:VAL:HG21 | 1.96 | 0.47 |
| 4:V:10:PHE:HB3 | 4:V:22:ILE:HG12 | 1.95 | 0.47 |
| 1:n:86:PHE:CE2 | 1:n:88:ALA:HB2 | 2.49 | 0.47 |
| 1:p:164:ASN:O | 1:p:164:ASN:ND2 | 2.47 | 0.47 |
| 8:r:134:VAL:HG21 | 8:r:188:TRP:CE3 | 2.49 | 0.47 |
| 2:2:432:ALA:HB2 | 2:2:440:ASN:ND2 | 2.28 | 0.47 |
| 2:5:272:GLY:O | 2:5:274:GLN:NE2 | 2.45 | 0.47 |
| 5:A0:291:ASN:OD1 | 7:BE:299:LEU:HD13 | 2.14 | 0.47 |
| 5:A0:423:LYS:HG3 | 5:A0:437:TRP:CD1 | 2.49 | 0.47 |
| 5:A2:12:TRP:CG | 5:A2:234:ALA:HB2 | 2.49 | 0.47 |
| 6:A4:147:MET:HE3 | 6:A4:366:ARG:HH12 | 1.79 | 0.47 |
| 7:A6:18:ARG:HA | 7:A6:22:ALA:HA | 1.97 | 0.47 |
| 6:A9:414:ALA:HB3 | 6:A9:423:VAL:HG13 | 1.96 | 0.47 |
| 8:AB:216:PHE:CE1 | 2:AD:561:LYS:HG2 | 2.49 | 0.47 |
| 2:AD:455:LYS:HD2 | 2:AD:502:VAL:HG22 | 1.96 | 0.47 |
| 3:AF:97:ASN:HA | 3:Bm:3:VAL:HG12 | 1.97 | 0.47 |
| 3:AJ:23:VAL:HG22 | 3:AJ:36:CYS:SG | 2.54 | 0.47 |
| 2:AL:456:TYR:HB3 | 2:AL:504:LYS:HB3 | 1.95 | 0.47 |
| 2:AN:264:THR:HB | 2:AN:267:ALA:HB3 | 1.96 | 0.47 |
| 2:AO:116:ILE:HD11 | 2:AO:131:ILE:HG13 | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AP:37:PRO:HG2 | 2:AP:42:LYS:HD3 | 1.96 | 0.47 |
| 6:AX:278:LEU:HD12 | 6:AX:284:MET:HB2 | 1.95 | 0.47 |
| 7:Aa:305:GLY:HA2 | 5:BB:304:VAL:HG13 | 1.95 | 0.47 |
| 7:Ab:159:PRO:HB3 | 7:Ab:174:GLY:O | 2.14 | 0.47 |
| 6:Ae:355:PHE:HB2 | 6:Ay:398:GLN:HE22 | 1.79 | 0.47 |
| 6:An:93:PRO:HG3 | 7:Aq:98:MET:HE2 | 1.96 | 0.47 |
| 6:Ap:278:LEU:HD12 | 6:Ap:284:MET:HB2 | 1.96 | 0.47 |
| 7:Ar:88:LEU:HD11 | 7:Ar:185:GLU:HB2 | 1.95 | 0.47 |
| 5:Av:38:ASP:OD2 | 5:Av:186:ARG:NH2 | 2.47 | 0.47 |
| 6:Aw:142:GLU:H | 6:Aw:490:GLN:HG2 | 1.79 | 0.47 |
| 2:B4:654:LEU:HD22 | 2:B4:655:THR:H | 1.78 | 0.47 |
| 2:B6:33:PHE:HA | 2:B6:61:THR:HG23 | 1.96 | 0.47 |
| 2:B7:101:TYR:CE2 | 2:B7:143:ILE:HG12 | 2.49 | 0.47 |
| 2:B7:308:ASN:ND2 | 2:B7:313:ASP:OD2 | 2.48 | 0.47 |
| 2:B7:455:LYS:HD3 | 2:B7:502:VAL:HG13 | 1.95 | 0.47 |
| 5:BA:182:VAL:HG22 | 5:BA:208:TYR:HD1 | 1.78 | 0.47 |
| 5:BD:213:GLU:HA | 5:BD:221:MET:HE1 | 1.96 | 0.47 |
| 6:BI:120:PRO:HD3 | 6:BI:453:TYR:CZ | 2.49 | 0.47 |
| 6:BJ:180:HIS:CE1 | 6:BJ:212:ILE:HD12 | 2.49 | 0.47 |
| 3:BZ:114:ARG:HG2 | 3:BZ:126:GLU:HG2 | 1.96 | 0.47 |
| 3:Ba:83:GLN:NE2 | 3:Ba:87:ASP:OD1 | 2.47 | 0.47 |
| 3:Bf:103:LYS:N | 3:Bf:106:GLU:OE2 | 2.46 | 0.47 |
| 2:Bp:332:GLU:H | 2:Bp:332:GLU:CD | 2.22 | 0.47 |
| 2:Bq:42:LYS:NZ | 2:Bq:43:GLN:O | 2.47 | 0.47 |
| 2:Bv:3:LEU:HG | 2:Bv:9:GLU:HB2 | 1.97 | 0.47 |
| 2:Bv:256:PRO:HG2 | 2:Bv:339:THR:H | 1.79 | 0.47 |
| 2:Bz:89:ALA:HA | 2:Bz:345:SER:HA | 1.95 | 0.47 |
| 8:t:61:SER:O | 8:t:62:GLN:HB2 | 2.13 | 0.47 |
| 9:v:168:LYS:HB3 | 9:v:173:ILE:HD11 | 1.95 | 0.47 |
| 1:0:63:ARG:HH12 | 8:q:125:ARG:HH22 | 1.62 | 0.47 |
| 2:4:451:ASP:HB2 | 2:4:471:ALA:HB2 | 1.96 | 0.47 |
| 2:5:28:ALA:HB2 | 2:5:370:VAL:HG21 | 1.95 | 0.47 |
| 3:6:83:GLN:HA | 3:6:86:VAL:HG22 | 1.95 | 0.47 |
| 5:A2:370:TYR:HD2 | 5:A2:375:VAL:HB | 1.78 | 0.47 |
| 6:A5:131:TYR:HD2 | 6:A5:250:MET:HE3 | 1.79 | 0.47 |
| 6:A9:345:TRP:CD1 | 6:A9:345:TRP:H | 2.32 | 0.47 |
| 3:AA:86:VAL:HG12 | 3:AA:137:VAL:HG21 | 1.96 | 0.47 |
| 8:AB:84:TYR:CZ | 8:q:143:PRO:HD3 | 2.49 | 0.47 |
| 2:AD:559:MET:O | 2:AD:563:ASN:ND2 | 2.47 | 0.47 |
| 3:AI:54:MET:HE1 | 3:Bm:22:GLN:HG3 | 1.96 | 0.47 |
| 3:AI:94:GLY:HA3 | 3:AI:100:THR:OG1 | 2.13 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AK:110:TYR:CD1 | 2:AK:177:GLY:HA3 | 2.50 | 0.47 |
| 2:AM:353:GLY:HA2 | 2:AM:356:MET:HE2 | 1.96 | 0.47 |
| 2:AO:109:ASN:N | 2:AO:138:GLY:HA3 | 2.30 | 0.47 |
| 6:AW:317:GLY:HA3 | 6:AW:516:VAL:HG22 | 1.95 | 0.47 |
| 6:AW:502:SER:O | 6:AW:506:SER:OG | 2.32 | 0.47 |
| 6:Ae:247:TRP:CG | 6:Ay:267:LYS:HD3 | 2.50 | 0.47 |
| 7:Ar:193:ASP:O | 7:Ar:242:TYR:OH | 2.33 | 0.47 |
| 7:Ar:307:LEU:HB2 | 5:Ax:335:TRP:HB2 | 1.95 | 0.47 |
| 7:At:159:PRO:HB3 | 7:At:174:GLY:O | 2.15 | 0.47 |
| 6:Aw:260:GLU:OE2 | 6:BM:72:HIS:ND1 | 2.46 | 0.47 |
| 6:Aw:344:ARG:HH21 | 6:BM:345:TRP:CD1 | 2.32 | 0.47 |
| 2:B5:57:PRO:O | 2:B5:462:ASN:ND2 | 2.43 | 0.47 |
| 2:B6:2:THR:OG1 | 2:B6:3:LEU:N | 2.47 | 0.47 |
| 2:B6:651:PHE:HE2 | 2:B7:630:GLN:HB2 | 1.80 | 0.47 |
| 7:BC:85:THR:HG21 | 7:BC:187:TRP:HE1 | 1.78 | 0.47 |
| 7:BC:147:TYR:OH | 5:BG:269:ASP:OD2 | 2.32 | 0.47 |
| 7:BC:200:ASN:OD1 | 7:BC:229:ARG:NH2 | 2.46 | 0.47 |
| 5:BF:310:ASN:ND2 | 5:BF:323:ASN:HD21 | 2.12 | 0.47 |
| 3:BX:64:ARG:NH1 | 3:Ba:95:GLN:HB3 | 2.30 | 0.47 |
| 3:Bc:95:GLN:OE1 | 3:Bc:95:GLN:N | 2.47 | 0.47 |
| 3:Be:125:LYS:NZ | 3:Bh:83:GLN:OE1 | 2.45 | 0.47 |
| 3:Bl:119:ASP:OD1 | 3:Bn:101:GLY:N | 2.47 | 0.47 |
| 3:Bo:14:ASP:OD1 | 3:Bo:14:ASP:N | 2.46 | 0.47 |
| 2:By:470:LEU:HD11 | 2:By:499:ILE:HG21 | 1.96 | 0.47 |
| 2:Bz:24:THR:O | 2:Bz:483:ASN:ND2 | 2.42 | 0.47 |
| 8:t:99:GLN:HB3 | 8:t:243:ASP:HB3 | 1.95 | 0.47 |
| 2:1:398:ASP:O | 2:1:401:GLN:HG2 | 2.14 | 0.47 |
| 2:4:569:LYS:O | 2:4:572:LEU:HB2 | 2.15 | 0.47 |
| 5:A0:426:LEU:HD13 | 5:A0:432:ILE:HD12 | 1.96 | 0.47 |
| 5:A2:99:ALA:O | 5:A2:411:GLN:NE2 | 2.48 | 0.47 |
| 5:A2:221:MET:HE1 | 5:BD:190:THR:HG21 | 1.96 | 0.47 |
| 5:A3:105:ASP:N | 5:A3:105:ASP:OD1 | 2.47 | 0.47 |
| 6:A8:452:PRO:HA | 6:A8:477:TYR:HA | 1.95 | 0.47 |
| 6:A9:467:PHE:CD2 | 6:An:459:LEU:HB3 | 2.50 | 0.47 |
| 8:AB:264:PRO:O | 2:AD:620:ARG:NH2 | 2.47 | 0.47 |
| 3:AE:70:THR:HG22 | 3:AE:156:THR:HG22 | 1.94 | 0.47 |
| 2:AL:414:VAL:HG23 | 2:AL:422:ALA:HB1 | 1.96 | 0.47 |
| 2:AN:430:ARG:HH21 | 2:AN:442:ASN:HA | 1.78 | 0.47 |
| 6:AZ:131:TYR:HA | 6:AZ:250:MET:HA | 1.96 | 0.47 |
| 7:Aa:55:LYS:HE2 | 7:As:173:MET:HE1 | 1.96 | 0.47 |
| 6:Ac:322:THR:HG21 | 6:Ac:363:GLU:HB2 | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ah:107:ILE:C | 6:Ah:303:ASN:HD21 | 2.22 | 0.47 |
| 6:Ah:383:VAL:HG12 | 6:Ah:406:THR:HG22 | 1.96 | 0.47 |
| 7:Al:13:LYS:HG3 | 7:Al:34:ILE:HG21 | 1.95 | 0.47 |
| 6:An:344:ARG:HE | 6:BK:344:ARG:NH1 | 2.12 | 0.47 |
| 6:Ao:490:GLN:OE1 | 6:Ao:490:GLN:N | 2.47 | 0.47 |
| 7:Aq:173:MET:HE1 | 7:As:55:LYS:HE2 | 1.96 | 0.47 |
| 7:At:75:ASP:OD1 | 7:At:75:ASP:N | 2.45 | 0.47 |
| 7:At:91:ASN:H | 5:BA:316:ALA:HB2 | 1.79 | 0.47 |
| 2:B2:89:ALA:HA | 2:B2:345:SER:HA | 1.96 | 0.47 |
| 2:B2:518:TYR:HE1 | 2:B2:537:GLY:HA3 | 1.79 | 0.47 |
| 2:B2:523:ASN:OD1 | 2:B2:539:LYS:N | 2.40 | 0.47 |
| 2:B3:244:TYR:CZ | 2:B3:266:LYS:HG2 | 2.49 | 0.47 |
| 2:B3:271:TYR:OH | 2:Bz:549:ASP:OD2 | 2.21 | 0.47 |
| 2:B5:57:PRO:HB3 | 2:B5:62:ALA:HA | 1.95 | 0.47 |
| 2:B7:69:MET:O | 2:B7:73:GLN:HG2 | 2.14 | 0.47 |
| 5:BD:72:THR:OG1 | 5:BD:155:ARG:NH2 | 2.42 | 0.47 |
| 7:BE:173:MET:HB3 | 5:BG:321:ILE:HD13 | 1.97 | 0.47 |
| 5:BF:182:VAL:HG22 | 5:BF:208:TYR:HD1 | 1.78 | 0.47 |
| 5:BG:94:GLU:OE2 | 5:BG:379:ARG:NE | 2.46 | 0.47 |
| 6:BI:157:GLN:N | 6:BI:227:GLY:O | 2.47 | 0.47 |
| 3:BY:19:ASN:OD1 | 3:BY:19:ASN:N | 2.37 | 0.47 |
| 3:BZ:100:THR:OG1 | 3:BZ:101:GLY:N | 2.47 | 0.47 |
| 3:Bc:64:ARG:NH2 | 3:Bf:93:ALA:HB3 | 2.29 | 0.47 |
| 3:Bd:70:THR:HG22 | 3:Bd:156:THR:HG22 | 1.95 | 0.47 |
| 2:Bp:37:PRO:HG3 | 2:Bp:226:TYR:CZ | 2.49 | 0.47 |
| 2:Bq:549:ASP:OD2 | 2:Bt:271:TYR:OH | 2.21 | 0.47 |
| 2:Bz:131:ILE:HG12 | 2:Bz:143:ILE:HG22 | 1.96 | 0.47 |
| 1:k:40:GLN:NE2 | 1:k:161:LEU:O | 2.47 | 0.47 |
| 8:s:92:ILE:HD12 | 8:t:142:GLN:HG3 | 1.95 | 0.47 |
| 2:1:252:LEU:HB3 | 2:1:336:GLY:HA2 | 1.96 | 0.47 |
| 2:2:36:GLY:O | 2:2:82:ARG:NH1 | 2.38 | 0.47 |
| 2:4:639:THR:HB | 2:AL:624:VAL:HG12 | 1.95 | 0.47 |
| 2:5:561:LYS:HG2 | 8:u:216:PHE:CE1 | 2.50 | 0.47 |
| 3:8:148:ASN:OD1 | 3:8:148:ASN:N | 2.47 | 0.47 |
| 3:9:115:GLN:HG2 | 3:AA:79:HIS:CE1 | 2.50 | 0.47 |
| 5:A1:419:LEU:HD13 | 5:A1:441:ILE:HD11 | 1.96 | 0.47 |
| 5:A3:26:GLU:HG2 | 5:A3:28:LEU:HG | 1.97 | 0.47 |
| 6:A5:286:ALA:N | 6:A5:289:GLU:OE1 | 2.47 | 0.47 |
| 6:A7:264:ARG:NH1 | 6:A7:477:TYR:HH | 2.12 | 0.47 |
| 6:A7:344:ARG:HG3 | 10:AU:306:TRP:HZ2 | 1.78 | 0.47 |
| 6:A8:374:ASN:ND2 | 6:A8:439:LYS:O | 2.39 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:572:LEU:HD12 | 2:AD:572:LEU:HA | 1.75 | 0.47 |
| 2:AL:406:LEU:HD13 | 2:AL:475:ALA:HB2 | 1.96 | 0.47 |
| 2:AP:457:GLN:HA | 2:AP:503:ILE:HG23 | 1.96 | 0.47 |
| 6:AV:225:ALA:HB3 | 6:Ap:305:GLU:HA | 1.95 | 0.47 |
| 6:AV:402:THR:HG22 | 6:AZ:420:LYS:HD2 | 1.96 | 0.47 |
| 6:AZ:449:TYR:CZ | 6:AZ:482:ASN:HB2 | 2.49 | 0.47 |
| 6:Af:93:PRO:HA | 6:Aj:121:THR:O | 2.15 | 0.47 |
| 6:Ah:377:ILE:HG23 | 6:Ah:435:THR:HB | 1.97 | 0.47 |
| 6:Aj:273:GLU:OE1 | 6:Aj:273:GLU:N | 2.48 | 0.47 |
| 6:Ak:319:SER:HA | 6:Ak:323:LEU:HB2 | 1.96 | 0.47 |
| 7:Aq:12:LEU:HD12 | 7:Aq:242:TYR:HD2 | 1.79 | 0.47 |
| 5:Av:86:TYR:C | 5:Av:88:VAL:H | 2.23 | 0.47 |
| 5:Ax:145:ASP:OD2 | 5:BA:413:LYS:NZ | 2.36 | 0.47 |
| 2:B1:153:LYS:HB3 | 2:B1:167:TRP:HH2 | 1.80 | 0.47 |
| 2:B2:642:PHE:CZ | 2:B3:561:LYS:HG2 | 2.49 | 0.47 |
| 2:B3:193:ILE:HD11 | 2:B3:205:MET:HG2 | 1.97 | 0.47 |
| 2:B3:438:ASP:OD1 | 2:B3:438:ASP:N | 2.45 | 0.47 |
| 2:B4:346:SER:O | 2:B4:350:VAL:HG23 | 2.15 | 0.47 |
| 5:BB:254:LEU:O | 5:BB:258:VAL:HG23 | 2.14 | 0.47 |
| 5:BG:494:THR:OG1 | 5:BG:495:ASP:N | 2.48 | 0.47 |
| 6:BI:345:TRP:CD1 | 6:BI:346:ALA:H | 2.31 | 0.47 |
| 6:BK:241:GLY:HA3 | 11:BP:43:GLY:HA2 | 1.96 | 0.47 |
| 3:Bc:103:LYS:O | 3:Bc:106:GLU:HG2 | 2.14 | 0.47 |
| 3:Bg:39:THR:HG22 | 3:Bg:71:VAL:HG22 | 1.97 | 0.47 |
| 3:Bl:41:LEU:HB3 | 3:Bo:140:LEU:HB3 | 1.95 | 0.47 |
| 2:Bs:107:GLY:H | 2:Bs:140:ILE:HG12 | 1.79 | 0.47 |
| 2:Bw:91:ASN:N | 2:Bw:91:ASN:OD1 | 2.47 | 0.47 |
| 2:Bw:539:LYS:HG3 | 2:Bw:541:ALA:H | 1.78 | 0.47 |
| 1:l:201:LEU:HB3 | 1:l:205:ARG:HH21 | 1.79 | 0.47 |
| 8:t:152:GLN:HE21 | 8:t:152:GLN:HB3 | 1.56 | 0.47 |
| 2:1:57:PRO:HG3 | 2:1:65:PHE:CD1 | 2.50 | 0.47 |
| 2:3:57:PRO:HG3 | 2:3:65:PHE:CD2 | 2.50 | 0.47 |
| 3:9:74:MET:HA | 3:9:152:THR:HG22 | 1.96 | 0.47 |
| 5:A1:91:ALA:HB1 | 5:A1:375:VAL:HG21 | 1.96 | 0.47 |
| 5:A1:215:TYR:HD2 | 5:A1:221:MET:HE1 | 1.78 | 0.47 |
| 5:A2:69:MET:C | 5:A2:71:THR:H | 2.23 | 0.47 |
| 7:A6:129:TYR:HD1 | 7:Al:105:PRO:HG2 | 1.79 | 0.47 |
| 3:AA:75:ASN:ND2 | 3:AA:151:GLN:OE1 | 2.48 | 0.47 |
| 2:AD:417:ILE:HB | 2:AD:421:ARG:HB3 | 1.97 | 0.47 |
| 2:AN:364:ASP:O | 2:AN:367:SER:N | 2.48 | 0.47 |
| 10:AQ:314:GLU:O | 10:AQ:318:MET:HG2 | 2.14 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:AW:319:SER:HA | 6:AW:323:LEU:HB2 | 1.96 | 0.47 |
| 6:AX:377:ILE:HG23 | 6:AX:435:THR:HB | 1.96 | 0.47 |
| 6:Ad:131:TYR:HD2 | 6:Ad:250:MET:HE3 | 1.80 | 0.47 |
| 6:Ag:456:LEU:HA | 6:Ag:475:THR:HG22 | 1.97 | 0.47 |
| 6:Ak:327:SER:OG | 6:Ak:328:LYS:N | 2.47 | 0.47 |
| 7:Al:25:ILE:HD12 | 7:BE:265:ARG:HG2 | 1.96 | 0.47 |
| 6:An:264:ARG:NH1 | 6:An:477:TYR:OH | 2.48 | 0.47 |
| 6:Ao:176:ASP:OD1 | 6:Ao:177:ILE:N | 2.47 | 0.47 |
| 6:Ap:120:PRO:HD3 | 6:Ap:453:TYR:CZ | 2.50 | 0.47 |
| 7:As:30:THR:C | 7:As:32:ASP:H | 2.22 | 0.47 |
| 6:Aw:105:ASN:HB2 | 6:Aw:412:VAL:HG13 | 1.96 | 0.47 |
| 6:Aw:490:GLN:OE1 | 6:Aw:490:GLN:N | 2.47 | 0.47 |
| 2:B1:252:LEU:HD21 | 2:B1:263:SER:HB3 | 1.97 | 0.47 |
| 2:B1:550:ARG:HB3 | 2:B1:553:VAL:HG12 | 1.97 | 0.47 |
| 2:B1:624:VAL:HG12 | 2:Bz:639:THR:HB | 1.97 | 0.47 |
| 6:BJ:153:MET:HE1 | 6:BJ:226:GLU:HG2 | 1.97 | 0.47 |
| 6:BK:84:THR:OG1 | 6:BK:88:VAL:O | 2.32 | 0.47 |
| 6:BM:481:ILE:HD13 | 6:BM:506:SER:HB3 | 1.95 | 0.47 |
| 11:BT:38:VAL:HG11 | 11:BT:69:ILE:HG12 | 1.96 | 0.47 |
| 3:Ba:7:THR:HG22 | 2:Bv:598:LEU:HD21 | 1.95 | 0.47 |
| 3:Bi:136:ASN:O | 3:Bi:136:ASN:ND2 | 2.46 | 0.47 |
| 3:Bl:129:ILE:HG21 | 3:Bl:159:LEU:HD22 | 1.95 | 0.47 |
| 3:Bm:4:ASP:OD1 | 3:Bm:4:ASP:N | 2.42 | 0.47 |
| 2:Br:110:TYR:CD1 | 2:Br:177:GLY:HA3 | 2.50 | 0.47 |
| 2:Br:609:ASP:N | 2:Br:609:ASP:OD1 | 2.48 | 0.47 |
| 2:Bt:32:LYS:HD2 | 2:Bt:355:LEU:HD21 | 1.96 | 0.47 |
| 2:Bt:44:VAL:HG11 | 2:Bt:50:LEU:HB2 | 1.96 | 0.47 |
| 2:Bz:116:ILE:HD13 | 2:Bz:171:ILE:HA | 1.96 | 0.47 |
| 4:I:62:ILE:HD12 | 4:T:58:LEU:HD22 | 1.96 | 0.47 |
| 4:a:44:MET:HE3 | 4:f:44:MET:HE3 | 1.97 | 0.47 |
| 1:0:3:THR:HG21 | 1:p:122:LEU:HA | 1.96 | 0.47 |
| 1:0:27:LEU:HG | 1:p:57:GLU:HG3 | 1.96 | 0.47 |
| 1:0:50:SER:OG | 7:Ar:269:MET:SD | 2.72 | 0.47 |
| 2:1:63:ASP:OD2 | 2:1:379:ALA:HB3 | 2.14 | 0.47 |
| 2:2:61:THR:O | 2:2:63:ASP:N | 2.48 | 0.47 |
| 2:2:634:SER:HB2 | 2:AP:574:GLU:N | 2.30 | 0.47 |
| 2:3:561:LYS:HD3 | 8:s:231:GLU:HG2 | 1.96 | 0.47 |
| 2:3:623:PHE:HB3 | 8:s:212:THR:HG22 | 1.97 | 0.47 |
| 2:4:398:ASP:O | 2:4:401:GLN:HG2 | 2.14 | 0.47 |
| 2:4:447:TYR:OH | 8:t:231:GLU:OE2 | 2.32 | 0.47 |
| 2:5:228:GLY:HA2 | 2:5:345:SER:HB3 | 1.97 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:5:256:PRO:HG2 | 2:5:339:THR:H | 1.79 | 0.47 |
| 2:5:389:VAL:O | 2:5:393:VAL:HG23 | 2.13 | 0.47 |
| 3:6:54:MET:C | 3:6:56:ARG:H | 2.22 | 0.47 |
| 3:9:70:THR:HG22 | 3:9:156:THR:HG22 | 1.97 | 0.47 |
| 4:A:23:SER:HB3 | 4:A:46:ARG:HD2 | 1.95 | 0.47 |
| 5:A1:456:GLU:OE2 | 5:BB:492:GLN:NE2 | 2.48 | 0.47 |
| 5:A2:166:ARG:H | 5:A2:166:ARG:HG3 | 1.35 | 0.47 |
| 5:A3:134:LEU:O | 5:A3:137:LEU:C | 2.57 | 0.47 |
| 5:A3:321:ILE:HG22 | 7:Al:173:MET:HB3 | 1.97 | 0.47 |
| 6:A4:254:ILE:HD12 | 6:A4:254:ILE:HA | 1.76 | 0.47 |
| 6:A5:258:VAL:O | 6:A5:499:GLY:N | 2.41 | 0.47 |
| 6:A7:363:GLU:OE2 | 6:A7:367:GLN:NE2 | 2.45 | 0.47 |
| 3:AA:48:LYS:NZ | 3:o:68:ASP:OD1 | 2.45 | 0.47 |
| 2:AD:641:ASN:HB2 | 2:AN:626:THR:HG22 | 1.95 | 0.47 |
| 3:AE:23:VAL:HG22 | 3:AE:36:CYS:SG | 2.54 | 0.47 |
| 3:AF:37:LYS:HE3 | 3:AF:74:MET:HE2 | 1.97 | 0.47 |
| 3:AG:30:GLN:O | 3:AG:30:GLN:NE2 | 2.46 | 0.47 |
| 2:AL:35:TRP:HH2 | 2:AL:224:ALA:HB1 | 1.78 | 0.47 |
| 2:AM:131:ILE:HD13 | 2:AM:140:ILE:HG21 | 1.97 | 0.47 |
| 2:AM:644:ALA:HA | 2:By:557:PHE:CZ | 2.50 | 0.47 |
| 2:AO:641:ASN:HB2 | 2:B5:626:THR:HG22 | 1.96 | 0.47 |
| 2:AP:37:PRO:HG3 | 2:AP:226:TYR:CZ | 2.49 | 0.47 |
| 6:AV:76:ALA:HA | 6:AZ:258:VAL:HG21 | 1.95 | 0.47 |
| 7:Aa:30:THR:HG22 | 7:Aa:33:GLN:NE2 | 2.29 | 0.47 |
| 7:Ab:95:ILE:HD12 | 7:Ab:96:THR:HG23 | 1.97 | 0.47 |
| 6:Ac:237:GLU:N | 6:Ac:245:ASN:O | 2.40 | 0.47 |
| 6:Ag:184:GLU:HB2 | 6:Ag:366:ARG:HH22 | 1.80 | 0.47 |
| 6:Ah:351:LYS:NZ | 6:Ah:394:SER:O | 2.48 | 0.47 |
| 6:Aj:120:PRO:HD3 | 6:Aj:453:TYR:CZ | 2.50 | 0.47 |
| 7:Al:81:VAL:HA | 7:Al:188:THR:HA | 1.97 | 0.47 |
| 7:Ar:34:ILE:O | 7:Ar:38:ILE:HG12 | 2.14 | 0.47 |
| 7:Ar:109:ASP:HB2 | 6:Au:476:ARG:HH12 | 1.80 | 0.47 |
| 7:At:231:VAL:HB | 4:H:31:ILE:HD11 | 1.97 | 0.47 |
| 6:Au:228:MET:HG2 | 6:BJ:263:SER:O | 2.14 | 0.47 |
| 2:B2:131:ILE:HD13 | 2:B2:140:ILE:HG21 | 1.96 | 0.47 |
| 2:B2:484:VAL:HG13 | 2:B2:485:SER:H | 1.80 | 0.47 |
| 2:B3:115:LYS:NZ | 2:B3:127:THR:O | 2.47 | 0.47 |
| 2:B3:391:LYS:HG2 | 2:B3:443:ILE:HD13 | 1.96 | 0.47 |
| 2:B5:41:ILE:HD13 | 2:B5:81:VAL:HB | 1.96 | 0.47 |
| 2:B5:505:LEU:HD21 | 2:B5:525:VAL:HB | 1.96 | 0.47 |
| 2:B6:284:ARG:HG2 | 2:B6:289:ILE:HD13 | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B7:642:PHE:HE1 | 2:Br:10:LEU:HD22 | 1.80 | 0.47 |
| 5:BG:125:MET:O | 5:BG:129:GLU:HG2 | 2.15 | 0.47 |
| 5:BH:115:LYS:HD3 | 5:BH:445:LYS:HE2 | 1.96 | 0.47 |
| 3:BY:147:ASN:ND2 | 3:Bm:63:ASP:OD2 | 2.41 | 0.47 |
| 3:Bb:97:ASN:HA | 3:Bo:3:VAL:HG12 | 1.95 | 0.47 |
| 3:Bc:83:GLN:NE2 | 3:Bc:87:ASP:OD1 | 2.47 | 0.47 |
| 3:Bg:75:ASN:ND2 | 3:Bg:151:GLN:OE1 | 2.41 | 0.47 |
| 3:Bg:82:ARG:NH1 | 3:Bg:138:GLY:HA2 | 2.29 | 0.47 |
| 3:Bh:94:GLY:HA3 | 3:Bh:100:THR:OG1 | 2.15 | 0.47 |
| 3:Bi:23:VAL:HG12 | 3:Bi:113:VAL:HB | 1.97 | 0.47 |
| 3:Bk:136:ASN:O | 3:Bk:136:ASN:ND2 | 2.45 | 0.47 |
| 3:Bo:38:ALA:N | 3:Bo:72:THR:OG1 | 2.47 | 0.47 |
| 2:Bp:639:THR:HB | 2:Bq:624:VAL:HG12 | 1.96 | 0.47 |
| 2:Bq:163:LEU:HD12 | 2:Bq:186:LYS:HA | 1.95 | 0.47 |
| 2:Br:45:THR:HA | 2:Br:76:ASN:O | 2.14 | 0.47 |
| 2:Br:47:GLU:OE2 | 2:Br:461:TYR:OH | 2.25 | 0.47 |
| 2:Br:57:PRO:HA | 2:Br:61:THR:HB | 1.97 | 0.47 |
| 2:Br:151:ILE:O | 2:Br:155:LYS:HG2 | 2.15 | 0.47 |
| 2:Bt:95:ILE:HG12 | 2:Bt:219:ILE:HD11 | 1.97 | 0.47 |
| 2:Bt:209:ASP:OD1 | 2:Bt:209:ASP:N | 2.46 | 0.47 |
| 2:Bt:299:ARG:HD2 | 2:Bt:299:ARG:H | 1.79 | 0.47 |
| 2:Bw:252:LEU:HD22 | 2:Bw:335:SER:HB3 | 1.95 | 0.47 |
| 2:Bw:546:SER:HA | 2:Bz:304:ILE:HG21 | 1.97 | 0.47 |
| 2:Bz:57:PRO:HG3 | 2:Bz:65:PHE:CD1 | 2.50 | 0.47 |
| 4:e:52:LEU:HD21 | 4:j:12:ASP:HB2 | 1.95 | 0.47 |
| 4:h:5:LEU:HD11 | 4:h:65:LEU:HD21 | 1.96 | 0.47 |
| 1:l:146:LEU:HD13 | 1:l:174:PHE:HD2 | 1.79 | 0.47 |
| 1:l:198:GLU:O | 1:l:205:ARG:NH2 | 2.48 | 0.47 |
| 8:r:28:ARG:NH2 | 8:r:129:ASP:OD2 | 2.48 | 0.47 |
| 8:t:91:ASN:O | 8:t:110:ASN:ND2 | 2.46 | 0.47 |
| 9:v:97:TYR:HB3 | 9:z:56:LEU:O | 2.14 | 0.47 |
| 9:z:37:VAL:HG22 | 9:z:73:VAL:HG13 | 1.97 | 0.47 |
| 1:0:2:ALA:N | 1:0:23:GLU:OE2 | 2.48 | 0.47 |
| 2:1:31:GLY:HA3 | 2:1:64:TYR:CD1 | 2.49 | 0.47 |
| 2:2:373:PHE:HB2 | 2:2:405:VAL:HG22 | 1.96 | 0.47 |
| 2:3:642:PHE:CE2 | 2:AK:561:LYS:HG2 | 2.50 | 0.47 |
| 2:4:410:PRO:O | 2:4:413:THR:HG22 | 2.15 | 0.47 |
| 5:A1:61:ILE:HG23 | 5:A1:227:LYS:HG3 | 1.96 | 0.47 |
| 5:A3:141:ARG:NH2 | 5:BF:444:ILE:O | 2.48 | 0.47 |
| 5:A3:311:ARG:HG3 | 5:A3:312:VAL:H | 1.80 | 0.47 |
| 6:A4:262:LYS:HE3 | 6:A4:500:MET:HE1 | 1.95 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A4:265:GLN:HB2 | 6:A5:247:TRP:CZ3 | 2.50 | 0.47 |
| 6:A4:267:LYS:HE3 | 6:A4:470:VAL:HG21 | 1.96 | 0.47 |
| 6:A8:494:SER:C | 6:A8:496:ILE:H | 2.23 | 0.47 |
| 8:AB:134:VAL:HG21 | 8:AB:188:TRP:CE3 | 2.50 | 0.47 |
| 3:AE:117:ALA:HB3 | 3:AE:122:THR:HB | 1.96 | 0.47 |
| 3:AH:118:ARG:N | 3:AI:77:GLU:OE2 | 2.43 | 0.47 |
| 2:AK:3:LEU:HD22 | 2:AP:511:GLN:HE21 | 1.79 | 0.47 |
| 2:AL:655:THR:HA | 2:AM:19:VAL:HG21 | 1.96 | 0.47 |
| 2:AM:110:TYR:H | 2:AM:138:GLY:HA3 | 1.79 | 0.47 |
| 2:AO:39:PHE:HB3 | 2:AO:361:PHE:CE1 | 2.49 | 0.47 |
| 2:AP:10:LEU:HD22 | 2:B5:561:LYS:HG2 | 1.97 | 0.47 |
| 2:AP:195:LEU:HD23 | 2:AP:195:LEU:H | 1.79 | 0.47 |
| 2:AP:368:VAL:HG12 | 2:AP:370:VAL:HG22 | 1.96 | 0.47 |
| 2:AP:560:LEU:HD21 | 2:AP:592:LEU:HD11 | 1.96 | 0.47 |
| 10:AQ:300:ARG:NH2 | 10:AQ:352:ASP:OD2 | 2.47 | 0.47 |
| 6:AZ:494:SER:C | 6:AZ:496:ILE:H | 2.22 | 0.47 |
| 6:Ag:184:GLU:O | 6:Ag:185:THR:OG1 | 2.29 | 0.47 |
| 6:Ak:105:ASN:O | 6:Ak:427:GLN:NE2 | 2.48 | 0.47 |
| 6:An:465:LYS:HD2 | 6:An:465:LYS:H | 1.79 | 0.47 |
| 7:As:236:ASN:HB3 | 4:j:36:THR:HG23 | 1.97 | 0.47 |
| 5:Av:39:GLY:HA3 | 5:Av:250:ILE:HG12 | 1.97 | 0.47 |
| 5:Av:398:ARG:HH12 | 5:BB:390:PHE:HB2 | 1.79 | 0.47 |
| 5:Ax:209:ASP:OD1 | 5:Ax:209:ASP:N | 2.46 | 0.47 |
| 2:B5:458:TYR:HD1 | 2:B6:317:LYS:HZ1 | 1.61 | 0.47 |
| 2:B6:40:GLN:H | 2:B6:81:VAL:HG23 | 1.79 | 0.47 |
| 2:B7:302:LYS:HA | 2:B7:308:ASN:HA | 1.97 | 0.47 |
| 7:BC:160:ASP:OD1 | 7:BC:160:ASP:N | 2.43 | 0.47 |
| 3:Bd:23:VAL:HG22 | 3:Bd:36:CYS:SG | 2.55 | 0.47 |
| 3:Bi:22:GLN:HB2 | 3:Bi:116:TYR:HE1 | 1.80 | 0.47 |
| 2:Bp:451:ASP:OD1 | 2:Bp:452:GLY:N | 2.40 | 0.47 |
| 2:Bp:514:ARG:NH1 | 2:Bq:364:ASP:OD1 | 2.41 | 0.47 |
| 2:Bq:427:VAL:HG22 | 2:Bq:520:GLU:HG3 | 1.96 | 0.47 |
| 2:Br:406:LEU:HD22 | 2:Br:474:ILE:HG13 | 1.97 | 0.47 |
| 2:Bu:90:LYS:HD2 | 2:Bu:192:GLY:H | 1.79 | 0.47 |
| 2:Bx:102:THR:HB | 2:Bx:183:THR:HB | 1.97 | 0.47 |
| 2:Bz:36:GLY:O | 2:Bz:82:ARG:NH1 | 2.42 | 0.47 |
| 2:Bz:46:ASN:OD1 | 2:Bz:47:GLU:N | 2.48 | 0.47 |
| 2:Bz:166:ASN:N | 2:Bz:166:ASN:OD1 | 2.45 | 0.47 |
| 4:J:34:ALA:N | 4:K:25:ILE:O | 2.42 | 0.47 |
| 1:l:5:ASP:OD2 | 1:l:8:LEU:N | 2.48 | 0.47 |
| 1:m:117:SER:HA | 1:m:168:LYS:HA | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:122:LEU:HA | 1:n:3:THR:HG21 | 1.97 | 0.47 |
| 8:t:168:MET:HG3 | 8:t:193:GLU:HB2 | 1.96 | 0.47 |
| 2:4:383:LEU:HD11 | 2:4:436:TYR:CD2 | 2.49 | 0.47 |
| 3:8:83:GLN:HA | 3:8:86:VAL:HG22 | 1.96 | 0.47 |
| 5:A0:398:ARG:HG2 | 5:BH:379:ARG:HD2 | 1.97 | 0.47 |
| 6:A5:267:LYS:HB2 | 6:AW:247:TRP:CE3 | 2.50 | 0.47 |
| 6:A8:319:SER:HA | 6:A8:323:LEU:HB2 | 1.97 | 0.47 |
| 2:AO:272:GLY:O | 2:AO:274:GLN:NE2 | 2.48 | 0.47 |
| 6:AV:396:ALA:O | 6:AZ:395:TYR:HA | 2.15 | 0.47 |
| 7:AY:191:TYR:HA | 7:AY:239:GLN:HE21 | 1.79 | 0.47 |
| 6:AZ:249:GLU:OE1 | 6:Am:66:ALA:N | 2.48 | 0.47 |
| 7:Aa:303:PRO:HG3 | 5:BB:289:THR:HG22 | 1.96 | 0.47 |
| 6:Ae:117:MET:HG3 | 6:Ae:451:ALA:HB1 | 1.97 | 0.47 |
| 6:Ae:133:LYS:HG2 | 6:Ae:249:GLU:HB2 | 1.97 | 0.47 |
| 6:Ae:155:SER:OG | 6:Ay:301:GLU:OE1 | 2.27 | 0.47 |
| 6:Ae:258:VAL:O | 6:Ae:499:GLY:N | 2.29 | 0.47 |
| 6:Ag:232:ILE:O | 6:Ag:236:GLN:HG2 | 2.15 | 0.47 |
| 6:Ah:163:PHE:HB2 | 6:Ah:179:THR:HG23 | 1.97 | 0.47 |
| 6:Ah:236:GLN:HB3 | 6:Ah:247:TRP:NE1 | 2.30 | 0.47 |
| 6:Ai:456:LEU:HD23 | 6:Ai:475:THR:HB | 1.97 | 0.47 |
| 6:An:232:ILE:O | 6:An:236:GLN:HG2 | 2.15 | 0.47 |
| 6:Ao:199:ASP:HB2 | 6:Ao:211:GLU:HG2 | 1.97 | 0.47 |
| 6:Ao:450:TYR:CE1 | 6:Ao:477:TYR:HB2 | 2.50 | 0.47 |
| 2:B1:147:THR:HG22 | 2:B1:150:ILE:HD12 | 1.96 | 0.47 |
| 2:B2:252:LEU:HB3 | 2:B2:336:GLY:HA2 | 1.97 | 0.47 |
| 2:B4:278:GLN:HG2 | 2:B4:296:SER:HB3 | 1.96 | 0.47 |
| 2:B6:130:LYS:HZ3 | 2:B6:132:THR:HA | 1.79 | 0.47 |
| 2:B7:44:VAL:HG11 | 2:B7:50:LEU:HB2 | 1.96 | 0.47 |
| 5:BD:497:GLU:OE1 | 5:BD:500:GLN:NE2 | 2.48 | 0.47 |
| 5:BF:457:LEU:HD13 | 5:BF:457:LEU:HA | 1.82 | 0.47 |
| 6:BI:404:PHE:HZ | 6:BI:417:LEU:HA | 1.79 | 0.47 |
| 6:BM:486:GLU:HB2 | 6:BM:509:LYS:HB3 | 1.97 | 0.47 |
| 11:BO:11:LYS:HG3 | 11:BO:27:GLU:HG2 | 1.97 | 0.47 |
| 3:BY:90:SER:HA | 3:BY:94:GLY:HA2 | 1.96 | 0.47 |
| 3:Bg:23:VAL:HG22 | 3:Bg:36:CYS:SG | 2.54 | 0.47 |
| 3:Bm:49:ILE:HG23 | 3:Bm:60:VAL:HG13 | 1.95 | 0.47 |
| 2:Bu:440:ASN:OD1 | 2:Bu:440:ASN:N | 2.48 | 0.47 |
| 2:Bu:482:ASP:HB2 | 2:Bu:487:THR:HG22 | 1.96 | 0.47 |
| 2:Bw:157:VAL:HG23 | 2:Bw:159:GLU:H | 1.80 | 0.47 |
| 4:P:9:PRO:HD3 | 4:P:57:VAL:HG21 | 1.95 | 0.47 |
| 4:P:62:ILE:HD12 | 4:U:58:LEU:HD22 | 1.97 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:k:170:THR:HG21 | 8:r:181:LEU:HD22 | 1.96 | 0.47 |
| 1:m:44:ASP:HB2 | 1:m:163:GLN:NE2 | 2.29 | 0.47 |
| 1:m:213:ILE:HD13 | 8:t:70:THR:HG22 | 1.96 | 0.47 |
| 2:1:306:ASP:O | 8:AB:221:ARG:NE | 2.42 | 0.47 |
| 2:5:163:LEU:HD22 | 2:5:167:TRP:CE2 | 2.49 | 0.47 |
| 3:7:20:LEU:HA | 9:AC:54:PHE:CD2 | 2.50 | 0.47 |
| 5:A2:181:GLN:HE22 | 5:A2:213:GLU:HA | 1.80 | 0.47 |
| 5:A3:81:ASN:HD21 | 7:Al:127:ARG:HB3 | 1.80 | 0.47 |
| 6:A4:406:THR:OG1 | 6:A5:372:GLU:OE2 | 2.30 | 0.47 |
| 6:A9:502:SER:O | 6:A9:506:SER:OG | 2.27 | 0.47 |
| 8:AB:26:ILE:HG12 | 8:AB:37:ILE:HG13 | 1.97 | 0.47 |
| 3:AF:96:GLY:O | 3:AJ:56:ARG:NH2 | 2.40 | 0.47 |
| 3:AG:97:ASN:HA | 3:BX:3:VAL:HG12 | 1.97 | 0.47 |
| 2:AK:151:ILE:O | 2:AK:155:LYS:HG2 | 2.15 | 0.47 |
| 2:AL:645:THR:OG1 | 2:Bv:629:ILE:O | 2.32 | 0.47 |
| 2:AM:228:GLY:HA2 | 2:AM:345:SER:HB3 | 1.95 | 0.47 |
| 2:AN:560:LEU:O | 2:AN:564:ILE:HG12 | 2.14 | 0.47 |
| 10:AQ:319:THR:HG23 | 10:AQ:325:TRP:HB3 | 1.97 | 0.47 |
| 6:AV:304:ARG:NH1 | 6:AV:426:ASP:OD1 | 2.47 | 0.47 |
| 7:AY:40:ARG:HH21 | 7:AY:254:LEU:HD22 | 1.81 | 0.47 |
| 6:Ae:235:LEU:HA | 6:Ae:239:PHE:HB3 | 1.97 | 0.47 |
| 6:Af:71:ASP:OD1 | 6:Af:72:HIS:N | 2.45 | 0.47 |
| 6:Am:267:LYS:HD3 | 6:BJ:247:TRP:HE3 | 1.80 | 0.47 |
| 6:An:381:ASN:HB3 | 6:An:521:ILE:HG21 | 1.96 | 0.47 |
| 5:Ax:105:ASP:OD1 | 5:BH:492:GLN:NE2 | 2.48 | 0.47 |
| 6:Ay:136:VAL:HG22 | 6:Ay:253:ARG:HD3 | 1.97 | 0.47 |
| 2:B2:527:GLY:HA2 | 2:B2:533:TYR:CD2 | 2.50 | 0.47 |
| 2:B6:346:SER:O | 2:B6:350:VAL:HG23 | 2.15 | 0.47 |
| 5:BA:189:ILE:O | 5:BA:189:ILE:HG13 | 2.15 | 0.47 |
| 5:BA:393:GLY:O | 5:BA:454:PHE:HB2 | 2.13 | 0.47 |
| 5:BB:87:GLU:OE2 | 5:BB:366:ARG:NH1 | 2.43 | 0.47 |
| 5:BB:411:GLN:O | 5:BB:415:GLU:HG3 | 2.15 | 0.47 |
| 7:BE:124:SER:HB3 | 7:BE:127:ARG:HH12 | 1.80 | 0.47 |
| 7:BL:193:ASP:O | 7:BL:242:TYR:OH | 2.31 | 0.47 |
| 3:BZ:142:LEU:HB3 | 3:Bo:21:PHE:CD1 | 2.50 | 0.47 |
| 3:Bi:4:ASP:OD1 | 3:Bi:4:ASP:N | 2.42 | 0.47 |
| 2:Bw:470:LEU:O | 2:Bw:474:ILE:HG12 | 2.15 | 0.47 |
| 2:Bw:569:LYS:HB2 | 2:By:8:ILE:HD11 | 1.97 | 0.47 |
| 2:By:373:PHE:HB2 | 2:By:405:VAL:HG22 | 1.97 | 0.47 |
| 1:m:45:VAL:HG11 | 1:n:9:PHE:CE2 | 2.50 | 0.47 |
| 1:m:101:SER:HA | 1:m:110:VAL:HA | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:176:TYR:HD1 | 8:t:71:ILE:HG23 | 1.79 | 0.47 |
| 8:u:151:GLU:OE1 | 8:u:199:TYR:OH | 2.27 | 0.47 |
| 9:w:37:VAL:HG22 | 9:w:73:VAL:HG13 | 1.97 | 0.47 |
| 2:5:244:TYR:HE2 | 2:5:272:GLY:H | 1.62 | 0.46 |
| 3:7:86:VAL:HG12 | 3:7:137:VAL:HG21 | 1.97 | 0.46 |
| 3:7:97:ASN:ND2 | 3:7:97:ASN:O | 2.47 | 0.46 |
| 5:A0:41:ARG:HD3 | 5:A0:65:TYR:CZ | 2.50 | 0.46 |
| 5:A1:220:ARG:HH11 | 5:A1:221:MET:H | 1.63 | 0.46 |
| 5:A3:482:SER:HA | 5:BG:505:ILE:HD11 | 1.96 | 0.46 |
| 6:A7:261:ALA:HA | 6:A7:478:GLY:HA3 | 1.97 | 0.46 |
| 6:A8:328:LYS:NZ | 6:A8:333:ASP:OD2 | 2.39 | 0.46 |
| 3:AE:1:MET:SD | 3:AF:22:GLN:NE2 | 2.88 | 0.46 |
| 2:AL:209:ASP:O | 2:AL:213:ASN:ND2 | 2.29 | 0.46 |
| 7:Aa:202:VAL:HG13 | 4:i:31:ILE:HG22 | 1.96 | 0.46 |
| 6:Aj:336:ASP:HB3 | 6:Aj:339:ASP:HB2 | 1.97 | 0.46 |
| 6:Ak:383:VAL:HG12 | 6:Ak:406:THR:HG22 | 1.97 | 0.46 |
| 6:An:176:ASP:OD1 | 6:An:177:ILE:N | 2.47 | 0.46 |
| 6:Ao:400:LEU:HD11 | 6:BM:417:LEU:HG | 1.96 | 0.46 |
| 7:Aq:80:ASN:OD1 | 7:Aq:80:ASN:N | 2.47 | 0.46 |
| 7:Ar:234:ASP:N | 7:Ar:234:ASP:OD1 | 2.47 | 0.46 |
| 5:Ax:213:GLU:H | 5:Ax:213:GLU:HG3 | 1.57 | 0.46 |
| 6:Ay:121:THR:HA | 6:Ay:259:ILE:O | 2.14 | 0.46 |
| 6:Ay:481:ILE:N | 6:Ay:499:GLY:O | 2.44 | 0.46 |
| 2:B3:609:ASP:OD1 | 2:B3:611:THR:OG1 | 2.31 | 0.46 |
| 2:B4:252:LEU:HB3 | 2:B4:336:GLY:HA2 | 1.96 | 0.46 |
| 2:B7:101:TYR:O | 2:B7:216:LYS:NZ | 2.37 | 0.46 |
| 7:BC:55:LYS:HB3 | 7:BC:187:TRP:CE3 | 2.50 | 0.46 |
| 7:BE:231:VAL:HG12 | 4:G:29:GLU:O | 2.15 | 0.46 |
| 5:BG:184:TYR:OH | 5:BG:204:GLU:OE1 | 2.32 | 0.46 |
| 5:BG:462:ILE:O | 5:BG:466:ARG:HG3 | 2.15 | 0.46 |
| 7:BL:128:PHE:H | 7:BL:128:PHE:HD1 | 1.63 | 0.46 |
| 7:BL:199:GLY:O | 7:BL:204:TYR:OH | 2.33 | 0.46 |
| 3:BZ:25:ILE:HD12 | 3:BZ:28:LEU:HD12 | 1.96 | 0.46 |
| 2:Bp:390:GLN:HB3 | 2:Bp:441:PHE:HE1 | 1.80 | 0.46 |
| 2:Bs:470:LEU:O | 2:Bs:474:ILE:HG12 | 2.15 | 0.46 |
| 2:Bu:456:TYR:CE1 | 2:Bu:465:ASN:HB3 | 2.50 | 0.46 |
| 2:Bw:272:GLY:O | 2:Bw:274:GLN:NE2 | 2.47 | 0.46 |
| 2:Bw:417:ILE:H | 2:Bw:417:ILE:HD13 | 1.80 | 0.46 |
| 2:By:617:VAL:HG22 | 2:By:622:GLU:HB2 | 1.97 | 0.46 |
| 2:Bz:455:LYS:HD3 | 2:Bz:457:GLN:HB2 | 1.97 | 0.46 |
| 4:D:47:PRO:HB2 | 4:T:48:THR:HG21 | 1.97 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:H:69:LEU:HD21 | 4:S:68:SER:HB3 | 1.97 | 0.46 |
| 4:I:48:THR:HG21 | 4:T:47:PRO:HB2 | 1.97 | 0.46 |
| 8:r:76:ASN:ND2 | 8:r:121:SER:HB2 | 2.30 | 0.46 |
| 9:v:74:ARG:HH11 | 9:v:154:VAL:HG11 | 1.79 | 0.46 |
| 2:1:23:SER:OG | 2:1:483:ASN:OD1 | 2.33 | 0.46 |
| 2:1:302:LYS:NZ | 2:1:306:ASP:OD1 | 2.49 | 0.46 |
| 3:6:23:VAL:HG13 | 3:6:36:CYS:SG | 2.55 | 0.46 |
| 4:A:10:PHE:HB3 | 4:A:22:ILE:HG12 | 1.98 | 0.46 |
| 5:A3:367:GLN:HA | 5:A3:377:LEU:HD11 | 1.97 | 0.46 |
| 6:A5:231:SER:HB3 | 6:A9:71:ASP:HB3 | 1.97 | 0.46 |
| 6:A7:274:LEU:HD13 | 6:Au:69:GLY:HA2 | 1.97 | 0.46 |
| 6:A7:380:ARG:NH2 | 6:A7:408:THR:OG1 | 2.40 | 0.46 |
| 6:A7:467:PHE:HB3 | 6:Ay:459:LEU:HD22 | 1.97 | 0.46 |
| 8:AB:231:GLU:OE2 | 2:AD:561:LYS:NZ | 2.32 | 0.46 |
| 2:AD:304:ILE:HG13 | 2:AD:305:TYR:H | 1.79 | 0.46 |
| 2:AD:498:GLN:HG2 | 2:AD:534:VAL:HG12 | 1.97 | 0.46 |
| 2:AD:594:GLY:HA2 | 3:o:8:ARG:HH11 | 1.80 | 0.46 |
| 3:AF:98:GLU:OE1 | 3:AF:98:GLU:N | 2.47 | 0.46 |
| 2:AP:299:ARG:H | 2:AP:299:ARG:HD2 | 1.80 | 0.46 |
| 10:AR:306:TRP:HB3 | 6:Ak:337:PRO:HB3 | 1.97 | 0.46 |
| 10:AS:299:HIS:H | 10:AS:299:HIS:CD2 | 2.32 | 0.46 |
| 6:AV:244:ASP:HB2 | 11:BV:13:PHE:HE2 | 1.80 | 0.46 |
| 6:AW:383:VAL:HG12 | 6:AW:406:THR:HG22 | 1.97 | 0.46 |
| 7:Aa:246:TRP:CE2 | 7:Aa:297:LEU:HB2 | 2.50 | 0.46 |
| 6:Ac:117:MET:HG3 | 6:Ac:451:ALA:HB1 | 1.97 | 0.46 |
| 6:Ag:71:ASP:OD1 | 6:Ag:72:HIS:N | 2.48 | 0.46 |
| 6:Ag:507:LEU:O | 6:Ag:509:LYS:NZ | 2.33 | 0.46 |
| 6:Aj:390:ASP:H | 6:Aj:397:ALA:HB3 | 1.80 | 0.46 |
| 6:Ak:79:ILE:HG23 | 6:Ao:121:THR:HB | 1.97 | 0.46 |
| 6:An:364:ILE:HD12 | 6:An:436:VAL:HG23 | 1.97 | 0.46 |
| 6:Ap:358:ASP:OD1 | 6:Ap:420:LYS:NZ | 2.48 | 0.46 |
| 7:Aq:40:ARG:HH21 | 7:Aq:254:LEU:HD22 | 1.80 | 0.46 |
| 7:Aq:213:TRP:HE3 | 7:Aq:217:GLU:HG2 | 1.80 | 0.46 |
| 7:Ar:161:PHE:HA | 7:Ar:171:LYS:O | 2.15 | 0.46 |
| 5:Av:408:ARG:HE | 5:Av:450:ARG:HH21 | 1.64 | 0.46 |
| 6:Aw:147:MET:HE3 | 6:Aw:366:ARG:HH12 | 1.80 | 0.46 |
| 5:Ax:39:GLY:HA3 | 5:Ax:250:ILE:HG13 | 1.97 | 0.46 |
| 2:B4:406:LEU:HD22 | 2:B4:474:ILE:HG13 | 1.95 | 0.46 |
| 2:B4:453:ASN:ND2 | 2:B4:505:LEU:HG | 2.28 | 0.46 |
| 2:B5:37:PRO:HG3 | 2:B5:226:TYR:CZ | 2.50 | 0.46 |
| 2:B5:315:PHE:HE1 | 2:B5:323:ILE:HG13 | 1.80 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B7:456:TYR:O | 2:B7:503:ILE:HG12 | 2.14 | 0.46 |
| 7:BC:193:ASP:OD1 | 7:BC:193:ASP:N | 2.49 | 0.46 |
| 5:BD:275:ARG:NH1 | 5:BD:355:ASN:HB2 | 2.30 | 0.46 |
| 5:BG:454:PHE:HA | 5:BG:457:LEU:HB2 | 1.96 | 0.46 |
| 7:BL:91:ASN:ND2 | 7:BL:101:ASN:OD1 | 2.48 | 0.46 |
| 3:Bc:115:GLN:NE2 | 3:Bc:116:TYR:O | 2.48 | 0.46 |
| 3:Bj:117:ALA:HB3 | 3:Bj:122:THR:HB | 1.96 | 0.46 |
| 2:Bp:509:THR:O | 2:Bp:514:ARG:NH1 | 2.47 | 0.46 |
| 2:Br:479:ALA:O | 2:Br:483:ASN:ND2 | 2.48 | 0.46 |
| 2:Bs:240:SER:OG | 2:Bs:243:ASP:OD1 | 2.33 | 0.46 |
| 2:Bt:29:LEU:O | 2:Bt:80:VAL:HA | 2.15 | 0.46 |
| 2:Bw:268:VAL:HG21 | 2:Bw:282:ILE:HD13 | 1.97 | 0.46 |
| 2:Bx:283:VAL:HB | 2:Bx:291:GLN:HB3 | 1.97 | 0.46 |
| 2:By:480:ARG:C | 2:By:482:ASP:H | 2.23 | 0.46 |
| 2:Bz:332:GLU:N | 2:Bz:332:GLU:OE1 | 2.44 | 0.46 |
| 1:k:136:ASP:N | 1:k:136:ASP:OD1 | 2.48 | 0.46 |
| 1:k:151:TRP:HZ2 | 8:q:59:ILE:HD12 | 1.80 | 0.46 |
| 1:m:112:ASP:HB2 | 1:m:173:LYS:HD3 | 1.97 | 0.46 |
| 1:p:140:PHE:HB2 | 1:p:147:PHE:HE1 | 1.80 | 0.46 |
| 8:q:151:GLU:OE1 | 8:q:199:TYR:OH | 2.24 | 0.46 |
| 9:v:168:LYS:HD2 | 9:w:85:ILE:HG21 | 1.97 | 0.46 |
| 2:2:375:ALA:HB3 | 2:2:407:CYS:HA | 1.97 | 0.46 |
| 2:2:417:ILE:HD13 | 2:2:417:ILE:H | 1.79 | 0.46 |
| 2:2:642:PHE:CZ | 2:AP:561:LYS:HG2 | 2.51 | 0.46 |
| 2:3:413:THR:OG1 | 2:3:425:ASN:HB3 | 2.16 | 0.46 |
| 2:4:35:TRP:HB2 | 2:4:230:LEU:HD12 | 1.97 | 0.46 |
| 2:5:494:TYR:OH | 2:5:528:THR:OG1 | 2.31 | 0.46 |
| 4:A:24:TRP:HB3 | 4:Q:45:ASN:ND2 | 2.29 | 0.46 |
| 5:A0:29:VAL:HG13 | 5:BH:8:LEU:HD23 | 1.97 | 0.46 |
| 5:A1:72:THR:HG23 | 5:A1:155:ARG:NH2 | 2.30 | 0.46 |
| 5:A1:477:ILE:HA | 5:A1:481:ILE:HG22 | 1.97 | 0.46 |
| 6:A4:420:LYS:HD3 | 6:A9:400:LEU:HD23 | 1.96 | 0.46 |
| 8:AB:42:THR:HB | 8:AB:46:LYS:NZ | 2.31 | 0.46 |
| 8:AB:68:VAL:HG11 | 1:p:207:LEU:HD11 | 1.97 | 0.46 |
| 3:AI:18:PRO:HG3 | 3:AJ:149:GLU:HB2 | 1.98 | 0.46 |
| 2:AK:491:PRO:HG3 | 2:AK:555:ARG:HH11 | 1.81 | 0.46 |
| 2:AM:642:PHE:CZ | 2:By:561:LYS:HG2 | 2.50 | 0.46 |
| 2:AN:193:ILE:HD12 | 2:AN:193:ILE:HA | 1.83 | 0.46 |
| 2:AO:29:LEU:O | 2:AO:80:VAL:HA | 2.16 | 0.46 |
| 6:AX:454:VAL:O | 6:AX:475:THR:OG1 | 2.25 | 0.46 |
| 7:Aa:138:LEU:HB3 | 5:Av:273:ILE:HD11 | 1.98 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ac:121:THR:HB | 6:Aw:79:ILE:HG23 | 1.95 | 0.46 |
| 7:Al:12:LEU:HD21 | 7:Al:248:LYS:HG2 | 1.96 | 0.46 |
| 6:Am:265:GLN:HG3 | 6:BJ:247:TRP:NE1 | 2.31 | 0.46 |
| 6:Ao:114:VAL:N | 6:Ao:443:GLU:OE2 | 2.42 | 0.46 |
| 7:At:71:THR:HG21 | 7:BC:216:SER:HB3 | 1.97 | 0.46 |
| 5:Av:379:ARG:NE | 5:Av:400:GLU:OE2 | 2.48 | 0.46 |
| 2:B2:480:ARG:O | 2:B2:484:VAL:HG12 | 2.15 | 0.46 |
| 2:B2:636:ASN:H | 2:B3:621:ASN:HB3 | 1.81 | 0.46 |
| 2:B5:655:THR:HB | 2:Bp:19:VAL:HB | 1.97 | 0.46 |
| 2:B7:46:ASN:OD1 | 2:B7:47:GLU:N | 2.48 | 0.46 |
| 7:BC:162:TRP:NE1 | 7:BE:54:ASN:HA | 2.30 | 0.46 |
| 6:BI:190:LEU:HB3 | 6:BI:221:LEU:HB3 | 1.96 | 0.46 |
| 6:BI:261:ALA:HA | 6:BI:478:GLY:HA3 | 1.96 | 0.46 |
| 7:BL:34:ILE:O | 7:BL:38:ILE:HG12 | 2.15 | 0.46 |
| 7:BL:201:THR:HA | 4:M:30:GLU:HA | 1.96 | 0.46 |
| 6:BM:147:MET:SD | 6:BM:487:SER:OG | 2.65 | 0.46 |
| 11:BQ:38:VAL:HG11 | 11:BQ:69:ILE:HG12 | 1.97 | 0.46 |
| 3:BX:140:LEU:HD21 | 3:BX:151:GLN:OE1 | 2.15 | 0.46 |
| 3:Bb:114:ARG:HD2 | 3:Bb:123:VAL:HG11 | 1.97 | 0.46 |
| 3:Bg:9:ALA:HB2 | 3:Bj:34:PHE:HB2 | 1.96 | 0.46 |
| 3:Bl:98:GLU:OE1 | 3:Bl:98:GLU:N | 2.47 | 0.46 |
| 2:Bq:28:ALA:HB2 | 2:Bq:370:VAL:HG21 | 1.96 | 0.46 |
| 2:Br:34:GLN:HB3 | 2:Br:55:GLY:HA3 | 1.97 | 0.46 |
| 2:Br:373:PHE:HB2 | 2:Br:405:VAL:HG22 | 1.97 | 0.46 |
| 2:Bs:217:TYR:HB2 | 2:Bs:219:ILE:HD12 | 1.96 | 0.46 |
| 4:g:10:PHE:O | 4:g:54:ASN:ND2 | 2.36 | 0.46 |
| 1:l:185:LEU:HD22 | 1:l:197:SER:HB2 | 1.96 | 0.46 |
| 8:t:72:LEU:O | 8:t:74:ARG:N | 2.48 | 0.46 |
| 9:y:51:THR:HG22 | 9:y:59:ALA:HB2 | 1.98 | 0.46 |
| 2:1:600:GLY:O | 2:1:632:ALA:HB2 | 2.15 | 0.46 |
| 2:2:107:GLY:HA3 | 2:2:110:TYR:HE2 | 1.79 | 0.46 |
| 2:2:605:ARG:HB3 | 2:2:628:TYR:CD1 | 2.50 | 0.46 |
| 2:3:202:GLU:OE1 | 2:3:203:ALA:N | 2.48 | 0.46 |
| 2:3:246:LYS:HG3 | 2:3:250:ALA:HB2 | 1.98 | 0.46 |
| 2:4:373:PHE:HB2 | 2:4:405:VAL:HG22 | 1.97 | 0.46 |
| 3:7:138:GLY:HA2 | 3:7:154:GLU:O | 2.15 | 0.46 |
| 6:A4:426:ASP:OD2 | 6:A4:433:TYR:OH | 2.24 | 0.46 |
| 6:A9:245:ASN:N | 6:A9:245:ASN:OD1 | 2.47 | 0.46 |
| 8:AB:71:ILE:HG23 | 1:p:176:TYR:CD1 | 2.50 | 0.46 |
| 2:AD:443:ILE:HG22 | 2:AD:445:SER:H | 1.81 | 0.46 |
| 3:AF:28:LEU:HD22 | 3:AF:84:LYS:HB3 | 1.98 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AO:69:MET:O | 2:AO:73:GLN:HG2 | 2.15 | 0.46 |
| 2:AO:157:VAL:HG23 | 2:AO:159:GLU:H | 1.80 | 0.46 |
| 2:AO:601:ILE:HG21 | 2:AO:604:TYR:HB3 | 1.98 | 0.46 |
| 2:AP:644:ALA:HA | 2:Bp:557:PHE:HZ | 1.79 | 0.46 |
| 6:AV:279:ARG:HH22 | 5:BG:65:TYR:HA | 1.80 | 0.46 |
| 6:Af:244:ASP:N | 6:Af:244:ASP:OD1 | 2.48 | 0.46 |
| 6:Ak:261:ALA:HA | 6:Ak:478:GLY:HA3 | 1.98 | 0.46 |
| 6:Ao:88:VAL:HG13 | 6:BM:258:VAL:HG21 | 1.96 | 0.46 |
| 6:Ao:384:ASN:HD21 | 6:BM:362:VAL:HG11 | 1.79 | 0.46 |
| 6:Ap:152:ALA:HA | 6:BI:301:GLU:HG2 | 1.96 | 0.46 |
| 7:Aq:162:TRP:CD1 | 7:As:54:ASN:HA | 2.50 | 0.46 |
| 7:As:213:TRP:CE3 | 7:As:217:GLU:HG2 | 2.51 | 0.46 |
| 7:As:272:PRO:HD3 | 1:l:47:VAL:HG13 | 1.98 | 0.46 |
| 7:At:191:TYR:HA | 7:At:239:GLN:HE21 | 1.80 | 0.46 |
| 5:Av:287:VAL:HG22 | 5:Av:345:THR:HG23 | 1.97 | 0.46 |
| 6:Az:336:ASP:O | 6:Az:340:ILE:HG12 | 2.16 | 0.46 |
| 2:B1:137:ASP:OD1 | 2:B1:137:ASP:N | 2.47 | 0.46 |
| 2:B3:430:ARG:HH21 | 2:B3:541:ALA:HB1 | 1.80 | 0.46 |
| 2:B3:480:ARG:C | 2:B3:482:ASP:H | 2.22 | 0.46 |
| 2:B6:47:GLU:HG3 | 2:B6:69:MET:HG3 | 1.97 | 0.46 |
| 2:B6:644:ALA:HA | 2:B7:557:PHE:HZ | 1.81 | 0.46 |
| 5:BB:396:ILE:HG22 | 5:BB:401:LEU:HG | 1.97 | 0.46 |
| 5:BG:454:PHE:CE2 | 5:BG:458:LYS:HD2 | 2.51 | 0.46 |
| 3:BY:25:ILE:HG22 | 3:BY:27:TYR:H | 1.81 | 0.46 |
| 3:Ba:124:THR:OG1 | 3:Bd:77:GLU:O | 2.24 | 0.46 |
| 3:Bc:118:ARG:N | 3:Bf:77:GLU:OE2 | 2.49 | 0.46 |
| 3:Be:118:ARG:NH2 | 3:Bg:92:ALA:O | 2.48 | 0.46 |
| 2:Bs:118:VAL:HB | 2:Bs:126:GLU:HB3 | 1.98 | 0.46 |
| 2:Bs:556:LEU:HD23 | 2:Bs:560:LEU:HD13 | 1.96 | 0.46 |
| 2:Bs:604:TYR:HB2 | 2:Bs:629:ILE:HG22 | 1.96 | 0.46 |
| 2:Bt:561:LYS:HD3 | 2:Bv:10:LEU:HD13 | 1.97 | 0.46 |
| 2:Bu:414:VAL:HG23 | 2:Bu:422:ALA:HB1 | 1.98 | 0.46 |
| 2:Bz:147:THR:HG22 | 2:Bz:150:ILE:HD12 | 1.96 | 0.46 |
| 1:l:51:ILE:HD12 | 1:l:119:ASN:HB2 | 1.97 | 0.46 |
| 9:v:102:ASN:O | 9:v:105:GLN:NE2 | 2.37 | 0.46 |
| 2:2:163:LEU:HD22 | 2:2:167:TRP:CE2 | 2.51 | 0.46 |
| 2:2:225:LEU:HB3 | 2:2:324:PHE:HB2 | 1.97 | 0.46 |
| 2:2:538:ASP:N | 2:2:538:ASP:OD1 | 2.48 | 0.46 |
| 2:3:624:VAL:HG12 | 8:s:213:TYR:HB2 | 1.97 | 0.46 |
| 2:5:373:PHE:HB2 | 2:5:405:VAL:HG22 | 1.97 | 0.46 |
| 3:8:134:PRO:HA | 3:8:157:LEU:HA | 1.98 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A9:380:ARG:HE | 6:A9:408:THR:HG21 | 1.81 | 0.46 |
| 2:AD:487:THR:HG21 | 2:AD:559:MET:HE3 | 1.97 | 0.46 |
| 3:AG:69:TRP:HB2 | 3:AG:159:LEU:HD23 | 1.98 | 0.46 |
| 3:AH:43:ALA:O | 3:AH:162:TRP:NE1 | 2.43 | 0.46 |
| 2:AK:116:ILE:HG12 | 2:AK:130:LYS:HA | 1.96 | 0.46 |
| 2:AK:310:TYR:O | 2:AK:314:PHE:HB3 | 2.15 | 0.46 |
| 2:AL:32:LYS:HD2 | 2:AL:355:LEU:HD21 | 1.97 | 0.46 |
| 2:AM:66:MET:HG2 | 2:AM:468:VAL:HG21 | 1.98 | 0.46 |
| 2:AN:406:LEU:HD13 | 2:AN:475:ALA:HB2 | 1.96 | 0.46 |
| 6:AW:236:GLN:HB3 | 6:AW:247:TRP:NE1 | 2.30 | 0.46 |
| 7:AY:55:LYS:HD3 | 7:BL:173:MET:HE3 | 1.97 | 0.46 |
| 7:Aa:196:LYS:HB3 | 7:Aa:226:LEU:HD11 | 1.96 | 0.46 |
| 7:Ab:66:GLU:HA | 7:Ab:69:TYR:HB3 | 1.97 | 0.46 |
| 6:Ad:387:ALA:HB2 | 6:Ad:404:PHE:HB2 | 1.97 | 0.46 |
| 6:Ad:445:ASP:N | 6:Ad:445:ASP:OD1 | 2.48 | 0.46 |
| 6:Ae:127:LEU:HD11 | 6:Ae:252:PHE:HB2 | 1.96 | 0.46 |
| 6:Ae:350:PHE:HB2 | 6:Ae:389:VAL:HG11 | 1.97 | 0.46 |
| 7:Al:210:GLN:OE1 | 7:Al:218:ARG:NH2 | 2.45 | 0.46 |
| 7:Aq:210:GLN:HA | 7:Aq:227:VAL:HG13 | 1.97 | 0.46 |
| 6:Au:458:PRO:HB3 | 6:Au:473:PHE:CE2 | 2.51 | 0.46 |
| 6:Au:459:LEU:HD21 | 6:Au:474:LYS:HD2 | 1.97 | 0.46 |
| 6:Az:266:LEU:HB3 | 6:Az:294:LEU:HD22 | 1.98 | 0.46 |
| 2:B3:159:GLU:HB3 | 2:B3:163:LEU:HD23 | 1.98 | 0.46 |
| 2:B4:617:VAL:HG23 | 2:B4:622:GLU:HB2 | 1.96 | 0.46 |
| 5:BH:80:ARG:NH2 | 5:BH:153:ASP:OD2 | 2.39 | 0.46 |
| 7:BL:206:THR:HG21 | 7:BL:213:TRP:HE1 | 1.79 | 0.46 |
| 6:BM:317:GLY:HA2 | 6:BM:514:ARG:HE | 1.80 | 0.46 |
| 6:BM:414:ALA:HB3 | 6:BM:423:VAL:HG13 | 1.98 | 0.46 |
| 11:BR:9:ASN:HB3 | 11:BR:56:TYR:CE2 | 2.50 | 0.46 |
| 3:Bk:58:ILE:HD13 | 3:Bk:58:ILE:H | 1.79 | 0.46 |
| 3:Bn:40:ALA:H | 3:Bn:69:TRP:HE1 | 1.63 | 0.46 |
| 3:Bn:136:ASN:ND2 | 3:Bn:136:ASN:O | 2.49 | 0.46 |
| 2:Bp:41:ILE:HD13 | 2:Bp:81:VAL:HB | 1.98 | 0.46 |
| 2:Bp:281:ILE:O | 2:Bp:292:SER:HA | 2.15 | 0.46 |
| 2:Br:32:LYS:HD2 | 2:Br:32:LYS:H | 1.81 | 0.46 |
| 2:Br:557:PHE:HB3 | 2:Br:561:LYS:NZ | 2.29 | 0.46 |
| 2:Bs:119:LYS:HE3 | 2:Bs:119:LYS:HB2 | 1.84 | 0.46 |
| 2:Bt:100:GLU:HB3 | 2:Bt:188:ILE:HD11 | 1.98 | 0.46 |
| 2:Bt:128:GLU:HB2 | 2:Bt:146:PRO:HG2 | 1.97 | 0.46 |
| 2:Bu:417:ILE:HB | 2:Bu:421:ARG:HB3 | 1.98 | 0.46 |
| 2:Bv:427:VAL:HG13 | 2:Bv:520:GLU:HG3 | 1.96 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:By:102:THR:N | 2:By:183:THR:O | 2.45 | 0.46 |
| 3:o:54:MET:C | 3:o:56:ARG:H | 2.22 | 0.46 |
| 8:q:13:TYR:CD2 | 8:q:116:MET:HE1 | 2.49 | 0.46 |
| 2:1:10:LEU:HD13 | 2:AN:561:LYS:HB3 | 1.96 | 0.46 |
| 2:1:117:THR:HG23 | 2:1:127:THR:HG22 | 1.98 | 0.46 |
| 2:2:131:ILE:HD13 | 2:2:140:ILE:HG21 | 1.97 | 0.46 |
| 2:2:310:TYR:O | 2:2:314:PHE:HB2 | 2.15 | 0.46 |
| 2:3:241:LYS:O | 2:3:244:TYR:CB | 2.63 | 0.46 |
| 2:3:453:ASN:HB2 | 2:3:506:ALA:HB3 | 1.98 | 0.46 |
| 2:4:240:SER:OG | 2:4:334:PHE:O | 2.24 | 0.46 |
| 2:4:430:ARG:HG3 | 2:4:522:ILE:HD11 | 1.97 | 0.46 |
| 2:5:66:MET:HG2 | 2:5:468:VAL:HG21 | 1.97 | 0.46 |
| 4:A:26:LYS:NZ | 4:Q:37:GLN:O | 2.49 | 0.46 |
| 5:A0:125:MET:O | 5:A0:129:GLU:HG2 | 2.16 | 0.46 |
| 5:A1:366:ARG:NH1 | 5:A1:382:GLN:OE1 | 2.48 | 0.46 |
| 5:A2:213:GLU:CD | 5:A2:214:SER:H | 2.24 | 0.46 |
| 5:A2:339:ARG:HB3 | 5:A2:342:LYS:HZ3 | 1.80 | 0.46 |
| 6:A4:79:ILE:HG23 | 6:A5:121:THR:HG22 | 1.98 | 0.46 |
| 6:A5:96:MET:HB2 | 6:AW:124:VAL:HB | 1.96 | 0.46 |
| 6:A8:107:ILE:O | 6:A8:303:ASN:ND2 | 2.45 | 0.46 |
| 3:AG:39:THR:HG22 | 3:AG:71:VAL:HG22 | 1.97 | 0.46 |
| 2:AK:57:PRO:HG3 | 2:AK:65:PHE:CD1 | 2.51 | 0.46 |
| 2:AO:644:ALA:HA | 2:B5:557:PHE:CZ | 2.51 | 0.46 |
| 7:Ab:17:LEU:HD23 | 1:l:12:LEU:HD12 | 1.98 | 0.46 |
| 7:Ab:122:GLY:N | 7:Ab:137:ASP:OD2 | 2.39 | 0.46 |
| 7:Ab:271:LEU:HB3 | 7:Ab:272:PRO:HD2 | 1.96 | 0.46 |
| 6:Ac:71:ASP:OD1 | 6:Ac:72:HIS:N | 2.48 | 0.46 |
| 6:Ad:232:ILE:O | 6:Ad:236:GLN:HG2 | 2.16 | 0.46 |
| 6:Af:123:GLN:HB3 | 6:Af:258:VAL:HG12 | 1.98 | 0.46 |
| 6:Ak:274:LEU:HD13 | 6:BK:69:GLY:HA2 | 1.98 | 0.46 |
| 7:Al:138:LEU:HD21 | 7:BE:151:MET:HB2 | 1.98 | 0.46 |
| 7:Al:216:SER:HB3 | 7:BE:71:THR:HG21 | 1.98 | 0.46 |
| 6:Am:204:ASP:OD1 | 6:Am:205:ALA:N | 2.48 | 0.46 |
| 6:Ao:263:SER:O | 6:BM:228:MET:HG2 | 2.16 | 0.46 |
| 6:Ap:311:ASN:O | 6:Ap:515:ARG:NH1 | 2.49 | 0.46 |
| 7:As:23:PRO:HB3 | 1:m:17:GLY:HA2 | 1.96 | 0.46 |
| 6:Au:314:ALA:HA | 6:Au:513:PHE:HB2 | 1.98 | 0.46 |
| 5:Ax:45:VAL:HG11 | 5:Ax:57:ALA:HB2 | 1.97 | 0.46 |
| 5:Ax:373:LEU:HD23 | 5:Ax:373:LEU:HA | 1.84 | 0.46 |
| 6:Az:379:SER:OG | 6:Az:432:ASP:OD1 | 2.29 | 0.46 |
| 2:B1:569:LYS:HG3 | 2:Bz:494:TYR:CZ | 2.50 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B2:44:VAL:HG11 | 2:B2:50:LEU:HB2 | 1.98 | 0.46 |
| 2:B6:36:GLY:O | 2:B6:82:ARG:NH1 | 2.48 | 0.46 |
| 5:BA:18:ARG:O | 5:BA:21:LYS:HG3 | 2.16 | 0.46 |
| 5:BD:125:MET:O | 5:BD:129:GLU:HG2 | 2.15 | 0.46 |
| 7:BE:66:GLU:HA | 7:BE:69:TYR:HB3 | 1.98 | 0.46 |
| 5:BF:82:LEU:HD22 | 5:BF:258:VAL:HG22 | 1.97 | 0.46 |
| 5:BF:86:TYR:C | 5:BF:88:VAL:H | 2.24 | 0.46 |
| 5:BF:366:ARG:NH2 | 5:BF:383:ASP:OD1 | 2.45 | 0.46 |
| 5:BG:69:MET:O | 5:BG:72:THR:HG22 | 2.16 | 0.46 |
| 6:BJ:383:VAL:HG12 | 6:BJ:406:THR:HG22 | 1.97 | 0.46 |
| 3:Bf:70:THR:HG22 | 3:Bf:156:THR:HG22 | 1.98 | 0.46 |
| 3:Bh:70:THR:HG22 | 3:Bh:156:THR:HG22 | 1.98 | 0.46 |
| 2:Bq:511:GLN:OE1 | 2:Bt:5:SER:OG | 2.33 | 0.46 |
| 2:Br:135:ASP:N | 2:Br:139:LYS:O | 2.47 | 0.46 |
| 2:Br:480:ARG:O | 2:Br:484:VAL:HG12 | 2.15 | 0.46 |
| 2:Bt:69:MET:O | 2:Bt:73:GLN:HG2 | 2.15 | 0.46 |
| 2:Bt:131:ILE:HD11 | 2:Bt:171:ILE:HD13 | 1.97 | 0.46 |
| 2:Bv:44:VAL:HG11 | 2:Bv:50:LEU:HB2 | 1.97 | 0.46 |
| 2:Bv:432:ALA:HB2 | 2:Bv:440:ASN:HD22 | 1.80 | 0.46 |
| 2:Bx:26:THR:HA | 2:Bx:77:ASP:O | 2.15 | 0.46 |
| 4:J:12:ASP:HB2 | 4:L:52:LEU:HD21 | 1.97 | 0.46 |
| 4:i:59:ASP:O | 4:i:62:ILE:HG22 | 2.16 | 0.46 |
| 1:n:188:ASN:OD1 | 1:n:189:GLU:N | 2.42 | 0.46 |
| 1:p:63:ARG:H | 1:p:136:ASP:HB3 | 1.81 | 0.46 |
| 2:1:605:ARG:HG2 | 2:1:607:VAL:HG23 | 1.97 | 0.46 |
| 2:2:639:THR:HG23 | 2:3:11:LYS:HD3 | 1.97 | 0.46 |
| 3:7:80:ASP:OD1 | 3:7:84:LYS:NZ | 2.49 | 0.46 |
| 3:9:148:ASN:HA | 9:w:47:THR:HG22 | 1.97 | 0.46 |
| 5:A0:137:LEU:HG | 5:A0:174:LEU:HD12 | 1.98 | 0.46 |
| 5:A1:290:GLY:HA2 | 5:BD:340:ASP:H | 1.81 | 0.46 |
| 5:A2:304:VAL:HG13 | 7:AY:305:GLY:HA2 | 1.97 | 0.46 |
| 6:A4:136:VAL:HG22 | 6:A4:253:ARG:HG3 | 1.97 | 0.46 |
| 6:A8:120:PRO:HD3 | 6:A8:453:TYR:CZ | 2.50 | 0.46 |
| 6:A8:133:LYS:HA | 6:A8:249:GLU:HB2 | 1.98 | 0.46 |
| 6:A8:322:THR:HG22 | 6:A8:359:LYS:HG2 | 1.97 | 0.46 |
| 3:AA:7:THR:HG23 | 3:AA:14:ASP:H | 1.80 | 0.46 |
| 3:AH:87:ASP:O | 3:AH:91:ILE:HG13 | 2.15 | 0.46 |
| 2:AK:417:ILE:HD13 | 2:AK:417:ILE:H | 1.81 | 0.46 |
| 2:AK:521:ALA:HB1 | 2:AK:541:ALA:HA | 1.98 | 0.46 |
| 2:AK:612:ASN:HB3 | 2:AK:624:VAL:HG23 | 1.97 | 0.46 |
| 2:AL:134:VAL:HA | 2:AL:140:ILE:HA | 1.96 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AL:411:ARG:O | 2:AL:415:VAL:HB | 2.16 | 0.46 |
| 2:AL:477:LEU:HD11 | 2:AL:497:GLY:HA2 | 1.97 | 0.46 |
| 2:AN:57:PRO:HG3 | 2:AN:65:PHE:HB3 | 1.98 | 0.46 |
| 2:AP:28:ALA:HB2 | 2:AP:370:VAL:HG21 | 1.98 | 0.46 |
| 2:AP:247:GLY:O | 2:AP:263:SER:OG | 2.34 | 0.46 |
| 2:AP:494:TYR:OH | 2:AP:528:THR:OG1 | 2.27 | 0.46 |
| 7:Aa:88:LEU:HD13 | 7:Aa:183:ILE:HG22 | 1.98 | 0.46 |
| 6:Ac:163:PHE:HB2 | 6:Ac:179:THR:HG23 | 1.97 | 0.46 |
| 6:Ae:380:ARG:H | 6:Ae:380:ARG:HG2 | 1.60 | 0.46 |
| 6:Ah:154:PHE:CE2 | 6:Ah:248:ASN:HB3 | 2.51 | 0.46 |
| 6:Am:154:PHE:O | 6:Am:248:ASN:ND2 | 2.46 | 0.46 |
| 6:Am:484:PHE:O | 6:Am:487:SER:OG | 2.32 | 0.46 |
| 7:As:23:PRO:HA | 1:m:17:GLY:HA2 | 1.98 | 0.46 |
| 7:At:114:MET:HG2 | 5:BH:266:LEU:HG | 1.97 | 0.46 |
| 7:At:203:GLY:HA2 | 4:S:32:LEU:HD23 | 1.98 | 0.46 |
| 5:Av:350:LEU:HD21 | 5:BB:283:ARG:NH1 | 2.30 | 0.46 |
| 2:B2:453:ASN:ND2 | 2:B2:505:LEU:HG | 2.30 | 0.46 |
| 2:B2:654:LEU:HD22 | 2:B3:605:ARG:HD3 | 1.97 | 0.46 |
| 2:B3:195:LEU:HD11 | 2:B3:225:LEU:HA | 1.97 | 0.46 |
| 2:B5:222:VAL:HG22 | 2:B5:325:ALA:HB2 | 1.98 | 0.46 |
| 7:BE:99:ASP:N | 7:BE:99:ASP:OD1 | 2.48 | 0.46 |
| 5:BG:497:GLU:O | 5:BG:501:GLU:HG2 | 2.16 | 0.46 |
| 5:BH:454:PHE:CE2 | 5:BH:458:LYS:HD2 | 2.50 | 0.46 |
| 11:BO:9:ASN:HB3 | 11:BO:56:TYR:CE2 | 2.51 | 0.46 |
| 3:Bh:43:ALA:HA | 3:Bk:138:GLY:HA3 | 1.98 | 0.46 |
| 3:Bl:23:VAL:HG22 | 3:Bl:36:CYS:SG | 2.56 | 0.46 |
| 2:Bq:26:THR:HA | 2:Bq:77:ASP:O | 2.16 | 0.46 |
| 2:Bt:244:TYR:CZ | 2:Bt:266:LYS:HD2 | 2.50 | 0.46 |
| 2:Bv:131:ILE:HA | 2:Bv:143:ILE:HG22 | 1.98 | 0.46 |
| 2:Bv:238:ILE:HG12 | 2:Bv:281:ILE:HG12 | 1.97 | 0.46 |
| 2:Bv:526:THR:OG1 | 2:Bw:366:GLU:OE1 | 2.32 | 0.46 |
| 2:Bw:69:MET:O | 2:Bw:73:GLN:HG2 | 2.16 | 0.46 |
| 4:F:48:THR:HG21 | 4:Q:47:PRO:HB2 | 1.98 | 0.46 |
| 1:l:215:ILE:HG23 | 8:s:56:TRP:CH2 | 2.51 | 0.46 |
| 1:m:213:ILE:O | 8:t:55:LYS:HD2 | 2.16 | 0.46 |
| 1:n:83:ALA:HB2 | 1:n:183:PRO:HB3 | 1.98 | 0.46 |
| 1:p:146:LEU:HD13 | 1:p:174:PHE:HD2 | 1.80 | 0.46 |
| 8:u:62:GLN:HB3 | 8:u:63:GLU:H | 1.49 | 0.46 |
| 2:5:490:SER:OG | 2:5:538:ASP:OD2 | 2.28 | 0.46 |
| 2:5:514:ARG:NH2 | 2:AM:364:ASP:OD1 | 2.42 | 0.46 |
| 3:6:140:LEU:HD11 | 3:6:151:GLN:HB2 | 1.97 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:8:132:LEU:HD21 | 3:8:157:LEU:HD13 | 1.97 | 0.46 |
| 5:A1:318:THR:O | 7:Aq:70:LYS:NZ | 2.43 | 0.46 |
| 5:A1:393:GLY:HA2 | 5:A1:457:LEU:HD12 | 1.98 | 0.46 |
| 5:A2:239:HIS:CD2 | 5:A2:241:GLY:H | 2.34 | 0.46 |
| 5:A3:12:TRP:CD1 | 5:A3:234:ALA:HB2 | 2.51 | 0.46 |
| 5:A3:160:LYS:HE3 | 5:A3:236:VAL:HG22 | 1.97 | 0.46 |
| 6:A7:69:GLY:N | 6:A9:234:GLU:OE2 | 2.48 | 0.46 |
| 3:AF:143:ASP:OD1 | 3:AF:144:TRP:N | 2.49 | 0.46 |
| 3:AH:6:VAL:HG21 | 3:o:58:ILE:HG12 | 1.96 | 0.46 |
| 2:AL:99:ILE:HD13 | 2:AL:184:LEU:HD22 | 1.97 | 0.46 |
| 2:AP:12:GLU:H | 2:AP:12:GLU:HG2 | 1.58 | 0.46 |
| 10:AQ:297:LEU:HB3 | 6:Af:328:LYS:NZ | 2.29 | 0.46 |
| 6:AV:401:ALA:O | 6:AZ:420:LYS:NZ | 2.41 | 0.46 |
| 7:AY:200:ASN:ND2 | 7:AY:233:GLN:O | 2.49 | 0.46 |
| 6:AZ:204:ASP:OD1 | 6:AZ:205:ALA:N | 2.48 | 0.46 |
| 6:Ak:139:GLY:O | 6:Ak:141:LYS:NZ | 2.37 | 0.46 |
| 7:Al:98:MET:HB3 | 6:BM:459:LEU:HD23 | 1.98 | 0.46 |
| 6:An:276:GLN:HG2 | 7:Aq:151:MET:SD | 2.56 | 0.46 |
| 6:An:337:PRO:HA | 6:An:340:ILE:HG12 | 1.98 | 0.46 |
| 6:Ao:278:LEU:HG | 6:Ao:284:MET:HB2 | 1.98 | 0.46 |
| 6:Ap:131:TYR:CE1 | 6:Ap:141:LYS:HB2 | 2.49 | 0.46 |
| 7:As:230:VAL:HB | 7:As:233:GLN:HG2 | 1.97 | 0.46 |
| 7:At:30:THR:OG1 | 7:At:33:GLN:OE1 | 2.17 | 0.46 |
| 6:Au:267:LYS:O | 6:Ay:249:GLU:HA | 2.16 | 0.46 |
| 5:Av:158:PHE:HB2 | 5:Av:236:VAL:HB | 1.98 | 0.46 |
| 6:Ay:262:LYS:HE3 | 6:Ay:500:MET:HE2 | 1.96 | 0.46 |
| 6:Ay:404:PHE:HB3 | 6:Ay:414:ALA:HB1 | 1.97 | 0.46 |
| 2:B2:514:ARG:NH1 | 2:B3:366:GLU:OE2 | 2.49 | 0.46 |
| 2:B2:642:PHE:HB3 | 2:B3:557:PHE:HE2 | 1.81 | 0.46 |
| 2:B3:116:ILE:HB | 2:B3:129:GLY:HA3 | 1.98 | 0.46 |
| 2:B4:550:ARG:HB3 | 2:B4:553:VAL:HG12 | 1.97 | 0.46 |
| 5:BA:111:LEU:HD11 | 5:BA:444:ILE:HD11 | 1.98 | 0.46 |
| 7:BC:261:GLN:OE1 | 7:BE:256:LYS:NZ | 2.49 | 0.46 |
| 7:BE:161:PHE:HA | 7:BE:171:LYS:O | 2.16 | 0.46 |
| 6:BJ:363:GLU:HA | 6:BJ:366:ARG:HG2 | 1.97 | 0.46 |
| 7:BL:296:GLU:O | 7:BL:299:LEU:HD12 | 2.16 | 0.46 |
| 11:BU:14:GLU:HB3 | 11:BU:25:GLY:H | 1.80 | 0.46 |
| 3:BY:8:ARG:HA | 3:BY:11:GLU:HG2 | 1.97 | 0.46 |
| 3:BY:83:GLN:HA | 3:BY:86:VAL:HG22 | 1.98 | 0.46 |
| 3:Be:69:TRP:CZ3 | 3:Be:132:LEU:HD21 | 2.50 | 0.46 |
| 2:Bs:148:ALA:O | 2:Bs:151:ILE:HG13 | 2.16 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bs:153:LYS:HB3 | 2:Bs:167:TRP:HH2 | 1.81 | 0.46 |
| 2:Bx:40:GLN:H | 2:Bx:81:VAL:HG23 | 1.81 | 0.46 |
| 2:By:49:ASP:N | 2:By:49:ASP:OD1 | 2.46 | 0.46 |
| 2:By:617:VAL:HG23 | 2:By:620:ARG:HD2 | 1.98 | 0.46 |
| 2:Bz:57:PRO:O | 2:Bz:462:ASN:ND2 | 2.47 | 0.46 |
| 2:Bz:427:VAL:HG13 | 2:Bz:520:GLU:HG3 | 1.97 | 0.46 |
| 4:C:48:THR:HG21 | 4:H:47:PRO:HB2 | 1.98 | 0.46 |
| 4:H:6:ASN:HB2 | 4:H:57:VAL:HG13 | 1.98 | 0.46 |
| 4:a:10:PHE:O | 4:a:54:ASN:ND2 | 2.49 | 0.46 |
| 8:t:105:VAL:HG23 | 8:t:205:ALA:HB3 | 1.98 | 0.46 |
| 8:u:8:SER:O | 8:u:12:ARG:HG2 | 2.15 | 0.46 |
| 9:x:137:ASP:OD1 | 9:x:138:LEU:N | 2.49 | 0.46 |
| 2:1:152:ALA:O | 2:1:156:GLU:HG2 | 2.16 | 0.46 |
| 2:2:154:ALA:HB2 | 2:2:163:LEU:HD11 | 1.98 | 0.46 |
| 2:2:623:PHE:HB3 | 8:r:212:THR:HG22 | 1.97 | 0.46 |
| 2:4:600:GLY:O | 2:4:632:ALA:HB2 | 2.16 | 0.46 |
| 2:5:379:ALA:HB2 | 2:5:411:ARG:HB2 | 1.97 | 0.46 |
| 3:8:41:LEU:N | 3:9:140:LEU:O | 2.41 | 0.46 |
| 3:9:131:GLY:O | 3:9:159:LEU:HA | 2.15 | 0.46 |
| 5:A0:207:ILE:HD11 | 5:A0:227:LYS:HB3 | 1.98 | 0.46 |
| 5:A1:175:ARG:NH1 | 5:BB:30:SER:OG | 2.48 | 0.46 |
| 5:A1:304:VAL:O | 5:A1:308:MET:HB3 | 2.15 | 0.46 |
| 5:A2:6:LEU:HD11 | 5:A2:228:ILE:HD13 | 1.98 | 0.46 |
| 5:A2:160:LYS:NZ | 5:A2:424:THR:OG1 | 2.35 | 0.46 |
| 5:A3:345:THR:HG21 | 7:A6:306:ILE:HD11 | 1.98 | 0.46 |
| 7:A6:163:PHE:HA | 7:A6:170:LEU:HA | 1.97 | 0.46 |
| 8:AB:43:TYR:HD1 | 8:AB:45:SER:H | 1.64 | 0.46 |
| 3:AG:103:LYS:H | 3:AG:103:LYS:HD2 | 1.81 | 0.46 |
| 3:AI:97:ASN:O | 3:Bd:3:VAL:N | 2.44 | 0.46 |
| 2:AM:547:PRO:HD3 | 2:AN:304:ILE:HB | 1.98 | 0.46 |
| 2:AN:239:VAL:HG22 | 2:AN:280:ALA:HB3 | 1.98 | 0.46 |
| 2:AP:24:THR:HB | 2:AP:483:ASN:OD1 | 2.16 | 0.46 |
| 2:AP:82:ARG:NH1 | 2:AP:227:PRO:O | 2.47 | 0.46 |
| 6:AV:454:VAL:HG21 | 7:BE:112:LEU:HD13 | 1.97 | 0.46 |
| 6:AW:318:LYS:NZ | 6:AW:356:GLN:OE1 | 2.37 | 0.46 |
| 7:Ab:54:ASN:OD1 | 7:Ab:188:THR:OG1 | 2.33 | 0.46 |
| 6:Ag:426:ASP:OD2 | 6:Ag:433:TYR:OH | 2.19 | 0.46 |
| 6:Ao:398:GLN:HG2 | 6:Ao:399:GLY:H | 1.81 | 0.46 |
| 6:Ap:337:PRO:HA | 6:Ap:340:ILE:HG12 | 1.98 | 0.46 |
| 7:Ar:159:PRO:HB3 | 7:Ar:174:GLY:O | 2.16 | 0.46 |
| 7:At:12:LEU:O | 7:At:16:ILE:HG12 | 2.14 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:At:112:LEU:HD21 | 7:At:129:TYR:CE2 | 2.49 | 0.46 |
| 6:Au:236:GLN:HG3 | 6:BJ:265:GLN:NE2 | 2.31 | 0.46 |
| 6:Aw:145:HIS:HD2 | 6:Aw:148:TYR:CD2 | 2.34 | 0.46 |
| 5:Ax:212:HIS:O | 5:Ax:214:SER:N | 2.47 | 0.46 |
| 2:B1:557:PHE:HE1 | 2:Bz:642:PHE:HB3 | 1.80 | 0.46 |
| 2:B2:105:THR:HB | 2:B2:181:VAL:HB | 1.98 | 0.46 |
| 2:B5:102:THR:HB | 2:B5:183:THR:HB | 1.97 | 0.46 |
| 2:B7:351:THR:OG1 | 2:B7:352:ALA:N | 2.48 | 0.46 |
| 5:BG:295:ARG:HA | 5:BG:295:ARG:HD3 | 1.82 | 0.46 |
| 3:Bd:64:ARG:NH2 | 3:Bg:93:ALA:HB3 | 2.31 | 0.46 |
| 3:Bl:51:VAL:HG23 | 3:Bl:58:ILE:HG12 | 1.98 | 0.46 |
| 2:Bs:514:ARG:NH1 | 2:Bt:366:GLU:OE2 | 2.49 | 0.46 |
| 2:Bs:642:PHE:CZ | 2:Bt:564:ILE:HD11 | 2.50 | 0.46 |
| 2:Bu:26:THR:HA | 2:Bu:77:ASP:O | 2.15 | 0.46 |
| 1:m:147:PHE:HE1 | 1:m:173:LYS:HD2 | 1.80 | 0.46 |
| 1:n:176:TYR:HA | 8:u:71:ILE:HA | 1.98 | 0.46 |
| 8:s:259:VAL:HG12 | 8:s:260:ASN:H | 1.81 | 0.46 |
| 9:v:56:LEU:O | 9:x:97:TYR:HB3 | 2.16 | 0.46 |
| 9:w:15:THR:OG1 | 9:w:16:ASN:N | 2.46 | 0.46 |
| 2:3:498:GLN:HA | 2:3:534:VAL:HA | 1.98 | 0.46 |
| 3:7:6:VAL:HG13 | 3:7:7:THR:H | 1.80 | 0.46 |
| 3:9:37:LYS:O | 3:AA:144:TRP:N | 2.46 | 0.46 |
| 5:A0:183:GLN:HB3 | 5:A0:207:ILE:HG23 | 1.98 | 0.46 |
| 5:A1:426:LEU:HD13 | 5:A1:432:ILE:HG21 | 1.97 | 0.46 |
| 5:A2:278:ARG:HD2 | 5:BF:283:ARG:HE | 1.81 | 0.46 |
| 6:A4:255:ASP:N | 6:A4:255:ASP:OD1 | 2.49 | 0.46 |
| 6:A5:153:MET:HE2 | 6:A5:189:TYR:CG | 2.51 | 0.46 |
| 6:A7:131:TYR:HD2 | 6:A7:250:MET:HE3 | 1.80 | 0.46 |
| 6:A8:450:TYR:CE1 | 6:A8:477:TYR:HB2 | 2.51 | 0.46 |
| 8:AB:13:TYR:CD2 | 8:AB:116:MET:HE1 | 2.51 | 0.46 |
| 2:AK:487:THR:HG21 | 2:AK:559:MET:HE3 | 1.98 | 0.46 |
| 2:AM:140:ILE:O | 2:AM:141:LYS:NZ | 2.47 | 0.46 |
| 2:AO:154:ALA:HA | 2:AO:157:VAL:HG22 | 1.98 | 0.46 |
| 6:AV:216:MET:HE1 | 6:Ap:430:LYS:HG3 | 1.98 | 0.46 |
| 6:AX:74:TYR:HA | 6:AX:79:ILE:HD11 | 1.98 | 0.46 |
| 6:AX:344:ARG:HG2 | 6:AX:345:TRP:H | 1.81 | 0.46 |
| 6:AZ:131:TYR:HD2 | 6:AZ:250:MET:HE3 | 1.81 | 0.46 |
| 6:AZ:379:SER:OG | 6:AZ:432:ASP:OD1 | 2.30 | 0.46 |
| 6:Ac:107:ILE:HA | 6:Ac:412:VAL:HG21 | 1.98 | 0.46 |
| 6:Ad:367:GLN:HB3 | 6:Ad:511:ALA:HB1 | 1.96 | 0.46 |
| 6:Aj:98:MET:HE2 | 6:An:127:LEU:HB2 | 1.98 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Al:210:GLN:O | 7:Al:210:GLN:NE2 | 2.49 | 0.46 |
| 6:An:91:ILE:HG13 | 6:BK:123:GLN:HE22 | 1.81 | 0.46 |
| 6:Ap:345:TRP:CD1 | 6:Ap:348:GLU:HG3 | 2.51 | 0.46 |
| 7:Ar:43:GLU:O | 7:Ar:47:GLU:HG2 | 2.16 | 0.46 |
| 5:Ax:329:SER:O | 5:BA:282:ARG:NH2 | 2.35 | 0.46 |
| 2:B1:131:ILE:HA | 2:B1:143:ILE:HG22 | 1.98 | 0.46 |
| 2:B4:538:ASP:O | 2:B4:550:ARG:HA | 2.15 | 0.46 |
| 2:B5:30:ALA:HB3 | 2:B5:359:TRP:CE2 | 2.51 | 0.46 |
| 2:B6:89:ALA:HA | 2:B6:345:SER:HA | 1.98 | 0.46 |
| 2:B7:118:VAL:HB | 2:B7:126:GLU:HB3 | 1.98 | 0.46 |
| 2:B7:375:ALA:HB1 | 2:B7:390:GLN:HG2 | 1.97 | 0.46 |
| 2:B7:521:ALA:HB1 | 2:B7:541:ALA:HA | 1.97 | 0.46 |
| 5:BF:278:ARG:HH11 | 5:BG:331:THR:HA | 1.80 | 0.46 |
| 5:BG:121:LYS:HB3 | 5:BG:121:LYS:HE2 | 1.77 | 0.46 |
| 5:BH:328:MET:HE2 | 5:BH:328:MET:HB3 | 1.81 | 0.46 |
| 6:BK:332:PHE:HB3 | 6:BK:518:VAL:HG12 | 1.97 | 0.46 |
| 6:BM:314:ALA:HA | 6:BM:513:PHE:HB2 | 1.97 | 0.46 |
| 3:Bf:17:ARG:HH11 | 3:Bf:118:ARG:HH11 | 1.63 | 0.46 |
| 3:Bg:37:LYS:HZ2 | 3:Bg:74:MET:HG2 | 1.81 | 0.46 |
| 3:Bg:64:ARG:NH1 | 3:Bj:95:GLN:HG2 | 2.31 | 0.46 |
| 3:Bn:114:ARG:HB3 | 3:Bn:123:VAL:HG13 | 1.96 | 0.46 |
| 2:Bp:379:ALA:HB2 | 2:Bp:454:TYR:HE2 | 1.81 | 0.46 |
| 2:Br:130:LYS:HZ3 | 2:Br:132:THR:HA | 1.81 | 0.46 |
| 2:Br:239:VAL:HG22 | 2:Br:280:ALA:HB3 | 1.98 | 0.46 |
| 2:Br:420:THR:HG22 | 2:Br:513:GLN:HE22 | 1.81 | 0.46 |
| 2:Bs:37:PRO:HG3 | 2:Bs:226:TYR:CZ | 2.51 | 0.46 |
| 2:Bs:414:VAL:HG23 | 2:Bs:422:ALA:HB1 | 1.97 | 0.46 |
| 2:Bs:480:ARG:C | 2:Bs:482:ASP:H | 2.23 | 0.46 |
| 2:Bu:641:ASN:OD1 | 2:Bu:641:ASN:N | 2.49 | 0.46 |
| 2:Bv:41:ILE:HD11 | 2:Bv:361:PHE:HB3 | 1.97 | 0.46 |
| 4:f:10:PHE:HB3 | 4:f:22:ILE:HG12 | 1.98 | 0.46 |
| 1:m:220:GLU:CD | 8:t:46:LYS:HZ1 | 2.24 | 0.46 |
| 1:n:233:GLU:HG3 | 1:n:234:PRO:HD2 | 1.97 | 0.46 |
| 8:q:128:ASP:O | 8:q:132:GLN:HG3 | 2.16 | 0.46 |
| 8:r:142:GLN:O | 8:r:143:PRO:C | 2.59 | 0.46 |
| 2:1:538:ASP:OD1 | 2:1:538:ASP:N | 2.48 | 0.45 |
| 2:2:413:THR:OG1 | 2:2:425:ASN:HB3 | 2.16 | 0.45 |
| 2:3:131:ILE:HD13 | 2:3:140:ILE:HG21 | 1.98 | 0.45 |
| 2:4:560:LEU:HD22 | 2:4:629:ILE:HD13 | 1.98 | 0.45 |
| 2:4:616:SER:O | 2:4:620:ARG:HG2 | 2.16 | 0.45 |
| 5:A1:461:GLU:HG3 | 5:BB:465:ARG:HH22 | 1.81 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A3:45:VAL:HG21 | 5:A3:187:GLU:HB2 | 1.98 | 0.45 |
| 6:A7:107:ILE:HD13 | 6:A7:424:TYR:HB3 | 1.98 | 0.45 |
| 2:AD:374:ILE:HG23 | 2:AD:471:ALA:O | 2.16 | 0.45 |
| 2:AD:528:THR:HA | 2:AN:367:SER:HA | 1.97 | 0.45 |
| 2:AK:91:ASN:OD1 | 2:AK:91:ASN:N | 2.49 | 0.45 |
| 2:AL:44:VAL:HG11 | 2:AL:50:LEU:HB2 | 1.98 | 0.45 |
| 2:AP:131:ILE:HG12 | 2:AP:143:ILE:HG22 | 1.97 | 0.45 |
| 7:Aa:12:LEU:HD12 | 7:Aa:242:TYR:HD2 | 1.81 | 0.45 |
| 6:Ac:333:ASP:HB3 | 6:Ac:336:ASP:HB2 | 1.97 | 0.45 |
| 6:Ac:345:TRP:HB3 | 6:Ag:343:ALA:HA | 1.97 | 0.45 |
| 6:Ad:350:PHE:HB2 | 6:Ad:389:VAL:HG11 | 1.97 | 0.45 |
| 6:Af:261:ALA:HA | 6:Af:478:GLY:HA3 | 1.98 | 0.45 |
| 6:Ai:255:ASP:OD1 | 6:Ai:255:ASP:N | 2.48 | 0.45 |
| 6:Aj:263:SER:O | 6:An:228:MET:N | 2.43 | 0.45 |
| 6:Ak:515:ARG:NH2 | 6:Ak:517:TYR:OH | 2.37 | 0.45 |
| 6:Am:133:LYS:HB2 | 6:Am:249:GLU:HG3 | 1.96 | 0.45 |
| 6:An:378:ALA:HB1 | 6:An:382:VAL:HB | 1.99 | 0.45 |
| 7:Aq:85:THR:HG21 | 7:Aq:187:TRP:HE1 | 1.81 | 0.45 |
| 7:Aq:91:ASN:O | 7:Aq:94:SER:N | 2.48 | 0.45 |
| 7:Ar:104:TYR:CZ | 6:Au:120:PRO:HB3 | 2.51 | 0.45 |
| 7:As:50:PHE:HB3 | 7:As:302:PRO:HD3 | 1.97 | 0.45 |
| 6:Au:148:TYR:HA | 6:Au:186:GLY:H | 1.80 | 0.45 |
| 5:Av:10:ALA:HB3 | 5:Av:11:PRO:HD3 | 1.98 | 0.45 |
| 5:Ax:60:THR:O | 5:Ax:64:SER:OG | 2.29 | 0.45 |
| 2:B1:454:TYR:H | 2:B1:506:ALA:HB2 | 1.79 | 0.45 |
| 2:B1:569:LYS:HG3 | 2:Bz:494:TYR:CE1 | 2.51 | 0.45 |
| 2:B4:205:MET:O | 2:B4:211:GLN:NE2 | 2.49 | 0.45 |
| 2:B5:617:VAL:HG22 | 2:B5:622:GLU:HB2 | 1.98 | 0.45 |
| 2:B6:222:VAL:HG21 | 2:B6:238:ILE:HD11 | 1.99 | 0.45 |
| 2:B7:159:GLU:OE2 | 2:B7:166:ASN:ND2 | 2.45 | 0.45 |
| 2:B7:642:PHE:H | 2:Br:12:GLU:HA | 1.81 | 0.45 |
| 5:BB:458:LYS:O | 5:BB:461:GLU:HG3 | 2.16 | 0.45 |
| 5:BD:70:LYS:HA | 5:BD:70:LYS:HD2 | 1.71 | 0.45 |
| 7:BE:20:LEU:HD23 | 7:BE:20:LEU:HA | 1.80 | 0.45 |
| 5:BH:37:ASP:OD1 | 5:BH:37:ASP:N | 2.48 | 0.45 |
| 6:BI:131:TYR:HA | 6:BI:250:MET:HA | 1.98 | 0.45 |
| 6:BJ:466:ASN:OD1 | 6:BJ:466:ASN:N | 2.47 | 0.45 |
| 3:BZ:63:ASP:OD1 | 3:BZ:64:ARG:N | 2.44 | 0.45 |
| 3:Ba:61:ALA:HA | 3:Bd:133:TRP:CH2 | 2.51 | 0.45 |
| 2:Bp:315:PHE:HE1 | 2:Bp:323:ILE:HG13 | 1.80 | 0.45 |
| 2:Bs:106:PRO:HB3 | 2:Bs:139:LYS:HZ3 | 1.81 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bt:332:GLU:OE1 | 2:Bt:332:GLU:N | 2.44 | 0.45 |
| 2:Bu:237:GLU:HB3 | 2:Bu:282:ILE:HG13 | 1.98 | 0.45 |
| 2:Bv:151:ILE:O | 2:Bv:155:LYS:HG2 | 2.15 | 0.45 |
| 2:By:346:SER:O | 2:By:350:VAL:HG23 | 2.16 | 0.45 |
| 2:By:639:THR:HB | 2:Bz:624:VAL:HG12 | 1.98 | 0.45 |
| 2:Bz:2:THR:OG1 | 2:Bz:3:LEU:N | 2.49 | 0.45 |
| 2:Bz:477:LEU:HD21 | 2:Bz:497:GLY:HA2 | 1.97 | 0.45 |
| 1:k:220:GLU:OE2 | 8:r:46:LYS:NZ | 2.41 | 0.45 |
| 1:l:169:ILE:H | 1:l:169:ILE:HG12 | 1.61 | 0.45 |
| 8:q:91:ASN:O | 8:q:110:ASN:ND2 | 2.48 | 0.45 |
| 2:2:317:LYS:HE3 | 2:2:317:LYS:HB2 | 1.82 | 0.45 |
| 2:2:372:LEU:HA | 2:2:372:LEU:HD12 | 1.80 | 0.45 |
| 5:A3:210:THR:O | 5:A3:224:ALA:HB1 | 2.16 | 0.45 |
| 7:A6:24:ILE:HG13 | 7:Al:262:ILE:HD13 | 1.99 | 0.45 |
| 6:A8:236:GLN:HE21 | 6:A8:247:TRP:HD1 | 1.63 | 0.45 |
| 6:A9:279:ARG:NH2 | 5:Av:227:LYS:HG3 | 2.31 | 0.45 |
| 8:AB:174:GLU:OE1 | 8:u:78:HIS:NE2 | 2.35 | 0.45 |
| 2:AD:91:ASN:N | 2:AD:91:ASN:OD1 | 2.49 | 0.45 |
| 3:AI:94:GLY:HA3 | 3:AI:100:THR:HG1 | 1.81 | 0.45 |
| 3:AJ:83:GLN:HA | 3:AJ:86:VAL:HG22 | 1.98 | 0.45 |
| 2:AK:164:GLY:H | 2:AK:167:TRP:CD1 | 2.34 | 0.45 |
| 10:AR:331:ASP:OD1 | 10:AR:331:ASP:N | 2.40 | 0.45 |
| 6:Ae:182:PHE:HB2 | 6:Ae:184:GLU:O | 2.17 | 0.45 |
| 6:Ae:315:GLN:OE1 | 6:Ae:514:ARG:NH1 | 2.49 | 0.45 |
| 6:Ag:279:ARG:HD3 | 6:Ag:285:ASP:HA | 1.98 | 0.45 |
| 6:Ah:76:ALA:HB1 | 6:BI:497:GLN:HA | 1.98 | 0.45 |
| 7:As:309:GLY:HA3 | 5:BB:305:MET:HE3 | 1.98 | 0.45 |
| 2:B1:57:PRO:HD2 | 2:B1:461:TYR:HD2 | 1.81 | 0.45 |
| 2:B2:642:PHE:CZ | 2:B3:564:ILE:HD11 | 2.51 | 0.45 |
| 2:B3:26:THR:HA | 2:B3:77:ASP:O | 2.16 | 0.45 |
| 2:B3:650:ASP:O | 2:B3:653:GLU:HG2 | 2.16 | 0.45 |
| 2:B4:227:PRO:HB2 | 2:B4:345:SER:HB3 | 1.98 | 0.45 |
| 2:B4:237:GLU:OE1 | 2:B4:284:ARG:NH1 | 2.42 | 0.45 |
| 2:B4:592:LEU:HD23 | 2:B4:604:TYR:HB2 | 1.98 | 0.45 |
| 2:B6:487:THR:HG21 | 2:B6:559:MET:HE3 | 1.99 | 0.45 |
| 2:B7:223:VAL:HA | 2:B7:340:LEU:HD11 | 1.98 | 0.45 |
| 2:B7:365:ARG:HB2 | 2:B7:400:ARG:HG2 | 1.97 | 0.45 |
| 2:B7:572:LEU:HB3 | 2:B7:573:PHE:H | 1.68 | 0.45 |
| 5:BB:125:MET:O | 5:BB:129:GLU:HG2 | 2.16 | 0.45 |
| 5:BB:366:ARG:HG2 | 5:BB:380:ILE:HD12 | 1.99 | 0.45 |
| 5:BB:399:ASP:OD1 | 5:BB:399:ASP:N | 2.49 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BE:50:PHE:HB3 | 7:BE:302:PRO:HD3 | 1.97 | 0.45 |
| 6:BJ:426:ASP:OD2 | 6:BJ:433:TYR:OH | 2.19 | 0.45 |
| 11:BS:26:LYS:NZ | 11:BS:74:ASP:OD1 | 2.42 | 0.45 |
| 3:BY:118:ARG:N | 3:Bb:77:GLU:OE2 | 2.48 | 0.45 |
| 3:Bd:32:PHE:HZ | 3:Bd:71:VAL:HG11 | 1.80 | 0.45 |
| 3:Bf:16:ALA:HB2 | 3:Bi:76:ASP:O | 2.17 | 0.45 |
| 3:Bf:16:ALA:HB3 | 3:Bi:151:GLN:HB2 | 1.98 | 0.45 |
| 3:Bk:59:ASN:ND2 | 3:Bn:159:LEU:O | 2.49 | 0.45 |
| 2:Br:406:LEU:HD13 | 2:Br:475:ALA:HB2 | 1.98 | 0.45 |
| 2:Bt:351:THR:OG1 | 2:Bt:352:ALA:N | 2.49 | 0.45 |
| 2:Bu:244:TYR:CZ | 2:Bu:266:LYS:HD2 | 2.51 | 0.45 |
| 2:Bv:526:THR:OG1 | 2:Bv:527:GLY:N | 2.48 | 0.45 |
| 1:m:60:TYR:OH | 1:m:136:ASP:OD2 | 2.30 | 0.45 |
| 1:m:202:ASN:HA | 1:m:205:ARG:HE | 1.81 | 0.45 |
| 1:p:147:PHE:HD2 | 1:p:172:GLY:O | 2.00 | 0.45 |
| 2:1:94:PRO:HB2 | 2:1:219:ILE:HD12 | 1.97 | 0.45 |
| 2:3:373:PHE:HB2 | 2:3:405:VAL:HG22 | 1.99 | 0.45 |
| 3:7:54:MET:C | 3:7:56:ARG:H | 2.22 | 0.45 |
| 4:A:26:LYS:HA | 4:Q:34:ALA:HB3 | 1.98 | 0.45 |
| 5:A0:278:ARG:HD2 | 5:BH:283:ARG:HH21 | 1.81 | 0.45 |
| 5:A2:292:MET:O | 5:A2:294:ALA:N | 2.45 | 0.45 |
| 6:A7:107:ILE:HG21 | 6:A7:424:TYR:HB3 | 1.98 | 0.45 |
| 6:A7:362:VAL:HG21 | 6:AW:384:ASN:HD21 | 1.81 | 0.45 |
| 6:A7:521:ILE:O | 6:A8:341:ARG:NH2 | 2.49 | 0.45 |
| 6:A8:426:ASP:OD2 | 6:A8:433:TYR:OH | 2.29 | 0.45 |
| 2:AK:550:ARG:HB3 | 2:AK:553:VAL:HG12 | 1.97 | 0.45 |
| 2:AN:642:PHE:CZ | 2:B2:564:ILE:HD11 | 2.50 | 0.45 |
| 2:AP:455:LYS:NZ | 2:AP:457:GLN:OE1 | 2.49 | 0.45 |
| 6:AV:263:SER:HA | 6:AV:476:ARG:HA | 1.98 | 0.45 |
| 6:AV:274:LEU:HD13 | 6:Am:69:GLY:HA2 | 1.98 | 0.45 |
| 6:AZ:350:PHE:HB3 | 6:AZ:389:VAL:HG21 | 1.98 | 0.45 |
| 6:Ad:309:TRP:HZ2 | 6:Ah:226:GLU:HB3 | 1.82 | 0.45 |
| 6:Ae:481:ILE:HG13 | 6:Ae:499:GLY:O | 2.16 | 0.45 |
| 6:Aj:134:ASP:HB3 | 6:Aj:137:ALA:HB2 | 1.98 | 0.45 |
| 6:Ak:344:ARG:H | 6:Ak:344:ARG:NE | 2.15 | 0.45 |
| 6:Ao:450:TYR:HE1 | 6:Ao:477:TYR:HB2 | 1.81 | 0.45 |
| 6:Ap:390:ASP:OD1 | 6:Ap:391:THR:N | 2.49 | 0.45 |
| 6:Au:317:GLY:HA2 | 6:Au:514:ARG:HE | 1.81 | 0.45 |
| 2:B1:332:GLU:H | 2:B1:332:GLU:CD | 2.24 | 0.45 |
| 2:B1:455:LYS:HD2 | 2:B1:502:VAL:HG22 | 1.98 | 0.45 |
| 2:B1:510:ARG:HG2 | 2:B1:511:GLN:H | 1.81 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B3:250:ALA:HB3 | 2:B3:263:SER:OG | 2.17 | 0.45 |
| 2:B5:430:ARG:HG3 | 2:B5:522:ILE:HD11 | 1.98 | 0.45 |
| 5:BA:125:MET:HB3 | 5:BA:431:ILE:HD13 | 1.99 | 0.45 |
| 7:BE:58:HIS:ND1 | 7:BE:186:SER:OG | 2.49 | 0.45 |
| 5:BF:494:THR:O | 5:BF:498:ILE:HG12 | 2.16 | 0.45 |
| 6:BJ:204:ASP:OD1 | 6:BJ:205:ALA:N | 2.50 | 0.45 |
| 11:BN:64:GLN:O | 11:BN:66:THR:N | 2.50 | 0.45 |
| 3:BY:41:LEU:HD13 | 3:Bb:140:LEU:HD23 | 1.97 | 0.45 |
| 3:Be:1:MET:SD | 3:Bh:22:GLN:NE2 | 2.89 | 0.45 |
| 3:Bf:124:THR:HB | 3:Bi:78:ALA:HA | 1.97 | 0.45 |
| 3:Bm:1:MET:HE2 | 3:Bm:1:MET:HB3 | 1.81 | 0.45 |
| 2:Bp:22:ASN:HB2 | 2:Bp:76:ASN:HD21 | 1.80 | 0.45 |
| 2:Bp:97:GLY:O | 2:Bp:147:THR:OG1 | 2.24 | 0.45 |
| 2:Bq:365:ARG:HA | 2:Bq:400:ARG:NH2 | 2.31 | 0.45 |
| 2:Bv:157:VAL:HG23 | 2:Bv:159:GLU:H | 1.81 | 0.45 |
| 2:Bw:394:VAL:HG11 | 2:Bw:443:ILE:HD12 | 1.99 | 0.45 |
| 2:Bz:134:VAL:HG12 | 2:Bz:140:ILE:HG22 | 1.98 | 0.45 |
| 2:Bz:539:LYS:HD3 | 2:Bz:550:ARG:HH21 | 1.81 | 0.45 |
| 1:l:152:VAL:HG13 | 1:l:169:ILE:HD13 | 1.98 | 0.45 |
| 1:l:177:SER:HB2 | 1:l:207:LEU:HB3 | 1.96 | 0.45 |
| 1:m:239:ASN:N | 1:m:239:ASN:OD1 | 2.49 | 0.45 |
| 8:r:162:ASP:OD1 | 8:r:162:ASP:N | 2.49 | 0.45 |
| 8:r:165:ILE:HG23 | 8:r:194:VAL:HG22 | 1.99 | 0.45 |
| 2:1:51:VAL:HG22 | 2:1:65:PHE:HZ | 1.82 | 0.45 |
| 2:4:132:THR:HB | 2:4:142:LYS:HB3 | 1.98 | 0.45 |
| 2:4:554:ARG:NH1 | 8:t:231:GLU:OE2 | 2.47 | 0.45 |
| 3:6:79:HIS:CE1 | 3:o:115:GLN:HG2 | 2.52 | 0.45 |
| 5:A0:41:ARG:HG3 | 5:A0:183:GLN:NE2 | 2.31 | 0.45 |
| 5:A0:80:ARG:NH2 | 5:A0:153:ASP:OD2 | 2.50 | 0.45 |
| 5:A1:338:ARG:NH2 | 5:BB:346:GLU:OE1 | 2.49 | 0.45 |
| 5:A3:282:ARG:HA | 5:BF:278:ARG:NH2 | 2.31 | 0.45 |
| 7:A6:112:LEU:HD21 | 7:A6:131:PRO:HG3 | 1.98 | 0.45 |
| 6:A9:133:LYS:HG2 | 6:A9:249:GLU:HB3 | 1.99 | 0.45 |
| 9:AC:64:VAL:O | 9:AC:65:THR:OG1 | 2.34 | 0.45 |
| 2:AP:498:GLN:HA | 2:AP:534:VAL:HG12 | 1.98 | 0.45 |
| 10:AT:318:MET:HE1 | 10:AT:328:ASP:HB3 | 1.98 | 0.45 |
| 6:AV:149:GLY:H | 6:AV:186:GLY:HA2 | 1.81 | 0.45 |
| 7:Ab:59:VAL:HG12 | 7:Ab:183:ILE:HG12 | 1.97 | 0.45 |
| 6:Ac:448:ILE:HD11 | 6:Ac:479:ILE:HD12 | 1.99 | 0.45 |
| 6:Ae:74:TYR:CE2 | 6:Ai:260:GLU:HG2 | 2.52 | 0.45 |
| 6:Aj:164:PRO:HG2 | 6:Aj:178:TYR:CD1 | 2.52 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ak:72:HIS:ND1 | 6:Ao:260:GLU:OE2 | 2.48 | 0.45 |
| 6:Am:305:GLU:OE1 | 6:Am:477:TYR:OH | 2.23 | 0.45 |
| 6:Ao:374:ASN:ND2 | 6:Ao:439:LYS:O | 2.34 | 0.45 |
| 6:Ao:382:VAL:HG22 | 6:Ao:518:VAL:HG21 | 1.99 | 0.45 |
| 6:Au:238:GLY:HA2 | 6:Au:242:SER:O | 2.17 | 0.45 |
| 6:Ay:448:ILE:HD11 | 6:Ay:479:ILE:HD11 | 1.98 | 0.45 |
| 2:B3:91:ASN:OD1 | 2:B3:91:ASN:N | 2.50 | 0.45 |
| 2:B3:209:ASP:OD1 | 2:B3:209:ASP:N | 2.49 | 0.45 |
| 2:B6:456:TYR:O | 2:B6:503:ILE:HG12 | 2.17 | 0.45 |
| 2:B7:104:SER:HB2 | 2:B7:181:VAL:HB | 1.98 | 0.45 |
| 5:BA:76:ILE:HD13 | 5:BA:179:PRO:HB2 | 1.98 | 0.45 |
| 5:BH:153:ASP:OD1 | 5:BH:153:ASP:N | 2.50 | 0.45 |
| 5:BH:157:PHE:HB2 | 5:BH:177:LEU:HB2 | 1.99 | 0.45 |
| 6:BJ:336:ASP:HB3 | 6:BJ:339:ASP:HB2 | 1.98 | 0.45 |
| 11:BU:11:LYS:HG3 | 11:BU:27:GLU:HG2 | 1.99 | 0.45 |
| 3:Bi:143:ASP:OD1 | 3:Bi:144:TRP:N | 2.50 | 0.45 |
| 3:Bm:11:GLU:OE1 | 2:Bp:486:GLN:NE2 | 2.46 | 0.45 |
| 2:Bq:69:MET:O | 2:Bq:73:GLN:HG2 | 2.15 | 0.45 |
| 2:Br:412:GLU:N | 2:Br:412:GLU:OE1 | 2.48 | 0.45 |
| 2:Bs:355:LEU:HD12 | 2:Bs:389:VAL:HG21 | 1.97 | 0.45 |
| 2:Bt:72:LEU:HD12 | 2:Bt:72:LEU:HA | 1.82 | 0.45 |
| 2:By:89:ALA:HA | 2:By:345:SER:HA | 1.97 | 0.45 |
| 2:By:462:ASN:OD1 | 2:By:466:ARG:NH1 | 2.44 | 0.45 |
| 2:By:487:THR:HG21 | 2:By:559:MET:HE3 | 1.98 | 0.45 |
| 2:By:635:ILE:HD11 | 2:Bz:576:ASN:ND2 | 2.30 | 0.45 |
| 2:By:637:TYR:HB2 | 2:Bz:622:GLU:HG2 | 1.99 | 0.45 |
| 1:k:235:TYR:OH | 8:r:19:ASP:OD2 | 2.28 | 0.45 |
| 1:l:235:TYR:OH | 8:s:19:ASP:OD2 | 2.31 | 0.45 |
| 1:m:44:ASP:HB2 | 1:m:163:GLN:HE22 | 1.81 | 0.45 |
| 3:o:39:THR:HG1 | 3:o:69:TRP:NE1 | 2.15 | 0.45 |
| 8:t:257:SER:O | 8:t:259:VAL:N | 2.46 | 0.45 |
| 9:z:5:LEU:H | 9:z:5:LEU:HD12 | 1.80 | 0.45 |
| 2:1:467:TRP:HZ3 | 2:AO:199:GLU:HB2 | 1.82 | 0.45 |
| 2:3:576:ASN:HB3 | 2:3:618:ILE:HG13 | 1.98 | 0.45 |
| 2:4:69:MET:O | 2:4:73:GLN:HG2 | 2.17 | 0.45 |
| 3:7:161:TYR:CZ | 3:8:97:ASN:HB2 | 2.52 | 0.45 |
| 5:A0:501:GLU:OE2 | 5:BG:482:SER:N | 2.30 | 0.45 |
| 5:A2:399:ASP:OD1 | 5:A2:399:ASP:N | 2.48 | 0.45 |
| 5:A3:223:GLU:CD | 5:A3:224:ALA:H | 2.22 | 0.45 |
| 5:A3:377:LEU:HD13 | 5:A3:377:LEU:HA | 1.78 | 0.45 |
| 6:A4:247:TRP:CD1 | 6:A9:265:GLN:HG2 | 2.51 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A5:435:THR:HG23 | 6:A5:515:ARG:HB3 | 1.97 | 0.45 |
| 6:A8:494:SER:HA | 11:BS:37:ASP:CG | 2.42 | 0.45 |
| 8:AB:262:PRO:HD3 | 8:AB:271:ARG:HG2 | 1.99 | 0.45 |
| 2:AD:51:VAL:HG21 | 2:AD:461:TYR:CZ | 2.51 | 0.45 |
| 2:AK:302:LYS:O | 2:AK:307:SER:N | 2.50 | 0.45 |
| 2:AM:406:LEU:HD13 | 2:AM:475:ALA:HB2 | 1.98 | 0.45 |
| 6:AX:96:MET:HB2 | 6:Az:123:GLN:O | 2.15 | 0.45 |
| 6:Ac:108:ALA:O | 6:Ac:110:ASP:N | 2.47 | 0.45 |
| 6:Ad:430:LYS:HG2 | 6:Ah:216:MET:HE1 | 1.98 | 0.45 |
| 6:Ai:380:ARG:HB3 | 6:Am:362:VAL:HG11 | 1.99 | 0.45 |
| 6:Ak:304:ARG:HD3 | 6:Ak:428:TYR:HD2 | 1.81 | 0.45 |
| 7:Al:55:LYS:HE2 | 7:BE:162:TRP:CD1 | 2.52 | 0.45 |
| 6:An:430:LYS:HD3 | 6:An:430:LYS:HA | 1.81 | 0.45 |
| 7:As:163:PHE:HA | 7:As:170:LEU:HA | 1.98 | 0.45 |
| 6:Au:133:LYS:HA | 6:Au:249:GLU:HB2 | 1.97 | 0.45 |
| 2:B1:33:PHE:HB2 | 2:B1:82:ARG:HG3 | 1.99 | 0.45 |
| 2:B1:100:GLU:HA | 2:B1:217:TYR:HE1 | 1.80 | 0.45 |
| 2:B4:383:LEU:HD11 | 2:B4:436:TYR:HE2 | 1.81 | 0.45 |
| 2:B5:92:SER:HB3 | 2:B5:340:LEU:HB3 | 1.98 | 0.45 |
| 11:BU:9:ASN:HB3 | 11:BU:56:TYR:CE2 | 2.51 | 0.45 |
| 3:Bh:67:ASP:OD1 | 3:Bh:67:ASP:N | 2.47 | 0.45 |
| 3:Bi:114:ARG:HB3 | 3:Bi:123:VAL:HG13 | 1.97 | 0.45 |
| 3:Bn:24:GLU:OE2 | 3:Bn:33:THR:OG1 | 2.34 | 0.45 |
| 2:Bp:247:GLY:HA2 | 2:Bp:266:LYS:HD3 | 1.98 | 0.45 |
| 2:Bs:566:ARG:HA | 2:Bs:569:LYS:HB3 | 1.98 | 0.45 |
| 2:Bu:375:ALA:HB3 | 2:Bu:407:CYS:HB3 | 1.97 | 0.45 |
| 2:Bv:254:ILE:HG13 | 2:Bv:337:ILE:HB | 1.99 | 0.45 |
| 2:Bw:32:LYS:HE2 | 2:Bw:350:VAL:HG11 | 1.97 | 0.45 |
| 2:By:254:ILE:HG13 | 2:By:337:ILE:HB | 1.98 | 0.45 |
| 2:Bz:110:TYR:CE1 | 2:Bz:171:ILE:HD12 | 2.52 | 0.45 |
| 4:C:2:ASP:OD1 | 4:C:3:ILE:N | 2.50 | 0.45 |
| 1:0:126:GLN:O | 1:0:188:ASN:ND2 | 2.49 | 0.45 |
| 2:4:417:ILE:HD13 | 2:4:417:ILE:H | 1.81 | 0.45 |
| 2:4:575:LEU:HD11 | 8:t:97:LEU:HD21 | 1.99 | 0.45 |
| 2:5:304:ILE:HG13 | 2:5:305:TYR:H | 1.81 | 0.45 |
| 3:8:147:ASN:HB3 | 9:v:45:PRO:HG3 | 1.99 | 0.45 |
| 5:A2:397:THR:OG1 | 5:A2:399:ASP:OD1 | 2.27 | 0.45 |
| 6:A5:128:ARG:NH1 | 6:A5:490:GLN:O | 2.50 | 0.45 |
| 6:A5:244:ASP:HB2 | 11:BT:13:PHE:HE2 | 1.81 | 0.45 |
| 6:A8:301:GLU:OE1 | 6:A9:155:SER:OG | 2.33 | 0.45 |
| 8:AB:71:ILE:HG23 | 1:p:176:TYR:HD1 | 1.82 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:291:GLN:HE22 | 2:AD:320:SER:HB2 | 1.81 | 0.45 |
| 3:AE:125:LYS:HD3 | 3:AE:125:LYS:HA | 1.46 | 0.45 |
| 2:AK:560:LEU:O | 2:AK:564:ILE:HG12 | 2.15 | 0.45 |
| 2:AM:159:GLU:O | 2:AM:162:THR:N | 2.50 | 0.45 |
| 6:AV:69:GLY:HA2 | 6:Am:274:LEU:HD13 | 1.99 | 0.45 |
| 6:AW:123:GLN:HB3 | 6:AW:258:VAL:HG12 | 1.99 | 0.45 |
| 6:AX:484:PHE:O | 6:AX:487:SER:OG | 2.32 | 0.45 |
| 7:AY:53:LEU:HD11 | 7:AY:82:PHE:HB3 | 1.99 | 0.45 |
| 6:Ac:184:GLU:O | 6:Ac:185:THR:OG1 | 2.29 | 0.45 |
| 6:Ae:101:ARG:HD2 | 6:Ai:146:PRO:HD3 | 1.97 | 0.45 |
| 6:Ae:259:ILE:HA | 6:Ae:500:MET:HE2 | 1.99 | 0.45 |
| 6:Af:176:ASP:OD1 | 6:Af:177:ILE:N | 2.46 | 0.45 |
| 6:Ai:345:TRP:CD1 | 6:Ai:346:ALA:H | 2.34 | 0.45 |
| 6:Ai:426:ASP:HB3 | 6:Ai:429:ALA:HB2 | 1.97 | 0.45 |
| 6:Aj:154:PHE:CE2 | 6:Aj:248:ASN:HB3 | 2.52 | 0.45 |
| 6:Am:250:MET:HE2 | 6:Am:250:MET:HB3 | 1.87 | 0.45 |
| 6:Ao:452:PRO:HA | 6:Ao:477:TYR:HA | 1.97 | 0.45 |
| 7:Ar:87:ILE:HD13 | 7:Ar:158:ILE:HB | 1.98 | 0.45 |
| 7:At:301:ASP:OD2 | 5:BA:339:ARG:NH1 | 2.50 | 0.45 |
| 6:Au:344:ARG:HE | 6:BJ:345:TRP:NE1 | 2.13 | 0.45 |
| 5:Av:136:HIS:NE2 | 5:Av:171:ILE:O | 2.49 | 0.45 |
| 6:Aw:494:SER:C | 6:Aw:496:ILE:H | 2.24 | 0.45 |
| 5:Ax:86:TYR:C | 5:Ax:88:VAL:H | 2.24 | 0.45 |
| 2:B1:419:VAL:HG22 | 2:B1:507:ILE:HB | 1.99 | 0.45 |
| 2:B3:112:VAL:HG13 | 2:B3:134:VAL:HG22 | 1.99 | 0.45 |
| 2:B3:311:ILE:HB | 2:B3:327:ALA:HB2 | 1.99 | 0.45 |
| 2:B3:409:PRO:O | 2:B3:454:TYR:OH | 2.33 | 0.45 |
| 2:B4:251:LEU:HB3 | 2:B4:260:THR:HB | 1.99 | 0.45 |
| 2:B5:496:ARG:NH2 | 2:B6:573:PHE:O | 2.49 | 0.45 |
| 2:B5:521:ALA:HB1 | 2:B5:541:ALA:HA | 1.99 | 0.45 |
| 2:B6:628:TYR:OH | 2:Bp:15:VAL:O | 2.34 | 0.45 |
| 2:B7:66:MET:HG2 | 2:B7:468:VAL:HG11 | 1.98 | 0.45 |
| 7:BC:30:THR:C | 7:BC:32:ASP:H | 2.25 | 0.45 |
| 5:BD:254:LEU:O | 5:BD:258:VAL:HG23 | 2.16 | 0.45 |
| 5:BF:211:ALA:HB2 | 5:BF:225:GLY:HA3 | 1.98 | 0.45 |
| 5:BG:161:ILE:HB | 5:BG:173:GLU:HB3 | 1.98 | 0.45 |
| 5:BG:207:ILE:HD12 | 5:BG:228:ILE:O | 2.17 | 0.45 |
| 5:BG:457:LEU:HD12 | 5:BG:457:LEU:HA | 1.86 | 0.45 |
| 5:BH:44:GLU:HA | 5:BH:188:ILE:O | 2.16 | 0.45 |
| 6:BJ:378:ALA:HB1 | 6:BJ:382:VAL:HB | 1.98 | 0.45 |
| 3:Ba:98:GLU:HA | 3:Bn:2:PHE:HA | 1.99 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bg:114:ARG:HG2 | 3:Bg:126:GLU:HG2 | 1.97 | 0.45 |
| 3:Bi:24:GLU:OE1 | 3:Bi:33:THR:OG1 | 2.35 | 0.45 |
| 3:Bk:28:LEU:HD22 | 3:Bk:84:LYS:HB3 | 1.99 | 0.45 |
| 3:Bk:90:SER:HA | 3:Bk:94:GLY:H | 1.81 | 0.45 |
| 3:Bl:41:LEU:N | 3:Bo:140:LEU:O | 2.40 | 0.45 |
| 2:Bq:110:TYR:CD1 | 2:Bq:177:GLY:HA3 | 2.52 | 0.45 |
| 2:Bq:510:ARG:HG2 | 2:Bq:511:GLN:H | 1.82 | 0.45 |
| 2:Bs:57:PRO:HG3 | 2:Bs:65:PHE:CD1 | 2.52 | 0.45 |
| 2:Bt:195:LEU:HD23 | 2:Bt:195:LEU:H | 1.82 | 0.45 |
| 2:Bu:152:ALA:O | 2:Bu:156:GLU:HG2 | 2.17 | 0.45 |
| 2:Bv:57:PRO:HB2 | 2:Bv:62:ALA:HA | 1.99 | 0.45 |
| 2:Bw:101:TYR:CZ | 2:Bw:143:ILE:HG12 | 2.52 | 0.45 |
| 2:By:406:LEU:HD13 | 2:By:475:ALA:HB2 | 1.99 | 0.45 |
| 1:k:70:LEU:O | 8:q:46:LYS:NZ | 2.40 | 0.45 |
| 1:l:27:LEU:HD23 | 1:l:27:LEU:HA | 1.80 | 0.45 |
| 1:m:86:PHE:CE2 | 1:m:88:ALA:HB2 | 2.51 | 0.45 |
| 8:u:72:LEU:HD12 | 8:u:125:ARG:HB2 | 1.98 | 0.45 |
| 9:x:139:SER:HB3 | 9:x:156:THR:H | 1.82 | 0.45 |
| 2:2:451:ASP:OD1 | 2:2:452:GLY:N | 2.39 | 0.45 |
| 2:3:538:ASP:OD1 | 2:3:538:ASP:N | 2.48 | 0.45 |
| 3:7:37:LYS:NZ | 3:7:152:THR:HG21 | 2.31 | 0.45 |
| 3:9:104:PRO:HA | 3:9:107:TYR:CE2 | 2.52 | 0.45 |
| 6:A4:133:LYS:HG2 | 6:A4:249:GLU:HB2 | 1.98 | 0.45 |
| 6:A4:496:ILE:HG12 | 6:A9:76:ALA:HB1 | 1.97 | 0.45 |
| 6:A5:71:ASP:OD1 | 6:A5:72:HIS:N | 2.50 | 0.45 |
| 7:A6:69:TYR:CD1 | 7:A6:177:GLN:HA | 2.51 | 0.45 |
| 7:A6:85:THR:OG1 | 7:A6:187:TRP:NE1 | 2.49 | 0.45 |
| 7:A6:187:TRP:CE2 | 5:BF:295:ARG:HD2 | 2.52 | 0.45 |
| 6:A7:344:ARG:H | 6:A7:344:ARG:HD3 | 1.81 | 0.45 |
| 6:A8:503:ILE:HG13 | 6:A8:507:LEU:HD13 | 1.98 | 0.45 |
| 3:AG:113:VAL:HG13 | 3:AG:127:ILE:HG12 | 1.99 | 0.45 |
| 3:AJ:103:LYS:NZ | 3:Bm:77:GLU:OE1 | 2.43 | 0.45 |
| 2:AK:429:TRP:CZ2 | 2:AK:441:PHE:HB2 | 2.52 | 0.45 |
| 2:AK:432:ALA:HB2 | 2:AK:440:ASN:HD22 | 1.82 | 0.45 |
| 2:AN:373:PHE:HB2 | 2:AN:405:VAL:HG22 | 1.97 | 0.45 |
| 6:AW:74:TYR:HA | 6:AW:79:ILE:HD11 | 1.99 | 0.45 |
| 6:AZ:117:MET:HB3 | 6:AZ:119:SER:O | 2.16 | 0.45 |
| 7:Ab:230:VAL:HB | 7:Ab:233:GLN:HG2 | 1.97 | 0.45 |
| 6:Ac:380:ARG:HH21 | 6:Ag:366:ARG:HH11 | 1.64 | 0.45 |
| 6:Af:131:TYR:HB2 | 6:Af:154:PHE:CZ | 2.52 | 0.45 |
| 6:Ag:151:ASP:HB3 | 6:Ag:154:PHE:HB2 | 1.98 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Aj:365:ALA:HB2 | 6:Aj:372:GLU:HA | 1.98 | 0.45 |
| 6:An:123:GLN:HB3 | 6:An:258:VAL:HG12 | 1.99 | 0.45 |
| 6:Aw:145:HIS:ND1 | 6:Aw:146:PRO:HD2 | 2.32 | 0.45 |
| 6:Az:106:LEU:HB3 | 6:Az:303:ASN:ND2 | 2.32 | 0.45 |
| 2:B1:278:GLN:HG2 | 2:B1:296:SER:HB3 | 1.98 | 0.45 |
| 2:B1:636:ASN:OD1 | 2:B1:636:ASN:N | 2.49 | 0.45 |
| 2:B2:593:GLN:NE2 | 3:Bg:4:ASP:OD2 | 2.43 | 0.45 |
| 2:B3:644:ALA:O | 2:B3:645:THR:OG1 | 2.34 | 0.45 |
| 2:B5:498:GLN:HG2 | 2:B5:534:VAL:HG12 | 1.99 | 0.45 |
| 7:BC:36:ASP:OD2 | 7:BE:18:ARG:NH1 | 2.48 | 0.45 |
| 5:BH:157:PHE:HB3 | 5:BH:177:LEU:HD12 | 1.99 | 0.45 |
| 5:BH:383:ASP:N | 5:BH:383:ASP:OD1 | 2.50 | 0.45 |
| 6:BK:121:THR:HG22 | 6:BK:260:GLU:HG3 | 1.99 | 0.45 |
| 3:BZ:17:ARG:O | 3:Bc:151:GLN:NE2 | 2.50 | 0.45 |
| 3:Bf:10:PHE:HD2 | 3:Bf:13:GLY:HA2 | 1.82 | 0.45 |
| 3:Bh:120:ALA:HB2 | 3:Bj:99:ILE:O | 2.16 | 0.45 |
| 3:Bi:3:VAL:HG12 | 3:Bn:97:ASN:HA | 1.98 | 0.45 |
| 3:Bn:37:LYS:NZ | 3:Bn:152:THR:OG1 | 2.46 | 0.45 |
| 2:Bp:302:LYS:HD2 | 2:Bp:306:ASP:HA | 1.98 | 0.45 |
| 2:Bx:46:ASN:OD1 | 2:Bx:47:GLU:N | 2.50 | 0.45 |
| 2:Bx:110:TYR:H | 2:Bx:138:GLY:HA3 | 1.82 | 0.45 |
| 2:Bx:456:TYR:HB3 | 2:Bx:503:ILE:HG23 | 1.99 | 0.45 |
| 4:D:48:THR:HG21 | 4:I:47:PRO:HB2 | 1.99 | 0.45 |
| 4:M:44:MET:HG2 | 4:O:44:MET:HE1 | 1.97 | 0.45 |
| 1:n:223:GLN:NE2 | 1:p:69:ASP:OD1 | 2.48 | 0.45 |
| 1:p:198:GLU:O | 1:p:205:ARG:NH2 | 2.50 | 0.45 |
| 8:r:60:ASN:OD1 | 8:r:60:ASN:N | 2.50 | 0.45 |
| 1:0:144:ASN:O | 1:0:144:ASN:ND2 | 2.50 | 0.45 |
| 1:0:245:PHE:CE1 | 8:q:38:ARG:HD3 | 2.51 | 0.45 |
| 2:4:413:THR:OG1 | 2:4:425:ASN:HB3 | 2.17 | 0.45 |
| 3:8:125:LYS:HG2 | 3:9:79:HIS:CG | 2.52 | 0.45 |
| 5:A1:335:TRP:HB2 | 7:As:307:LEU:HB2 | 1.98 | 0.45 |
| 5:A3:30:SER:HB2 | 5:BG:161:ILE:HD11 | 1.99 | 0.45 |
| 5:A3:440:GLU:OE1 | 5:A3:443:ASN:ND2 | 2.34 | 0.45 |
| 6:A4:249:GLU:HG2 | 6:A9:267:LYS:HG3 | 1.99 | 0.45 |
| 6:A7:91:ILE:HA | 6:Ay:125:PHE:HZ | 1.81 | 0.45 |
| 6:A9:183:GLN:N | 6:A9:209:ASP:OD2 | 2.40 | 0.45 |
| 6:A9:476:ARG:NH1 | 7:Aa:105:PRO:HD3 | 2.32 | 0.45 |
| 9:AC:15:THR:O | 9:AC:17:PHE:HD1 | 2.00 | 0.45 |
| 2:AD:237:GLU:OE1 | 2:AD:284:ARG:NH1 | 2.48 | 0.45 |
| 2:AD:550:ARG:HB3 | 2:AD:553:VAL:HG12 | 1.99 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:AE:90:SER:HA | 3:AE:94:GLY:H | 1.82 | 0.45 |
| 3:AG:55:ASN:HA | 3:Bg:19:ASN:HD22 | 1.82 | 0.45 |
| 2:AN:234:ILE:HB | 2:AN:340:LEU:HD12 | 1.99 | 0.45 |
| 2:AN:556:LEU:HD23 | 2:AN:560:LEU:HD13 | 1.98 | 0.45 |
| 2:AO:368:VAL:HG12 | 2:AO:370:VAL:HG22 | 1.99 | 0.45 |
| 10:AR:307:CYS:HB2 | 10:AR:312:MET:HE2 | 1.99 | 0.45 |
| 6:AW:127:LEU:HD12 | 6:AW:254:ILE:HD11 | 1.99 | 0.45 |
| 6:AX:312:TYR:CE2 | 6:AX:507:LEU:HD12 | 2.52 | 0.45 |
| 6:Af:211:GLU:OE2 | 6:Af:215:GLN:NE2 | 2.38 | 0.45 |
| 6:Ag:284:MET:HE1 | 6:Ak:127:LEU:HD13 | 1.97 | 0.45 |
| 6:Aj:301:GLU:HG2 | 6:An:152:ALA:HA | 1.99 | 0.45 |
| 6:Ak:72:HIS:C | 6:Ak:74:TYR:H | 2.25 | 0.45 |
| 6:Ak:376:ILE:HG12 | 6:Ak:436:VAL:HG22 | 1.99 | 0.45 |
| 7:Aq:43:GLU:HG2 | 7:As:245:ARG:HB2 | 1.98 | 0.45 |
| 7:Aq:154:MET:HE3 | 7:Aq:154:MET:HB3 | 1.76 | 0.45 |
| 7:Aq:160:ASP:OD1 | 7:Aq:160:ASP:N | 2.38 | 0.45 |
| 7:Aq:163:PHE:HA | 7:Aq:170:LEU:HA | 1.98 | 0.45 |
| 7:Aq:189:LYS:H | 7:Aq:189:LYS:HG2 | 1.54 | 0.45 |
| 6:Au:387:ALA:HB2 | 6:Au:404:PHE:HB2 | 1.97 | 0.45 |
| 6:Aw:244:ASP:O | 6:Aw:245:ASN:C | 2.59 | 0.45 |
| 6:Az:452:PRO:HA | 6:Az:477:TYR:HA | 1.99 | 0.45 |
| 2:B4:222:VAL:HG21 | 2:B4:238:ILE:HD11 | 1.99 | 0.45 |
| 2:B5:652:ASP:HB3 | 2:Bp:458:TYR:CE2 | 2.52 | 0.45 |
| 2:B7:391:LYS:HG2 | 2:B7:443:ILE:HD13 | 1.99 | 0.45 |
| 6:BI:153:MET:HB2 | 6:BI:189:TYR:CE2 | 2.52 | 0.45 |
| 6:BJ:105:ASN:ND2 | 6:BJ:409:THR:O | 2.46 | 0.45 |
| 6:BJ:404:PHE:HZ | 6:BJ:417:LEU:HA | 1.81 | 0.45 |
| 7:BL:128:PHE:N | 7:BL:128:PHE:CD1 | 2.85 | 0.45 |
| 11:BP:12:THR:HG22 | 11:BP:46:TYR:HB3 | 1.99 | 0.45 |
| 3:BX:30:GLN:O | 3:BX:30:GLN:NE2 | 2.48 | 0.45 |
| 3:Be:16:ALA:HB1 | 3:Be:115:GLN:HE22 | 1.82 | 0.45 |
| 3:Bf:43:ALA:HB2 | 3:Bi:139:GLU:H | 1.82 | 0.45 |
| 3:Bh:14:ASP:N | 3:Bh:14:ASP:OD1 | 2.48 | 0.45 |
| 3:Bj:82:ARG:O | 3:Bj:86:VAL:HG13 | 2.17 | 0.45 |
| 2:Bp:28:ALA:HB1 | 2:Bp:362:PHE:CE2 | 2.52 | 0.45 |
| 2:Bp:70:ASN:OD1 | 2:Bp:457:GLN:NE2 | 2.47 | 0.45 |
| 2:Bq:82:ARG:NH1 | 2:Bq:227:PRO:O | 2.45 | 0.45 |
| 2:Bq:148:ALA:HB2 | 2:Bq:258:GLY:HA3 | 1.99 | 0.45 |
| 2:Br:653:GLU:HB2 | 2:Bu:16:GLN:HA | 1.98 | 0.45 |
| 2:Bt:104:SER:OG | 2:Bt:183:THR:OG1 | 2.32 | 0.45 |
| 2:By:92:SER:HB3 | 2:By:340:LEU:HB3 | 1.99 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bz:234:ILE:HB | 2:Bz:340:LEU:HD12 | 1.99 | 0.45 |
| 2:Bz:478:CYS:O | 2:Bz:555:ARG:NH1 | 2.47 | 0.45 |
| 4:W:23:SER:HB3 | 4:W:46:ARG:HE | 1.82 | 0.45 |
| 4:Y:54:ASN:HB3 | 4:i:55:VAL:HG11 | 1.99 | 0.45 |
| 1:n:152:VAL:HG13 | 1:n:169:ILE:HD13 | 1.98 | 0.45 |
| 8:q:27:LYS:HG3 | 8:q:36:PHE:HE1 | 1.82 | 0.45 |
| 8:t:236:GLU:HG3 | 8:t:237:VAL:N | 2.32 | 0.45 |
| 8:t:238:VAL:HG13 | 8:t:239:PRO:HD2 | 1.99 | 0.45 |
| 9:w:106:LYS:HG3 | 9:w:107:THR:HG23 | 1.98 | 0.45 |
| 2:4:413:THR:HG23 | 2:4:414:VAL:HG23 | 1.97 | 0.45 |
| 2:5:538:ASP:N | 2:5:538:ASP:OD1 | 2.49 | 0.45 |
| 5:A0:7:SER:OG | 5:A0:8:LEU:N | 2.49 | 0.45 |
| 5:A2:215:TYR:CD2 | 5:A2:219:GLY:HA2 | 2.52 | 0.45 |
| 6:A7:88:VAL:HG11 | 6:Au:278:LEU:HD21 | 1.99 | 0.45 |
| 6:A7:176:ASP:OD1 | 6:A7:177:ILE:N | 2.50 | 0.45 |
| 3:AA:114:ARG:HB3 | 3:AA:123:VAL:HG13 | 1.99 | 0.45 |
| 2:AK:90:LYS:NZ | 2:AK:190:ASP:OD1 | 2.48 | 0.45 |
| 2:AK:438:ASP:OD1 | 2:AK:438:ASP:N | 2.48 | 0.45 |
| 10:AQ:313:ASP:OD2 | 10:AQ:357:ARG:NH2 | 2.50 | 0.45 |
| 10:AR:299:HIS:CE1 | 6:Ag:328:LYS:HE2 | 2.51 | 0.45 |
| 6:AV:354:LEU:HD22 | 6:Ap:400:LEU:HD21 | 1.99 | 0.45 |
| 6:AW:324:THR:OG1 | 6:AW:327:SER:HB2 | 2.16 | 0.45 |
| 6:AZ:380:ARG:NH2 | 6:AZ:427:GLN:HB2 | 2.32 | 0.45 |
| 6:Ae:236:GLN:HG3 | 6:Ay:265:GLN:NE2 | 2.31 | 0.45 |
| 6:Af:131:TYR:HB3 | 6:Af:250:MET:HG2 | 1.98 | 0.45 |
| 6:Am:265:GLN:HG3 | 6:BJ:247:TRP:HE1 | 1.81 | 0.45 |
| 6:An:133:LYS:HG2 | 6:An:249:GLU:HB2 | 1.98 | 0.45 |
| 6:An:367:GLN:HB3 | 6:An:511:ALA:HB1 | 1.98 | 0.45 |
| 6:Au:365:ALA:HB2 | 6:Au:372:GLU:HA | 1.99 | 0.45 |
| 5:Av:114:ASP:N | 5:Av:114:ASP:OD1 | 2.49 | 0.45 |
| 5:Av:462:ILE:HG13 | 5:BB:453:TYR:CG | 2.52 | 0.45 |
| 2:B1:418:PRO:HD2 | 2:B1:421:ARG:NH1 | 2.32 | 0.45 |
| 2:B3:406:LEU:HD13 | 2:B3:475:ALA:HB2 | 1.99 | 0.45 |
| 2:B4:151:ILE:O | 2:B4:155:LYS:HG2 | 2.17 | 0.45 |
| 2:B5:410:PRO:O | 2:B5:413:THR:HG22 | 2.16 | 0.45 |
| 5:BB:401:LEU:O | 5:BB:405:LYS:HG2 | 2.16 | 0.45 |
| 7:BC:2:SER:OG | 7:BC:3:GLY:N | 2.48 | 0.45 |
| 5:BF:125:MET:O | 5:BF:129:GLU:HG2 | 2.17 | 0.45 |
| 5:BF:259:LYS:HB3 | 5:BF:260:PRO:HD3 | 1.99 | 0.45 |
| 5:BG:171:ILE:HD13 | 5:BG:171:ILE:H | 1.82 | 0.45 |
| 6:BI:430:LYS:HA | 6:BI:430:LYS:HD3 | 1.81 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:BM:131:TYR:CZ | 6:BM:143:ALA:HA | 2.52 | 0.45 |
| 11:BR:29:SER:HB2 | 11:BR:59:VAL:HG22 | 1.98 | 0.45 |
| 11:BS:9:ASN:HB3 | 11:BS:56:TYR:CE2 | 2.52 | 0.45 |
| 3:BX:17:ARG:HG3 | 3:BX:20:LEU:HD12 | 1.99 | 0.45 |
| 3:BX:72:THR:HG22 | 3:BX:154:GLU:HG3 | 1.98 | 0.45 |
| 3:BY:80:ASP:O | 3:BY:84:LYS:HG3 | 2.17 | 0.45 |
| 3:Bd:64:ARG:NH1 | 3:Bg:95:GLN:OE1 | 2.50 | 0.45 |
| 3:Bg:104:PRO:HA | 3:Bg:107:TYR:CZ | 2.52 | 0.45 |
| 3:Bj:82:ARG:HH12 | 3:Bj:138:GLY:HA2 | 1.82 | 0.45 |
| 2:Bp:373:PHE:HB2 | 2:Bp:405:VAL:HG22 | 1.99 | 0.45 |
| 2:Br:509:THR:HB | 2:Br:513:GLN:HB2 | 1.99 | 0.45 |
| 2:Bs:84:VAL:HG13 | 2:Bs:346:SER:HB3 | 1.98 | 0.45 |
| 2:Bt:446:THR:OG1 | 2:Bt:554:ARG:NH2 | 2.50 | 0.45 |
| 2:Bu:332:GLU:CD | 2:Bu:332:GLU:H | 2.25 | 0.45 |
| 2:Bv:72:LEU:HD13 | 2:Bv:72:LEU:HA | 1.85 | 0.45 |
| 2:By:351:THR:OG1 | 2:By:352:ALA:N | 2.50 | 0.45 |
| 2:Bz:334:PHE:HZ | 2:Bz:338:LEU:HD21 | 1.81 | 0.45 |
| 4:X:62:ILE:HD11 | 4:c:62:ILE:HG13 | 1.98 | 0.45 |
| 1:p:60:TYR:HB2 | 1:p:86:PHE:CD1 | 2.52 | 0.45 |
| 8:q:56:TRP:HB3 | 8:q:65:VAL:HG21 | 1.99 | 0.45 |
| 8:r:147:THR:HG23 | 8:r:163:ILE:HG12 | 1.98 | 0.45 |
| 8:t:198:MET:SD | 8:u:135:GLU:HG2 | 2.57 | 0.45 |
| 9:x:42:ILE:HD11 | 9:y:138:LEU:HD23 | 1.99 | 0.45 |
| 2:1:33:PHE:HD2 | 2:1:82:ARG:HG3 | 1.81 | 0.45 |
| 2:1:157:VAL:HG23 | 2:1:159:GLU:H | 1.82 | 0.45 |
| 2:1:374:ILE:HG23 | 2:1:471:ALA:O | 2.17 | 0.45 |
| 2:1:644:ALA:HA | 2:AO:557:PHE:HZ | 1.81 | 0.45 |
| 2:2:374:ILE:HG23 | 2:2:471:ALA:O | 2.17 | 0.45 |
| 2:5:39:PHE:HD2 | 2:5:361:PHE:HE1 | 1.65 | 0.45 |
| 2:5:411:ARG:HG3 | 2:5:415:VAL:HG21 | 1.98 | 0.45 |
| 3:8:23:VAL:HG13 | 3:8:36:CYS:SG | 2.57 | 0.45 |
| 5:A2:160:LYS:HA | 5:A2:174:LEU:HD23 | 1.99 | 0.45 |
| 6:A4:432:ASP:HB3 | 6:A4:518:VAL:HG23 | 1.99 | 0.45 |
| 7:A6:257:GLU:OE1 | 7:A6:290:LYS:NZ | 2.46 | 0.45 |
| 6:A7:115:GLN:NE2 | 6:A7:444:MET:SD | 2.90 | 0.45 |
| 9:AC:119:ASN:HB2 | 9:v:79:GLU:HG3 | 1.98 | 0.45 |
| 2:AD:100:GLU:HB3 | 2:AD:188:ILE:HD11 | 1.99 | 0.45 |
| 3:AH:136:ASN:ND2 | 3:AH:136:ASN:O | 2.49 | 0.45 |
| 3:AJ:90:SER:HA | 3:AJ:94:GLY:H | 1.82 | 0.45 |
| 2:AK:596:LYS:HG2 | 2:AK:601:ILE:O | 2.17 | 0.45 |
| 2:AL:378:CYS:SG | 2:AL:454:TYR:OH | 2.55 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AM:410:PRO:O | 2:AM:413:THR:HG22 | 2.17 | 0.45 |
| 2:AN:57:PRO:HA | 2:AN:61:THR:HB | 1.99 | 0.45 |
| 2:AN:110:TYR:H | 2:AN:138:GLY:HA3 | 1.81 | 0.45 |
| 2:AO:455:LYS:HB3 | 2:AO:470:LEU:HD11 | 1.98 | 0.45 |
| 2:AP:99:ILE:HD13 | 2:AP:184:LEU:HD22 | 1.99 | 0.45 |
| 2:AP:118:VAL:H | 2:AP:126:GLU:HB3 | 1.81 | 0.45 |
| 2:AP:332:GLU:OE1 | 2:AP:332:GLU:N | 2.37 | 0.45 |
| 2:AP:391:LYS:HG2 | 2:AP:443:ILE:HD13 | 1.98 | 0.45 |
| 6:AV:437:GLY:HA2 | 6:AV:512:TYR:O | 2.17 | 0.45 |
| 6:AX:348:GLU:HB3 | 6:AX:396:ALA:HB2 | 1.99 | 0.45 |
| 7:AY:217:GLU:HB3 | 7:AY:224:HIS:HD2 | 1.80 | 0.45 |
| 6:AZ:363:GLU:OE2 | 6:AZ:366:ARG:NH1 | 2.50 | 0.45 |
| 7:Ab:34:ILE:O | 7:Ab:38:ILE:HG12 | 2.17 | 0.45 |
| 6:Ae:68:ILE:HG22 | 6:Ae:70:GLY:H | 1.81 | 0.45 |
| 6:Ah:456:LEU:H | 6:Ah:475:THR:HG22 | 1.82 | 0.45 |
| 6:Ak:314:ALA:HA | 6:Ak:513:PHE:HB2 | 1.98 | 0.45 |
| 6:An:460:ARG:HH22 | 6:An:471:MET:HE2 | 1.82 | 0.45 |
| 7:As:89:ARG:NH1 | 7:As:156:SER:O | 2.50 | 0.45 |
| 6:Au:245:ASN:OD1 | 6:Au:245:ASN:N | 2.49 | 0.45 |
| 2:B1:34:GLN:O | 2:B1:82:ARG:NH2 | 2.50 | 0.45 |
| 2:B1:451:ASP:OD1 | 2:B1:452:GLY:N | 2.40 | 0.45 |
| 2:B7:35:TRP:CE2 | 2:B7:226:TYR:HB2 | 2.52 | 0.45 |
| 5:BA:411:GLN:O | 5:BA:415:GLU:HG3 | 2.16 | 0.45 |
| 5:BD:150:TRP:HD1 | 5:BD:156:ILE:HG22 | 1.82 | 0.45 |
| 5:BF:52:SER:HB3 | 5:BF:55:ASN:HB3 | 1.97 | 0.45 |
| 5:BF:184:TYR:HE1 | 5:BF:204:GLU:HB3 | 1.82 | 0.45 |
| 6:BK:117:MET:HG3 | 6:BK:453:TYR:HB2 | 1.98 | 0.45 |
| 7:BL:61:TYR:O | 7:BL:68:ARG:NH1 | 2.50 | 0.45 |
| 3:BY:136:ASN:O | 3:BY:136:ASN:ND2 | 2.50 | 0.45 |
| 3:Bi:104:PRO:HA | 3:Bi:107:TYR:CZ | 2.52 | 0.45 |
| 2:Bq:547:PRO:HB3 | 2:Bt:305:TYR:CZ | 2.52 | 0.45 |
| 2:Br:269:PHE:CZ | 2:Br:280:ALA:HB1 | 2.52 | 0.45 |
| 2:Bs:480:ARG:O | 2:Bs:484:VAL:HG12 | 2.17 | 0.45 |
| 2:Bu:468:VAL:HG12 | 2:Bu:469:PRO:HD2 | 1.99 | 0.45 |
| 2:Bx:368:VAL:HG12 | 2:Bx:370:VAL:HG22 | 1.98 | 0.45 |
| 2:Bx:576:ASN:HB3 | 2:Bx:618:ILE:HG23 | 1.99 | 0.45 |
| 4:W:25:ILE:HD13 | 4:g:44:MET:HE2 | 1.98 | 0.45 |
| 4:Y:44:MET:HE3 | 4:i:44:MET:HE3 | 1.99 | 0.45 |
| 1:m:152:VAL:HG22 | 1:m:169:ILE:HG23 | 1.97 | 0.45 |
| 1:n:238:VAL:HG11 | 9:y:121:LYS:HB2 | 1.99 | 0.45 |
| 8:q:48:HIS:NE2 | 8:r:176:ILE:O | 2.41 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:y:15:THR:OG1 | 9:y:16:ASN:N | 2.49 | 0.45 |
| 1:0:160:GLN:HA | 7:BC:273:GLY:HA3 | 1.99 | 0.44 |
| 2:1:614:THR:O | 2:1:616:SER:N | 2.46 | 0.44 |
| 2:2:592:LEU:HD23 | 2:2:604:TYR:HB2 | 1.99 | 0.44 |
| 2:3:107:GLY:HA3 | 2:3:110:TYR:CE2 | 2.50 | 0.44 |
| 2:3:647:THR:OG1 | 2:AK:633:ARG:NH1 | 2.45 | 0.44 |
| 2:5:63:ASP:OD2 | 2:5:379:ALA:HB3 | 2.16 | 0.44 |
| 2:5:101:TYR:CZ | 2:5:143:ILE:HG12 | 2.52 | 0.44 |
| 3:8:101:GLY:N | 3:AJ:119:ASP:OD1 | 2.50 | 0.44 |
| 5:A1:495:ASP:OD1 | 5:A1:495:ASP:N | 2.49 | 0.44 |
| 6:A4:409:THR:HG21 | 6:A5:371:GLY:N | 2.32 | 0.44 |
| 6:A8:445:ASP:OD1 | 6:A8:445:ASP:N | 2.50 | 0.44 |
| 6:A9:318:LYS:NZ | 6:A9:339:ASP:OD1 | 2.50 | 0.44 |
| 2:AK:488:TRP:HB3 | 2:AK:556:LEU:HD12 | 1.98 | 0.44 |
| 2:AK:496:ARG:NH2 | 2:Bs:573:PHE:O | 2.39 | 0.44 |
| 2:AL:29:LEU:O | 2:AL:80:VAL:HA | 2.16 | 0.44 |
| 2:AL:424:ASP:OD1 | 2:AL:516:ARG:NH2 | 2.50 | 0.44 |
| 2:AN:163:LEU:HD11 | 2:AN:187:ILE:HG12 | 1.99 | 0.44 |
| 2:AP:237:GLU:OE1 | 2:AP:284:ARG:NH2 | 2.36 | 0.44 |
| 2:AP:467:TRP:CH2 | 2:Bp:199:GLU:HB2 | 2.53 | 0.44 |
| 6:AV:117:MET:HG2 | 6:AV:451:ALA:HB1 | 1.99 | 0.44 |
| 6:AX:204:ASP:OD1 | 6:AX:205:ALA:N | 2.50 | 0.44 |
| 7:AY:53:LEU:HG | 7:AY:187:TRP:HB3 | 2.00 | 0.44 |
| 6:AZ:190:LEU:HB3 | 6:AZ:221:LEU:HB3 | 1.99 | 0.44 |
| 6:Ae:153:MET:HB3 | 6:Ae:158:GLY:H | 1.81 | 0.44 |
| 6:Af:494:SER:C | 6:Af:496:ILE:H | 2.25 | 0.44 |
| 6:Am:84:THR:HG21 | 6:Am:90:GLN:HE21 | 1.82 | 0.44 |
| 6:Am:345:TRP:CG | 6:Am:346:ALA:N | 2.85 | 0.44 |
| 6:Ap:444:MET:O | 6:Ap:449:TYR:OH | 2.25 | 0.44 |
| 7:Aq:127:ARG:HH21 | 5:BB:71:THR:HB | 1.82 | 0.44 |
| 2:B2:538:ASP:HB2 | 2:B2:551:ILE:HB | 1.98 | 0.44 |
| 2:B4:252:LEU:HD21 | 2:B4:263:SER:HB3 | 1.98 | 0.44 |
| 2:B5:222:VAL:HG21 | 2:B5:238:ILE:HD11 | 1.98 | 0.44 |
| 2:B7:162:THR:O | 2:B7:186:LYS:HB3 | 2.16 | 0.44 |
| 2:B7:220:PRO:HG2 | 2:B7:338:LEU:HD11 | 1.99 | 0.44 |
| 5:BB:10:ALA:HB3 | 5:BB:11:PRO:HD3 | 1.99 | 0.44 |
| 6:BI:327:SER:OG | 6:BI:328:LYS:N | 2.48 | 0.44 |
| 6:BK:147:MET:SD | 6:BK:487:SER:OG | 2.69 | 0.44 |
| 6:BM:487:SER:OG | 6:BM:488:ALA:N | 2.49 | 0.44 |
| 11:BV:10:ILE:HG12 | 11:BV:48:THR:HB | 1.99 | 0.44 |
| 3:BX:104:PRO:HA | 3:BX:107:TYR:CZ | 2.52 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bb:48:LYS:HE2 | 3:Be:158:ALA:HB2 | 1.99 | 0.44 |
| 3:Bi:80:ASP:O | 3:Bi:84:LYS:HG3 | 2.17 | 0.44 |
| 2:Bp:109:ASN:N | 2:Bp:138:GLY:HA3 | 2.32 | 0.44 |
| 2:Br:432:ALA:HB2 | 2:Br:440:ASN:HD22 | 1.82 | 0.44 |
| 2:Bt:37:PRO:HG3 | 2:Bt:226:TYR:CZ | 2.52 | 0.44 |
| 2:Bt:64:TYR:HE1 | 2:Bt:377:SER:HA | 1.81 | 0.44 |
| 2:Bu:377:SER:O | 2:Bu:381:GLU:HG3 | 2.16 | 0.44 |
| 2:Bw:550:ARG:HB3 | 2:Bw:553:VAL:HG12 | 1.97 | 0.44 |
| 2:Bx:159:GLU:O | 2:Bx:162:THR:N | 2.49 | 0.44 |
| 4:D:59:ASP:HB2 | 4:I:58:LEU:HD21 | 1.99 | 0.44 |
| 4:a:10:PHE:HB3 | 4:a:22:ILE:HG12 | 1.99 | 0.44 |
| 4:d:9:PRO:HA | 4:d:19:GLN:HA | 1.99 | 0.44 |
| 1:l:243:LYS:H | 8:r:4:TYR:H | 1.65 | 0.44 |
| 1:m:118:ILE:HD12 | 1:m:167:ARG:HB3 | 1.98 | 0.44 |
| 8:t:243:ASP:OD1 | 8:t:243:ASP:N | 2.51 | 0.44 |
| 2:1:303:ASP:OD1 | 2:1:304:ILE:N | 2.50 | 0.44 |
| 2:1:557:PHE:CZ | 2:1:629:ILE:HD11 | 2.52 | 0.44 |
| 2:2:244:TYR:CZ | 2:2:272:GLY:HA3 | 2.52 | 0.44 |
| 2:5:110:TYR:HB2 | 2:5:138:GLY:O | 2.18 | 0.44 |
| 3:8:25:ILE:HD12 | 3:8:28:LEU:HD13 | 1.99 | 0.44 |
| 7:A6:275:VAL:HG11 | 7:Al:268:GLY:O | 2.17 | 0.44 |
| 6:A8:398:GLN:NE2 | 6:A9:355:PHE:HB2 | 2.33 | 0.44 |
| 9:AC:37:VAL:HG22 | 9:AC:73:VAL:HG13 | 1.99 | 0.44 |
| 3:AG:62:GLY:O | 3:Bd:118:ARG:NH2 | 2.50 | 0.44 |
| 3:AJ:85:PHE:HB3 | 3:AJ:137:VAL:HG21 | 1.99 | 0.44 |
| 3:AJ:118:ARG:HA | 3:AJ:118:ARG:HD2 | 1.90 | 0.44 |
| 2:AM:8:ILE:HD11 | 2:Bv:569:LYS:HB2 | 1.97 | 0.44 |
| 2:AM:373:PHE:HB2 | 2:AM:405:VAL:HG22 | 1.99 | 0.44 |
| 2:AN:121:VAL:HG22 | 2:AN:166:ASN:HB3 | 1.99 | 0.44 |
| 2:AN:406:LEU:HD22 | 2:AN:474:ILE:HG13 | 1.99 | 0.44 |
| 2:AO:104:SER:HB2 | 2:AO:181:VAL:HB | 1.98 | 0.44 |
| 2:AP:222:VAL:HG21 | 2:AP:238:ILE:HD11 | 1.99 | 0.44 |
| 7:AY:265:ARG:HA | 7:AY:265:ARG:HD3 | 1.88 | 0.44 |
| 6:Ac:365:ALA:HB2 | 6:Ac:372:GLU:HG2 | 1.99 | 0.44 |
| 6:Af:264:ARG:HG3 | 6:Af:477:TYR:HE1 | 1.82 | 0.44 |
| 6:Ag:447:GLY:O | 6:Ag:510:ASN:ND2 | 2.43 | 0.44 |
| 6:Ap:147:MET:HE2 | 6:Ap:367:GLN:HG2 | 1.99 | 0.44 |
| 6:Ap:481:ILE:N | 6:Ap:499:GLY:O | 2.46 | 0.44 |
| 6:Aw:228:MET:HG2 | 6:Aw:233:ALA:HB2 | 1.98 | 0.44 |
| 5:Ax:254:LEU:O | 5:Ax:258:VAL:HG23 | 2.17 | 0.44 |
| 5:Ax:413:LYS:HA | 5:Ax:413:LYS:HD3 | 1.75 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B1:220:PRO:HD2 | 2:B1:338:LEU:HD21 | 2.00 | 0.44 |
| 2:B2:23:SER:O | 2:B2:76:ASN:HB2 | 2.18 | 0.44 |
| 2:B2:371:GLN:OE1 | 2:B2:562:THR:OG1 | 2.28 | 0.44 |
| 2:B3:355:LEU:HD12 | 2:B3:389:VAL:HG21 | 1.98 | 0.44 |
| 2:B3:368:VAL:HG12 | 2:B3:370:VAL:HG22 | 2.00 | 0.44 |
| 2:B6:92:SER:HB3 | 2:B6:340:LEU:HB3 | 1.99 | 0.44 |
| 5:BB:408:ARG:HH21 | 5:BB:450:ARG:CZ | 2.30 | 0.44 |
| 7:BC:230:VAL:HG21 | 7:BC:233:GLN:HB2 | 1.99 | 0.44 |
| 6:BK:490:GLN:OE1 | 6:BK:490:GLN:N | 2.49 | 0.44 |
| 11:BW:18:ASP:HB3 | 11:BW:21:LYS:HD3 | 1.98 | 0.44 |
| 3:Bc:48:LYS:HE3 | 3:Bc:48:LYS:HB3 | 1.80 | 0.44 |
| 2:Bp:246:LYS:HD2 | 2:Bp:250:ALA:HB2 | 1.98 | 0.44 |
| 2:Bt:237:GLU:OE1 | 2:Bt:284:ARG:NH1 | 2.37 | 0.44 |
| 2:Bu:238:ILE:HB | 2:Bu:334:PHE:HE2 | 1.81 | 0.44 |
| 2:Bx:453:ASN:HB3 | 2:Bx:507:ILE:HG12 | 1.99 | 0.44 |
| 2:By:69:MET:O | 2:By:73:GLN:HG2 | 2.17 | 0.44 |
| 2:By:225:LEU:HD13 | 2:By:324:PHE:HB2 | 1.98 | 0.44 |
| 1:l:60:TYR:OH | 1:l:136:ASP:OD2 | 2.23 | 0.44 |
| 1:n:60:TYR:OH | 1:n:136:ASP:OD2 | 2.26 | 0.44 |
| 3:o:20:LEU:HA | 9:y:54:PHE:CD1 | 2.52 | 0.44 |
| 1:p:202:ASN:HA | 1:p:205:ARG:HB2 | 1.99 | 0.44 |
| 9:v:38:PRO:HB3 | 9:w:142:GLU:HA | 1.98 | 0.44 |
| 9:w:13:ASN:H | 9:w:16:ASN:ND2 | 2.15 | 0.44 |
| 1:0:146:LEU:HB3 | 8:q:68:VAL:HG12 | 1.99 | 0.44 |
| 2:1:384:GLU:HA | 2:1:439:ASN:CG | 2.42 | 0.44 |
| 2:2:356:MET:HB2 | 2:2:392:HIS:CD2 | 2.52 | 0.44 |
| 2:4:45:THR:OG1 | 2:4:46:ASN:OD1 | 2.30 | 0.44 |
| 2:5:193:ILE:HD12 | 2:5:193:ILE:HA | 1.85 | 0.44 |
| 2:5:225:LEU:H | 2:5:225:LEU:HD23 | 1.82 | 0.44 |
| 2:5:252:LEU:HG | 2:5:263:SER:HB2 | 1.99 | 0.44 |
| 6:A7:253:ARG:HH21 | 6:A7:492:PRO:HG2 | 1.82 | 0.44 |
| 6:A8:279:ARG:NH2 | 7:Ab:122:GLY:O | 2.50 | 0.44 |
| 6:A9:159:ALA:HB3 | 6:A9:228:MET:HE2 | 1.99 | 0.44 |
| 9:AC:139:SER:HB3 | 9:AC:156:THR:H | 1.81 | 0.44 |
| 3:AH:57:LYS:HE2 | 3:Bm:147:ASN:HD21 | 1.83 | 0.44 |
| 2:AL:477:LEU:HD21 | 2:AL:497:GLY:HA2 | 1.99 | 0.44 |
| 2:AL:612:ASN:HB3 | 2:AL:624:VAL:HG23 | 1.99 | 0.44 |
| 10:AT:284:ALA:HB2 | 10:AT:342:GLN:HE22 | 1.82 | 0.44 |
| 6:AV:270:TYR:HB3 | 6:AV:290:LEU:HD12 | 1.99 | 0.44 |
| 7:AY:103:THR:HG21 | 6:Ao:462:SER:O | 2.18 | 0.44 |
| 7:AY:217:GLU:HB3 | 7:AY:224:HIS:CD2 | 2.51 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AY:246:TRP:NE1 | 7:AY:297:LEU:HB2 | 2.32 | 0.44 |
| 6:Af:123:GLN:O | 6:Az:96:MET:N | 2.50 | 0.44 |
| 6:Ah:204:ASP:OD1 | 6:Ah:205:ALA:N | 2.46 | 0.44 |
| 6:Ai:131:TYR:HA | 6:Ai:250:MET:HA | 1.98 | 0.44 |
| 6:Ai:324:THR:OG1 | 6:Ai:327:SER:HB2 | 2.16 | 0.44 |
| 6:Aj:71:ASP:OD1 | 6:Aj:72:HIS:N | 2.50 | 0.44 |
| 6:Am:148:TYR:HA | 6:Am:185:THR:HA | 1.99 | 0.44 |
| 6:Ao:381:ASN:HB3 | 6:Ao:521:ILE:HG21 | 1.99 | 0.44 |
| 6:Ap:455:ALA:HB1 | 5:BF:65:TYR:H | 1.82 | 0.44 |
| 7:Ar:200:ASN:HB3 | 4:X:31:ILE:HB | 1.99 | 0.44 |
| 5:Ax:335:TRP:HH2 | 5:BA:308:MET:HG2 | 1.83 | 0.44 |
| 2:B1:521:ALA:HB1 | 2:B1:541:ALA:HA | 1.99 | 0.44 |
| 2:B2:514:ARG:HH12 | 2:B3:364:ASP:CG | 2.25 | 0.44 |
| 2:B2:548:PHE:HE2 | 2:B2:557:PHE:CG | 2.35 | 0.44 |
| 2:B6:432:ALA:HB2 | 2:B6:440:ASN:HD22 | 1.83 | 0.44 |
| 2:B7:76:ASN:O | 2:B7:76:ASN:ND2 | 2.46 | 0.44 |
| 5:BB:46:SER:OG | 5:BB:49:GLU:OE1 | 2.32 | 0.44 |
| 7:BE:29:LEU:HD11 | 7:BE:258:LEU:HB3 | 1.98 | 0.44 |
| 5:BF:189:ILE:HG12 | 5:BF:200:LYS:HB2 | 2.00 | 0.44 |
| 5:BG:477:ILE:H | 5:BG:477:ILE:HG13 | 1.63 | 0.44 |
| 6:BJ:151:ASP:HB3 | 6:BJ:154:PHE:HB2 | 1.98 | 0.44 |
| 6:BM:456:LEU:H | 6:BM:475:THR:HB | 1.82 | 0.44 |
| 3:BX:82:ARG:NH1 | 3:BX:138:GLY:HA2 | 2.32 | 0.44 |
| 3:BZ:138:GLY:HA3 | 3:Bo:43:ALA:HA | 1.99 | 0.44 |
| 3:Bd:58:ILE:HD13 | 3:Bd:58:ILE:H | 1.82 | 0.44 |
| 3:Bi:37:LYS:HB2 | 3:Bi:37:LYS:HZ2 | 1.82 | 0.44 |
| 3:Bk:39:THR:HG22 | 3:Bk:71:VAL:HA | 1.99 | 0.44 |
| 2:Bq:222:VAL:HG22 | 2:Bq:325:ALA:HB2 | 1.98 | 0.44 |
| 2:Br:40:GLN:H | 2:Br:81:VAL:HG23 | 1.82 | 0.44 |
| 2:Bs:346:SER:O | 2:Bs:350:VAL:HG23 | 2.17 | 0.44 |
| 2:Bt:30:ALA:HB3 | 2:Bt:359:TRP:CE2 | 2.52 | 0.44 |
| 2:Bu:44:VAL:HG11 | 2:Bu:50:LEU:HD13 | 1.99 | 0.44 |
| 2:Bu:45:THR:OG1 | 2:Bu:49:ASP:OD2 | 2.31 | 0.44 |
| 2:Bu:90:LYS:NZ | 2:Bu:190:ASP:OD1 | 2.36 | 0.44 |
| 2:Bu:222:VAL:HG21 | 2:Bu:238:ILE:HD11 | 1.99 | 0.44 |
| 2:Bw:66:MET:SD | 2:Bw:459:ASP:HB2 | 2.57 | 0.44 |
| 2:Bw:639:THR:HB | 2:Bx:624:VAL:HG12 | 1.98 | 0.44 |
| 2:Bz:159:GLU:OE2 | 2:Bz:166:ASN:ND2 | 2.50 | 0.44 |
| 2:Bz:225:LEU:HD13 | 2:Bz:324:PHE:HB2 | 1.99 | 0.44 |
| 1:k:176:TYR:HD2 | 8:r:73:PRO:HD3 | 1.82 | 0.44 |
| 1:l:62:PRO:HG3 | 1:l:84:TRP:HZ3 | 1.81 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:s:69:GLU:HG2 | 8:s:70:THR:H | 1.82 | 0.44 |
| 1:0:221:VAL:HG13 | 8:q:22:SER:HB2 | 2.00 | 0.44 |
| 2:1:389:VAL:O | 2:1:393:VAL:HG23 | 2.18 | 0.44 |
| 2:2:268:VAL:HG21 | 2:2:282:ILE:HD11 | 1.99 | 0.44 |
| 2:2:368:VAL:O | 2:2:400:ARG:NH2 | 2.50 | 0.44 |
| 2:4:389:VAL:O | 2:4:393:VAL:HG23 | 2.17 | 0.44 |
| 2:4:590:GLN:NE2 | 9:y:163:TYR:OH | 2.50 | 0.44 |
| 3:7:18:PRO:HB2 | 3:8:146:SER:HB2 | 2.00 | 0.44 |
| 5:A1:93:SER:OG | 5:BB:374:ARG:NH2 | 2.50 | 0.44 |
| 5:A3:300:HIS:HE1 | 7:A6:50:PHE:HB2 | 1.82 | 0.44 |
| 6:A4:444:MET:HE2 | 6:A4:444:MET:HB3 | 1.89 | 0.44 |
| 6:A5:430:LYS:HE2 | 6:AW:188:VAL:HG13 | 2.00 | 0.44 |
| 3:AA:10:PHE:CE1 | 3:o:35:GLN:HG2 | 2.52 | 0.44 |
| 8:AB:56:TRP:HB3 | 8:AB:65:VAL:HG21 | 1.98 | 0.44 |
| 2:AD:66:MET:HG2 | 2:AD:468:VAL:HG21 | 1.98 | 0.44 |
| 2:AD:538:ASP:HB2 | 2:AD:551:ILE:HB | 1.98 | 0.44 |
| 3:AI:99:ILE:O | 3:Bg:120:ALA:HB2 | 2.18 | 0.44 |
| 2:AK:247:GLY:O | 2:AK:263:SER:OG | 2.34 | 0.44 |
| 2:AL:116:ILE:HD13 | 2:AL:171:ILE:HG23 | 1.98 | 0.44 |
| 2:AM:101:TYR:CE1 | 2:AM:143:ILE:HG12 | 2.52 | 0.44 |
| 2:AM:202:GLU:H | 2:AM:202:GLU:HG3 | 1.59 | 0.44 |
| 2:AM:644:ALA:O | 2:AM:645:THR:OG1 | 2.36 | 0.44 |
| 2:AN:110:TYR:CE2 | 2:AN:177:GLY:HA3 | 2.52 | 0.44 |
| 2:AN:206:THR:HA | 2:AN:211:GLN:HE21 | 1.83 | 0.44 |
| 2:AN:252:LEU:HB2 | 2:AN:337:ILE:HG12 | 1.99 | 0.44 |
| 2:AO:97:GLY:N | 2:AO:188:ILE:O | 2.50 | 0.44 |
| 2:AO:378:CYS:HG | 2:AO:454:TYR:HH | 1.59 | 0.44 |
| 2:AO:480:ARG:O | 2:AO:484:VAL:HG12 | 2.18 | 0.44 |
| 6:AV:238:GLY:HA2 | 6:AV:242:SER:O | 2.17 | 0.44 |
| 6:AX:142:GLU:HB2 | 6:AX:490:GLN:HB3 | 2.00 | 0.44 |
| 6:Ae:344:ARG:HB2 | 6:Ae:348:GLU:CD | 2.43 | 0.44 |
| 6:Ak:84:THR:OG1 | 6:Ak:88:VAL:O | 2.35 | 0.44 |
| 6:Am:263:SER:HA | 6:Am:476:ARG:HA | 1.98 | 0.44 |
| 6:Ap:494:SER:HA | 11:BW:37:ASP:CG | 2.42 | 0.44 |
| 7:As:231:VAL:HG12 | 4:P:29:GLU:O | 2.17 | 0.44 |
| 6:Au:378:ALA:HB1 | 6:Au:382:VAL:HB | 2.00 | 0.44 |
| 6:Aw:125:PHE:CZ | 6:BI:91:ILE:HA | 2.50 | 0.44 |
| 6:Ay:486:GLU:HA | 6:Ay:509:LYS:O | 2.17 | 0.44 |
| 6:Az:131:TYR:HD2 | 6:Az:250:MET:HE3 | 1.81 | 0.44 |
| 6:Az:147:MET:SD | 6:Az:366:ARG:NH1 | 2.90 | 0.44 |
| 2:B2:28:ALA:HB2 | 2:B2:370:VAL:HG21 | 1.97 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B4:516:ARG:O | 2:B4:520:GLU:HG2 | 2.18 | 0.44 |
| 2:B6:188:ILE:H | 2:B6:188:ILE:HG13 | 1.28 | 0.44 |
| 2:B6:368:VAL:HG12 | 2:B6:370:VAL:HG22 | 1.99 | 0.44 |
| 2:B7:110:TYR:CE2 | 2:B7:171:ILE:HG21 | 2.45 | 0.44 |
| 5:BB:408:ARG:HE | 5:BB:450:ARG:NH2 | 2.14 | 0.44 |
| 7:BC:20:LEU:HD11 | 7:BC:255:ALA:HB1 | 2.00 | 0.44 |
| 7:BC:54:ASN:HD22 | 7:BC:54:ASN:C | 2.24 | 0.44 |
| 7:BC:309:GLY:HA2 | 5:BH:332:GLU:HG2 | 1.99 | 0.44 |
| 5:BD:354:ASP:N | 5:BD:354:ASP:OD1 | 2.46 | 0.44 |
| 7:BE:187:TRP:CE2 | 5:BG:295:ARG:HD2 | 2.53 | 0.44 |
| 5:BG:82:LEU:HD22 | 5:BG:258:VAL:HG22 | 1.99 | 0.44 |
| 7:BL:112:LEU:HD22 | 7:BL:114:MET:HE2 | 2.00 | 0.44 |
| 3:Ba:113:VAL:HG13 | 3:Ba:127:ILE:HG23 | 1.98 | 0.44 |
| 3:Bf:1:MET:HE3 | 3:Bf:1:MET:HB2 | 1.91 | 0.44 |
| 2:Bp:39:PHE:HB3 | 2:Bp:361:PHE:CE2 | 2.53 | 0.44 |
| 2:Bs:315:PHE:HE2 | 2:Bs:323:ILE:HG13 | 1.82 | 0.44 |
| 2:Bv:219:ILE:HB | 2:Bv:338:LEU:HD21 | 1.99 | 0.44 |
| 2:Bv:220:PRO:HG2 | 2:Bv:338:LEU:HD11 | 1.97 | 0.44 |
| 2:Bv:538:ASP:O | 2:Bv:551:ILE:N | 2.30 | 0.44 |
| 2:Bx:487:THR:HG21 | 2:Bx:559:MET:HE3 | 1.99 | 0.44 |
| 4:Y:12:ASP:HB2 | 4:i:52:LEU:HD21 | 1.99 | 0.44 |
| 4:j:35:ASP:N | 4:j:41:GLU:OE2 | 2.45 | 0.44 |
| 3:o:23:VAL:HB | 3:o:113:VAL:HB | 2.00 | 0.44 |
| 8:q:248:ASP:OD1 | 8:q:248:ASP:N | 2.50 | 0.44 |
| 9:x:51:THR:OG1 | 9:x:56:LEU:O | 2.36 | 0.44 |
| 9:y:168:LYS:HB3 | 9:y:173:ILE:HD11 | 1.98 | 0.44 |
| 2:1:406:LEU:HD22 | 2:1:474:ILE:HG13 | 1.98 | 0.44 |
| 2:2:438:ASP:N | 2:2:438:ASP:OD1 | 2.51 | 0.44 |
| 2:4:129:GLY:HA2 | 2:4:146:PRO:HD3 | 1.98 | 0.44 |
| 2:4:429:TRP:CD1 | 2:4:440:ASN:HA | 2.53 | 0.44 |
| 5:A0:301:MET:HE2 | 7:BC:304:PHE:HZ | 1.82 | 0.44 |
| 5:A0:332:GLU:HG2 | 7:BE:309:GLY:HA2 | 1.99 | 0.44 |
| 5:A1:162:ILE:HD13 | 5:A1:163:ASP:N | 2.33 | 0.44 |
| 5:A1:329:SER:HB2 | 7:As:150:MET:HE2 | 1.99 | 0.44 |
| 5:A2:188:ILE:HG22 | 5:A2:202:TYR:HB3 | 1.98 | 0.44 |
| 5:A2:376:PRO:HG3 | 5:A2:403:PHE:HB2 | 1.99 | 0.44 |
| 6:A4:348:GLU:HB3 | 6:A4:396:ALA:HB2 | 1.99 | 0.44 |
| 6:A5:363:GLU:OE2 | 6:A5:366:ARG:NH1 | 2.51 | 0.44 |
| 6:A7:345:TRP:NE1 | 6:A8:348:GLU:HB2 | 2.32 | 0.44 |
| 6:A9:277:ASP:OD1 | 6:An:476:ARG:NH2 | 2.46 | 0.44 |
| 3:AA:25:ILE:HD12 | 3:AA:28:LEU:HD22 | 2.00 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:AB:72:LEU:HD23 | 8:AB:72:LEU:HA | 1.66 | 0.44 |
| 2:AD:417:ILE:HD13 | 2:AD:417:ILE:H | 1.82 | 0.44 |
| 2:AK:511:GLN:OE1 | 2:AK:514:ARG:NH2 | 2.50 | 0.44 |
| 2:AL:100:GLU:HG3 | 2:AL:185:GLY:HA3 | 1.99 | 0.44 |
| 2:AL:234:ILE:HB | 2:AL:340:LEU:HD12 | 2.00 | 0.44 |
| 2:AL:494:TYR:CE1 | 2:Bv:569:LYS:HG3 | 2.51 | 0.44 |
| 2:AM:11:LYS:HG2 | 2:AM:13:THR:HG23 | 1.99 | 0.44 |
| 2:AP:471:ALA:HA | 2:AP:474:ILE:HG12 | 2.00 | 0.44 |
| 2:AP:494:TYR:CZ | 2:Bp:569:LYS:HD3 | 2.53 | 0.44 |
| 7:Ab:30:THR:C | 7:Ab:32:ASP:H | 2.25 | 0.44 |
| 6:Ac:109:PHE:CZ | 6:Ac:303:ASN:HA | 2.53 | 0.44 |
| 6:Ad:106:LEU:HB2 | 6:Ad:303:ASN:ND2 | 2.32 | 0.44 |
| 6:Af:354:LEU:HD22 | 6:Az:400:LEU:HD21 | 1.99 | 0.44 |
| 6:Ak:346:ALA:HB2 | 6:Ao:341:ARG:HB3 | 2.00 | 0.44 |
| 6:Ao:466:ASN:HB3 | 7:BL:93:GLY:HA2 | 1.99 | 0.44 |
| 6:Ap:236:GLN:HG3 | 6:BI:265:GLN:HE21 | 1.83 | 0.44 |
| 7:Aq:202:VAL:O | 4:Z:27:ASN:HA | 2.17 | 0.44 |
| 7:Ar:175:ASN:OD1 | 5:BA:323:ASN:N | 2.47 | 0.44 |
| 6:Au:131:TYR:HB3 | 6:Au:250:MET:HE2 | 1.98 | 0.44 |
| 5:Av:308:MET:HG2 | 5:BB:335:TRP:HH2 | 1.83 | 0.44 |
| 5:Ax:76:ILE:HD12 | 5:Ax:180:ARG:HB3 | 2.00 | 0.44 |
| 2:B3:28:ALA:HB2 | 2:B3:370:VAL:HG21 | 1.99 | 0.44 |
| 5:BD:398:ARG:HD2 | 5:BD:398:ARG:HA | 1.70 | 0.44 |
| 7:BE:30:THR:C | 7:BE:32:ASP:H | 2.25 | 0.44 |
| 7:BE:68:ARG:HD2 | 7:BE:74:PHE:CE2 | 2.53 | 0.44 |
| 5:BF:379:ARG:H | 5:BF:379:ARG:HG2 | 1.46 | 0.44 |
| 5:BG:311:ARG:HG3 | 5:BG:312:VAL:H | 1.82 | 0.44 |
| 11:BP:10:ILE:HD11 | 11:BP:35:TYR:CE1 | 2.53 | 0.44 |
| 11:BQ:26:LYS:HD2 | 11:BQ:75:LEU:HD23 | 1.98 | 0.44 |
| 3:BZ:37:LYS:NZ | 3:BZ:74:MET:HG2 | 2.32 | 0.44 |
| 3:Bc:143:ASP:OD1 | 3:Bc:144:TRP:N | 2.51 | 0.44 |
| 3:Bd:23:VAL:HG11 | 3:Bd:39:THR:HG21 | 1.99 | 0.44 |
| 3:Be:83:GLN:HA | 3:Be:86:VAL:HG22 | 1.99 | 0.44 |
| 2:Bp:444:SER:HB3 | 2:Bp:543:SER:H | 1.82 | 0.44 |
| 2:Bt:394:VAL:HG11 | 2:Bt:443:ILE:HD12 | 1.99 | 0.44 |
| 2:Bu:154:ALA:HA | 2:Bu:157:VAL:HG22 | 1.99 | 0.44 |
| 2:Bv:572:LEU:HD12 | 2:Bv:572:LEU:HA | 1.77 | 0.44 |
| 2:Bw:119:LYS:HE3 | 2:Bw:122:SER:HA | 2.00 | 0.44 |
| 2:Bw:365:ARG:HA | 2:Bw:400:ARG:NH2 | 2.32 | 0.44 |
| 2:Bx:495:ASN:OD1 | 2:Bx:495:ASN:N | 2.50 | 0.44 |
| 2:By:488:TRP:O | 2:By:552:ASN:ND2 | 2.50 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:m:173:LYS:HB3 | 8:t:69:GLU:HB2 | 1.98 | 0.44 |
| 1:p:11:LYS:H | 1:p:11:LYS:HD2 | 1.83 | 0.44 |
| 8:q:217:HIS:HA | 8:q:229:VAL:HB | 2.00 | 0.44 |
| 9:x:168:LYS:HD3 | 9:x:173:ILE:HD11 | 2.00 | 0.44 |
| 2:2:51:VAL:HG22 | 2:2:65:PHE:HZ | 1.83 | 0.44 |
| 2:2:202:GLU:HA | 2:2:205:MET:HG2 | 1.98 | 0.44 |
| 2:3:525:VAL:HG22 | 2:3:535:LEU:HD23 | 1.98 | 0.44 |
| 2:4:545:PRO:HG3 | 2:5:271:TYR:HB2 | 1.99 | 0.44 |
| 5:A0:420:ASP:HB3 | 5:A0:421:PRO:HD3 | 2.00 | 0.44 |
| 5:A1:66:GLU:HB2 | 6:BK:288:ALA:HB2 | 1.99 | 0.44 |
| 5:A2:28:LEU:HD11 | 5:BF:172:LYS:HG2 | 1.99 | 0.44 |
| 8:AB:60:ASN:N | 8:AB:60:ASN:OD1 | 2.50 | 0.44 |
| 2:AD:130:LYS:HE3 | 2:AD:130:LYS:HB2 | 1.85 | 0.44 |
| 2:AO:355:LEU:HD12 | 2:AO:389:VAL:HG21 | 2.00 | 0.44 |
| 2:AP:151:ILE:O | 2:AP:155:LYS:HG2 | 2.17 | 0.44 |
| 7:Aa:16:ILE:HD12 | 7:Aa:252:THR:HG23 | 1.99 | 0.44 |
| 7:Ab:53:LEU:HD12 | 7:Ab:53:LEU:HA | 1.75 | 0.44 |
| 6:Ad:503:ILE:HA | 6:Ad:507:LEU:HB2 | 1.98 | 0.44 |
| 6:Au:269:ALA:HB2 | 6:Au:470:VAL:HG13 | 1.99 | 0.44 |
| 6:Ay:322:THR:O | 6:Ay:322:THR:OG1 | 2.29 | 0.44 |
| 6:Az:417:LEU:HB3 | 6:Az:421:TYR:HB2 | 2.00 | 0.44 |
| 2:B1:222:VAL:HG21 | 2:B1:238:ILE:HD11 | 1.99 | 0.44 |
| 2:B1:313:ASP:N | 2:B1:313:ASP:OD1 | 2.50 | 0.44 |
| 2:B2:560:LEU:O | 2:B2:564:ILE:HG12 | 2.18 | 0.44 |
| 2:B3:510:ARG:O | 2:B3:514:ARG:HB2 | 2.17 | 0.44 |
| 2:B4:116:ILE:N | 2:B4:129:GLY:O | 2.50 | 0.44 |
| 2:B4:560:LEU:O | 2:B4:564:ILE:HG12 | 2.18 | 0.44 |
| 5:BA:337:GLN:HB3 | 5:BA:344:VAL:HB | 2.00 | 0.44 |
| 5:BB:86:TYR:O | 5:BB:87:GLU:HB2 | 2.16 | 0.44 |
| 5:BB:423:LYS:HG3 | 5:BB:437:TRP:CD1 | 2.52 | 0.44 |
| 7:BC:99:ASP:OD1 | 7:BC:100:GLY:N | 2.51 | 0.44 |
| 5:BD:218:ASP:OD1 | 5:BD:218:ASP:N | 2.51 | 0.44 |
| 5:BF:327:ASN:ND2 | 7:BL:142:THR:O | 2.51 | 0.44 |
| 5:BF:366:ARG:NH1 | 5:BF:382:GLN:OE1 | 2.51 | 0.44 |
| 7:BL:53:LEU:HD12 | 7:BL:53:LEU:HA | 1.87 | 0.44 |
| 7:BL:97:SER:OG | 7:BL:101:ASN:OD1 | 2.34 | 0.44 |
| 6:BM:146:PRO:HB3 | 6:BM:369:GLY:HA3 | 2.00 | 0.44 |
| 6:BM:309:TRP:CD1 | 6:BM:479:ILE:HD13 | 2.53 | 0.44 |
| 11:BQ:9:ASN:HB3 | 11:BQ:56:TYR:CE2 | 2.52 | 0.44 |
| 3:BY:77:GLU:HG2 | 3:Bn:124:THR:HG21 | 2.00 | 0.44 |
| 3:Bb:99:ILE:HG12 | 3:Bn:56:ARG:HG3 | 1.99 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bi:103:LYS:O | 3:Bi:106:GLU:HG2 | 2.17 | 0.44 |
| 2:Bs:28:ALA:HB1 | 2:Bs:362:PHE:CE2 | 2.53 | 0.44 |
| 2:Bs:411:ARG:O | 2:Bs:415:VAL:HB | 2.18 | 0.44 |
| 2:By:495:ASN:OD1 | 2:By:495:ASN:N | 2.49 | 0.44 |
| 4:g:8:LEU:O | 4:g:19:GLN:NE2 | 2.50 | 0.44 |
| 1:m:59:TYR:HB2 | 1:m:139:TYR:HB3 | 1.99 | 0.44 |
| 8:q:22:SER:O | 8:q:38:ARG:NH1 | 2.51 | 0.44 |
| 8:q:215:ASP:N | 8:q:215:ASP:OD1 | 2.51 | 0.44 |
| 8:r:91:ASN:OD1 | 8:r:92:ILE:N | 2.50 | 0.44 |
| 1:0:33:PHE:HE1 | 7:BC:277:ILE:HD12 | 1.83 | 0.44 |
| 3:8:5:ASP:HB3 | 3:8:8:ARG:HB2 | 1.99 | 0.44 |
| 5:A3:39:GLY:H | 5:A3:250:ILE:HD11 | 1.83 | 0.44 |
| 6:A4:414:ALA:HB3 | 6:A4:423:VAL:HB | 1.99 | 0.44 |
| 6:A7:337:PRO:HA | 6:A7:340:ILE:HG12 | 2.00 | 0.44 |
| 6:A9:85:SER:HB2 | 11:BT:35:TYR:HE2 | 1.82 | 0.44 |
| 9:AC:78:ASP:HA | 9:z:11:GLN:HA | 2.00 | 0.44 |
| 3:AF:64:ARG:NH1 | 3:AG:95:GLN:HB3 | 2.32 | 0.44 |
| 3:AH:83:GLN:HA | 3:AH:86:VAL:HG22 | 2.00 | 0.44 |
| 2:AK:32:LYS:HD2 | 2:AK:64:TYR:HE2 | 1.82 | 0.44 |
| 2:AM:131:ILE:HA | 2:AM:143:ILE:HA | 1.99 | 0.44 |
| 2:AM:406:LEU:HA | 2:AM:449:ALA:O | 2.18 | 0.44 |
| 2:AN:104:SER:HB2 | 2:AN:181:VAL:HB | 2.00 | 0.44 |
| 6:Ae:448:ILE:HD11 | 6:Ae:479:ILE:HD12 | 2.00 | 0.44 |
| 6:Af:305:GLU:HA | 6:Aj:225:ALA:HB3 | 1.99 | 0.44 |
| 6:Ag:100:ARG:HD3 | 6:Ak:127:LEU:HD22 | 2.00 | 0.44 |
| 6:Ag:262:LYS:NZ | 6:Ak:226:GLU:OE1 | 2.50 | 0.44 |
| 6:Ai:406:THR:OG1 | 6:Am:372:GLU:OE2 | 2.23 | 0.44 |
| 7:Al:30:THR:O | 7:Al:32:ASP:N | 2.48 | 0.44 |
| 7:Al:117:ILE:HD13 | 7:Al:117:ILE:H | 1.82 | 0.44 |
| 6:Ao:90:GLN:HE21 | 6:Ao:90:GLN:HB2 | 1.59 | 0.44 |
| 6:Ao:445:ASP:OD1 | 6:Ao:445:ASP:N | 2.49 | 0.44 |
| 7:Aq:40:ARG:HH21 | 7:Aq:254:LEU:HB3 | 1.81 | 0.44 |
| 7:As:98:MET:H | 7:As:102:ALA:HB3 | 1.81 | 0.44 |
| 7:At:29:LEU:O | 1:k:10:ALA:N | 2.49 | 0.44 |
| 6:Az:145:HIS:ND1 | 6:Az:146:PRO:O | 2.50 | 0.44 |
| 2:B5:213:ASN:O | 2:B5:217:TYR:HD1 | 1.99 | 0.44 |
| 2:B7:18:THR:HG21 | 2:B7:48:VAL:HG22 | 1.99 | 0.44 |
| 2:B7:57:PRO:HG3 | 2:B7:65:PHE:HB3 | 1.99 | 0.44 |
| 2:B7:153:LYS:O | 2:B7:157:VAL:HG22 | 2.18 | 0.44 |
| 2:B7:209:ASP:OD1 | 2:B7:210:PHE:N | 2.51 | 0.44 |
| 5:BA:29:VAL:HG23 | 5:BA:199:VAL:O | 2.18 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BD:76:ILE:O | 5:BD:80:ARG:HG2 | 2.18 | 0.44 |
| 5:BD:454:PHE:CE2 | 5:BD:458:LYS:HD2 | 2.52 | 0.44 |
| 7:BE:194:THR:O | 7:BE:198:VAL:HG23 | 2.18 | 0.44 |
| 3:Bn:42:PRO:HG2 | 3:Bn:127:ILE:HD11 | 1.99 | 0.44 |
| 2:Bp:32:LYS:HG3 | 2:Bp:350:VAL:HG21 | 2.00 | 0.44 |
| 2:Bp:285:ARG:NH1 | 2:Bp:286:ASN:OD1 | 2.51 | 0.44 |
| 2:Bs:455:LYS:HB3 | 2:Bs:470:LEU:HD13 | 1.98 | 0.44 |
| 2:Bs:509:THR:O | 2:Bs:514:ARG:NH1 | 2.50 | 0.44 |
| 2:Bt:379:ALA:HB2 | 2:Bt:469:PRO:HD3 | 2.00 | 0.44 |
| 2:Bw:273:PRO:HD3 | 2:Bw:280:ALA:HB2 | 1.99 | 0.44 |
| 2:Bx:351:THR:OG1 | 2:Bx:352:ALA:N | 2.50 | 0.44 |
| 2:By:151:ILE:O | 2:By:155:LYS:HG2 | 2.17 | 0.44 |
| 2:By:254:ILE:HG22 | 2:By:257:GLY:H | 1.83 | 0.44 |
| 2:By:454:TYR:HB3 | 2:By:467:TRP:CD1 | 2.53 | 0.44 |
| 4:L:8:LEU:HD22 | 4:L:54:ASN:HB3 | 1.99 | 0.44 |
| 4:Z:9:PRO:HD3 | 4:Z:57:VAL:HG21 | 1.98 | 0.44 |
| 4:a:24:TRP:O | 4:a:46:ARG:NH2 | 2.49 | 0.44 |
| 1:m:61:VAL:HB | 1:m:137:LEU:HB2 | 1.99 | 0.44 |
| 3:o:94:GLY:HA3 | 3:o:100:THR:HB | 2.00 | 0.44 |
| 8:r:72:LEU:HD12 | 8:r:125:ARG:HB2 | 2.00 | 0.44 |
| 8:r:99:GLN:HB3 | 8:r:243:ASP:HB3 | 1.98 | 0.44 |
| 8:s:237:VAL:HG13 | 8:s:247:TRP:CZ3 | 2.52 | 0.44 |
| 2:1:373:PHE:HB2 | 2:1:405:VAL:HG22 | 2.00 | 0.44 |
| 2:2:44:VAL:HG11 | 2:2:50:LEU:HB2 | 1.99 | 0.44 |
| 2:4:406:LEU:HD22 | 2:4:474:ILE:HG13 | 1.99 | 0.44 |
| 2:5:510:ARG:HG2 | 2:5:511:GLN:H | 1.83 | 0.44 |
| 3:6:18:PRO:HB2 | 3:7:146:SER:HB2 | 2.00 | 0.44 |
| 3:8:64:ARG:HH21 | 3:9:95:GLN:HB2 | 1.83 | 0.44 |
| 5:A0:76:ILE:HD13 | 5:A0:179:PRO:HB2 | 1.99 | 0.44 |
| 5:A1:301:MET:HE2 | 7:Aq:304:PHE:HZ | 1.83 | 0.44 |
| 5:A1:321:ILE:O | 7:Aq:174:GLY:HA2 | 2.17 | 0.44 |
| 5:A1:328:MET:HB3 | 5:BB:282:ARG:HH12 | 1.82 | 0.44 |
| 5:A3:311:ARG:HH21 | 5:A3:326:HIS:CD2 | 2.36 | 0.44 |
| 6:A7:270:TYR:HB3 | 6:A7:290:LEU:HD22 | 2.00 | 0.44 |
| 2:AD:299:ARG:HG2 | 2:AD:310:TYR:CZ | 2.52 | 0.44 |
| 3:AG:43:ALA:HA | 3:AH:139:GLU:H | 1.83 | 0.44 |
| 3:AI:42:PRO:HB2 | 3:AI:43:ALA:H | 1.55 | 0.44 |
| 3:AJ:11:GLU:H | 3:AJ:11:GLU:HG2 | 1.56 | 0.44 |
| 3:AJ:97:ASN:O | 3:Bg:3:VAL:N | 2.46 | 0.44 |
| 3:AJ:103:LYS:HG3 | 3:Bj:13:GLY:HA3 | 2.00 | 0.44 |
| 2:AK:139:LYS:HB3 | 2:AK:141:LYS:NZ | 2.33 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AM:284:ARG:HG2 | 2:AM:289:ILE:HD13 | 2.00 | 0.44 |
| 2:AN:510:ARG:HG2 | 2:AN:511:GLN:H | 1.83 | 0.44 |
| 2:AO:572:LEU:HD12 | 2:AO:572:LEU:HA | 1.84 | 0.44 |
| 6:AX:267:LYS:HE2 | 6:Az:247:TRP:HB2 | 1.98 | 0.44 |
| 6:AX:351:LYS:NZ | 6:AX:394:SER:O | 2.51 | 0.44 |
| 6:Ac:155:SER:OG | 6:Aw:301:GLU:OE1 | 2.33 | 0.44 |
| 6:Af:131:TYR:HE2 | 6:Af:143:ALA:HA | 1.83 | 0.44 |
| 6:Af:366:ARG:HD2 | 6:Az:380:ARG:HH21 | 1.82 | 0.44 |
| 6:Ai:184:GLU:O | 6:Ai:185:THR:OG1 | 2.30 | 0.44 |
| 6:Ai:345:TRP:HZ2 | 6:Am:351:LYS:HD2 | 1.83 | 0.44 |
| 6:Ak:267:LYS:HD3 | 6:Ao:247:TRP:CE3 | 2.53 | 0.44 |
| 6:Ak:278:LEU:HD23 | 6:Ak:286:ALA:HB2 | 2.00 | 0.44 |
| 7:Al:271:LEU:HD21 | 1:n:54:ARG:HD3 | 2.00 | 0.44 |
| 5:Ax:289:THR:HB | 5:Ax:292:MET:HE3 | 1.99 | 0.44 |
| 2:B1:612:ASN:OD1 | 2:B1:612:ASN:N | 2.50 | 0.44 |
| 2:B3:351:THR:HG23 | 2:B3:354:ASP:H | 1.82 | 0.44 |
| 2:B4:283:VAL:O | 2:B4:290:VAL:HG12 | 2.18 | 0.44 |
| 2:B4:453:ASN:ND2 | 2:B4:454:TYR:O | 2.49 | 0.44 |
| 5:BF:11:PRO:HA | 5:BF:14:LYS:HE3 | 2.00 | 0.44 |
| 6:BK:141:LYS:HA | 6:BK:490:GLN:HG2 | 2.00 | 0.44 |
| 7:BL:128:PHE:CD2 | 7:BL:129:TYR:HD2 | 2.36 | 0.44 |
| 3:BX:69:TRP:HB2 | 3:BX:159:LEU:HD23 | 1.99 | 0.44 |
| 3:BZ:8:ARG:HA | 3:BZ:11:GLU:HG2 | 2.00 | 0.44 |
| 3:Be:124:THR:HB | 3:Bh:78:ALA:HA | 2.00 | 0.44 |
| 3:Bi:21:PHE:HZ | 3:Bi:38:ALA:HA | 1.82 | 0.44 |
| 2:Bp:647:THR:O | 2:Bq:630:GLN:NE2 | 2.51 | 0.44 |
| 2:Bt:33:PHE:HA | 2:Bt:61:THR:HG23 | 1.99 | 0.44 |
| 2:Bt:302:LYS:O | 2:Bt:307:SER:N | 2.50 | 0.44 |
| 2:Bv:269:PHE:CZ | 2:Bv:280:ALA:HB1 | 2.52 | 0.44 |
| 2:By:498:GLN:HA | 2:By:534:VAL:HG12 | 1.99 | 0.44 |
| 2:Bz:351:THR:OG1 | 2:Bz:352:ALA:N | 2.49 | 0.44 |
| 4:K:24:TRP:O | 4:K:26:LYS:NZ | 2.51 | 0.44 |
| 4:b:44:MET:HE2 | 4:b:44:MET:HB3 | 1.89 | 0.44 |
| 8:s:218:ALA:H | 8:s:229:VAL:HG21 | 1.83 | 0.44 |
| 8:t:13:TYR:CD2 | 8:t:116:MET:HE1 | 2.53 | 0.44 |
| 8:t:81:ASP:OD1 | 8:t:82:PHE:N | 2.50 | 0.44 |
| 9:w:19:VAL:HG11 | 9:w:37:VAL:HG21 | 1.99 | 0.44 |
| 9:y:168:LYS:HD2 | 9:z:85:ILE:HG21 | 1.99 | 0.44 |
| 9:z:83:SER:O | 9:z:87:MET:HG2 | 2.18 | 0.44 |
| 1:0:176:TYR:HA | 8:q:71:ILE:HA | 2.00 | 0.44 |
| 2:1:406:LEU:H | 2:1:406:LEU:HG | 1.67 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:246:LYS:HG3 | 2:2:250:ALA:HB2 | 1.98 | 0.44 |
| 2:5:374:ILE:HG23 | 2:5:471:ALA:O | 2.18 | 0.44 |
| 3:9:118:ARG:NH2 | 9:y:94:THR:O | 2.51 | 0.44 |
| 5:A1:41:ARG:NH2 | 5:A1:64:SER:OG | 2.51 | 0.44 |
| 5:A3:236:VAL:HG13 | 5:A3:420:ASP:HB3 | 2.00 | 0.44 |
| 6:A9:462:SER:N | 7:As:102:ALA:O | 2.35 | 0.44 |
| 3:AE:39:THR:HG22 | 3:AE:71:VAL:HG22 | 1.99 | 0.44 |
| 3:AF:56:ARG:HB3 | 3:AF:56:ARG:HH11 | 1.82 | 0.44 |
| 2:AL:527:GLY:HA2 | 2:AL:533:TYR:CD2 | 2.53 | 0.44 |
| 2:AM:462:ASN:HB2 | 2:AM:464:VAL:HG22 | 1.99 | 0.44 |
| 7:Al:53:LEU:HD12 | 7:Al:53:LEU:HA | 1.87 | 0.44 |
| 6:Am:387:ALA:HB2 | 6:Am:404:PHE:HB2 | 1.99 | 0.44 |
| 6:Ap:476:ARG:NH2 | 6:BM:277:ASP:OD1 | 2.49 | 0.44 |
| 7:Aq:163:PHE:HB2 | 7:Aq:170:LEU:HB2 | 2.00 | 0.44 |
| 5:Av:93:SER:HA | 5:Av:148:ARG:HH21 | 1.82 | 0.44 |
| 6:Aw:184:GLU:O | 6:Aw:185:THR:OG1 | 2.29 | 0.44 |
| 5:Ax:283:ARG:HD3 | 5:BA:350:LEU:HD21 | 1.99 | 0.44 |
| 2:B1:404:LEU:HD22 | 2:B1:404:LEU:HA | 1.83 | 0.44 |
| 2:B2:456:TYR:O | 2:B2:503:ILE:HG12 | 2.17 | 0.44 |
| 5:BB:376:PRO:HB3 | 5:BB:399:ASP:HB2 | 2.00 | 0.44 |
| 5:BB:383:ASP:N | 5:BB:383:ASP:OD1 | 2.51 | 0.44 |
| 5:BB:474:GLU:HG3 | 5:BB:475:PRO:HD3 | 2.00 | 0.44 |
| 7:BC:269:MET:HE1 | 7:BE:272:PRO:HG2 | 2.00 | 0.44 |
| 5:BD:5:VAL:N | 5:BD:9:PHE:HD1 | 2.15 | 0.44 |
| 3:Bb:23:VAL:HG11 | 3:Bb:39:THR:HG21 | 2.00 | 0.44 |
| 3:Bo:103:LYS:O | 3:Bo:106:GLU:HG2 | 2.18 | 0.44 |
| 2:Bp:34:GLN:OE1 | 2:Bp:58:THR:OG1 | 2.35 | 0.44 |
| 2:Bp:450:ILE:HD13 | 2:Bp:522:ILE:HG12 | 2.00 | 0.44 |
| 2:Bq:481:THR:HG23 | 2:Bq:496:ARG:HD3 | 1.99 | 0.44 |
| 2:Br:470:LEU:O | 2:Br:474:ILE:HG12 | 2.18 | 0.44 |
| 2:Bs:110:TYR:CD1 | 2:Bs:177:GLY:HA3 | 2.53 | 0.44 |
| 2:Bw:148:ALA:O | 2:Bw:151:ILE:HG13 | 2.18 | 0.44 |
| 2:Bx:346:SER:O | 2:Bx:350:VAL:HG23 | 2.18 | 0.44 |
| 2:Bz:130:LYS:HE2 | 2:Bz:130:LYS:HB2 | 1.78 | 0.44 |
| 2:Bz:454:TYR:HB3 | 2:Bz:467:TRP:HD1 | 1.83 | 0.44 |
| 4:H:76:ILE:HD11 | 4:S:76:ILE:HG13 | 1.99 | 0.44 |
| 4:I:27:ASN:HB3 | 4:i:38:TYR:CE2 | 2.53 | 0.44 |
| 8:s:85:ASN:H | 8:s:114:ILE:HA | 1.83 | 0.44 |
| 8:u:144:HIS:HB2 | 8:u:164:LYS:HB3 | 2.00 | 0.44 |
| 2:3:297:THR:HG22 | 2:3:311:ILE:HD12 | 1.99 | 0.43 |
| 2:3:410:PRO:O | 2:3:413:THR:HG22 | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:4:285:ARG:HG2 | 2:4:286:ASN:ND2 | 2.33 | 0.43 |
| 2:4:371:GLN:HB2 | 2:4:403:CYS:HA | 1.99 | 0.43 |
| 2:4:654:LEU:HD22 | 2:5:17:SER:H | 1.82 | 0.43 |
| 3:8:99:ILE:HD11 | 3:AI:1:MET:HE3 | 1.99 | 0.43 |
| 4:A:57:VAL:HA | 4:A:60:LYS:HE2 | 2.00 | 0.43 |
| 5:A0:227:LYS:HA | 5:A0:227:LYS:HD3 | 1.91 | 0.43 |
| 5:A1:401:LEU:HD22 | 5:A1:405:LYS:HE2 | 2.00 | 0.43 |
| 5:A3:461:GLU:O | 5:A3:465:ARG:HG2 | 2.17 | 0.43 |
| 6:A5:301:GLU:OE1 | 6:AW:155:SER:OG | 2.29 | 0.43 |
| 7:A6:90:THR:O | 7:A6:96:THR:HA | 2.18 | 0.43 |
| 7:A6:133:ALA:HA | 7:A6:136:ALA:HB2 | 1.99 | 0.43 |
| 6:A7:154:PHE:CE2 | 6:A7:248:ASN:HB3 | 2.53 | 0.43 |
| 2:AD:310:TYR:O | 2:AD:314:PHE:CB | 2.66 | 0.43 |
| 2:AK:66:MET:HB3 | 2:AK:468:VAL:HG11 | 1.99 | 0.43 |
| 2:AK:359:TRP:HZ3 | 2:AK:373:PHE:HD2 | 1.66 | 0.43 |
| 2:AL:93:SER:HB3 | 2:AL:191:SER:HB2 | 1.99 | 0.43 |
| 2:AM:404:LEU:HD22 | 2:AM:404:LEU:HA | 1.87 | 0.43 |
| 2:AM:633:ARG:HD2 | 2:AM:633:ARG:HA | 1.88 | 0.43 |
| 2:AM:644:ALA:HA | 2:By:557:PHE:HZ | 1.83 | 0.43 |
| 2:AP:51:VAL:HG22 | 2:AP:65:PHE:CZ | 2.53 | 0.43 |
| 6:AX:452:PRO:HA | 6:AX:477:TYR:HA | 2.00 | 0.43 |
| 7:AY:117:ILE:HD12 | 7:AY:118:ASN:H | 1.83 | 0.43 |
| 7:Ab:80:ASN:HB2 | 7:Ab:189:LYS:HD3 | 1.99 | 0.43 |
| 6:Ac:380:ARG:HH21 | 6:Ag:366:ARG:HD2 | 1.83 | 0.43 |
| 6:Ah:345:TRP:CD1 | 6:BI:348:GLU:HB3 | 2.53 | 0.43 |
| 6:Aj:380:ARG:CZ | 6:An:366:ARG:HB3 | 2.48 | 0.43 |
| 6:Ak:190:LEU:HD13 | 6:Ak:221:LEU:HD13 | 1.98 | 0.43 |
| 6:An:153:MET:HE1 | 6:An:226:GLU:HG2 | 2.00 | 0.43 |
| 6:Ap:393:ILE:HG22 | 6:BI:397:ALA:HB1 | 2.00 | 0.43 |
| 7:Aq:258:LEU:HD22 | 7:Aq:258:LEU:HA | 1.89 | 0.43 |
| 7:As:161:PHE:O | 5:BB:303:HIS:NE2 | 2.51 | 0.43 |
| 5:Ax:508:GLU:OE1 | 5:BA:482:SER:OG | 2.35 | 0.43 |
| 6:Az:128:ARG:NH1 | 6:Az:490:GLN:O | 2.51 | 0.43 |
| 6:Az:363:GLU:OE2 | 6:Az:366:ARG:NH1 | 2.50 | 0.43 |
| 2:B1:46:ASN:O | 2:B1:50:LEU:HD23 | 2.18 | 0.43 |
| 2:B3:480:ARG:O | 2:B3:484:VAL:HG12 | 2.18 | 0.43 |
| 2:B6:371:GLN:HE21 | 2:B6:371:GLN:HB3 | 1.58 | 0.43 |
| 5:BA:336:LEU:HD11 | 5:BA:347:VAL:HG12 | 2.00 | 0.43 |
| 5:BD:115:LYS:HD3 | 5:BD:445:LYS:HE3 | 2.00 | 0.43 |
| 5:BG:210:THR:O | 5:BG:225:GLY:HA2 | 2.18 | 0.43 |
| 5:BH:56:ALA:O | 5:BH:60:THR:N | 2.51 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BH:111:LEU:HD11 | 5:BH:444:ILE:HD11 | 2.00 | 0.43 |
| 6:BI:131:TYR:HD2 | 6:BI:250:MET:HE3 | 1.83 | 0.43 |
| 7:BL:29:LEU:HD21 | 7:BL:259:ASN:HB2 | 2.00 | 0.43 |
| 11:BP:14:GLU:HB3 | 11:BP:25:GLY:N | 2.33 | 0.43 |
| 11:BT:9:ASN:HB3 | 11:BT:56:TYR:CE2 | 2.52 | 0.43 |
| 11:BW:10:ILE:HD13 | 11:BW:41:ILE:HG21 | 2.00 | 0.43 |
| 3:Bg:137:VAL:HB | 3:Bg:155:VAL:HG13 | 2.00 | 0.43 |
| 3:Bm:19:ASN:OD1 | 3:Bm:19:ASN:N | 2.46 | 0.43 |
| 3:Bn:14:ASP:N | 3:Bn:14:ASP:OD1 | 2.51 | 0.43 |
| 2:Bp:151:ILE:O | 2:Bp:155:LYS:HG2 | 2.17 | 0.43 |
| 2:Bu:527:GLY:HA2 | 2:Bu:533:TYR:HD1 | 1.83 | 0.43 |
| 2:Bw:74:TYR:CD2 | 2:Bw:476:GLY:HA3 | 2.52 | 0.43 |
| 2:Bx:2:THR:OG1 | 2:Bx:3:LEU:N | 2.51 | 0.43 |
| 2:Bx:39:PHE:HE1 | 2:Bx:84:VAL:H | 1.66 | 0.43 |
| 4:M:75:ASP:OD2 | 4:O:80:GLN:NE2 | 2.51 | 0.43 |
| 4:V:7:ASP:OD1 | 4:V:7:ASP:N | 2.51 | 0.43 |
| 1:p:59:TYR:HB2 | 1:p:139:TYR:HB3 | 1.98 | 0.43 |
| 2:1:410:PRO:O | 2:1:413:THR:HG22 | 2.17 | 0.43 |
| 2:3:100:GLU:HG2 | 2:3:186:LYS:O | 2.18 | 0.43 |
| 2:5:99:ILE:O | 2:5:100:GLU:HG3 | 2.18 | 0.43 |
| 2:5:225:LEU:HB3 | 2:5:324:PHE:HB2 | 2.00 | 0.43 |
| 3:8:41:LEU:HD22 | 3:9:140:LEU:HD23 | 2.00 | 0.43 |
| 3:9:97:ASN:O | 3:9:97:ASN:ND2 | 2.44 | 0.43 |
| 5:A1:208:TYR:HB2 | 5:A1:230:ILE:HD11 | 2.00 | 0.43 |
| 5:A3:427:LEU:HD21 | 5:A3:434:GLU:HG3 | 1.98 | 0.43 |
| 6:A4:264:ARG:NH1 | 6:A4:477:TYR:OH | 2.47 | 0.43 |
| 3:AA:89:GLN:NE2 | 3:AA:135:THR:O | 2.51 | 0.43 |
| 8:AB:132:GLN:HG2 | 8:u:6:TYR:CD1 | 2.54 | 0.43 |
| 2:AD:41:ILE:HA | 2:AD:81:VAL:HG22 | 2.00 | 0.43 |
| 2:AD:654:LEU:HD21 | 2:AN:628:TYR:CZ | 2.53 | 0.43 |
| 3:AH:137:VAL:HG23 | 3:AH:155:VAL:HG22 | 2.00 | 0.43 |
| 2:AM:108:SER:O | 2:AM:177:GLY:HA2 | 2.18 | 0.43 |
| 2:AM:332:GLU:CD | 2:AM:332:GLU:H | 2.26 | 0.43 |
| 2:AM:563:ASN:OD1 | 2:AM:591:TYR:OH | 2.24 | 0.43 |
| 2:AO:94:PRO:HD3 | 2:AO:222:VAL:O | 2.18 | 0.43 |
| 2:AP:31:GLY:O | 2:AP:82:ARG:HA | 2.18 | 0.43 |
| 2:AP:365:ARG:HG3 | 2:AP:402:ASP:CG | 2.43 | 0.43 |
| 6:AV:264:ARG:NE | 6:AV:477:TYR:OH | 2.43 | 0.43 |
| 7:AY:115:ALA:HB2 | 6:Ao:272:ILE:HG12 | 2.00 | 0.43 |
| 7:Ab:309:GLY:O | 5:Ax:309:LYS:NZ | 2.38 | 0.43 |
| 6:Ah:184:GLU:O | 6:Ah:185:THR:OG1 | 2.33 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ah:267:LYS:HE2 | 6:BI:247:TRP:HB2 | 2.01 | 0.43 |
| 6:Ah:395:TYR:HD1 | 6:Ah:396:ALA:H | 1.66 | 0.43 |
| 7:Al:215:LEU:HD11 | 7:BE:75:ASP:HB3 | 1.99 | 0.43 |
| 6:Am:261:ALA:HA | 6:Am:478:GLY:HA3 | 2.00 | 0.43 |
| 6:An:365:ALA:HB2 | 6:An:372:GLU:HA | 2.00 | 0.43 |
| 6:Ao:345:TRP:CD1 | 6:Ao:346:ALA:N | 2.85 | 0.43 |
| 7:Ar:192:ILE:HD11 | 7:Ar:226:LEU:HG | 1.99 | 0.43 |
| 7:As:12:LEU:HD12 | 7:As:242:TYR:CD2 | 2.47 | 0.43 |
| 7:At:187:TRP:CE2 | 5:BH:295:ARG:HD2 | 2.52 | 0.43 |
| 6:Au:190:LEU:HB3 | 6:Au:221:LEU:HB3 | 1.99 | 0.43 |
| 6:Aw:264:ARG:NH1 | 6:Aw:477:TYR:OH | 2.49 | 0.43 |
| 6:Az:202:ALA:HA | 6:Az:207:LYS:HE2 | 2.00 | 0.43 |
| 2:B1:256:PRO:HG2 | 2:B1:339:THR:HB | 2.00 | 0.43 |
| 2:B2:15:VAL:HG11 | 2:Bz:626:THR:HG21 | 2.00 | 0.43 |
| 2:B2:35:TRP:CE3 | 2:B2:230:LEU:HB3 | 2.53 | 0.43 |
| 2:B3:108:SER:O | 2:B3:177:GLY:HA2 | 2.18 | 0.43 |
| 2:B3:458:TYR:CE2 | 2:Bz:652:ASP:HB3 | 2.53 | 0.43 |
| 2:B5:284:ARG:HG2 | 2:B5:289:ILE:HD13 | 2.00 | 0.43 |
| 2:B6:406:LEU:HD13 | 2:B6:475:ALA:HB2 | 1.99 | 0.43 |
| 2:B6:643:VAL:HG21 | 2:B7:628:TYR:CZ | 2.53 | 0.43 |
| 2:B7:101:TYR:CZ | 2:B7:143:ILE:HG12 | 2.53 | 0.43 |
| 5:BF:502:ALA:O | 5:BF:506:GLU:HG2 | 2.18 | 0.43 |
| 11:BQ:18:ASP:HB3 | 11:BQ:21:LYS:HD3 | 1.99 | 0.43 |
| 3:BZ:14:ASP:N | 3:BZ:14:ASP:OD1 | 2.50 | 0.43 |
| 3:Bd:28:LEU:HD22 | 3:Bd:84:LYS:HB3 | 2.00 | 0.43 |
| 3:Bf:64:ARG:NH1 | 3:Bi:94:GLY:O | 2.50 | 0.43 |
| 2:Bp:355:LEU:HD12 | 2:Bp:389:VAL:HG21 | 2.00 | 0.43 |
| 2:Bs:283:VAL:HB | 2:Bs:291:GLN:HB3 | 2.00 | 0.43 |
| 2:Bu:137:ASP:OD1 | 2:Bu:137:ASP:N | 2.49 | 0.43 |
| 2:Bv:485:SER:OG | 2:Bv:486:GLN:N | 2.50 | 0.43 |
| 2:Bv:490:SER:O | 2:Bv:496:ARG:NH1 | 2.34 | 0.43 |
| 2:Bw:467:TRP:CH2 | 2:Bx:199:GLU:HB2 | 2.52 | 0.43 |
| 2:By:550:ARG:HB3 | 2:By:553:VAL:HG12 | 1.99 | 0.43 |
| 1:p:151:TRP:CZ2 | 8:u:59:ILE:HD12 | 2.51 | 0.43 |
| 8:u:72:LEU:HB3 | 8:u:73:PRO:CD | 2.48 | 0.43 |
| 8:u:163:ILE:HD13 | 8:u:163:ILE:H | 1.83 | 0.43 |
| 2:1:109:ASN:N | 2:1:138:GLY:HA3 | 2.33 | 0.43 |
| 2:2:126:GLU:HG2 | 2:2:146:PRO:HD2 | 1.99 | 0.43 |
| 2:4:211:GLN:OE1 | 2:4:329:ASN:ND2 | 2.39 | 0.43 |
| 2:5:454:TYR:CD2 | 2:5:467:TRP:HB3 | 2.53 | 0.43 |
| 5:A3:83:MET:HE3 | 5:A3:83:MET:HB3 | 1.90 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A5:72:HIS:CE1 | 6:A5:90:GLN:HG3 | 2.53 | 0.43 |
| 6:A5:176:ASP:OD1 | 6:A5:177:ILE:N | 2.44 | 0.43 |
| 6:A5:383:VAL:HG12 | 6:A5:406:THR:HG22 | 2.00 | 0.43 |
| 7:A6:55:LYS:HE2 | 7:A6:187:TRP:CH2 | 2.53 | 0.43 |
| 8:AB:242:ILE:HD12 | 8:AB:247:TRP:HB3 | 2.00 | 0.43 |
| 2:AD:411:ARG:HG3 | 2:AD:415:VAL:HG21 | 1.99 | 0.43 |
| 3:AJ:42:PRO:HD3 | 3:AJ:69:TRP:CD1 | 2.53 | 0.43 |
| 2:AK:365:ARG:HA | 2:AK:400:ARG:NH2 | 2.33 | 0.43 |
| 2:AL:637:TYR:HB2 | 2:Bv:622:GLU:HG2 | 2.00 | 0.43 |
| 2:AN:368:VAL:O | 2:AN:400:ARG:NH2 | 2.51 | 0.43 |
| 2:AO:46:ASN:OD1 | 2:AO:47:GLU:N | 2.51 | 0.43 |
| 2:AO:220:PRO:HG2 | 2:AO:338:LEU:HD11 | 2.00 | 0.43 |
| 2:AP:480:ARG:NH2 | 2:AP:498:GLN:O | 2.52 | 0.43 |
| 10:AT:330:PRO:HA | 10:AT:335:TYR:CE1 | 2.54 | 0.43 |
| 6:AV:346:ALA:HB1 | 6:AV:350:PHE:CE2 | 2.54 | 0.43 |
| 6:AV:476:ARG:NH2 | 6:AZ:230:THR:HG23 | 2.33 | 0.43 |
| 7:Aa:161:PHE:O | 5:Av:303:HIS:NE2 | 2.51 | 0.43 |
| 7:Aa:231:VAL:HG11 | 4:d:25:ILE:HG22 | 2.01 | 0.43 |
| 7:Ab:150:MET:SD | 5:BA:273:ILE:HD12 | 2.58 | 0.43 |
| 6:Ac:365:ALA:HB2 | 6:Ac:372:GLU:HA | 1.99 | 0.43 |
| 6:Aj:253:ARG:HH21 | 6:Aj:492:PRO:HG2 | 1.83 | 0.43 |
| 7:Ar:117:ILE:HG13 | 5:BH:255:HIS:CE1 | 2.54 | 0.43 |
| 7:Ar:217:GLU:HG3 | 7:Ar:224:HIS:CD2 | 2.53 | 0.43 |
| 5:Av:464:GLU:HB2 | 5:Ax:469:MET:HE1 | 2.00 | 0.43 |
| 5:Ax:501:GLU:OE1 | 5:BA:485:THR:OG1 | 2.22 | 0.43 |
| 6:Ay:449:TYR:CZ | 6:Ay:482:ASN:HB2 | 2.53 | 0.43 |
| 2:B3:538:ASP:HA | 2:B3:551:ILE:HD12 | 2.00 | 0.43 |
| 2:B4:211:GLN:HE22 | 2:B4:326:THR:HG21 | 1.83 | 0.43 |
| 2:B4:426:LEU:HD22 | 2:B4:522:ILE:HD13 | 2.00 | 0.43 |
| 2:B5:115:LYS:HD2 | 2:B5:115:LYS:HA | 1.82 | 0.43 |
| 2:B5:641:ASN:HB2 | 2:B6:626:THR:HA | 2.00 | 0.43 |
| 2:B6:47:GLU:O | 2:B6:51:VAL:HG23 | 2.18 | 0.43 |
| 2:B6:620:ARG:HB2 | 2:B6:622:GLU:HG3 | 2.00 | 0.43 |
| 2:B7:250:ALA:HB3 | 2:B7:263:SER:OG | 2.18 | 0.43 |
| 5:BA:256:ARG:O | 5:BA:372:ALA:HB1 | 2.18 | 0.43 |
| 7:BC:200:ASN:HA | 7:BC:229:ARG:HH22 | 1.82 | 0.43 |
| 7:BE:196:LYS:HD3 | 7:BE:226:LEU:HD11 | 2.00 | 0.43 |
| 5:BG:29:VAL:HG21 | 5:BG:198:ILE:HD12 | 2.01 | 0.43 |
| 5:BG:82:LEU:HD11 | 5:BG:261:ALA:HB3 | 2.00 | 0.43 |
| 6:BI:184:GLU:O | 6:BI:185:THR:OG1 | 2.29 | 0.43 |
| 3:BZ:128:GLU:HB3 | 3:BZ:130:LYS:HE2 | 1.99 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bg:63:ASP:CG | 3:Bk:147:ASN:HB3 | 2.43 | 0.43 |
| 3:Bh:25:ILE:C | 3:Bh:27:TYR:H | 2.25 | 0.43 |
| 3:Bi:118:ARG:HG3 | 3:Bk:101:GLY:HA3 | 2.00 | 0.43 |
| 3:Bj:58:ILE:H | 3:Bj:58:ILE:HD13 | 1.83 | 0.43 |
| 3:Bj:136:ASN:O | 3:Bj:136:ASN:ND2 | 2.51 | 0.43 |
| 3:Bl:40:ALA:O | 3:Bl:69:TRP:NE1 | 2.45 | 0.43 |
| 2:Bp:222:VAL:HG21 | 2:Bp:238:ILE:HD11 | 1.99 | 0.43 |
| 2:Bp:277:SER:O | 2:Bp:297:THR:OG1 | 2.35 | 0.43 |
| 2:Bp:480:ARG:O | 2:Bp:482:ASP:N | 2.50 | 0.43 |
| 2:Bp:480:ARG:O | 2:Bp:484:VAL:HG12 | 2.19 | 0.43 |
| 2:Bt:137:ASP:OD1 | 2:Bt:137:ASP:N | 2.52 | 0.43 |
| 2:Bt:637:TYR:HB3 | 2:Bw:3:LEU:HB2 | 1.99 | 0.43 |
| 2:Bu:100:GLU:HB3 | 2:Bu:188:ILE:HD11 | 2.01 | 0.43 |
| 2:Bu:346:SER:O | 2:Bu:350:VAL:HG23 | 2.19 | 0.43 |
| 2:Bu:378:CYS:SG | 2:Bu:454:TYR:OH | 2.58 | 0.43 |
| 2:Bv:43:GLN:NE2 | 2:Bv:77:ASP:OD2 | 2.51 | 0.43 |
| 2:Bz:413:THR:OG1 | 2:Bz:425:ASN:HB3 | 2.18 | 0.43 |
| 1:k:147:PHE:HD1 | 1:k:172:GLY:O | 2.01 | 0.43 |
| 1:p:44:ASP:HB2 | 1:p:163:GLN:NE2 | 2.34 | 0.43 |
| 1:p:97:GLU:O | 1:p:113:GLU:HB3 | 2.18 | 0.43 |
| 9:z:87:MET:HB2 | 9:z:138:LEU:HD21 | 2.00 | 0.43 |
| 2:1:102:THR:N | 2:1:183:THR:O | 2.51 | 0.43 |
| 2:2:239:VAL:HG21 | 2:2:265:ALA:HB2 | 2.00 | 0.43 |
| 2:4:498:GLN:HB3 | 2:4:534:VAL:HG12 | 1.99 | 0.43 |
| 2:4:564:ILE:HD11 | 8:t:216:PHE:CZ | 2.53 | 0.43 |
| 3:6:118:ARG:NH1 | 9:AC:64:VAL:HG13 | 2.33 | 0.43 |
| 3:8:46:VAL:HG22 | 3:8:64:ARG:HD2 | 2.01 | 0.43 |
| 5:A0:328:MET:SD | 5:BG:282:ARG:NH1 | 2.91 | 0.43 |
| 5:A0:379:ARG:NH2 | 5:A0:400:GLU:OE1 | 2.51 | 0.43 |
| 5:A1:254:LEU:O | 5:A1:258:VAL:HG23 | 2.18 | 0.43 |
| 5:A3:166:ARG:NH2 | 5:BF:26:GLU:OE1 | 2.51 | 0.43 |
| 6:A5:93:PRO:HB3 | 6:AW:121:THR:O | 2.19 | 0.43 |
| 6:A7:237:GLU:N | 6:A7:245:ASN:O | 2.50 | 0.43 |
| 6:A8:273:GLU:OE2 | 5:Av:324:GLN:NE2 | 2.51 | 0.43 |
| 6:A9:253:ARG:NH2 | 6:A9:495:ARG:HG2 | 2.33 | 0.43 |
| 3:AE:103:LYS:O | 3:AE:106:GLU:HG2 | 2.18 | 0.43 |
| 3:AF:4:ASP:OD1 | 3:o:97:ASN:ND2 | 2.46 | 0.43 |
| 3:AG:117:ALA:HB3 | 3:AG:122:THR:HB | 2.00 | 0.43 |
| 2:AL:89:ALA:HA | 2:AL:344:LEU:HB3 | 2.00 | 0.43 |
| 2:AM:455:LYS:HB3 | 2:AM:470:LEU:HD13 | 2.00 | 0.43 |
| 2:AN:494:TYR:CE1 | 2:B2:569:LYS:HG3 | 2.52 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AN:639:THR:HG23 | 2:AO:11:LYS:HD3 | 2.00 | 0.43 |
| 2:AO:310:TYR:CE2 | 2:AO:312:ASP:HB2 | 2.52 | 0.43 |
| 2:AP:160:TYR:HA | 2:AP:161:PRO:HA | 1.86 | 0.43 |
| 6:AV:79:ILE:HD11 | 6:AZ:260:GLU:HG3 | 2.01 | 0.43 |
| 6:AV:485:ALA:C | 6:AV:487:SER:H | 2.27 | 0.43 |
| 7:AY:12:LEU:HD12 | 7:AY:242:TYR:CD2 | 2.52 | 0.43 |
| 6:AZ:135:PRO:HG3 | 6:Am:67:GLU:HG2 | 2.01 | 0.43 |
| 7:Ab:80:ASN:HD21 | 7:Ab:222:PRO:HG2 | 1.83 | 0.43 |
| 7:Al:92:ILE:H | 7:Al:92:ILE:HD12 | 1.84 | 0.43 |
| 7:Al:264:ALA:HA | 7:Al:267:GLN:HB2 | 1.99 | 0.43 |
| 6:Am:71:ASP:HB2 | 6:Au:230:THR:HB | 2.00 | 0.43 |
| 7:Ar:80:ASN:OD1 | 7:Ar:80:ASN:N | 2.51 | 0.43 |
| 7:Ar:98:MET:HE2 | 7:Ar:148:MET:HG3 | 2.00 | 0.43 |
| 7:As:53:LEU:HD12 | 7:As:53:LEU:HA | 1.88 | 0.43 |
| 5:Av:292:MET:O | 5:Av:294:ALA:N | 2.44 | 0.43 |
| 6:Ay:257:GLN:HG2 | 6:Ay:499:GLY:HA2 | 1.99 | 0.43 |
| 6:Az:346:ALA:HA | 6:Az:349:SER:HB3 | 2.01 | 0.43 |
| 2:B1:29:LEU:HD13 | 2:B1:374:ILE:HB | 2.01 | 0.43 |
| 2:B2:220:PRO:HG2 | 2:B2:338:LEU:HD11 | 1.99 | 0.43 |
| 2:B3:101:TYR:CE2 | 2:B3:143:ILE:HG12 | 2.53 | 0.43 |
| 2:B4:195:LEU:HD12 | 2:B4:201:ALA:HB1 | 1.99 | 0.43 |
| 2:B4:614:THR:O | 2:B4:616:SER:N | 2.47 | 0.43 |
| 2:B7:481:THR:HG23 | 2:B7:496:ARG:HD3 | 2.00 | 0.43 |
| 2:B7:596:LYS:HG2 | 2:B7:601:ILE:O | 2.18 | 0.43 |
| 5:BA:21:LYS:NZ | 5:BA:22:ASP:OD1 | 2.36 | 0.43 |
| 7:BC:306:ILE:HD11 | 5:BH:345:THR:HG21 | 2.00 | 0.43 |
| 6:BK:318:LYS:O | 6:BK:329:ALA:HA | 2.19 | 0.43 |
| 3:BX:80:ASP:O | 3:BX:84:LYS:HG3 | 2.18 | 0.43 |
| 3:Bb:1:MET:HE3 | 3:Bb:1:MET:HB2 | 1.82 | 0.43 |
| 3:Bi:137:VAL:HG23 | 3:Bi:155:VAL:HG22 | 2.00 | 0.43 |
| 2:Bp:24:THR:O | 2:Bp:483:ASN:ND2 | 2.40 | 0.43 |
| 2:Bq:164:GLY:H | 2:Bq:167:TRP:CD1 | 2.36 | 0.43 |
| 2:Bq:571:ARG:HA | 2:Bq:571:ARG:HD3 | 1.88 | 0.43 |
| 2:Bq:637:TYR:HB2 | 2:Br:622:GLU:HG2 | 1.99 | 0.43 |
| 2:Bs:110:TYR:H | 2:Bs:138:GLY:HA3 | 1.83 | 0.43 |
| 2:Bs:383:LEU:HD11 | 2:Bs:436:TYR:CE2 | 2.53 | 0.43 |
| 2:Bt:39:PHE:HE1 | 2:Bt:86:ARG:HD2 | 1.84 | 0.43 |
| 2:Bt:464:VAL:HG12 | 2:Bu:313:ASP:HB3 | 2.00 | 0.43 |
| 2:Bt:510:ARG:HG2 | 2:Bt:511:GLN:H | 1.83 | 0.43 |
| 2:Bu:57:PRO:HB3 | 2:Bu:62:ALA:HA | 2.01 | 0.43 |
| 2:Bv:32:LYS:HG2 | 2:Bv:350:VAL:HG21 | 2.00 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bw:29:LEU:O | 2:Bw:80:VAL:HA | 2.18 | 0.43 |
| 2:Bw:49:ASP:OD1 | 2:Bw:49:ASP:N | 2.50 | 0.43 |
| 2:Bx:540:THR:HG22 | 2:Bx:551:ILE:HG23 | 2.00 | 0.43 |
| 2:By:205:MET:HE1 | 2:By:221:GLY:O | 2.17 | 0.43 |
| 2:By:455:LYS:HB2 | 2:By:470:LEU:HD13 | 1.99 | 0.43 |
| 4:O:9:PRO:HD3 | 4:O:57:VAL:HG21 | 1.99 | 0.43 |
| 1:l:87:ALA:HB2 | 1:m:26:ILE:HG23 | 1.99 | 0.43 |
| 1:n:231:TYR:CZ | 8:u:12:ARG:HD2 | 2.53 | 0.43 |
| 8:r:75:ILE:HG12 | 8:r:122:ILE:HG12 | 2.00 | 0.43 |
| 2:2:117:THR:HG23 | 2:2:127:THR:HG22 | 2.00 | 0.43 |
| 3:7:41:LEU:HD12 | 3:7:41:LEU:HA | 1.81 | 0.43 |
| 5:A0:306:ASN:CG | 5:A0:310:ASN:HD21 | 2.26 | 0.43 |
| 5:A1:371:MET:HG2 | 5:BD:90:ASN:ND2 | 2.33 | 0.43 |
| 5:A2:26:GLU:HG3 | 5:A2:28:LEU:HD13 | 2.00 | 0.43 |
| 5:A2:411:GLN:O | 5:A2:415:GLU:HG3 | 2.18 | 0.43 |
| 5:A3:396:ILE:HG21 | 5:A3:401:LEU:HG | 1.99 | 0.43 |
| 7:A6:30:THR:HA | 1:p:8:LEU:O | 2.19 | 0.43 |
| 3:AA:47:GLU:HG2 | 3:AH:148:ASN:ND2 | 2.34 | 0.43 |
| 8:AB:229:VAL:HG13 | 2:AD:547:PRO:HG2 | 2.00 | 0.43 |
| 2:AK:164:GLY:H | 2:AK:167:TRP:HD1 | 1.66 | 0.43 |
| 2:AN:103:ILE:HD13 | 2:AN:182:ILE:HG22 | 1.99 | 0.43 |
| 6:AV:149:GLY:H | 6:AV:186:GLY:CA | 2.31 | 0.43 |
| 6:AX:365:ALA:HB2 | 6:AX:372:GLU:HA | 2.00 | 0.43 |
| 7:Aa:137:ASP:O | 7:Aa:139:GLY:N | 2.52 | 0.43 |
| 7:Aa:262:ILE:HA | 7:Ab:25:ILE:HD13 | 2.00 | 0.43 |
| 6:Ac:426:ASP:OD2 | 6:Ac:433:TYR:OH | 2.30 | 0.43 |
| 6:Ag:100:ARG:HB3 | 6:Ak:127:LEU:HB3 | 2.01 | 0.43 |
| 6:Ag:265:GLN:HA | 6:Ag:473:PHE:O | 2.19 | 0.43 |
| 6:Aj:304:ARG:HD2 | 6:Aj:304:ARG:HA | 1.92 | 0.43 |
| 6:Ao:466:ASN:OD1 | 6:Ao:466:ASN:N | 2.51 | 0.43 |
| 6:Ap:180:HIS:NE2 | 6:Ap:209:ASP:OD1 | 2.41 | 0.43 |
| 7:Aq:121:MET:HE1 | 7:Aq:129:TYR:CE1 | 2.52 | 0.43 |
| 6:Aw:259:ILE:HG12 | 6:Aw:260:GLU:H | 1.82 | 0.43 |
| 6:Az:120:PRO:HD3 | 6:Az:453:TYR:CZ | 2.53 | 0.43 |
| 2:B1:478:CYS:O | 2:B1:555:ARG:NH1 | 2.51 | 0.43 |
| 2:B2:391:LYS:HG2 | 2:B2:443:ILE:HD13 | 2.00 | 0.43 |
| 2:B3:412:GLU:OE1 | 2:B3:412:GLU:N | 2.49 | 0.43 |
| 2:B4:536:TYR:HD1 | 2:B4:536:TYR:HA | 1.76 | 0.43 |
| 2:B5:108:SER:O | 2:B5:177:GLY:HA2 | 2.18 | 0.43 |
| 2:B6:57:PRO:HG3 | 2:B6:65:PHE:HB3 | 2.00 | 0.43 |
| 2:B6:163:LEU:HD11 | 2:B6:187:ILE:HG12 | 2.00 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B7:346:SER:O | 2:B7:350:VAL:HG23 | 2.19 | 0.43 |
| 5:BB:289:THR:HB | 5:BB:292:MET:HE2 | 2.00 | 0.43 |
| 5:BG:121:LYS:O | 5:BG:125:MET:HG3 | 2.19 | 0.43 |
| 5:BG:275:ARG:CZ | 5:BG:355:ASN:HB2 | 2.48 | 0.43 |
| 5:BH:411:GLN:O | 5:BH:415:GLU:HG3 | 2.18 | 0.43 |
| 5:BH:423:LYS:HB2 | 5:BH:437:TRP:CE2 | 2.53 | 0.43 |
| 6:BK:181:PHE:CD1 | 6:BK:187:THR:HB | 2.50 | 0.43 |
| 6:BK:374:ASN:OD1 | 6:BK:374:ASN:N | 2.47 | 0.43 |
| 11:BR:10:ILE:HD11 | 11:BR:35:TYR:HE1 | 1.84 | 0.43 |
| 3:Ba:60:VAL:HG22 | 3:Ba:61:ALA:H | 1.84 | 0.43 |
| 3:Bd:83:GLN:HA | 3:Bd:86:VAL:HG22 | 2.00 | 0.43 |
| 3:Bk:4:ASP:OD1 | 3:Bk:4:ASP:N | 2.48 | 0.43 |
| 3:Bn:17:ARG:HG3 | 3:Bn:20:LEU:HD12 | 2.00 | 0.43 |
| 2:Bp:463:ASP:HB3 | 2:Bq:308:ASN:HB2 | 1.99 | 0.43 |
| 2:Bs:567:SER:O | 2:Bs:571:ARG:HG2 | 2.18 | 0.43 |
| 2:Bt:242:ALA:O | 2:Bt:246:LYS:HG3 | 2.18 | 0.43 |
| 2:Bt:478:CYS:O | 2:Bt:555:ARG:NH1 | 2.44 | 0.43 |
| 2:Bw:37:PRO:HG3 | 2:Bw:226:TYR:CZ | 2.54 | 0.43 |
| 2:Bw:550:ARG:HA | 2:Bw:550:ARG:HE | 1.83 | 0.43 |
| 2:By:202:GLU:H | 2:By:202:GLU:HG3 | 1.69 | 0.43 |
| 2:Bz:195:LEU:HD23 | 2:Bz:195:LEU:H | 1.83 | 0.43 |
| 1:k:156:ASP:HB3 | 1:k:157:PRO:HD3 | 2.00 | 0.43 |
| 1:p:239:ASN:OD1 | 1:p:239:ASN:N | 2.51 | 0.43 |
| 8:r:62:GLN:HB3 | 8:r:63:GLU:H | 1.55 | 0.43 |
| 8:r:116:MET:HG2 | 8:r:194:VAL:O | 2.19 | 0.43 |
| 8:s:99:GLN:HB3 | 8:s:243:ASP:HB3 | 1.99 | 0.43 |
| 9:x:46:VAL:HG13 | 9:y:134:TRP:HZ2 | 1.84 | 0.43 |
| 2:2:556:LEU:HD23 | 2:2:560:LEU:HD13 | 2.01 | 0.43 |
| 2:4:229:GLU:N | 2:4:345:SER:OG | 2.52 | 0.43 |
| 2:5:635:ILE:HG22 | 2:AM:572:LEU:HA | 2.01 | 0.43 |
| 5:A2:197:LYS:NZ | 5:BF:215:TYR:OH | 2.41 | 0.43 |
| 5:A3:376:PRO:HD3 | 5:A3:403:PHE:CD1 | 2.53 | 0.43 |
| 5:A3:398:ARG:HA | 5:A3:398:ARG:HD2 | 1.71 | 0.43 |
| 5:A3:470:LEU:HD22 | 5:A3:491:LEU:HD21 | 2.01 | 0.43 |
| 5:A3:503:LYS:HD2 | 5:A3:503:LYS:HA | 1.77 | 0.43 |
| 6:A4:486:GLU:HA | 6:A4:509:LYS:O | 2.18 | 0.43 |
| 7:A6:101:ASN:OD1 | 7:A6:106:TRP:N | 2.50 | 0.43 |
| 6:A8:99:VAL:HG22 | 6:A9:444:MET:HB3 | 2.01 | 0.43 |
| 6:A8:328:LYS:HB2 | 6:A8:331:VAL:HG13 | 2.00 | 0.43 |
| 3:AA:21:PHE:CD1 | 3:o:142:LEU:HB3 | 2.54 | 0.43 |
| 9:AC:22:PRO:HB2 | 2:AD:571:ARG:NH1 | 2.34 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:594:GLY:HA2 | 3:o:8:ARG:HD3 | 2.00 | 0.43 |
| 2:AK:641:ASN:HB2 | 2:Bs:626:THR:HG22 | 2.00 | 0.43 |
| 2:AL:46:ASN:OD1 | 2:AL:47:GLU:N | 2.51 | 0.43 |
| 2:AM:515:ASP:OD1 | 2:AN:5:SER:N | 2.51 | 0.43 |
| 2:AN:223:VAL:O | 2:AN:324:PHE:N | 2.48 | 0.43 |
| 2:AN:654:LEU:HD23 | 2:AN:655:THR:H | 1.84 | 0.43 |
| 2:AO:480:ARG:C | 2:AO:482:ASP:H | 2.27 | 0.43 |
| 6:AV:108:ALA:HB1 | 6:AV:306:VAL:HB | 2.00 | 0.43 |
| 6:AV:263:SER:O | 6:AZ:228:MET:N | 2.52 | 0.43 |
| 6:AV:502:SER:O | 6:AV:506:SER:OG | 2.34 | 0.43 |
| 6:AZ:191:GLN:HB2 | 6:AZ:224:ILE:HG21 | 2.00 | 0.43 |
| 6:AZ:358:ASP:O | 6:AZ:362:VAL:HG23 | 2.19 | 0.43 |
| 6:Af:385:VAL:HG21 | 6:Af:521:ILE:HD12 | 1.99 | 0.43 |
| 6:Aj:343:ALA:HB1 | 6:Aj:348:GLU:HG3 | 2.01 | 0.43 |
| 7:Al:55:LYS:HD3 | 7:Al:187:TRP:CZ2 | 2.54 | 0.43 |
| 6:An:131:TYR:CE1 | 6:An:141:LYS:HB2 | 2.48 | 0.43 |
| 7:Aq:162:TRP:CD1 | 7:As:55:LYS:H | 2.36 | 0.43 |
| 2:B1:47:GLU:OE1 | 2:B1:461:TYR:OH | 2.36 | 0.43 |
| 2:B2:241:LYS:HD3 | 2:B2:273:PRO:HB2 | 2.00 | 0.43 |
| 2:B3:100:GLU:HG3 | 2:B3:185:GLY:HA3 | 2.00 | 0.43 |
| 2:B6:46:ASN:OD1 | 2:B6:47:GLU:N | 2.51 | 0.43 |
| 2:B6:373:PHE:HB2 | 2:B6:405:VAL:HG22 | 2.00 | 0.43 |
| 2:B7:557:PHE:CZ | 2:B7:629:ILE:HD11 | 2.54 | 0.43 |
| 7:BE:134:PHE:O | 5:BG:265:LYS:NZ | 2.41 | 0.43 |
| 7:BE:189:LYS:O | 7:BE:222:PRO:HG3 | 2.18 | 0.43 |
| 5:BF:423:LYS:HB2 | 5:BF:437:TRP:CE2 | 2.54 | 0.43 |
| 6:BJ:286:ALA:N | 6:BJ:289:GLU:OE1 | 2.52 | 0.43 |
| 6:BM:223:GLU:CD | 6:BM:223:GLU:H | 2.26 | 0.43 |
| 11:BW:9:ASN:HB3 | 11:BW:56:TYR:CE2 | 2.52 | 0.43 |
| 3:BX:24:GLU:HB2 | 3:BX:114:ARG:HH12 | 1.83 | 0.43 |
| 3:BX:93:ALA:HB3 | 3:Bm:64:ARG:NH2 | 2.33 | 0.43 |
| 3:Bb:17:ARG:C | 3:Be:151:GLN:HG3 | 2.44 | 0.43 |
| 3:Bc:23:VAL:HG22 | 3:Bc:36:CYS:SG | 2.58 | 0.43 |
| 3:Bj:23:VAL:HG11 | 3:Bj:39:THR:HG21 | 2.00 | 0.43 |
| 2:Bq:57:PRO:HA | 2:Bq:61:THR:HB | 2.00 | 0.43 |
| 2:Bq:332:GLU:OE1 | 2:Bq:332:GLU:N | 2.50 | 0.43 |
| 2:Br:195:LEU:H | 2:Br:195:LEU:HD23 | 1.84 | 0.43 |
| 2:Br:295:LEU:HB3 | 2:Br:311:ILE:HG12 | 2.01 | 0.43 |
| 2:Bs:57:PRO:HB3 | 2:Bs:62:ALA:HA | 2.01 | 0.43 |
| 2:Bt:49:ASP:OD1 | 2:Bt:49:ASP:N | 2.50 | 0.43 |
| 2:Bv:77:ASP:OD1 | 2:Bv:78:LEU:N | 2.51 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bv:264:THR:HG22 | 2:Bv:267:ALA:HB3 | 2.01 | 0.43 |
| 2:Bw:642:PHE:CE1 | 2:Bx:561:LYS:HG2 | 2.54 | 0.43 |
| 1:k:159:TYR:HD2 | 1:k:162:GLY:HA2 | 1.83 | 0.43 |
| 1:n:221:VAL:HG13 | 8:u:22:SER:HB2 | 2.01 | 0.43 |
| 2:2:281:ILE:HD12 | 2:2:295:LEU:HD12 | 2.01 | 0.43 |
| 2:3:556:LEU:HD23 | 2:3:560:LEU:HD13 | 2.00 | 0.43 |
| 2:4:101:TYR:CG | 2:4:143:ILE:HD11 | 2.54 | 0.43 |
| 2:4:362:PHE:HD1 | 2:4:368:VAL:HG21 | 1.83 | 0.43 |
| 3:7:17:ARG:O | 3:8:151:GLN:NE2 | 2.50 | 0.43 |
| 5:A2:10:ALA:HB3 | 5:A2:11:PRO:HD3 | 2.00 | 0.43 |
| 5:A2:167:PRO:HB2 | 5:A2:428:LEU:HD12 | 2.01 | 0.43 |
| 6:A5:379:SER:HB2 | 6:A5:380:ARG:NH1 | 2.34 | 0.43 |
| 6:A5:502:SER:H | 6:A5:505:ASN:HB2 | 1.84 | 0.43 |
| 7:A6:23:PRO:HD2 | 7:Al:33:GLN:NE2 | 2.34 | 0.43 |
| 7:A6:301:ASP:OD1 | 7:A6:301:ASP:N | 2.46 | 0.43 |
| 6:A7:258:VAL:HG11 | 6:AW:80:ALA:HB2 | 2.01 | 0.43 |
| 3:AA:62:GLY:O | 3:AG:118:ARG:NH2 | 2.52 | 0.43 |
| 2:AD:413:THR:C | 2:AD:417:ILE:HD11 | 2.44 | 0.43 |
| 3:AG:69:TRP:CE3 | 3:AG:132:LEU:HD21 | 2.54 | 0.43 |
| 3:AG:136:ASN:O | 3:AG:136:ASN:ND2 | 2.52 | 0.43 |
| 3:AI:82:ARG:O | 3:AI:86:VAL:HG13 | 2.18 | 0.43 |
| 2:AK:412:GLU:HA | 2:AK:415:VAL:HG12 | 2.00 | 0.43 |
| 2:AL:162:THR:O | 2:AL:186:LYS:HB3 | 2.19 | 0.43 |
| 2:AN:653:GLU:H | 2:AN:653:GLU:HG2 | 1.68 | 0.43 |
| 2:AP:514:ARG:NH1 | 2:Bp:364:ASP:OD2 | 2.46 | 0.43 |
| 10:AU:320:GLU:HG3 | 10:AU:376:PRO:O | 2.19 | 0.43 |
| 6:Ae:145:HIS:HD2 | 6:Ae:490:GLN:HG3 | 1.83 | 0.43 |
| 6:Af:96:MET:HB2 | 6:Aj:123:GLN:O | 2.19 | 0.43 |
| 6:Af:264:ARG:NH1 | 6:Af:477:TYR:HH | 2.16 | 0.43 |
| 6:Ai:377:ILE:HG23 | 6:Ai:435:THR:HB | 2.01 | 0.43 |
| 6:Ak:318:LYS:HE3 | 6:Ak:327:SER:OG | 2.19 | 0.43 |
| 6:An:107:ILE:O | 6:An:303:ASN:ND2 | 2.44 | 0.43 |
| 6:An:265:GLN:NE2 | 6:BK:236:GLN:HG3 | 2.34 | 0.43 |
| 6:Ap:133:LYS:NZ | 6:Ap:249:GLU:OE2 | 2.51 | 0.43 |
| 7:Ar:250:TYR:OH | 7:Ar:294:ARG:NH2 | 2.49 | 0.43 |
| 7:At:271:LEU:N | 7:At:275:VAL:O | 2.50 | 0.43 |
| 6:Au:290:LEU:HG | 6:Ay:252:PHE:HE1 | 1.83 | 0.43 |
| 6:Ay:494:SER:HA | 11:BO:37:ASP:CG | 2.44 | 0.43 |
| 2:B2:236:ILE:HD11 | 2:B2:323:ILE:HG21 | 2.00 | 0.43 |
| 2:B2:455:LYS:HD3 | 2:B2:502:VAL:HG13 | 2.01 | 0.43 |
| 2:B3:432:ALA:HB1 | 2:B3:440:ASN:HD22 | 1.84 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B6:171:ILE:H | 2:B6:171:ILE:HG12 | 1.56 | 0.43 |
| 2:B7:110:TYR:CE2 | 2:B7:177:GLY:HA3 | 2.53 | 0.43 |
| 2:B7:237:GLU:OE1 | 2:B7:284:ARG:NH2 | 2.41 | 0.43 |
| 5:BB:182:VAL:HG22 | 5:BB:208:TYR:HD1 | 1.82 | 0.43 |
| 5:BB:212:HIS:ND1 | 5:BB:212:HIS:O | 2.51 | 0.43 |
| 5:BH:398:ARG:HD2 | 5:BH:398:ARG:HA | 1.78 | 0.43 |
| 6:BJ:287:ASP:OD2 | 6:BJ:460:ARG:NH2 | 2.52 | 0.43 |
| 6:BJ:348:GLU:HB3 | 6:BJ:396:ALA:HB1 | 2.01 | 0.43 |
| 6:BK:487:SER:OG | 6:BK:488:ALA:N | 2.49 | 0.43 |
| 7:BL:127:ARG:HD3 | 6:BM:444:MET:HG2 | 2.00 | 0.43 |
| 11:BP:8:VAL:HG11 | 11:BP:35:TYR:CE2 | 2.53 | 0.43 |
| 11:BW:27:GLU:O | 11:BW:58:THR:OG1 | 2.36 | 0.43 |
| 3:Be:41:LEU:HB3 | 3:Bh:140:LEU:HB3 | 2.00 | 0.43 |
| 3:Bi:41:LEU:H | 3:Bi:41:LEU:HD12 | 1.84 | 0.43 |
| 3:Bi:46:VAL:HG22 | 3:Bi:64:ARG:HB2 | 2.00 | 0.43 |
| 2:Bs:44:VAL:HG11 | 2:Bs:50:LEU:HB2 | 2.00 | 0.43 |
| 2:Bu:130:LYS:HG3 | 2:Bu:144:ASN:HB3 | 1.99 | 0.43 |
| 2:Bu:387:SER:HB3 | 2:Bu:391:LYS:NZ | 2.34 | 0.43 |
| 2:Bv:159:GLU:HB3 | 2:Bv:163:LEU:HA | 2.00 | 0.43 |
| 2:Bv:406:LEU:HD13 | 2:Bv:475:ALA:HB2 | 1.99 | 0.43 |
| 2:Bx:315:PHE:HB3 | 2:Bx:324:PHE:CD1 | 2.54 | 0.43 |
| 4:J:44:MET:HE1 | 4:K:44:MET:HG2 | 1.99 | 0.43 |
| 4:S:8:LEU:O | 4:S:19:GLN:NE2 | 2.52 | 0.43 |
| 1:l:176:TYR:CD1 | 8:s:71:ILE:HG23 | 2.53 | 0.43 |
| 1:m:224:ILE:HG13 | 1:n:71:ILE:HD12 | 2.00 | 0.43 |
| 1:m:243:LYS:N | 8:s:4:TYR:H | 2.16 | 0.43 |
| 3:o:24:GLU:CD | 3:o:114:ARG:HH12 | 2.27 | 0.43 |
| 1:p:11:LYS:HE2 | 1:p:11:LYS:HB3 | 1.92 | 0.43 |
| 8:q:232:SER:OG | 8:q:271:ARG:NH1 | 2.52 | 0.43 |
| 2:4:33:PHE:HA | 2:4:61:THR:HG21 | 2.01 | 0.43 |
| 2:4:110:TYR:CZ | 2:4:177:GLY:HA2 | 2.54 | 0.43 |
| 2:4:233:LYS:HE2 | 2:4:233:LYS:HB3 | 1.90 | 0.43 |
| 2:4:654:LEU:HD22 | 2:5:17:SER:HB3 | 2.01 | 0.43 |
| 2:5:96:ALA:HA | 2:5:188:ILE:HB | 2.00 | 0.43 |
| 2:5:614:THR:C | 2:5:616:SER:H | 2.26 | 0.43 |
| 3:6:10:PHE:O | 3:6:11:GLU:HB2 | 2.18 | 0.43 |
| 3:8:20:LEU:HD21 | 9:v:56:LEU:HD21 | 2.01 | 0.43 |
| 5:A0:19:ASN:O | 5:A0:23:GLN:HG2 | 2.18 | 0.43 |
| 5:A0:134:LEU:O | 5:A0:137:LEU:C | 2.61 | 0.43 |
| 5:A0:228:ILE:HG12 | 5:BG:196:THR:HG21 | 2.00 | 0.43 |
| 5:A1:186:ARG:HB2 | 5:A1:204:GLU:OE1 | 2.19 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A2:227:LYS:H | 5:A2:227:LYS:HG2 | 1.56 | 0.43 |
| 5:A3:49:GLU:O | 5:A3:52:SER:OG | 2.33 | 0.43 |
| 5:A3:501:GLU:O | 5:BF:482:SER:OG | 2.37 | 0.43 |
| 6:A7:93:PRO:HB2 | 6:A8:123:GLN:HB3 | 2.00 | 0.43 |
| 6:A8:344:ARG:HD2 | 6:A9:344:ARG:NH1 | 2.34 | 0.43 |
| 6:A9:350:PHE:HD2 | 6:A9:389:VAL:HG13 | 1.83 | 0.43 |
| 3:AG:25:ILE:HG23 | 3:AG:111:ALA:HB2 | 1.99 | 0.43 |
| 2:AK:31:GLY:O | 2:AK:82:ARG:HA | 2.18 | 0.43 |
| 2:AL:400:ARG:HD3 | 2:AL:403:CYS:SG | 2.59 | 0.43 |
| 2:AM:94:PRO:HD3 | 2:AM:340:LEU:HD22 | 2.01 | 0.43 |
| 2:AM:101:TYR:CZ | 2:AM:143:ILE:HG12 | 2.54 | 0.43 |
| 2:AO:284:ARG:HE | 2:AO:289:ILE:HD13 | 1.82 | 0.43 |
| 2:AO:510:ARG:HG2 | 2:AO:511:GLN:H | 1.83 | 0.43 |
| 2:AP:51:VAL:HG22 | 2:AP:65:PHE:HZ | 1.83 | 0.43 |
| 2:AP:536:TYR:HD1 | 2:AP:536:TYR:HA | 1.69 | 0.43 |
| 10:AT:324:ASP:OD1 | 10:AT:324:ASP:N | 2.51 | 0.43 |
| 6:AV:343:ALA:HB1 | 6:AV:348:GLU:HB2 | 2.01 | 0.43 |
| 6:AV:486:GLU:HG3 | 6:AV:509:LYS:HB3 | 2.00 | 0.43 |
| 7:AY:120:GLY:HA3 | 5:BD:78:THR:HG23 | 2.01 | 0.43 |
| 6:Ad:250:MET:HE2 | 6:Ad:250:MET:HB3 | 1.91 | 0.43 |
| 6:Ad:261:ALA:HA | 6:Ad:478:GLY:HA3 | 2.00 | 0.43 |
| 6:Ad:346:ALA:HA | 6:Ad:349:SER:HB3 | 2.00 | 0.43 |
| 6:Ae:151:ASP:HB3 | 6:Ae:154:PHE:HB2 | 2.01 | 0.43 |
| 6:Aj:278:LEU:HD23 | 6:Aj:286:ALA:HB2 | 2.00 | 0.43 |
| 7:Al:92:ILE:HD11 | 6:Ap:465:LYS:HA | 1.99 | 0.43 |
| 7:Al:96:THR:HA | 7:Al:106:TRP:CZ3 | 2.53 | 0.43 |
| 7:Al:306:ILE:HB | 5:BG:308:MET:HG3 | 2.00 | 0.43 |
| 6:An:332:PHE:HB3 | 6:An:518:VAL:HG12 | 2.00 | 0.43 |
| 6:An:356:GLN:O | 6:An:360:GLU:HG2 | 2.19 | 0.43 |
| 6:Ao:459:LEU:HB3 | 6:BK:467:PHE:CD2 | 2.53 | 0.43 |
| 6:Aw:381:ASN:HB3 | 6:Aw:521:ILE:HD13 | 2.01 | 0.43 |
| 6:Aw:383:VAL:HG12 | 6:Aw:406:THR:HG22 | 1.99 | 0.43 |
| 5:Ax:338:ARG:HG2 | 5:Ax:343:ALA:HA | 2.00 | 0.43 |
| 6:Ay:261:ALA:HA | 6:Ay:478:GLY:HA3 | 2.00 | 0.43 |
| 6:Ay:310:ILE:HG12 | 6:Ay:448:ILE:HG21 | 2.01 | 0.43 |
| 2:B3:31:GLY:O | 2:B3:82:ARG:HA | 2.19 | 0.43 |
| 2:B3:109:ASN:N | 2:B3:138:GLY:HA3 | 2.34 | 0.43 |
| 2:B3:429:TRP:CZ2 | 2:B3:441:PHE:HB2 | 2.54 | 0.43 |
| 2:B4:240:SER:OG | 2:B4:243:ASP:OD1 | 2.37 | 0.43 |
| 2:B6:3:LEU:HD11 | 2:B6:9:GLU:HB2 | 2.00 | 0.43 |
| 2:B7:2:THR:OG1 | 2:B7:3:LEU:N | 2.42 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BF:367:GLN:HA | 5:BF:377:LEU:HD11 | 2.01 | 0.43 |
| 6:BJ:445:ASP:N | 6:BJ:445:ASP:OD1 | 2.49 | 0.43 |
| 7:BL:263:LEU:HD13 | 7:BL:277:ILE:HG21 | 1.99 | 0.43 |
| 3:Ba:24:GLU:OE1 | 3:Ba:33:THR:OG1 | 2.36 | 0.43 |
| 3:Bb:23:VAL:HG22 | 3:Bb:36:CYS:SG | 2.58 | 0.43 |
| 3:Bf:2:PHE:HB3 | 3:Bk:97:ASN:HB3 | 2.01 | 0.43 |
| 3:Bj:143:ASP:OD2 | 3:Bj:145:ASP:HB2 | 2.19 | 0.43 |
| 2:Bq:108:SER:O | 2:Bq:177:GLY:HA2 | 2.18 | 0.43 |
| 2:Bq:458:TYR:HE1 | 2:Bq:460:LYS:HA | 1.83 | 0.43 |
| 2:Bs:256:PRO:HG2 | 2:Bs:339:THR:H | 1.82 | 0.43 |
| 2:Bt:47:GLU:OE1 | 2:Bt:461:TYR:OH | 2.34 | 0.43 |
| 2:Bt:171:ILE:HG22 | 2:Bt:172:SER:H | 1.84 | 0.43 |
| 2:Bt:596:LYS:HG2 | 2:Bt:601:ILE:O | 2.19 | 0.43 |
| 2:Bw:389:VAL:O | 2:Bw:393:VAL:HG23 | 2.18 | 0.43 |
| 2:Bw:406:LEU:HD13 | 2:Bw:475:ALA:HB2 | 2.01 | 0.43 |
| 2:Bz:57:PRO:CB | 2:Bz:62:ALA:HA | 2.49 | 0.43 |
| 2:Bz:121:VAL:HG13 | 2:Bz:166:ASN:HB3 | 2.01 | 0.43 |
| 4:P:27:ASN:HB3 | 4:j:38:TYR:CE2 | 2.53 | 0.43 |
| 4:c:36:THR:OG1 | 4:c:39:GLY:N | 2.45 | 0.43 |
| 1:n:95:GLY:HA2 | 1:p:158:PHE:CD1 | 2.54 | 0.43 |
| 8:q:47:GLU:HB2 | 8:r:184:ARG:CZ | 2.49 | 0.43 |
| 9:y:37:VAL:HG22 | 9:y:73:VAL:HG13 | 2.01 | 0.43 |
| 2:1:143:ILE:HD12 | 2:1:145:ILE:HD11 | 2.00 | 0.43 |
| 2:1:297:THR:HG21 | 2:1:330:TRP:CG | 2.54 | 0.43 |
| 2:1:317:LYS:HE3 | 2:1:317:LYS:HB2 | 1.80 | 0.43 |
| 2:1:538:ASP:O | 2:1:550:ARG:HD3 | 2.18 | 0.43 |
| 2:3:31:GLY:HA3 | 2:3:64:TYR:CD1 | 2.54 | 0.43 |
| 2:5:372:LEU:HD21 | 2:5:475:ALA:O | 2.18 | 0.43 |
| 5:A3:125:MET:O | 5:A3:129:GLU:HG2 | 2.18 | 0.43 |
| 5:A3:293:PRO:O | 5:A3:295:ARG:N | 2.51 | 0.43 |
| 7:A6:43:GLU:O | 7:A6:47:GLU:HG2 | 2.19 | 0.43 |
| 6:A7:318:LYS:NZ | 6:A7:356:GLN:OE1 | 2.36 | 0.43 |
| 6:A8:432:ASP:HB3 | 6:A8:518:VAL:HG23 | 2.00 | 0.43 |
| 2:AD:574:GLU:HB3 | 2:AD:580:THR:HG21 | 2.01 | 0.43 |
| 3:AE:9:ALA:HB2 | 3:AF:34:PHE:HB2 | 2.01 | 0.43 |
| 3:AE:83:GLN:HA | 3:AE:86:VAL:HG22 | 2.00 | 0.43 |
| 3:AF:43:ALA:O | 3:AF:162:TRP:NE1 | 2.51 | 0.43 |
| 3:AG:85:PHE:HB3 | 3:AG:137:VAL:HG21 | 2.00 | 0.43 |
| 3:AJ:143:ASP:OD2 | 3:AJ:146:SER:N | 2.52 | 0.43 |
| 2:AK:121:VAL:HG22 | 2:AK:166:ASN:HB3 | 2.01 | 0.43 |
| 2:AK:456:TYR:CE1 | 2:AK:465:ASN:HB3 | 2.54 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AL:410:PRO:O | 2:AL:413:THR:HG22 | 2.19 | 0.43 |
| 2:AM:137:ASP:OD1 | 2:AM:137:ASP:N | 2.47 | 0.43 |
| 2:AM:147:THR:HG22 | 2:AM:150:ILE:HD12 | 2.01 | 0.43 |
| 2:AM:505:LEU:HD21 | 2:AM:525:VAL:HG12 | 2.00 | 0.43 |
| 2:AP:51:VAL:HG21 | 2:AP:461:TYR:OH | 2.19 | 0.43 |
| 2:AP:430:ARG:NH2 | 2:AP:443:ILE:O | 2.52 | 0.43 |
| 10:AS:309:TRP:HB3 | 10:AS:356:SER:HB3 | 2.01 | 0.43 |
| 6:AV:376:ILE:HG12 | 6:AV:436:VAL:HG22 | 1.99 | 0.43 |
| 6:AX:379:SER:OG | 6:AX:432:ASP:OD1 | 2.32 | 0.43 |
| 6:AZ:71:ASP:HB3 | 6:Ah:230:THR:HB | 2.01 | 0.43 |
| 6:Ag:131:TYR:HA | 6:Ag:250:MET:HA | 2.01 | 0.43 |
| 7:Al:88:LEU:HD13 | 7:Al:183:ILE:HG22 | 2.00 | 0.43 |
| 7:Al:305:GLY:HA2 | 5:BG:304:VAL:HG13 | 2.01 | 0.43 |
| 6:Am:356:GLN:O | 6:Am:360:GLU:HG2 | 2.18 | 0.43 |
| 7:Aq:18:ARG:HA | 7:Aq:22:ALA:HA | 2.00 | 0.43 |
| 7:Aq:110:PHE:HA | 7:Aq:115:ALA:HB3 | 2.01 | 0.43 |
| 5:Ax:160:LYS:HE2 | 5:Ax:424:THR:OG1 | 2.19 | 0.43 |
| 5:Ax:504:GLN:OE1 | 5:BA:484:ARG:NH2 | 2.39 | 0.43 |
| 2:B1:644:ALA:O | 2:B1:645:THR:OG1 | 2.29 | 0.43 |
| 2:B6:332:GLU:OE1 | 2:B6:332:GLU:N | 2.34 | 0.43 |
| 2:B7:246:LYS:HB2 | 2:B7:250:ALA:HB2 | 2.01 | 0.43 |
| 2:B7:254:ILE:HG22 | 2:B7:257:GLY:H | 1.83 | 0.43 |
| 2:B7:268:VAL:HG21 | 2:B7:282:ILE:HD13 | 2.01 | 0.43 |
| 2:B7:446:THR:OG1 | 2:B7:554:ARG:NH2 | 2.49 | 0.43 |
| 2:B7:607:VAL:HB | 2:B7:626:THR:OG1 | 2.18 | 0.43 |
| 5:BA:10:ALA:HB3 | 5:BA:11:PRO:HD3 | 2.01 | 0.43 |
| 5:BB:32:THR:OG1 | 5:BB:35:LYS:NZ | 2.52 | 0.43 |
| 5:BB:260:PRO:O | 5:BB:369:LEU:HB2 | 2.18 | 0.43 |
| 5:BD:470:LEU:HD23 | 5:BD:470:LEU:HA | 1.86 | 0.43 |
| 6:BM:442:ASN:OD1 | 6:BM:443:GLU:N | 2.52 | 0.43 |
| 11:BQ:12:THR:HG22 | 11:BQ:46:TYR:HB3 | 2.01 | 0.43 |
| 3:BX:44:GLY:HA3 | 3:Ba:89:GLN:HE22 | 1.84 | 0.43 |
| 3:Bc:132:LEU:HD13 | 3:Bc:159:LEU:HB3 | 2.01 | 0.43 |
| 3:Bf:22:GLN:HB2 | 3:Bf:116:TYR:HE1 | 1.84 | 0.43 |
| 3:Bh:23:VAL:HG12 | 3:Bh:113:VAL:HB | 2.01 | 0.43 |
| 3:Bi:43:ALA:O | 3:Bi:162:TRP:NE1 | 2.51 | 0.43 |
| 3:Bl:17:ARG:HG3 | 3:Bl:20:LEU:HD12 | 2.01 | 0.43 |
| 2:Br:90:LYS:HD2 | 2:Br:192:GLY:H | 1.84 | 0.43 |
| 2:Bu:57:PRO:HG3 | 2:Bu:65:PHE:HB3 | 1.99 | 0.43 |
| 2:Bv:451:ASP:OD2 | 2:Bv:470:LEU:HB3 | 2.19 | 0.43 |
| 2:By:601:ILE:H | 2:By:601:ILE:HG13 | 1.62 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:h:8:LEU:O | 4:h:19:GLN:NE2 | 2.51 | 0.43 |
| 4:h:9:PRO:HD3 | 4:h:57:VAL:HG21 | 2.01 | 0.43 |
| 1:l:154:PRO:HG2 | 1:l:155:TYR:CD2 | 2.54 | 0.43 |
| 1:l:159:TYR:HB3 | 1:l:162:GLY:HA2 | 2.00 | 0.43 |
| 1:p:147:PHE:HB3 | 1:p:171:ALA:HB1 | 2.01 | 0.43 |
| 2:1:28:ALA:HB2 | 2:1:370:VAL:HG21 | 2.01 | 0.43 |
| 2:3:401:GLN:OE1 | 8:s:257:SER:OG | 2.31 | 0.43 |
| 2:3:600:GLY:O | 2:3:632:ALA:HB2 | 2.19 | 0.43 |
| 2:3:620:ARG:NH2 | 8:s:266:GLU:O | 2.51 | 0.43 |
| 2:4:225:LEU:HB3 | 2:4:324:PHE:HB2 | 2.01 | 0.43 |
| 2:4:480:ARG:C | 2:4:482:ASP:H | 2.27 | 0.43 |
| 2:5:368:VAL:O | 2:5:400:ARG:NH2 | 2.51 | 0.43 |
| 3:6:97:ASN:HD21 | 3:AG:4:ASP:CG | 2.27 | 0.43 |
| 3:7:46:VAL:HG22 | 3:7:64:ARG:HD2 | 2.00 | 0.43 |
| 5:A2:62:PHE:CE1 | 5:A2:227:LYS:HG3 | 2.54 | 0.43 |
| 5:A3:158:PHE:HB2 | 5:A3:236:VAL:HB | 1.99 | 0.43 |
| 7:A6:12:LEU:HD21 | 7:A6:248:LYS:HG2 | 2.01 | 0.43 |
| 6:A8:267:LYS:HD3 | 6:A9:247:TRP:CG | 2.54 | 0.43 |
| 6:A8:430:LYS:HD2 | 6:A9:182:PHE:HE2 | 1.82 | 0.43 |
| 3:AE:21:PHE:HZ | 3:AE:38:ALA:HA | 1.84 | 0.43 |
| 3:AG:16:ALA:HB2 | 3:AH:76:ASP:O | 2.18 | 0.43 |
| 3:AG:83:GLN:HA | 3:AG:86:VAL:HG22 | 2.01 | 0.43 |
| 2:AL:33:PHE:HA | 2:AL:61:THR:HG23 | 2.01 | 0.43 |
| 2:AL:332:GLU:OE1 | 2:AL:332:GLU:N | 2.50 | 0.43 |
| 2:AL:642:PHE:CZ | 2:Bv:564:ILE:HD11 | 2.54 | 0.43 |
| 2:AM:637:TYR:HD2 | 2:By:622:GLU:HG2 | 1.83 | 0.43 |
| 2:AO:137:ASP:OD1 | 2:AO:137:ASP:N | 2.47 | 0.43 |
| 2:AO:209:ASP:OD1 | 2:AO:210:PHE:N | 2.52 | 0.43 |
| 2:AP:130:LYS:HD3 | 2:AP:144:ASN:HB3 | 2.00 | 0.43 |
| 6:AX:133:LYS:HG2 | 6:AX:249:GLU:HB3 | 2.00 | 0.43 |
| 7:Aa:257:GLU:OE1 | 7:Aa:290:LYS:NZ | 2.40 | 0.43 |
| 6:Ad:147:MET:O | 6:Ad:185:THR:N | 2.52 | 0.43 |
| 6:Ad:179:THR:HG22 | 6:Ad:189:TYR:CD2 | 2.54 | 0.43 |
| 6:Ae:158:GLY:HA2 | 6:Ae:163:PHE:HE2 | 1.84 | 0.43 |
| 6:Ae:247:TRP:CZ3 | 6:Ay:265:GLN:HB2 | 2.54 | 0.43 |
| 6:Ag:128:ARG:CZ | 6:Ag:491:ALA:H | 2.32 | 0.43 |
| 6:Aj:191:GLN:HB2 | 6:Aj:224:ILE:HG21 | 2.00 | 0.43 |
| 6:Ak:130:VAL:HG12 | 6:Ak:142:GLU:HA | 2.01 | 0.43 |
| 6:An:265:GLN:NE2 | 6:BK:236:GLN:HE21 | 2.17 | 0.43 |
| 6:Ao:337:PRO:HA | 6:Ao:340:ILE:HG12 | 2.00 | 0.43 |
| 6:Ap:90:GLN:HG3 | 7:BE:96:THR:O | 2.19 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:At:254:LEU:HD23 | 7:At:290:LYS:NZ | 2.34 | 0.43 |
| 5:Ax:292:MET:HG2 | 5:Ax:293:PRO:HD2 | 2.01 | 0.43 |
| 5:Ax:411:GLN:O | 5:Ax:415:GLU:HG3 | 2.19 | 0.43 |
| 2:B4:391:LYS:NZ | 2:B4:440:ASN:O | 2.47 | 0.43 |
| 2:B5:66:MET:HG2 | 2:B5:468:VAL:HG21 | 2.00 | 0.43 |
| 2:B5:510:ARG:HG2 | 2:B5:511:GLN:H | 1.83 | 0.43 |
| 2:B6:131:ILE:HD13 | 2:B6:140:ILE:HG21 | 2.01 | 0.43 |
| 2:B6:495:ASN:HB2 | 2:B6:496:ARG:HE | 1.83 | 0.43 |
| 2:B6:538:ASP:HA | 2:B6:551:ILE:HD12 | 2.00 | 0.43 |
| 2:B7:517:LEU:HG | 2:B7:522:ILE:HB | 2.01 | 0.43 |
| 7:BC:222:PRO:O | 7:BC:225:ASN:ND2 | 2.40 | 0.43 |
| 5:BG:366:ARG:NH2 | 5:BG:382:GLN:HG2 | 2.34 | 0.43 |
| 6:BJ:259:ILE:HG21 | 6:BJ:480:GLY:HA3 | 2.00 | 0.43 |
| 7:BL:163:PHE:HA | 7:BL:170:LEU:HA | 2.00 | 0.43 |
| 3:Bd:56:ARG:HG3 | 3:Bj:99:ILE:HG12 | 2.00 | 0.43 |
| 2:Bp:130:LYS:HE2 | 2:Bp:130:LYS:HB2 | 1.84 | 0.43 |
| 2:Bq:135:ASP:OD1 | 2:Bq:136:ALA:N | 2.52 | 0.43 |
| 2:Bq:252:LEU:HB3 | 2:Bq:336:GLY:HA2 | 2.01 | 0.43 |
| 2:Bq:416:GLY:H | 2:Bq:417:ILE:HD13 | 1.83 | 0.43 |
| 2:Bq:617:VAL:HG22 | 2:Bq:622:GLU:HB2 | 2.01 | 0.43 |
| 2:Bs:527:GLY:HA2 | 2:Bs:533:TYR:CD1 | 2.54 | 0.43 |
| 2:Bt:237:GLU:HB3 | 2:Bt:282:ILE:HB | 2.01 | 0.43 |
| 2:Bt:413:THR:C | 2:Bt:417:ILE:HD11 | 2.44 | 0.43 |
| 2:Bt:637:TYR:HB3 | 2:Bw:3:LEU:HD12 | 2.00 | 0.43 |
| 2:Bx:157:VAL:HG23 | 2:Bx:159:GLU:H | 1.84 | 0.43 |
| 2:By:102:THR:HB | 2:By:183:THR:HB | 2.01 | 0.43 |
| 4:M:9:PRO:HD3 | 4:M:57:VAL:HG21 | 1.99 | 0.43 |
| 4:U:47:PRO:O | 4:U:51:VAL:HG23 | 2.19 | 0.43 |
| 4:d:62:ILE:HD12 | 4:i:58:LEU:HD22 | 1.99 | 0.43 |
| 1:k:49:GLU:HG3 | 1:k:50:SER:N | 2.34 | 0.43 |
| 8:q:26:ILE:HD12 | 8:q:129:ASP:HB3 | 2.00 | 0.43 |
| 8:q:217:HIS:CD2 | 8:q:229:VAL:HG23 | 2.54 | 0.43 |
| 8:s:46:LYS:HB3 | 8:s:51:MET:CG | 2.49 | 0.43 |
| 8:s:91:ASN:O | 8:s:110:ASN:ND2 | 2.51 | 0.43 |
| 1:0:242:GLY:HA3 | 8:AB:4:TYR:H | 1.83 | 0.42 |
| 2:3:293:VAL:HG22 | 2:3:294:VAL:H | 1.84 | 0.42 |
| 2:4:191:SER:HB3 | 2:4:342:GLY:HA3 | 2.01 | 0.42 |
| 2:4:498:GLN:HA | 2:4:534:VAL:HA | 1.99 | 0.42 |
| 2:4:528:THR:HA | 2:AL:367:SER:HA | 2.01 | 0.42 |
| 2:4:628:TYR:HD2 | 8:t:217:HIS:HB2 | 1.84 | 0.42 |
| 2:5:117:THR:HG23 | 2:5:127:THR:HG22 | 2.01 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:8:3:VAL:HG11 | 3:8:9:ALA:HB2 | 2.02 | 0.42 |
| 3:9:20:LEU:HD23 | 9:w:54:PHE:HB3 | 2.01 | 0.42 |
| 4:A:47:PRO:HB2 | 4:Q:48:THR:HG21 | 2.00 | 0.42 |
| 5:A3:465:ARG:NH2 | 5:BG:464:GLU:OE1 | 2.49 | 0.42 |
| 5:A3:508:GLU:HG2 | 5:BF:483:HIS:HB3 | 2.01 | 0.42 |
| 6:A8:435:THR:HB | 6:A8:515:ARG:HB2 | 2.01 | 0.42 |
| 2:AD:303:ASP:OD1 | 2:AD:304:ILE:N | 2.51 | 0.42 |
| 3:AH:54:MET:SD | 3:Bg:1:MET:HE1 | 2.59 | 0.42 |
| 2:AM:37:PRO:HG3 | 2:AM:226:TYR:CZ | 2.54 | 0.42 |
| 2:AO:142:LYS:HE2 | 2:AO:142:LYS:HB2 | 1.83 | 0.42 |
| 2:AP:205:MET:HE3 | 2:AP:324:PHE:HD1 | 1.83 | 0.42 |
| 10:AU:309:TRP:H | 10:AU:356:SER:HB3 | 1.83 | 0.42 |
| 6:AW:265:GLN:HA | 6:AW:473:PHE:O | 2.19 | 0.42 |
| 6:AX:258:VAL:HG21 | 6:BK:76:ALA:HA | 2.00 | 0.42 |
| 6:AX:260:GLU:OE2 | 6:BK:72:HIS:ND1 | 2.48 | 0.42 |
| 6:AX:337:PRO:HA | 6:AX:340:ILE:HG12 | 2.01 | 0.42 |
| 6:AX:346:ALA:HB2 | 6:Az:341:ARG:HB2 | 2.01 | 0.42 |
| 6:AX:383:VAL:HG12 | 6:AX:406:THR:HG22 | 2.01 | 0.42 |
| 6:Ac:265:GLN:HG2 | 6:Ac:474:LYS:HB3 | 2.00 | 0.42 |
| 6:Ae:267:LYS:HE3 | 6:Ai:247:TRP:CD2 | 2.54 | 0.42 |
| 6:Ae:452:PRO:HB3 | 6:Ae:477:TYR:HD1 | 1.83 | 0.42 |
| 6:Ah:345:TRP:CE2 | 6:BI:348:GLU:HG2 | 2.54 | 0.42 |
| 6:Ai:154:PHE:CE2 | 6:Ai:248:ASN:HB3 | 2.54 | 0.42 |
| 6:Am:151:ASP:HB3 | 6:Am:154:PHE:HB2 | 2.00 | 0.42 |
| 6:Am:430:LYS:HA | 6:Am:430:LYS:HD3 | 1.84 | 0.42 |
| 6:Ap:363:GLU:OE2 | 6:Ap:367:GLN:NE2 | 2.52 | 0.42 |
| 5:Av:287:VAL:HB | 5:Av:301:MET:SD | 2.59 | 0.42 |
| 5:Av:484:ARG:HE | 5:BB:504:GLN:NE2 | 2.17 | 0.42 |
| 6:Aw:123:GLN:CD | 6:BM:93:PRO:HG2 | 2.44 | 0.42 |
| 6:Aw:133:LYS:HB2 | 6:Aw:133:LYS:HE3 | 1.83 | 0.42 |
| 6:Aw:344:ARG:NE | 6:Aw:348:GLU:OE2 | 2.52 | 0.42 |
| 2:B1:64:TYR:CE1 | 2:B1:377:SER:HA | 2.54 | 0.42 |
| 2:B1:238:ILE:HG12 | 2:B1:281:ILE:HG23 | 2.00 | 0.42 |
| 2:B2:110:TYR:H | 2:B2:138:GLY:CA | 2.31 | 0.42 |
| 2:B2:116:ILE:HD11 | 2:B2:131:ILE:HG13 | 2.01 | 0.42 |
| 2:B3:614:THR:O | 2:B3:616:SER:N | 2.46 | 0.42 |
| 2:B5:371:GLN:OE1 | 2:B5:562:THR:OG1 | 2.23 | 0.42 |
| 2:B5:488:TRP:O | 2:B5:552:ASN:OD1 | 2.36 | 0.42 |
| 2:B5:549:ASP:O | 2:B5:550:ARG:NE | 2.50 | 0.42 |
| 2:B7:100:GLU:HG3 | 2:B7:185:GLY:HA3 | 2.00 | 0.42 |
| 5:BA:117:LYS:HD3 | 5:BA:117:LYS:HA | 1.88 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BA:292:MET:O | 5:BA:294:ALA:N | 2.46 | 0.42 |
| 5:BB:160:LYS:NZ | 5:BB:233:ALA:O | 2.52 | 0.42 |
| 5:BB:191:GLU:N | 5:BB:198:ILE:O | 2.52 | 0.42 |
| 7:BC:59:VAL:HG12 | 7:BC:183:ILE:HG13 | 2.01 | 0.42 |
| 5:BD:259:LYS:HB3 | 5:BD:260:PRO:HD3 | 2.01 | 0.42 |
| 5:BF:244:ASP:HB2 | 5:BF:251:ILE:HD12 | 2.02 | 0.42 |
| 6:BM:234:GLU:HB3 | 6:BM:235:LEU:HD12 | 2.01 | 0.42 |
| 3:BZ:114:ARG:HH21 | 3:BZ:116:TYR:HH | 1.64 | 0.42 |
| 2:Bs:410:PRO:O | 2:Bs:413:THR:HG22 | 2.18 | 0.42 |
| 2:By:654:LEU:HD13 | 2:Bz:605:ARG:HD3 | 2.01 | 0.42 |
| 2:Bz:103:ILE:HD13 | 2:Bz:182:ILE:HG22 | 2.00 | 0.42 |
| 1:p:61:VAL:HB | 1:p:137:LEU:HB2 | 2.01 | 0.42 |
| 8:u:238:VAL:HG13 | 8:u:239:PRO:HD2 | 2.01 | 0.42 |
| 9:v:13:ASN:HD22 | 9:v:15:THR:H | 1.67 | 0.42 |
| 2:1:202:GLU:OE1 | 2:1:203:ALA:N | 2.53 | 0.42 |
| 2:3:32:LYS:HD2 | 2:3:347:ASN:HB3 | 2.01 | 0.42 |
| 2:3:96:ALA:HB2 | 2:3:191:SER:HA | 2.01 | 0.42 |
| 2:5:22:ASN:N | 2:5:22:ASN:OD1 | 2.52 | 0.42 |
| 2:5:601:ILE:HD13 | 2:5:629:ILE:HB | 2.00 | 0.42 |
| 5:A0:243:VAL:HG12 | 5:A0:250:ILE:HG12 | 2.01 | 0.42 |
| 5:A2:301:MET:HE2 | 7:BL:304:PHE:HZ | 1.84 | 0.42 |
| 5:A3:226:THR:HG21 | 5:BF:196:THR:HG22 | 2.01 | 0.42 |
| 6:A4:355:PHE:CE2 | 6:A4:359:LYS:HD2 | 2.54 | 0.42 |
| 6:A5:346:ALA:HB2 | 6:AW:341:ARG:HD3 | 2.01 | 0.42 |
| 6:A7:236:GLN:HB2 | 6:A7:247:TRP:CZ2 | 2.54 | 0.42 |
| 8:AB:79:LEU:HD12 | 8:AB:118:TYR:CZ | 2.54 | 0.42 |
| 2:AD:381:GLU:HB3 | 2:AD:385:THR:HG23 | 2.01 | 0.42 |
| 3:AE:106:GLU:O | 3:AE:109:LYS:NZ | 2.52 | 0.42 |
| 3:AI:23:VAL:HG22 | 3:AI:36:CYS:SG | 2.59 | 0.42 |
| 2:AK:545:PRO:HB2 | 2:AL:304:ILE:HD13 | 2.00 | 0.42 |
| 2:AM:427:VAL:O | 2:AM:431:THR:OG1 | 2.35 | 0.42 |
| 2:AO:373:PHE:HB2 | 2:AO:405:VAL:HG22 | 2.00 | 0.42 |
| 2:AP:510:ARG:HG2 | 2:AP:511:GLN:H | 1.84 | 0.42 |
| 6:AV:87:ALA:O | 6:BJ:495:ARG:NH2 | 2.51 | 0.42 |
| 6:AX:253:ARG:NH2 | 6:AX:255:ASP:OD2 | 2.53 | 0.42 |
| 7:Ab:95:ILE:HG22 | 7:Ar:108:THR:HG23 | 2.00 | 0.42 |
| 6:Ae:230:THR:O | 6:Ae:234:GLU:HG2 | 2.18 | 0.42 |
| 6:Ag:494:SER:C | 6:Ag:496:ILE:H | 2.27 | 0.42 |
| 6:Ah:223:GLU:CD | 6:Ah:223:GLU:H | 2.28 | 0.42 |
| 6:Aj:145:HIS:NE2 | 6:Aj:487:SER:O | 2.52 | 0.42 |
| 6:Ak:80:ALA:HA | 6:Ak:93:PRO:HG3 | 2.00 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Am:112:CYS:SG | 6:Am:310:ILE:HD11 | 2.59 | 0.42 |
| 6:Am:279:ARG:NH2 | 6:Am:285:ASP:OD1 | 2.52 | 0.42 |
| 6:An:387:ALA:HB2 | 6:An:404:PHE:HB2 | 2.00 | 0.42 |
| 6:Ap:118:ASN:OD1 | 6:Ap:118:ASN:N | 2.48 | 0.42 |
| 7:Ar:221:ASN:HB3 | 7:Ar:224:HIS:CD2 | 2.54 | 0.42 |
| 5:Ax:218:ASP:OD1 | 5:Ax:219:GLY:N | 2.52 | 0.42 |
| 6:Ay:141:LYS:HA | 6:Ay:490:GLN:HG2 | 2.01 | 0.42 |
| 2:B1:438:ASP:OD1 | 2:B1:438:ASP:N | 2.39 | 0.42 |
| 2:B4:455:LYS:HB3 | 2:B4:470:LEU:HD13 | 2.01 | 0.42 |
| 2:B7:31:GLY:O | 2:B7:82:ARG:HA | 2.19 | 0.42 |
| 5:BB:366:ARG:NH2 | 5:BB:382:GLN:HG2 | 2.34 | 0.42 |
| 7:BC:171:LYS:HD2 | 7:BE:219:TYR:CE2 | 2.54 | 0.42 |
| 5:BF:50:ALA:HA | 5:BF:55:ASN:ND2 | 2.34 | 0.42 |
| 5:BG:212:HIS:HD1 | 5:BG:222:TYR:HA | 1.84 | 0.42 |
| 5:BH:94:GLU:HG3 | 5:BH:379:ARG:HH21 | 1.83 | 0.42 |
| 7:BL:234:ASP:N | 7:BL:234:ASP:OD1 | 2.52 | 0.42 |
| 3:Bd:140:LEU:HD21 | 3:Bd:151:GLN:NE2 | 2.33 | 0.42 |
| 3:Bl:16:ALA:HB2 | 3:Bo:76:ASP:O | 2.20 | 0.42 |
| 3:Bl:42:PRO:HG2 | 3:Bl:127:ILE:HD11 | 2.02 | 0.42 |
| 3:Bl:60:VAL:HG21 | 3:Bo:104:PRO:HG3 | 2.01 | 0.42 |
| 3:Bl:109:LYS:O | 3:Bl:132:LEU:N | 2.47 | 0.42 |
| 3:Bn:70:THR:HG22 | 3:Bn:156:THR:HG22 | 2.00 | 0.42 |
| 3:Bn:94:GLY:HA3 | 3:Bn:100:THR:OG1 | 2.20 | 0.42 |
| 2:Bq:495:ASN:HD22 | 2:Bq:495:ASN:H | 1.66 | 0.42 |
| 2:Br:131:ILE:HD13 | 2:Br:140:ILE:HG21 | 2.00 | 0.42 |
| 2:Bu:547:PRO:HG3 | 2:Bx:305:TYR:CE1 | 2.54 | 0.42 |
| 2:Bw:131:ILE:HD13 | 2:Bw:140:ILE:HG21 | 2.01 | 0.42 |
| 2:Bx:109:ASN:HA | 2:Bx:137:ASP:HB2 | 2.00 | 0.42 |
| 4:I:10:PHE:HA | 4:I:20:SER:O | 2.20 | 0.42 |
| 4:U:9:PRO:O | 4:U:20:SER:N | 2.52 | 0.42 |
| 1:k:220:GLU:CD | 8:r:46:LYS:HZ1 | 2.26 | 0.42 |
| 1:l:103:PHE:CD1 | 8:s:51:MET:HE3 | 2.53 | 0.42 |
| 1:l:223:GLN:NE2 | 1:m:69:ASP:OD1 | 2.51 | 0.42 |
| 1:m:45:VAL:HG11 | 1:n:9:PHE:HE2 | 1.83 | 0.42 |
| 1:n:213:ILE:O | 8:u:55:LYS:HD2 | 2.19 | 0.42 |
| 3:o:10:PHE:O | 3:o:11:GLU:HB2 | 2.20 | 0.42 |
| 1:p:26:ILE:HG22 | 1:p:27:LEU:HB2 | 2.00 | 0.42 |
| 1:p:27:LEU:HD22 | 1:p:27:LEU:HA | 1.88 | 0.42 |
| 1:p:56:VAL:N | 1:p:88:ALA:O | 2.42 | 0.42 |
| 8:q:232:SER:HB2 | 8:q:256:THR:OG1 | 2.19 | 0.42 |
| 8:s:61:SER:OG | 8:s:62:GLN:N | 2.52 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:u:134:VAL:HG21 | 8:u:188:TRP:CE3 | 2.54 | 0.42 |
| 1:0:44:ASP:HB2 | 1:0:163:GLN:NE2 | 2.33 | 0.42 |
| 2:1:451:ASP:OD1 | 2:1:452:GLY:N | 2.45 | 0.42 |
| 2:1:594:GLY:HA2 | 3:6:8:ARG:HD3 | 2.01 | 0.42 |
| 2:3:226:TYR:HA | 2:3:227:PRO:HD3 | 1.90 | 0.42 |
| 2:3:598:LEU:HD23 | 2:3:598:LEU:HA | 1.92 | 0.42 |
| 2:3:614:THR:C | 2:3:616:SER:H | 2.28 | 0.42 |
| 2:4:4:LEU:HG | 2:4:5:SER:H | 1.85 | 0.42 |
| 2:4:638:ILE:HB | 2:5:8:ILE:HG22 | 2.00 | 0.42 |
| 3:8:138:GLY:HA3 | 3:8:153:PHE:HB2 | 2.01 | 0.42 |
| 3:9:125:LYS:HG2 | 3:AA:79:HIS:CD2 | 2.55 | 0.42 |
| 5:A2:248:LYS:HD3 | 5:BF:217:CYS:H | 1.83 | 0.42 |
| 5:A3:320:LYS:HE3 | 5:A3:322:LYS:HG2 | 2.00 | 0.42 |
| 7:A6:161:PHE:HB2 | 7:A6:170:LEU:HD11 | 2.00 | 0.42 |
| 6:A7:430:LYS:HA | 6:A7:430:LYS:HD3 | 1.91 | 0.42 |
| 6:A8:128:ARG:NE | 6:A8:492:PRO:HD3 | 2.35 | 0.42 |
| 3:AE:138:GLY:HA3 | 3:AJ:43:ALA:HA | 2.01 | 0.42 |
| 3:AF:94:GLY:HA3 | 3:AF:100:THR:OG1 | 2.19 | 0.42 |
| 2:AK:455:LYS:HD2 | 2:AK:502:VAL:HG22 | 2.02 | 0.42 |
| 2:AL:254:ILE:HG22 | 2:AL:257:GLY:H | 1.84 | 0.42 |
| 2:AL:289:ILE:H | 2:AL:289:ILE:HG12 | 1.65 | 0.42 |
| 6:AV:245:ASN:OD1 | 6:AV:245:ASN:N | 2.52 | 0.42 |
| 6:AV:269:ALA:HA | 6:AV:470:VAL:HA | 2.00 | 0.42 |
| 6:AX:269:ALA:HA | 6:AX:470:VAL:HA | 2.01 | 0.42 |
| 7:Aa:55:LYS:HB3 | 7:Aa:187:TRP:CE3 | 2.54 | 0.42 |
| 7:Ab:126:ASN:OD1 | 7:Ab:126:ASN:N | 2.52 | 0.42 |
| 7:Ab:189:LYS:HE2 | 7:Ab:189:LYS:HB3 | 1.77 | 0.42 |
| 7:Ab:221:ASN:HB3 | 7:Ab:224:HIS:CE1 | 2.54 | 0.42 |
| 6:Ac:244:ASP:HB2 | 11:BW:13:PHE:HE2 | 1.84 | 0.42 |
| 6:Ag:398:GLN:HG3 | 6:Ak:351:LYS:HD3 | 2.01 | 0.42 |
| 6:Ag:515:ARG:NH2 | 6:Ag:517:TYR:OH | 2.44 | 0.42 |
| 6:Ah:380:ARG:HB3 | 6:BI:362:VAL:HG11 | 2.01 | 0.42 |
| 6:Ah:384:ASN:HD21 | 6:BI:362:VAL:HG21 | 1.85 | 0.42 |
| 6:Am:344:ARG:NH2 | 6:Am:348:GLU:OE1 | 2.52 | 0.42 |
| 6:Am:355:PHE:CE2 | 6:Am:359:LYS:HD2 | 2.55 | 0.42 |
| 6:Am:379:SER:OG | 6:Am:432:ASP:OD1 | 2.34 | 0.42 |
| 6:Am:397:ALA:HA | 6:BJ:394:SER:O | 2.18 | 0.42 |
| 6:Ao:313:SER:HB2 | 6:Ao:510:ASN:HB2 | 2.00 | 0.42 |
| 6:Ao:378:ALA:HB1 | 6:Ao:382:VAL:HB | 2.00 | 0.42 |
| 5:Av:292:MET:HE3 | 5:Av:297:ALA:HA | 2.01 | 0.42 |
| 6:Az:181:PHE:HD1 | 6:Az:187:THR:HB | 1.84 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B1:153:LYS:HB3 | 2:B1:167:TRP:CH2 | 2.54 | 0.42 |
| 2:B3:567:SER:O | 2:B3:571:ARG:HG2 | 2.19 | 0.42 |
| 2:B6:410:PRO:O | 2:B6:413:THR:HG22 | 2.19 | 0.42 |
| 2:B7:101:TYR:OH | 2:B7:143:ILE:O | 2.26 | 0.42 |
| 7:BC:61:TYR:CZ | 7:BC:181:LEU:HD21 | 2.54 | 0.42 |
| 7:BE:154:MET:HE3 | 7:BE:154:MET:HB3 | 1.92 | 0.42 |
| 5:BG:496:GLU:CD | 5:BG:496:GLU:H | 2.28 | 0.42 |
| 5:BH:277:THR:HG23 | 5:BH:278:ARG:HG3 | 2.01 | 0.42 |
| 6:BI:311:ASN:ND2 | 6:BI:433:TYR:OH | 2.52 | 0.42 |
| 6:BM:503:ILE:HA | 6:BM:507:LEU:HB2 | 2.02 | 0.42 |
| 2:Bq:450:ILE:HG21 | 2:Bq:522:ILE:HG12 | 2.01 | 0.42 |
| 2:Br:89:ALA:HA | 2:Br:345:SER:O | 2.19 | 0.42 |
| 2:Bs:160:TYR:HA | 2:Bs:161:PRO:HA | 1.87 | 0.42 |
| 2:Bt:410:PRO:O | 2:Bt:413:THR:HG22 | 2.19 | 0.42 |
| 2:Bu:101:TYR:CG | 2:Bu:143:ILE:HD11 | 2.54 | 0.42 |
| 2:Bv:39:PHE:HB3 | 2:Bv:361:PHE:CE2 | 2.54 | 0.42 |
| 2:Bv:234:ILE:HB | 2:Bv:340:LEU:HD12 | 2.00 | 0.42 |
| 2:Bw:70:ASN:OD1 | 2:Bw:457:GLN:NE2 | 2.52 | 0.42 |
| 2:Bx:374:ILE:HG22 | 2:Bx:376:GLY:H | 1.83 | 0.42 |
| 2:Bz:26:THR:HB | 2:Bz:77:ASP:HB3 | 2.01 | 0.42 |
| 1:l:66:VAL:O | 1:l:77:LYS:HB2 | 2.18 | 0.42 |
| 1:p:122:LEU:HD11 | 1:p:126:GLN:HE21 | 1.84 | 0.42 |
| 8:t:128:ASP:O | 8:t:132:GLN:HG3 | 2.18 | 0.42 |
| 2:5:261:ARG:NH2 | 2:5:337:ILE:HD13 | 2.34 | 0.42 |
| 2:5:295:LEU:HB3 | 2:5:311:ILE:HG12 | 2.01 | 0.42 |
| 5:A0:105:ASP:N | 5:A0:105:ASP:OD1 | 2.51 | 0.42 |
| 5:A1:196:THR:OG1 | 5:A1:197:LYS:N | 2.52 | 0.42 |
| 5:A3:68:GLY:HA2 | 6:AV:116:PRO:HG3 | 2.01 | 0.42 |
| 5:A3:467:ILE:HD13 | 5:BF:473:ALA:HB2 | 2.02 | 0.42 |
| 6:A4:247:TRP:CH2 | 7:As:98:MET:HG2 | 2.51 | 0.42 |
| 6:A4:247:TRP:CZ3 | 7:As:99:ASP:HB2 | 2.55 | 0.42 |
| 6:A5:482:ASN:HB3 | 6:A5:485:ALA:HB2 | 2.01 | 0.42 |
| 6:A8:265:GLN:NE2 | 6:A9:236:GLN:HG3 | 2.35 | 0.42 |
| 3:AA:10:PHE:HE1 | 3:o:35:GLN:HG2 | 1.84 | 0.42 |
| 3:AE:136:ASN:ND2 | 3:AE:136:ASN:O | 2.52 | 0.42 |
| 3:AF:2:PHE:HA | 3:o:98:GLU:HA | 2.01 | 0.42 |
| 2:AK:311:ILE:HB | 2:AK:327:ALA:HB2 | 2.01 | 0.42 |
| 2:AL:463:ASP:OD1 | 2:Bv:317:LYS:NZ | 2.46 | 0.42 |
| 2:AM:222:VAL:HG21 | 2:AM:238:ILE:HD11 | 2.00 | 0.42 |
| 2:AN:220:PRO:HD3 | 2:AN:334:PHE:CE2 | 2.54 | 0.42 |
| 2:AN:642:PHE:CZ | 2:B2:561:LYS:HG2 | 2.54 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AO:642:PHE:CZ | 2:B5:564:ILE:HD11 | 2.54 | 0.42 |
| 6:AW:84:THR:OG1 | 6:AW:88:VAL:O | 2.37 | 0.42 |
| 6:AZ:344:ARG:HG3 | 6:Ad:344:ARG:NH1 | 2.34 | 0.42 |
| 6:AZ:365:ALA:HB2 | 6:AZ:372:GLU:HA | 2.00 | 0.42 |
| 6:Ac:190:LEU:HD23 | 6:Ac:223:GLU:HA | 2.00 | 0.42 |
| 6:Ad:111:ILE:HD12 | 6:Ad:377:ILE:HD11 | 2.01 | 0.42 |
| 6:Ae:121:THR:HB | 6:Ay:79:ILE:HG23 | 2.01 | 0.42 |
| 6:Ag:324:THR:OG1 | 6:Ag:327:SER:HB2 | 2.19 | 0.42 |
| 6:Ai:93:PRO:HA | 6:Am:121:THR:O | 2.20 | 0.42 |
| 6:Am:71:ASP:OD1 | 6:Am:72:HIS:N | 2.52 | 0.42 |
| 6:Am:374:ASN:HD21 | 6:Am:439:LYS:C | 2.26 | 0.42 |
| 6:Au:309:TRP:CD1 | 6:Au:479:ILE:HD13 | 2.55 | 0.42 |
| 6:Aw:245:ASN:C | 6:Aw:247:TRP:N | 2.77 | 0.42 |
| 6:Ay:345:TRP:CD1 | 6:Ay:346:ALA:N | 2.88 | 0.42 |
| 2:B1:577:ASN:ND2 | 2:B1:579:PHE:H | 2.17 | 0.42 |
| 2:B1:591:TYR:HD2 | 2:B1:592:LEU:HD12 | 1.83 | 0.42 |
| 2:B3:400:ARG:NH1 | 2:B3:402:ASP:OD1 | 2.52 | 0.42 |
| 2:B5:14:THR:HG21 | 2:B6:306:ASP:HB2 | 2.00 | 0.42 |
| 2:B6:35:TRP:HB2 | 2:B6:230:LEU:HD12 | 2.01 | 0.42 |
| 2:B6:642:PHE:CZ | 2:B7:564:ILE:HD11 | 2.55 | 0.42 |
| 5:BF:38:ASP:N | 5:BF:38:ASP:OD1 | 2.52 | 0.42 |
| 5:BF:267:LEU:HD12 | 5:BF:365:PHE:HD2 | 1.83 | 0.42 |
| 5:BF:375:VAL:HG12 | 5:BF:379:ARG:HG3 | 2.01 | 0.42 |
| 5:BG:397:THR:HG23 | 5:BG:400:GLU:HB2 | 2.02 | 0.42 |
| 5:BH:282:ARG:HA | 5:BH:282:ARG:HD3 | 1.90 | 0.42 |
| 6:BI:314:ALA:HA | 6:BI:513:PHE:HB2 | 2.01 | 0.42 |
| 6:BJ:444:MET:O | 6:BJ:449:TYR:OH | 2.26 | 0.42 |
| 6:BK:366:ARG:NH1 | 6:BK:367:GLN:HG3 | 2.35 | 0.42 |
| 6:BM:269:ALA:HA | 6:BM:470:VAL:HA | 2.01 | 0.42 |
| 6:BM:494:SER:C | 6:BM:496:ILE:H | 2.27 | 0.42 |
| 11:BS:11:LYS:NZ | 11:BS:27:GLU:OE2 | 2.44 | 0.42 |
| 11:BT:30:VAL:HG11 | 11:BT:68:TRP:CD2 | 2.55 | 0.42 |
| 3:BY:23:VAL:HG22 | 3:BY:36:CYS:SG | 2.60 | 0.42 |
| 3:BZ:143:ASP:OD2 | 3:BZ:145:ASP:HB2 | 2.20 | 0.42 |
| 3:Bk:19:ASN:OD1 | 3:Bk:19:ASN:N | 2.36 | 0.42 |
| 3:Bn:137:VAL:HG23 | 3:Bn:155:VAL:HG22 | 2.02 | 0.42 |
| 2:Bp:188:ILE:H | 2:Bp:188:ILE:HG12 | 1.59 | 0.42 |
| 2:Bq:269:PHE:CZ | 2:Bq:292:SER:HB2 | 2.53 | 0.42 |
| 2:Bq:642:PHE:CZ | 2:Br:561:LYS:HG2 | 2.54 | 0.42 |
| 2:Br:254:ILE:HG22 | 2:Br:257:GLY:H | 1.84 | 0.42 |
| 2:Bs:66:MET:HG2 | 2:Bs:468:VAL:HG21 | 2.00 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bs:536:TYR:HD1 | 2:Bs:536:TYR:HA | 1.72 | 0.42 |
| 2:Bt:154:ALA:HB1 | 2:Bt:160:TYR:HB2 | 2.02 | 0.42 |
| 2:Bt:254:ILE:HG13 | 2:Bt:337:ILE:HB | 2.02 | 0.42 |
| 2:Bw:3:LEU:HD21 | 2:Bw:9:GLU:HB2 | 2.02 | 0.42 |
| 2:Bw:441:PHE:CZ | 2:Bw:443:ILE:HD11 | 2.54 | 0.42 |
| 2:Bx:576:ASN:ND2 | 2:Bx:622:GLU:O | 2.52 | 0.42 |
| 2:Bz:49:ASP:OD1 | 2:Bz:49:ASP:N | 2.48 | 0.42 |
| 2:Bz:110:TYR:CG | 2:Bz:177:GLY:HA3 | 2.55 | 0.42 |
| 4:h:66:LYS:HE3 | 4:h:66:LYS:HB3 | 1.93 | 0.42 |
| 1:k:59:TYR:HD2 | 1:k:139:TYR:HD2 | 1.68 | 0.42 |
| 8:q:212:THR:OG1 | 8:q:235:SER:OG | 2.19 | 0.42 |
| 8:s:151:GLU:OE1 | 8:s:199:TYR:OH | 2.35 | 0.42 |
| 9:x:163:TYR:HE1 | 9:x:165:GLN:HE21 | 1.67 | 0.42 |
| 2:2:118:VAL:HG22 | 2:2:169:ALA:HB2 | 2.02 | 0.42 |
| 2:2:241:LYS:HB2 | 2:2:273:PRO:HB2 | 2.02 | 0.42 |
| 2:3:9:GLU:HG2 | 2:3:11:LYS:HG3 | 2.00 | 0.42 |
| 2:3:454:TYR:HB3 | 2:3:467:TRP:CD1 | 2.55 | 0.42 |
| 2:4:356:MET:HG3 | 2:4:392:HIS:CD2 | 2.54 | 0.42 |
| 2:5:136:ALA:HB3 | 2:5:139:LYS:HE2 | 2.01 | 0.42 |
| 3:8:97:ASN:HD21 | 3:AI:4:ASP:CG | 2.27 | 0.42 |
| 5:A0:96:VAL:HG22 | 5:A0:147:PHE:HD2 | 1.84 | 0.42 |
| 5:A0:292:MET:O | 5:A0:294:ALA:N | 2.48 | 0.42 |
| 5:A1:31:ILE:HG22 | 5:A1:198:ILE:HG22 | 2.02 | 0.42 |
| 6:A4:379:SER:OG | 6:A4:432:ASP:OD1 | 2.32 | 0.42 |
| 7:A6:54:ASN:HA | 7:Al:162:TRP:HE1 | 1.82 | 0.42 |
| 7:A6:71:THR:HG21 | 7:BL:216:SER:HB3 | 2.02 | 0.42 |
| 9:AC:172:ILE:HD13 | 9:AC:172:ILE:HA | 1.79 | 0.42 |
| 2:AD:356:MET:SD | 2:AD:392:HIS:ND1 | 2.92 | 0.42 |
| 2:AL:26:THR:HA | 2:AL:77:ASP:O | 2.20 | 0.42 |
| 2:AL:361:PHE:HD1 | 2:AL:361:PHE:HA | 1.71 | 0.42 |
| 2:AN:32:LYS:HG2 | 2:AN:350:VAL:HG21 | 2.00 | 0.42 |
| 2:AO:37:PRO:HG3 | 2:AO:226:TYR:CZ | 2.54 | 0.42 |
| 6:AV:230:THR:HB | 6:BI:71:ASP:CG | 2.44 | 0.42 |
| 6:AV:374:ASN:O | 6:AV:422:ARG:HD3 | 2.19 | 0.42 |
| 7:AY:117:ILE:H | 7:AY:117:ILE:HG13 | 1.47 | 0.42 |
| 7:AY:164:ASN:ND2 | 7:Aq:51:ASP:OD1 | 2.52 | 0.42 |
| 6:AZ:145:HIS:ND1 | 6:AZ:146:PRO:HD2 | 2.34 | 0.42 |
| 6:Ak:252:PHE:N | 6:Ak:252:PHE:CD1 | 2.87 | 0.42 |
| 6:An:466:ASN:OD1 | 6:An:466:ASN:N | 2.52 | 0.42 |
| 6:Ap:125:PHE:HZ | 6:BM:91:ILE:HA | 1.83 | 0.42 |
| 6:Ap:357:ILE:HG12 | 6:Ap:434:PHE:CE2 | 2.54 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Ar:86:ARG:NH1 | 5:Ax:311:ARG:HD2 | 2.34 | 0.42 |
| 5:Av:236:VAL:HG21 | 5:Av:421:PRO:HG3 | 2.02 | 0.42 |
| 5:Av:400:GLU:OE1 | 5:Ax:398:ARG:NH2 | 2.52 | 0.42 |
| 5:Ax:249:ASN:OD1 | 5:Ax:250:ILE:N | 2.52 | 0.42 |
| 6:Ay:331:VAL:HA | 6:Ay:517:TYR:O | 2.19 | 0.42 |
| 2:B2:234:ILE:HG12 | 2:B2:285:ARG:HD3 | 2.02 | 0.42 |
| 2:B4:57:PRO:HG3 | 2:B4:65:PHE:CG | 2.53 | 0.42 |
| 2:B4:94:PRO:HD2 | 2:B4:223:VAL:HG12 | 2.02 | 0.42 |
| 2:B6:91:ASN:ND2 | 2:B6:225:LEU:O | 2.52 | 0.42 |
| 2:B6:331:PRO:HB2 | 2:B6:334:PHE:HB2 | 2.02 | 0.42 |
| 7:BC:280:GLN:OE1 | 7:BC:280:GLN:N | 2.52 | 0.42 |
| 5:BD:161:ILE:HB | 5:BD:173:GLU:HB3 | 2.01 | 0.42 |
| 5:BG:290:GLY:C | 5:BG:291:ASN:HD22 | 2.22 | 0.42 |
| 5:BH:94:GLU:CG | 5:BH:379:ARG:HH21 | 2.33 | 0.42 |
| 6:BK:269:ALA:HA | 6:BK:470:VAL:HA | 2.00 | 0.42 |
| 6:BK:291:SER:HB2 | 6:BK:471:MET:SD | 2.59 | 0.42 |
| 6:BM:269:ALA:HB2 | 6:BM:470:VAL:HG13 | 2.02 | 0.42 |
| 11:BQ:9:ASN:ND2 | 11:BQ:51:SER:OG | 2.52 | 0.42 |
| 11:BW:41:ILE:HD13 | 11:BW:46:TYR:CE2 | 2.55 | 0.42 |
| 3:Ba:90:SER:HA | 3:Ba:94:GLY:H | 1.85 | 0.42 |
| 3:Bc:25:ILE:HD12 | 3:Bc:28:LEU:HD12 | 2.01 | 0.42 |
| 2:Bp:281:ILE:HG13 | 2:Bp:295:LEU:HD12 | 2.02 | 0.42 |
| 2:Bp:571:ARG:NH2 | 2:Bp:587:GLU:OE1 | 2.41 | 0.42 |
| 2:Bq:410:PRO:O | 2:Bq:413:THR:HG22 | 2.19 | 0.42 |
| 2:Bq:609:ASP:OD1 | 2:Bq:611:THR:OG1 | 2.28 | 0.42 |
| 2:Br:23:SER:O | 2:Br:76:ASN:HB2 | 2.20 | 0.42 |
| 2:Br:202:GLU:H | 2:Br:202:GLU:HG3 | 1.60 | 0.42 |
| 2:Br:394:VAL:HG21 | 2:Br:443:ILE:HD12 | 2.02 | 0.42 |
| 2:Bt:57:PRO:HB3 | 2:Bt:65:PHE:HB3 | 2.02 | 0.42 |
| 2:Bu:278:GLN:HG2 | 2:Bu:296:SER:HB3 | 2.01 | 0.42 |
| 2:Bu:510:ARG:HB2 | 2:Bu:513:GLN:HE21 | 1.83 | 0.42 |
| 2:Bv:398:ASP:O | 2:Bv:401:GLN:HG3 | 2.19 | 0.42 |
| 2:Bv:490:SER:OG | 2:Bv:538:ASP:OD2 | 2.31 | 0.42 |
| 2:Bx:34:GLN:NE2 | 2:Bx:56:GLN:H | 2.18 | 0.42 |
| 2:Bz:264:THR:HG21 | 2:Bz:284:ARG:HH22 | 1.84 | 0.42 |
| 3:o:70:THR:HG22 | 3:o:156:THR:HG22 | 2.00 | 0.42 |
| 8:r:41:ILE:HA | 8:r:75:ILE:O | 2.18 | 0.42 |
| 8:r:142:GLN:O | 8:r:144:HIS:N | 2.53 | 0.42 |
| 9:v:14:THR:HB | 9:w:151:PRO:HD2 | 2.01 | 0.42 |
| 2:1:30:ALA:HB3 | 2:1:359:TRP:CE2 | 2.54 | 0.42 |
| 2:1:313:ASP:OD1 | 2:1:313:ASP:N | 2.51 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:197:GLU:HB3 | 2:2:199:GLU:HG2 | 2.01 | 0.42 |
| 2:4:423:VAL:HG21 | 2:4:513:GLN:HB3 | 2.02 | 0.42 |
| 3:8:10:PHE:O | 3:8:11:GLU:HB2 | 2.20 | 0.42 |
| 3:9:161:TYR:CZ | 3:AA:97:ASN:HB2 | 2.55 | 0.42 |
| 5:A0:175:ARG:NH1 | 5:BG:30:SER:OG | 2.52 | 0.42 |
| 5:A0:286:TYR:HB3 | 5:BH:338:ARG:HD2 | 2.01 | 0.42 |
| 5:A0:408:ARG:CZ | 5:A0:450:ARG:HH21 | 2.33 | 0.42 |
| 5:A2:182:VAL:HG22 | 5:A2:208:TYR:CD1 | 2.52 | 0.42 |
| 6:A4:265:GLN:OE1 | 6:A5:236:GLN:HG3 | 2.19 | 0.42 |
| 6:A5:381:ASN:HB3 | 6:A5:521:ILE:HG21 | 2.00 | 0.42 |
| 7:A6:72:GLY:O | 7:A6:171:LYS:HA | 2.20 | 0.42 |
| 6:A8:117:MET:HE3 | 6:A8:451:ALA:HB3 | 2.01 | 0.42 |
| 6:A9:458:PRO:HB3 | 6:A9:473:PHE:CE2 | 2.54 | 0.42 |
| 2:AD:11:LYS:HE2 | 2:AD:11:LYS:HB2 | 1.89 | 0.42 |
| 2:AD:654:LEU:H | 2:AD:654:LEU:HD12 | 1.84 | 0.42 |
| 3:AE:64:ARG:HG2 | 3:AF:93:ALA:HB1 | 2.02 | 0.42 |
| 3:AG:114:ARG:NH2 | 3:AG:116:TYR:OH | 2.36 | 0.42 |
| 3:AH:124:THR:HB | 3:AI:78:ALA:HA | 2.02 | 0.42 |
| 2:AK:94:PRO:HD2 | 2:AK:223:VAL:HG12 | 2.01 | 0.42 |
| 2:AO:171:ILE:H | 2:AO:171:ILE:HG12 | 1.65 | 0.42 |
| 2:AO:514:ARG:NH1 | 2:B5:366:GLU:OE2 | 2.52 | 0.42 |
| 2:AP:109:ASN:N | 2:AP:138:GLY:HA3 | 2.34 | 0.42 |
| 6:AX:94:ALA:O | 6:AX:95:VAL:HG13 | 2.20 | 0.42 |
| 6:AX:426:ASP:OD2 | 6:AX:433:TYR:OH | 2.24 | 0.42 |
| 6:AZ:122:GLY:N | 6:AZ:259:ILE:HG22 | 2.35 | 0.42 |
| 6:AZ:127:LEU:HD12 | 6:AZ:253:ARG:O | 2.20 | 0.42 |
| 6:AZ:285:ASP:OD2 | 6:AZ:288:ALA:N | 2.42 | 0.42 |
| 6:AZ:387:ALA:HB2 | 6:AZ:404:PHE:HB2 | 2.01 | 0.42 |
| 6:Ac:503:ILE:HG23 | 6:Ac:507:LEU:HD12 | 2.02 | 0.42 |
| 6:Ah:264:ARG:HD2 | 6:Ah:477:TYR:HE1 | 1.84 | 0.42 |
| 6:Ai:498:SER:O | 6:Ai:505:ASN:ND2 | 2.52 | 0.42 |
| 6:Aj:142:GLU:HB2 | 6:Aj:490:GLN:HB2 | 2.02 | 0.42 |
| 6:Aj:384:ASN:HD21 | 6:An:362:VAL:HG21 | 1.85 | 0.42 |
| 6:Ak:66:ALA:N | 6:BK:269:ALA:O | 2.51 | 0.42 |
| 6:Ak:252:PHE:HD1 | 6:Ak:252:PHE:N | 2.17 | 0.42 |
| 6:Am:120:PRO:HD3 | 6:Am:453:TYR:CE1 | 2.53 | 0.42 |
| 6:Am:345:TRP:HD1 | 6:Am:348:GLU:HG3 | 1.85 | 0.42 |
| 6:Ao:107:ILE:HD12 | 6:Ao:307:VAL:HG21 | 2.02 | 0.42 |
| 7:As:298:TYR:HD1 | 7:As:298:TYR:HA | 1.74 | 0.42 |
| 6:Au:247:TRP:HB2 | 6:BJ:267:LYS:HE2 | 2.01 | 0.42 |
| 5:Av:29:VAL:HG22 | 5:BB:8:LEU:HD21 | 2.00 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:Av:254:LEU:O | 5:Av:258:VAL:HG23 | 2.20 | 0.42 |
| 5:Av:448:PHE:O | 5:Av:450:ARG:NH1 | 2.52 | 0.42 |
| 6:Aw:131:TYR:HA | 6:Aw:250:MET:HA | 2.01 | 0.42 |
| 5:Ax:282:ARG:HD3 | 5:Ax:282:ARG:HA | 1.87 | 0.42 |
| 5:Ax:451:ASP:OD2 | 5:BA:405:LYS:NZ | 2.52 | 0.42 |
| 6:Ay:128:ARG:NH1 | 6:Ay:490:GLN:O | 2.53 | 0.42 |
| 6:Az:268:ALA:HB2 | 6:Az:294:LEU:HD11 | 2.01 | 0.42 |
| 2:B1:556:LEU:HD11 | 2:B1:601:ILE:HG12 | 2.02 | 0.42 |
| 2:B3:365:ARG:HA | 2:B3:400:ARG:NH2 | 2.34 | 0.42 |
| 2:B3:379:ALA:HB2 | 2:B3:454:TYR:CE2 | 2.53 | 0.42 |
| 2:B3:641:ASN:HB2 | 2:B4:626:THR:HG22 | 2.01 | 0.42 |
| 2:B4:222:VAL:HA | 2:B4:325:ALA:HB2 | 2.00 | 0.42 |
| 2:B4:365:ARG:HG3 | 2:B4:402:ASP:CG | 2.44 | 0.42 |
| 2:B4:653:GLU:O | 2:B7:17:SER:OG | 2.26 | 0.42 |
| 5:BA:275:ARG:HD3 | 5:BA:355:ASN:CG | 2.44 | 0.42 |
| 5:BB:398:ARG:HB2 | 5:BB:398:ARG:HH11 | 1.85 | 0.42 |
| 5:BD:78:THR:HG21 | 7:BL:134:PHE:CZ | 2.53 | 0.42 |
| 5:BF:43:PHE:O | 5:BF:187:GLU:HA | 2.19 | 0.42 |
| 5:BF:86:TYR:O | 5:BF:87:GLU:HB2 | 2.19 | 0.42 |
| 6:BJ:146:PRO:HB3 | 6:BJ:369:GLY:HA3 | 2.02 | 0.42 |
| 6:BK:131:TYR:CE1 | 6:BK:141:LYS:HB2 | 2.54 | 0.42 |
| 3:Bb:55:ASN:HD21 | 3:Bf:20:LEU:HD11 | 1.84 | 0.42 |
| 3:Bg:82:ARG:HG3 | 3:Bg:153:PHE:CE1 | 2.54 | 0.42 |
| 3:Bn:106:GLU:O | 3:Bn:109:LYS:NZ | 2.41 | 0.42 |
| 2:Bp:609:ASP:N | 2:Bp:609:ASP:OD1 | 2.53 | 0.42 |
| 2:Br:131:ILE:HG12 | 2:Br:143:ILE:HG22 | 2.01 | 0.42 |
| 2:Bs:159:GLU:OE1 | 2:Bs:162:THR:OG1 | 2.36 | 0.42 |
| 2:Bt:438:ASP:OD1 | 2:Bt:438:ASP:N | 2.51 | 0.42 |
| 4:M:5:LEU:HB3 | 4:M:61:ASN:HD21 | 1.85 | 0.42 |
| 1:m:101:SER:HB2 | 8:u:180:ASN:OD1 | 2.20 | 0.42 |
| 8:r:217:HIS:ND1 | 8:r:229:VAL:O | 2.53 | 0.42 |
| 9:w:78:ASP:OD2 | 9:w:82:LYS:NZ | 2.42 | 0.42 |
| 1:0:146:LEU:HB2 | 8:q:66:ALA:HB1 | 2.00 | 0.42 |
| 2:1:454:TYR:HD2 | 2:1:467:TRP:CD1 | 2.34 | 0.42 |
| 2:1:459:ASP:OD2 | 2:1:462:ASN:N | 2.45 | 0.42 |
| 2:3:654:LEU:HD13 | 2:AK:605:ARG:NH1 | 2.35 | 0.42 |
| 2:4:510:ARG:HB3 | 2:4:513:GLN:HG2 | 2.01 | 0.42 |
| 2:5:346:SER:O | 2:5:350:VAL:HG23 | 2.19 | 0.42 |
| 2:5:633:ARG:H | 2:5:633:ARG:HG2 | 1.67 | 0.42 |
| 5:A0:78:THR:HA | 5:A0:81:ASN:HD21 | 1.85 | 0.42 |
| 5:A1:469:MET:HE3 | 5:A1:469:MET:HB2 | 1.85 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A2:58:PHE:CZ | 5:A2:62:PHE:HE2 | 2.37 | 0.42 |
| 5:A2:310:ASN:HA | 5:A2:326:HIS:H | 1.85 | 0.42 |
| 5:A3:292:MET:O | 5:A3:294:ALA:N | 2.45 | 0.42 |
| 7:A6:34:ILE:O | 7:A6:38:ILE:HG12 | 2.19 | 0.42 |
| 6:A9:274:LEU:HD13 | 6:Aj:69:GLY:HA2 | 2.01 | 0.42 |
| 2:AD:109:ASN:N | 2:AD:138:GLY:HA3 | 2.34 | 0.42 |
| 3:AG:82:ARG:NH1 | 3:AG:138:GLY:HA2 | 2.35 | 0.42 |
| 3:AJ:39:THR:HG22 | 3:AJ:71:VAL:HG22 | 2.01 | 0.42 |
| 2:AK:135:ASP:OD1 | 2:AK:136:ALA:N | 2.51 | 0.42 |
| 2:AL:32:LYS:NZ | 2:AL:60:GLU:OE2 | 2.52 | 0.42 |
| 2:AN:454:TYR:HB3 | 2:AN:467:TRP:HD1 | 1.84 | 0.42 |
| 2:AO:444:SER:OG | 2:AO:543:SER:OG | 2.25 | 0.42 |
| 10:AU:299:HIS:ND1 | 10:AU:300:ARG:HG3 | 2.35 | 0.42 |
| 6:AX:154:PHE:CE2 | 6:AX:248:ASN:HB3 | 2.55 | 0.42 |
| 6:AX:323:LEU:HD13 | 6:AX:329:ALA:HA | 2.01 | 0.42 |
| 7:AY:115:ALA:HB1 | 6:Ao:275:ALA:HB3 | 2.00 | 0.42 |
| 7:AY:155:LEU:HD21 | 7:Aq:133:ALA:HB1 | 2.01 | 0.42 |
| 6:AZ:490:GLN:OE1 | 6:AZ:490:GLN:N | 2.51 | 0.42 |
| 7:Ab:107:PHE:O | 7:Ab:111:LEU:HG | 2.19 | 0.42 |
| 6:Ad:176:ASP:OD1 | 6:Ad:177:ILE:N | 2.46 | 0.42 |
| 6:Af:454:VAL:HB | 6:Af:476:ARG:H | 1.83 | 0.42 |
| 6:Ag:84:THR:OG1 | 6:Ag:88:VAL:O | 2.30 | 0.42 |
| 6:Ag:128:ARG:NH1 | 6:Ag:491:ALA:H | 2.17 | 0.42 |
| 7:Al:300:LEU:HD23 | 5:BG:292:MET:HG2 | 2.02 | 0.42 |
| 6:Am:199:ASP:HB2 | 6:Am:211:GLU:HG2 | 2.00 | 0.42 |
| 6:Ao:98:MET:HB2 | 6:Ao:282:HIS:CE1 | 2.55 | 0.42 |
| 6:Ao:383:VAL:HG12 | 6:Ao:406:THR:HG22 | 2.00 | 0.42 |
| 5:Av:183:GLN:HB3 | 5:Av:207:ILE:HD11 | 2.02 | 0.42 |
| 5:Av:458:LYS:HB3 | 5:Av:458:LYS:HE2 | 1.83 | 0.42 |
| 5:Ax:219:GLY:O | 5:Ax:221:MET:N | 2.53 | 0.42 |
| 6:Ay:381:ASN:HB3 | 6:Ay:521:ILE:HD13 | 2.01 | 0.42 |
| 2:B1:253:PRO:HD2 | 2:B1:336:GLY:HA2 | 2.01 | 0.42 |
| 2:B2:130:LYS:HE2 | 2:B2:130:LYS:HB2 | 1.88 | 0.42 |
| 2:B2:131:ILE:HA | 2:B2:143:ILE:HA | 2.01 | 0.42 |
| 2:B4:30:ALA:HB3 | 2:B4:359:TRP:NE1 | 2.34 | 0.42 |
| 2:B5:346:SER:O | 2:B5:350:VAL:HG23 | 2.19 | 0.42 |
| 2:B6:77:ASP:OD2 | 2:B6:79:ARG:NH1 | 2.52 | 0.42 |
| 5:BA:310:ASN:OD1 | 5:BA:323:ASN:ND2 | 2.37 | 0.42 |
| 5:BG:237:TYR:CZ | 5:BG:239:HIS:HB3 | 2.54 | 0.42 |
| 5:BH:267:LEU:HD22 | 5:BH:267:LEU:HA | 1.92 | 0.42 |
| 6:BI:154:PHE:CE2 | 6:BI:248:ASN:HB3 | 2.55 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:BK:145:HIS:CE1 | 6:BK:147:MET:HB2 | 2.55 | 0.42 |
| 6:BM:278:LEU:HD23 | 6:BM:278:LEU:HA | 1.93 | 0.42 |
| 6:BM:318:LYS:O | 6:BM:329:ALA:HA | 2.20 | 0.42 |
| 3:BX:137:VAL:O | 3:Bm:44:GLY:N | 2.43 | 0.42 |
| 3:Bb:30:GLN:HB2 | 2:Bu:579:PHE:CE2 | 2.55 | 0.42 |
| 3:Bd:39:THR:HG22 | 3:Bd:71:VAL:HG22 | 2.00 | 0.42 |
| 2:Bp:171:ILE:H | 2:Bp:171:ILE:HG12 | 1.71 | 0.42 |
| 2:Bs:379:ALA:HB2 | 2:Bs:454:TYR:CE2 | 2.55 | 0.42 |
| 2:Bs:382:SER:OG | 2:Bs:385:THR:HG22 | 2.20 | 0.42 |
| 2:Bs:406:LEU:HD13 | 2:Bs:475:ALA:HB2 | 2.01 | 0.42 |
| 2:Bu:45:THR:HA | 2:Bu:76:ASN:O | 2.19 | 0.42 |
| 2:Bu:651:PHE:HD1 | 2:Bu:651:PHE:HA | 1.69 | 0.42 |
| 2:Bv:538:ASP:OD1 | 2:Bv:538:ASP:N | 2.53 | 0.42 |
| 2:Bx:74:TYR:OH | 2:Bx:500:LEU:N | 2.52 | 0.42 |
| 2:Bx:95:ILE:HD12 | 2:Bx:210:PHE:CE1 | 2.55 | 0.42 |
| 2:By:2:THR:OG1 | 2:By:3:LEU:N | 2.51 | 0.42 |
| 2:By:116:ILE:HD13 | 2:By:171:ILE:HG23 | 2.02 | 0.42 |
| 2:Bz:308:ASN:ND2 | 2:Bz:313:ASP:OD2 | 2.52 | 0.42 |
| 2:Bz:454:TYR:HB3 | 2:Bz:467:TRP:CD1 | 2.54 | 0.42 |
| 4:J:26:LYS:HA | 4:L:34:ALA:HB3 | 2.01 | 0.42 |
| 1:n:239:ASN:OD1 | 1:n:239:ASN:N | 2.52 | 0.42 |
| 8:r:72:LEU:HA | 8:r:72:LEU:HD23 | 1.65 | 0.42 |
| 8:t:111:PRO:HG2 | 8:t:197:TRP:CE3 | 2.55 | 0.42 |
| 9:z:118:ASP:HB2 | 9:z:125:VAL:HG13 | 2.01 | 0.42 |
| 1:0:5:ASP:OD2 | 1:0:8:LEU:N | 2.52 | 0.42 |
| 1:0:87:ALA:HB2 | 1:k:26:ILE:HG23 | 2.01 | 0.42 |
| 2:1:561:LYS:HG2 | 8:q:216:PHE:CE1 | 2.55 | 0.42 |
| 2:2:505:LEU:HD12 | 2:2:505:LEU:HA | 1.88 | 0.42 |
| 2:4:457:GLN:HG2 | 2:4:458:TYR:H | 1.85 | 0.42 |
| 2:4:644:ALA:HA | 2:AL:557:PHE:HZ | 1.84 | 0.42 |
| 2:5:383:LEU:HD23 | 2:5:410:PRO:HG2 | 2.02 | 0.42 |
| 2:5:594:GLY:HA2 | 3:AA:8:ARG:HD3 | 2.02 | 0.42 |
| 3:8:140:LEU:HD11 | 3:8:151:GLN:HB2 | 2.01 | 0.42 |
| 5:A0:382:GLN:NE2 | 5:BG:367:GLN:OE1 | 2.53 | 0.42 |
| 5:A0:453:TYR:HD2 | 5:BG:458:LYS:HZ1 | 1.66 | 0.42 |
| 5:A2:155:ARG:HH12 | 5:A2:250:ILE:HB | 1.85 | 0.42 |
| 5:A2:155:ARG:HD2 | 5:A2:157:PHE:HE1 | 1.85 | 0.42 |
| 6:A5:147:MET:SD | 6:A5:367:GLN:HG2 | 2.60 | 0.42 |
| 7:A6:129:TYR:CD1 | 7:Al:105:PRO:HG2 | 2.55 | 0.42 |
| 6:A7:264:ARG:NH1 | 6:A7:305:GLU:OE1 | 2.52 | 0.42 |
| 6:A8:262:LYS:HE3 | 6:A8:500:MET:HE2 | 2.01 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A8:504:LEU:O | 6:A8:509:LYS:NZ | 2.48 | 0.42 |
| 3:AA:21:PHE:CE1 | 3:o:142:LEU:HB3 | 2.55 | 0.42 |
| 3:AA:48:LYS:HE2 | 3:AA:48:LYS:HB3 | 1.90 | 0.42 |
| 9:AC:138:LEU:HD12 | 9:AC:138:LEU:HA | 1.84 | 0.42 |
| 9:AC:145:TYR:OH | 9:z:17:PHE:O | 2.32 | 0.42 |
| 9:AC:167:GLU:OE2 | 2:AD:586:THR:HB | 2.19 | 0.42 |
| 2:AL:455:LYS:HB2 | 2:AL:470:LEU:HD13 | 2.01 | 0.42 |
| 2:AM:69:MET:O | 2:AM:73:GLN:HG2 | 2.20 | 0.42 |
| 2:AM:456:TYR:O | 2:AM:503:ILE:HG12 | 2.19 | 0.42 |
| 2:AM:527:GLY:HA2 | 2:AM:533:TYR:HD1 | 1.84 | 0.42 |
| 2:AO:389:VAL:O | 2:AO:393:VAL:HG23 | 2.20 | 0.42 |
| 2:AP:373:PHE:HB2 | 2:AP:405:VAL:HG22 | 2.01 | 0.42 |
| 2:AP:400:ARG:HB2 | 2:AP:403:CYS:SG | 2.60 | 0.42 |
| 2:AP:540:THR:OG1 | 2:AP:550:ARG:N | 2.53 | 0.42 |
| 10:AR:317:LYS:HG3 | 10:AR:321:GLU:CD | 2.44 | 0.42 |
| 7:Ab:268:GLY:HA3 | 7:Ar:275:VAL:HA | 2.00 | 0.42 |
| 6:Ae:354:LEU:HD22 | 6:Ay:400:LEU:HD21 | 2.01 | 0.42 |
| 6:Ap:350:PHE:HB2 | 6:Ap:389:VAL:HG11 | 2.02 | 0.42 |
| 7:As:309:GLY:O | 5:BB:309:LYS:HE3 | 2.20 | 0.42 |
| 7:At:22:ALA:HB1 | 7:At:23:PRO:HD2 | 2.01 | 0.42 |
| 7:At:298:TYR:HD1 | 7:At:298:TYR:HA | 1.74 | 0.42 |
| 5:Av:283:ARG:O | 5:BB:333:ASP:HB3 | 2.20 | 0.42 |
| 6:Aw:452:PRO:HA | 6:Aw:477:TYR:HA | 2.01 | 0.42 |
| 6:Ay:151:ASP:HB3 | 6:Ay:154:PHE:HB2 | 2.02 | 0.42 |
| 6:Az:380:ARG:HD3 | 6:Az:380:ARG:H | 1.84 | 0.42 |
| 2:B1:116:ILE:HD11 | 2:B1:131:ILE:HG13 | 2.02 | 0.42 |
| 2:B1:406:LEU:HD13 | 2:B1:475:ALA:HB2 | 2.02 | 0.42 |
| 2:B1:536:TYR:HD1 | 2:B1:536:TYR:HA | 1.74 | 0.42 |
| 2:B3:261:ARG:HG2 | 2:B3:262:ALA:H | 1.84 | 0.42 |
| 2:B4:653:GLU:HB2 | 2:B7:16:GLN:HA | 2.01 | 0.42 |
| 2:B5:365:ARG:HA | 2:B5:400:ARG:NH2 | 2.34 | 0.42 |
| 2:B5:510:ARG:H | 2:B5:513:GLN:NE2 | 2.14 | 0.42 |
| 2:B6:69:MET:O | 2:B6:73:GLN:HG2 | 2.19 | 0.42 |
| 5:BA:243:VAL:HB | 5:BA:247:GLY:HA2 | 2.02 | 0.42 |
| 5:BB:398:ARG:HA | 5:BB:398:ARG:HD3 | 1.78 | 0.42 |
| 5:BD:314:TYR:CD1 | 5:BD:316:ALA:HB2 | 2.55 | 0.42 |
| 5:BF:285:TRP:CZ3 | 5:BF:347:VAL:HB | 2.55 | 0.42 |
| 5:BF:295:ARG:HA | 5:BF:295:ARG:HD3 | 1.88 | 0.42 |
| 5:BG:354:ASP:OD1 | 5:BG:354:ASP:N | 2.52 | 0.42 |
| 5:BH:496:GLU:H | 5:BH:496:GLU:CD | 2.28 | 0.42 |
| 7:BL:90:THR:O | 7:BL:96:THR:HA | 2.20 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:BP:2:ALA:N | 11:BP:61:GLU:OE2 | 2.52 | 0.42 |
| 11:BS:22:LYS:NZ | 11:BS:80:GLY:O | 2.53 | 0.42 |
| 3:BY:40:ALA:H | 3:BY:69:TRP:HE1 | 1.68 | 0.42 |
| 3:Bc:23:VAL:HG11 | 3:Bc:39:THR:HG21 | 2.01 | 0.42 |
| 3:Bg:136:ASN:O | 3:Bg:136:ASN:ND2 | 2.53 | 0.42 |
| 3:Bk:41:LEU:HD23 | 3:Bn:140:LEU:HB3 | 2.02 | 0.42 |
| 3:Bm:82:ARG:NH1 | 3:Bm:138:GLY:HA2 | 2.31 | 0.42 |
| 3:Bm:83:GLN:HA | 3:Bm:86:VAL:HG22 | 2.02 | 0.42 |
| 2:Bq:116:ILE:HG12 | 2:Bq:171:ILE:HG12 | 2.00 | 0.42 |
| 2:Bq:383:LEU:HD11 | 2:Bq:436:TYR:HE1 | 1.84 | 0.42 |
| 2:Bq:406:LEU:HD13 | 2:Bq:475:ALA:HB2 | 2.02 | 0.42 |
| 2:Br:299:ARG:H | 2:Br:299:ARG:HD2 | 1.84 | 0.42 |
| 2:Br:409:PRO:HB3 | 2:Br:426:LEU:HD21 | 2.01 | 0.42 |
| 2:Bs:538:ASP:OD1 | 2:Bs:538:ASP:N | 2.51 | 0.42 |
| 2:Bs:614:THR:C | 2:Bs:616:SER:H | 2.27 | 0.42 |
| 2:Bw:39:PHE:HB3 | 2:Bw:361:PHE:CE1 | 2.55 | 0.42 |
| 2:Bw:528:THR:HA | 2:Bx:367:SER:HA | 2.01 | 0.42 |
| 2:Bx:89:ALA:HA | 2:Bx:345:SER:HA | 2.01 | 0.42 |
| 2:Bx:120:TYR:CD2 | 2:Bx:121:VAL:HG22 | 2.54 | 0.42 |
| 2:Bz:152:ALA:O | 2:Bz:156:GLU:HG2 | 2.19 | 0.42 |
| 2:Bz:510:ARG:HG2 | 2:Bz:511:GLN:H | 1.85 | 0.42 |
| 4:D:23:SER:HB3 | 4:D:46:ARG:HE | 1.85 | 0.42 |
| 3:o:48:LYS:HG3 | 3:o:59:ASN:HB3 | 2.01 | 0.42 |
| 1:p:166:ILE:HD13 | 1:p:166:ILE:HA | 1.91 | 0.42 |
| 8:r:6:TYR:CD1 | 8:s:132:GLN:HG2 | 2.55 | 0.42 |
| 8:u:252:LYS:NZ | 8:u:270:PRO:HG2 | 2.35 | 0.42 |
| 2:1:480:ARG:C | 2:1:482:ASP:H | 2.27 | 0.42 |
| 2:2:30:ALA:HB3 | 2:2:359:TRP:CE2 | 2.55 | 0.42 |
| 2:2:121:VAL:HG22 | 2:2:166:ASN:HB3 | 2.02 | 0.42 |
| 3:9:125:LYS:HG2 | 3:AA:79:HIS:CG | 2.54 | 0.42 |
| 5:A0:412:HIS:HB3 | 5:BH:141:ARG:HG3 | 2.02 | 0.42 |
| 5:A1:282:ARG:O | 5:A1:350:LEU:HB3 | 2.20 | 0.42 |
| 5:A1:373:LEU:HD23 | 5:A1:373:LEU:HA | 1.89 | 0.42 |
| 5:A3:134:LEU:O | 5:A3:137:LEU:O | 2.37 | 0.42 |
| 5:A3:220:ARG:HG3 | 5:A3:221:MET:H | 1.84 | 0.42 |
| 5:A3:350:LEU:HD12 | 5:A3:351:PRO:HD2 | 2.01 | 0.42 |
| 6:A5:257:GLN:NE2 | 6:A5:481:ILE:O | 2.52 | 0.42 |
| 7:A6:33:GLN:HE22 | 7:A6:262:ILE:HD11 | 1.85 | 0.42 |
| 6:A8:91:ILE:HD13 | 6:A8:281:VAL:HG13 | 2.02 | 0.42 |
| 6:A9:147:MET:O | 6:A9:185:THR:HB | 2.20 | 0.42 |
| 3:AA:43:ALA:HB2 | 3:o:139:GLU:HA | 2.01 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:AC:167:GLU:OE1 | 2:AD:582:SER:OG | 2.37 | 0.42 |
| 3:AI:25:ILE:HD12 | 3:AI:28:LEU:HD12 | 2.02 | 0.42 |
| 2:AL:10:LEU:HD13 | 2:Bs:561:LYS:HD2 | 2.01 | 0.42 |
| 2:AL:467:TRP:HH2 | 2:Bv:199:GLU:HB2 | 1.85 | 0.42 |
| 2:AL:510:ARG:HG2 | 2:AL:511:GLN:H | 1.84 | 0.42 |
| 2:AM:383:LEU:HD22 | 2:AM:439:ASN:HB2 | 2.01 | 0.42 |
| 2:AP:285:ARG:NH1 | 2:AP:286:ASN:OD1 | 2.53 | 0.42 |
| 10:AS:328:ASP:OD1 | 10:AS:329:ASP:N | 2.53 | 0.42 |
| 6:AV:91:ILE:HA | 6:BJ:125:PHE:HZ | 1.84 | 0.42 |
| 6:AV:129:ALA:HB3 | 6:AV:143:ALA:HB3 | 2.02 | 0.42 |
| 6:AV:290:LEU:HD23 | 6:AV:290:LEU:HA | 1.85 | 0.42 |
| 7:AY:301:ASP:N | 7:AY:301:ASP:OD1 | 2.50 | 0.42 |
| 6:AZ:93:PRO:O | 6:Ad:123:GLN:NE2 | 2.53 | 0.42 |
| 6:AZ:104:PRO:HD2 | 6:AZ:300:LEU:HD21 | 2.02 | 0.42 |
| 6:AZ:494:SER:HA | 11:BN:37:ASP:CG | 2.45 | 0.42 |
| 7:Aa:69:TYR:HE1 | 7:Aa:177:GLN:HA | 1.85 | 0.42 |
| 7:Ab:306:ILE:HD11 | 5:Av:345:THR:HG21 | 2.01 | 0.42 |
| 6:Ad:304:ARG:HD3 | 6:Ad:428:TYR:HD2 | 1.84 | 0.42 |
| 6:Af:317:GLY:O | 6:Af:330:GLY:HA2 | 2.20 | 0.42 |
| 6:Ah:261:ALA:HA | 6:Ah:478:GLY:HA3 | 2.02 | 0.42 |
| 6:Ak:355:PHE:CE2 | 6:Ak:359:LYS:HD2 | 2.55 | 0.42 |
| 6:An:494:SER:HA | 11:BT:37:ASP:CG | 2.45 | 0.42 |
| 7:Aq:7:GLN:HB3 | 7:Aq:239:GLN:H | 1.85 | 0.42 |
| 7:As:138:LEU:HD12 | 5:BB:273:ILE:HD11 | 2.02 | 0.42 |
| 5:Av:36:LEU:HB3 | 5:Av:38:ASP:OD2 | 2.20 | 0.42 |
| 5:Av:398:ARG:HG2 | 5:BB:379:ARG:HD2 | 2.02 | 0.42 |
| 5:Av:485:THR:O | 5:Av:489:ASP:HB3 | 2.20 | 0.42 |
| 6:Ay:383:VAL:HG12 | 6:Ay:406:THR:HG22 | 2.01 | 0.42 |
| 6:Az:127:LEU:HD11 | 6:Az:252:PHE:HB2 | 2.01 | 0.42 |
| 6:Az:437:GLY:HA3 | 6:Az:513:PHE:HD1 | 1.85 | 0.42 |
| 2:B1:169:ALA:HB2 | 2:B1:184:LEU:HD11 | 2.02 | 0.42 |
| 2:B1:563:ASN:OD1 | 2:B1:591:TYR:OH | 2.38 | 0.42 |
| 2:B2:304:ILE:HG21 | 2:By:545:PRO:O | 2.19 | 0.42 |
| 2:B2:430:ARG:HG3 | 2:B2:522:ILE:HD11 | 2.01 | 0.42 |
| 2:B2:481:THR:HB | 2:B2:555:ARG:HH12 | 1.84 | 0.42 |
| 2:B4:241:LYS:NZ | 2:B4:274:GLN:O | 2.50 | 0.42 |
| 2:B4:455:LYS:HE3 | 2:B4:455:LYS:HB2 | 1.89 | 0.42 |
| 2:B5:414:VAL:HG23 | 2:B5:422:ALA:HB1 | 2.02 | 0.42 |
| 5:BA:154:SER:OG | 5:BA:155:ARG:NH1 | 2.53 | 0.42 |
| 5:BB:285:TRP:HZ3 | 5:BB:336:LEU:HD21 | 1.84 | 0.42 |
| 5:BD:86:TYR:C | 5:BD:88:VAL:H | 2.26 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BH:434:GLU:CD | 5:BH:434:GLU:H | 2.28 | 0.42 |
| 6:BI:471:MET:HE3 | 6:BI:471:MET:HB3 | 1.93 | 0.42 |
| 6:BI:494:SER:C | 6:BI:496:ILE:H | 2.28 | 0.42 |
| 6:BJ:128:ARG:NE | 6:BJ:492:PRO:HD3 | 2.35 | 0.42 |
| 6:BJ:314:ALA:HA | 6:BJ:513:PHE:HB2 | 2.00 | 0.42 |
| 6:BJ:433:TYR:HA | 6:BJ:517:TYR:HA | 2.01 | 0.42 |
| 7:BL:13:LYS:HG3 | 7:BL:34:ILE:HG21 | 2.02 | 0.42 |
| 11:BR:10:ILE:HD11 | 11:BR:35:TYR:CE1 | 2.54 | 0.42 |
| 3:BX:89:GLN:NE2 | 3:Bm:46:VAL:HG23 | 2.34 | 0.42 |
| 3:BX:137:VAL:HB | 3:BX:155:VAL:HG13 | 2.02 | 0.42 |
| 3:Bd:41:LEU:HD13 | 3:Bg:140:LEU:HD23 | 2.01 | 0.42 |
| 3:Bf:120:ALA:HB2 | 3:Bh:99:ILE:O | 2.20 | 0.42 |
| 3:Bf:133:TRP:CZ3 | 3:Bf:135:THR:HG22 | 2.54 | 0.42 |
| 2:Bp:315:PHE:CE2 | 2:Bp:325:ALA:HB3 | 2.55 | 0.42 |
| 2:Bp:557:PHE:CZ | 2:Bp:629:ILE:HD11 | 2.55 | 0.42 |
| 2:Br:29:LEU:O | 2:Br:80:VAL:HA | 2.19 | 0.42 |
| 2:Br:130:LYS:HE2 | 2:Br:130:LYS:HB2 | 1.89 | 0.42 |
| 2:Bt:456:TYR:HB3 | 2:Bt:503:ILE:HG23 | 2.02 | 0.42 |
| 2:Bt:655:THR:HB | 2:Bw:19:VAL:HG21 | 2.02 | 0.42 |
| 2:Bu:253:PRO:HB3 | 2:Bu:260:THR:HG22 | 2.02 | 0.42 |
| 2:Bv:222:VAL:HG21 | 2:Bv:238:ILE:HD11 | 2.01 | 0.42 |
| 2:Bz:163:LEU:HD12 | 2:Bz:186:LYS:HA | 2.02 | 0.42 |
| 2:Bz:209:ASP:OD1 | 2:Bz:209:ASP:N | 2.52 | 0.42 |
| 4:C:62:ILE:HD12 | 4:H:58:LEU:HD22 | 2.01 | 0.42 |
| 4:U:29:GLU:HG2 | 4:U:30:GLU:H | 1.83 | 0.42 |
| 1:l:168:LYS:HE3 | 1:l:168:LYS:HB2 | 1.77 | 0.42 |
| 1:m:41:ILE:HD13 | 1:n:5:ASP:HB2 | 2.01 | 0.42 |
| 8:q:61:SER:OG | 8:q:62:GLN:N | 2.41 | 0.42 |
| 8:s:8:SER:O | 8:s:12:ARG:HG3 | 2.20 | 0.42 |
| 8:t:212:THR:OG1 | 8:t:235:SER:OG | 2.14 | 0.42 |
| 8:u:60:ASN:OD1 | 8:u:60:ASN:N | 2.51 | 0.42 |
| 1:0:26:ILE:HG22 | 1:0:27:LEU:HB2 | 2.02 | 0.42 |
| 2:1:269:PHE:CE2 | 2:1:280:ALA:HB1 | 2.55 | 0.42 |
| 2:2:584:PHE:CE2 | 2:2:627:PHE:HZ | 2.38 | 0.42 |
| 2:3:90:LYS:H | 2:3:344:LEU:HB3 | 1.85 | 0.42 |
| 2:3:216:LYS:HB3 | 2:3:216:LYS:HE2 | 1.85 | 0.42 |
| 3:7:16:ALA:O | 3:8:151:GLN:HG2 | 2.19 | 0.42 |
| 3:9:56:ARG:NH2 | 3:o:94:GLY:O | 2.52 | 0.42 |
| 3:9:59:ASN:OD1 | 3:9:59:ASN:N | 2.53 | 0.42 |
| 5:A1:160:LYS:NZ | 5:A1:424:THR:OG1 | 2.38 | 0.42 |
| 5:A2:380:ILE:HD12 | 5:A2:381:PRO:HD2 | 2.02 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A2:440:GLU:O | 5:A2:444:ILE:HG22 | 2.19 | 0.42 |
| 5:A3:214:SER:HB3 | 5:A3:215:TYR:CE2 | 2.55 | 0.42 |
| 5:A3:333:ASP:OD1 | 5:A3:333:ASP:N | 2.51 | 0.42 |
| 6:A4:253:ARG:O | 6:A4:254:ILE:HB | 2.19 | 0.42 |
| 6:A8:378:ALA:HB1 | 6:A8:382:VAL:HB | 2.01 | 0.42 |
| 8:AB:111:PRO:HB2 | 8:AB:197:TRP:HB3 | 2.01 | 0.42 |
| 2:AD:538:ASP:OD1 | 2:AD:538:ASP:N | 2.52 | 0.42 |
| 3:AG:97:ASN:O | 3:BX:3:VAL:N | 2.49 | 0.42 |
| 3:AI:37:LYS:HB2 | 3:AI:37:LYS:HZ2 | 1.85 | 0.42 |
| 2:AK:455:LYS:HG3 | 2:AK:502:VAL:HG13 | 2.02 | 0.42 |
| 2:AK:617:VAL:CG2 | 2:AK:622:GLU:HB2 | 2.49 | 0.42 |
| 2:AN:284:ARG:HG2 | 2:AN:289:ILE:HD13 | 2.02 | 0.42 |
| 2:AN:365:ARG:HA | 2:AN:400:ARG:NH2 | 2.35 | 0.42 |
| 6:AV:363:GLU:HA | 6:AV:366:ARG:HG2 | 2.02 | 0.42 |
| 6:AW:154:PHE:CZ | 6:AW:248:ASN:HB3 | 2.55 | 0.42 |
| 6:AX:258:VAL:O | 6:AX:499:GLY:N | 2.40 | 0.42 |
| 7:AY:271:LEU:HB3 | 7:AY:272:PRO:HD2 | 2.02 | 0.42 |
| 7:Aa:221:ASN:HB3 | 7:Aa:224:HIS:CE1 | 2.54 | 0.42 |
| 7:Ab:52:GLY:O | 7:Ab:189:LYS:HA | 2.20 | 0.42 |
| 7:Ab:232:GLY:HA3 | 4:i:38:TYR:HE2 | 1.84 | 0.42 |
| 6:Ad:313:SER:HA | 6:Ad:506:SER:O | 2.19 | 0.42 |
| 6:Af:278:LEU:HD11 | 6:Aj:252:PHE:HE2 | 1.85 | 0.42 |
| 6:Af:345:TRP:CE2 | 6:Aj:348:GLU:HB2 | 2.55 | 0.42 |
| 6:Ag:350:PHE:HD2 | 6:Ag:389:VAL:HG13 | 1.84 | 0.42 |
| 6:Ah:264:ARG:HD2 | 6:Ah:477:TYR:CE1 | 2.55 | 0.42 |
| 6:Ah:344:ARG:HE | 6:BI:344:ARG:NH1 | 2.17 | 0.42 |
| 6:Ah:500:MET:O | 6:Ah:505:ASN:ND2 | 2.48 | 0.42 |
| 6:Ai:153:MET:HG3 | 6:Ai:225:ALA:HA | 2.01 | 0.42 |
| 6:Ao:123:GLN:NE2 | 6:BK:91:ILE:HG23 | 2.35 | 0.42 |
| 7:Ar:29:LEU:HD11 | 7:Ar:258:LEU:HD12 | 2.02 | 0.42 |
| 6:Au:290:LEU:HD21 | 6:Ay:251:GLY:HA2 | 2.00 | 0.42 |
| 6:Au:290:LEU:HD23 | 6:Au:290:LEU:HA | 1.83 | 0.42 |
| 6:Au:485:ALA:O | 6:Au:486:GLU:HB3 | 2.20 | 0.42 |
| 2:B1:626:THR:HG22 | 2:Bz:641:ASN:HB2 | 2.00 | 0.42 |
| 2:B2:400:ARG:NH1 | 2:B2:402:ASP:OD1 | 2.53 | 0.42 |
| 2:B2:653:GLU:HB2 | 2:B5:16:GLN:HA | 2.02 | 0.42 |
| 2:B3:29:LEU:O | 2:B3:80:VAL:HA | 2.20 | 0.42 |
| 2:B6:557:PHE:HB3 | 2:B6:561:LYS:HZ1 | 1.85 | 0.42 |
| 2:B7:505:LEU:HB2 | 2:B7:533:TYR:CE2 | 2.54 | 0.42 |
| 5:BA:333:ASP:CG | 5:BH:283:ARG:HB3 | 2.45 | 0.42 |
| 7:BC:95:ILE:HG13 | 7:BC:148:MET:HE1 | 2.02 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BC:207:VAL:HG23 | 4:g:29:GLU:O | 2.20 | 0.42 |
| 5:BD:82:LEU:HD22 | 5:BD:258:VAL:HG22 | 2.02 | 0.42 |
| 5:BG:242:LEU:HB3 | 5:BG:251:ILE:HG13 | 2.02 | 0.42 |
| 5:BH:329:SER:N | 5:BH:332:GLU:OE1 | 2.52 | 0.42 |
| 6:BI:149:GLY:H | 6:BI:185:THR:C | 2.28 | 0.42 |
| 11:BN:38:VAL:HG21 | 11:BN:65:ARG:HH12 | 1.83 | 0.42 |
| 3:BX:99:ILE:HG12 | 3:Bj:56:ARG:HG3 | 2.02 | 0.42 |
| 3:Be:48:LYS:HB3 | 3:Be:48:LYS:HE3 | 1.82 | 0.42 |
| 3:Bf:41:LEU:HD22 | 3:Bi:140:LEU:HD23 | 2.02 | 0.42 |
| 2:Bp:11:LYS:HG2 | 2:Bp:13:THR:HG23 | 2.01 | 0.42 |
| 2:Bp:566:ARG:HA | 2:Bp:569:LYS:HE2 | 2.01 | 0.42 |
| 2:Bq:121:VAL:HG13 | 2:Bq:166:ASN:HB3 | 2.02 | 0.42 |
| 2:Bq:412:GLU:HA | 2:Bq:415:VAL:HG12 | 2.01 | 0.42 |
| 2:Bq:413:THR:C | 2:Bq:417:ILE:HD11 | 2.45 | 0.42 |
| 2:Br:57:PRO:HB3 | 2:Br:65:PHE:HB3 | 2.02 | 0.42 |
| 2:Br:256:PRO:HG2 | 2:Br:339:THR:H | 1.85 | 0.42 |
| 2:Br:414:VAL:HG23 | 2:Br:422:ALA:HB1 | 2.01 | 0.42 |
| 2:Bs:166:ASN:OD1 | 2:Bs:166:ASN:N | 2.53 | 0.42 |
| 2:Bt:639:THR:HB | 2:Bu:624:VAL:HG12 | 2.01 | 0.42 |
| 2:Bu:33:PHE:O | 2:Bu:82:ARG:NE | 2.53 | 0.42 |
| 2:Bu:82:ARG:NH1 | 2:Bu:227:PRO:O | 2.51 | 0.42 |
| 2:Bu:237:GLU:OE1 | 2:Bu:284:ARG:NH1 | 2.53 | 0.42 |
| 2:Bv:239:VAL:HG22 | 2:Bv:280:ALA:HB3 | 2.01 | 0.42 |
| 2:Bw:94:PRO:HG3 | 2:Bw:338:LEU:HD13 | 2.01 | 0.42 |
| 2:By:130:LYS:HE2 | 2:By:130:LYS:HB2 | 1.73 | 0.42 |
| 2:Bz:481:THR:HG23 | 2:Bz:496:ARG:HD2 | 2.01 | 0.42 |
| 4:U:10:PHE:HB3 | 4:U:22:ILE:HG13 | 2.02 | 0.42 |
| 1:l:146:LEU:HB3 | 8:s:68:VAL:HG12 | 2.01 | 0.42 |
| 8:r:13:TYR:CG | 8:r:116:MET:HE1 | 2.55 | 0.42 |
| 8:r:237:VAL:HG13 | 8:r:240:ARG:HA | 2.00 | 0.42 |
| 8:s:164:LYS:HD3 | 9:w:13:ASN:OD1 | 2.19 | 0.42 |
| 9:w:117:LEU:HD13 | 9:w:121:LYS:HA | 2.02 | 0.42 |
| 9:z:127:SER:OG | 9:z:167:GLU:HB3 | 2.19 | 0.42 |
| 2:3:237:GLU:OE1 | 2:3:284:ARG:NH1 | 2.53 | 0.41 |
| 2:4:140:ILE:H | 2:4:140:ILE:HG13 | 1.72 | 0.41 |
| 2:5:561:LYS:NZ | 8:u:231:GLU:OE2 | 2.39 | 0.41 |
| 3:6:79:HIS:CG | 3:o:125:LYS:HG2 | 2.55 | 0.41 |
| 3:6:82:ARG:O | 3:6:86:VAL:HG13 | 2.19 | 0.41 |
| 5:A1:66:GLU:HB3 | 5:A1:67:PRO:HD3 | 2.00 | 0.41 |
| 5:A1:161:ILE:HD11 | 5:BB:30:SER:HB3 | 2.02 | 0.41 |
| 5:A3:278:ARG:HD2 | 5:BG:283:ARG:HE | 1.85 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A4:377:ILE:HG23 | 6:A4:435:THR:HB | 2.01 | 0.41 |
| 6:A5:147:MET:O | 6:A5:185:THR:N | 2.52 | 0.41 |
| 6:A5:304:ARG:HD2 | 6:A5:304:ARG:HA | 1.93 | 0.41 |
| 6:A8:390:ASP:HB2 | 6:A8:397:ALA:HB3 | 2.01 | 0.41 |
| 6:A8:482:ASN:HD22 | 6:A8:484:PHE:H | 1.67 | 0.41 |
| 3:AA:10:PHE:O | 3:AA:11:GLU:HB2 | 2.20 | 0.41 |
| 3:AA:140:LEU:HD11 | 3:AA:151:GLN:HB2 | 2.01 | 0.41 |
| 3:AF:58:ILE:HD13 | 3:AF:58:ILE:H | 1.84 | 0.41 |
| 2:AK:406:LEU:HD13 | 2:AK:475:ALA:HB2 | 2.00 | 0.41 |
| 2:AM:310:TYR:CE2 | 2:AM:312:ASP:HB2 | 2.55 | 0.41 |
| 2:AN:2:THR:OG1 | 2:AN:3:LEU:N | 2.53 | 0.41 |
| 2:AP:365:ARG:HH21 | 2:AP:401:GLN:HB2 | 1.85 | 0.41 |
| 10:AR:310:TRP:CD1 | 10:AR:311:VAL:HG23 | 2.55 | 0.41 |
| 6:AV:267:LYS:HE3 | 6:AV:470:VAL:HG11 | 2.01 | 0.41 |
| 6:AX:449:TYR:OH | 6:AX:482:ASN:ND2 | 2.38 | 0.41 |
| 7:AY:45:TYR:OH | 7:AY:51:ASP:O | 2.23 | 0.41 |
| 7:Ab:162:TRP:CZ3 | 7:Ar:54:ASN:HA | 2.55 | 0.41 |
| 6:Ae:166:LEU:HA | 6:Ae:166:LEU:HD23 | 1.82 | 0.41 |
| 6:Ag:107:ILE:N | 6:Ag:303:ASN:OD1 | 2.53 | 0.41 |
| 6:Ah:304:ARG:HD2 | 6:Ah:304:ARG:HA | 1.95 | 0.41 |
| 6:Ah:345:TRP:NE1 | 6:Ah:346:ALA:O | 2.53 | 0.41 |
| 6:Am:454:VAL:O | 6:Am:475:THR:OG1 | 2.35 | 0.41 |
| 6:Ap:304:ARG:HD2 | 6:Ap:304:ARG:HA | 1.94 | 0.41 |
| 7:Aq:102:ALA:HB1 | 6:BK:120:PRO:HG2 | 2.02 | 0.41 |
| 7:Ar:162:TRP:CD1 | 7:At:54:ASN:HA | 2.54 | 0.41 |
| 7:Ar:207:VAL:HG23 | 4:h:29:GLU:O | 2.20 | 0.41 |
| 7:At:249:ASP:O | 7:At:252:THR:OG1 | 2.33 | 0.41 |
| 6:Au:337:PRO:HA | 6:Au:340:ILE:HG12 | 2.02 | 0.41 |
| 5:Av:135:ASN:ND2 | 5:Ax:439:ASP:O | 2.53 | 0.41 |
| 5:Av:190:THR:HB | 5:Av:199:VAL:HG12 | 2.01 | 0.41 |
| 5:Av:288:ASP:HA | 5:BB:338:ARG:O | 2.20 | 0.41 |
| 5:Av:381:PRO:HB2 | 5:Ax:377:LEU:HD23 | 2.02 | 0.41 |
| 6:Aw:94:ALA:O | 6:Aw:95:VAL:HG13 | 2.20 | 0.41 |
| 6:Aw:123:GLN:HB3 | 6:BM:93:PRO:HB2 | 2.02 | 0.41 |
| 2:B1:110:TYR:H | 2:B1:138:GLY:CA | 2.32 | 0.41 |
| 2:B1:561:LYS:HG2 | 2:Bz:642:PHE:CZ | 2.54 | 0.41 |
| 2:B2:10:LEU:HD22 | 2:By:642:PHE:HE1 | 1.85 | 0.41 |
| 2:B2:69:MET:O | 2:B2:73:GLN:HG2 | 2.20 | 0.41 |
| 2:B3:527:GLY:HA2 | 2:B3:533:TYR:CD2 | 2.55 | 0.41 |
| 2:B3:572:LEU:HD12 | 2:B3:572:LEU:HA | 1.72 | 0.41 |
| 2:B4:548:PHE:HE1 | 2:B4:557:PHE:CG | 2.37 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B5:315:PHE:CE1 | 2:B5:323:ILE:HG13 | 2.55 | 0.41 |
| 2:B6:536:TYR:HD1 | 2:B6:536:TYR:HA | 1.70 | 0.41 |
| 5:BA:231:PRO:O | 5:BA:233:ALA:N | 2.53 | 0.41 |
| 7:BE:263:LEU:HD22 | 7:BE:277:ILE:HG12 | 2.02 | 0.41 |
| 5:BF:55:ASN:O | 5:BF:59:GLN:HG2 | 2.20 | 0.41 |
| 5:BG:115:LYS:HD3 | 5:BG:445:LYS:HE3 | 2.02 | 0.41 |
| 6:BI:204:ASP:OD1 | 6:BI:205:ALA:N | 2.53 | 0.41 |
| 6:BK:264:ARG:O | 6:BK:474:LYS:HA | 2.20 | 0.41 |
| 11:BU:65:ARG:HB3 | 11:BU:66:THR:H | 1.70 | 0.41 |
| 3:Bd:82:ARG:HH22 | 3:Bd:138:GLY:HA2 | 1.85 | 0.41 |
| 3:Bg:51:VAL:HG23 | 3:Bg:58:ILE:HG12 | 2.02 | 0.41 |
| 3:Bh:48:LYS:HB3 | 3:Bh:48:LYS:HE3 | 1.82 | 0.41 |
| 3:Bj:128:GLU:HB2 | 3:Bj:163:GLU:HB2 | 2.00 | 0.41 |
| 2:Bp:91:ASN:OD1 | 2:Bp:91:ASN:N | 2.53 | 0.41 |
| 2:Bp:372:LEU:HD21 | 2:Bp:478:CYS:HB2 | 2.02 | 0.41 |
| 2:Bp:412:GLU:CD | 2:Bp:412:GLU:H | 2.28 | 0.41 |
| 2:Bq:200:ASN:OD1 | 2:Bq:200:ASN:N | 2.51 | 0.41 |
| 2:Br:33:PHE:HA | 2:Br:61:THR:HG23 | 2.02 | 0.41 |
| 2:Br:379:ALA:HB2 | 2:Br:454:TYR:HE2 | 1.85 | 0.41 |
| 2:Bt:493:GLY:O | 2:Bt:497:GLY:N | 2.50 | 0.41 |
| 2:Bu:550:ARG:HD3 | 2:Bu:550:ARG:HA | 1.94 | 0.41 |
| 2:Bw:455:LYS:HE2 | 2:Bw:502:VAL:HG22 | 2.01 | 0.41 |
| 2:Bx:116:ILE:HD11 | 2:Bx:131:ILE:HG13 | 2.02 | 0.41 |
| 2:Bx:131:ILE:HG12 | 2:Bx:143:ILE:HG22 | 2.01 | 0.41 |
| 2:Bx:315:PHE:CD1 | 2:Bx:324:PHE:HA | 2.55 | 0.41 |
| 2:By:227:PRO:HB2 | 2:By:345:SER:HB3 | 2.01 | 0.41 |
| 2:Bz:202:GLU:H | 2:Bz:202:GLU:HG3 | 1.59 | 0.41 |
| 2:Bz:269:PHE:CE1 | 2:Bz:280:ALA:HB1 | 2.54 | 0.41 |
| 2:Bz:446:THR:OG1 | 2:Bz:554:ARG:NH2 | 2.53 | 0.41 |
| 1:n:2:ALA:HB3 | 1:n:6:LYS:HB2 | 2.02 | 0.41 |
| 1:p:201:LEU:O | 1:p:204:VAL:HG12 | 2.20 | 0.41 |
| 8:r:215:ASP:OD1 | 8:r:215:ASP:N | 2.53 | 0.41 |
| 8:s:46:LYS:HD3 | 8:s:46:LYS:HA | 1.84 | 0.41 |
| 8:s:76:ASN:ND2 | 8:s:121:SER:HB2 | 2.35 | 0.41 |
| 9:v:168:LYS:HD3 | 9:v:173:ILE:HD11 | 2.01 | 0.41 |
| 1:0:49:GLU:OE2 | 7:Ar:265:ARG:NH1 | 2.53 | 0.41 |
| 2:1:545:PRO:HG3 | 2:2:271:TYR:HB3 | 2.01 | 0.41 |
| 3:7:21:PHE:CD1 | 3:8:142:LEU:HB3 | 2.55 | 0.41 |
| 3:8:125:LYS:HD2 | 3:8:125:LYS:HA | 1.80 | 0.41 |
| 5:A0:119:SER:HB2 | 5:A0:122:ILE:HD13 | 2.02 | 0.41 |
| 5:A0:324:GLN:HB3 | 7:BE:99:ASP:HB3 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A1:273:ILE:HD11 | 7:Aq:138:LEU:HB3 | 2.02 | 0.41 |
| 5:A1:495:ASP:OD2 | 5:BD:123:LYS:NZ | 2.49 | 0.41 |
| 5:A2:429:LYS:HE3 | 5:A2:429:LYS:HB2 | 1.92 | 0.41 |
| 5:A3:54:TYR:CZ | 6:AV:410:LYS:HD3 | 2.54 | 0.41 |
| 5:A3:376:PRO:HG3 | 5:A3:403:PHE:HB2 | 2.02 | 0.41 |
| 6:A4:319:SER:HA | 6:A4:323:LEU:HB2 | 2.02 | 0.41 |
| 2:AD:465:ASN:OD1 | 2:AD:465:ASN:N | 2.53 | 0.41 |
| 3:AI:103:LYS:O | 3:AI:106:GLU:HG2 | 2.20 | 0.41 |
| 2:AK:30:ALA:HB3 | 2:AK:359:TRP:NE1 | 2.35 | 0.41 |
| 2:AL:366:GLU:OE1 | 2:AL:367:SER:N | 2.52 | 0.41 |
| 2:AN:153:LYS:O | 2:AN:157:VAL:HG22 | 2.21 | 0.41 |
| 2:AO:95:ILE:HG22 | 2:AO:188:ILE:HG21 | 2.02 | 0.41 |
| 2:AP:202:GLU:H | 2:AP:202:GLU:HG3 | 1.62 | 0.41 |
| 10:AQ:328:ASP:O | 10:AQ:338:ARG:NH1 | 2.53 | 0.41 |
| 6:AX:497:GLN:HE21 | 6:AX:497:GLN:HB3 | 1.65 | 0.41 |
| 7:Aa:59:VAL:HG12 | 7:Aa:183:ILE:HG13 | 2.00 | 0.41 |
| 7:Aa:80:ASN:OD1 | 7:Aa:80:ASN:N | 2.53 | 0.41 |
| 6:Ad:453:TYR:CD2 | 6:Ad:454:VAL:HG23 | 2.55 | 0.41 |
| 6:Ae:278:LEU:HD23 | 6:Ae:278:LEU:HA | 1.89 | 0.41 |
| 6:Ag:154:PHE:CE2 | 6:Ag:248:ASN:HB3 | 2.54 | 0.41 |
| 6:Ag:264:ARG:NH1 | 6:Ag:305:GLU:OE1 | 2.52 | 0.41 |
| 6:Aj:164:PRO:HG2 | 6:Aj:178:TYR:HD1 | 1.84 | 0.41 |
| 6:Ao:430:LYS:HD3 | 6:Ao:430:LYS:HA | 1.81 | 0.41 |
| 6:Ap:123:GLN:HB3 | 6:BI:93:PRO:HB2 | 2.01 | 0.41 |
| 6:Ap:225:ALA:HB3 | 6:BI:305:GLU:HA | 2.00 | 0.41 |
| 7:As:217:GLU:HG3 | 7:As:224:HIS:HD1 | 1.85 | 0.41 |
| 6:Az:398:GLN:HG2 | 6:Az:399:GLY:H | 1.84 | 0.41 |
| 2:B1:351:THR:OG1 | 2:B1:352:ALA:N | 2.54 | 0.41 |
| 2:B1:557:PHE:HZ | 2:Bz:644:ALA:HA | 1.85 | 0.41 |
| 2:B4:411:ARG:HB2 | 2:B4:454:TYR:HE2 | 1.85 | 0.41 |
| 2:B5:107:GLY:HA3 | 2:B5:110:TYR:CE2 | 2.55 | 0.41 |
| 2:B5:160:TYR:CE1 | 2:B5:187:ILE:HG21 | 2.54 | 0.41 |
| 2:B7:617:VAL:HG22 | 2:B7:622:GLU:HB2 | 2.02 | 0.41 |
| 5:BB:187:GLU:OE1 | 5:BB:205:TYR:OH | 2.32 | 0.41 |
| 5:BG:99:ALA:HB2 | 5:BG:407:ILE:HD12 | 2.02 | 0.41 |
| 6:BI:191:GLN:HB2 | 6:BI:224:ILE:HG21 | 2.02 | 0.41 |
| 6:BK:85:SER:HB2 | 11:BU:35:TYR:CE2 | 2.55 | 0.41 |
| 6:BK:238:GLY:HA2 | 6:BK:242:SER:O | 2.20 | 0.41 |
| 6:BM:157:GLN:NE2 | 6:BM:227:GLY:O | 2.51 | 0.41 |
| 11:BN:38:VAL:HG11 | 11:BN:69:ILE:HG12 | 2.01 | 0.41 |
| 3:BZ:133:TRP:CH2 | 3:Bo:61:ALA:HA | 2.56 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bb:139:GLU:OE2 | 3:Bb:141:GLN:NE2 | 2.52 | 0.41 |
| 3:Be:119:ASP:OD1 | 3:Bg:101:GLY:N | 2.53 | 0.41 |
| 3:Bi:75:ASN:HD21 | 3:Bi:79:HIS:CG | 2.38 | 0.41 |
| 2:Bq:274:GLN:N | 2:Bq:278:GLN:OE1 | 2.37 | 0.41 |
| 2:Bs:57:PRO:O | 2:Bs:462:ASN:ND2 | 2.36 | 0.41 |
| 2:Bu:69:MET:O | 2:Bu:73:GLN:HG2 | 2.20 | 0.41 |
| 2:Bu:654:LEU:HD23 | 2:Bu:654:LEU:HA | 1.96 | 0.41 |
| 2:Bv:455:LYS:HG3 | 2:Bv:502:VAL:HG13 | 2.02 | 0.41 |
| 2:Bv:467:TRP:CZ3 | 2:Bw:199:GLU:HB2 | 2.56 | 0.41 |
| 2:Bv:505:LEU:HD21 | 2:Bv:525:VAL:HG12 | 2.03 | 0.41 |
| 2:Bw:614:THR:C | 2:Bw:616:SER:H | 2.29 | 0.41 |
| 2:Bx:92:SER:HB3 | 2:Bx:340:LEU:HB3 | 2.02 | 0.41 |
| 2:Bz:32:LYS:HD3 | 2:Bz:64:TYR:HE2 | 1.85 | 0.41 |
| 2:Bz:572:LEU:HD12 | 2:Bz:572:LEU:HA | 1.85 | 0.41 |
| 4:S:9:PRO:HD3 | 4:S:57:VAL:HG21 | 2.02 | 0.41 |
| 1:k:152:VAL:HG13 | 1:k:169:ILE:HD13 | 2.02 | 0.41 |
| 1:l:90:LEU:HA | 1:l:90:LEU:HD23 | 1.80 | 0.41 |
| 1:m:61:VAL:HG22 | 1:m:83:ALA:HB2 | 2.02 | 0.41 |
| 1:m:74:GLU:HB2 | 8:t:126:TYR:HD1 | 1.85 | 0.41 |
| 1:m:81:THR:HG23 | 1:m:82:LYS:HG3 | 2.01 | 0.41 |
| 3:o:52:GLY:HA3 | 3:o:57:LYS:HZ3 | 1.85 | 0.41 |
| 8:q:99:GLN:NE2 | 8:q:102:ALA:HA | 2.35 | 0.41 |
| 8:r:81:ASP:OD1 | 8:r:82:PHE:N | 2.53 | 0.41 |
| 8:t:76:ASN:HD22 | 8:t:121:SER:HB2 | 1.85 | 0.41 |
| 9:v:119:ASN:HB2 | 9:w:79:GLU:HG3 | 2.02 | 0.41 |
| 1:0:152:VAL:HG13 | 1:0:169:ILE:HD13 | 2.02 | 0.41 |
| 2:2:614:THR:C | 2:2:616:SER:H | 2.27 | 0.41 |
| 2:3:378:CYS:HB2 | 2:3:454:TYR:OH | 2.20 | 0.41 |
| 2:5:51:VAL:HG22 | 2:5:65:PHE:HZ | 1.84 | 0.41 |
| 2:5:116:ILE:HD11 | 2:5:131:ILE:HG12 | 2.01 | 0.41 |
| 2:5:157:VAL:HG23 | 2:5:159:GLU:H | 1.85 | 0.41 |
| 5:A2:420:ASP:HB3 | 5:A2:421:PRO:HD3 | 2.02 | 0.41 |
| 5:A3:279:ALA:N | 5:A3:280:PRO:HD2 | 2.35 | 0.41 |
| 6:A4:155:SER:OG | 6:A9:301:GLU:OE1 | 2.26 | 0.41 |
| 6:A9:304:ARG:HD2 | 6:A9:304:ARG:HA | 1.79 | 0.41 |
| 6:A9:502:SER:HB3 | 6:A9:505:ASN:ND2 | 2.35 | 0.41 |
| 3:AA:37:LYS:HB3 | 3:AA:74:MET:HE3 | 2.01 | 0.41 |
| 9:AC:113:THR:HG22 | 9:AC:129:ASN:HD22 | 1.84 | 0.41 |
| 2:AK:61:THR:HG22 | 2:AK:65:PHE:HB2 | 2.02 | 0.41 |
| 2:AL:430:ARG:NH2 | 2:AL:541:ALA:HB1 | 2.35 | 0.41 |
| 2:AM:23:SER:O | 2:AM:76:ASN:HB2 | 2.21 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AM:383:LEU:HD11 | 2:AM:436:TYR:CD1 | 2.45 | 0.41 |
| 2:AN:39:PHE:HB3 | 2:AN:361:PHE:CE1 | 2.55 | 0.41 |
| 2:AN:152:ALA:O | 2:AN:156:GLU:HG2 | 2.19 | 0.41 |
| 2:AP:376:GLY:HA3 | 2:AP:471:ALA:HB3 | 2.03 | 0.41 |
| 6:AW:450:TYR:CE1 | 6:AW:477:TYR:HB2 | 2.54 | 0.41 |
| 6:AX:67:GLU:H | 6:AX:67:GLU:HG3 | 1.58 | 0.41 |
| 7:AY:166:ALA:N | 7:Aq:51:ASP:OD2 | 2.54 | 0.41 |
| 7:AY:191:TYR:HA | 7:AY:239:GLN:NE2 | 2.36 | 0.41 |
| 7:Ab:92:ILE:HD12 | 7:Ab:93:GLY:H | 1.85 | 0.41 |
| 7:Ab:138:LEU:HD23 | 7:Ab:138:LEU:HA | 1.91 | 0.41 |
| 6:Ac:127:LEU:HD11 | 6:Ac:252:PHE:HB2 | 2.01 | 0.41 |
| 6:Ad:75:ASN:OD1 | 6:Ad:76:ALA:N | 2.53 | 0.41 |
| 6:Ae:345:TRP:HD1 | 6:Ai:344:ARG:HH12 | 1.66 | 0.41 |
| 6:Af:117:MET:HB2 | 6:Af:453:TYR:CD1 | 2.54 | 0.41 |
| 6:Af:351:LYS:NZ | 6:Af:395:TYR:O | 2.53 | 0.41 |
| 6:Ak:105:ASN:ND2 | 6:Ak:409:THR:O | 2.47 | 0.41 |
| 6:Ak:318:LYS:N | 6:Ak:360:GLU:OE2 | 2.41 | 0.41 |
| 7:Aq:60:PHE:HZ | 7:Aq:76:LEU:HD21 | 1.85 | 0.41 |
| 7:Ar:89:ARG:HB3 | 7:Ar:97:SER:HB3 | 2.01 | 0.41 |
| 7:Ar:147:TYR:HE2 | 7:Ar:151:MET:HE3 | 1.84 | 0.41 |
| 5:Av:69:MET:C | 5:Av:71:THR:H | 2.28 | 0.41 |
| 5:Av:86:TYR:O | 5:Av:87:GLU:HB2 | 2.19 | 0.41 |
| 5:Ax:383:ASP:OD1 | 5:Ax:383:ASP:N | 2.49 | 0.41 |
| 6:Ay:454:VAL:O | 6:Ay:475:THR:OG1 | 2.31 | 0.41 |
| 6:Az:137:ALA:HB3 | 6:Az:140:ALA:HB2 | 2.02 | 0.41 |
| 2:B1:163:LEU:HB3 | 2:B1:164:GLY:H | 1.74 | 0.41 |
| 2:B1:315:PHE:CD1 | 2:B1:324:PHE:HA | 2.56 | 0.41 |
| 2:B2:94:PRO:HB3 | 2:B2:338:LEU:HB3 | 2.01 | 0.41 |
| 2:B2:159:GLU:HB3 | 2:B2:163:LEU:HD23 | 2.03 | 0.41 |
| 2:B2:650:ASP:C | 2:B2:652:ASP:H | 2.28 | 0.41 |
| 2:B4:116:ILE:HA | 2:B4:171:ILE:HA | 2.01 | 0.41 |
| 2:B6:489:MET:HE1 | 2:B7:575:LEU:HD13 | 2.02 | 0.41 |
| 5:BA:399:ASP:OD1 | 5:BA:399:ASP:N | 2.52 | 0.41 |
| 5:BB:315:ASP:HB2 | 5:BB:322:LYS:HG3 | 2.02 | 0.41 |
| 5:BD:55:ASN:O | 5:BD:59:GLN:HG2 | 2.20 | 0.41 |
| 5:BD:474:GLU:HA | 5:BD:477:ILE:HG23 | 2.02 | 0.41 |
| 7:BE:6:PRO:HG3 | 7:BE:15:VAL:HG21 | 2.02 | 0.41 |
| 5:BH:454:PHE:O | 5:BH:458:LYS:HG3 | 2.20 | 0.41 |
| 6:BJ:125:PHE:CD2 | 6:BJ:256:LYS:HB3 | 2.55 | 0.41 |
| 6:BJ:337:PRO:HA | 6:BJ:340:ILE:HG12 | 2.02 | 0.41 |
| 6:BK:340:ILE:HD12 | 6:BK:343:ALA:HB3 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:BX:75:ASN:OD1 | 3:BX:79:HIS:HA | 2.21 | 0.41 |
| 3:Be:10:PHE:HD2 | 3:Be:13:GLY:HA2 | 1.84 | 0.41 |
| 3:Bh:21:PHE:HZ | 3:Bh:38:ALA:HA | 1.85 | 0.41 |
| 3:Bi:14:ASP:OD1 | 3:Bi:14:ASP:N | 2.51 | 0.41 |
| 3:Bi:64:ARG:NH1 | 3:Bl:95:GLN:HG3 | 2.35 | 0.41 |
| 2:Bp:32:LYS:HE2 | 2:Bp:350:VAL:HB | 2.02 | 0.41 |
| 2:Bq:115:LYS:HD2 | 2:Bq:115:LYS:HA | 1.83 | 0.41 |
| 2:Bq:374:ILE:HG22 | 2:Bq:376:GLY:H | 1.86 | 0.41 |
| 2:Br:69:MET:O | 2:Br:73:GLN:HG2 | 2.21 | 0.41 |
| 2:Bt:36:GLY:O | 2:Bt:82:ARG:NH1 | 2.46 | 0.41 |
| 2:Bu:593:GLN:OE1 | 2:Bu:604:TYR:OH | 2.29 | 0.41 |
| 2:Bw:117:THR:HG23 | 2:Bw:127:THR:HG22 | 2.01 | 0.41 |
| 2:Bx:154:ALA:HA | 2:Bx:157:VAL:HG22 | 2.02 | 0.41 |
| 2:Bx:273:PRO:HB3 | 2:Bx:278:GLN:HB2 | 2.02 | 0.41 |
| 2:Bx:609:ASP:OD1 | 2:Bx:611:THR:OG1 | 2.30 | 0.41 |
| 2:By:31:GLY:HA3 | 2:By:64:TYR:CE2 | 2.55 | 0.41 |
| 1:m:211:HIS:HA | 8:t:71:ILE:HG21 | 2.02 | 0.41 |
| 8:t:248:ASP:OD1 | 8:t:248:ASP:N | 2.53 | 0.41 |
| 9:x:11:GLN:HA | 9:y:78:ASP:HA | 2.01 | 0.41 |
| 2:2:574:GLU:OE2 | 9:v:2:SER:N | 2.53 | 0.41 |
| 2:2:642:PHE:CZ | 2:AP:564:ILE:HD11 | 2.55 | 0.41 |
| 2:3:643:VAL:N | 2:AK:627:PHE:O | 2.53 | 0.41 |
| 2:4:390:GLN:HB3 | 2:4:441:PHE:HE2 | 1.84 | 0.41 |
| 2:4:456:TYR:O | 2:4:503:ILE:HG12 | 2.20 | 0.41 |
| 5:A0:239:HIS:HB2 | 5:A0:250:ILE:HD13 | 2.03 | 0.41 |
| 5:A1:162:ILE:HD13 | 5:A1:163:ASP:H | 1.85 | 0.41 |
| 5:A3:82:LEU:HD22 | 5:A3:258:VAL:HG22 | 2.02 | 0.41 |
| 5:A3:411:GLN:O | 5:A3:415:GLU:HG3 | 2.19 | 0.41 |
| 5:A3:454:PHE:CZ | 5:A3:458:LYS:HD2 | 2.55 | 0.41 |
| 6:A4:264:ARG:NH1 | 6:A4:305:GLU:OE1 | 2.53 | 0.41 |
| 6:A5:453:TYR:CD2 | 6:A5:454:VAL:HG23 | 2.55 | 0.41 |
| 6:A7:159:ALA:HB3 | 6:A7:228:MET:HE2 | 2.02 | 0.41 |
| 6:A8:128:ARG:NH1 | 6:A8:490:GLN:O | 2.53 | 0.41 |
| 6:A8:456:LEU:HD12 | 5:BA:65:TYR:HD2 | 1.84 | 0.41 |
| 8:AB:230:PHE:HB3 | 8:AB:258:ASN:HA | 2.03 | 0.41 |
| 3:AE:41:LEU:HD13 | 3:AF:142:LEU:HD22 | 2.01 | 0.41 |
| 3:AF:120:ALA:HB3 | 3:AF:121:LYS:HD2 | 2.02 | 0.41 |
| 3:AG:14:ASP:OD1 | 3:o:103:LYS:HA | 2.21 | 0.41 |
| 3:AJ:67:ASP:OD1 | 3:AJ:67:ASP:N | 2.53 | 0.41 |
| 2:AK:455:LYS:HB2 | 2:AK:470:LEU:HD13 | 2.02 | 0.41 |
| 2:AL:130:LYS:HD3 | 2:AL:132:THR:HG22 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AL:503:ILE:HG13 | 2:AL:504:LYS:N | 2.32 | 0.41 |
| 2:AN:160:TYR:HA | 2:AN:161:PRO:HA | 1.90 | 0.41 |
| 2:AN:450:ILE:O | 2:AN:523:ASN:ND2 | 2.52 | 0.41 |
| 2:AN:494:TYR:CZ | 2:B2:569:LYS:HG3 | 2.56 | 0.41 |
| 2:AP:636:ASN:HD22 | 2:Bp:621:ASN:HB3 | 1.85 | 0.41 |
| 6:AV:204:ASP:OD1 | 6:AV:205:ALA:N | 2.54 | 0.41 |
| 6:AV:250:MET:HE3 | 6:AV:250:MET:HB2 | 1.91 | 0.41 |
| 6:AV:331:VAL:HG11 | 6:AV:519:LYS:HE2 | 2.01 | 0.41 |
| 6:AW:237:GLU:HB2 | 6:AW:247:TRP:HE1 | 1.86 | 0.41 |
| 6:AX:131:TYR:CE1 | 6:AX:141:LYS:HB2 | 2.56 | 0.41 |
| 6:AX:431:GLN:HG3 | 6:AX:432:ASP:H | 1.84 | 0.41 |
| 7:AY:73:VAL:HG11 | 7:Aq:216:SER:HA | 2.01 | 0.41 |
| 7:AY:81:VAL:HG22 | 7:AY:188:THR:HG22 | 2.03 | 0.41 |
| 7:Ab:308:VAL:HG11 | 5:Av:328:MET:HG2 | 2.01 | 0.41 |
| 6:Ac:456:LEU:N | 6:Ac:475:THR:HG22 | 2.32 | 0.41 |
| 6:Ae:498:SER:HB3 | 6:Ae:500:MET:HE3 | 2.02 | 0.41 |
| 6:Af:456:LEU:HD23 | 6:Af:456:LEU:HA | 1.89 | 0.41 |
| 6:An:143:ALA:HB2 | 6:An:250:MET:HE1 | 2.03 | 0.41 |
| 7:Ar:2:SER:N | 4:T:30:GLU:OE2 | 2.54 | 0.41 |
| 6:Au:328:LYS:HD2 | 6:Au:328:LYS:HA | 1.87 | 0.41 |
| 5:Av:96:VAL:HG22 | 5:Av:147:PHE:HD2 | 1.85 | 0.41 |
| 5:Av:160:LYS:NZ | 5:Av:233:ALA:O | 2.31 | 0.41 |
| 6:Aw:431:GLN:HG3 | 6:Aw:432:ASP:H | 1.85 | 0.41 |
| 6:Ay:431:GLN:HG3 | 6:Ay:432:ASP:H | 1.85 | 0.41 |
| 2:B2:332:GLU:CD | 2:B2:332:GLU:H | 2.27 | 0.41 |
| 2:B3:110:TYR:H | 2:B3:138:GLY:HA3 | 1.84 | 0.41 |
| 2:B3:451:ASP:OD1 | 2:B3:452:GLY:N | 2.41 | 0.41 |
| 2:B3:464:VAL:HG12 | 2:B4:313:ASP:HB3 | 2.02 | 0.41 |
| 2:B4:438:ASP:OD1 | 2:B4:438:ASP:N | 2.53 | 0.41 |
| 2:B4:451:ASP:OD2 | 2:B4:470:LEU:HB3 | 2.20 | 0.41 |
| 2:B4:550:ARG:HA | 2:B4:550:ARG:HE | 1.85 | 0.41 |
| 2:B5:451:ASP:HB2 | 2:B5:474:ILE:HD13 | 2.02 | 0.41 |
| 2:B6:379:ALA:HB2 | 2:B6:469:PRO:HD3 | 2.03 | 0.41 |
| 2:B7:104:SER:HG | 2:B7:183:THR:HG1 | 1.61 | 0.41 |
| 5:BB:158:PHE:HB2 | 5:BB:236:VAL:HB | 2.01 | 0.41 |
| 5:BB:248:LYS:HA | 5:BB:248:LYS:HD3 | 1.85 | 0.41 |
| 5:BG:259:LYS:HB3 | 5:BG:260:PRO:HD3 | 2.02 | 0.41 |
| 5:BH:85:ASN:CG | 5:BH:265:LYS:HE2 | 2.45 | 0.41 |
| 5:BH:86:TYR:C | 5:BH:88:VAL:H | 2.28 | 0.41 |
| 6:BI:131:TYR:CE1 | 6:BI:141:LYS:HB2 | 2.56 | 0.41 |
| 6:BI:274:LEU:HD23 | 6:BM:67:GLU:HB3 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:BI:481:ILE:HG12 | 6:BI:499:GLY:O | 2.20 | 0.41 |
| 6:BJ:312:TYR:CE2 | 6:BJ:507:LEU:HD13 | 2.55 | 0.41 |
| 3:BY:77:GLU:OE2 | 3:Bn:118:ARG:N | 2.54 | 0.41 |
| 3:Bf:17:ARG:O | 3:Bi:151:GLN:NE2 | 2.53 | 0.41 |
| 3:Bo:104:PRO:HA | 3:Bo:107:TYR:CZ | 2.55 | 0.41 |
| 2:Bp:159:GLU:OE2 | 2:Bp:166:ASN:ND2 | 2.53 | 0.41 |
| 2:Bv:510:ARG:HG2 | 2:Bv:511:GLN:H | 1.84 | 0.41 |
| 2:Bv:549:ASP:OD1 | 2:By:271:TYR:OH | 2.32 | 0.41 |
| 2:Bw:379:ALA:HB2 | 2:Bw:454:TYR:CE2 | 2.55 | 0.41 |
| 2:By:30:ALA:HB3 | 2:By:359:TRP:CD1 | 2.56 | 0.41 |
| 2:By:32:LYS:HZ3 | 2:By:350:VAL:HB | 1.84 | 0.41 |
| 2:By:44:VAL:HG11 | 2:By:50:LEU:HB2 | 2.02 | 0.41 |
| 1:p:36:TYR:HD1 | 1:p:36:TYR:HA | 1.75 | 0.41 |
| 8:t:142:GLN:O | 8:t:144:HIS:N | 2.54 | 0.41 |
| 1:0:61:VAL:HG22 | 1:0:83:ALA:HB2 | 2.03 | 0.41 |
| 2:1:272:GLY:O | 2:1:274:GLN:NE2 | 2.42 | 0.41 |
| 2:2:303:ASP:OD1 | 2:2:304:ILE:N | 2.53 | 0.41 |
| 2:2:612:ASN:HB3 | 2:2:624:VAL:HG23 | 2.03 | 0.41 |
| 2:4:131:ILE:HD13 | 2:4:140:ILE:HG21 | 2.03 | 0.41 |
| 3:8:99:ILE:HD11 | 3:AI:1:MET:HB2 | 2.03 | 0.41 |
| 4:A:44:MET:HE2 | 4:A:44:MET:HB3 | 1.92 | 0.41 |
| 5:A0:121:LYS:O | 5:A0:125:MET:HG2 | 2.21 | 0.41 |
| 5:A3:82:LEU:HD11 | 5:A3:261:ALA:HB3 | 2.02 | 0.41 |
| 5:A3:481:ILE:HG13 | 5:A3:485:THR:HB | 2.01 | 0.41 |
| 7:A6:127:ARG:HA | 7:A6:127:ARG:NH1 | 2.36 | 0.41 |
| 6:A8:124:VAL:HG21 | 6:A8:444:MET:HE1 | 2.03 | 0.41 |
| 3:AA:36:CYS:HA | 3:AA:73:VAL:HA | 2.03 | 0.41 |
| 3:AA:89:GLN:HG3 | 3:AA:134:PRO:HG2 | 2.01 | 0.41 |
| 3:AF:140:LEU:HD21 | 3:AF:151:GLN:OE1 | 2.19 | 0.41 |
| 3:AI:87:ASP:O | 3:AI:91:ILE:HG13 | 2.20 | 0.41 |
| 2:AL:430:ARG:NH2 | 2:AL:443:ILE:O | 2.52 | 0.41 |
| 2:AL:494:TYR:O | 2:AL:498:GLN:NE2 | 2.52 | 0.41 |
| 2:AL:642:PHE:HB3 | 2:Bv:557:PHE:HE2 | 1.84 | 0.41 |
| 2:AN:256:PRO:HG2 | 2:AN:339:THR:H | 1.85 | 0.41 |
| 2:AO:254:ILE:HG22 | 2:AO:257:GLY:H | 1.85 | 0.41 |
| 2:AO:373:PHE:HZ | 2:AO:400:ARG:HH11 | 1.67 | 0.41 |
| 2:AP:381:GLU:HB3 | 2:AP:385:THR:HG23 | 2.01 | 0.41 |
| 6:AV:400:LEU:HD12 | 6:AV:400:LEU:HA | 1.94 | 0.41 |
| 6:AX:421:TYR:HE2 | 6:BK:400:LEU:HD11 | 1.85 | 0.41 |
| 7:Aa:70:LYS:NZ | 5:Av:318:THR:O | 2.50 | 0.41 |
| 6:Ag:291:SER:HB2 | 6:Ag:471:MET:HE1 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ag:328:LYS:HB2 | 6:Ag:331:VAL:HG13 | 2.02 | 0.41 |
| 6:Ag:426:ASP:HB3 | 6:Ag:429:ALA:HB2 | 2.02 | 0.41 |
| 6:Ai:133:LYS:NZ | 6:Ai:249:GLU:OE2 | 2.53 | 0.41 |
| 6:Aj:515:ARG:NH1 | 6:Aj:517:TYR:OH | 2.54 | 0.41 |
| 6:Ak:426:ASP:OD2 | 6:Ak:433:TYR:OH | 2.31 | 0.41 |
| 6:Am:449:TYR:OH | 6:Am:482:ASN:OD1 | 2.33 | 0.41 |
| 6:An:278:LEU:HD12 | 6:An:284:MET:HB2 | 2.03 | 0.41 |
| 6:An:318:LYS:HD3 | 6:An:356:GLN:CD | 2.45 | 0.41 |
| 6:Ao:97:GLY:HA3 | 6:BM:444:MET:HE2 | 2.03 | 0.41 |
| 6:Ap:270:TYR:HB3 | 6:Ap:290:LEU:CD1 | 2.50 | 0.41 |
| 7:Ar:53:LEU:HD21 | 7:Ar:82:PHE:CD2 | 2.55 | 0.41 |
| 6:Au:350:PHE:HD2 | 6:Au:389:VAL:HG13 | 1.86 | 0.41 |
| 5:Av:440:GLU:O | 5:Av:444:ILE:HG22 | 2.21 | 0.41 |
| 6:Aw:348:GLU:HB3 | 6:Aw:396:ALA:HB2 | 2.03 | 0.41 |
| 5:Ax:420:ASP:HB3 | 5:Ax:421:PRO:HD3 | 2.03 | 0.41 |
| 6:Az:121:THR:HG22 | 6:Az:260:GLU:HG3 | 2.01 | 0.41 |
| 2:B1:572:LEU:HA | 2:B1:572:LEU:HD12 | 1.76 | 0.41 |
| 2:B4:32:LYS:HZ2 | 2:B4:64:TYR:HE2 | 1.67 | 0.41 |
| 2:B4:412:GLU:H | 2:B4:412:GLU:CD | 2.29 | 0.41 |
| 2:B4:567:SER:O | 2:B4:571:ARG:HG2 | 2.20 | 0.41 |
| 2:B7:510:ARG:HG2 | 2:B7:511:GLN:H | 1.85 | 0.41 |
| 5:BB:295:ARG:HA | 5:BB:295:ARG:HD3 | 1.86 | 0.41 |
| 5:BB:304:VAL:O | 5:BB:308:MET:HB3 | 2.20 | 0.41 |
| 5:BB:420:ASP:HB3 | 5:BB:421:PRO:HD3 | 2.03 | 0.41 |
| 7:BE:301:ASP:OD1 | 7:BE:301:ASP:N | 2.53 | 0.41 |
| 5:BG:420:ASP:HB3 | 5:BG:421:PRO:HD3 | 2.03 | 0.41 |
| 6:BJ:408:THR:HG22 | 6:BJ:425:ILE:HG21 | 2.03 | 0.41 |
| 3:BY:47:GLU:HB2 | 3:Bc:148:ASN:OD1 | 2.20 | 0.41 |
| 3:Bd:83:GLN:NE2 | 3:Bd:87:ASP:OD1 | 2.53 | 0.41 |
| 3:Be:98:GLU:OE1 | 3:Be:98:GLU:N | 2.44 | 0.41 |
| 3:Bg:54:MET:O | 3:Bg:56:ARG:N | 2.53 | 0.41 |
| 3:Bg:70:THR:HG22 | 3:Bg:156:THR:HG22 | 2.02 | 0.41 |
| 2:Bp:137:ASP:OD1 | 2:Bp:137:ASP:N | 2.54 | 0.41 |
| 2:Br:95:ILE:HG23 | 2:Br:217:TYR:HE2 | 1.85 | 0.41 |
| 2:Br:389:VAL:O | 2:Br:393:VAL:HG23 | 2.21 | 0.41 |
| 2:Bs:220:PRO:HG2 | 2:Bs:338:LEU:HD11 | 2.01 | 0.41 |
| 2:Bt:115:LYS:HD2 | 2:Bt:115:LYS:HA | 1.86 | 0.41 |
| 2:Bt:283:VAL:O | 2:Bt:290:VAL:HG12 | 2.18 | 0.41 |
| 2:Bw:106:PRO:HB3 | 2:Bw:139:LYS:HD2 | 2.02 | 0.41 |
| 2:By:205:MET:HE2 | 2:By:205:MET:HB3 | 1.93 | 0.41 |
| 2:By:560:LEU:HD21 | 2:By:601:ILE:HD11 | 2.03 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bz:57:PRO:HG3 | 2:Bz:65:PHE:CG | 2.55 | 0.41 |
| 2:Bz:633:ARG:HD2 | 2:Bz:633:ARG:HA | 1.97 | 0.41 |
| 4:T:10:PHE:HB3 | 4:T:22:ILE:HG12 | 2.02 | 0.41 |
| 1:m:152:VAL:HG13 | 1:m:169:ILE:HD13 | 2.03 | 0.41 |
| 8:r:84:TYR:OH | 8:s:143:PRO:HD3 | 2.20 | 0.41 |
| 1:0:176:TYR:HA | 8:q:71:ILE:HG13 | 2.02 | 0.41 |
| 2:2:45:THR:HA | 2:2:76:ASN:O | 2.19 | 0.41 |
| 2:3:612:ASN:HB3 | 2:3:624:VAL:HG23 | 2.01 | 0.41 |
| 2:4:430:ARG:NH2 | 2:4:443:ILE:H | 2.19 | 0.41 |
| 2:4:561:LYS:HG2 | 8:t:216:PHE:CE1 | 2.56 | 0.41 |
| 2:5:310:TYR:HD2 | 2:5:313:ASP:HB2 | 1.84 | 0.41 |
| 3:6:95:GLN:OE1 | 3:o:64:ARG:NH2 | 2.54 | 0.41 |
| 3:8:125:LYS:HG2 | 3:9:79:HIS:CD2 | 2.55 | 0.41 |
| 3:9:125:LYS:HG2 | 3:AA:79:HIS:HB2 | 2.02 | 0.41 |
| 5:A0:160:LYS:HA | 5:A0:174:LEU:HD23 | 2.01 | 0.41 |
| 5:A0:308:MET:HE1 | 5:A0:334:TYR:HE1 | 1.85 | 0.41 |
| 5:A3:36:LEU:HB3 | 5:A3:38:ASP:OD2 | 2.21 | 0.41 |
| 5:A3:481:ILE:HD12 | 5:A3:481:ILE:HA | 1.95 | 0.41 |
| 6:A5:426:ASP:OD2 | 6:A5:433:TYR:OH | 2.32 | 0.41 |
| 6:A5:444:MET:HE2 | 6:A5:444:MET:HB3 | 1.82 | 0.41 |
| 7:A6:23:PRO:HD3 | 1:p:12:LEU:HD21 | 2.03 | 0.41 |
| 9:AC:140:GLU:H | 9:AC:140:GLU:HG3 | 1.55 | 0.41 |
| 2:AD:131:ILE:HD13 | 2:AD:140:ILE:HG21 | 2.00 | 0.41 |
| 2:AD:310:TYR:O | 2:AD:314:PHE:HB2 | 2.20 | 0.41 |
| 2:AD:635:ILE:O | 2:AN:573:PHE:HA | 2.20 | 0.41 |
| 3:AE:77:GLU:HA | 3:AJ:16:ALA:HB2 | 2.02 | 0.41 |
| 3:AF:83:GLN:HA | 3:AF:86:VAL:HG22 | 2.03 | 0.41 |
| 3:AH:56:ARG:HB3 | 3:AH:56:ARG:NH1 | 2.35 | 0.41 |
| 3:AI:91:ILE:HG22 | 3:AI:107:TYR:HB3 | 2.03 | 0.41 |
| 2:AL:66:MET:HG2 | 2:AL:468:VAL:HG21 | 2.01 | 0.41 |
| 2:AL:494:TYR:CZ | 2:Bv:569:LYS:HG3 | 2.56 | 0.41 |
| 2:AN:195:LEU:HD22 | 2:AN:205:MET:HE3 | 2.03 | 0.41 |
| 2:AO:108:SER:O | 2:AO:177:GLY:HA2 | 2.20 | 0.41 |
| 10:AS:325:TRP:HA | 10:AS:338:ARG:HH21 | 1.85 | 0.41 |
| 10:AT:372:ILE:HG22 | 10:AT:373:TYR:HD1 | 1.84 | 0.41 |
| 6:AV:228:MET:HG2 | 6:Ap:263:SER:O | 2.21 | 0.41 |
| 6:AV:322:THR:OG1 | 6:AV:514:ARG:NH2 | 2.54 | 0.41 |
| 7:AY:280:GLN:O | 7:AY:284:GLU:HG2 | 2.20 | 0.41 |
| 6:AZ:133:LYS:HG2 | 6:AZ:249:GLU:HB2 | 2.02 | 0.41 |
| 7:Aa:266:HIS:O | 1:k:54:ARG:NH2 | 2.36 | 0.41 |
| 6:Ac:346:ALA:HB2 | 6:Ag:341:ARG:HD3 | 2.01 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ag:344:ARG:HH21 | 6:Ak:344:ARG:HH12 | 1.68 | 0.41 |
| 6:Ak:131:TYR:HA | 6:Ak:250:MET:HA | 2.02 | 0.41 |
| 6:Ap:404:PHE:HZ | 6:Ap:417:LEU:HG | 1.85 | 0.41 |
| 7:Aq:273:GLY:O | 1:m:160:GLN:NE2 | 2.51 | 0.41 |
| 7:Ar:52:GLY:HA2 | 7:Ar:190:SER:OG | 2.20 | 0.41 |
| 7:At:6:PRO:HG3 | 7:At:15:VAL:HG21 | 2.01 | 0.41 |
| 6:Aw:407:ASP:OD1 | 6:Aw:409:THR:N | 2.53 | 0.41 |
| 6:Ay:345:TRP:HB3 | 6:Ay:348:GLU:HG2 | 2.01 | 0.41 |
| 2:B1:134:VAL:HG12 | 2:B1:140:ILE:HA | 2.03 | 0.41 |
| 2:B1:193:ILE:HB | 2:B1:210:PHE:CD1 | 2.56 | 0.41 |
| 2:B2:163:LEU:HD12 | 2:B2:186:LYS:HA | 2.02 | 0.41 |
| 2:B2:404:LEU:HD12 | 2:B2:406:LEU:HG | 2.02 | 0.41 |
| 2:B2:655:THR:HB | 2:B5:19:VAL:HG21 | 2.01 | 0.41 |
| 2:B4:241:LYS:HB2 | 2:B4:273:PRO:HB2 | 2.02 | 0.41 |
| 2:B4:428:ASN:HA | 2:B4:433:ALA:HB3 | 2.02 | 0.41 |
| 2:B5:406:LEU:HD13 | 2:B5:475:ALA:HB2 | 2.01 | 0.41 |
| 2:B6:134:VAL:HG12 | 2:B6:140:ILE:HG22 | 2.02 | 0.41 |
| 2:B6:404:LEU:HD22 | 2:B6:404:LEU:HA | 1.93 | 0.41 |
| 5:BB:160:LYS:HE2 | 5:BB:424:THR:OG1 | 2.21 | 0.41 |
| 7:BE:28:GLU:OE1 | 1:p:42:LEU:HD11 | 2.21 | 0.41 |
| 7:BE:36:ASP:OD1 | 7:BE:40:ARG:NH1 | 2.53 | 0.41 |
| 7:BE:124:SER:HB3 | 7:BE:127:ARG:NH1 | 2.36 | 0.41 |
| 6:BJ:384:ASN:C | 6:BJ:384:ASN:HD22 | 2.28 | 0.41 |
| 6:BK:345:TRP:O | 6:BK:347:GLY:N | 2.53 | 0.41 |
| 6:BK:486:GLU:HA | 6:BK:509:LYS:O | 2.20 | 0.41 |
| 6:BM:133:LYS:HG3 | 6:BM:249:GLU:CD | 2.45 | 0.41 |
| 6:BM:170:THR:HG22 | 6:BM:198:ILE:HG21 | 2.02 | 0.41 |
| 3:BZ:20:LEU:HA | 3:Bn:54:MET:HE3 | 2.01 | 0.41 |
| 3:BZ:94:GLY:O | 3:Bo:64:ARG:NH1 | 2.54 | 0.41 |
| 3:Bd:20:LEU:HD11 | 3:Bd:118:ARG:HD2 | 2.01 | 0.41 |
| 2:Bp:607:VAL:HB | 2:Bp:626:THR:OG1 | 2.20 | 0.41 |
| 2:Bq:101:TYR:CE2 | 2:Bq:143:ILE:HG12 | 2.55 | 0.41 |
| 2:Bs:266:LYS:HE3 | 2:Bs:266:LYS:HB3 | 1.93 | 0.41 |
| 2:Bt:46:ASN:OD1 | 2:Bt:47:GLU:N | 2.53 | 0.41 |
| 2:Bt:151:ILE:O | 2:Bt:155:LYS:HG2 | 2.20 | 0.41 |
| 2:Bw:114:ASP:OD2 | 2:Bw:131:ILE:HD12 | 2.21 | 0.41 |
| 2:Bw:255:TYR:HB2 | 2:Bw:256:PRO:HD3 | 2.03 | 0.41 |
| 2:Bx:269:PHE:CZ | 2:Bx:280:ALA:HB1 | 2.56 | 0.41 |
| 2:By:284:ARG:HG2 | 2:By:289:ILE:HG12 | 2.02 | 0.41 |
| 2:Bz:518:TYR:CZ | 2:Bz:539:LYS:HE2 | 2.56 | 0.41 |
| 4:G:52:LEU:HD21 | 4:R:12:ASP:HB2 | 2.01 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:K:44:MET:HE2 | 4:K:44:MET:HB3 | 1.87 | 0.41 |
| 1:m:74:GLU:HB2 | 8:t:126:TYR:CD1 | 2.56 | 0.41 |
| 1:m:156:ASP:HB3 | 1:m:157:PRO:HD3 | 2.03 | 0.41 |
| 1:n:207:LEU:O | 1:n:210:ILE:HG13 | 2.21 | 0.41 |
| 8:u:72:LEU:HD23 | 8:u:72:LEU:HA | 1.68 | 0.41 |
| 9:x:46:VAL:HG22 | 9:y:134:TRP:CH2 | 2.55 | 0.41 |
| 9:z:37:VAL:HG13 | 9:z:73:VAL:HG22 | 2.03 | 0.41 |
| 1:0:243:LYS:N | 8:AB:4:TYR:H | 2.17 | 0.41 |
| 2:1:638:ILE:HG23 | 2:AO:623:PHE:HD2 | 1.86 | 0.41 |
| 2:2:157:VAL:HG23 | 2:2:159:GLU:H | 1.86 | 0.41 |
| 2:2:569:LYS:O | 2:2:572:LEU:HB2 | 2.21 | 0.41 |
| 2:3:394:VAL:HG21 | 2:3:441:PHE:HZ | 1.86 | 0.41 |
| 2:5:423:VAL:HG21 | 2:5:513:GLN:HB3 | 2.02 | 0.41 |
| 5:A0:220:ARG:HB2 | 6:BJ:452:PRO:HG2 | 2.03 | 0.41 |
| 5:A1:285:TRP:HZ3 | 5:A1:336:LEU:HD21 | 1.84 | 0.41 |
| 5:A3:61:ILE:HG23 | 5:A3:227:LYS:HB2 | 2.03 | 0.41 |
| 5:A3:216:ALA:O | 5:A3:218:ASP:N | 2.53 | 0.41 |
| 5:A3:477:ILE:HA | 5:A3:481:ILE:HG22 | 2.01 | 0.41 |
| 6:A4:312:TYR:CZ | 6:A4:507:LEU:HG | 2.56 | 0.41 |
| 6:A7:182:PHE:HB2 | 6:A7:184:GLU:O | 2.20 | 0.41 |
| 6:A8:481:ILE:HD11 | 6:A8:501:PRO:HB3 | 2.03 | 0.41 |
| 6:A9:161:LYS:HE3 | 6:A9:163:PHE:CE1 | 2.56 | 0.41 |
| 8:AB:97:LEU:HD21 | 2:AD:575:LEU:HD11 | 2.03 | 0.41 |
| 3:AI:22:GLN:HB2 | 3:AI:116:TYR:HE1 | 1.85 | 0.41 |
| 3:AJ:54:MET:SD | 3:Bm:1:MET:HE1 | 2.60 | 0.41 |
| 2:AK:410:PRO:O | 2:AK:413:THR:HG22 | 2.20 | 0.41 |
| 2:AL:413:THR:C | 2:AL:417:ILE:HD11 | 2.45 | 0.41 |
| 2:AL:535:LEU:HD23 | 2:AL:536:TYR:H | 1.85 | 0.41 |
| 2:AM:454:TYR:HB3 | 2:AM:467:TRP:CD1 | 2.54 | 0.41 |
| 2:AN:252:LEU:HD22 | 2:AN:335:SER:O | 2.21 | 0.41 |
| 2:AO:110:TYR:CD1 | 2:AO:177:GLY:HA3 | 2.55 | 0.41 |
| 2:AP:430:ARG:O | 2:AP:430:ARG:HD3 | 2.21 | 0.41 |
| 10:AR:295:HIS:NE2 | 6:Ag:333:ASP:OD2 | 2.53 | 0.41 |
| 6:AW:232:ILE:O | 6:AW:236:GLN:HG2 | 2.20 | 0.41 |
| 6:AW:310:ILE:HG12 | 6:AW:448:ILE:HG21 | 2.02 | 0.41 |
| 7:AY:23:PRO:HA | 1:n:17:GLY:HA2 | 2.03 | 0.41 |
| 6:Ac:181:PHE:HD1 | 6:Ac:187:THR:HB | 1.85 | 0.41 |
| 6:Ae:486:GLU:CD | 6:Ae:486:GLU:H | 2.28 | 0.41 |
| 6:Af:285:ASP:OD1 | 6:Af:285:ASP:N | 2.37 | 0.41 |
| 6:Ag:255:ASP:OD1 | 6:Ag:255:ASP:N | 2.52 | 0.41 |
| 6:Ah:123:GLN:HB3 | 6:Ah:258:VAL:HG12 | 2.01 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ah:272:ILE:HG13 | 6:Ah:469:PRO:HD3 | 2.03 | 0.41 |
| 6:Ah:376:ILE:HB | 6:Ah:423:VAL:HG22 | 2.01 | 0.41 |
| 6:Ak:237:GLU:N | 6:Ak:245:ASN:O | 2.48 | 0.41 |
| 6:Ak:374:ASN:ND2 | 6:Ak:439:LYS:O | 2.48 | 0.41 |
| 6:Am:304:ARG:NH2 | 6:Am:308:ASP:OD1 | 2.54 | 0.41 |
| 6:Ao:191:GLN:HB2 | 6:Ao:224:ILE:HG21 | 2.02 | 0.41 |
| 6:Ap:131:TYR:HB2 | 6:Ap:154:PHE:CZ | 2.55 | 0.41 |
| 6:Ap:378:ALA:HB1 | 6:Ap:382:VAL:HB | 2.02 | 0.41 |
| 6:Au:249:GLU:HA | 6:BJ:267:LYS:O | 2.21 | 0.41 |
| 5:Av:420:ASP:HB3 | 5:Av:421:PRO:HD3 | 2.02 | 0.41 |
| 5:Av:427:LEU:HD21 | 5:Av:434:GLU:HG3 | 2.03 | 0.41 |
| 6:Aw:107:ILE:C | 6:Aw:303:ASN:HD21 | 2.28 | 0.41 |
| 5:Ax:283:ARG:HH11 | 5:BA:350:LEU:HD21 | 1.86 | 0.41 |
| 5:Ax:451:ASP:O | 5:BA:458:LYS:NZ | 2.30 | 0.41 |
| 6:Az:183:GLN:HG2 | 6:Az:209:ASP:OD2 | 2.21 | 0.41 |
| 2:B1:110:TYR:CE1 | 2:B1:171:ILE:HG21 | 2.52 | 0.41 |
| 2:B2:151:ILE:O | 2:B2:155:LYS:HG2 | 2.21 | 0.41 |
| 2:B3:112:VAL:HG13 | 2:B3:134:VAL:HG13 | 2.03 | 0.41 |
| 2:B3:389:VAL:O | 2:B3:393:VAL:HG23 | 2.21 | 0.41 |
| 2:B5:269:PHE:CE1 | 2:B5:280:ALA:HB1 | 2.55 | 0.41 |
| 2:B5:423:VAL:HG21 | 2:B5:513:GLN:HB3 | 2.03 | 0.41 |
| 2:B5:511:GLN:NE2 | 2:B5:515:ASP:OD1 | 2.53 | 0.41 |
| 2:B6:252:LEU:HB3 | 2:B6:336:GLY:HA2 | 2.03 | 0.41 |
| 5:BA:413:LYS:HA | 5:BA:413:LYS:HD2 | 1.89 | 0.41 |
| 5:BB:71:THR:O | 5:BB:74:GLU:HG3 | 2.20 | 0.41 |
| 5:BD:206:PHE:HE2 | 5:BD:232:LYS:HG2 | 1.86 | 0.41 |
| 5:BD:484:ARG:HA | 5:BD:487:MET:HE2 | 2.02 | 0.41 |
| 5:BD:497:GLU:HA | 5:BD:500:GLN:HG2 | 2.03 | 0.41 |
| 7:BE:28:GLU:H | 7:BE:28:GLU:HG2 | 1.59 | 0.41 |
| 7:BE:269:MET:HE3 | 7:BE:277:ILE:HG21 | 2.03 | 0.41 |
| 5:BF:396:ILE:HD12 | 5:BF:396:ILE:HA | 1.91 | 0.41 |
| 5:BG:26:GLU:O | 5:BG:28:LEU:HG | 2.21 | 0.41 |
| 5:BG:366:ARG:HG2 | 5:BG:380:ILE:HD12 | 2.03 | 0.41 |
| 5:BH:206:PHE:HZ | 5:BH:237:TYR:HB2 | 1.86 | 0.41 |
| 6:BK:108:ALA:HB2 | 6:BK:303:ASN:HB2 | 2.03 | 0.41 |
| 3:Ba:154:GLU:N | 3:Ba:154:GLU:OE1 | 2.53 | 0.41 |
| 3:Bb:67:ASP:N | 3:Bb:67:ASP:OD1 | 2.53 | 0.41 |
| 3:Bb:114:ARG:HB3 | 3:Bb:123:VAL:HG13 | 2.02 | 0.41 |
| 3:Bc:83:GLN:HA | 3:Bc:86:VAL:HG22 | 2.02 | 0.41 |
| 3:Bh:140:LEU:HD21 | 3:Bh:151:GLN:OE1 | 2.20 | 0.41 |
| 3:Bj:64:ARG:HH12 | 3:Bm:95:GLN:NE2 | 2.19 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bm:123:VAL:HG12 | 3:Bm:126:GLU:HB2 | 2.03 | 0.41 |
| 3:Bn:90:SER:HA | 3:Bn:94:GLY:H | 1.84 | 0.41 |
| 2:Bp:365:ARG:HA | 2:Bp:400:ARG:CZ | 2.51 | 0.41 |
| 2:Bp:394:VAL:HG11 | 2:Bp:443:ILE:HD12 | 2.03 | 0.41 |
| 2:Bq:126:GLU:HB2 | 2:Bq:150:ILE:HD11 | 2.03 | 0.41 |
| 2:Bq:238:ILE:HG12 | 2:Bq:281:ILE:HG23 | 2.02 | 0.41 |
| 2:Bq:470:LEU:O | 2:Bq:474:ILE:HG12 | 2.20 | 0.41 |
| 2:Bs:38:ALA:HB3 | 2:Bs:196:ALA:HB1 | 2.02 | 0.41 |
| 2:Bs:222:VAL:HA | 2:Bs:325:ALA:HB2 | 2.03 | 0.41 |
| 2:Bs:519:GLN:HE21 | 2:Bv:4:LEU:HD13 | 1.85 | 0.41 |
| 2:Bv:229:GLU:OE1 | 2:Bv:344:LEU:HD22 | 2.20 | 0.41 |
| 2:Bv:251:LEU:HB3 | 2:Bv:260:THR:HB | 2.02 | 0.41 |
| 2:Bx:92:SER:OG | 2:Bx:232:ASP:OD1 | 2.29 | 0.41 |
| 2:By:414:VAL:HG23 | 2:By:422:ALA:HB1 | 2.02 | 0.41 |
| 2:By:473:ASP:HB3 | 2:By:499:ILE:HG23 | 2.03 | 0.41 |
| 4:G:9:PRO:O | 4:G:20:SER:N | 2.54 | 0.41 |
| 4:K:44:MET:HE1 | 4:L:44:MET:HG2 | 2.02 | 0.41 |
| 4:Z:66:LYS:HE3 | 4:Z:66:LYS:HB3 | 1.91 | 0.41 |
| 4:b:6:ASN:HB2 | 4:b:57:VAL:HG13 | 2.01 | 0.41 |
| 4:b:23:SER:HB3 | 4:b:46:ARG:HD2 | 2.01 | 0.41 |
| 1:k:109:GLN:HA | 8:r:70:THR:HG23 | 2.03 | 0.41 |
| 1:m:154:PRO:HA | 1:m:167:ARG:HD3 | 2.01 | 0.41 |
| 8:s:87:PRO:HA | 9:y:146:THR:HB | 2.01 | 0.41 |
| 8:t:88:PHE:CE1 | 9:y:152:ALA:HB2 | 2.55 | 0.41 |
| 1:0:17:GLY:HA2 | 7:BE:23:PRO:HA | 2.03 | 0.41 |
| 1:0:55:GLY:HA2 | 1:0:89:TYR:HA | 2.01 | 0.41 |
| 2:1:346:SER:O | 2:1:350:VAL:HG23 | 2.21 | 0.41 |
| 2:1:505:LEU:HA | 2:1:505:LEU:HD12 | 1.80 | 0.41 |
| 2:2:639:THR:HB | 2:AP:624:VAL:HG12 | 2.02 | 0.41 |
| 3:6:18:PRO:HG2 | 3:7:149:GLU:HB3 | 2.02 | 0.41 |
| 3:8:109:LYS:O | 3:8:132:LEU:N | 2.39 | 0.41 |
| 5:A0:161:ILE:HD11 | 5:A0:175:ARG:HG3 | 2.02 | 0.41 |
| 5:A2:428:LEU:HD13 | 5:A2:428:LEU:HA | 1.90 | 0.41 |
| 5:A3:66:GLU:N | 5:A3:69:MET:HE3 | 2.34 | 0.41 |
| 5:A3:379:ARG:NE | 5:A3:400:GLU:OE2 | 2.54 | 0.41 |
| 6:A5:118:ASN:OD1 | 6:A5:118:ASN:N | 2.44 | 0.41 |
| 7:A6:99:ASP:O | 7:A6:145:THR:HG23 | 2.20 | 0.41 |
| 6:A7:142:GLU:HB2 | 6:A7:490:GLN:HB2 | 2.03 | 0.41 |
| 6:A8:259:ILE:HG21 | 6:A8:480:GLY:HA3 | 2.03 | 0.41 |
| 6:A8:314:ALA:HA | 6:A8:513:PHE:HB2 | 2.02 | 0.41 |
| 6:A9:485:ALA:C | 6:A9:487:SER:H | 2.28 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:66:MET:HE1 | 2:AD:459:ASP:OD1 | 2.21 | 0.41 |
| 3:AI:16:ALA:HB2 | 3:AJ:76:ASP:O | 2.21 | 0.41 |
| 3:AI:17:ARG:O | 3:AI:115:GLN:NE2 | 2.54 | 0.41 |
| 2:AK:147:THR:HG22 | 2:AK:150:ILE:HD12 | 2.03 | 0.41 |
| 2:AK:188:ILE:H | 2:AK:188:ILE:HG13 | 1.66 | 0.41 |
| 2:AK:494:TYR:OH | 2:Bs:569:LYS:NZ | 2.50 | 0.41 |
| 2:AM:42:LYS:HE3 | 2:AM:42:LYS:HB3 | 1.92 | 0.41 |
| 2:AM:44:VAL:HG11 | 2:AM:50:LEU:HB2 | 2.03 | 0.41 |
| 2:AN:526:THR:OG1 | 2:B2:366:GLU:OE1 | 2.39 | 0.41 |
| 2:AO:269:PHE:CZ | 2:AO:292:SER:HB2 | 2.56 | 0.41 |
| 10:AQ:292:PRO:HD2 | 10:AQ:340:THR:OG1 | 2.20 | 0.41 |
| 10:AS:320:GLU:HG3 | 10:AS:376:PRO:O | 2.20 | 0.41 |
| 6:AV:236:GLN:HG3 | 6:Ap:265:GLN:HE21 | 1.84 | 0.41 |
| 6:AV:383:VAL:HG21 | 6:AV:425:ILE:HG12 | 2.03 | 0.41 |
| 7:AY:117:ILE:HA | 7:AY:121:MET:HE3 | 2.02 | 0.41 |
| 6:AZ:211:GLU:O | 6:AZ:215:GLN:HG2 | 2.21 | 0.41 |
| 6:AZ:267:LYS:HE3 | 6:AZ:470:VAL:HG21 | 2.02 | 0.41 |
| 7:Aa:104:TYR:O | 7:Aa:104:TYR:CG | 2.71 | 0.41 |
| 6:Ad:71:ASP:OD1 | 6:Ad:72:HIS:N | 2.54 | 0.41 |
| 6:Ad:285:ASP:HB3 | 6:Ad:287:ASP:OD1 | 2.20 | 0.41 |
| 6:Ae:264:ARG:NH2 | 6:Ai:152:ALA:O | 2.47 | 0.41 |
| 6:Ag:481:ILE:HD13 | 6:Ag:506:SER:HB3 | 2.01 | 0.41 |
| 6:Ah:106:LEU:HB2 | 6:Ah:303:ASN:CG | 2.45 | 0.41 |
| 6:Ah:384:ASN:ND2 | 6:Ah:406:THR:HG21 | 2.35 | 0.41 |
| 6:Aj:72:HIS:C | 6:Aj:74:TYR:H | 2.29 | 0.41 |
| 6:Aj:314:ALA:HA | 6:Aj:513:PHE:HB2 | 2.01 | 0.41 |
| 6:Ak:153:MET:HE2 | 6:Ak:226:GLU:HG2 | 2.03 | 0.41 |
| 6:Ak:336:ASP:O | 6:Ak:340:ILE:HG12 | 2.21 | 0.41 |
| 7:Al:63:GLY:O | 7:Al:179:TYR:N | 2.41 | 0.41 |
| 6:Am:363:GLU:OE2 | 6:Am:366:ARG:NH2 | 2.34 | 0.41 |
| 6:An:454:VAL:HG22 | 6:An:476:ARG:HB2 | 2.02 | 0.41 |
| 6:Ap:317:GLY:HA2 | 6:Ap:514:ARG:NH1 | 2.36 | 0.41 |
| 7:Aq:6:PRO:HB3 | 7:Aq:11:GLU:HB3 | 2.03 | 0.41 |
| 7:Aq:109:ASP:OD2 | 6:BK:453:TYR:OH | 2.30 | 0.41 |
| 7:Ar:84:VAL:HG13 | 7:Ar:184:VAL:HB | 2.02 | 0.41 |
| 7:As:12:LEU:O | 7:As:16:ILE:HG12 | 2.21 | 0.41 |
| 5:Av:256:ARG:NH2 | 5:Av:372:ALA:O | 2.48 | 0.41 |
| 2:B1:130:LYS:HE2 | 2:B1:130:LYS:HB2 | 1.93 | 0.41 |
| 2:B1:564:ILE:HD11 | 2:Bz:642:PHE:CE2 | 2.56 | 0.41 |
| 2:B3:510:ARG:NH2 | 2:B4:360:ASP:HB3 | 2.35 | 0.41 |
| 2:B3:645:THR:OG1 | 2:B4:629:ILE:O | 2.36 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B4:39:PHE:HA | 2:B4:81:VAL:HG23 | 2.03 | 0.41 |
| 2:B4:638:ILE:HD12 | 2:B7:8:ILE:HD11 | 2.02 | 0.41 |
| 2:B5:106:PRO:HB3 | 2:B5:139:LYS:HA | 2.02 | 0.41 |
| 2:B5:524:PRO:O | 2:B5:535:LEU:HD23 | 2.20 | 0.41 |
| 2:B5:598:LEU:HD23 | 2:B5:598:LEU:HA | 1.88 | 0.41 |
| 5:BA:9:PHE:HB3 | 5:BA:12:TRP:HD1 | 1.86 | 0.41 |
| 5:BA:330:MET:HG2 | 5:BH:280:PRO:HG2 | 2.03 | 0.41 |
| 5:BB:31:ILE:H | 5:BB:31:ILE:HG12 | 1.61 | 0.41 |
| 7:BC:34:ILE:O | 7:BC:38:ILE:HG12 | 2.20 | 0.41 |
| 7:BC:50:PHE:HE2 | 7:BC:300:LEU:HD22 | 1.85 | 0.41 |
| 5:BG:212:HIS:ND1 | 5:BG:222:TYR:HA | 2.35 | 0.41 |
| 6:BJ:163:PHE:HB2 | 6:BJ:179:THR:HG23 | 2.01 | 0.41 |
| 6:BK:170:THR:H | 6:BK:198:ILE:HG22 | 1.85 | 0.41 |
| 6:BM:104:PRO:HG2 | 6:BM:300:LEU:HD21 | 2.02 | 0.41 |
| 6:BM:202:ALA:HA | 6:BM:207:LYS:HD3 | 2.02 | 0.41 |
| 3:BX:22:GLN:HB2 | 3:BX:116:TYR:HE1 | 1.86 | 0.41 |
| 3:BX:42:PRO:O | 3:BX:43:ALA:HB2 | 2.20 | 0.41 |
| 3:Bd:67:ASP:OD1 | 3:Bd:67:ASP:N | 2.54 | 0.41 |
| 3:Bg:56:ARG:HB3 | 3:Bg:56:ARG:HH11 | 1.86 | 0.41 |
| 3:Bk:87:ASP:O | 3:Bk:91:ILE:HG13 | 2.21 | 0.41 |
| 3:Bm:137:VAL:HG23 | 3:Bm:155:VAL:HG22 | 2.03 | 0.41 |
| 3:Bo:83:GLN:HA | 3:Bo:86:VAL:HG22 | 2.01 | 0.41 |
| 2:Bq:641:ASN:HB2 | 2:Br:626:THR:HG23 | 2.03 | 0.41 |
| 2:Bt:26:THR:HA | 2:Bt:77:ASP:O | 2.20 | 0.41 |
| 2:Bu:33:PHE:HD2 | 2:Bu:82:ARG:HA | 1.86 | 0.41 |
| 2:Bu:110:TYR:CE1 | 2:Bu:177:GLY:HA3 | 2.56 | 0.41 |
| 2:Bu:557:PHE:CZ | 2:Bu:629:ILE:HD11 | 2.56 | 0.41 |
| 2:Bv:228:GLY:HA2 | 2:Bv:345:SER:HB3 | 2.03 | 0.41 |
| 2:Bv:253:PRO:HD2 | 2:Bv:335:SER:O | 2.21 | 0.41 |
| 2:Bw:382:SER:HB3 | 2:Bw:385:THR:HG22 | 2.03 | 0.41 |
| 2:Bx:130:LYS:HB2 | 2:Bx:130:LYS:HE2 | 1.85 | 0.41 |
| 2:Bx:229:GLU:H | 2:Bx:229:GLU:CD | 2.28 | 0.41 |
| 2:By:427:VAL:HG13 | 2:By:520:GLU:HG3 | 2.02 | 0.41 |
| 2:By:538:ASP:OD1 | 2:By:538:ASP:N | 2.52 | 0.41 |
| 2:Bz:193:ILE:HG12 | 2:Bz:223:VAL:HG21 | 2.03 | 0.41 |
| 4:e:10:PHE:HB3 | 4:e:22:ILE:HG12 | 2.02 | 0.41 |
| 8:r:238:VAL:HG13 | 8:r:239:PRO:HD2 | 2.03 | 0.41 |
| 8:s:243:ASP:OD1 | 8:s:243:ASP:N | 2.54 | 0.41 |
| 8:s:244:PRO:HB2 | 9:w:5:LEU:HD11 | 2.03 | 0.41 |
| 8:t:134:VAL:HG21 | 8:t:188:TRP:CE3 | 2.56 | 0.41 |
| 8:u:187:GLU:C | 8:u:188:TRP:HD1 | 2.28 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:y:149:SER:O | 9:y:151:PRO:HD3 | 2.20 | 0.41 |
| 2:1:237:GLU:OE1 | 2:1:284:ARG:NH1 | 2.54 | 0.41 |
| 2:1:374:ILE:HA | 2:1:406:LEU:HD12 | 2.02 | 0.41 |
| 2:2:422:ALA:O | 2:2:426:LEU:HG | 2.21 | 0.41 |
| 2:3:193:ILE:HG12 | 2:3:205:MET:HA | 2.03 | 0.41 |
| 2:3:564:ILE:HD11 | 8:s:216:PHE:CZ | 2.56 | 0.41 |
| 2:4:160:TYR:HA | 2:4:161:PRO:HA | 1.89 | 0.41 |
| 2:5:240:SER:O | 2:5:244:TYR:HB2 | 2.21 | 0.41 |
| 2:5:360:ASP:OD1 | 2:5:392:HIS:NE2 | 2.46 | 0.41 |
| 3:6:21:PHE:HZ | 3:6:38:ALA:HA | 1.85 | 0.41 |
| 3:6:95:GLN:HG3 | 3:o:66:PHE:HZ | 1.86 | 0.41 |
| 3:7:118:ARG:HA | 3:7:118:ARG:HD2 | 1.91 | 0.41 |
| 3:9:41:LEU:HD23 | 3:AA:82:ARG:NH2 | 2.36 | 0.41 |
| 5:A0:104:ASP:OD2 | 5:BG:450:ARG:NH1 | 2.35 | 0.41 |
| 5:A0:232:LYS:HE2 | 5:A0:233:ALA:H | 1.85 | 0.41 |
| 5:A0:295:ARG:HD2 | 7:BC:187:TRP:CE2 | 2.55 | 0.41 |
| 5:A0:440:GLU:O | 5:A0:444:ILE:HG22 | 2.21 | 0.41 |
| 5:A1:55:ASN:O | 5:A1:59:GLN:HB2 | 2.20 | 0.41 |
| 5:A1:128:ASP:O | 5:A1:131:SER:OG | 2.32 | 0.41 |
| 5:A1:382:GLN:NE2 | 5:BB:367:GLN:OE1 | 2.54 | 0.41 |
| 5:A2:89:ASP:OD2 | 5:BD:256:ARG:NH1 | 2.54 | 0.41 |
| 5:A2:345:THR:HG21 | 7:AY:306:ILE:HD11 | 2.02 | 0.41 |
| 5:A3:160:LYS:NZ | 5:A3:233:ALA:O | 2.49 | 0.41 |
| 5:A3:439:ASP:O | 5:BG:135:ASN:ND2 | 2.54 | 0.41 |
| 6:A4:262:LYS:NZ | 6:A5:226:GLU:OE2 | 2.41 | 0.41 |
| 6:A5:166:LEU:HD22 | 6:A5:198:ILE:HD12 | 2.02 | 0.41 |
| 6:A5:312:TYR:CZ | 6:A5:507:LEU:HG | 2.55 | 0.41 |
| 7:A6:126:ASN:HB2 | 7:A6:129:TYR:HE2 | 1.86 | 0.41 |
| 7:A6:160:ASP:HB3 | 5:BF:306:ASN:OD1 | 2.21 | 0.41 |
| 6:A7:78:ASN:ND2 | 11:BO:5:ARG:O | 2.53 | 0.41 |
| 6:A7:105:ASN:ND2 | 6:A7:408:THR:O | 2.53 | 0.41 |
| 6:A7:356:GLN:O | 6:A7:360:GLU:HG2 | 2.21 | 0.41 |
| 6:A8:350:PHE:HB3 | 6:A8:389:VAL:HG11 | 2.02 | 0.41 |
| 6:A9:285:ASP:HA | 5:Av:65:TYR:CE2 | 2.53 | 0.41 |
| 3:AA:94:GLY:HA3 | 3:AA:100:THR:HB | 2.03 | 0.41 |
| 8:AB:96:ASN:N | 8:AB:96:ASN:OD1 | 2.53 | 0.41 |
| 9:AC:35:GLN:HA | 9:v:145:TYR:HD2 | 1.86 | 0.41 |
| 2:AD:26:THR:HA | 2:AD:77:ASP:O | 2.21 | 0.41 |
| 2:AD:406:LEU:HD13 | 2:AD:475:ALA:HB2 | 2.03 | 0.41 |
| 2:AD:554:ARG:O | 2:AD:554:ARG:HD3 | 2.20 | 0.41 |
| 3:AH:94:GLY:HA3 | 3:AH:100:THR:OG1 | 2.21 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:AI:98:GLU:HG2 | 3:AI:100:THR:HG23 | 2.03 | 0.41 |
| 2:AK:35:TRP:CG | 2:AK:36:GLY:H | 2.38 | 0.41 |
| 2:AK:592:LEU:HD23 | 2:AK:604:TYR:HB2 | 2.03 | 0.41 |
| 2:AK:643:VAL:HG22 | 2:AL:15:VAL:H | 1.86 | 0.41 |
| 2:AL:153:LYS:HD3 | 2:AL:153:LYS:HA | 1.88 | 0.41 |
| 2:AL:228:GLY:HA2 | 2:AL:345:SER:HB3 | 2.02 | 0.41 |
| 2:AL:592:LEU:HD13 | 2:AL:592:LEU:HA | 1.89 | 0.41 |
| 2:AL:638:ILE:HG21 | 2:Bv:568:SER:HB2 | 2.02 | 0.41 |
| 2:AM:413:THR:C | 2:AM:417:ILE:HD11 | 2.46 | 0.41 |
| 2:AM:470:LEU:HD12 | 2:AM:470:LEU:HA | 1.93 | 0.41 |
| 2:AM:538:ASP:HA | 2:AM:551:ILE:HD12 | 2.03 | 0.41 |
| 2:AM:576:ASN:O | 2:AM:576:ASN:ND2 | 2.45 | 0.41 |
| 2:AN:166:ASN:OD1 | 2:AN:166:ASN:N | 2.54 | 0.41 |
| 2:AN:349:GLU:O | 2:AN:350:VAL:C | 2.64 | 0.41 |
| 2:AO:31:GLY:O | 2:AO:82:ARG:HA | 2.21 | 0.41 |
| 2:AO:518:TYR:CE2 | 2:AP:6:PRO:HD3 | 2.55 | 0.41 |
| 2:AP:188:ILE:H | 2:AP:188:ILE:HG13 | 1.69 | 0.41 |
| 2:AP:351:THR:OG1 | 2:AP:352:ALA:N | 2.53 | 0.41 |
| 2:AP:477:LEU:HD21 | 2:AP:497:GLY:HA2 | 2.02 | 0.41 |
| 2:AP:651:PHE:HD1 | 2:AP:651:PHE:HA | 1.70 | 0.41 |
| 6:AV:334:PHE:HD2 | 6:AV:349:SER:HB3 | 1.86 | 0.41 |
| 6:AX:71:ASP:HB3 | 6:Af:230:THR:HB | 2.02 | 0.41 |
| 6:AX:131:TYR:HE1 | 6:AX:141:LYS:HB2 | 1.86 | 0.41 |
| 6:AX:373:GLY:HA2 | 6:AX:438:TYR:HB2 | 2.03 | 0.41 |
| 7:AY:175:ASN:H | 5:BD:320:LYS:HZ1 | 1.69 | 0.41 |
| 7:AY:199:GLY:HA2 | 7:AY:229:ARG:HH21 | 1.86 | 0.41 |
| 6:AZ:94:ALA:O | 6:AZ:95:VAL:HG13 | 2.21 | 0.41 |
| 6:AZ:254:ILE:HG22 | 6:Am:89:THR:HG22 | 2.02 | 0.41 |
| 6:AZ:336:ASP:HB3 | 6:AZ:339:ASP:HB2 | 2.01 | 0.41 |
| 6:AZ:344:ARG:HG3 | 6:Ad:344:ARG:HH11 | 1.85 | 0.41 |
| 6:AZ:345:TRP:CD1 | 6:Ad:348:GLU:HB3 | 2.56 | 0.41 |
| 7:Aa:104:TYR:O | 7:Aa:105:PRO:C | 2.64 | 0.41 |
| 7:Aa:204:TYR:O | 4:i:31:ILE:HB | 2.19 | 0.41 |
| 7:Ab:55:LYS:HB2 | 7:Ab:187:TRP:CZ3 | 2.56 | 0.41 |
| 6:Ac:114:VAL:HG12 | 6:Ac:116:PRO:HD3 | 2.03 | 0.41 |
| 6:Ac:290:LEU:HD23 | 6:Ac:290:LEU:HA | 1.91 | 0.41 |
| 6:Ac:305:GLU:HA | 6:Ag:225:ALA:HB3 | 2.03 | 0.41 |
| 6:Ad:106:LEU:HB2 | 6:Ad:303:ASN:HD22 | 1.86 | 0.41 |
| 6:Ae:147:MET:HE3 | 6:Ae:147:MET:HB2 | 1.88 | 0.41 |
| 6:Af:161:LYS:HE3 | 6:Af:161:LYS:HB2 | 1.94 | 0.41 |
| 6:Ag:210:ALA:O | 6:Ag:214:LYS:HG3 | 2.20 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ah:80:ALA:HB2 | 6:BI:258:VAL:HG11 | 2.03 | 0.41 |
| 6:Ah:490:GLN:CD | 6:Ah:490:GLN:H | 2.28 | 0.41 |
| 7:Al:52:GLY:HA2 | 7:Al:190:SER:OG | 2.21 | 0.41 |
| 7:Al:55:LYS:HB3 | 7:Al:187:TRP:CE3 | 2.56 | 0.41 |
| 7:Al:171:LYS:HD3 | 7:Al:173:MET:HE2 | 2.03 | 0.41 |
| 6:An:414:ALA:HB2 | 6:An:425:ILE:HG13 | 2.03 | 0.41 |
| 6:An:466:ASN:HB2 | 6:An:468:GLN:HG2 | 2.02 | 0.41 |
| 6:Ao:123:GLN:HE22 | 6:BK:91:ILE:HG23 | 1.86 | 0.41 |
| 6:Ap:379:SER:OG | 6:Ap:432:ASP:OD1 | 2.34 | 0.41 |
| 7:Aq:52:GLY:HA2 | 7:Aq:190:SER:OG | 2.21 | 0.41 |
| 7:Aq:193:ASP:O | 7:Aq:242:TYR:OH | 2.35 | 0.41 |
| 7:Ar:96:THR:HB | 6:BJ:91:ILE:HA | 2.03 | 0.41 |
| 7:Ar:138:LEU:HG | 5:BA:273:ILE:HD11 | 2.03 | 0.41 |
| 7:Ar:221:ASN:HD22 | 7:Ar:224:HIS:CE1 | 2.39 | 0.41 |
| 7:As:58:HIS:ND1 | 7:As:186:SER:OG | 2.50 | 0.41 |
| 7:At:189:LYS:H | 7:At:189:LYS:HG2 | 1.70 | 0.41 |
| 7:At:217:GLU:HG3 | 7:At:224:HIS:ND1 | 2.36 | 0.41 |
| 6:Au:204:ASP:OD1 | 6:Au:205:ALA:N | 2.53 | 0.41 |
| 6:Au:223:GLU:H | 6:Au:223:GLU:CD | 2.28 | 0.41 |
| 6:Au:303:ASN:HD22 | 6:Au:303:ASN:C | 2.29 | 0.41 |
| 5:Av:12:TRP:CD1 | 5:Av:234:ALA:HB2 | 2.56 | 0.41 |
| 5:Av:150:TRP:HD1 | 5:Av:156:ILE:HG22 | 1.86 | 0.41 |
| 6:Aw:153:MET:HE1 | 6:Aw:226:GLU:HB2 | 2.03 | 0.41 |
| 6:Ay:133:LYS:HA | 6:Ay:249:GLU:HB2 | 2.02 | 0.41 |
| 6:Ay:182:PHE:HE1 | 6:Ay:188:VAL:HG11 | 1.84 | 0.41 |
| 6:Ay:279:ARG:HA | 6:Ay:279:ARG:HD3 | 1.91 | 0.41 |
| 6:Az:116:PRO:HA | 6:Az:452:PRO:HD2 | 2.02 | 0.41 |
| 6:Az:145:HIS:HD2 | 6:Az:490:GLN:HG3 | 1.86 | 0.41 |
| 6:Az:264:ARG:NH1 | 6:Az:305:GLU:OE1 | 2.53 | 0.41 |
| 6:Az:344:ARG:NH2 | 6:Az:348:GLU:OE2 | 2.53 | 0.41 |
| 2:B2:538:ASP:OD1 | 2:B2:538:ASP:N | 2.54 | 0.41 |
| 2:B4:654:LEU:HD23 | 2:B4:654:LEU:HA | 1.92 | 0.41 |
| 2:B6:30:ALA:HB3 | 2:B6:359:TRP:CE2 | 2.56 | 0.41 |
| 2:B6:612:ASN:OD1 | 2:B6:612:ASN:N | 2.53 | 0.41 |
| 2:B7:283:VAL:HG21 | 2:B7:323:ILE:HD13 | 2.03 | 0.41 |
| 5:BA:44:GLU:H | 5:BA:44:GLU:HG2 | 1.66 | 0.41 |
| 5:BA:477:ILE:HD13 | 5:BA:483:HIS:NE2 | 2.36 | 0.41 |
| 5:BB:150:TRP:HD1 | 5:BB:156:ILE:HG22 | 1.84 | 0.41 |
| 5:BD:47:SER:O | 5:BD:49:GLU:N | 2.54 | 0.41 |
| 5:BD:432:ILE:HD12 | 5:BD:432:ILE:HA | 1.94 | 0.41 |
| 5:BF:21:LYS:HE3 | 5:BF:21:LYS:HB3 | 1.86 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:BG:182:VAL:HG22 | 5:BG:208:TYR:CD1 | 2.56 | 0.41 |
| 5:BG:267:LEU:HD11 | 5:BG:361:ASP:OD1 | 2.21 | 0.41 |
| 5:BG:408:ARG:HE | 5:BG:450:ARG:HH21 | 1.69 | 0.41 |
| 5:BH:83:MET:HG3 | 5:BH:152:VAL:HG22 | 2.03 | 0.41 |
| 5:BH:136:HIS:HB3 | 5:BH:174:LEU:HD13 | 2.03 | 0.41 |
| 6:BI:154:PHE:O | 6:BI:248:ASN:ND2 | 2.39 | 0.41 |
| 6:BI:278:LEU:HD12 | 6:BI:278:LEU:HA | 1.90 | 0.41 |
| 6:BI:378:ALA:HB1 | 6:BI:382:VAL:HB | 2.03 | 0.41 |
| 6:BK:191:GLN:HB2 | 6:BK:224:ILE:HG21 | 2.03 | 0.41 |
| 6:BK:445:ASP:OD1 | 6:BK:445:ASP:N | 2.53 | 0.41 |
| 7:BL:68:ARG:HD2 | 7:BL:74:PHE:CE2 | 2.56 | 0.41 |
| 7:BL:270:MET:HA | 7:BL:276:THR:HG23 | 2.02 | 0.41 |
| 11:BQ:10:ILE:HD11 | 11:BQ:35:TYR:HE1 | 1.86 | 0.41 |
| 11:BS:27:GLU:HB3 | 11:BS:56:TYR:CG | 2.55 | 0.41 |
| 11:BU:27:GLU:HB3 | 11:BU:56:TYR:CG | 2.56 | 0.41 |
| 3:Bc:3:VAL:N | 3:Bh:97:ASN:O | 2.52 | 0.41 |
| 3:Bc:129:ILE:HG21 | 3:Bc:132:LEU:HD13 | 2.02 | 0.41 |
| 3:Bd:140:LEU:HD12 | 3:Bd:140:LEU:HA | 1.91 | 0.41 |
| 3:Be:104:PRO:HA | 3:Be:107:TYR:CE2 | 2.55 | 0.41 |
| 3:Bf:136:ASN:O | 3:Bf:136:ASN:ND2 | 2.54 | 0.41 |
| 3:Bh:98:GLU:OE1 | 3:Bh:98:GLU:N | 2.40 | 0.41 |
| 3:Bi:48:LYS:HE3 | 3:Bi:48:LYS:HB3 | 1.87 | 0.41 |
| 3:Bo:15:PHE:HB2 | 3:Bo:17:ARG:NH2 | 2.35 | 0.41 |
| 2:Bp:390:GLN:OE1 | 2:Bp:407:CYS:HB3 | 2.20 | 0.41 |
| 2:Bp:505:LEU:HD12 | 2:Bp:505:LEU:HA | 1.88 | 0.41 |
| 2:Bp:620:ARG:HB2 | 2:Bp:622:GLU:HG3 | 2.03 | 0.41 |
| 2:Br:2:THR:OG1 | 2:Br:3:LEU:N | 2.53 | 0.41 |
| 2:Bs:441:PHE:CZ | 2:Bs:443:ILE:HD11 | 2.56 | 0.41 |
| 2:Bs:652:ASP:OD2 | 2:Bv:458:TYR:OH | 2.31 | 0.41 |
| 2:Bs:653:GLU:HA | 2:Bv:16:GLN:HG3 | 2.03 | 0.41 |
| 2:Bs:654:LEU:HD22 | 2:Bt:605:ARG:HD3 | 2.01 | 0.41 |
| 2:Bt:614:THR:O | 2:Bt:616:SER:N | 2.52 | 0.41 |
| 2:Bv:365:ARG:HA | 2:Bv:400:ARG:CZ | 2.51 | 0.41 |
| 2:Bx:110:TYR:CZ | 2:Bx:180:ALA:HB2 | 2.56 | 0.41 |
| 2:Bx:142:LYS:HE2 | 2:Bx:142:LYS:HB2 | 1.95 | 0.41 |
| 2:Bx:233:LYS:HE2 | 2:Bx:233:LYS:HB3 | 1.94 | 0.41 |
| 2:Bx:459:ASP:OD2 | 2:Bx:466:ARG:NH1 | 2.53 | 0.41 |
| 2:By:291:GLN:HE22 | 2:By:320:SER:HB2 | 1.84 | 0.41 |
| 2:By:593:GLN:HB2 | 2:By:604:TYR:OH | 2.21 | 0.41 |
| 2:Bz:221:GLY:O | 2:Bz:325:ALA:HA | 2.21 | 0.41 |
| 2:Bz:450:ILE:HD13 | 2:Bz:522:ILE:HG12 | 2.03 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:n:12:LEU:H | 1:n:12:LEU:HD12 | 1.86 | 0.41 |
| 3:o:57:LYS:HZ3 | 3:o:57:LYS:HB3 | 1.85 | 0.41 |
| 1:p:117:SER:HA | 1:p:168:LYS:HA | 2.02 | 0.41 |
| 1:p:144:ASN:O | 1:p:144:ASN:ND2 | 2.54 | 0.41 |
| 8:q:111:PRO:HB2 | 8:q:197:TRP:HB3 | 2.02 | 0.41 |
| 8:q:144:HIS:ND1 | 9:v:150:ASP:OD2 | 2.54 | 0.41 |
| 8:q:198:MET:SD | 8:r:135:GLU:HG2 | 2.60 | 0.41 |
| 8:q:223:LEU:O | 8:q:224:PRO:C | 2.64 | 0.41 |
| 8:t:232:SER:HB2 | 8:t:256:THR:OG1 | 2.20 | 0.41 |
| 8:u:63:GLU:HB3 | 8:u:64:ASP:H | 1.69 | 0.41 |
| 8:u:168:MET:HG3 | 8:u:193:GLU:HB2 | 2.02 | 0.41 |
| 9:z:2:SER:OG | 9:z:3:GLN:N | 2.50 | 0.41 |
| 1:0:6:LYS:NZ | 1:0:23:GLU:OE2 | 2.54 | 0.41 |
| 2:1:72:LEU:HD13 | 2:1:72:LEU:HA | 1.94 | 0.41 |
| 2:1:310:TYR:CE2 | 2:1:312:ASP:HB3 | 2.56 | 0.41 |
| 2:2:523:ASN:OD1 | 2:2:539:LYS:N | 2.51 | 0.41 |
| 2:2:573:PHE:CE2 | 8:r:237:VAL:HG21 | 2.54 | 0.41 |
| 2:3:493:GLY:HA2 | 2:AK:572:LEU:HD23 | 2.02 | 0.41 |
| 2:3:547:PRO:HD3 | 2:4:304:ILE:HB | 2.03 | 0.41 |
| 2:3:602:TYR:CD1 | 2:3:632:ALA:HA | 2.56 | 0.41 |
| 2:5:487:THR:O | 2:5:555:ARG:NH1 | 2.54 | 0.41 |
| 3:9:24:GLU:CD | 3:9:114:ARG:HH12 | 2.29 | 0.41 |
| 5:A1:118:PHE:CZ | 5:A1:432:ILE:HD11 | 2.56 | 0.41 |
| 5:A1:508:GLU:HG2 | 5:BB:483:HIS:HB3 | 2.03 | 0.41 |
| 5:A3:47:SER:OG | 5:A3:190:THR:O | 2.30 | 0.41 |
| 5:A3:413:LYS:HD2 | 5:A3:413:LYS:HA | 1.77 | 0.41 |
| 6:A4:106:LEU:HB3 | 6:A4:300:LEU:HD12 | 2.02 | 0.41 |
| 6:A5:309:TRP:HZ2 | 6:AW:226:GLU:HB3 | 1.85 | 0.41 |
| 6:A5:458:PRO:HB3 | 6:A5:473:PHE:CE2 | 2.56 | 0.41 |
| 7:A6:55:LYS:H | 7:Al:162:TRP:CD1 | 2.39 | 0.41 |
| 7:A6:160:ASP:OD1 | 7:A6:160:ASP:N | 2.43 | 0.41 |
| 6:A8:145:HIS:CG | 6:A8:146:PRO:HD2 | 2.56 | 0.41 |
| 2:AD:100:GLU:HG2 | 2:AD:186:LYS:O | 2.20 | 0.41 |
| 3:AE:97:ASN:HA | 3:Bj:3:VAL:HG12 | 2.03 | 0.41 |
| 3:AF:51:VAL:N | 3:AF:58:ILE:O | 2.54 | 0.41 |
| 3:AF:132:LEU:HD13 | 3:AF:159:LEU:HB3 | 2.03 | 0.41 |
| 3:AJ:49:ILE:HD11 | 3:BX:150:ILE:HG22 | 2.03 | 0.41 |
| 3:AJ:51:VAL:HG11 | 3:Bm:15:PHE:CE1 | 2.56 | 0.41 |
| 2:AM:46:ASN:OD1 | 2:AM:47:GLU:N | 2.54 | 0.41 |
| 2:AM:57:PRO:HB3 | 2:AM:65:PHE:HB3 | 2.02 | 0.41 |
| 2:AO:494:TYR:CZ | 2:B5:569:LYS:HD3 | 2.56 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AP:66:MET:HG2 | 2:AP:468:VAL:HG21 | 2.03 | 0.41 |
| 10:AU:335:TYR:HA | 10:AU:338:ARG:HD3 | 2.03 | 0.41 |
| 6:AV:75:ASN:OD1 | 6:AV:76:ALA:N | 2.54 | 0.41 |
| 6:AV:93:PRO:HG2 | 6:AZ:123:GLN:CD | 2.45 | 0.41 |
| 6:AV:394:SER:O | 6:Ap:397:ALA:HA | 2.20 | 0.41 |
| 6:AX:125:PHE:HB2 | 6:BK:98:MET:HA | 2.03 | 0.41 |
| 6:AX:269:ALA:HB2 | 6:AX:470:VAL:HG23 | 2.03 | 0.41 |
| 6:AZ:93:PRO:HB2 | 6:Ad:123:GLN:HB3 | 2.03 | 0.41 |
| 7:Aa:54:ASN:HB2 | 7:Aa:219:TYR:CZ | 2.56 | 0.41 |
| 7:Ab:302:PRO:HB3 | 5:Av:300:HIS:CE1 | 2.56 | 0.41 |
| 6:Ah:93:PRO:O | 6:BI:123:GLN:NE2 | 2.54 | 0.41 |
| 6:Ah:129:ALA:O | 6:Ah:143:ALA:N | 2.42 | 0.41 |
| 6:Ah:153:MET:HB2 | 6:Ah:189:TYR:CE2 | 2.56 | 0.41 |
| 6:Ah:408:THR:HG21 | 6:Ah:427:GLN:HB3 | 2.03 | 0.41 |
| 6:Ai:372:GLU:OE1 | 6:Ai:372:GLU:N | 2.41 | 0.41 |
| 7:Al:2:SER:OG | 7:Al:3:GLY:N | 2.51 | 0.41 |
| 6:Am:72:HIS:C | 6:Am:74:TYR:H | 2.28 | 0.41 |
| 6:Am:314:ALA:HA | 6:Am:513:PHE:HB2 | 2.03 | 0.41 |
| 6:An:100:ARG:HG3 | 6:BK:127:LEU:HD22 | 2.03 | 0.41 |
| 6:Ao:108:ALA:O | 6:Ao:109:PHE:HB2 | 2.21 | 0.41 |
| 7:Aq:45:TYR:OH | 7:Aq:51:ASP:O | 2.22 | 0.41 |
| 6:Aw:131:TYR:HB2 | 6:Aw:154:PHE:CZ | 2.56 | 0.41 |
| 6:Aw:437:GLY:HA2 | 6:Aw:512:TYR:O | 2.21 | 0.41 |
| 6:Ay:304:ARG:HA | 6:Ay:304:ARG:HD2 | 1.90 | 0.41 |
| 6:Az:238:GLY:HA2 | 6:Az:242:SER:O | 2.21 | 0.41 |
| 6:Az:364:ILE:HD11 | 6:Az:514:ARG:HG3 | 2.03 | 0.41 |
| 2:B2:85:ASP:H | 2:B2:346:SER:HB3 | 1.86 | 0.41 |
| 2:B2:130:LYS:HG3 | 2:B2:144:ASN:HB3 | 2.03 | 0.41 |
| 2:B3:35:TRP:HB2 | 2:B3:230:LEU:HD12 | 2.02 | 0.41 |
| 2:B3:116:ILE:HD13 | 2:B3:171:ILE:HG23 | 2.03 | 0.41 |
| 2:B5:13:THR:HB | 2:B5:14:THR:H | 1.72 | 0.41 |
| 2:B6:44:VAL:HG11 | 2:B6:50:LEU:HB2 | 2.02 | 0.41 |
| 2:B6:195:LEU:HD12 | 2:B6:198:ILE:HD11 | 2.02 | 0.41 |
| 5:BA:236:VAL:HG13 | 5:BA:420:ASP:HB3 | 2.03 | 0.41 |
| 5:BA:367:GLN:HA | 5:BA:377:LEU:HD11 | 2.03 | 0.41 |
| 5:BB:39:GLY:HA3 | 5:BB:250:ILE:HG12 | 2.02 | 0.41 |
| 7:BC:155:LEU:HD21 | 7:BE:117:ILE:HG12 | 2.01 | 0.41 |
| 5:BG:411:GLN:O | 5:BG:415:GLU:HG3 | 2.21 | 0.41 |
| 5:BH:183:GLN:HB3 | 5:BH:207:ILE:HG23 | 2.03 | 0.41 |
| 5:BH:339:ARG:O | 5:BH:342:LYS:HG3 | 2.21 | 0.41 |
| 6:BK:357:ILE:HG12 | 6:BK:434:PHE:CE1 | 2.55 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:BL:92:ILE:HG13 | 7:BL:181:LEU:HB2 | 2.02 | 0.41 |
| 11:BV:40:LYS:HB3 | 11:BV:72:ASN:OD1 | 2.20 | 0.41 |
| 3:Ba:56:ARG:HG3 | 3:Bg:99:ILE:HG12 | 2.02 | 0.41 |
| 3:Bb:16:ALA:HB3 | 3:Be:75:ASN:HB3 | 2.03 | 0.41 |
| 3:Be:16:ALA:HB3 | 3:Bh:75:ASN:HB3 | 2.02 | 0.41 |
| 3:Be:23:VAL:HG22 | 3:Be:36:CYS:SG | 2.61 | 0.41 |
| 3:Bf:16:ALA:HB3 | 3:Bi:75:ASN:HB3 | 2.03 | 0.41 |
| 3:Bg:57:LYS:HE2 | 3:Bn:147:ASN:HD21 | 1.85 | 0.41 |
| 2:Bq:169:ALA:HB2 | 2:Bq:184:LEU:HD11 | 2.03 | 0.41 |
| 2:Bq:211:GLN:NE2 | 2:Bq:329:ASN:OD1 | 2.51 | 0.41 |
| 2:Bq:484:VAL:HG13 | 2:Bq:485:SER:H | 1.85 | 0.41 |
| 2:Br:375:ALA:HB1 | 2:Br:390:GLN:HG2 | 2.03 | 0.41 |
| 2:Bt:371:GLN:OE1 | 2:Bt:562:THR:OG1 | 2.38 | 0.41 |
| 2:Bu:89:ALA:HB3 | 2:Bu:194:LEU:HG | 2.02 | 0.41 |
| 2:Bv:26:THR:HA | 2:Bv:77:ASP:O | 2.20 | 0.41 |
| 2:Bv:130:LYS:HE2 | 2:Bv:130:LYS:HB2 | 1.84 | 0.41 |
| 2:Bv:455:LYS:HB2 | 2:Bv:470:LEU:HD13 | 2.03 | 0.41 |
| 2:Bw:238:ILE:HG12 | 2:Bw:281:ILE:HD12 | 2.01 | 0.41 |
| 2:Bz:202:GLU:OE1 | 2:Bz:203:ALA:N | 2.54 | 0.41 |
| 4:D:15:PRO:HG3 | 4:D:21:ARG:HB2 | 2.02 | 0.41 |
| 4:M:26:LYS:HG2 | 4:O:34:ALA:HB3 | 2.03 | 0.41 |
| 1:m:122:LEU:HD11 | 1:m:126:GLN:HE21 | 1.86 | 0.41 |
| 8:q:40:PRO:HG2 | 8:q:74:ARG:HG2 | 2.03 | 0.41 |
| 8:r:187:GLU:C | 8:r:188:TRP:HD1 | 2.29 | 0.41 |
| 8:s:108:GLN:OE1 | 8:s:152:GLN:NE2 | 2.54 | 0.41 |
| 9:v:64:VAL:O | 9:v:65:THR:OG1 | 2.32 | 0.41 |
| 9:y:42:ILE:HG22 | 9:y:68:TYR:HB3 | 2.03 | 0.41 |
| 9:z:118:ASP:HB3 | 9:z:123:GLU:HG3 | 2.02 | 0.41 |
| 1:0:207:LEU:O | 1:0:210:ILE:HG13 | 2.22 | 0.40 |
| 2:1:23:SER:OG | 2:1:24:THR:N | 2.54 | 0.40 |
| 2:1:195:LEU:HD12 | 2:1:225:LEU:HA | 2.02 | 0.40 |
| 2:2:464:VAL:HG12 | 2:AP:313:ASP:HB3 | 2.03 | 0.40 |
| 2:3:154:ALA:HB1 | 2:3:160:TYR:HB2 | 2.02 | 0.40 |
| 2:3:187:ILE:HD13 | 2:3:187:ILE:HA | 1.93 | 0.40 |
| 2:5:252:LEU:HB3 | 2:5:336:GLY:HA2 | 2.02 | 0.40 |
| 3:9:43:ALA:HB2 | 3:AA:139:GLU:HA | 2.03 | 0.40 |
| 5:A0:36:LEU:HB2 | 5:A0:38:ASP:OD2 | 2.21 | 0.40 |
| 5:A0:293:PRO:HB3 | 7:BC:47:GLU:O | 2.21 | 0.40 |
| 5:A0:423:LYS:HB2 | 5:A0:437:TRP:CZ2 | 2.55 | 0.40 |
| 7:A6:105:PRO:HG3 | 6:Aw:234:GLU:HG3 | 2.02 | 0.40 |
| 6:A7:267:LYS:HB2 | 6:A8:247:TRP:CE3 | 2.57 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A7:401:ALA:O | 6:A8:420:LYS:NZ | 2.33 | 0.40 |
| 6:A9:148:TYR:HA | 6:A9:186:GLY:H | 1.86 | 0.40 |
| 3:AH:99:ILE:O | 3:Bd:120:ALA:HB2 | 2.22 | 0.40 |
| 2:AL:252:LEU:HB3 | 2:AL:336:GLY:HA2 | 2.03 | 0.40 |
| 2:AM:390:GLN:NE2 | 2:AM:408:SER:O | 2.30 | 0.40 |
| 2:AO:213:ASN:O | 2:AO:217:TYR:HD2 | 2.04 | 0.40 |
| 6:AV:267:LYS:O | 6:AZ:249:GLU:HA | 2.21 | 0.40 |
| 6:AV:270:TYR:HB3 | 6:AV:290:LEU:CD1 | 2.51 | 0.40 |
| 6:AV:450:TYR:HB2 | 6:AV:479:ILE:HB | 2.02 | 0.40 |
| 6:AW:337:PRO:HA | 6:AW:340:ILE:HG12 | 2.02 | 0.40 |
| 7:Ab:250:TYR:HA | 7:Ab:293:LEU:HD13 | 2.03 | 0.40 |
| 6:Ah:121:THR:HA | 6:Ah:259:ILE:O | 2.21 | 0.40 |
| 6:Ah:311:ASN:ND2 | 6:Ah:433:TYR:OH | 2.47 | 0.40 |
| 6:Ak:147:MET:O | 6:Ak:185:THR:HA | 2.21 | 0.40 |
| 7:Al:192:ILE:HG23 | 7:Al:197:MET:HE2 | 2.02 | 0.40 |
| 7:Al:202:VAL:O | 4:V:27:ASN:HA | 2.21 | 0.40 |
| 6:Ap:430:LYS:HD3 | 6:Ap:430:LYS:HA | 1.84 | 0.40 |
| 7:Ar:53:LEU:HA | 7:Ar:53:LEU:HD12 | 1.82 | 0.40 |
| 7:At:115:ALA:HB1 | 5:BH:81:ASN:OD1 | 2.21 | 0.40 |
| 7:At:246:TRP:NE1 | 7:At:297:LEU:HB2 | 2.36 | 0.40 |
| 5:Ax:37:ASP:OD1 | 5:Ax:37:ASP:N | 2.53 | 0.40 |
| 5:Ax:161:ILE:HD12 | 5:Ax:173:GLU:HB3 | 2.03 | 0.40 |
| 6:Az:298:ILE:HG21 | 6:Az:456:LEU:HD21 | 2.02 | 0.40 |
| 6:Az:323:LEU:HD13 | 6:Az:329:ALA:HA | 2.02 | 0.40 |
| 2:B2:451:ASP:OD2 | 2:B2:470:LEU:HB3 | 2.21 | 0.40 |
| 2:B4:101:TYR:CE1 | 2:B4:143:ILE:HG12 | 2.57 | 0.40 |
| 2:B4:131:ILE:HG23 | 2:B4:143:ILE:HG22 | 2.03 | 0.40 |
| 2:B5:654:LEU:HD13 | 2:B6:605:ARG:HD3 | 2.03 | 0.40 |
| 2:B6:490:SER:O | 2:B6:496:ARG:NH1 | 2.40 | 0.40 |
| 2:B7:605:ARG:NH2 | 2:B7:606:VAL:O | 2.54 | 0.40 |
| 5:BA:376:PRO:HB3 | 5:BA:399:ASP:HB2 | 2.03 | 0.40 |
| 5:BA:488:LYS:HE3 | 5:BA:488:LYS:HB2 | 1.87 | 0.40 |
| 7:BC:162:TRP:HE1 | 7:BE:54:ASN:HA | 1.85 | 0.40 |
| 7:BC:296:GLU:O | 7:BC:299:LEU:HD12 | 2.22 | 0.40 |
| 5:BH:429:LYS:HE3 | 5:BH:429:LYS:HB2 | 1.94 | 0.40 |
| 6:BI:270:TYR:HA | 6:BM:67:GLU:HB2 | 2.03 | 0.40 |
| 6:BJ:276:GLN:HG3 | 6:BJ:279:ARG:HH22 | 1.85 | 0.40 |
| 7:BL:127:ARG:HG2 | 6:BM:442:ASN:HD21 | 1.85 | 0.40 |
| 11:BN:64:GLN:HG3 | 11:BN:67:GLU:HB2 | 2.03 | 0.40 |
| 11:BS:34:LEU:HD11 | 11:BS:65:ARG:HA | 2.03 | 0.40 |
| 3:BY:3:VAL:N | 3:Bd:97:ASN:O | 2.49 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bc:104:PRO:HA | 3:Bc:107:TYR:CZ | 2.56 | 0.40 |
| 3:Bd:53:PHE:HE2 | 3:Be:5:ASP:HB2 | 1.85 | 0.40 |
| 3:Bg:48:LYS:HB2 | 3:Bj:133:TRP:CZ2 | 2.56 | 0.40 |
| 3:Bo:137:VAL:HG23 | 3:Bo:155:VAL:HG22 | 2.03 | 0.40 |
| 2:Bp:252:LEU:HG | 2:Bp:263:SER:HB3 | 2.03 | 0.40 |
| 2:Bp:261:ARG:CZ | 2:Bp:337:ILE:HD13 | 2.51 | 0.40 |
| 2:Bq:3:LEU:HD11 | 2:Bq:9:GLU:HB2 | 2.03 | 0.40 |
| 2:Bq:462:ASN:HB2 | 2:Bq:464:VAL:HG22 | 2.03 | 0.40 |
| 2:Br:44:VAL:HG11 | 2:Br:50:LEU:HB2 | 2.03 | 0.40 |
| 2:Bs:572:LEU:HD12 | 2:Bs:572:LEU:HA | 1.78 | 0.40 |
| 2:Bt:474:ILE:H | 2:Bt:474:ILE:HG12 | 1.68 | 0.40 |
| 2:Bu:536:TYR:HD1 | 2:Bu:536:TYR:HA | 1.77 | 0.40 |
| 2:Bv:456:TYR:O | 2:Bv:503:ILE:HG22 | 2.21 | 0.40 |
| 2:Bw:510:ARG:HG2 | 2:Bw:511:GLN:H | 1.86 | 0.40 |
| 2:Bw:557:PHE:CE1 | 2:Bw:629:ILE:HD11 | 2.56 | 0.40 |
| 2:By:596:LYS:HG2 | 2:By:601:ILE:O | 2.21 | 0.40 |
| 2:Bz:215:LYS:HB2 | 2:Bz:329:ASN:HD22 | 1.86 | 0.40 |
| 4:M:44:MET:HE3 | 4:N:44:MET:HE3 | 2.02 | 0.40 |
| 4:V:35:ASP:OD1 | 4:a:27:ASN:ND2 | 2.54 | 0.40 |
| 1:k:11:LYS:HB3 | 1:k:11:LYS:HE2 | 1.91 | 0.40 |
| 1:k:122:LEU:HA | 1:l:3:THR:HG21 | 2.03 | 0.40 |
| 1:l:142:MET:HE3 | 1:l:142:MET:HB3 | 1.98 | 0.40 |
| 8:q:47:GLU:OE1 | 8:r:184:ARG:NH2 | 2.53 | 0.40 |
| 8:s:128:ASP:O | 8:s:132:GLN:HG3 | 2.21 | 0.40 |
| 9:v:42:ILE:HG22 | 9:v:68:TYR:HB3 | 2.02 | 0.40 |
| 2:1:310:TYR:HD2 | 2:1:313:ASP:H | 1.69 | 0.40 |
| 2:1:383:LEU:HD13 | 2:1:439:ASN:HB2 | 2.02 | 0.40 |
| 2:2:644:ALA:O | 2:2:645:THR:OG1 | 2.38 | 0.40 |
| 2:3:193:ILE:HD12 | 2:3:193:ILE:HA | 1.91 | 0.40 |
| 2:4:252:LEU:HA | 2:4:253:PRO:HD3 | 1.96 | 0.40 |
| 2:5:91:ASN:ND2 | 2:5:225:LEU:O | 2.53 | 0.40 |
| 2:5:430:ARG:HD3 | 2:5:520:GLU:O | 2.20 | 0.40 |
| 2:5:450:ILE:HD13 | 2:5:522:ILE:HG12 | 2.03 | 0.40 |
| 3:9:45:ILE:HG23 | 3:9:65:THR:O | 2.21 | 0.40 |
| 5:A2:282:ARG:O | 5:A2:350:LEU:HB3 | 2.20 | 0.40 |
| 5:A3:31:ILE:H | 5:A3:31:ILE:HD13 | 1.86 | 0.40 |
| 5:A3:477:ILE:H | 5:A3:477:ILE:HG13 | 1.71 | 0.40 |
| 6:A7:450:TYR:HA | 6:A7:479:ILE:HG12 | 2.02 | 0.40 |
| 6:A8:232:ILE:O | 6:A8:236:GLN:HG2 | 2.21 | 0.40 |
| 6:A8:406:THR:OG1 | 6:A9:372:GLU:OE2 | 2.27 | 0.40 |
| 6:A8:416:VAL:HG12 | 6:A8:419:GLY:H | 1.87 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:A9:111:ILE:HD12 | 6:A9:377:ILE:HD11 | 2.03 | 0.40 |
| 3:AA:46:VAL:HG22 | 3:AA:64:ARG:HD2 | 2.02 | 0.40 |
| 8:AB:58:SER:O | 8:AB:61:SER:HB2 | 2.20 | 0.40 |
| 8:AB:101:GLY:C | 8:AB:103:THR:H | 2.29 | 0.40 |
| 2:AK:33:PHE:HA | 2:AK:61:THR:HG23 | 2.02 | 0.40 |
| 2:AK:57:PRO:HG3 | 2:AK:65:PHE:CG | 2.56 | 0.40 |
| 2:AL:253:PRO:HA | 2:AL:260:THR:HG22 | 2.03 | 0.40 |
| 2:AL:576:ASN:ND2 | 2:AL:576:ASN:O | 2.54 | 0.40 |
| 2:AO:415:VAL:HG13 | 2:AO:416:GLY:H | 1.85 | 0.40 |
| 2:AP:30:ALA:HB3 | 2:AP:359:TRP:CE2 | 2.56 | 0.40 |
| 10:AQ:304:TYR:CD1 | 6:Af:337:PRO:HD3 | 2.57 | 0.40 |
| 10:AR:332:SER:HB2 | 10:AR:338:ARG:HH22 | 1.87 | 0.40 |
| 6:AV:273:GLU:OE2 | 6:BJ:474:LYS:HD3 | 2.20 | 0.40 |
| 6:AV:355:PHE:CE2 | 6:AV:359:LYS:HD2 | 2.56 | 0.40 |
| 6:AW:106:LEU:HD23 | 6:AW:300:LEU:HD23 | 2.02 | 0.40 |
| 6:AX:494:SER:HA | 11:BQ:37:ASP:CG | 2.45 | 0.40 |
| 7:AY:165:SER:O | 7:AY:168:GLU:HG3 | 2.21 | 0.40 |
| 7:Aa:60:PHE:CE2 | 7:Aa:170:LEU:HD21 | 2.56 | 0.40 |
| 7:Ab:95:ILE:H | 7:Ab:95:ILE:HG13 | 1.50 | 0.40 |
| 7:Ab:162:TRP:CD1 | 7:Ar:55:LYS:HD2 | 2.56 | 0.40 |
| 6:Ad:112:CYS:HA | 6:Ad:446:ALA:HB1 | 2.03 | 0.40 |
| 6:Ae:160:ALA:HB2 | 6:Ae:232:ILE:HG21 | 2.04 | 0.40 |
| 6:Ae:351:LYS:HB3 | 6:Ay:398:GLN:OE1 | 2.22 | 0.40 |
| 6:Ae:387:ALA:HB2 | 6:Ae:404:PHE:HB2 | 2.03 | 0.40 |
| 6:Af:265:GLN:HB3 | 6:Aj:247:TRP:CZ3 | 2.56 | 0.40 |
| 6:Ak:318:LYS:NZ | 6:Ak:356:GLN:OE1 | 2.34 | 0.40 |
| 7:Al:12:LEU:HD12 | 7:Al:242:TYR:CD2 | 2.51 | 0.40 |
| 7:Al:80:ASN:H | 7:Al:221:ASN:HD21 | 1.70 | 0.40 |
| 7:Aq:53:LEU:HD21 | 7:Aq:82:PHE:CD2 | 2.56 | 0.40 |
| 7:Aq:307:LEU:HD23 | 7:Aq:307:LEU:HA | 1.88 | 0.40 |
| 6:Au:74:TYR:HD1 | 6:Ay:500:MET:HE1 | 1.87 | 0.40 |
| 6:Au:131:TYR:HB2 | 6:Au:154:PHE:CZ | 2.56 | 0.40 |
| 5:Ax:115:LYS:HE2 | 5:Ax:115:LYS:HB3 | 1.82 | 0.40 |
| 5:Ax:477:ILE:HA | 5:Ax:481:ILE:HG23 | 2.02 | 0.40 |
| 6:Ay:207:LYS:O | 6:Ay:211:GLU:HG2 | 2.21 | 0.40 |
| 6:Az:495:ARG:HE | 6:Az:495:ARG:HB3 | 1.77 | 0.40 |
| 2:B1:313:ASP:HB3 | 2:Bz:464:VAL:HG12 | 2.03 | 0.40 |
| 2:B2:464:VAL:HG12 | 2:B3:313:ASP:HB3 | 2.04 | 0.40 |
| 2:B3:10:LEU:HD23 | 2:Bz:640:LEU:HB2 | 2.03 | 0.40 |
| 2:B3:110:TYR:CG | 2:B3:177:GLY:HA3 | 2.56 | 0.40 |
| 2:B3:253:PRO:HG2 | 2:B3:255:TYR:HE1 | 1.87 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B3:413:THR:C | 2:B3:417:ILE:HD11 | 2.46 | 0.40 |
| 2:B3:477:LEU:HD13 | 2:B3:499:ILE:HD13 | 2.03 | 0.40 |
| 2:B4:596:LYS:HG3 | 2:B4:601:ILE:O | 2.21 | 0.40 |
| 2:B5:69:MET:O | 2:B5:73:GLN:HG2 | 2.21 | 0.40 |
| 5:BA:401:LEU:HD23 | 5:BA:401:LEU:HA | 1.83 | 0.40 |
| 5:BB:86:TYR:C | 5:BB:88:VAL:H | 2.29 | 0.40 |
| 5:BB:267:LEU:HD12 | 5:BB:365:PHE:CD2 | 2.57 | 0.40 |
| 5:BB:328:MET:HE1 | 5:BB:334:TYR:CZ | 2.55 | 0.40 |
| 5:BF:41:ARG:HE | 5:BF:66:GLU:CD | 2.30 | 0.40 |
| 5:BF:423:LYS:HG3 | 5:BF:437:TRP:CD1 | 2.56 | 0.40 |
| 6:BJ:304:ARG:NH2 | 6:BJ:308:ASP:OD1 | 2.54 | 0.40 |
| 6:BK:242:SER:HB2 | 6:BK:245:ASN:HD21 | 1.86 | 0.40 |
| 11:BO:62:GLU:HG2 | 11:BS:4:THR:HG21 | 2.03 | 0.40 |
| 11:BT:72:ASN:OD1 | 11:BT:73:GLU:N | 2.54 | 0.40 |
| 3:BZ:25:ILE:HG23 | 3:BZ:111:ALA:HB2 | 2.02 | 0.40 |
| 3:BZ:83:GLN:HA | 3:BZ:86:VAL:HG22 | 2.02 | 0.40 |
| 3:Ba:46:VAL:HG22 | 3:Ba:64:ARG:HA | 2.04 | 0.40 |
| 3:Bb:48:LYS:HE3 | 3:Bb:48:LYS:HB3 | 1.84 | 0.40 |
| 3:Bc:128:GLU:HB3 | 3:Bc:130:LYS:HE2 | 2.04 | 0.40 |
| 3:Be:2:PHE:HA | 3:Bj:98:GLU:HA | 2.02 | 0.40 |
| 3:Bh:17:ARG:HD2 | 3:Bh:118:ARG:HD3 | 2.03 | 0.40 |
| 3:Bh:131:GLY:O | 3:Bh:159:LEU:HA | 2.21 | 0.40 |
| 3:Bn:43:ALA:O | 3:Bn:162:TRP:NE1 | 2.52 | 0.40 |
| 2:Bq:30:ALA:HB3 | 2:Bq:359:TRP:CE2 | 2.56 | 0.40 |
| 2:Br:57:PRO:HB2 | 2:Br:62:ALA:HA | 2.02 | 0.40 |
| 2:Br:252:LEU:HD22 | 2:Br:335:SER:O | 2.21 | 0.40 |
| 2:Br:269:PHE:CE2 | 2:Br:282:ILE:HG13 | 2.56 | 0.40 |
| 2:Bt:205:MET:O | 2:Bt:211:GLN:NE2 | 2.34 | 0.40 |
| 2:Bt:413:THR:OG1 | 2:Bt:425:ASN:HB3 | 2.21 | 0.40 |
| 2:Bt:642:PHE:CZ | 2:Bu:561:LYS:HG2 | 2.57 | 0.40 |
| 2:Bu:28:ALA:HB2 | 2:Bu:370:VAL:HG11 | 2.02 | 0.40 |
| 2:Bu:459:ASP:HB3 | 2:Bu:464:VAL:HG23 | 2.03 | 0.40 |
| 4:G:66:LYS:HE3 | 4:G:66:LYS:HB3 | 1.91 | 0.40 |
| 4:K:66:LYS:HD3 | 4:L:5:LEU:HD12 | 2.03 | 0.40 |
| 4:Z:5:LEU:HD23 | 4:Z:5:LEU:HA | 1.94 | 0.40 |
| 4:e:16:ALA:H | 4:e:19:GLN:HB2 | 1.86 | 0.40 |
| 1:k:176:TYR:CE1 | 1:k:179:GLU:HG3 | 2.56 | 0.40 |
| 1:m:151:TRP:CG | 8:t:180:ASN:HB3 | 2.57 | 0.40 |
| 8:q:144:HIS:HB2 | 8:q:164:LYS:HB3 | 2.03 | 0.40 |
| 8:r:128:ASP:O | 8:r:132:GLN:HG3 | 2.22 | 0.40 |
| 8:u:42:THR:O | 8:u:76:ASN:HA | 2.21 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:228:ALA:HA | 1:0:231:TYR:CE2 | 2.57 | 0.40 |
| 2:2:91:ASN:HD21 | 2:2:195:LEU:HG | 1.87 | 0.40 |
| 2:3:35:TRP:NE1 | 2:3:226:TYR:HD2 | 2.20 | 0.40 |
| 2:4:273:PRO:HB3 | 2:4:278:GLN:HB2 | 2.02 | 0.40 |
| 2:5:26:THR:HA | 2:5:77:ASP:O | 2.22 | 0.40 |
| 2:5:401:GLN:O | 2:5:561:LYS:NZ | 2.54 | 0.40 |
| 3:6:104:PRO:O | 3:6:108:LYS:HB2 | 2.21 | 0.40 |
| 3:8:52:GLY:HA2 | 3:8:57:LYS:HA | 2.02 | 0.40 |
| 3:8:131:GLY:O | 3:8:159:LEU:HA | 2.21 | 0.40 |
| 3:9:20:LEU:HD21 | 9:w:56:LEU:HD21 | 2.03 | 0.40 |
| 3:9:55:ASN:ND2 | 3:9:55:ASN:O | 2.55 | 0.40 |
| 5:A1:328:MET:SD | 5:A1:334:TYR:OH | 2.67 | 0.40 |
| 5:A1:337:GLN:HE21 | 5:A1:344:VAL:HG11 | 1.87 | 0.40 |
| 5:A3:315:ASP:OD2 | 5:A3:318:THR:OG1 | 2.28 | 0.40 |
| 6:A4:117:MET:HB2 | 6:A4:451:ALA:HB1 | 2.04 | 0.40 |
| 6:A5:290:LEU:HD23 | 6:A5:290:LEU:HA | 1.92 | 0.40 |
| 6:A7:123:GLN:O | 6:AW:96:MET:HB2 | 2.22 | 0.40 |
| 6:A8:199:ASP:HB2 | 6:A8:211:GLU:HG2 | 2.02 | 0.40 |
| 6:A9:265:GLN:HG3 | 6:A9:266:LEU:N | 2.36 | 0.40 |
| 8:AB:222:ASP:HA | 2:AD:605:ARG:NH2 | 2.36 | 0.40 |
| 3:AE:113:VAL:HG13 | 3:AE:127:ILE:HG12 | 2.04 | 0.40 |
| 3:AE:140:LEU:HD11 | 3:AE:151:GLN:HB3 | 2.03 | 0.40 |
| 3:AI:90:SER:HA | 3:AI:94:GLY:H | 1.86 | 0.40 |
| 2:AK:378:CYS:SG | 2:AK:454:TYR:OH | 2.60 | 0.40 |
| 2:AL:384:GLU:HG2 | 2:AL:439:ASN:OD1 | 2.22 | 0.40 |
| 2:AN:237:GLU:HB3 | 2:AN:282:ILE:HB | 2.04 | 0.40 |
| 2:AN:638:ILE:HD13 | 2:B2:568:SER:HB2 | 2.03 | 0.40 |
| 2:AO:355:LEU:HD23 | 2:AO:355:LEU:HA | 1.92 | 0.40 |
| 2:AP:32:LYS:HD3 | 2:AP:32:LYS:H | 1.87 | 0.40 |
| 10:AU:319:THR:HG23 | 10:AU:325:TRP:HB3 | 2.03 | 0.40 |
| 7:Aa:265:ARG:NH2 | 7:Ab:26:ASN:O | 2.55 | 0.40 |
| 7:Ab:29:LEU:HD21 | 7:Ab:259:ASN:HB2 | 2.04 | 0.40 |
| 7:Ab:189:LYS:O | 7:Ab:222:PRO:HG3 | 2.22 | 0.40 |
| 6:Ac:444:MET:HE2 | 6:Ac:444:MET:HB3 | 1.92 | 0.40 |
| 6:Ag:191:GLN:HB2 | 6:Ag:224:ILE:HG21 | 2.02 | 0.40 |
| 6:Ai:390:ASP:HB2 | 6:Ai:397:ALA:HB3 | 2.03 | 0.40 |
| 6:Aj:439:LYS:NZ | 6:Aj:440:GLY:O | 2.49 | 0.40 |
| 7:Al:24:ILE:HG22 | 7:Al:25:ILE:HG23 | 2.04 | 0.40 |
| 7:Al:160:ASP:OD1 | 7:Al:173:MET:HB2 | 2.21 | 0.40 |
| 6:Ao:376:ILE:O | 6:Ao:423:VAL:HA | 2.22 | 0.40 |
| 6:Ao:404:PHE:HZ | 6:Ao:417:LEU:HG | 1.85 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:Aq:6:PRO:HG2 | 7:Aq:248:LYS:HD3 | 2.04 | 0.40 |
| 7:Ar:65:ASP:HB3 | 7:Ar:68:ARG:HB2 | 2.03 | 0.40 |
| 7:At:112:LEU:HB2 | 7:At:116:GLY:H | 1.87 | 0.40 |
| 6:Au:93:PRO:HG2 | 6:Ay:123:GLN:CD | 2.45 | 0.40 |
| 6:Ay:114:VAL:HG23 | 6:Ay:115:GLN:H | 1.86 | 0.40 |
| 6:Ay:449:TYR:OH | 6:Ay:482:ASN:HB2 | 2.21 | 0.40 |
| 2:B1:10:LEU:HD22 | 2:Bx:642:PHE:HE1 | 1.86 | 0.40 |
| 2:B1:115:LYS:HD2 | 2:B1:115:LYS:HA | 1.94 | 0.40 |
| 2:B2:57:PRO:HB3 | 2:B2:62:ALA:CA | 2.46 | 0.40 |
| 2:B2:293:VAL:HG22 | 2:B2:294:VAL:H | 1.85 | 0.40 |
| 2:B3:579:PHE:CE2 | 3:Bj:30:GLN:HB2 | 2.57 | 0.40 |
| 2:B4:612:ASN:OD1 | 2:B4:612:ASN:N | 2.54 | 0.40 |
| 2:B4:614:THR:C | 2:B4:616:SER:H | 2.29 | 0.40 |
| 2:B4:654:LEU:HD13 | 2:B4:655:THR:HG22 | 2.03 | 0.40 |
| 2:B5:46:ASN:OD1 | 2:B5:47:GLU:N | 2.51 | 0.40 |
| 2:B5:225:LEU:HD12 | 2:B5:324:PHE:HB2 | 2.03 | 0.40 |
| 2:B5:310:TYR:CE2 | 2:B5:312:ASP:HB2 | 2.56 | 0.40 |
| 2:B6:28:ALA:HB1 | 2:B6:362:PHE:CZ | 2.57 | 0.40 |
| 2:B6:583:SER:HB3 | 3:Bm:26:SER:HB2 | 2.03 | 0.40 |
| 5:BA:113:LEU:HD21 | 5:BA:444:ILE:HG13 | 2.03 | 0.40 |
| 5:BB:208:TYR:HB3 | 5:BB:228:ILE:HG22 | 2.02 | 0.40 |
| 5:BH:413:LYS:HA | 5:BH:413:LYS:HD2 | 1.82 | 0.40 |
| 5:BH:477:ILE:HD12 | 5:BH:483:HIS:CE1 | 2.56 | 0.40 |
| 7:BL:118:ASN:ND2 | 6:BM:118:ASN:O | 2.50 | 0.40 |
| 6:BM:204:ASP:OD1 | 6:BM:205:ALA:N | 2.53 | 0.40 |
| 3:Bb:48:LYS:HG3 | 3:Bb:59:ASN:HB3 | 2.03 | 0.40 |
| 3:Bj:91:ILE:HG22 | 3:Bj:107:TYR:HB3 | 2.04 | 0.40 |
| 3:Bk:30:GLN:O | 3:Bk:30:GLN:NE2 | 2.41 | 0.40 |
| 2:Bq:193:ILE:HB | 2:Bq:210:PHE:CZ | 2.56 | 0.40 |
| 2:Br:90:LYS:HA | 2:Br:90:LYS:HD3 | 1.87 | 0.40 |
| 2:Bs:137:ASP:OD1 | 2:Bs:137:ASP:N | 2.55 | 0.40 |
| 2:Bs:413:THR:C | 2:Bs:417:ILE:HD11 | 2.46 | 0.40 |
| 2:Bs:510:ARG:HG2 | 2:Bs:511:GLN:H | 1.87 | 0.40 |
| 2:Bs:643:VAL:HG12 | 2:Bs:645:THR:HG23 | 2.03 | 0.40 |
| 2:Bt:108:SER:O | 2:Bt:177:GLY:HA2 | 2.20 | 0.40 |
| 2:Bt:642:PHE:CZ | 2:Bu:564:ILE:HD11 | 2.55 | 0.40 |
| 2:Bu:107:GLY:H | 2:Bu:140:ILE:HG12 | 1.86 | 0.40 |
| 2:Bv:299:ARG:H | 2:Bv:299:ARG:HD2 | 1.87 | 0.40 |
| 2:Bw:110:TYR:CE1 | 2:Bw:171:ILE:HG21 | 2.54 | 0.40 |
| 2:Bw:195:LEU:HD23 | 2:Bw:195:LEU:H | 1.85 | 0.40 |
| 2:Bw:572:LEU:O | 2:Bw:573:PHE:C | 2.64 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bw:595:ILE:HG22 | 2:Bw:601:ILE:HG12 | 2.03 | 0.40 |
| 2:Bx:295:LEU:HD11 | 2:Bx:315:PHE:HE2 | 1.87 | 0.40 |
| 2:Bx:477:LEU:HD11 | 2:Bx:497:GLY:HA2 | 2.03 | 0.40 |
| 2:By:91:ASN:OD1 | 2:By:91:ASN:N | 2.53 | 0.40 |
| 2:Bz:291:GLN:HE22 | 2:Bz:320:SER:HB2 | 1.85 | 0.40 |
| 4:F:27:ASN:HB3 | 4:f:38:TYR:CE2 | 2.57 | 0.40 |
| 4:W:41:GLU:O | 4:W:45:ASN:ND2 | 2.54 | 0.40 |
| 1:m:221:VAL:HG13 | 8:t:22:SER:HB2 | 2.03 | 0.40 |
| 8:t:124:THR:HG22 | 8:t:126:TYR:H | 1.85 | 0.40 |
| 9:v:83:SER:O | 9:v:87:MET:HG2 | 2.21 | 0.40 |
| 2:1:306:ASP:HB3 | 8:AB:219:ASN:ND2 | 2.37 | 0.40 |
| 2:2:401:GLN:NE2 | 8:r:257:SER:OG | 2.54 | 0.40 |
| 2:4:202:GLU:O | 2:4:206:THR:OG1 | 2.36 | 0.40 |
| 2:4:642:PHE:CZ | 2:AL:564:ILE:HD11 | 2.56 | 0.40 |
| 2:5:509:THR:O | 2:5:514:ARG:NH1 | 2.54 | 0.40 |
| 3:6:2:PHE:HA | 9:AC:53:PRO:HG3 | 2.04 | 0.40 |
| 3:6:16:ALA:O | 3:7:151:GLN:HG2 | 2.21 | 0.40 |
| 5:A1:283:ARG:NH1 | 5:A1:334:TYR:OH | 2.54 | 0.40 |
| 5:A2:126:MET:HG2 | 5:A2:426:LEU:HD11 | 2.03 | 0.40 |
| 5:A3:366:ARG:HG2 | 5:A3:380:ILE:HD12 | 2.03 | 0.40 |
| 7:A6:127:ARG:HA | 7:A6:127:ARG:CZ | 2.51 | 0.40 |
| 6:A7:106:LEU:HD21 | 6:A7:300:LEU:HG | 2.03 | 0.40 |
| 6:A7:245:ASN:N | 6:A7:245:ASN:OD1 | 2.54 | 0.40 |
| 6:A9:317:GLY:HA2 | 6:A9:514:ARG:NE | 2.36 | 0.40 |
| 6:A9:459:LEU:HD22 | 7:As:98:MET:HG3 | 2.02 | 0.40 |
| 3:AA:103:LYS:O | 3:AA:106:GLU:HG2 | 2.22 | 0.40 |
| 3:AA:130:LYS:HE2 | 3:AA:130:LYS:HB3 | 1.95 | 0.40 |
| 2:AD:450:ILE:HG22 | 2:AD:541:ALA:HB2 | 2.03 | 0.40 |
| 2:AD:528:THR:HB | 2:AN:366:GLU:HB2 | 2.03 | 0.40 |
| 3:AH:98:GLU:H | 3:AH:98:GLU:CD | 2.30 | 0.40 |
| 2:AK:32:LYS:NZ | 2:AK:347:ASN:O | 2.54 | 0.40 |
| 2:AN:614:THR:C | 2:AN:616:SER:H | 2.30 | 0.40 |
| 2:AO:391:LYS:HZ3 | 2:AO:443:ILE:HD13 | 1.86 | 0.40 |
| 2:AP:404:LEU:HD22 | 2:AP:404:LEU:HA | 1.91 | 0.40 |
| 10:AQ:351:VAL:O | 10:AQ:363:HIS:HA | 2.21 | 0.40 |
| 10:AU:348:TYR:HA | 10:AU:349:PRO:HD3 | 1.89 | 0.40 |
| 6:AZ:131:TYR:CE1 | 6:AZ:141:LYS:HB2 | 2.45 | 0.40 |
| 6:AZ:169:SER:HB3 | 6:AZ:200:ALA:HB2 | 2.04 | 0.40 |
| 6:Ac:131:TYR:HA | 6:Ac:250:MET:HA | 2.03 | 0.40 |
| 6:Af:380:ARG:NH1 | 6:Af:427:GLN:O | 2.51 | 0.40 |
| 6:Ag:377:ILE:HG23 | 6:Ag:435:THR:HB | 2.04 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Ag:385:VAL:HG21 | 6:Ag:521:ILE:HD12 | 2.02 | 0.40 |
| 6:Ah:304:ARG:NH2 | 6:Ah:308:ASP:OD1 | 2.55 | 0.40 |
| 6:Ai:131:TYR:HE1 | 6:Ai:141:LYS:HB2 | 1.86 | 0.40 |
| 6:Ai:180:HIS:NE2 | 6:Ai:209:ASP:OD1 | 2.46 | 0.40 |
| 6:Aj:169:SER:HB3 | 6:Aj:200:ALA:HB2 | 2.02 | 0.40 |
| 6:Ao:351:LYS:NZ | 6:Ao:395:TYR:O | 2.48 | 0.40 |
| 6:Ap:123:GLN:HB3 | 6:Ap:258:VAL:HG12 | 2.02 | 0.40 |
| 7:Ar:204:TYR:CD1 | 7:Ar:226:LEU:HD13 | 2.57 | 0.40 |
| 7:Ar:204:TYR:O | 4:h:31:ILE:HB | 2.20 | 0.40 |
| 7:At:125:CYS:O | 7:At:127:ARG:N | 2.54 | 0.40 |
| 5:Ax:111:LEU:HD12 | 5:Ax:111:LEU:HA | 1.92 | 0.40 |
| 6:Ay:453:TYR:CD2 | 6:Ay:454:VAL:HG23 | 2.55 | 0.40 |
| 6:Az:163:PHE:HB2 | 6:Az:179:THR:HG23 | 2.03 | 0.40 |
| 6:Az:304:ARG:HA | 6:Az:304:ARG:HD2 | 1.87 | 0.40 |
| 2:B1:143:ILE:HD12 | 2:B1:145:ILE:HD11 | 2.02 | 0.40 |
| 2:B1:446:THR:OG1 | 2:B1:554:ARG:NH2 | 2.53 | 0.40 |
| 2:B4:275:THR:OG1 | 2:B4:278:GLN:HG3 | 2.22 | 0.40 |
| 2:B6:621:ASN:OD1 | 2:B6:621:ASN:N | 2.55 | 0.40 |
| 2:B7:577:ASN:HA | 2:B7:581:ARG:HH21 | 1.87 | 0.40 |
| 5:BA:420:ASP:HB3 | 5:BA:421:PRO:HD3 | 2.03 | 0.40 |
| 5:BB:244:ASP:O | 5:BB:245:CYS:C | 2.64 | 0.40 |
| 7:BC:269:MET:HE2 | 7:BC:269:MET:HB3 | 1.82 | 0.40 |
| 5:BF:463:LEU:HD12 | 5:BF:463:LEU:HA | 1.85 | 0.40 |
| 5:BH:99:ALA:HB2 | 5:BH:407:ILE:HD12 | 2.03 | 0.40 |
| 7:BL:204:TYR:O | 4:O:31:ILE:HB | 2.21 | 0.40 |
| 6:BM:263:SER:HA | 6:BM:476:ARG:HA | 2.02 | 0.40 |
| 6:BM:312:TYR:CZ | 6:BM:507:LEU:HD13 | 2.56 | 0.40 |
| 11:BN:10:ILE:HD11 | 11:BN:35:TYR:CE1 | 2.57 | 0.40 |
| 3:BY:133:TRP:CH2 | 3:Bn:61:ALA:HA | 2.57 | 0.40 |
| 3:BY:140:LEU:HD13 | 3:BY:153:PHE:HB3 | 2.03 | 0.40 |
| 3:BZ:144:TRP:CE2 | 3:Bk:54:MET:HG2 | 2.57 | 0.40 |
| 3:Bd:56:ARG:HB3 | 3:Bd:56:ARG:HH11 | 1.87 | 0.40 |
| 3:Bd:134:PRO:HA | 3:Bd:157:LEU:HA | 2.03 | 0.40 |
| 3:Bf:132:LEU:HD13 | 3:Bf:132:LEU:HA | 1.88 | 0.40 |
| 3:Bh:124:THR:OG1 | 3:Bk:78:ALA:HA | 2.21 | 0.40 |
| 3:Bk:17:ARG:C | 3:Bn:151:GLN:HG3 | 2.47 | 0.40 |
| 3:Bn:23:VAL:HG22 | 3:Bn:36:CYS:SG | 2.61 | 0.40 |
| 2:Bp:383:LEU:HD11 | 2:Bp:436:TYR:CD1 | 2.57 | 0.40 |
| 2:Bq:130:LYS:HE2 | 2:Bq:130:LYS:HB2 | 1.87 | 0.40 |
| 2:Bq:193:ILE:HD13 | 2:Bq:205:MET:HE3 | 2.02 | 0.40 |
| 2:Bu:240:SER:OG | 2:Bu:243:ASP:OD1 | 2.39 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Bv:32:LYS:HD2 | 2:Bv:64:TYR:CE2 | 2.57 | 0.40 |
| 2:Bv:332:GLU:H | 2:Bv:332:GLU:CD | 2.28 | 0.40 |
| 2:Bv:592:LEU:HD12 | 2:Bv:592:LEU:HA | 1.96 | 0.40 |
| 2:Bx:35:TRP:CG | 2:Bx:36:GLY:H | 2.38 | 0.40 |
| 2:Bx:302:LYS:O | 2:Bx:307:SER:N | 2.55 | 0.40 |
| 2:By:642:PHE:CZ | 2:Bz:561:LYS:HG2 | 2.56 | 0.40 |
| 4:W:31:ILE:HG23 | 4:W:44:MET:SD | 2.61 | 0.40 |
| 1:m:63:ARG:HD3 | 1:m:78:ASN:HD22 | 1.87 | 0.40 |
| 1:p:243:LYS:H | 8:u:4:TYR:H | 1.70 | 0.40 |
| 8:s:81:ASP:OD1 | 8:s:82:PHE:N | 2.53 | 0.40 |
| 8:s:187:GLU:C | 8:s:188:TRP:HD1 | 2.29 | 0.40 |
| 8:u:73:PRO:HD3 | 8:u:124:THR:HG23 | 2.03 | 0.40 |
| 9:z:10:ASN:OD1 | 9:z:10:ASN:N | 2.50 | 0.40 |
| 2:1:614:THR:C | 2:1:616:SER:H | 2.30 | 0.40 |
| 2:3:374:ILE:HG23 | 2:3:471:ALA:O | 2.21 | 0.40 |
| 2:3:609:ASP:HB2 | 2:3:611:THR:HG22 | 2.03 | 0.40 |
| 2:4:66:MET:HB2 | 2:4:66:MET:HE3 | 1.81 | 0.40 |
| 3:8:150:ILE:H | 3:8:150:ILE:HD13 | 1.86 | 0.40 |
| 3:9:125:LYS:HD2 | 3:9:125:LYS:HA | 1.89 | 0.40 |
| 5:A0:200:LYS:HB3 | 5:A0:200:LYS:HE2 | 1.87 | 0.40 |
| 5:A0:423:LYS:HB2 | 5:A0:437:TRP:CE2 | 2.57 | 0.40 |
| 6:A4:71:ASP:HB3 | 6:AW:230:THR:HB | 2.04 | 0.40 |
| 6:A4:131:TYR:CE1 | 6:A4:141:LYS:HB2 | 2.57 | 0.40 |
| 6:A4:431:GLN:HG3 | 6:A4:432:ASP:H | 1.87 | 0.40 |
| 6:A5:151:ASP:HB3 | 6:A5:154:PHE:HB2 | 2.02 | 0.40 |
| 3:AA:5:ASP:HB3 | 3:AA:8:ARG:HB2 | 2.03 | 0.40 |
| 8:AB:46:LYS:O | 8:AB:51:MET:HE2 | 2.22 | 0.40 |
| 3:AF:131:GLY:O | 3:AF:159:LEU:HA | 2.22 | 0.40 |
| 3:AG:8:ARG:HD2 | 3:AH:34:PHE:CE1 | 2.57 | 0.40 |
| 3:AG:99:ILE:O | 3:Ba:120:ALA:HB2 | 2.22 | 0.40 |
| 2:AL:346:SER:O | 2:AL:350:VAL:HG23 | 2.21 | 0.40 |
| 2:AL:364:ASP:O | 2:AL:367:SER:N | 2.50 | 0.40 |
| 2:AL:422:ALA:O | 2:AL:426:LEU:HG | 2.21 | 0.40 |
| 2:AN:126:GLU:HB2 | 2:AN:150:ILE:HD11 | 2.03 | 0.40 |
| 2:AO:102:THR:HB | 2:AO:183:THR:HB | 2.02 | 0.40 |
| 2:AO:110:TYR:CG | 2:AO:177:GLY:HA3 | 2.57 | 0.40 |
| 2:AO:299:ARG:H | 2:AO:299:ARG:HD2 | 1.87 | 0.40 |
| 10:AQ:299:HIS:NE2 | 6:Af:328:LYS:O | 2.54 | 0.40 |
| 6:AV:486:GLU:HA | 6:AV:509:LYS:O | 2.22 | 0.40 |
| 6:AW:131:TYR:HD2 | 6:AW:250:MET:HE3 | 1.87 | 0.40 |
| 6:AX:309:TRP:CZ3 | 6:Az:224:ILE:HD11 | 2.57 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:AY:155:LEU:O | 7:Aq:97:SER:HB2 | 2.21 | 0.40 |
| 6:AZ:347:GLY:O | 6:AZ:351:LYS:HG2 | 2.20 | 0.40 |
| 7:Aa:84:VAL:HG13 | 7:Aa:184:VAL:HB | 2.04 | 0.40 |
| 7:Aa:207:VAL:HG23 | 4:i:29:GLU:O | 2.22 | 0.40 |
| 6:Ac:398:GLN:O | 6:Ag:351:LYS:HD3 | 2.21 | 0.40 |
| 6:Ac:430:LYS:HG2 | 6:Ag:216:MET:HE1 | 2.02 | 0.40 |
| 6:Ad:284:MET:HE1 | 6:Ah:127:LEU:HD13 | 2.04 | 0.40 |
| 6:Ag:105:ASN:ND2 | 6:Ag:411:SER:HA | 2.37 | 0.40 |
| 6:Ag:383:VAL:HG12 | 6:Ag:406:THR:HG22 | 2.04 | 0.40 |
| 6:Ah:69:GLY:O | 6:Ah:86:GLY:HA3 | 2.21 | 0.40 |
| 6:Ak:176:ASP:OD1 | 6:Ak:177:ILE:N | 2.51 | 0.40 |
| 7:Al:267:GLN:HG3 | 7:Al:279:GLY:H | 1.87 | 0.40 |
| 6:Am:304:ARG:HD2 | 6:Am:304:ARG:HA | 1.83 | 0.40 |
| 6:An:117:MET:HG3 | 6:An:451:ALA:HB1 | 2.02 | 0.40 |
| 6:Ap:117:MET:HE3 | 6:Ap:451:ALA:HB3 | 2.03 | 0.40 |
| 7:Ar:12:LEU:HD12 | 7:Ar:242:TYR:CD2 | 2.52 | 0.40 |
| 6:Aw:331:VAL:HG11 | 6:Aw:519:LYS:HD2 | 2.03 | 0.40 |
| 6:Aw:456:LEU:HD23 | 6:Aw:456:LEU:HA | 1.88 | 0.40 |
| 5:Ax:197:LYS:HE2 | 5:Ax:197:LYS:HB3 | 1.98 | 0.40 |
| 6:Az:131:TYR:HB2 | 6:Az:154:PHE:CZ | 2.57 | 0.40 |
| 2:B2:284:ARG:HG3 | 2:B2:289:ILE:HD13 | 2.03 | 0.40 |
| 2:B4:432:ALA:HB2 | 2:B4:440:ASN:HD22 | 1.87 | 0.40 |
| 2:B5:187:ILE:HD13 | 2:B5:187:ILE:HA | 1.97 | 0.40 |
| 2:B5:269:PHE:CZ | 2:B5:292:SER:HB2 | 2.56 | 0.40 |
| 2:B6:23:SER:O | 2:B6:76:ASN:HB2 | 2.22 | 0.40 |
| 2:B6:66:MET:HG2 | 2:B6:468:VAL:HG11 | 2.04 | 0.40 |
| 2:B6:557:PHE:HB3 | 2:B6:561:LYS:NZ | 2.37 | 0.40 |
| 2:B7:153:LYS:HB3 | 2:B7:167:TRP:HH2 | 1.87 | 0.40 |
| 7:BC:53:LEU:HD12 | 7:BC:53:LEU:HA | 1.90 | 0.40 |
| 5:BF:182:VAL:HG22 | 5:BF:208:TYR:CD1 | 2.57 | 0.40 |
| 5:BF:320:LYS:HE3 | 5:BF:320:LYS:HB2 | 1.82 | 0.40 |
| 6:BJ:159:ALA:HB3 | 6:BJ:228:MET:HE1 | 2.03 | 0.40 |
| 6:BK:131:TYR:HB3 | 6:BK:250:MET:HE2 | 2.03 | 0.40 |
| 3:BY:34:PHE:CE2 | 3:Bn:8:ARG:HD2 | 2.57 | 0.40 |
| 3:BY:149:GLU:HB3 | 3:Bn:18:PRO:HG3 | 2.02 | 0.40 |
| 3:BZ:89:GLN:HE21 | 3:BZ:89:GLN:HB2 | 1.74 | 0.40 |
| 3:Ba:1:MET:HE2 | 3:Ba:1:MET:HB3 | 1.85 | 0.40 |
| 3:Bb:83:GLN:HA | 3:Bb:86:VAL:HG22 | 2.03 | 0.40 |
| 3:Bc:114:ARG:HB3 | 3:Bc:123:VAL:HG13 | 2.03 | 0.40 |
| 3:Be:9:ALA:O | 3:Bh:35:GLN:NE2 | 2.55 | 0.40 |
| 3:Bf:18:PRO:HA | 3:Bi:151:GLN:HE21 | 1.87 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Bl:55:ASN:HB3 | 3:Bl:56:ARG:H | 1.76 | 0.40 |
| 3:Bo:40:ALA:H | 3:Bo:69:TRP:HE1 | 1.69 | 0.40 |
| 2:Bq:456:TYR:O | 2:Bq:503:ILE:HG12 | 2.22 | 0.40 |
| 2:Bs:34:GLN:O | 2:Bs:82:ARG:NH2 | 2.55 | 0.40 |
| 2:Bs:100:GLU:HG2 | 2:Bs:186:LYS:O | 2.22 | 0.40 |
| 2:Bs:159:GLU:O | 2:Bs:162:THR:N | 2.36 | 0.40 |
| 2:Bt:482:ASP:HB2 | 2:Bt:487:THR:HG22 | 2.03 | 0.40 |
| 2:Bu:211:GLN:HB3 | 2:Bu:329:ASN:ND2 | 2.37 | 0.40 |
| 2:Bv:28:ALA:HB1 | 2:Bv:362:PHE:CE2 | 2.56 | 0.40 |
| 2:Bv:642:PHE:HE1 | 2:By:10:LEU:HD22 | 1.87 | 0.40 |
| 2:Bx:554:ARG:HD3 | 2:Bx:554:ARG:HA | 1.78 | 0.40 |
| 2:By:74:TYR:CD1 | 2:By:476:GLY:HA3 | 2.57 | 0.40 |
| 2:By:209:ASP:OD1 | 2:By:209:ASP:N | 2.48 | 0.40 |
| 2:Bz:526:THR:HG22 | 2:Bz:534:VAL:O | 2.22 | 0.40 |
| 4:C:44:MET:HE3 | 4:H:44:MET:HE3 | 2.03 | 0.40 |
| 4:Y:44:MET:HE1 | 4:d:44:MET:HG2 | 2.03 | 0.40 |
| 1:k:15:ARG:HD2 | 1:k:15:ARG:N | 2.37 | 0.40 |
| 1:k:99:ALA:HB3 | 1:k:111:GLN:HG3 | 2.04 | 0.40 |
| 8:r:108:GLN:HE22 | 8:r:199:TYR:HB3 | 1.86 | 0.40 |
| 8:u:243:ASP:OD1 | 8:u:243:ASP:N | 2.51 | 0.40 |
| 9:v:126:MET:HE3 | 9:v:166:VAL:HG13 | 2.04 | 0.40 |
| 9:z:40:PRO:HG3 | 9:z:130:PHE:HE2 | 1.87 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 242/256 (94%) | 210 (87%) | 31 (13%) | 1 (0%) | 30 | 62 |
| 1 | k | 242/256 (94%) | 206 (85%) | 35 (14%) | 1 (0%) | 30 | 62 |
| 1 | l | 242/256 (94%) | 205 (85%) | 35 (14%) | 2 (1%) | 16 | 48 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | m | 242/256 (94%) | 213 (88%) | 28 (12%) | 1 (0%) | 30 | 62 |
| 1 | n | 242/256 (94%) | 210 (87%) | 31 (13%) | 1 (0%) | 30 | 62 |
| 1 | p | 242/256 (94%) | 211 (87%) | 30 (12%) | 1 (0%) | 30 | 62 |
| 2 | 1 | 651/659 (99%) | 586 (90%) | 62 (10%) | 3 (0%) | 24 | 57 |
| 2 | 2 | 651/659 (99%) | 590 (91%) | 58 (9%) | 3 (0%) | 24 | 57 |
| 2 | 3 | 651/659 (99%) | 584 (90%) | 64 (10%) | 3 (0%) | 24 | 57 |
| 2 | 4 | 651/659 (99%) | 584 (90%) | 65 (10%) | 2 (0%) | 36 | 67 |
| 2 | 5 | 651/659 (99%) | 588 (90%) | 61 (9%) | 2 (0%) | 36 | 67 |
| 2 | AD | 651/659 (99%) | 589 (90%) | 60 (9%) | 2 (0%) | 36 | 67 |
| 2 | AK | 653/659 (99%) | 586 (90%) | 63 (10%) | 4 (1%) | 21 | 54 |
| 2 | AL | 653/659 (99%) | 592 (91%) | 58 (9%) | 3 (0%) | 24 | 57 |
| 2 | AM | 653/659 (99%) | 584 (89%) | 67 (10%) | 2 (0%) | 36 | 67 |
| 2 | AN | 653/659 (99%) | 586 (90%) | 62 (10%) | 5 (1%) | 16 | 48 |
| 2 | AO | 653/659 (99%) | 596 (91%) | 55 (8%) | 2 (0%) | 36 | 67 |
| 2 | AP | 653/659 (99%) | 585 (90%) | 64 (10%) | 4 (1%) | 21 | 54 |
| 2 | B1 | 653/659 (99%) | 590 (90%) | 60 (9%) | 3 (0%) | 24 | 57 |
| 2 | B2 | 653/659 (99%) | 594 (91%) | 55 (8%) | 4 (1%) | 21 | 54 |
| 2 | B3 | 653/659 (99%) | 592 (91%) | 58 (9%) | 3 (0%) | 24 | 57 |
| 2 | B4 | 653/659 (99%) | 586 (90%) | 65 (10%) | 2 (0%) | 36 | 67 |
| 2 | B5 | 653/659 (99%) | 595 (91%) | 54 (8%) | 4 (1%) | 21 | 54 |
| 2 | B6 | 653/659 (99%) | 579 (89%) | 72 (11%) | 2 (0%) | 36 | 67 |
| 2 | B7 | 653/659 (99%) | 583 (89%) | 67 (10%) | 3 (0%) | 24 | 57 |
| 2 | Bp | 653/659 (99%) | 587 (90%) | 63 (10%) | 3 (0%) | 24 | 57 |
| 2 | Bq | 653/659 (99%) | 591 (90%) | 59 (9%) | 3 (0%) | 24 | 57 |
| 2 | Br | 653/659 (99%) | 588 (90%) | 61 (9%) | 4 (1%) | 21 | 54 |
| 2 | Bs | 653/659 (99%) | 585 (90%) | 66 (10%) | 2 (0%) | 36 | 67 |
| 2 | Bt | 653/659 (99%) | 585 (90%) | 65 (10%) | 3 (0%) | 24 | 57 |
| 2 | Bu | 653/659 (99%) | 592 (91%) | 59 (9%) | 2 (0%) | 36 | 67 |
| 2 | Bv | 653/659 (99%) | 589 (90%) | 63 (10%) | 1 (0%) | 43 | 73 |
| 2 | Bw | 653/659 (99%) | 585 (90%) | 66 (10%) | 2 (0%) | 36 | 67 |
| 2 | Bx | 653/659 (99%) | 591 (90%) | 61 (9%) | 1 (0%) | 43 | 73 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 2 | By | 653/659 (99%) | 587 (90%) | 63 (10%) | 3 (0%) | 24 57 |
| 2 | Bz | 653/659 (99%) | 581 (89%) | 70 (11%) | 2 (0%) | 36 67 |
| 3 | 6 | 160/163 (98%) | 138 (86%) | 18 (11%) | 4 (2%) | 4 28 |
| 3 | 7 | 160/163 (98%) | 141 (88%) | 16 (10%) | 3 (2%) | 6 32 |
| 3 | 8 | 160/163 (98%) | 139 (87%) | 19 (12%) | 2 (1%) | 9 38 |
| 3 | 9 | 160/163 (98%) | 140 (88%) | 17 (11%) | 3 (2%) | 6 32 |
| 3 | AA | 160/163 (98%) | 142 (89%) | 13 (8%) | 5 (3%) | 3 25 |
| 3 | AE | 161/163 (99%) | 138 (86%) | 21 (13%) | 2 (1%) | 10 40 |
| 3 | AF | 161/163 (99%) | 142 (88%) | 18 (11%) | 1 (1%) | 21 54 |
| 3 | AG | 161/163 (99%) | 140 (87%) | 20 (12%) | 1 (1%) | 21 54 |
| 3 | AH | 161/163 (99%) | 141 (88%) | 19 (12%) | 1 (1%) | 21 54 |
| 3 | AI | 161/163 (99%) | 141 (88%) | 18 (11%) | 2 (1%) | 10 40 |
| 3 | AJ | 161/163 (99%) | 141 (88%) | 19 (12%) | 1 (1%) | 21 54 |
| 3 | BX | 161/163 (99%) | 141 (88%) | 17 (11%) | 3 (2%) | 6 32 |
| 3 | BY | 161/163 (99%) | 141 (88%) | 18 (11%) | 2 (1%) | 10 40 |
| 3 | BZ | 161/163 (99%) | 141 (88%) | 18 (11%) | 2 (1%) | 10 40 |
| 3 | Ba | 161/163 (99%) | 140 (87%) | 20 (12%) | 1 (1%) | 21 54 |
| 3 | Bb | 161/163 (99%) | 141 (88%) | 20 (12%) | 0 | 100 100 |
| 3 | Bc | 161/163 (99%) | 138 (86%) | 21 (13%) | 2 (1%) | 10 40 |
| 3 | Bd | 161/163 (99%) | 143 (89%) | 17 (11%) | 1 (1%) | 21 54 |
| 3 | Be | 161/163 (99%) | 142 (88%) | 18 (11%) | 1 (1%) | 21 54 |
| 3 | Bf | 161/163 (99%) | 143 (89%) | 18 (11%) | 0 | 100 100 |
| 3 | Bg | 161/163 (99%) | 138 (86%) | 22 (14%) | 1 (1%) | 21 54 |
| 3 | Bh | 161/163 (99%) | 137 (85%) | 23 (14%) | 1 (1%) | 21 54 |
| 3 | Bi | 161/163 (99%) | 141 (88%) | 19 (12%) | 1 (1%) | 21 54 |
| 3 | Bj | 161/163 (99%) | 142 (88%) | 19 (12%) | 0 | 100 100 |
| 3 | Bk | 161/163 (99%) | 137 (85%) | 24 (15%) | 0 | 100 100 |
| 3 | Bl | 161/163 (99%) | 133 (83%) | 27 (17%) | 1 (1%) | 21 54 |
| 3 | Bm | 161/163 (99%) | 142 (88%) | 17 (11%) | 2 (1%) | 10 40 |
| 3 | Bn | 161/163 (99%) | 140 (87%) | 18 (11%) | 3 (2%) | 6 32 |
| 3 | Bo | 161/163 (99%) | 135 (84%) | 25 (16%) | 1 (1%) | 21 54 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | o | 160/163 (98%) | 143 (89%) | 15 (9%) | 2 (1%) | 9 | 38 |
| 4 | A | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | B | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | C | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | D | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | E | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | F | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | G | 77/487 (16%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | H | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | I | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | J | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | K | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | L | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | M | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | N | 77/487 (16%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | O | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | P | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | Q | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | R | 77/487 (16%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | S | 77/487 (16%) | 74 (96%) | 3 (4%) | 0 | 100 | 100 |
| 4 | T | 77/487 (16%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | U | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | V | 77/487 (16%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | W | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | X | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | Y | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | Z | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | a | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | b | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | c | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | d | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | e | 77/487 (16%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | f | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | g | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | h | 77/487 (16%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | i | 77/487 (16%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 4 | j | 77/487 (16%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | A0 | 505/524 (96%) | 444 (88%) | 54 (11%) | 7 (1%) | 9 | 37 |
| 5 | A1 | 505/524 (96%) | 459 (91%) | 40 (8%) | 6 (1%) | 10 | 40 |
| 5 | A2 | 504/524 (96%) | 454 (90%) | 43 (8%) | 7 (1%) | 9 | 37 |
| 5 | A3 | 504/524 (96%) | 440 (87%) | 56 (11%) | 8 (2%) | 7 | 35 |
| 5 | Av | 504/524 (96%) | 455 (90%) | 44 (9%) | 5 (1%) | 12 | 43 |
| 5 | Ax | 504/524 (96%) | 461 (92%) | 40 (8%) | 3 (1%) | 21 | 54 |
| 5 | BA | 496/524 (95%) | 445 (90%) | 45 (9%) | 6 (1%) | 10 | 40 |
| 5 | BB | 484/524 (92%) | 445 (92%) | 38 (8%) | 1 (0%) | 43 | 73 |
| 5 | BD | 504/524 (96%) | 459 (91%) | 42 (8%) | 3 (1%) | 21 | 54 |
| 5 | BF | 504/524 (96%) | 463 (92%) | 39 (8%) | 2 (0%) | 30 | 62 |
| 5 | BG | 493/524 (94%) | 447 (91%) | 44 (9%) | 2 (0%) | 30 | 62 |
| 5 | BH | 504/524 (96%) | 467 (93%) | 34 (7%) | 3 (1%) | 21 | 54 |
| 6 | A4 | 454/521 (87%) | 413 (91%) | 40 (9%) | 1 (0%) | 43 | 73 |
| 6 | A5 | 454/521 (87%) | 423 (93%) | 31 (7%) | 0 | 100 | 100 |
| 6 | A7 | 454/521 (87%) | 420 (92%) | 34 (8%) | 0 | 100 | 100 |
| 6 | A8 | 438/521 (84%) | 396 (90%) | 41 (9%) | 1 (0%) | 43 | 73 |
| 6 | A9 | 454/521 (87%) | 413 (91%) | 41 (9%) | 0 | 100 | 100 |
| 6 | AV | 454/521 (87%) | 413 (91%) | 41 (9%) | 0 | 100 | 100 |
| 6 | AW | 454/521 (87%) | 419 (92%) | 35 (8%) | 0 | 100 | 100 |
| 6 | AX | 454/521 (87%) | 419 (92%) | 35 (8%) | 0 | 100 | 100 |
| 6 | AZ | 454/521 (87%) | 423 (93%) | 30 (7%) | 1 (0%) | 43 | 73 |
| 6 | Ac | 454/521 (87%) | 415 (91%) | 39 (9%) | 0 | 100 | 100 |
| 6 | Ad | 454/521 (87%) | 424 (93%) | 30 (7%) | 0 | 100 | 100 |
| 6 | Ae | 454/521 (87%) | 422 (93%) | 32 (7%) | 0 | 100 | 100 |
| 6 | Af | 454/521 (87%) | 414 (91%) | 40 (9%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 6 | Ag | 454/521 (87%) | 419 (92%) | 34 (8%) | 1 (0%) | 43 73 |
| 6 | Ah | 454/521 (87%) | 420 (92%) | 34 (8%) | 0 | 100 100 |
| 6 | Ai | 454/521 (87%) | 417 (92%) | 37 (8%) | 0 | 100 100 |
| 6 | Aj | 454/521 (87%) | 415 (91%) | 38 (8%) | 1 (0%) | 43 73 |
| 6 | Ak | 454/521 (87%) | 413 (91%) | 40 (9%) | 1 (0%) | 43 73 |
| 6 | Am | 454/521 (87%) | 420 (92%) | 33 (7%) | 1 (0%) | 43 73 |
| 6 | An | 438/521 (84%) | 404 (92%) | 34 (8%) | 0 | 100 100 |
| 6 | Ao | 435/521 (84%) | 397 (91%) | 36 (8%) | 2 (0%) | 24 57 |
| 6 | Ap | 438/521 (84%) | 406 (93%) | 31 (7%) | 1 (0%) | 43 73 |
| 6 | Au | 454/521 (87%) | 419 (92%) | 35 (8%) | 0 | 100 100 |
| 6 | Aw | 454/521 (87%) | 424 (93%) | 29 (6%) | 1 (0%) | 43 73 |
| 6 | Ay | 454/521 (87%) | 421 (93%) | 32 (7%) | 1 (0%) | 43 73 |
| 6 | Az | 454/521 (87%) | 422 (93%) | 32 (7%) | 0 | 100 100 |
| 6 | BI | 454/521 (87%) | 420 (92%) | 34 (8%) | 0 | 100 100 |
| 6 | BJ | 435/521 (84%) | 398 (92%) | 36 (8%) | 1 (0%) | 43 73 |
| 6 | BK | 454/521 (87%) | 415 (91%) | 39 (9%) | 0 | 100 100 |
| 6 | BM | 454/521 (87%) | 422 (93%) | 31 (7%) | 1 (0%) | 43 73 |
| 7 | A6 | 306/309 (99%) | 286 (94%) | 20 (6%) | 0 | 100 100 |
| 7 | AY | 306/309 (99%) | 276 (90%) | 28 (9%) | 2 (1%) | 18 51 |
| 7 | Aa | 306/309 (99%) | 269 (88%) | 34 (11%) | 3 (1%) | 12 43 |
| 7 | Ab | 306/309 (99%) | 284 (93%) | 21 (7%) | 1 (0%) | 36 67 |
| 7 | Al | 306/309 (99%) | 268 (88%) | 36 (12%) | 2 (1%) | 18 51 |
| 7 | Aq | 306/309 (99%) | 266 (87%) | 37 (12%) | 3 (1%) | 12 43 |
| 7 | Ar | 286/309 (93%) | 254 (89%) | 31 (11%) | 1 (0%) | 36 67 |
| 7 | As | 306/309 (99%) | 276 (90%) | 29 (10%) | 1 (0%) | 36 67 |
| 7 | At | 294/309 (95%) | 264 (90%) | 27 (9%) | 3 (1%) | 12 43 |
| 7 | BC | 306/309 (99%) | 273 (89%) | 32 (10%) | 1 (0%) | 36 67 |
| 7 | BE | 306/309 (99%) | 284 (93%) | 20 (6%) | 2 (1%) | 18 51 |
| 7 | BL | 306/309 (99%) | 267 (87%) | 37 (12%) | 2 (1%) | 18 51 |
| 8 | AB | 270/272 (99%) | 235 (87%) | 31 (12%) | 4 (2%) | 8 36 |
| 8 | q | 270/272 (99%) | 237 (88%) | 28 (10%) | 5 (2%) | 6 32 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 8 | r | 270/272 (99%) | 236 (87%) | 31 (12%) | 3 (1%) | 11 41 |
| 8 | s | 270/272 (99%) | 240 (89%) | 28 (10%) | 2 (1%) | 18 51 |
| 8 | t | 270/272 (99%) | 238 (88%) | 29 (11%) | 3 (1%) | 11 41 |
| 8 | u | 270/272 (99%) | 237 (88%) | 28 (10%) | 5 (2%) | 6 32 |
| 9 | AC | 173/176 (98%) | 152 (88%) | 19 (11%) | 2 (1%) | 10 40 |
| 9 | v | 173/176 (98%) | 156 (90%) | 15 (9%) | 2 (1%) | 10 40 |
| 9 | w | 173/176 (98%) | 157 (91%) | 15 (9%) | 1 (1%) | 21 54 |
| 9 | x | 173/176 (98%) | 158 (91%) | 14 (8%) | 1 (1%) | 21 54 |
| 9 | y | 173/176 (98%) | 155 (90%) | 16 (9%) | 2 (1%) | 10 40 |
| 9 | z | 173/176 (98%) | 157 (91%) | 14 (8%) | 2 (1%) | 10 40 |
| 10 | AQ | 94/376 (25%) | 86 (92%) | 8 (8%) | 0 | 100 100 |
| 10 | AR | 94/376 (25%) | 88 (94%) | 5 (5%) | 1 (1%) | 11 41 |
| 10 | AS | 94/376 (25%) | 85 (90%) | 9 (10%) | 0 | 100 100 |
| 10 | AT | 94/376 (25%) | 81 (86%) | 12 (13%) | 1 (1%) | 11 41 |
| 10 | AU | 94/376 (25%) | 83 (88%) | 11 (12%) | 0 | 100 100 |
| 11 | BN | 77/80 (96%) | 71 (92%) | 5 (6%) | 1 (1%) | 9 38 |
| 11 | BO | 77/80 (96%) | 72 (94%) | 4 (5%) | 1 (1%) | 9 38 |
| 11 | BP | 77/80 (96%) | 69 (90%) | 7 (9%) | 1 (1%) | 9 38 |
| 11 | BQ | 77/80 (96%) | 70 (91%) | 6 (8%) | 1 (1%) | 9 38 |
| 11 | BR | 77/80 (96%) | 69 (90%) | 7 (9%) | 1 (1%) | 9 38 |
| 11 | BS | 77/80 (96%) | 73 (95%) | 3 (4%) | 1 (1%) | 9 38 |
| 11 | BT | 77/80 (96%) | 67 (87%) | 9 (12%) | 1 (1%) | 9 38 |
| 11 | BU | 77/80 (96%) | 68 (88%) | 9 (12%) | 0 | 100 100 |
| 11 | BV | 77/80 (96%) | 69 (90%) | 7 (9%) | 1 (1%) | 9 38 |
| 11 | BW | 77/80 (96%) | 69 (90%) | 7 (9%) | 1 (1%) | 9 38 |
| All | All | 55709/74722 (75%) | 50476 (91%) | 4964 (9%) | 269 (0%) | 26 57 |

All (269) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 62 | ALA |
| 2 | 1 | 552 | ASN |
| 2 | 2 | 62 | ALA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 4 | 552 | ASN |
| 2 | 5 | 62 | ALA |
| 2 | 5 | 552 | ASN |
| 3 | 6 | 6 | VAL |
| 3 | 6 | 11 | GLU |
| 3 | 7 | 6 | VAL |
| 3 | 7 | 11 | GLU |
| 3 | 8 | 6 | VAL |
| 3 | 8 | 11 | GLU |
| 3 | 9 | 6 | VAL |
| 3 | 9 | 11 | GLU |
| 5 | A0 | 10 | ALA |
| 5 | A0 | 217 | CYS |
| 5 | A0 | 233 | ALA |
| 5 | A2 | 45 | VAL |
| 5 | A2 | 392 | SER |
| 5 | A2 | 481 | ILE |
| 5 | A3 | 224 | ALA |
| 5 | A3 | 233 | ALA |
| 5 | A3 | 384 | GLN |
| 5 | A3 | 396 | ILE |
| 6 | A8 | 90 | GLN |
| 3 | AA | 6 | VAL |
| 3 | AA | 11 | GLU |
| 8 | AB | 143 | PRO |
| 8 | AB | 224 | PRO |
| 8 | AB | 239 | PRO |
| 9 | AC | 28 | SER |
| 2 | AD | 552 | ASN |
| 3 | AE | 42 | PRO |
| 3 | AG | 43 | ALA |
| 3 | AI | 42 | PRO |
| 3 | AJ | 42 | PRO |
| 2 | AK | 121 | VAL |
| 2 | AK | 265 | ALA |
| 2 | AK | 552 | ASN |
| 2 | AL | 265 | ALA |
| 2 | AM | 265 | ALA |
| 2 | AM | 552 | ASN |
| 2 | AN | 121 | VAL |
| 2 | AN | 346 | SER |
| 2 | AN | 350 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AN | 552 | ASN |
| 2 | AO | 265 | ALA |
| 2 | AO | 552 | ASN |
| 2 | AP | 121 | VAL |
| 7 | AY | 25 | ILE |
| 7 | Aa | 105 | PRO |
| 6 | Aj | 346 | ALA |
| 7 | Al | 193 | ASP |
| 6 | Am | 108 | ALA |
| 7 | Aq | 92 | ILE |
| 7 | At | 121 | MET |
| 5 | Av | 7 | SER |
| 5 | Av | 233 | ALA |
| 5 | Av | 294 | ALA |
| 5 | Ax | 374 | ARG |
| 2 | B1 | 265 | ALA |
| 2 | B1 | 552 | ASN |
| 2 | B2 | 265 | ALA |
| 2 | B3 | 552 | ASN |
| 2 | B7 | 265 | ALA |
| 2 | B7 | 552 | ASN |
| 5 | BA | 10 | ALA |
| 5 | BF | 317 | SER |
| 5 | BF | 374 | ARG |
| 5 | BG | 245 | CYS |
| 5 | BG | 374 | ARG |
| 5 | BH | 374 | ARG |
| 7 | BL | 193 | ASP |
| 11 | BO | 65 | ARG |
| 11 | BP | 65 | ARG |
| 11 | BQ | 65 | ARG |
| 11 | BR | 65 | ARG |
| 11 | BS | 65 | ARG |
| 11 | BT | 65 | ARG |
| 11 | BV | 65 | ARG |
| 3 | BY | 120 | ALA |
| 3 | BZ | 42 | PRO |
| 3 | BZ | 120 | ALA |
| 3 | Bc | 42 | PRO |
| 3 | Be | 42 | PRO |
| 3 | Bh | 42 | PRO |
| 3 | Bl | 42 | PRO |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Bn | 42 | PRO |
| 3 | Bo | 42 | PRO |
| 2 | Bp | 13 | THR |
| 2 | Bp | 552 | ASN |
| 2 | Bq | 552 | ASN |
| 2 | Br | 265 | ALA |
| 2 | Br | 552 | ASN |
| 2 | Bs | 265 | ALA |
| 2 | Bs | 552 | ASN |
| 2 | Bt | 552 | ASN |
| 2 | Bu | 552 | ASN |
| 2 | Bx | 552 | ASN |
| 2 | By | 265 | ALA |
| 2 | By | 552 | ASN |
| 3 | o | 6 | VAL |
| 3 | o | 11 | GLU |
| 8 | q | 62 | GLN |
| 8 | q | 143 | PRO |
| 8 | q | 224 | PRO |
| 8 | q | 239 | PRO |
| 8 | r | 62 | GLN |
| 8 | r | 156 | ASP |
| 8 | r | 239 | PRO |
| 8 | s | 239 | PRO |
| 8 | t | 62 | GLN |
| 8 | t | 156 | ASP |
| 8 | t | 239 | PRO |
| 8 | u | 62 | GLN |
| 8 | u | 73 | PRO |
| 8 | u | 156 | ASP |
| 8 | u | 224 | PRO |
| 8 | u | 239 | PRO |
| 9 | v | 28 | SER |
| 9 | w | 28 | SER |
| 9 | y | 28 | SER |
| 9 | z | 28 | SER |
| 2 | 2 | 552 | ASN |
| 2 | 3 | 552 | ASN |
| 5 | A0 | 8 | LEU |
| 5 | A0 | 294 | ALA |
| 5 | A1 | 45 | VAL |
| 5 | A1 | 141 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A1 | 228 | ILE |
| 5 | A2 | 294 | ALA |
| 5 | A2 | 394 | THR |
| 5 | A3 | 45 | VAL |
| 2 | AL | 552 | ASN |
| 2 | AP | 552 | ASN |
| 7 | Aa | 138 | LEU |
| 7 | Ab | 22 | ALA |
| 6 | Ag | 346 | ALA |
| 6 | Ak | 391 | THR |
| 6 | Ao | 108 | ALA |
| 7 | Aq | 193 | ASP |
| 7 | As | 22 | ALA |
| 5 | Av | 10 | ALA |
| 5 | Av | 45 | VAL |
| 5 | Ax | 211 | ALA |
| 5 | Ax | 220 | ARG |
| 2 | B2 | 552 | ASN |
| 2 | B3 | 265 | ALA |
| 2 | B4 | 552 | ASN |
| 2 | B5 | 265 | ALA |
| 2 | B5 | 552 | ASN |
| 2 | B6 | 552 | ASN |
| 5 | BA | 8 | LEU |
| 5 | BA | 45 | VAL |
| 5 | BA | 232 | LYS |
| 5 | BD | 154 | SER |
| 5 | BD | 211 | ALA |
| 5 | BD | 398 | ARG |
| 7 | BE | 125 | CYS |
| 5 | BH | 66 | GLU |
| 11 | BN | 65 | ARG |
| 11 | BW | 65 | ARG |
| 3 | BX | 55 | ASN |
| 3 | BY | 55 | ASN |
| 2 | Bp | 482 | ASP |
| 2 | Br | 121 | VAL |
| 2 | Br | 482 | ASP |
| 2 | Bv | 552 | ASN |
| 2 | Bw | 552 | ASN |
| 2 | Bw | 645 | THR |
| 2 | By | 121 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bz | 552 | ASN |
| 5 | A3 | 217 | CYS |
| 6 | A4 | 254 | ILE |
| 3 | AE | 55 | ASN |
| 3 | AH | 125 | LYS |
| 2 | AL | 13 | THR |
| 2 | AN | 347 | ASN |
| 2 | AP | 265 | ALA |
| 7 | AY | 22 | ALA |
| 7 | Aa | 22 | ALA |
| 2 | B2 | 163 | LEU |
| 2 | B3 | 654 | LEU |
| 2 | B6 | 265 | ALA |
| 5 | BA | 51 | ALA |
| 5 | BB | 214 | SER |
| 7 | BE | 22 | ALA |
| 3 | BX | 43 | ALA |
| 3 | BX | 125 | LYS |
| 3 | Bc | 125 | LYS |
| 3 | Bd | 55 | ASN |
| 3 | Bg | 55 | ASN |
| 3 | Bn | 55 | ASN |
| 2 | Bt | 645 | THR |
| 1 | l | 188 | ASN |
| 8 | s | 156 | ASP |
| 3 | 6 | 43 | ALA |
| 3 | 6 | 125 | LYS |
| 3 | 9 | 43 | ALA |
| 5 | A0 | 45 | VAL |
| 5 | A1 | 104 | ASP |
| 3 | AA | 14 | ASP |
| 3 | AA | 125 | LYS |
| 8 | AB | 156 | ASP |
| 3 | AI | 125 | LYS |
| 6 | Ao | 91 | ILE |
| 7 | Ar | 22 | ALA |
| 7 | At | 129 | TYR |
| 6 | Ay | 121 | THR |
| 2 | B4 | 645 | THR |
| 2 | B7 | 572 | LEU |
| 5 | BA | 294 | ALA |
| 7 | BC | 22 | ALA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BH | 61 | ILE |
| 7 | BL | 22 | ALA |
| 3 | Ba | 125 | LYS |
| 8 | q | 156 | ASP |
| 5 | A0 | 328 | MET |
| 5 | A1 | 67 | PRO |
| 5 | A1 | 207 | ILE |
| 5 | A2 | 216 | ALA |
| 5 | A3 | 294 | ALA |
| 3 | AA | 43 | ALA |
| 2 | AK | 13 | THR |
| 6 | AZ | 245 | ASN |
| 7 | At | 22 | ALA |
| 2 | B1 | 645 | THR |
| 3 | Bm | 55 | ASN |
| 2 | Bq | 121 | VAL |
| 2 | Bq | 265 | ALA |
| 1 | n | 236 | VAL |
| 1 | p | 236 | VAL |
| 2 | 3 | 62 | ALA |
| 3 | 7 | 43 | ALA |
| 5 | A2 | 328 | MET |
| 5 | A3 | 328 | MET |
| 3 | AF | 55 | ASN |
| 2 | AP | 13 | THR |
| 7 | Al | 22 | ALA |
| 6 | Ap | 346 | ALA |
| 7 | Aq | 22 | ALA |
| 6 | Aw | 246 | PRO |
| 2 | B2 | 39 | PHE |
| 2 | B5 | 13 | THR |
| 6 | BJ | 91 | ILE |
| 6 | BM | 345 | TRP |
| 3 | Bi | 55 | ASN |
| 3 | Bn | 125 | LYS |
| 2 | Bt | 350 | VAL |
| 2 | Bu | 39 | PHE |
| 2 | Bz | 163 | LEU |
| 1 | l | 236 | VAL |
| 2 | 3 | 20 | VAL |
| 10 | AT | 375 | TYR |
| 1 | m | 236 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | AR | 375 | TYR |
| 1 | k | 236 | VAL |
| 9 | x | 173 | ILE |
| 1 | 0 | 236 | VAL |
| 2 | 4 | 20 | VAL |
| 9 | AC | 173 | ILE |
| 2 | 1 | 20 | VAL |
| 2 | 2 | 20 | VAL |
| 2 | AD | 20 | VAL |
| 9 | v | 173 | ILE |
| 2 | B5 | 121 | VAL |
| 3 | Bm | 42 | PRO |
| 9 | y | 173 | ILE |
| 9 | z | 173 | ILE |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 0 | 217/229 (95%) | 191 (88%) | 26 (12%) | 5 21 |
| 1 | k | 217/229 (95%) | 189 (87%) | 28 (13%) | 4 20 |
| 1 | l | 217/229 (95%) | 193 (89%) | 24 (11%) | 6 24 |
| 1 | m | 217/229 (95%) | 196 (90%) | 21 (10%) | 8 29 |
| 1 | n | 217/229 (95%) | 196 (90%) | 21 (10%) | 8 29 |
| 1 | p | 217/229 (95%) | 195 (90%) | 22 (10%) | 7 27 |
| 2 | 1 | 532/536 (99%) | 486 (91%) | 46 (9%) | 10 33 |
| 2 | 2 | 532/536 (99%) | 495 (93%) | 37 (7%) | 14 40 |
| 2 | 3 | 532/536 (99%) | 494 (93%) | 38 (7%) | 13 39 |
| 2 | 4 | 532/536 (99%) | 493 (93%) | 39 (7%) | 13 39 |
| 2 | 5 | 532/536 (99%) | 496 (93%) | 36 (7%) | 14 40 |
| 2 | AD | 532/536 (99%) | 492 (92%) | 40 (8%) | 12 38 |
| 2 | AK | 534/536 (100%) | 478 (90%) | 56 (10%) | 6 26 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | AL | 534/536 (100%) | 489 (92%) | 45 (8%) | 10 34 |
| 2 | AM | 534/536 (100%) | 487 (91%) | 47 (9%) | 9 33 |
| 2 | AN | 534/536 (100%) | 494 (92%) | 40 (8%) | 12 38 |
| 2 | AO | 534/536 (100%) | 487 (91%) | 47 (9%) | 9 33 |
| 2 | AP | 534/536 (100%) | 479 (90%) | 55 (10%) | 7 27 |
| 2 | B1 | 534/536 (100%) | 482 (90%) | 52 (10%) | 8 29 |
| 2 | B2 | 534/536 (100%) | 491 (92%) | 43 (8%) | 11 35 |
| 2 | B3 | 534/536 (100%) | 484 (91%) | 50 (9%) | 8 30 |
| 2 | B4 | 534/536 (100%) | 489 (92%) | 45 (8%) | 10 34 |
| 2 | B5 | 534/536 (100%) | 490 (92%) | 44 (8%) | 10 35 |
| 2 | B6 | 534/536 (100%) | 486 (91%) | 48 (9%) | 9 32 |
| 2 | B7 | 534/536 (100%) | 487 (91%) | 47 (9%) | 9 33 |
| 2 | Bp | 534/536 (100%) | 498 (93%) | 36 (7%) | 15 41 |
| 2 | Bq | 534/536 (100%) | 485 (91%) | 49 (9%) | 8 31 |
| 2 | Br | 534/536 (100%) | 484 (91%) | 50 (9%) | 8 30 |
| 2 | Bs | 534/536 (100%) | 494 (92%) | 40 (8%) | 12 38 |
| 2 | Bt | 534/536 (100%) | 482 (90%) | 52 (10%) | 8 29 |
| 2 | Bu | 534/536 (100%) | 481 (90%) | 53 (10%) | 7 28 |
| 2 | Bv | 534/536 (100%) | 484 (91%) | 50 (9%) | 8 30 |
| 2 | Bw | 534/536 (100%) | 478 (90%) | 56 (10%) | 6 26 |
| 2 | Bx | 534/536 (100%) | 489 (92%) | 45 (8%) | 10 34 |
| 2 | By | 534/536 (100%) | 484 (91%) | 50 (9%) | 8 30 |
| 2 | Bz | 534/536 (100%) | 493 (92%) | 41 (8%) | 12 37 |
| 3 | 6 | 136/137 (99%) | 120 (88%) | 16 (12%) | 5 22 |
| 3 | 7 | 136/137 (99%) | 120 (88%) | 16 (12%) | 5 22 |
| 3 | 8 | 136/137 (99%) | 119 (88%) | 17 (12%) | 4 21 |
| 3 | 9 | 136/137 (99%) | 116 (85%) | 20 (15%) | 3 17 |
| 3 | AA | 136/137 (99%) | 121 (89%) | 15 (11%) | 6 24 |
| 3 | AE | 137/137 (100%) | 118 (86%) | 19 (14%) | 3 18 |
| 3 | AF | 137/137 (100%) | 116 (85%) | 21 (15%) | 3 16 |
| 3 | AG | 137/137 (100%) | 119 (87%) | 18 (13%) | 4 20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | AH | 137/137 (100%) | 118 (86%) | 19 (14%) | 3 18 |
| 3 | AI | 137/137 (100%) | 123 (90%) | 14 (10%) | 7 27 |
| 3 | AJ | 137/137 (100%) | 118 (86%) | 19 (14%) | 3 18 |
| 3 | BX | 137/137 (100%) | 118 (86%) | 19 (14%) | 3 18 |
| 3 | BY | 137/137 (100%) | 120 (88%) | 17 (12%) | 4 21 |
| 3 | BZ | 137/137 (100%) | 117 (85%) | 20 (15%) | 3 17 |
| 3 | Ba | 137/137 (100%) | 120 (88%) | 17 (12%) | 4 21 |
| 3 | Bb | 137/137 (100%) | 122 (89%) | 15 (11%) | 6 25 |
| 3 | Bc | 137/137 (100%) | 125 (91%) | 12 (9%) | 9 33 |
| 3 | Bd | 137/137 (100%) | 120 (88%) | 17 (12%) | 4 21 |
| 3 | Be | 137/137 (100%) | 121 (88%) | 16 (12%) | 5 22 |
| 3 | Bf | 137/137 (100%) | 117 (85%) | 20 (15%) | 3 17 |
| 3 | Bg | 137/137 (100%) | 117 (85%) | 20 (15%) | 3 17 |
| 3 | Bh | 137/137 (100%) | 116 (85%) | 21 (15%) | 3 16 |
| 3 | Bi | 137/137 (100%) | 122 (89%) | 15 (11%) | 6 25 |
| 3 | Bj | 137/137 (100%) | 116 (85%) | 21 (15%) | 3 16 |
| 3 | Bk | 137/137 (100%) | 117 (85%) | 20 (15%) | 3 17 |
| 3 | Bl | 137/137 (100%) | 116 (85%) | 21 (15%) | 3 16 |
| 3 | Bm | 137/137 (100%) | 120 (88%) | 17 (12%) | 4 21 |
| 3 | Bn | 137/137 (100%) | 125 (91%) | 12 (9%) | 9 33 |
| 3 | Bo | 137/137 (100%) | 120 (88%) | 17 (12%) | 4 21 |
| 3 | o | 136/137 (99%) | 115 (85%) | 21 (15%) | 2 15 |
| 4 | A | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | B | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | C | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | D | 69/419 (16%) | 67 (97%) | 2 (3%) | 37 58 |
| 4 | E | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | F | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | G | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | H | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | I | 69/419 (16%) | 69 (100%) | 0 | 100 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 4 | J | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | K | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | L | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | M | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | N | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | O | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | P | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | Q | 69/419 (16%) | 67 (97%) | 2 (3%) | 37 58 |
| 4 | R | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | S | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | T | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | U | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | V | 69/419 (16%) | 67 (97%) | 2 (3%) | 37 58 |
| 4 | W | 69/419 (16%) | 67 (97%) | 2 (3%) | 37 58 |
| 4 | X | 69/419 (16%) | 66 (96%) | 3 (4%) | 26 50 |
| 4 | Y | 69/419 (16%) | 67 (97%) | 2 (3%) | 37 58 |
| 4 | Z | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | a | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | b | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | c | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | d | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | e | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | f | 69/419 (16%) | 67 (97%) | 2 (3%) | 37 58 |
| 4 | g | 69/419 (16%) | 68 (99%) | 1 (1%) | 59 70 |
| 4 | h | 69/419 (16%) | 67 (97%) | 2 (3%) | 37 58 |
| 4 | i | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 4 | j | 69/419 (16%) | 69 (100%) | 0 | 100 100 |
| 5 | A0 | 449/465 (97%) | 400 (89%) | 49 (11%) | 6 25 |
| 5 | A1 | 449/465 (97%) | 392 (87%) | 57 (13%) | 4 21 |
| 5 | A2 | 448/465 (96%) | 398 (89%) | 50 (11%) | 6 24 |
| 5 | A3 | 448/465 (96%) | 390 (87%) | 58 (13%) | 4 20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 5 | Av | 448/465 (96%) | 388 (87%) | 60 (13%) | 4 | 19 |
| 5 | Ax | 448/465 (96%) | 401 (90%) | 47 (10%) | 6 | 26 |
| 5 | BA | 441/465 (95%) | 394 (89%) | 47 (11%) | 6 | 25 |
| 5 | BB | 435/465 (94%) | 393 (90%) | 42 (10%) | 8 | 29 |
| 5 | BD | 448/465 (96%) | 385 (86%) | 63 (14%) | 3 | 18 |
| 5 | BF | 448/465 (96%) | 400 (89%) | 48 (11%) | 6 | 25 |
| 5 | BG | 436/465 (94%) | 385 (88%) | 51 (12%) | 5 | 22 |
| 5 | BH | 438/465 (94%) | 385 (88%) | 53 (12%) | 5 | 21 |
| 6 | A4 | 345/400 (86%) | 320 (93%) | 25 (7%) | 13 | 39 |
| 6 | A5 | 345/400 (86%) | 326 (94%) | 19 (6%) | 19 | 45 |
| 6 | A7 | 345/400 (86%) | 324 (94%) | 21 (6%) | 17 | 43 |
| 6 | A8 | 335/400 (84%) | 317 (95%) | 18 (5%) | 20 | 45 |
| 6 | A9 | 345/400 (86%) | 330 (96%) | 15 (4%) | 26 | 50 |
| 6 | AV | 345/400 (86%) | 321 (93%) | 24 (7%) | 14 | 40 |
| 6 | AW | 345/400 (86%) | 328 (95%) | 17 (5%) | 22 | 47 |
| 6 | AX | 345/400 (86%) | 314 (91%) | 31 (9%) | 9 | 32 |
| 6 | AZ | 345/400 (86%) | 312 (90%) | 33 (10%) | 8 | 29 |
| 6 | Ac | 345/400 (86%) | 324 (94%) | 21 (6%) | 17 | 43 |
| 6 | Ad | 345/400 (86%) | 323 (94%) | 22 (6%) | 16 | 42 |
| 6 | Ae | 345/400 (86%) | 319 (92%) | 26 (8%) | 12 | 38 |
| 6 | Af | 345/400 (86%) | 326 (94%) | 19 (6%) | 19 | 45 |
| 6 | Ag | 345/400 (86%) | 330 (96%) | 15 (4%) | 26 | 50 |
| 6 | Ah | 345/400 (86%) | 330 (96%) | 15 (4%) | 26 | 50 |
| 6 | Ai | 345/400 (86%) | 330 (96%) | 15 (4%) | 26 | 50 |
| 6 | Aj | 345/400 (86%) | 329 (95%) | 16 (5%) | 24 | 48 |
| 6 | Ak | 345/400 (86%) | 331 (96%) | 14 (4%) | 27 | 51 |
| 6 | Am | 345/400 (86%) | 327 (95%) | 18 (5%) | 21 | 46 |
| 6 | An | 335/400 (84%) | 317 (95%) | 18 (5%) | 20 | 45 |
| 6 | Ao | 333/400 (83%) | 312 (94%) | 21 (6%) | 16 | 42 |
| 6 | Ap | 335/400 (84%) | 314 (94%) | 21 (6%) | 16 | 42 |
| 6 | Au | 345/400 (86%) | 325 (94%) | 20 (6%) | 18 | 44 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 6 | Aw | 345/400 (86%) | 320 (93%) | 25 (7%) | 13 | 39 |
| 6 | Ay | 345/400 (86%) | 316 (92%) | 29 (8%) | 10 | 34 |
| 6 | Az | 345/400 (86%) | 322 (93%) | 23 (7%) | 15 | 41 |
| 6 | BI | 345/400 (86%) | 326 (94%) | 19 (6%) | 19 | 45 |
| 6 | BJ | 333/400 (83%) | 311 (93%) | 22 (7%) | 15 | 41 |
| 6 | BK | 345/400 (86%) | 329 (95%) | 16 (5%) | 24 | 48 |
| 6 | BM | 345/400 (86%) | 328 (95%) | 17 (5%) | 22 | 47 |
| 7 | A6 | 259/260 (100%) | 234 (90%) | 25 (10%) | 8 | 29 |
| 7 | AY | 258/260 (99%) | 234 (91%) | 24 (9%) | 8 | 30 |
| 7 | Aa | 259/260 (100%) | 235 (91%) | 24 (9%) | 8 | 30 |
| 7 | Ab | 259/260 (100%) | 234 (90%) | 25 (10%) | 8 | 29 |
| 7 | Al | 258/260 (99%) | 236 (92%) | 22 (8%) | 10 | 33 |
| 7 | Aq | 259/260 (100%) | 234 (90%) | 25 (10%) | 8 | 29 |
| 7 | Ar | 247/260 (95%) | 228 (92%) | 19 (8%) | 12 | 37 |
| 7 | As | 259/260 (100%) | 233 (90%) | 26 (10%) | 7 | 28 |
| 7 | At | 251/260 (96%) | 224 (89%) | 27 (11%) | 6 | 25 |
| 7 | BC | 259/260 (100%) | 235 (91%) | 24 (9%) | 8 | 30 |
| 7 | BE | 259/260 (100%) | 238 (92%) | 21 (8%) | 11 | 35 |
| 7 | BL | 259/260 (100%) | 230 (89%) | 29 (11%) | 6 | 24 |
| 8 | AB | 250/250 (100%) | 224 (90%) | 26 (10%) | 7 | 26 |
| 8 | q | 250/250 (100%) | 230 (92%) | 20 (8%) | 11 | 36 |
| 8 | r | 250/250 (100%) | 226 (90%) | 24 (10%) | 8 | 29 |
| 8 | s | 250/250 (100%) | 222 (89%) | 28 (11%) | 6 | 24 |
| 8 | t | 250/250 (100%) | 227 (91%) | 23 (9%) | 8 | 31 |
| 8 | u | 250/250 (100%) | 229 (92%) | 21 (8%) | 10 | 34 |
| 9 | AC | 156/157 (99%) | 144 (92%) | 12 (8%) | 12 | 37 |
| 9 | v | 156/157 (99%) | 148 (95%) | 8 (5%) | 21 | 46 |
| 9 | w | 156/157 (99%) | 147 (94%) | 9 (6%) | 18 | 44 |
| 9 | x | 156/157 (99%) | 145 (93%) | 11 (7%) | 13 | 39 |
| 9 | y | 156/157 (99%) | 144 (92%) | 12 (8%) | 12 | 37 |
| 9 | z | 156/157 (99%) | 145 (93%) | 11 (7%) | 13 | 39 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 10 | AQ | 87/319 (27%) | 85 (98%) | 2 (2%) | 44 | 63 |
| 10 | AR | 87/319 (27%) | 85 (98%) | 2 (2%) | 44 | 63 |
| 10 | AS | 87/319 (27%) | 84 (97%) | 3 (3%) | 32 | 55 |
| 10 | AT | 87/319 (27%) | 86 (99%) | 1 (1%) | 65 | 73 |
| 10 | AU | 87/319 (27%) | 86 (99%) | 1 (1%) | 65 | 73 |
| 11 | BN | 67/68 (98%) | 64 (96%) | 3 (4%) | 24 | 48 |
| 11 | BO | 67/68 (98%) | 63 (94%) | 4 (6%) | 17 | 43 |
| 11 | BP | 67/68 (98%) | 64 (96%) | 3 (4%) | 24 | 48 |
| 11 | BQ | 67/68 (98%) | 64 (96%) | 3 (4%) | 24 | 48 |
| 11 | BR | 67/68 (98%) | 64 (96%) | 3 (4%) | 24 | 48 |
| 11 | BS | 67/68 (98%) | 64 (96%) | 3 (4%) | 24 | 48 |
| 11 | BT | 67/68 (98%) | 63 (94%) | 4 (6%) | 17 | 43 |
| 11 | BU | 67/68 (98%) | 65 (97%) | 2 (3%) | 36 | 57 |
| 11 | BV | 67/68 (98%) | 64 (96%) | 3 (4%) | 24 | 48 |
| 11 | BW | 67/68 (98%) | 64 (96%) | 3 (4%) | 24 | 48 |
| All | All | 46157/62065 (74%) | 42302 (92%) | 3855 (8%) | 12 | 34 |

All (3855) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 8 | LEU |
| 1 | 0 | 11 | LYS |
| 1 | 0 | 15 | ARG |
| 1 | 0 | 27 | LEU |
| 1 | 0 | 51 | ILE |
| 1 | 0 | 57 | GLU |
| 1 | 0 | 75 | ASP |
| 1 | 0 | 78 | ASN |
| 1 | 0 | 90 | LEU |
| 1 | 0 | 94 | GLU |
| 1 | 0 | 108 | MET |
| 1 | 0 | 110 | VAL |
| 1 | 0 | 114 | VAL |
| 1 | 0 | 115 | THR |
| 1 | 0 | 127 | VAL |
| 1 | 0 | 128 | ASN |
| 1 | 0 | 146 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 166 | ILE |
| 1 | 0 | 175 | ILE |
| 1 | 0 | 182 | ASN |
| 1 | 0 | 213 | ILE |
| 1 | 0 | 214 | ASN |
| 1 | 0 | 230 | GLU |
| 1 | 0 | 233 | GLU |
| 1 | 0 | 238 | VAL |
| 1 | 0 | 245 | PHE |
| 2 | 1 | 4 | LEU |
| 2 | 1 | 14 | THR |
| 2 | 1 | 18 | THR |
| 2 | 1 | 70 | ASN |
| 2 | 1 | 72 | LEU |
| 2 | 1 | 88 | THR |
| 2 | 1 | 133 | GLU |
| 2 | 1 | 166 | ASN |
| 2 | 1 | 178 | LEU |
| 2 | 1 | 186 | LYS |
| 2 | 1 | 188 | ILE |
| 2 | 1 | 193 | ILE |
| 2 | 1 | 202 | GLU |
| 2 | 1 | 206 | THR |
| 2 | 1 | 246 | LYS |
| 2 | 1 | 255 | TYR |
| 2 | 1 | 284 | ARG |
| 2 | 1 | 286 | ASN |
| 2 | 1 | 303 | ASP |
| 2 | 1 | 317 | LYS |
| 2 | 1 | 339 | THR |
| 2 | 1 | 344 | LEU |
| 2 | 1 | 355 | LEU |
| 2 | 1 | 371 | GLN |
| 2 | 1 | 372 | LEU |
| 2 | 1 | 385 | THR |
| 2 | 1 | 404 | LEU |
| 2 | 1 | 406 | LEU |
| 2 | 1 | 417 | ILE |
| 2 | 1 | 430 | ARG |
| 2 | 1 | 450 | ILE |
| 2 | 1 | 464 | VAL |
| 2 | 1 | 477 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 494 | TYR |
| 2 | 1 | 501 | ASN |
| 2 | 1 | 508 | GLU |
| 2 | 1 | 523 | ASN |
| 2 | 1 | 528 | THR |
| 2 | 1 | 535 | LEU |
| 2 | 1 | 544 | VAL |
| 2 | 1 | 560 | LEU |
| 2 | 1 | 564 | ILE |
| 2 | 1 | 572 | LEU |
| 2 | 1 | 588 | THR |
| 2 | 1 | 611 | THR |
| 2 | 1 | 633 | ARG |
| 2 | 2 | 11 | LYS |
| 2 | 2 | 14 | THR |
| 2 | 2 | 18 | THR |
| 2 | 2 | 49 | ASP |
| 2 | 2 | 58 | THR |
| 2 | 2 | 66 | MET |
| 2 | 2 | 84 | VAL |
| 2 | 2 | 87 | ASP |
| 2 | 2 | 144 | ASN |
| 2 | 2 | 178 | LEU |
| 2 | 2 | 181 | VAL |
| 2 | 2 | 202 | GLU |
| 2 | 2 | 206 | THR |
| 2 | 2 | 255 | TYR |
| 2 | 2 | 303 | ASP |
| 2 | 2 | 355 | LEU |
| 2 | 2 | 404 | LEU |
| 2 | 2 | 406 | LEU |
| 2 | 2 | 417 | ILE |
| 2 | 2 | 430 | ARG |
| 2 | 2 | 443 | ILE |
| 2 | 2 | 494 | TYR |
| 2 | 2 | 503 | ILE |
| 2 | 2 | 509 | THR |
| 2 | 2 | 523 | ASN |
| 2 | 2 | 535 | LEU |
| 2 | 2 | 536 | TYR |
| 2 | 2 | 540 | THR |
| 2 | 2 | 552 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 2 | 553 | VAL |
| 2 | 2 | 564 | ILE |
| 2 | 2 | 575 | LEU |
| 2 | 2 | 601 | ILE |
| 2 | 2 | 611 | THR |
| 2 | 2 | 617 | VAL |
| 2 | 2 | 635 | ILE |
| 2 | 2 | 651 | PHE |
| 2 | 3 | 14 | THR |
| 2 | 3 | 47 | GLU |
| 2 | 3 | 66 | MET |
| 2 | 3 | 81 | VAL |
| 2 | 3 | 84 | VAL |
| 2 | 3 | 88 | THR |
| 2 | 3 | 91 | ASN |
| 2 | 3 | 133 | GLU |
| 2 | 3 | 134 | VAL |
| 2 | 3 | 195 | LEU |
| 2 | 3 | 202 | GLU |
| 2 | 3 | 205 | MET |
| 2 | 3 | 206 | THR |
| 2 | 3 | 229 | GLU |
| 2 | 3 | 236 | ILE |
| 2 | 3 | 255 | TYR |
| 2 | 3 | 271 | TYR |
| 2 | 3 | 303 | ASP |
| 2 | 3 | 337 | ILE |
| 2 | 3 | 344 | LEU |
| 2 | 3 | 350 | VAL |
| 2 | 3 | 355 | LEU |
| 2 | 3 | 368 | VAL |
| 2 | 3 | 383 | LEU |
| 2 | 3 | 406 | LEU |
| 2 | 3 | 417 | ILE |
| 2 | 3 | 430 | ARG |
| 2 | 3 | 431 | THR |
| 2 | 3 | 445 | SER |
| 2 | 3 | 454 | TYR |
| 2 | 3 | 467 | TRP |
| 2 | 3 | 505 | LEU |
| 2 | 3 | 513 | GLN |
| 2 | 3 | 536 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 3 | 572 | LEU |
| 2 | 3 | 588 | THR |
| 2 | 3 | 609 | ASP |
| 2 | 3 | 641 | ASN |
| 2 | 4 | 4 | LEU |
| 2 | 4 | 14 | THR |
| 2 | 4 | 58 | THR |
| 2 | 4 | 61 | THR |
| 2 | 4 | 66 | MET |
| 2 | 4 | 70 | ASN |
| 2 | 4 | 72 | LEU |
| 2 | 4 | 76 | ASN |
| 2 | 4 | 140 | ILE |
| 2 | 4 | 195 | LEU |
| 2 | 4 | 206 | THR |
| 2 | 4 | 290 | VAL |
| 2 | 4 | 303 | ASP |
| 2 | 4 | 344 | LEU |
| 2 | 4 | 350 | VAL |
| 2 | 4 | 355 | LEU |
| 2 | 4 | 370 | VAL |
| 2 | 4 | 383 | LEU |
| 2 | 4 | 406 | LEU |
| 2 | 4 | 412 | GLU |
| 2 | 4 | 413 | THR |
| 2 | 4 | 417 | ILE |
| 2 | 4 | 430 | ARG |
| 2 | 4 | 437 | THR |
| 2 | 4 | 439 | ASN |
| 2 | 4 | 454 | TYR |
| 2 | 4 | 473 | ASP |
| 2 | 4 | 483 | ASN |
| 2 | 4 | 484 | VAL |
| 2 | 4 | 494 | TYR |
| 2 | 4 | 495 | ASN |
| 2 | 4 | 513 | GLN |
| 2 | 4 | 523 | ASN |
| 2 | 4 | 535 | LEU |
| 2 | 4 | 536 | TYR |
| 2 | 4 | 560 | LEU |
| 2 | 4 | 572 | LEU |
| 2 | 4 | 611 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 4 | 624 | VAL |
| 2 | 5 | 14 | THR |
| 2 | 5 | 58 | THR |
| 2 | 5 | 66 | MET |
| 2 | 5 | 84 | VAL |
| 2 | 5 | 87 | ASP |
| 2 | 5 | 100 | GLU |
| 2 | 5 | 133 | GLU |
| 2 | 5 | 194 | LEU |
| 2 | 5 | 195 | LEU |
| 2 | 5 | 206 | THR |
| 2 | 5 | 268 | VAL |
| 2 | 5 | 269 | PHE |
| 2 | 5 | 303 | ASP |
| 2 | 5 | 350 | VAL |
| 2 | 5 | 355 | LEU |
| 2 | 5 | 378 | CYS |
| 2 | 5 | 385 | THR |
| 2 | 5 | 401 | GLN |
| 2 | 5 | 404 | LEU |
| 2 | 5 | 417 | ILE |
| 2 | 5 | 430 | ARG |
| 2 | 5 | 436 | TYR |
| 2 | 5 | 453 | ASN |
| 2 | 5 | 454 | TYR |
| 2 | 5 | 459 | ASP |
| 2 | 5 | 503 | ILE |
| 2 | 5 | 518 | TYR |
| 2 | 5 | 523 | ASN |
| 2 | 5 | 535 | LEU |
| 2 | 5 | 560 | LEU |
| 2 | 5 | 563 | ASN |
| 2 | 5 | 617 | VAL |
| 2 | 5 | 624 | VAL |
| 2 | 5 | 629 | ILE |
| 2 | 5 | 639 | THR |
| 2 | 5 | 653 | GLU |
| 3 | 6 | 7 | THR |
| 3 | 6 | 10 | PHE |
| 3 | 6 | 23 | VAL |
| 3 | 6 | 41 | LEU |
| 3 | 6 | 45 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 6 | 49 | ILE |
| 3 | 6 | 51 | VAL |
| 3 | 6 | 55 | ASN |
| 3 | 6 | 57 | LYS |
| 3 | 6 | 113 | VAL |
| 3 | 6 | 124 | THR |
| 3 | 6 | 127 | ILE |
| 3 | 6 | 137 | VAL |
| 3 | 6 | 150 | ILE |
| 3 | 6 | 159 | LEU |
| 3 | 6 | 160 | ASP |
| 3 | 7 | 4 | ASP |
| 3 | 7 | 23 | VAL |
| 3 | 7 | 41 | LEU |
| 3 | 7 | 45 | ILE |
| 3 | 7 | 49 | ILE |
| 3 | 7 | 51 | VAL |
| 3 | 7 | 55 | ASN |
| 3 | 7 | 63 | ASP |
| 3 | 7 | 64 | ARG |
| 3 | 7 | 71 | VAL |
| 3 | 7 | 112 | ILE |
| 3 | 7 | 113 | VAL |
| 3 | 7 | 127 | ILE |
| 3 | 7 | 137 | VAL |
| 3 | 7 | 150 | ILE |
| 3 | 7 | 157 | LEU |
| 3 | 8 | 10 | PHE |
| 3 | 8 | 15 | PHE |
| 3 | 8 | 23 | VAL |
| 3 | 8 | 41 | LEU |
| 3 | 8 | 45 | ILE |
| 3 | 8 | 49 | ILE |
| 3 | 8 | 57 | LYS |
| 3 | 8 | 63 | ASP |
| 3 | 8 | 64 | ARG |
| 3 | 8 | 100 | THR |
| 3 | 8 | 112 | ILE |
| 3 | 8 | 113 | VAL |
| 3 | 8 | 127 | ILE |
| 3 | 8 | 137 | VAL |
| 3 | 8 | 150 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 8 | 154 | GLU |
| 3 | 8 | 157 | LEU |
| 3 | 9 | 4 | ASP |
| 3 | 9 | 7 | THR |
| 3 | 9 | 10 | PHE |
| 3 | 9 | 23 | VAL |
| 3 | 9 | 41 | LEU |
| 3 | 9 | 45 | ILE |
| 3 | 9 | 48 | LYS |
| 3 | 9 | 49 | ILE |
| 3 | 9 | 51 | VAL |
| 3 | 9 | 57 | LYS |
| 3 | 9 | 58 | ILE |
| 3 | 9 | 59 | ASN |
| 3 | 9 | 63 | ASP |
| 3 | 9 | 97 | ASN |
| 3 | 9 | 98 | GLU |
| 3 | 9 | 112 | ILE |
| 3 | 9 | 113 | VAL |
| 3 | 9 | 123 | VAL |
| 3 | 9 | 127 | ILE |
| 3 | 9 | 150 | ILE |
| 4 | A | 11 | VAL |
| 5 | A0 | 6 | LEU |
| 5 | A0 | 26 | GLU |
| 5 | A0 | 28 | LEU |
| 5 | A0 | 31 | ILE |
| 5 | A0 | 41 | ARG |
| 5 | A0 | 45 | VAL |
| 5 | A0 | 87 | GLU |
| 5 | A0 | 88 | VAL |
| 5 | A0 | 89 | ASP |
| 5 | A0 | 106 | THR |
| 5 | A0 | 107 | GLU |
| 5 | A0 | 108 | VAL |
| 5 | A0 | 109 | VAL |
| 5 | A0 | 139 | PHE |
| 5 | A0 | 140 | GLN |
| 5 | A0 | 142 | LYS |
| 5 | A0 | 165 | LYS |
| 5 | A0 | 168 | LYS |
| 5 | A0 | 185 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A0 | 210 | THR |
| 5 | A0 | 217 | CYS |
| 5 | A0 | 220 | ARG |
| 5 | A0 | 223 | GLU |
| 5 | A0 | 232 | LYS |
| 5 | A0 | 242 | LEU |
| 5 | A0 | 248 | LYS |
| 5 | A0 | 267 | LEU |
| 5 | A0 | 278 | ARG |
| 5 | A0 | 301 | MET |
| 5 | A0 | 307 | THR |
| 5 | A0 | 308 | MET |
| 5 | A0 | 310 | ASN |
| 5 | A0 | 324 | GLN |
| 5 | A0 | 340 | ASP |
| 5 | A0 | 354 | ASP |
| 5 | A0 | 374 | ARG |
| 5 | A0 | 380 | ILE |
| 5 | A0 | 397 | THR |
| 5 | A0 | 401 | LEU |
| 5 | A0 | 405 | LYS |
| 5 | A0 | 417 | VAL |
| 5 | A0 | 441 | ILE |
| 5 | A0 | 445 | LYS |
| 5 | A0 | 450 | ARG |
| 5 | A0 | 451 | ASP |
| 5 | A0 | 462 | ILE |
| 5 | A0 | 503 | LYS |
| 5 | A0 | 506 | GLU |
| 5 | A0 | 508 | GLU |
| 5 | A1 | 14 | LYS |
| 5 | A1 | 24 | GLU |
| 5 | A1 | 31 | ILE |
| 5 | A1 | 45 | VAL |
| 5 | A1 | 59 | GLN |
| 5 | A1 | 61 | ILE |
| 5 | A1 | 62 | PHE |
| 5 | A1 | 86 | TYR |
| 5 | A1 | 101 | VAL |
| 5 | A1 | 119 | SER |
| 5 | A1 | 134 | LEU |
| 5 | A1 | 141 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A1 | 146 | HIS |
| 5 | A1 | 149 | ARG |
| 5 | A1 | 162 | ILE |
| 5 | A1 | 169 | GLU |
| 5 | A1 | 185 | VAL |
| 5 | A1 | 186 | ARG |
| 5 | A1 | 189 | ILE |
| 5 | A1 | 204 | GLU |
| 5 | A1 | 212 | HIS |
| 5 | A1 | 215 | TYR |
| 5 | A1 | 248 | LYS |
| 5 | A1 | 250 | ILE |
| 5 | A1 | 263 | GLN |
| 5 | A1 | 264 | LEU |
| 5 | A1 | 267 | LEU |
| 5 | A1 | 301 | MET |
| 5 | A1 | 308 | MET |
| 5 | A1 | 310 | ASN |
| 5 | A1 | 312 | VAL |
| 5 | A1 | 320 | LYS |
| 5 | A1 | 322 | LYS |
| 5 | A1 | 349 | THR |
| 5 | A1 | 359 | MET |
| 5 | A1 | 373 | LEU |
| 5 | A1 | 380 | ILE |
| 5 | A1 | 388 | VAL |
| 5 | A1 | 397 | THR |
| 5 | A1 | 401 | LEU |
| 5 | A1 | 426 | LEU |
| 5 | A1 | 434 | GLU |
| 5 | A1 | 445 | LYS |
| 5 | A1 | 456 | GLU |
| 5 | A1 | 459 | GLU |
| 5 | A1 | 462 | ILE |
| 5 | A1 | 469 | MET |
| 5 | A1 | 474 | GLU |
| 5 | A1 | 479 | LYS |
| 5 | A1 | 484 | ARG |
| 5 | A1 | 495 | ASP |
| 5 | A1 | 497 | GLU |
| 5 | A1 | 499 | GLU |
| 5 | A1 | 501 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A1 | 503 | LYS |
| 5 | A1 | 504 | GLN |
| 5 | A1 | 508 | GLU |
| 5 | A2 | 17 | GLU |
| 5 | A2 | 45 | VAL |
| 5 | A2 | 55 | ASN |
| 5 | A2 | 70 | LYS |
| 5 | A2 | 74 | GLU |
| 5 | A2 | 87 | GLU |
| 5 | A2 | 101 | VAL |
| 5 | A2 | 107 | GLU |
| 5 | A2 | 108 | VAL |
| 5 | A2 | 118 | PHE |
| 5 | A2 | 128 | ASP |
| 5 | A2 | 162 | ILE |
| 5 | A2 | 163 | ASP |
| 5 | A2 | 166 | ARG |
| 5 | A2 | 178 | ASP |
| 5 | A2 | 185 | VAL |
| 5 | A2 | 188 | ILE |
| 5 | A2 | 190 | THR |
| 5 | A2 | 198 | ILE |
| 5 | A2 | 200 | LYS |
| 5 | A2 | 212 | HIS |
| 5 | A2 | 215 | TYR |
| 5 | A2 | 217 | CYS |
| 5 | A2 | 223 | GLU |
| 5 | A2 | 227 | LYS |
| 5 | A2 | 242 | LEU |
| 5 | A2 | 267 | LEU |
| 5 | A2 | 278 | ARG |
| 5 | A2 | 301 | MET |
| 5 | A2 | 308 | MET |
| 5 | A2 | 310 | ASN |
| 5 | A2 | 320 | LYS |
| 5 | A2 | 322 | LYS |
| 5 | A2 | 328 | MET |
| 5 | A2 | 347 | VAL |
| 5 | A2 | 359 | MET |
| 5 | A2 | 380 | ILE |
| 5 | A2 | 385 | GLN |
| 5 | A2 | 389 | MET |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A2 | 397 | THR |
| 5 | A2 | 401 | LEU |
| 5 | A2 | 428 | LEU |
| 5 | A2 | 441 | ILE |
| 5 | A2 | 450 | ARG |
| 5 | A2 | 456 | GLU |
| 5 | A2 | 462 | ILE |
| 5 | A2 | 487 | MET |
| 5 | A2 | 495 | ASP |
| 5 | A2 | 499 | GLU |
| 5 | A2 | 510 | LYS |
| 5 | A3 | 17 | GLU |
| 5 | A3 | 28 | LEU |
| 5 | A3 | 29 | VAL |
| 5 | A3 | 31 | ILE |
| 5 | A3 | 36 | LEU |
| 5 | A3 | 45 | VAL |
| 5 | A3 | 54 | TYR |
| 5 | A3 | 60 | THR |
| 5 | A3 | 85 | ASN |
| 5 | A3 | 88 | VAL |
| 5 | A3 | 101 | VAL |
| 5 | A3 | 107 | GLU |
| 5 | A3 | 134 | LEU |
| 5 | A3 | 165 | LYS |
| 5 | A3 | 168 | LYS |
| 5 | A3 | 185 | VAL |
| 5 | A3 | 188 | ILE |
| 5 | A3 | 189 | ILE |
| 5 | A3 | 207 | ILE |
| 5 | A3 | 209 | ASP |
| 5 | A3 | 213 | GLU |
| 5 | A3 | 221 | MET |
| 5 | A3 | 223 | GLU |
| 5 | A3 | 226 | THR |
| 5 | A3 | 232 | LYS |
| 5 | A3 | 245 | CYS |
| 5 | A3 | 251 | ILE |
| 5 | A3 | 267 | LEU |
| 5 | A3 | 308 | MET |
| 5 | A3 | 310 | ASN |
| 5 | A3 | 327 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A3 | 328 | MET |
| 5 | A3 | 333 | ASP |
| 5 | A3 | 340 | ASP |
| 5 | A3 | 345 | THR |
| 5 | A3 | 359 | MET |
| 5 | A3 | 360 | GLU |
| 5 | A3 | 374 | ARG |
| 5 | A3 | 377 | LEU |
| 5 | A3 | 380 | ILE |
| 5 | A3 | 382 | GLN |
| 5 | A3 | 389 | MET |
| 5 | A3 | 396 | ILE |
| 5 | A3 | 397 | THR |
| 5 | A3 | 400 | GLU |
| 5 | A3 | 401 | LEU |
| 5 | A3 | 405 | LYS |
| 5 | A3 | 410 | LEU |
| 5 | A3 | 417 | VAL |
| 5 | A3 | 423 | LYS |
| 5 | A3 | 425 | ASN |
| 5 | A3 | 441 | ILE |
| 5 | A3 | 450 | ARG |
| 5 | A3 | 462 | ILE |
| 5 | A3 | 487 | MET |
| 5 | A3 | 495 | ASP |
| 5 | A3 | 497 | GLU |
| 5 | A3 | 499 | GLU |
| 6 | A4 | 67 | GLU |
| 6 | A4 | 68 | ILE |
| 6 | A4 | 95 | VAL |
| 6 | A4 | 107 | ILE |
| 6 | A4 | 114 | VAL |
| 6 | A4 | 131 | TYR |
| 6 | A4 | 136 | VAL |
| 6 | A4 | 235 | LEU |
| 6 | A4 | 254 | ILE |
| 6 | A4 | 259 | ILE |
| 6 | A4 | 265 | GLN |
| 6 | A4 | 303 | ASN |
| 6 | A4 | 318 | LYS |
| 6 | A4 | 345 | TRP |
| 6 | A4 | 358 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | A4 | 377 | ILE |
| 6 | A4 | 389 | VAL |
| 6 | A4 | 417 | LEU |
| 6 | A4 | 431 | GLN |
| 6 | A4 | 432 | ASP |
| 6 | A4 | 436 | VAL |
| 6 | A4 | 459 | LEU |
| 6 | A4 | 476 | ARG |
| 6 | A4 | 496 | ILE |
| 6 | A4 | 507 | LEU |
| 6 | A5 | 101 | ARG |
| 6 | A5 | 106 | LEU |
| 6 | A5 | 118 | ASN |
| 6 | A5 | 121 | THR |
| 6 | A5 | 208 | LEU |
| 6 | A5 | 221 | LEU |
| 6 | A5 | 259 | ILE |
| 6 | A5 | 322 | THR |
| 6 | A5 | 331 | VAL |
| 6 | A5 | 380 | ARG |
| 6 | A5 | 389 | VAL |
| 6 | A5 | 405 | SER |
| 6 | A5 | 417 | LEU |
| 6 | A5 | 436 | VAL |
| 6 | A5 | 449 | TYR |
| 6 | A5 | 450 | TYR |
| 6 | A5 | 471 | MET |
| 6 | A5 | 496 | ILE |
| 6 | A5 | 507 | LEU |
| 7 | A6 | 12 | LEU |
| 7 | A6 | 20 | LEU |
| 7 | A6 | 25 | ILE |
| 7 | A6 | 36 | ASP |
| 7 | A6 | 43 | GLU |
| 7 | A6 | 66 | GLU |
| 7 | A6 | 77 | ARG |
| 7 | A6 | 80 | ASN |
| 7 | A6 | 98 | MET |
| 7 | A6 | 101 | ASN |
| 7 | A6 | 106 | TRP |
| 7 | A6 | 137 | ASP |
| 7 | A6 | 138 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | A6 | 158 | ILE |
| 7 | A6 | 162 | TRP |
| 7 | A6 | 178 | LYS |
| 7 | A6 | 189 | LYS |
| 7 | A6 | 192 | ILE |
| 7 | A6 | 211 | ASP |
| 7 | A6 | 231 | VAL |
| 7 | A6 | 237 | VAL |
| 7 | A6 | 258 | LEU |
| 7 | A6 | 276 | THR |
| 7 | A6 | 297 | LEU |
| 7 | A6 | 299 | LEU |
| 6 | A7 | 95 | VAL |
| 6 | A7 | 101 | ARG |
| 6 | A7 | 106 | LEU |
| 6 | A7 | 110 | ASP |
| 6 | A7 | 117 | MET |
| 6 | A7 | 131 | TYR |
| 6 | A7 | 174 | VAL |
| 6 | A7 | 184 | GLU |
| 6 | A7 | 187 | THR |
| 6 | A7 | 188 | VAL |
| 6 | A7 | 208 | LEU |
| 6 | A7 | 265 | GLN |
| 6 | A7 | 289 | GLU |
| 6 | A7 | 315 | GLN |
| 6 | A7 | 324 | THR |
| 6 | A7 | 331 | VAL |
| 6 | A7 | 344 | ARG |
| 6 | A7 | 406 | THR |
| 6 | A7 | 412 | VAL |
| 6 | A7 | 448 | ILE |
| 6 | A7 | 476 | ARG |
| 6 | A8 | 111 | ILE |
| 6 | A8 | 174 | VAL |
| 6 | A8 | 185 | THR |
| 6 | A8 | 247 | TRP |
| 6 | A8 | 265 | GLN |
| 6 | A8 | 279 | ARG |
| 6 | A8 | 287 | ASP |
| 6 | A8 | 331 | VAL |
| 6 | A8 | 344 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | A8 | 376 | ILE |
| 6 | A8 | 377 | ILE |
| 6 | A8 | 395 | TYR |
| 6 | A8 | 435 | THR |
| 6 | A8 | 444 | MET |
| 6 | A8 | 466 | ASN |
| 6 | A8 | 471 | MET |
| 6 | A8 | 486 | GLU |
| 6 | A8 | 516 | VAL |
| 6 | A9 | 110 | ASP |
| 6 | A9 | 117 | MET |
| 6 | A9 | 124 | VAL |
| 6 | A9 | 174 | VAL |
| 6 | A9 | 187 | THR |
| 6 | A9 | 244 | ASP |
| 6 | A9 | 255 | ASP |
| 6 | A9 | 278 | LEU |
| 6 | A9 | 398 | GLN |
| 6 | A9 | 400 | LEU |
| 6 | A9 | 423 | VAL |
| 6 | A9 | 427 | GLN |
| 6 | A9 | 432 | ASP |
| 6 | A9 | 482 | ASN |
| 6 | A9 | 486 | GLU |
| 3 | AA | 4 | ASP |
| 3 | AA | 7 | THR |
| 3 | AA | 10 | PHE |
| 3 | AA | 23 | VAL |
| 3 | AA | 41 | LEU |
| 3 | AA | 45 | ILE |
| 3 | AA | 57 | LYS |
| 3 | AA | 60 | VAL |
| 3 | AA | 63 | ASP |
| 3 | AA | 72 | THR |
| 3 | AA | 113 | VAL |
| 3 | AA | 124 | THR |
| 3 | AA | 127 | ILE |
| 3 | AA | 137 | VAL |
| 3 | AA | 150 | ILE |
| 8 | AB | 20 | LEU |
| 8 | AB | 26 | ILE |
| 8 | AB | 35 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | AB | 59 | ILE |
| 8 | AB | 60 | ASN |
| 8 | AB | 72 | LEU |
| 8 | AB | 88 | PHE |
| 8 | AB | 96 | ASN |
| 8 | AB | 98 | LEU |
| 8 | AB | 105 | VAL |
| 8 | AB | 114 | ILE |
| 8 | AB | 142 | GLN |
| 8 | AB | 147 | THR |
| 8 | AB | 163 | ILE |
| 8 | AB | 164 | LYS |
| 8 | AB | 172 | ILE |
| 8 | AB | 187 | GLU |
| 8 | AB | 198 | MET |
| 8 | AB | 208 | LEU |
| 8 | AB | 214 | THR |
| 8 | AB | 229 | VAL |
| 8 | AB | 238 | VAL |
| 8 | AB | 241 | ASP |
| 8 | AB | 250 | THR |
| 8 | AB | 256 | THR |
| 8 | AB | 258 | ASN |
| 9 | AC | 5 | LEU |
| 9 | AC | 10 | ASN |
| 9 | AC | 11 | GLN |
| 9 | AC | 47 | THR |
| 9 | AC | 64 | VAL |
| 9 | AC | 68 | TYR |
| 9 | AC | 76 | ILE |
| 9 | AC | 129 | ASN |
| 9 | AC | 136 | SER |
| 9 | AC | 140 | GLU |
| 9 | AC | 156 | THR |
| 9 | AC | 172 | ILE |
| 2 | AD | 11 | LYS |
| 2 | AD | 14 | THR |
| 2 | AD | 58 | THR |
| 2 | AD | 66 | MET |
| 2 | AD | 84 | VAL |
| 2 | AD | 88 | THR |
| 2 | AD | 91 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AD | 187 | ILE |
| 2 | AD | 194 | LEU |
| 2 | AD | 255 | TYR |
| 2 | AD | 268 | VAL |
| 2 | AD | 302 | LYS |
| 2 | AD | 303 | ASP |
| 2 | AD | 344 | LEU |
| 2 | AD | 355 | LEU |
| 2 | AD | 360 | ASP |
| 2 | AD | 366 | GLU |
| 2 | AD | 401 | GLN |
| 2 | AD | 404 | LEU |
| 2 | AD | 408 | SER |
| 2 | AD | 417 | ILE |
| 2 | AD | 424 | ASP |
| 2 | AD | 430 | ARG |
| 2 | AD | 465 | ASN |
| 2 | AD | 483 | ASN |
| 2 | AD | 505 | LEU |
| 2 | AD | 513 | GLN |
| 2 | AD | 520 | GLU |
| 2 | AD | 523 | ASN |
| 2 | AD | 528 | THR |
| 2 | AD | 535 | LEU |
| 2 | AD | 536 | TYR |
| 2 | AD | 560 | LEU |
| 2 | AD | 564 | ILE |
| 2 | AD | 572 | LEU |
| 2 | AD | 588 | THR |
| 2 | AD | 611 | THR |
| 2 | AD | 629 | ILE |
| 2 | AD | 651 | PHE |
| 2 | AD | 654 | LEU |
| 3 | AE | 6 | VAL |
| 3 | AE | 17 | ARG |
| 3 | AE | 23 | VAL |
| 3 | AE | 31 | ASN |
| 3 | AE | 37 | LYS |
| 3 | AE | 45 | ILE |
| 3 | AE | 49 | ILE |
| 3 | AE | 54 | MET |
| 3 | AE | 56 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | AE | 57 | LYS |
| 3 | AE | 64 | ARG |
| 3 | AE | 112 | ILE |
| 3 | AE | 113 | VAL |
| 3 | AE | 121 | LYS |
| 3 | AE | 125 | LYS |
| 3 | AE | 126 | GLU |
| 3 | AE | 127 | ILE |
| 3 | AE | 137 | VAL |
| 3 | AE | 150 | ILE |
| 3 | AF | 6 | VAL |
| 3 | AF | 17 | ARG |
| 3 | AF | 19 | ASN |
| 3 | AF | 23 | VAL |
| 3 | AF | 31 | ASN |
| 3 | AF | 48 | LYS |
| 3 | AF | 49 | ILE |
| 3 | AF | 56 | ARG |
| 3 | AF | 57 | LYS |
| 3 | AF | 58 | ILE |
| 3 | AF | 72 | THR |
| 3 | AF | 112 | ILE |
| 3 | AF | 113 | VAL |
| 3 | AF | 115 | GLN |
| 3 | AF | 121 | LYS |
| 3 | AF | 122 | THR |
| 3 | AF | 127 | ILE |
| 3 | AF | 128 | GLU |
| 3 | AF | 136 | ASN |
| 3 | AF | 137 | VAL |
| 3 | AF | 142 | LEU |
| 3 | AG | 6 | VAL |
| 3 | AG | 19 | ASN |
| 3 | AG | 23 | VAL |
| 3 | AG | 31 | ASN |
| 3 | AG | 37 | LYS |
| 3 | AG | 45 | ILE |
| 3 | AG | 48 | LYS |
| 3 | AG | 49 | ILE |
| 3 | AG | 57 | LYS |
| 3 | AG | 58 | ILE |
| 3 | AG | 98 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | AG | 112 | ILE |
| 3 | AG | 113 | VAL |
| 3 | AG | 121 | LYS |
| 3 | AG | 127 | ILE |
| 3 | AG | 137 | VAL |
| 3 | AG | 143 | ASP |
| 3 | AG | 163 | GLU |
| 3 | AH | 5 | ASP |
| 3 | AH | 6 | VAL |
| 3 | AH | 17 | ARG |
| 3 | AH | 19 | ASN |
| 3 | AH | 23 | VAL |
| 3 | AH | 37 | LYS |
| 3 | AH | 45 | ILE |
| 3 | AH | 48 | LYS |
| 3 | AH | 49 | ILE |
| 3 | AH | 57 | LYS |
| 3 | AH | 58 | ILE |
| 3 | AH | 72 | THR |
| 3 | AH | 80 | ASP |
| 3 | AH | 112 | ILE |
| 3 | AH | 121 | LYS |
| 3 | AH | 127 | ILE |
| 3 | AH | 137 | VAL |
| 3 | AH | 142 | LEU |
| 3 | AH | 150 | ILE |
| 3 | AI | 6 | VAL |
| 3 | AI | 17 | ARG |
| 3 | AI | 37 | LYS |
| 3 | AI | 45 | ILE |
| 3 | AI | 48 | LYS |
| 3 | AI | 49 | ILE |
| 3 | AI | 54 | MET |
| 3 | AI | 57 | LYS |
| 3 | AI | 58 | ILE |
| 3 | AI | 63 | ASP |
| 3 | AI | 112 | ILE |
| 3 | AI | 113 | VAL |
| 3 | AI | 127 | ILE |
| 3 | AI | 128 | GLU |
| 3 | AJ | 6 | VAL |
| 3 | AJ | 11 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | AJ | 14 | ASP |
| 3 | AJ | 19 | ASN |
| 3 | AJ | 23 | VAL |
| 3 | AJ | 37 | LYS |
| 3 | AJ | 45 | ILE |
| 3 | AJ | 49 | ILE |
| 3 | AJ | 54 | MET |
| 3 | AJ | 57 | LYS |
| 3 | AJ | 58 | ILE |
| 3 | AJ | 64 | ARG |
| 3 | AJ | 70 | THR |
| 3 | AJ | 100 | THR |
| 3 | AJ | 112 | ILE |
| 3 | AJ | 113 | VAL |
| 3 | AJ | 127 | ILE |
| 3 | AJ | 136 | ASN |
| 3 | AJ | 142 | LEU |
| 2 | AK | 20 | VAL |
| 2 | AK | 42 | LYS |
| 2 | AK | 49 | ASP |
| 2 | AK | 66 | MET |
| 2 | AK | 88 | THR |
| 2 | AK | 91 | ASN |
| 2 | AK | 112 | VAL |
| 2 | AK | 115 | LYS |
| 2 | AK | 130 | LYS |
| 2 | AK | 133 | GLU |
| 2 | AK | 144 | ASN |
| 2 | AK | 149 | LYS |
| 2 | AK | 166 | ASN |
| 2 | AK | 170 | GLU |
| 2 | AK | 171 | ILE |
| 2 | AK | 186 | LYS |
| 2 | AK | 188 | ILE |
| 2 | AK | 195 | LEU |
| 2 | AK | 197 | GLU |
| 2 | AK | 202 | GLU |
| 2 | AK | 219 | ILE |
| 2 | AK | 229 | GLU |
| 2 | AK | 239 | VAL |
| 2 | AK | 255 | TYR |
| 2 | AK | 298 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AK | 302 | LYS |
| 2 | AK | 303 | ASP |
| 2 | AK | 344 | LEU |
| 2 | AK | 383 | LEU |
| 2 | AK | 404 | LEU |
| 2 | AK | 413 | THR |
| 2 | AK | 417 | ILE |
| 2 | AK | 426 | LEU |
| 2 | AK | 430 | ARG |
| 2 | AK | 446 | THR |
| 2 | AK | 456 | TYR |
| 2 | AK | 468 | VAL |
| 2 | AK | 487 | THR |
| 2 | AK | 503 | ILE |
| 2 | AK | 505 | LEU |
| 2 | AK | 523 | ASN |
| 2 | AK | 526 | THR |
| 2 | AK | 535 | LEU |
| 2 | AK | 540 | THR |
| 2 | AK | 548 | PHE |
| 2 | AK | 550 | ARG |
| 2 | AK | 572 | LEU |
| 2 | AK | 574 | GLU |
| 2 | AK | 596 | LYS |
| 2 | AK | 598 | LEU |
| 2 | AK | 606 | VAL |
| 2 | AK | 610 | THR |
| 2 | AK | 621 | ASN |
| 2 | AK | 650 | ASP |
| 2 | AK | 651 | PHE |
| 2 | AK | 655 | THR |
| 2 | AL | 14 | THR |
| 2 | AL | 32 | LYS |
| 2 | AL | 66 | MET |
| 2 | AL | 76 | ASN |
| 2 | AL | 80 | VAL |
| 2 | AL | 81 | VAL |
| 2 | AL | 112 | VAL |
| 2 | AL | 121 | VAL |
| 2 | AL | 130 | LYS |
| 2 | AL | 139 | LYS |
| 2 | AL | 149 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AL | 153 | LYS |
| 2 | AL | 170 | GLU |
| 2 | AL | 182 | ILE |
| 2 | AL | 183 | THR |
| 2 | AL | 186 | LYS |
| 2 | AL | 195 | LEU |
| 2 | AL | 199 | GLU |
| 2 | AL | 219 | ILE |
| 2 | AL | 230 | LEU |
| 2 | AL | 266 | LYS |
| 2 | AL | 290 | VAL |
| 2 | AL | 298 | LYS |
| 2 | AL | 303 | ASP |
| 2 | AL | 344 | LEU |
| 2 | AL | 361 | PHE |
| 2 | AL | 366 | GLU |
| 2 | AL | 384 | GLU |
| 2 | AL | 398 | ASP |
| 2 | AL | 404 | LEU |
| 2 | AL | 417 | ILE |
| 2 | AL | 430 | ARG |
| 2 | AL | 437 | THR |
| 2 | AL | 482 | ASP |
| 2 | AL | 503 | ILE |
| 2 | AL | 526 | THR |
| 2 | AL | 535 | LEU |
| 2 | AL | 536 | TYR |
| 2 | AL | 550 | ARG |
| 2 | AL | 572 | LEU |
| 2 | AL | 592 | LEU |
| 2 | AL | 606 | VAL |
| 2 | AL | 626 | THR |
| 2 | AL | 629 | ILE |
| 2 | AL | 651 | PHE |
| 2 | AM | 66 | MET |
| 2 | AM | 80 | VAL |
| 2 | AM | 81 | VAL |
| 2 | AM | 88 | THR |
| 2 | AM | 112 | VAL |
| 2 | AM | 130 | LYS |
| 2 | AM | 139 | LYS |
| 2 | AM | 143 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AM | 149 | LYS |
| 2 | AM | 171 | ILE |
| 2 | AM | 186 | LYS |
| 2 | AM | 195 | LEU |
| 2 | AM | 202 | GLU |
| 2 | AM | 219 | ILE |
| 2 | AM | 239 | VAL |
| 2 | AM | 252 | LEU |
| 2 | AM | 255 | TYR |
| 2 | AM | 298 | LYS |
| 2 | AM | 303 | ASP |
| 2 | AM | 332 | GLU |
| 2 | AM | 344 | LEU |
| 2 | AM | 366 | GLU |
| 2 | AM | 383 | LEU |
| 2 | AM | 385 | THR |
| 2 | AM | 398 | ASP |
| 2 | AM | 404 | LEU |
| 2 | AM | 417 | ILE |
| 2 | AM | 443 | ILE |
| 2 | AM | 446 | THR |
| 2 | AM | 451 | ASP |
| 2 | AM | 467 | TRP |
| 2 | AM | 482 | ASP |
| 2 | AM | 483 | ASN |
| 2 | AM | 484 | VAL |
| 2 | AM | 505 | LEU |
| 2 | AM | 522 | ILE |
| 2 | AM | 526 | THR |
| 2 | AM | 535 | LEU |
| 2 | AM | 536 | TYR |
| 2 | AM | 542 | THR |
| 2 | AM | 564 | ILE |
| 2 | AM | 576 | ASN |
| 2 | AM | 606 | VAL |
| 2 | AM | 617 | VAL |
| 2 | AM | 629 | ILE |
| 2 | AM | 650 | ASP |
| 2 | AM | 655 | THR |
| 2 | AN | 32 | LYS |
| 2 | AN | 42 | LYS |
| 2 | AN | 66 | MET |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AN | 88 | THR |
| 2 | AN | 91 | ASN |
| 2 | AN | 121 | VAL |
| 2 | AN | 130 | LYS |
| 2 | AN | 133 | GLU |
| 2 | AN | 141 | LYS |
| 2 | AN | 149 | LYS |
| 2 | AN | 166 | ASN |
| 2 | AN | 171 | ILE |
| 2 | AN | 178 | LEU |
| 2 | AN | 186 | LYS |
| 2 | AN | 190 | ASP |
| 2 | AN | 194 | LEU |
| 2 | AN | 219 | ILE |
| 2 | AN | 230 | LEU |
| 2 | AN | 255 | TYR |
| 2 | AN | 298 | LYS |
| 2 | AN | 303 | ASP |
| 2 | AN | 344 | LEU |
| 2 | AN | 365 | ARG |
| 2 | AN | 366 | GLU |
| 2 | AN | 406 | LEU |
| 2 | AN | 412 | GLU |
| 2 | AN | 417 | ILE |
| 2 | AN | 430 | ARG |
| 2 | AN | 443 | ILE |
| 2 | AN | 456 | TYR |
| 2 | AN | 467 | TRP |
| 2 | AN | 503 | ILE |
| 2 | AN | 535 | LEU |
| 2 | AN | 536 | TYR |
| 2 | AN | 542 | THR |
| 2 | AN | 572 | LEU |
| 2 | AN | 592 | LEU |
| 2 | AN | 596 | LYS |
| 2 | AN | 606 | VAL |
| 2 | AN | 654 | LEU |
| 2 | AO | 14 | THR |
| 2 | AO | 32 | LYS |
| 2 | AO | 76 | ASN |
| 2 | AO | 81 | VAL |
| 2 | AO | 116 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AO | 139 | LYS |
| 2 | AO | 149 | LYS |
| 2 | AO | 166 | ASN |
| 2 | AO | 171 | ILE |
| 2 | AO | 194 | LEU |
| 2 | AO | 195 | LEU |
| 2 | AO | 202 | GLU |
| 2 | AO | 215 | LYS |
| 2 | AO | 219 | ILE |
| 2 | AO | 239 | VAL |
| 2 | AO | 252 | LEU |
| 2 | AO | 289 | ILE |
| 2 | AO | 290 | VAL |
| 2 | AO | 298 | LYS |
| 2 | AO | 303 | ASP |
| 2 | AO | 317 | LYS |
| 2 | AO | 344 | LEU |
| 2 | AO | 365 | ARG |
| 2 | AO | 384 | GLU |
| 2 | AO | 398 | ASP |
| 2 | AO | 415 | VAL |
| 2 | AO | 417 | ILE |
| 2 | AO | 430 | ARG |
| 2 | AO | 437 | THR |
| 2 | AO | 443 | ILE |
| 2 | AO | 453 | ASN |
| 2 | AO | 455 | LYS |
| 2 | AO | 456 | TYR |
| 2 | AO | 467 | TRP |
| 2 | AO | 483 | ASN |
| 2 | AO | 518 | TYR |
| 2 | AO | 523 | ASN |
| 2 | AO | 535 | LEU |
| 2 | AO | 536 | TYR |
| 2 | AO | 542 | THR |
| 2 | AO | 550 | ARG |
| 2 | AO | 574 | GLU |
| 2 | AO | 606 | VAL |
| 2 | AO | 614 | THR |
| 2 | AO | 629 | ILE |
| 2 | AO | 633 | ARG |
| 2 | AO | 650 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AP | 12 | GLU |
| 2 | AP | 13 | THR |
| 2 | AP | 14 | THR |
| 2 | AP | 16 | GLN |
| 2 | AP | 32 | LYS |
| 2 | AP | 66 | MET |
| 2 | AP | 80 | VAL |
| 2 | AP | 91 | ASN |
| 2 | AP | 130 | LYS |
| 2 | AP | 149 | LYS |
| 2 | AP | 178 | LEU |
| 2 | AP | 182 | ILE |
| 2 | AP | 186 | LYS |
| 2 | AP | 197 | GLU |
| 2 | AP | 202 | GLU |
| 2 | AP | 215 | LYS |
| 2 | AP | 219 | ILE |
| 2 | AP | 239 | VAL |
| 2 | AP | 243 | ASP |
| 2 | AP | 252 | LEU |
| 2 | AP | 255 | TYR |
| 2 | AP | 290 | VAL |
| 2 | AP | 298 | LYS |
| 2 | AP | 299 | ARG |
| 2 | AP | 303 | ASP |
| 2 | AP | 366 | GLU |
| 2 | AP | 383 | LEU |
| 2 | AP | 398 | ASP |
| 2 | AP | 404 | LEU |
| 2 | AP | 417 | ILE |
| 2 | AP | 430 | ARG |
| 2 | AP | 438 | ASP |
| 2 | AP | 451 | ASP |
| 2 | AP | 453 | ASN |
| 2 | AP | 454 | TYR |
| 2 | AP | 473 | ASP |
| 2 | AP | 477 | LEU |
| 2 | AP | 503 | ILE |
| 2 | AP | 523 | ASN |
| 2 | AP | 536 | TYR |
| 2 | AP | 540 | THR |
| 2 | AP | 542 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AP | 550 | ARG |
| 2 | AP | 552 | ASN |
| 2 | AP | 553 | VAL |
| 2 | AP | 572 | LEU |
| 2 | AP | 574 | GLU |
| 2 | AP | 592 | LEU |
| 2 | AP | 606 | VAL |
| 2 | AP | 617 | VAL |
| 2 | AP | 624 | VAL |
| 2 | AP | 650 | ASP |
| 2 | AP | 651 | PHE |
| 2 | AP | 653 | GLU |
| 2 | AP | 655 | THR |
| 10 | AQ | 351 | VAL |
| 10 | AQ | 374 | THR |
| 10 | AR | 353 | VAL |
| 10 | AR | 374 | THR |
| 10 | AS | 314 | GLU |
| 10 | AS | 361 | ILE |
| 10 | AS | 362 | ILE |
| 10 | AT | 337 | HIS |
| 10 | AU | 307 | CYS |
| 6 | AV | 72 | HIS |
| 6 | AV | 110 | ASP |
| 6 | AV | 114 | VAL |
| 6 | AV | 115 | GLN |
| 6 | AV | 124 | VAL |
| 6 | AV | 174 | VAL |
| 6 | AV | 185 | THR |
| 6 | AV | 257 | GLN |
| 6 | AV | 265 | GLN |
| 6 | AV | 278 | LEU |
| 6 | AV | 287 | ASP |
| 6 | AV | 316 | VAL |
| 6 | AV | 331 | VAL |
| 6 | AV | 393 | ILE |
| 6 | AV | 395 | TYR |
| 6 | AV | 422 | ARG |
| 6 | AV | 423 | VAL |
| 6 | AV | 427 | GLN |
| 6 | AV | 439 | LYS |
| 6 | AV | 449 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | AV | 450 | TYR |
| 6 | AV | 476 | ARG |
| 6 | AV | 479 | ILE |
| 6 | AV | 521 | ILE |
| 6 | AW | 68 | ILE |
| 6 | AW | 106 | LEU |
| 6 | AW | 114 | VAL |
| 6 | AW | 188 | VAL |
| 6 | AW | 232 | ILE |
| 6 | AW | 255 | ASP |
| 6 | AW | 331 | VAL |
| 6 | AW | 351 | LYS |
| 6 | AW | 364 | ILE |
| 6 | AW | 377 | ILE |
| 6 | AW | 389 | VAL |
| 6 | AW | 432 | ASP |
| 6 | AW | 436 | VAL |
| 6 | AW | 439 | LYS |
| 6 | AW | 479 | ILE |
| 6 | AW | 495 | ARG |
| 6 | AW | 515 | ARG |
| 6 | AX | 67 | GLU |
| 6 | AX | 68 | ILE |
| 6 | AX | 77 | THR |
| 6 | AX | 88 | VAL |
| 6 | AX | 89 | THR |
| 6 | AX | 95 | VAL |
| 6 | AX | 112 | CYS |
| 6 | AX | 114 | VAL |
| 6 | AX | 131 | TYR |
| 6 | AX | 136 | VAL |
| 6 | AX | 183 | GLN |
| 6 | AX | 188 | VAL |
| 6 | AX | 243 | THR |
| 6 | AX | 259 | ILE |
| 6 | AX | 289 | GLU |
| 6 | AX | 334 | PHE |
| 6 | AX | 344 | ARG |
| 6 | AX | 356 | GLN |
| 6 | AX | 376 | ILE |
| 6 | AX | 377 | ILE |
| 6 | AX | 389 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | AX | 395 | TYR |
| 6 | AX | 430 | LYS |
| 6 | AX | 432 | ASP |
| 6 | AX | 436 | VAL |
| 6 | AX | 444 | MET |
| 6 | AX | 481 | ILE |
| 6 | AX | 486 | GLU |
| 6 | AX | 497 | GLN |
| 6 | AX | 503 | ILE |
| 6 | AX | 513 | PHE |
| 7 | AY | 12 | LEU |
| 7 | AY | 25 | ILE |
| 7 | AY | 28 | GLU |
| 7 | AY | 44 | LEU |
| 7 | AY | 51 | ASP |
| 7 | AY | 73 | VAL |
| 7 | AY | 87 | ILE |
| 7 | AY | 103 | THR |
| 7 | AY | 108 | THR |
| 7 | AY | 117 | ILE |
| 7 | AY | 121 | MET |
| 7 | AY | 138 | LEU |
| 7 | AY | 152 | GLN |
| 7 | AY | 162 | TRP |
| 7 | AY | 189 | LYS |
| 7 | AY | 192 | ILE |
| 7 | AY | 207 | VAL |
| 7 | AY | 227 | VAL |
| 7 | AY | 234 | ASP |
| 7 | AY | 252 | THR |
| 7 | AY | 258 | LEU |
| 7 | AY | 282 | LEU |
| 7 | AY | 297 | LEU |
| 7 | AY | 299 | LEU |
| 6 | AZ | 67 | GLU |
| 6 | AZ | 68 | ILE |
| 6 | AZ | 84 | THR |
| 6 | AZ | 95 | VAL |
| 6 | AZ | 106 | LEU |
| 6 | AZ | 107 | ILE |
| 6 | AZ | 114 | VAL |
| 6 | AZ | 121 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | AZ | 131 | TYR |
| 6 | AZ | 145 | HIS |
| 6 | AZ | 235 | LEU |
| 6 | AZ | 236 | GLN |
| 6 | AZ | 243 | THR |
| 6 | AZ | 259 | ILE |
| 6 | AZ | 260 | GLU |
| 6 | AZ | 278 | LEU |
| 6 | AZ | 300 | LEU |
| 6 | AZ | 324 | THR |
| 6 | AZ | 356 | GLN |
| 6 | AZ | 376 | ILE |
| 6 | AZ | 389 | VAL |
| 6 | AZ | 398 | GLN |
| 6 | AZ | 417 | LEU |
| 6 | AZ | 432 | ASP |
| 6 | AZ | 436 | VAL |
| 6 | AZ | 444 | MET |
| 6 | AZ | 448 | ILE |
| 6 | AZ | 470 | VAL |
| 6 | AZ | 476 | ARG |
| 6 | AZ | 482 | ASN |
| 6 | AZ | 496 | ILE |
| 6 | AZ | 503 | ILE |
| 6 | AZ | 521 | ILE |
| 7 | Aa | 12 | LEU |
| 7 | Aa | 53 | LEU |
| 7 | Aa | 90 | THR |
| 7 | Aa | 103 | THR |
| 7 | Aa | 106 | TRP |
| 7 | Aa | 111 | LEU |
| 7 | Aa | 112 | LEU |
| 7 | Aa | 121 | MET |
| 7 | Aa | 138 | LEU |
| 7 | Aa | 148 | MET |
| 7 | Aa | 150 | MET |
| 7 | Aa | 151 | MET |
| 7 | Aa | 168 | GLU |
| 7 | Aa | 175 | ASN |
| 7 | Aa | 210 | GLN |
| 7 | Aa | 215 | LEU |
| 7 | Aa | 229 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | Aa | 237 | VAL |
| 7 | Aa | 252 | THR |
| 7 | Aa | 258 | LEU |
| 7 | Aa | 265 | ARG |
| 7 | Aa | 290 | LYS |
| 7 | Aa | 297 | LEU |
| 7 | Aa | 299 | LEU |
| 7 | Ab | 12 | LEU |
| 7 | Ab | 28 | GLU |
| 7 | Ab | 40 | ARG |
| 7 | Ab | 44 | LEU |
| 7 | Ab | 53 | LEU |
| 7 | Ab | 66 | GLU |
| 7 | Ab | 87 | ILE |
| 7 | Ab | 92 | ILE |
| 7 | Ab | 95 | ILE |
| 7 | Ab | 98 | MET |
| 7 | Ab | 101 | ASN |
| 7 | Ab | 126 | ASN |
| 7 | Ab | 129 | TYR |
| 7 | Ab | 134 | PHE |
| 7 | Ab | 162 | TRP |
| 7 | Ab | 168 | GLU |
| 7 | Ab | 182 | ILE |
| 7 | Ab | 189 | LYS |
| 7 | Ab | 230 | VAL |
| 7 | Ab | 231 | VAL |
| 7 | Ab | 237 | VAL |
| 7 | Ab | 249 | ASP |
| 7 | Ab | 275 | VAL |
| 7 | Ab | 297 | LEU |
| 7 | Ab | 299 | LEU |
| 6 | Ac | 67 | GLU |
| 6 | Ac | 103 | ILE |
| 6 | Ac | 109 | PHE |
| 6 | Ac | 118 | ASN |
| 6 | Ac | 119 | SER |
| 6 | Ac | 130 | VAL |
| 6 | Ac | 134 | ASP |
| 6 | Ac | 208 | LEU |
| 6 | Ac | 259 | ILE |
| 6 | Ac | 331 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Ac | 389 | VAL |
| 6 | Ac | 391 | THR |
| 6 | Ac | 398 | GLN |
| 6 | Ac | 408 | THR |
| 6 | Ac | 417 | LEU |
| 6 | Ac | 432 | ASP |
| 6 | Ac | 436 | VAL |
| 6 | Ac | 449 | TYR |
| 6 | Ac | 450 | TYR |
| 6 | Ac | 516 | VAL |
| 6 | Ac | 518 | VAL |
| 6 | Ad | 91 | ILE |
| 6 | Ad | 106 | LEU |
| 6 | Ad | 124 | VAL |
| 6 | Ad | 208 | LEU |
| 6 | Ad | 215 | GLN |
| 6 | Ad | 259 | ILE |
| 6 | Ad | 263 | SER |
| 6 | Ad | 289 | GLU |
| 6 | Ad | 324 | THR |
| 6 | Ad | 331 | VAL |
| 6 | Ad | 338 | ILE |
| 6 | Ad | 380 | ARG |
| 6 | Ad | 384 | ASN |
| 6 | Ad | 389 | VAL |
| 6 | Ad | 398 | GLN |
| 6 | Ad | 417 | LEU |
| 6 | Ad | 430 | LYS |
| 6 | Ad | 436 | VAL |
| 6 | Ad | 445 | ASP |
| 6 | Ad | 479 | ILE |
| 6 | Ad | 486 | GLU |
| 6 | Ad | 516 | VAL |
| 6 | Ae | 67 | GLU |
| 6 | Ae | 71 | ASP |
| 6 | Ae | 111 | ILE |
| 6 | Ae | 141 | LYS |
| 6 | Ae | 184 | GLU |
| 6 | Ae | 187 | THR |
| 6 | Ae | 194 | VAL |
| 6 | Ae | 208 | LEU |
| 6 | Ae | 222 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Ae | 259 | ILE |
| 6 | Ae | 303 | ASN |
| 6 | Ae | 324 | THR |
| 6 | Ae | 331 | VAL |
| 6 | Ae | 338 | ILE |
| 6 | Ae | 348 | GLU |
| 6 | Ae | 389 | VAL |
| 6 | Ae | 398 | GLN |
| 6 | Ae | 417 | LEU |
| 6 | Ae | 430 | LYS |
| 6 | Ae | 444 | MET |
| 6 | Ae | 448 | ILE |
| 6 | Ae | 450 | TYR |
| 6 | Ae | 481 | ILE |
| 6 | Ae | 507 | LEU |
| 6 | Ae | 516 | VAL |
| 6 | Ae | 518 | VAL |
| 6 | Af | 68 | ILE |
| 6 | Af | 106 | LEU |
| 6 | Af | 107 | ILE |
| 6 | Af | 114 | VAL |
| 6 | Af | 117 | MET |
| 6 | Af | 147 | MET |
| 6 | Af | 187 | THR |
| 6 | Af | 242 | SER |
| 6 | Af | 244 | ASP |
| 6 | Af | 255 | ASP |
| 6 | Af | 287 | ASP |
| 6 | Af | 324 | THR |
| 6 | Af | 331 | VAL |
| 6 | Af | 377 | ILE |
| 6 | Af | 398 | GLN |
| 6 | Af | 430 | LYS |
| 6 | Af | 439 | LYS |
| 6 | Af | 471 | MET |
| 6 | Af | 479 | ILE |
| 6 | Ag | 68 | ILE |
| 6 | Ag | 79 | ILE |
| 6 | Ag | 95 | VAL |
| 6 | Ag | 106 | LEU |
| 6 | Ag | 107 | ILE |
| 6 | Ag | 110 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Ag | 114 | VAL |
| 6 | Ag | 124 | VAL |
| 6 | Ag | 188 | VAL |
| 6 | Ag | 331 | VAL |
| 6 | Ag | 344 | ARG |
| 6 | Ag | 374 | ASN |
| 6 | Ag | 377 | ILE |
| 6 | Ag | 389 | VAL |
| 6 | Ag | 456 | LEU |
| 6 | Ah | 68 | ILE |
| 6 | Ah | 84 | THR |
| 6 | Ah | 106 | LEU |
| 6 | Ah | 107 | ILE |
| 6 | Ah | 114 | VAL |
| 6 | Ah | 124 | VAL |
| 6 | Ah | 161 | LYS |
| 6 | Ah | 331 | VAL |
| 6 | Ah | 345 | TRP |
| 6 | Ah | 377 | ILE |
| 6 | Ah | 389 | VAL |
| 6 | Ah | 395 | TYR |
| 6 | Ah | 436 | VAL |
| 6 | Ah | 479 | ILE |
| 6 | Ah | 495 | ARG |
| 6 | Ai | 71 | ASP |
| 6 | Ai | 72 | HIS |
| 6 | Ai | 99 | VAL |
| 6 | Ai | 107 | ILE |
| 6 | Ai | 114 | VAL |
| 6 | Ai | 131 | TYR |
| 6 | Ai | 279 | ARG |
| 6 | Ai | 328 | LYS |
| 6 | Ai | 331 | VAL |
| 6 | Ai | 377 | ILE |
| 6 | Ai | 395 | TYR |
| 6 | Ai | 398 | GLN |
| 6 | Ai | 408 | THR |
| 6 | Ai | 436 | VAL |
| 6 | Ai | 439 | LYS |
| 6 | Aj | 72 | HIS |
| 6 | Aj | 101 | ARG |
| 6 | Aj | 107 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Aj | 110 | ASP |
| 6 | Aj | 117 | MET |
| 6 | Aj | 133 | LYS |
| 6 | Aj | 134 | ASP |
| 6 | Aj | 174 | VAL |
| 6 | Aj | 208 | LEU |
| 6 | Aj | 255 | ASP |
| 6 | Aj | 259 | ILE |
| 6 | Aj | 324 | THR |
| 6 | Aj | 331 | VAL |
| 6 | Aj | 345 | TRP |
| 6 | Aj | 395 | TYR |
| 6 | Aj | 421 | TYR |
| 6 | Ak | 106 | LEU |
| 6 | Ak | 109 | PHE |
| 6 | Ak | 110 | ASP |
| 6 | Ak | 170 | THR |
| 6 | Ak | 174 | VAL |
| 6 | Ak | 223 | GLU |
| 6 | Ak | 252 | PHE |
| 6 | Ak | 255 | ASP |
| 6 | Ak | 260 | GLU |
| 6 | Ak | 300 | LEU |
| 6 | Ak | 328 | LYS |
| 6 | Ak | 331 | VAL |
| 6 | Ak | 344 | ARG |
| 6 | Ak | 448 | ILE |
| 7 | Al | 12 | LEU |
| 7 | Al | 87 | ILE |
| 7 | Al | 92 | ILE |
| 7 | Al | 101 | ASN |
| 7 | Al | 106 | TRP |
| 7 | Al | 117 | ILE |
| 7 | Al | 127 | ARG |
| 7 | Al | 137 | ASP |
| 7 | Al | 138 | LEU |
| 7 | Al | 152 | GLN |
| 7 | Al | 192 | ILE |
| 7 | Al | 210 | GLN |
| 7 | Al | 215 | LEU |
| 7 | Al | 237 | VAL |
| 7 | Al | 238 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | Al | 258 | LEU |
| 7 | Al | 265 | ARG |
| 7 | Al | 266 | HIS |
| 7 | Al | 280 | GLN |
| 7 | Al | 297 | LEU |
| 7 | Al | 299 | LEU |
| 7 | Al | 304 | PHE |
| 6 | Am | 88 | VAL |
| 6 | Am | 95 | VAL |
| 6 | Am | 101 | ARG |
| 6 | Am | 106 | LEU |
| 6 | Am | 109 | PHE |
| 6 | Am | 131 | TYR |
| 6 | Am | 174 | VAL |
| 6 | Am | 249 | GLU |
| 6 | Am | 255 | ASP |
| 6 | Am | 265 | GLN |
| 6 | Am | 297 | GLU |
| 6 | Am | 331 | VAL |
| 6 | Am | 344 | ARG |
| 6 | Am | 406 | THR |
| 6 | Am | 448 | ILE |
| 6 | Am | 450 | TYR |
| 6 | Am | 490 | GLN |
| 6 | Am | 521 | ILE |
| 6 | An | 89 | THR |
| 6 | An | 106 | LEU |
| 6 | An | 131 | TYR |
| 6 | An | 136 | VAL |
| 6 | An | 185 | THR |
| 6 | An | 188 | VAL |
| 6 | An | 243 | THR |
| 6 | An | 279 | ARG |
| 6 | An | 331 | VAL |
| 6 | An | 376 | ILE |
| 6 | An | 377 | ILE |
| 6 | An | 395 | TYR |
| 6 | An | 432 | ASP |
| 6 | An | 435 | THR |
| 6 | An | 465 | LYS |
| 6 | An | 466 | ASN |
| 6 | An | 490 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | An | 516 | VAL |
| 6 | Ao | 88 | VAL |
| 6 | Ao | 90 | GLN |
| 6 | Ao | 105 | ASN |
| 6 | Ao | 124 | VAL |
| 6 | Ao | 131 | TYR |
| 6 | Ao | 142 | GLU |
| 6 | Ao | 174 | VAL |
| 6 | Ao | 185 | THR |
| 6 | Ao | 247 | TRP |
| 6 | Ao | 276 | GLN |
| 6 | Ao | 294 | LEU |
| 6 | Ao | 331 | VAL |
| 6 | Ao | 376 | ILE |
| 6 | Ao | 377 | ILE |
| 6 | Ao | 417 | LEU |
| 6 | Ao | 435 | THR |
| 6 | Ao | 436 | VAL |
| 6 | Ao | 463 | ASP |
| 6 | Ao | 486 | GLU |
| 6 | Ao | 507 | LEU |
| 6 | Ao | 516 | VAL |
| 6 | Ap | 88 | VAL |
| 6 | Ap | 95 | VAL |
| 6 | Ap | 114 | VAL |
| 6 | Ap | 131 | TYR |
| 6 | Ap | 185 | THR |
| 6 | Ap | 237 | GLU |
| 6 | Ap | 247 | TRP |
| 6 | Ap | 260 | GLU |
| 6 | Ap | 272 | ILE |
| 6 | Ap | 331 | VAL |
| 6 | Ap | 364 | ILE |
| 6 | Ap | 376 | ILE |
| 6 | Ap | 377 | ILE |
| 6 | Ap | 417 | LEU |
| 6 | Ap | 435 | THR |
| 6 | Ap | 443 | GLU |
| 6 | Ap | 444 | MET |
| 6 | Ap | 459 | LEU |
| 6 | Ap | 507 | LEU |
| 6 | Ap | 513 | PHE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Ap | 516 | VAL |
| 7 | Aq | 12 | LEU |
| 7 | Aq | 28 | GLU |
| 7 | Aq | 29 | LEU |
| 7 | Aq | 80 | ASN |
| 7 | Aq | 87 | ILE |
| 7 | Aq | 117 | ILE |
| 7 | Aq | 121 | MET |
| 7 | Aq | 125 | CYS |
| 7 | Aq | 127 | ARG |
| 7 | Aq | 141 | PHE |
| 7 | Aq | 148 | MET |
| 7 | Aq | 158 | ILE |
| 7 | Aq | 168 | GLU |
| 7 | Aq | 170 | LEU |
| 7 | Aq | 188 | THR |
| 7 | Aq | 189 | LYS |
| 7 | Aq | 192 | ILE |
| 7 | Aq | 215 | LEU |
| 7 | Aq | 237 | VAL |
| 7 | Aq | 238 | LYS |
| 7 | Aq | 252 | THR |
| 7 | Aq | 258 | LEU |
| 7 | Aq | 282 | LEU |
| 7 | Aq | 297 | LEU |
| 7 | Aq | 299 | LEU |
| 7 | Ar | 12 | LEU |
| 7 | Ar | 28 | GLU |
| 7 | Ar | 29 | LEU |
| 7 | Ar | 51 | ASP |
| 7 | Ar | 53 | LEU |
| 7 | Ar | 80 | ASN |
| 7 | Ar | 87 | ILE |
| 7 | Ar | 92 | ILE |
| 7 | Ar | 95 | ILE |
| 7 | Ar | 103 | THR |
| 7 | Ar | 108 | THR |
| 7 | Ar | 109 | ASP |
| 7 | Ar | 181 | LEU |
| 7 | Ar | 229 | ARG |
| 7 | Ar | 230 | VAL |
| 7 | Ar | 237 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | Ar | 258 | LEU |
| 7 | Ar | 265 | ARG |
| 7 | Ar | 297 | LEU |
| 7 | As | 12 | LEU |
| 7 | As | 17 | LEU |
| 7 | As | 28 | GLU |
| 7 | As | 33 | GLN |
| 7 | As | 36 | ASP |
| 7 | As | 51 | ASP |
| 7 | As | 66 | GLU |
| 7 | As | 80 | ASN |
| 7 | As | 109 | ASP |
| 7 | As | 118 | ASN |
| 7 | As | 127 | ARG |
| 7 | As | 129 | TYR |
| 7 | As | 134 | PHE |
| 7 | As | 138 | LEU |
| 7 | As | 148 | MET |
| 7 | As | 162 | TRP |
| 7 | As | 182 | ILE |
| 7 | As | 189 | LYS |
| 7 | As | 192 | ILE |
| 7 | As | 201 | THR |
| 7 | As | 207 | VAL |
| 7 | As | 231 | VAL |
| 7 | As | 234 | ASP |
| 7 | As | 258 | LEU |
| 7 | As | 298 | TYR |
| 7 | As | 299 | LEU |
| 7 | At | 12 | LEU |
| 7 | At | 24 | ILE |
| 7 | At | 28 | GLU |
| 7 | At | 32 | ASP |
| 7 | At | 33 | GLN |
| 7 | At | 40 | ARG |
| 7 | At | 47 | GLU |
| 7 | At | 51 | ASP |
| 7 | At | 66 | GLU |
| 7 | At | 80 | ASN |
| 7 | At | 107 | PHE |
| 7 | At | 108 | THR |
| 7 | At | 112 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | At | 118 | ASN |
| 7 | At | 121 | MET |
| 7 | At | 128 | PHE |
| 7 | At | 138 | LEU |
| 7 | At | 144 | LEU |
| 7 | At | 152 | GLN |
| 7 | At | 162 | TRP |
| 7 | At | 168 | GLU |
| 7 | At | 189 | LYS |
| 7 | At | 207 | VAL |
| 7 | At | 231 | VAL |
| 7 | At | 258 | LEU |
| 7 | At | 297 | LEU |
| 7 | At | 299 | LEU |
| 6 | Au | 71 | ASP |
| 6 | Au | 110 | ASP |
| 6 | Au | 117 | MET |
| 6 | Au | 124 | VAL |
| 6 | Au | 174 | VAL |
| 6 | Au | 187 | THR |
| 6 | Au | 257 | GLN |
| 6 | Au | 258 | VAL |
| 6 | Au | 289 | GLU |
| 6 | Au | 303 | ASN |
| 6 | Au | 316 | VAL |
| 6 | Au | 323 | LEU |
| 6 | Au | 389 | VAL |
| 6 | Au | 423 | VAL |
| 6 | Au | 432 | ASP |
| 6 | Au | 439 | LYS |
| 6 | Au | 448 | ILE |
| 6 | Au | 450 | TYR |
| 6 | Au | 459 | LEU |
| 6 | Au | 496 | ILE |
| 5 | Av | 28 | LEU |
| 5 | Av | 29 | VAL |
| 5 | Av | 31 | ILE |
| 5 | Av | 36 | LEU |
| 5 | Av | 45 | VAL |
| 5 | Av | 55 | ASN |
| 5 | Av | 58 | PHE |
| 5 | Av | 61 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | Av | 65 | TYR |
| 5 | Av | 69 | MET |
| 5 | Av | 70 | LYS |
| 5 | Av | 74 | GLU |
| 5 | Av | 85 | ASN |
| 5 | Av | 101 | VAL |
| 5 | Av | 108 | VAL |
| 5 | Av | 142 | LYS |
| 5 | Av | 165 | LYS |
| 5 | Av | 168 | LYS |
| 5 | Av | 174 | LEU |
| 5 | Av | 189 | ILE |
| 5 | Av | 190 | THR |
| 5 | Av | 191 | GLU |
| 5 | Av | 196 | THR |
| 5 | Av | 198 | ILE |
| 5 | Av | 209 | ASP |
| 5 | Av | 213 | GLU |
| 5 | Av | 223 | GLU |
| 5 | Av | 240 | SER |
| 5 | Av | 242 | LEU |
| 5 | Av | 248 | LYS |
| 5 | Av | 251 | ILE |
| 5 | Av | 263 | GLN |
| 5 | Av | 267 | LEU |
| 5 | Av | 308 | MET |
| 5 | Av | 310 | ASN |
| 5 | Av | 312 | VAL |
| 5 | Av | 318 | THR |
| 5 | Av | 320 | LYS |
| 5 | Av | 322 | LYS |
| 5 | Av | 332 | GLU |
| 5 | Av | 340 | ASP |
| 5 | Av | 359 | MET |
| 5 | Av | 374 | ARG |
| 5 | Av | 380 | ILE |
| 5 | Av | 382 | GLN |
| 5 | Av | 384 | GLN |
| 5 | Av | 397 | THR |
| 5 | Av | 398 | ARG |
| 5 | Av | 423 | LYS |
| 5 | Av | 441 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | Av | 445 | LYS |
| 5 | Av | 450 | ARG |
| 5 | Av | 451 | ASP |
| 5 | Av | 462 | ILE |
| 5 | Av | 483 | HIS |
| 5 | Av | 488 | LYS |
| 5 | Av | 495 | ASP |
| 5 | Av | 499 | GLU |
| 5 | Av | 503 | LYS |
| 5 | Av | 506 | GLU |
| 6 | Aw | 67 | GLU |
| 6 | Aw | 68 | ILE |
| 6 | Aw | 84 | THR |
| 6 | Aw | 95 | VAL |
| 6 | Aw | 106 | LEU |
| 6 | Aw | 107 | ILE |
| 6 | Aw | 114 | VAL |
| 6 | Aw | 124 | VAL |
| 6 | Aw | 131 | TYR |
| 6 | Aw | 136 | VAL |
| 6 | Aw | 145 | HIS |
| 6 | Aw | 183 | GLN |
| 6 | Aw | 234 | GLU |
| 6 | Aw | 243 | THR |
| 6 | Aw | 257 | GLN |
| 6 | Aw | 260 | GLU |
| 6 | Aw | 344 | ARG |
| 6 | Aw | 389 | VAL |
| 6 | Aw | 398 | GLN |
| 6 | Aw | 430 | LYS |
| 6 | Aw | 436 | VAL |
| 6 | Aw | 448 | ILE |
| 6 | Aw | 459 | LEU |
| 6 | Aw | 470 | VAL |
| 6 | Aw | 503 | ILE |
| 5 | Ax | 5 | VAL |
| 5 | Ax | 28 | LEU |
| 5 | Ax | 62 | PHE |
| 5 | Ax | 72 | THR |
| 5 | Ax | 85 | ASN |
| 5 | Ax | 94 | GLU |
| 5 | Ax | 101 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | Ax | 103 | GLU |
| 5 | Ax | 104 | ASP |
| 5 | Ax | 107 | GLU |
| 5 | Ax | 121 | LYS |
| 5 | Ax | 166 | ARG |
| 5 | Ax | 181 | GLN |
| 5 | Ax | 189 | ILE |
| 5 | Ax | 204 | GLU |
| 5 | Ax | 205 | TYR |
| 5 | Ax | 207 | ILE |
| 5 | Ax | 209 | ASP |
| 5 | Ax | 213 | GLU |
| 5 | Ax | 228 | ILE |
| 5 | Ax | 267 | LEU |
| 5 | Ax | 291 | ASN |
| 5 | Ax | 309 | LYS |
| 5 | Ax | 310 | ASN |
| 5 | Ax | 340 | ASP |
| 5 | Ax | 342 | LYS |
| 5 | Ax | 359 | MET |
| 5 | Ax | 374 | ARG |
| 5 | Ax | 379 | ARG |
| 5 | Ax | 380 | ILE |
| 5 | Ax | 382 | GLN |
| 5 | Ax | 384 | GLN |
| 5 | Ax | 390 | PHE |
| 5 | Ax | 397 | THR |
| 5 | Ax | 401 | LEU |
| 5 | Ax | 405 | LYS |
| 5 | Ax | 410 | LEU |
| 5 | Ax | 432 | ILE |
| 5 | Ax | 441 | ILE |
| 5 | Ax | 442 | ASN |
| 5 | Ax | 444 | ILE |
| 5 | Ax | 456 | GLU |
| 5 | Ax | 459 | GLU |
| 5 | Ax | 462 | ILE |
| 5 | Ax | 479 | LYS |
| 5 | Ax | 488 | LYS |
| 5 | Ax | 496 | GLU |
| 6 | Ay | 67 | GLU |
| 6 | Ay | 84 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Ay | 88 | VAL |
| 6 | Ay | 95 | VAL |
| 6 | Ay | 107 | ILE |
| 6 | Ay | 112 | CYS |
| 6 | Ay | 114 | VAL |
| 6 | Ay | 136 | VAL |
| 6 | Ay | 187 | THR |
| 6 | Ay | 235 | LEU |
| 6 | Ay | 237 | GLU |
| 6 | Ay | 243 | THR |
| 6 | Ay | 257 | GLN |
| 6 | Ay | 264 | ARG |
| 6 | Ay | 278 | LEU |
| 6 | Ay | 322 | THR |
| 6 | Ay | 376 | ILE |
| 6 | Ay | 377 | ILE |
| 6 | Ay | 389 | VAL |
| 6 | Ay | 432 | ASP |
| 6 | Ay | 436 | VAL |
| 6 | Ay | 444 | MET |
| 6 | Ay | 448 | ILE |
| 6 | Ay | 482 | ASN |
| 6 | Ay | 486 | GLU |
| 6 | Ay | 496 | ILE |
| 6 | Ay | 500 | MET |
| 6 | Ay | 503 | ILE |
| 6 | Ay | 518 | VAL |
| 6 | Az | 95 | VAL |
| 6 | Az | 111 | ILE |
| 6 | Az | 130 | VAL |
| 6 | Az | 131 | TYR |
| 6 | Az | 147 | MET |
| 6 | Az | 208 | LEU |
| 6 | Az | 234 | GLU |
| 6 | Az | 259 | ILE |
| 6 | Az | 278 | LEU |
| 6 | Az | 289 | GLU |
| 6 | Az | 324 | THR |
| 6 | Az | 331 | VAL |
| 6 | Az | 360 | GLU |
| 6 | Az | 380 | ARG |
| 6 | Az | 395 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Az | 416 | VAL |
| 6 | Az | 430 | LYS |
| 6 | Az | 432 | ASP |
| 6 | Az | 436 | VAL |
| 6 | Az | 450 | TYR |
| 6 | Az | 479 | ILE |
| 6 | Az | 516 | VAL |
| 6 | Az | 518 | VAL |
| 2 | B1 | 14 | THR |
| 2 | B1 | 32 | LYS |
| 2 | B1 | 42 | LYS |
| 2 | B1 | 47 | GLU |
| 2 | B1 | 50 | LEU |
| 2 | B1 | 66 | MET |
| 2 | B1 | 85 | ASP |
| 2 | B1 | 109 | ASN |
| 2 | B1 | 112 | VAL |
| 2 | B1 | 124 | ASP |
| 2 | B1 | 130 | LYS |
| 2 | B1 | 139 | LYS |
| 2 | B1 | 149 | LYS |
| 2 | B1 | 166 | ASN |
| 2 | B1 | 186 | LYS |
| 2 | B1 | 188 | ILE |
| 2 | B1 | 197 | GLU |
| 2 | B1 | 199 | GLU |
| 2 | B1 | 215 | LYS |
| 2 | B1 | 219 | ILE |
| 2 | B1 | 252 | LEU |
| 2 | B1 | 271 | TYR |
| 2 | B1 | 290 | VAL |
| 2 | B1 | 298 | LYS |
| 2 | B1 | 299 | ARG |
| 2 | B1 | 303 | ASP |
| 2 | B1 | 313 | ASP |
| 2 | B1 | 344 | LEU |
| 2 | B1 | 366 | GLU |
| 2 | B1 | 385 | THR |
| 2 | B1 | 398 | ASP |
| 2 | B1 | 404 | LEU |
| 2 | B1 | 412 | GLU |
| 2 | B1 | 415 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B1 | 417 | ILE |
| 2 | B1 | 437 | THR |
| 2 | B1 | 443 | ILE |
| 2 | B1 | 453 | ASN |
| 2 | B1 | 456 | TYR |
| 2 | B1 | 484 | VAL |
| 2 | B1 | 495 | ASN |
| 2 | B1 | 536 | TYR |
| 2 | B1 | 542 | THR |
| 2 | B1 | 550 | ARG |
| 2 | B1 | 552 | ASN |
| 2 | B1 | 569 | LYS |
| 2 | B1 | 606 | VAL |
| 2 | B1 | 612 | ASN |
| 2 | B1 | 617 | VAL |
| 2 | B1 | 629 | ILE |
| 2 | B1 | 633 | ARG |
| 2 | B1 | 636 | ASN |
| 2 | B2 | 8 | ILE |
| 2 | B2 | 14 | THR |
| 2 | B2 | 24 | THR |
| 2 | B2 | 32 | LYS |
| 2 | B2 | 47 | GLU |
| 2 | B2 | 49 | ASP |
| 2 | B2 | 66 | MET |
| 2 | B2 | 81 | VAL |
| 2 | B2 | 130 | LYS |
| 2 | B2 | 139 | LYS |
| 2 | B2 | 149 | LYS |
| 2 | B2 | 151 | ILE |
| 2 | B2 | 182 | ILE |
| 2 | B2 | 195 | LEU |
| 2 | B2 | 202 | GLU |
| 2 | B2 | 209 | ASP |
| 2 | B2 | 219 | ILE |
| 2 | B2 | 271 | TYR |
| 2 | B2 | 298 | LYS |
| 2 | B2 | 303 | ASP |
| 2 | B2 | 383 | LEU |
| 2 | B2 | 390 | GLN |
| 2 | B2 | 398 | ASP |
| 2 | B2 | 404 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B2 | 415 | VAL |
| 2 | B2 | 417 | ILE |
| 2 | B2 | 430 | ARG |
| 2 | B2 | 441 | PHE |
| 2 | B2 | 467 | TRP |
| 2 | B2 | 470 | LEU |
| 2 | B2 | 477 | LEU |
| 2 | B2 | 503 | ILE |
| 2 | B2 | 519 | GLN |
| 2 | B2 | 536 | TYR |
| 2 | B2 | 540 | THR |
| 2 | B2 | 553 | VAL |
| 2 | B2 | 586 | THR |
| 2 | B2 | 606 | VAL |
| 2 | B2 | 617 | VAL |
| 2 | B2 | 629 | ILE |
| 2 | B2 | 643 | VAL |
| 2 | B2 | 650 | ASP |
| 2 | B2 | 655 | THR |
| 2 | B3 | 14 | THR |
| 2 | B3 | 24 | THR |
| 2 | B3 | 32 | LYS |
| 2 | B3 | 41 | ILE |
| 2 | B3 | 42 | LYS |
| 2 | B3 | 49 | ASP |
| 2 | B3 | 66 | MET |
| 2 | B3 | 72 | LEU |
| 2 | B3 | 85 | ASP |
| 2 | B3 | 91 | ASN |
| 2 | B3 | 112 | VAL |
| 2 | B3 | 115 | LYS |
| 2 | B3 | 119 | LYS |
| 2 | B3 | 130 | LYS |
| 2 | B3 | 139 | LYS |
| 2 | B3 | 141 | LYS |
| 2 | B3 | 149 | LYS |
| 2 | B3 | 166 | ASN |
| 2 | B3 | 171 | ILE |
| 2 | B3 | 183 | THR |
| 2 | B3 | 195 | LEU |
| 2 | B3 | 202 | GLU |
| 2 | B3 | 215 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B3 | 219 | ILE |
| 2 | B3 | 239 | VAL |
| 2 | B3 | 271 | TYR |
| 2 | B3 | 298 | LYS |
| 2 | B3 | 302 | LYS |
| 2 | B3 | 303 | ASP |
| 2 | B3 | 417 | ILE |
| 2 | B3 | 430 | ARG |
| 2 | B3 | 431 | THR |
| 2 | B3 | 456 | TYR |
| 2 | B3 | 503 | ILE |
| 2 | B3 | 505 | LEU |
| 2 | B3 | 534 | VAL |
| 2 | B3 | 535 | LEU |
| 2 | B3 | 536 | TYR |
| 2 | B3 | 539 | LYS |
| 2 | B3 | 540 | THR |
| 2 | B3 | 542 | THR |
| 2 | B3 | 550 | ARG |
| 2 | B3 | 572 | LEU |
| 2 | B3 | 590 | GLN |
| 2 | B3 | 602 | TYR |
| 2 | B3 | 606 | VAL |
| 2 | B3 | 629 | ILE |
| 2 | B3 | 650 | ASP |
| 2 | B3 | 651 | PHE |
| 2 | B3 | 655 | THR |
| 2 | B4 | 14 | THR |
| 2 | B4 | 32 | LYS |
| 2 | B4 | 42 | LYS |
| 2 | B4 | 47 | GLU |
| 2 | B4 | 66 | MET |
| 2 | B4 | 76 | ASN |
| 2 | B4 | 81 | VAL |
| 2 | B4 | 88 | THR |
| 2 | B4 | 115 | LYS |
| 2 | B4 | 130 | LYS |
| 2 | B4 | 133 | GLU |
| 2 | B4 | 139 | LYS |
| 2 | B4 | 149 | LYS |
| 2 | B4 | 186 | LYS |
| 2 | B4 | 189 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B4 | 202 | GLU |
| 2 | B4 | 205 | MET |
| 2 | B4 | 219 | ILE |
| 2 | B4 | 252 | LEU |
| 2 | B4 | 268 | VAL |
| 2 | B4 | 290 | VAL |
| 2 | B4 | 298 | LYS |
| 2 | B4 | 302 | LYS |
| 2 | B4 | 303 | ASP |
| 2 | B4 | 312 | ASP |
| 2 | B4 | 344 | LEU |
| 2 | B4 | 417 | ILE |
| 2 | B4 | 426 | LEU |
| 2 | B4 | 430 | ARG |
| 2 | B4 | 455 | LYS |
| 2 | B4 | 456 | TYR |
| 2 | B4 | 482 | ASP |
| 2 | B4 | 484 | VAL |
| 2 | B4 | 503 | ILE |
| 2 | B4 | 505 | LEU |
| 2 | B4 | 535 | LEU |
| 2 | B4 | 536 | TYR |
| 2 | B4 | 538 | ASP |
| 2 | B4 | 542 | THR |
| 2 | B4 | 550 | ARG |
| 2 | B4 | 570 | TYR |
| 2 | B4 | 606 | VAL |
| 2 | B4 | 617 | VAL |
| 2 | B4 | 629 | ILE |
| 2 | B4 | 654 | LEU |
| 2 | B5 | 14 | THR |
| 2 | B5 | 32 | LYS |
| 2 | B5 | 66 | MET |
| 2 | B5 | 72 | LEU |
| 2 | B5 | 81 | VAL |
| 2 | B5 | 88 | THR |
| 2 | B5 | 112 | VAL |
| 2 | B5 | 130 | LYS |
| 2 | B5 | 139 | LYS |
| 2 | B5 | 143 | ILE |
| 2 | B5 | 149 | LYS |
| 2 | B5 | 151 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B5 | 195 | LEU |
| 2 | B5 | 199 | GLU |
| 2 | B5 | 202 | GLU |
| 2 | B5 | 205 | MET |
| 2 | B5 | 219 | ILE |
| 2 | B5 | 298 | LYS |
| 2 | B5 | 303 | ASP |
| 2 | B5 | 317 | LYS |
| 2 | B5 | 326 | THR |
| 2 | B5 | 383 | LEU |
| 2 | B5 | 398 | ASP |
| 2 | B5 | 404 | LEU |
| 2 | B5 | 411 | ARG |
| 2 | B5 | 417 | ILE |
| 2 | B5 | 430 | ARG |
| 2 | B5 | 453 | ASN |
| 2 | B5 | 460 | LYS |
| 2 | B5 | 499 | ILE |
| 2 | B5 | 503 | ILE |
| 2 | B5 | 535 | LEU |
| 2 | B5 | 536 | TYR |
| 2 | B5 | 540 | THR |
| 2 | B5 | 542 | THR |
| 2 | B5 | 550 | ARG |
| 2 | B5 | 556 | LEU |
| 2 | B5 | 560 | LEU |
| 2 | B5 | 572 | LEU |
| 2 | B5 | 574 | GLU |
| 2 | B5 | 606 | VAL |
| 2 | B5 | 617 | VAL |
| 2 | B5 | 629 | ILE |
| 2 | B5 | 633 | ARG |
| 2 | B6 | 14 | THR |
| 2 | B6 | 32 | LYS |
| 2 | B6 | 66 | MET |
| 2 | B6 | 76 | ASN |
| 2 | B6 | 130 | LYS |
| 2 | B6 | 149 | LYS |
| 2 | B6 | 151 | ILE |
| 2 | B6 | 166 | ASN |
| 2 | B6 | 171 | ILE |
| 2 | B6 | 186 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B6 | 188 | ILE |
| 2 | B6 | 194 | LEU |
| 2 | B6 | 195 | LEU |
| 2 | B6 | 199 | GLU |
| 2 | B6 | 205 | MET |
| 2 | B6 | 219 | ILE |
| 2 | B6 | 229 | GLU |
| 2 | B6 | 230 | LEU |
| 2 | B6 | 260 | THR |
| 2 | B6 | 290 | VAL |
| 2 | B6 | 298 | LYS |
| 2 | B6 | 303 | ASP |
| 2 | B6 | 344 | LEU |
| 2 | B6 | 370 | VAL |
| 2 | B6 | 371 | GLN |
| 2 | B6 | 385 | THR |
| 2 | B6 | 404 | LEU |
| 2 | B6 | 417 | ILE |
| 2 | B6 | 450 | ILE |
| 2 | B6 | 453 | ASN |
| 2 | B6 | 455 | LYS |
| 2 | B6 | 467 | TRP |
| 2 | B6 | 483 | ASN |
| 2 | B6 | 484 | VAL |
| 2 | B6 | 496 | ARG |
| 2 | B6 | 518 | TYR |
| 2 | B6 | 523 | ASN |
| 2 | B6 | 535 | LEU |
| 2 | B6 | 536 | TYR |
| 2 | B6 | 553 | VAL |
| 2 | B6 | 556 | LEU |
| 2 | B6 | 574 | GLU |
| 2 | B6 | 575 | LEU |
| 2 | B6 | 606 | VAL |
| 2 | B6 | 621 | ASN |
| 2 | B6 | 629 | ILE |
| 2 | B6 | 650 | ASP |
| 2 | B6 | 655 | THR |
| 2 | B7 | 10 | LEU |
| 2 | B7 | 32 | LYS |
| 2 | B7 | 49 | ASP |
| 2 | B7 | 60 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B7 | 66 | MET |
| 2 | B7 | 130 | LYS |
| 2 | B7 | 131 | ILE |
| 2 | B7 | 139 | LYS |
| 2 | B7 | 149 | LYS |
| 2 | B7 | 170 | GLU |
| 2 | B7 | 178 | LEU |
| 2 | B7 | 186 | LYS |
| 2 | B7 | 202 | GLU |
| 2 | B7 | 219 | ILE |
| 2 | B7 | 239 | VAL |
| 2 | B7 | 271 | TYR |
| 2 | B7 | 290 | VAL |
| 2 | B7 | 297 | THR |
| 2 | B7 | 298 | LYS |
| 2 | B7 | 302 | LYS |
| 2 | B7 | 303 | ASP |
| 2 | B7 | 340 | LEU |
| 2 | B7 | 365 | ARG |
| 2 | B7 | 383 | LEU |
| 2 | B7 | 398 | ASP |
| 2 | B7 | 404 | LEU |
| 2 | B7 | 415 | VAL |
| 2 | B7 | 417 | ILE |
| 2 | B7 | 426 | LEU |
| 2 | B7 | 439 | ASN |
| 2 | B7 | 453 | ASN |
| 2 | B7 | 461 | TYR |
| 2 | B7 | 484 | VAL |
| 2 | B7 | 518 | TYR |
| 2 | B7 | 523 | ASN |
| 2 | B7 | 535 | LEU |
| 2 | B7 | 536 | TYR |
| 2 | B7 | 538 | ASP |
| 2 | B7 | 540 | THR |
| 2 | B7 | 542 | THR |
| 2 | B7 | 552 | ASN |
| 2 | B7 | 556 | LEU |
| 2 | B7 | 569 | LYS |
| 2 | B7 | 605 | ARG |
| 2 | B7 | 621 | ASN |
| 2 | B7 | 653 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B7 | 654 | LEU |
| 5 | BA | 6 | LEU |
| 5 | BA | 21 | LYS |
| 5 | BA | 28 | LEU |
| 5 | BA | 29 | VAL |
| 5 | BA | 31 | ILE |
| 5 | BA | 36 | LEU |
| 5 | BA | 65 | TYR |
| 5 | BA | 69 | MET |
| 5 | BA | 70 | LYS |
| 5 | BA | 89 | ASP |
| 5 | BA | 134 | LEU |
| 5 | BA | 165 | LYS |
| 5 | BA | 168 | LYS |
| 5 | BA | 172 | LYS |
| 5 | BA | 189 | ILE |
| 5 | BA | 191 | GLU |
| 5 | BA | 199 | VAL |
| 5 | BA | 200 | LYS |
| 5 | BA | 207 | ILE |
| 5 | BA | 209 | ASP |
| 5 | BA | 212 | HIS |
| 5 | BA | 226 | THR |
| 5 | BA | 232 | LYS |
| 5 | BA | 242 | LEU |
| 5 | BA | 249 | ASN |
| 5 | BA | 267 | LEU |
| 5 | BA | 291 | ASN |
| 5 | BA | 301 | MET |
| 5 | BA | 308 | MET |
| 5 | BA | 312 | VAL |
| 5 | BA | 313 | VAL |
| 5 | BA | 320 | LYS |
| 5 | BA | 340 | ASP |
| 5 | BA | 347 | VAL |
| 5 | BA | 359 | MET |
| 5 | BA | 380 | ILE |
| 5 | BA | 382 | GLN |
| 5 | BA | 397 | THR |
| 5 | BA | 401 | LEU |
| 5 | BA | 423 | LYS |
| 5 | BA | 441 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BA | 454 | PHE |
| 5 | BA | 462 | ILE |
| 5 | BA | 477 | ILE |
| 5 | BA | 487 | MET |
| 5 | BA | 499 | GLU |
| 5 | BA | 505 | ILE |
| 5 | BB | 6 | LEU |
| 5 | BB | 31 | ILE |
| 5 | BB | 43 | PHE |
| 5 | BB | 49 | GLU |
| 5 | BB | 69 | MET |
| 5 | BB | 85 | ASN |
| 5 | BB | 106 | THR |
| 5 | BB | 107 | GLU |
| 5 | BB | 115 | LYS |
| 5 | BB | 166 | ARG |
| 5 | BB | 168 | LYS |
| 5 | BB | 171 | ILE |
| 5 | BB | 174 | LEU |
| 5 | BB | 185 | VAL |
| 5 | BB | 187 | GLU |
| 5 | BB | 204 | GLU |
| 5 | BB | 223 | GLU |
| 5 | BB | 226 | THR |
| 5 | BB | 228 | ILE |
| 5 | BB | 229 | LYS |
| 5 | BB | 243 | VAL |
| 5 | BB | 245 | CYS |
| 5 | BB | 263 | GLN |
| 5 | BB | 267 | LEU |
| 5 | BB | 276 | ILE |
| 5 | BB | 308 | MET |
| 5 | BB | 310 | ASN |
| 5 | BB | 321 | ILE |
| 5 | BB | 342 | LYS |
| 5 | BB | 359 | MET |
| 5 | BB | 380 | ILE |
| 5 | BB | 396 | ILE |
| 5 | BB | 398 | ARG |
| 5 | BB | 410 | LEU |
| 5 | BB | 413 | LYS |
| 5 | BB | 428 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BB | 432 | ILE |
| 5 | BB | 470 | LEU |
| 5 | BB | 479 | LYS |
| 5 | BB | 485 | THR |
| 5 | BB | 496 | GLU |
| 5 | BB | 504 | GLN |
| 7 | BC | 12 | LEU |
| 7 | BC | 28 | GLU |
| 7 | BC | 43 | GLU |
| 7 | BC | 53 | LEU |
| 7 | BC | 54 | ASN |
| 7 | BC | 64 | ASP |
| 7 | BC | 81 | VAL |
| 7 | BC | 87 | ILE |
| 7 | BC | 92 | ILE |
| 7 | BC | 114 | MET |
| 7 | BC | 126 | ASN |
| 7 | BC | 144 | LEU |
| 7 | BC | 168 | GLU |
| 7 | BC | 188 | THR |
| 7 | BC | 192 | ILE |
| 7 | BC | 193 | ASP |
| 7 | BC | 206 | THR |
| 7 | BC | 210 | GLN |
| 7 | BC | 229 | ARG |
| 7 | BC | 238 | LYS |
| 7 | BC | 258 | LEU |
| 7 | BC | 282 | LEU |
| 7 | BC | 297 | LEU |
| 7 | BC | 299 | LEU |
| 5 | BD | 6 | LEU |
| 5 | BD | 9 | PHE |
| 5 | BD | 15 | MET |
| 5 | BD | 24 | GLU |
| 5 | BD | 28 | LEU |
| 5 | BD | 31 | ILE |
| 5 | BD | 35 | LYS |
| 5 | BD | 41 | ARG |
| 5 | BD | 42 | GLU |
| 5 | BD | 54 | TYR |
| 5 | BD | 85 | ASN |
| 5 | BD | 87 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BD | 101 | VAL |
| 5 | BD | 103 | GLU |
| 5 | BD | 108 | VAL |
| 5 | BD | 121 | LYS |
| 5 | BD | 124 | ASN |
| 5 | BD | 134 | LEU |
| 5 | BD | 142 | LYS |
| 5 | BD | 165 | LYS |
| 5 | BD | 166 | ARG |
| 5 | BD | 169 | GLU |
| 5 | BD | 171 | ILE |
| 5 | BD | 181 | GLN |
| 5 | BD | 182 | VAL |
| 5 | BD | 185 | VAL |
| 5 | BD | 205 | TYR |
| 5 | BD | 226 | THR |
| 5 | BD | 228 | ILE |
| 5 | BD | 229 | LYS |
| 5 | BD | 239 | HIS |
| 5 | BD | 248 | LYS |
| 5 | BD | 267 | LEU |
| 5 | BD | 291 | ASN |
| 5 | BD | 306 | ASN |
| 5 | BD | 310 | ASN |
| 5 | BD | 312 | VAL |
| 5 | BD | 313 | VAL |
| 5 | BD | 327 | ASN |
| 5 | BD | 330 | MET |
| 5 | BD | 332 | GLU |
| 5 | BD | 342 | LYS |
| 5 | BD | 347 | VAL |
| 5 | BD | 380 | ILE |
| 5 | BD | 384 | GLN |
| 5 | BD | 388 | VAL |
| 5 | BD | 398 | ARG |
| 5 | BD | 401 | LEU |
| 5 | BD | 409 | GLU |
| 5 | BD | 423 | LYS |
| 5 | BD | 433 | THR |
| 5 | BD | 434 | GLU |
| 5 | BD | 441 | ILE |
| 5 | BD | 444 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BD | 445 | LYS |
| 5 | BD | 459 | GLU |
| 5 | BD | 462 | ILE |
| 5 | BD | 477 | ILE |
| 5 | BD | 479 | LYS |
| 5 | BD | 487 | MET |
| 5 | BD | 497 | GLU |
| 5 | BD | 499 | GLU |
| 5 | BD | 510 | LYS |
| 7 | BE | 12 | LEU |
| 7 | BE | 28 | GLU |
| 7 | BE | 29 | LEU |
| 7 | BE | 33 | GLN |
| 7 | BE | 36 | ASP |
| 7 | BE | 51 | ASP |
| 7 | BE | 66 | GLU |
| 7 | BE | 87 | ILE |
| 7 | BE | 90 | THR |
| 7 | BE | 92 | ILE |
| 7 | BE | 148 | MET |
| 7 | BE | 162 | TRP |
| 7 | BE | 177 | GLN |
| 7 | BE | 189 | LYS |
| 7 | BE | 192 | ILE |
| 7 | BE | 207 | VAL |
| 7 | BE | 237 | VAL |
| 7 | BE | 258 | LEU |
| 7 | BE | 280 | GLN |
| 7 | BE | 297 | LEU |
| 7 | BE | 299 | LEU |
| 5 | BF | 14 | LYS |
| 5 | BF | 28 | LEU |
| 5 | BF | 29 | VAL |
| 5 | BF | 42 | GLU |
| 5 | BF | 60 | THR |
| 5 | BF | 70 | LYS |
| 5 | BF | 72 | THR |
| 5 | BF | 89 | ASP |
| 5 | BF | 101 | VAL |
| 5 | BF | 107 | GLU |
| 5 | BF | 108 | VAL |
| 5 | BF | 121 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BF | 171 | ILE |
| 5 | BF | 181 | GLN |
| 5 | BF | 182 | VAL |
| 5 | BF | 185 | VAL |
| 5 | BF | 189 | ILE |
| 5 | BF | 205 | TYR |
| 5 | BF | 212 | HIS |
| 5 | BF | 213 | GLU |
| 5 | BF | 227 | LYS |
| 5 | BF | 229 | LYS |
| 5 | BF | 242 | LEU |
| 5 | BF | 243 | VAL |
| 5 | BF | 251 | ILE |
| 5 | BF | 267 | LEU |
| 5 | BF | 310 | ASN |
| 5 | BF | 313 | VAL |
| 5 | BF | 320 | LYS |
| 5 | BF | 321 | ILE |
| 5 | BF | 342 | LYS |
| 5 | BF | 347 | VAL |
| 5 | BF | 349 | THR |
| 5 | BF | 359 | MET |
| 5 | BF | 375 | VAL |
| 5 | BF | 379 | ARG |
| 5 | BF | 383 | ASP |
| 5 | BF | 394 | THR |
| 5 | BF | 401 | LEU |
| 5 | BF | 409 | GLU |
| 5 | BF | 423 | LYS |
| 5 | BF | 432 | ILE |
| 5 | BF | 441 | ILE |
| 5 | BF | 444 | ILE |
| 5 | BF | 445 | LYS |
| 5 | BF | 457 | LEU |
| 5 | BF | 462 | ILE |
| 5 | BF | 479 | LYS |
| 5 | BG | 14 | LYS |
| 5 | BG | 28 | LEU |
| 5 | BG | 29 | VAL |
| 5 | BG | 60 | THR |
| 5 | BG | 65 | TYR |
| 5 | BG | 101 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BG | 108 | VAL |
| 5 | BG | 121 | LYS |
| 5 | BG | 134 | LEU |
| 5 | BG | 156 | ILE |
| 5 | BG | 166 | ARG |
| 5 | BG | 171 | ILE |
| 5 | BG | 189 | ILE |
| 5 | BG | 190 | THR |
| 5 | BG | 207 | ILE |
| 5 | BG | 210 | THR |
| 5 | BG | 212 | HIS |
| 5 | BG | 228 | ILE |
| 5 | BG | 229 | LYS |
| 5 | BG | 248 | LYS |
| 5 | BG | 249 | ASN |
| 5 | BG | 256 | ARG |
| 5 | BG | 259 | LYS |
| 5 | BG | 267 | LEU |
| 5 | BG | 291 | ASN |
| 5 | BG | 310 | ASN |
| 5 | BG | 320 | LYS |
| 5 | BG | 321 | ILE |
| 5 | BG | 340 | ASP |
| 5 | BG | 342 | LYS |
| 5 | BG | 359 | MET |
| 5 | BG | 380 | ILE |
| 5 | BG | 384 | GLN |
| 5 | BG | 390 | PHE |
| 5 | BG | 397 | THR |
| 5 | BG | 401 | LEU |
| 5 | BG | 409 | GLU |
| 5 | BG | 413 | LYS |
| 5 | BG | 432 | ILE |
| 5 | BG | 433 | THR |
| 5 | BG | 441 | ILE |
| 5 | BG | 444 | ILE |
| 5 | BG | 445 | LYS |
| 5 | BG | 454 | PHE |
| 5 | BG | 457 | LEU |
| 5 | BG | 462 | ILE |
| 5 | BG | 470 | LEU |
| 5 | BG | 487 | MET |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BG | 495 | ASP |
| 5 | BG | 496 | GLU |
| 5 | BG | 497 | GLU |
| 5 | BH | 6 | LEU |
| 5 | BH | 8 | LEU |
| 5 | BH | 14 | LYS |
| 5 | BH | 18 | ARG |
| 5 | BH | 28 | LEU |
| 5 | BH | 41 | ARG |
| 5 | BH | 42 | GLU |
| 5 | BH | 54 | TYR |
| 5 | BH | 60 | THR |
| 5 | BH | 66 | GLU |
| 5 | BH | 69 | MET |
| 5 | BH | 81 | ASN |
| 5 | BH | 87 | GLU |
| 5 | BH | 101 | VAL |
| 5 | BH | 107 | GLU |
| 5 | BH | 109 | VAL |
| 5 | BH | 117 | LYS |
| 5 | BH | 134 | LEU |
| 5 | BH | 153 | ASP |
| 5 | BH | 166 | ARG |
| 5 | BH | 171 | ILE |
| 5 | BH | 181 | GLN |
| 5 | BH | 185 | VAL |
| 5 | BH | 189 | ILE |
| 5 | BH | 199 | VAL |
| 5 | BH | 204 | GLU |
| 5 | BH | 226 | THR |
| 5 | BH | 229 | LYS |
| 5 | BH | 250 | ILE |
| 5 | BH | 256 | ARG |
| 5 | BH | 267 | LEU |
| 5 | BH | 288 | ASP |
| 5 | BH | 291 | ASN |
| 5 | BH | 310 | ASN |
| 5 | BH | 321 | ILE |
| 5 | BH | 342 | LYS |
| 5 | BH | 379 | ARG |
| 5 | BH | 397 | THR |
| 5 | BH | 398 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BH | 401 | LEU |
| 5 | BH | 405 | LYS |
| 5 | BH | 433 | THR |
| 5 | BH | 434 | GLU |
| 5 | BH | 441 | ILE |
| 5 | BH | 457 | LEU |
| 5 | BH | 459 | GLU |
| 5 | BH | 462 | ILE |
| 5 | BH | 470 | LEU |
| 5 | BH | 479 | LYS |
| 5 | BH | 497 | GLU |
| 5 | BH | 499 | GLU |
| 5 | BH | 501 | GLU |
| 5 | BH | 503 | LYS |
| 6 | BI | 95 | VAL |
| 6 | BI | 107 | ILE |
| 6 | BI | 110 | ASP |
| 6 | BI | 134 | ASP |
| 6 | BI | 174 | VAL |
| 6 | BI | 208 | LEU |
| 6 | BI | 237 | GLU |
| 6 | BI | 249 | GLU |
| 6 | BI | 273 | GLU |
| 6 | BI | 324 | THR |
| 6 | BI | 331 | VAL |
| 6 | BI | 393 | ILE |
| 6 | BI | 398 | GLN |
| 6 | BI | 406 | THR |
| 6 | BI | 448 | ILE |
| 6 | BI | 449 | TYR |
| 6 | BI | 450 | TYR |
| 6 | BI | 471 | MET |
| 6 | BI | 496 | ILE |
| 6 | BJ | 89 | THR |
| 6 | BJ | 95 | VAL |
| 6 | BJ | 99 | VAL |
| 6 | BJ | 106 | LEU |
| 6 | BJ | 118 | ASN |
| 6 | BJ | 124 | VAL |
| 6 | BJ | 131 | TYR |
| 6 | BJ | 162 | LYS |
| 6 | BJ | 185 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | BJ | 187 | THR |
| 6 | BJ | 188 | VAL |
| 6 | BJ | 247 | TRP |
| 6 | BJ | 273 | GLU |
| 6 | BJ | 282 | HIS |
| 6 | BJ | 331 | VAL |
| 6 | BJ | 356 | GLN |
| 6 | BJ | 376 | ILE |
| 6 | BJ | 377 | ILE |
| 6 | BJ | 417 | LEU |
| 6 | BJ | 435 | THR |
| 6 | BJ | 444 | MET |
| 6 | BJ | 516 | VAL |
| 6 | BK | 107 | ILE |
| 6 | BK | 110 | ASP |
| 6 | BK | 124 | VAL |
| 6 | BK | 174 | VAL |
| 6 | BK | 185 | THR |
| 6 | BK | 254 | ILE |
| 6 | BK | 255 | ASP |
| 6 | BK | 278 | LEU |
| 6 | BK | 289 | GLU |
| 6 | BK | 303 | ASN |
| 6 | BK | 316 | VAL |
| 6 | BK | 432 | ASP |
| 6 | BK | 436 | VAL |
| 6 | BK | 445 | ASP |
| 6 | BK | 450 | TYR |
| 6 | BK | 504 | LEU |
| 7 | BL | 12 | LEU |
| 7 | BL | 32 | ASP |
| 7 | BL | 53 | LEU |
| 7 | BL | 87 | ILE |
| 7 | BL | 92 | ILE |
| 7 | BL | 95 | ILE |
| 7 | BL | 101 | ASN |
| 7 | BL | 103 | THR |
| 7 | BL | 112 | LEU |
| 7 | BL | 118 | ASN |
| 7 | BL | 127 | ARG |
| 7 | BL | 128 | PHE |
| 7 | BL | 144 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | BL | 148 | MET |
| 7 | BL | 158 | ILE |
| 7 | BL | 165 | SER |
| 7 | BL | 170 | LEU |
| 7 | BL | 181 | LEU |
| 7 | BL | 192 | ILE |
| 7 | BL | 215 | LEU |
| 7 | BL | 237 | VAL |
| 7 | BL | 238 | LYS |
| 7 | BL | 252 | THR |
| 7 | BL | 258 | LEU |
| 7 | BL | 265 | ARG |
| 7 | BL | 266 | HIS |
| 7 | BL | 297 | LEU |
| 7 | BL | 299 | LEU |
| 7 | BL | 300 | LEU |
| 6 | BM | 110 | ASP |
| 6 | BM | 124 | VAL |
| 6 | BM | 166 | LEU |
| 6 | BM | 174 | VAL |
| 6 | BM | 187 | THR |
| 6 | BM | 223 | GLU |
| 6 | BM | 259 | ILE |
| 6 | BM | 303 | ASN |
| 6 | BM | 316 | VAL |
| 6 | BM | 328 | LYS |
| 6 | BM | 358 | ASP |
| 6 | BM | 398 | GLN |
| 6 | BM | 432 | ASP |
| 6 | BM | 436 | VAL |
| 6 | BM | 439 | LYS |
| 6 | BM | 486 | GLU |
| 6 | BM | 496 | ILE |
| 11 | BN | 4 | THR |
| 11 | BN | 41 | ILE |
| 11 | BN | 64 | GLN |
| 11 | BO | 37 | ASP |
| 11 | BO | 41 | ILE |
| 11 | BO | 45 | HIS |
| 11 | BO | 48 | THR |
| 11 | BP | 41 | ILE |
| 11 | BP | 45 | HIS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | BP | 64 | GLN |
| 11 | BQ | 41 | ILE |
| 11 | BQ | 64 | GLN |
| 11 | BQ | 74 | ASP |
| 11 | BR | 41 | ILE |
| 11 | BR | 65 | ARG |
| 11 | BR | 72 | ASN |
| 11 | BS | 41 | ILE |
| 11 | BS | 72 | ASN |
| 11 | BS | 77 | LYS |
| 11 | BT | 8 | VAL |
| 11 | BT | 30 | VAL |
| 11 | BT | 41 | ILE |
| 11 | BT | 64 | GLN |
| 11 | BU | 30 | VAL |
| 11 | BU | 41 | ILE |
| 11 | BV | 41 | ILE |
| 11 | BV | 45 | HIS |
| 11 | BV | 72 | ASN |
| 11 | BW | 8 | VAL |
| 11 | BW | 41 | ILE |
| 11 | BW | 64 | GLN |
| 3 | BX | 6 | VAL |
| 3 | BX | 17 | ARG |
| 3 | BX | 19 | ASN |
| 3 | BX | 23 | VAL |
| 3 | BX | 25 | ILE |
| 3 | BX | 45 | ILE |
| 3 | BX | 48 | LYS |
| 3 | BX | 56 | ARG |
| 3 | BX | 57 | LYS |
| 3 | BX | 58 | ILE |
| 3 | BX | 112 | ILE |
| 3 | BX | 113 | VAL |
| 3 | BX | 118 | ARG |
| 3 | BX | 124 | THR |
| 3 | BX | 127 | ILE |
| 3 | BX | 137 | VAL |
| 3 | BX | 143 | ASP |
| 3 | BX | 148 | ASN |
| 3 | BX | 150 | ILE |
| 3 | BY | 4 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | BY | 17 | ARG |
| 3 | BY | 19 | ASN |
| 3 | BY | 23 | VAL |
| 3 | BY | 45 | ILE |
| 3 | BY | 49 | ILE |
| 3 | BY | 51 | VAL |
| 3 | BY | 56 | ARG |
| 3 | BY | 57 | LYS |
| 3 | BY | 58 | ILE |
| 3 | BY | 112 | ILE |
| 3 | BY | 113 | VAL |
| 3 | BY | 127 | ILE |
| 3 | BY | 137 | VAL |
| 3 | BY | 143 | ASP |
| 3 | BY | 149 | GLU |
| 3 | BY | 163 | GLU |
| 3 | BZ | 1 | MET |
| 3 | BZ | 4 | ASP |
| 3 | BZ | 7 | THR |
| 3 | BZ | 14 | ASP |
| 3 | BZ | 19 | ASN |
| 3 | BZ | 37 | LYS |
| 3 | BZ | 51 | VAL |
| 3 | BZ | 57 | LYS |
| 3 | BZ | 58 | ILE |
| 3 | BZ | 68 | ASP |
| 3 | BZ | 80 | ASP |
| 3 | BZ | 98 | GLU |
| 3 | BZ | 112 | ILE |
| 3 | BZ | 113 | VAL |
| 3 | BZ | 124 | THR |
| 3 | BZ | 125 | LYS |
| 3 | BZ | 127 | ILE |
| 3 | BZ | 137 | VAL |
| 3 | BZ | 156 | THR |
| 3 | BZ | 163 | GLU |
| 3 | Ba | 6 | VAL |
| 3 | Ba | 19 | ASN |
| 3 | Ba | 23 | VAL |
| 3 | Ba | 37 | LYS |
| 3 | Ba | 45 | ILE |
| 3 | Ba | 48 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Ba | 49 | ILE |
| 3 | Ba | 56 | ARG |
| 3 | Ba | 57 | LYS |
| 3 | Ba | 58 | ILE |
| 3 | Ba | 72 | THR |
| 3 | Ba | 112 | ILE |
| 3 | Ba | 113 | VAL |
| 3 | Ba | 124 | THR |
| 3 | Ba | 127 | ILE |
| 3 | Ba | 137 | VAL |
| 3 | Ba | 159 | LEU |
| 3 | Bb | 1 | MET |
| 3 | Bb | 17 | ARG |
| 3 | Bb | 25 | ILE |
| 3 | Bb | 48 | LYS |
| 3 | Bb | 49 | ILE |
| 3 | Bb | 54 | MET |
| 3 | Bb | 57 | LYS |
| 3 | Bb | 58 | ILE |
| 3 | Bb | 89 | GLN |
| 3 | Bb | 112 | ILE |
| 3 | Bb | 113 | VAL |
| 3 | Bb | 127 | ILE |
| 3 | Bb | 136 | ASN |
| 3 | Bb | 137 | VAL |
| 3 | Bb | 150 | ILE |
| 3 | Bc | 23 | VAL |
| 3 | Bc | 37 | LYS |
| 3 | Bc | 45 | ILE |
| 3 | Bc | 57 | LYS |
| 3 | Bc | 58 | ILE |
| 3 | Bc | 112 | ILE |
| 3 | Bc | 113 | VAL |
| 3 | Bc | 124 | THR |
| 3 | Bc | 127 | ILE |
| 3 | Bc | 137 | VAL |
| 3 | Bc | 145 | ASP |
| 3 | Bc | 150 | ILE |
| 3 | Bd | 6 | VAL |
| 3 | Bd | 19 | ASN |
| 3 | Bd | 23 | VAL |
| 3 | Bd | 45 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Bd | 49 | ILE |
| 3 | Bd | 56 | ARG |
| 3 | Bd | 57 | LYS |
| 3 | Bd | 58 | ILE |
| 3 | Bd | 106 | GLU |
| 3 | Bd | 112 | ILE |
| 3 | Bd | 113 | VAL |
| 3 | Bd | 127 | ILE |
| 3 | Bd | 128 | GLU |
| 3 | Bd | 136 | ASN |
| 3 | Bd | 137 | VAL |
| 3 | Bd | 141 | GLN |
| 3 | Bd | 143 | ASP |
| 3 | Be | 6 | VAL |
| 3 | Be | 7 | THR |
| 3 | Be | 17 | ARG |
| 3 | Be | 37 | LYS |
| 3 | Be | 49 | ILE |
| 3 | Be | 54 | MET |
| 3 | Be | 57 | LYS |
| 3 | Be | 58 | ILE |
| 3 | Be | 95 | GLN |
| 3 | Be | 112 | ILE |
| 3 | Be | 113 | VAL |
| 3 | Be | 127 | ILE |
| 3 | Be | 137 | VAL |
| 3 | Be | 143 | ASP |
| 3 | Be | 150 | ILE |
| 3 | Be | 156 | THR |
| 3 | Bf | 17 | ARG |
| 3 | Bf | 25 | ILE |
| 3 | Bf | 31 | ASN |
| 3 | Bf | 41 | LEU |
| 3 | Bf | 47 | GLU |
| 3 | Bf | 48 | LYS |
| 3 | Bf | 57 | LYS |
| 3 | Bf | 58 | ILE |
| 3 | Bf | 68 | ASP |
| 3 | Bf | 85 | PHE |
| 3 | Bf | 106 | GLU |
| 3 | Bf | 112 | ILE |
| 3 | Bf | 113 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Bf | 127 | ILE |
| 3 | Bf | 132 | LEU |
| 3 | Bf | 137 | VAL |
| 3 | Bf | 142 | LEU |
| 3 | Bf | 143 | ASP |
| 3 | Bf | 149 | GLU |
| 3 | Bf | 150 | ILE |
| 3 | Bg | 11 | GLU |
| 3 | Bg | 14 | ASP |
| 3 | Bg | 19 | ASN |
| 3 | Bg | 23 | VAL |
| 3 | Bg | 31 | ASN |
| 3 | Bg | 37 | LYS |
| 3 | Bg | 45 | ILE |
| 3 | Bg | 48 | LYS |
| 3 | Bg | 49 | ILE |
| 3 | Bg | 56 | ARG |
| 3 | Bg | 57 | LYS |
| 3 | Bg | 58 | ILE |
| 3 | Bg | 64 | ARG |
| 3 | Bg | 113 | VAL |
| 3 | Bg | 124 | THR |
| 3 | Bg | 127 | ILE |
| 3 | Bg | 128 | GLU |
| 3 | Bg | 135 | THR |
| 3 | Bg | 137 | VAL |
| 3 | Bg | 150 | ILE |
| 3 | Bh | 14 | ASP |
| 3 | Bh | 17 | ARG |
| 3 | Bh | 19 | ASN |
| 3 | Bh | 37 | LYS |
| 3 | Bh | 45 | ILE |
| 3 | Bh | 48 | LYS |
| 3 | Bh | 49 | ILE |
| 3 | Bh | 54 | MET |
| 3 | Bh | 57 | LYS |
| 3 | Bh | 58 | ILE |
| 3 | Bh | 59 | ASN |
| 3 | Bh | 68 | ASP |
| 3 | Bh | 95 | GLN |
| 3 | Bh | 112 | ILE |
| 3 | Bh | 113 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Bh | 124 | THR |
| 3 | Bh | 127 | ILE |
| 3 | Bh | 137 | VAL |
| 3 | Bh | 143 | ASP |
| 3 | Bh | 150 | ILE |
| 3 | Bh | 154 | GLU |
| 3 | Bi | 14 | ASP |
| 3 | Bi | 17 | ARG |
| 3 | Bi | 19 | ASN |
| 3 | Bi | 37 | LYS |
| 3 | Bi | 57 | LYS |
| 3 | Bi | 58 | ILE |
| 3 | Bi | 64 | ARG |
| 3 | Bi | 91 | ILE |
| 3 | Bi | 98 | GLU |
| 3 | Bi | 113 | VAL |
| 3 | Bi | 127 | ILE |
| 3 | Bi | 128 | GLU |
| 3 | Bi | 149 | GLU |
| 3 | Bi | 150 | ILE |
| 3 | Bi | 156 | THR |
| 3 | Bj | 5 | ASP |
| 3 | Bj | 17 | ARG |
| 3 | Bj | 19 | ASN |
| 3 | Bj | 23 | VAL |
| 3 | Bj | 37 | LYS |
| 3 | Bj | 49 | ILE |
| 3 | Bj | 51 | VAL |
| 3 | Bj | 56 | ARG |
| 3 | Bj | 57 | LYS |
| 3 | Bj | 58 | ILE |
| 3 | Bj | 80 | ASP |
| 3 | Bj | 100 | THR |
| 3 | Bj | 112 | ILE |
| 3 | Bj | 113 | VAL |
| 3 | Bj | 118 | ARG |
| 3 | Bj | 121 | LYS |
| 3 | Bj | 127 | ILE |
| 3 | Bj | 137 | VAL |
| 3 | Bj | 149 | GLU |
| 3 | Bj | 150 | ILE |
| 3 | Bj | 163 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Bk | 6 | VAL |
| 3 | Bk | 17 | ARG |
| 3 | Bk | 19 | ASN |
| 3 | Bk | 23 | VAL |
| 3 | Bk | 45 | ILE |
| 3 | Bk | 48 | LYS |
| 3 | Bk | 49 | ILE |
| 3 | Bk | 51 | VAL |
| 3 | Bk | 56 | ARG |
| 3 | Bk | 57 | LYS |
| 3 | Bk | 58 | ILE |
| 3 | Bk | 64 | ARG |
| 3 | Bk | 85 | PHE |
| 3 | Bk | 89 | GLN |
| 3 | Bk | 112 | ILE |
| 3 | Bk | 113 | VAL |
| 3 | Bk | 127 | ILE |
| 3 | Bk | 136 | ASN |
| 3 | Bk | 137 | VAL |
| 3 | Bk | 150 | ILE |
| 3 | Bl | 6 | VAL |
| 3 | Bl | 17 | ARG |
| 3 | Bl | 19 | ASN |
| 3 | Bl | 23 | VAL |
| 3 | Bl | 37 | LYS |
| 3 | Bl | 45 | ILE |
| 3 | Bl | 47 | GLU |
| 3 | Bl | 49 | ILE |
| 3 | Bl | 57 | LYS |
| 3 | Bl | 58 | ILE |
| 3 | Bl | 68 | ASP |
| 3 | Bl | 80 | ASP |
| 3 | Bl | 85 | PHE |
| 3 | Bl | 100 | THR |
| 3 | Bl | 112 | ILE |
| 3 | Bl | 114 | ARG |
| 3 | Bl | 127 | ILE |
| 3 | Bl | 129 | ILE |
| 3 | Bl | 142 | LEU |
| 3 | Bl | 143 | ASP |
| 3 | Bl | 150 | ILE |
| 3 | Bm | 17 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Bm | 19 | ASN |
| 3 | Bm | 23 | VAL |
| 3 | Bm | 37 | LYS |
| 3 | Bm | 45 | ILE |
| 3 | Bm | 49 | ILE |
| 3 | Bm | 56 | ARG |
| 3 | Bm | 57 | LYS |
| 3 | Bm | 58 | ILE |
| 3 | Bm | 76 | ASP |
| 3 | Bm | 112 | ILE |
| 3 | Bm | 113 | VAL |
| 3 | Bm | 124 | THR |
| 3 | Bm | 127 | ILE |
| 3 | Bm | 135 | THR |
| 3 | Bm | 136 | ASN |
| 3 | Bm | 141 | GLN |
| 3 | Bn | 17 | ARG |
| 3 | Bn | 37 | LYS |
| 3 | Bn | 45 | ILE |
| 3 | Bn | 49 | ILE |
| 3 | Bn | 57 | LYS |
| 3 | Bn | 58 | ILE |
| 3 | Bn | 113 | VAL |
| 3 | Bn | 124 | THR |
| 3 | Bn | 127 | ILE |
| 3 | Bn | 129 | ILE |
| 3 | Bn | 137 | VAL |
| 3 | Bn | 157 | LEU |
| 3 | Bo | 14 | ASP |
| 3 | Bo | 17 | ARG |
| 3 | Bo | 19 | ASN |
| 3 | Bo | 37 | LYS |
| 3 | Bo | 45 | ILE |
| 3 | Bo | 49 | ILE |
| 3 | Bo | 57 | LYS |
| 3 | Bo | 58 | ILE |
| 3 | Bo | 95 | GLN |
| 3 | Bo | 103 | LYS |
| 3 | Bo | 112 | ILE |
| 3 | Bo | 113 | VAL |
| 3 | Bo | 127 | ILE |
| 3 | Bo | 137 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Bo | 142 | LEU |
| 3 | Bo | 143 | ASP |
| 3 | Bo | 150 | ILE |
| 2 | Bp | 32 | LYS |
| 2 | Bp | 66 | MET |
| 2 | Bp | 80 | VAL |
| 2 | Bp | 81 | VAL |
| 2 | Bp | 88 | THR |
| 2 | Bp | 91 | ASN |
| 2 | Bp | 130 | LYS |
| 2 | Bp | 139 | LYS |
| 2 | Bp | 149 | LYS |
| 2 | Bp | 186 | LYS |
| 2 | Bp | 188 | ILE |
| 2 | Bp | 195 | LEU |
| 2 | Bp | 205 | MET |
| 2 | Bp | 215 | LYS |
| 2 | Bp | 219 | ILE |
| 2 | Bp | 239 | VAL |
| 2 | Bp | 260 | THR |
| 2 | Bp | 266 | LYS |
| 2 | Bp | 275 | THR |
| 2 | Bp | 297 | THR |
| 2 | Bp | 298 | LYS |
| 2 | Bp | 302 | LYS |
| 2 | Bp | 303 | ASP |
| 2 | Bp | 365 | ARG |
| 2 | Bp | 383 | LEU |
| 2 | Bp | 385 | THR |
| 2 | Bp | 390 | GLN |
| 2 | Bp | 404 | LEU |
| 2 | Bp | 417 | ILE |
| 2 | Bp | 443 | ILE |
| 2 | Bp | 535 | LEU |
| 2 | Bp | 536 | TYR |
| 2 | Bp | 550 | ARG |
| 2 | Bp | 574 | GLU |
| 2 | Bp | 592 | LEU |
| 2 | Bp | 606 | VAL |
| 2 | Bq | 42 | LYS |
| 2 | Bq | 66 | MET |
| 2 | Bq | 85 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bq | 86 | ARG |
| 2 | Bq | 112 | VAL |
| 2 | Bq | 130 | LYS |
| 2 | Bq | 139 | LYS |
| 2 | Bq | 166 | ASN |
| 2 | Bq | 170 | GLU |
| 2 | Bq | 178 | LEU |
| 2 | Bq | 186 | LYS |
| 2 | Bq | 190 | ASP |
| 2 | Bq | 199 | GLU |
| 2 | Bq | 202 | GLU |
| 2 | Bq | 205 | MET |
| 2 | Bq | 215 | LYS |
| 2 | Bq | 219 | ILE |
| 2 | Bq | 229 | GLU |
| 2 | Bq | 252 | LEU |
| 2 | Bq | 287 | ASP |
| 2 | Bq | 290 | VAL |
| 2 | Bq | 298 | LYS |
| 2 | Bq | 303 | ASP |
| 2 | Bq | 368 | VAL |
| 2 | Bq | 383 | LEU |
| 2 | Bq | 390 | GLN |
| 2 | Bq | 398 | ASP |
| 2 | Bq | 412 | GLU |
| 2 | Bq | 417 | ILE |
| 2 | Bq | 424 | ASP |
| 2 | Bq | 430 | ARG |
| 2 | Bq | 431 | THR |
| 2 | Bq | 437 | THR |
| 2 | Bq | 438 | ASP |
| 2 | Bq | 453 | ASN |
| 2 | Bq | 467 | TRP |
| 2 | Bq | 484 | VAL |
| 2 | Bq | 495 | ASN |
| 2 | Bq | 501 | ASN |
| 2 | Bq | 526 | THR |
| 2 | Bq | 536 | TYR |
| 2 | Bq | 538 | ASP |
| 2 | Bq | 542 | THR |
| 2 | Bq | 550 | ARG |
| 2 | Bq | 564 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bq | 606 | VAL |
| 2 | Bq | 619 | ASP |
| 2 | Bq | 629 | ILE |
| 2 | Bq | 655 | THR |
| 2 | Br | 14 | THR |
| 2 | Br | 32 | LYS |
| 2 | Br | 47 | GLU |
| 2 | Br | 66 | MET |
| 2 | Br | 81 | VAL |
| 2 | Br | 85 | ASP |
| 2 | Br | 88 | THR |
| 2 | Br | 112 | VAL |
| 2 | Br | 130 | LYS |
| 2 | Br | 139 | LYS |
| 2 | Br | 149 | LYS |
| 2 | Br | 166 | ASN |
| 2 | Br | 168 | THR |
| 2 | Br | 171 | ILE |
| 2 | Br | 178 | LEU |
| 2 | Br | 197 | GLU |
| 2 | Br | 202 | GLU |
| 2 | Br | 205 | MET |
| 2 | Br | 209 | ASP |
| 2 | Br | 219 | ILE |
| 2 | Br | 230 | LEU |
| 2 | Br | 283 | VAL |
| 2 | Br | 287 | ASP |
| 2 | Br | 290 | VAL |
| 2 | Br | 297 | THR |
| 2 | Br | 298 | LYS |
| 2 | Br | 303 | ASP |
| 2 | Br | 344 | LEU |
| 2 | Br | 349 | GLU |
| 2 | Br | 383 | LEU |
| 2 | Br | 398 | ASP |
| 2 | Br | 417 | ILE |
| 2 | Br | 430 | ARG |
| 2 | Br | 443 | ILE |
| 2 | Br | 453 | ASN |
| 2 | Br | 455 | LYS |
| 2 | Br | 487 | THR |
| 2 | Br | 503 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Br | 510 | ARG |
| 2 | Br | 518 | TYR |
| 2 | Br | 536 | TYR |
| 2 | Br | 540 | THR |
| 2 | Br | 542 | THR |
| 2 | Br | 564 | ILE |
| 2 | Br | 572 | LEU |
| 2 | Br | 577 | ASN |
| 2 | Br | 606 | VAL |
| 2 | Br | 607 | VAL |
| 2 | Br | 641 | ASN |
| 2 | Br | 651 | PHE |
| 2 | Bs | 13 | THR |
| 2 | Bs | 14 | THR |
| 2 | Bs | 32 | LYS |
| 2 | Bs | 66 | MET |
| 2 | Bs | 80 | VAL |
| 2 | Bs | 81 | VAL |
| 2 | Bs | 85 | ASP |
| 2 | Bs | 88 | THR |
| 2 | Bs | 91 | ASN |
| 2 | Bs | 112 | VAL |
| 2 | Bs | 114 | ASP |
| 2 | Bs | 119 | LYS |
| 2 | Bs | 130 | LYS |
| 2 | Bs | 139 | LYS |
| 2 | Bs | 149 | LYS |
| 2 | Bs | 166 | ASN |
| 2 | Bs | 168 | THR |
| 2 | Bs | 170 | GLU |
| 2 | Bs | 171 | ILE |
| 2 | Bs | 183 | THR |
| 2 | Bs | 186 | LYS |
| 2 | Bs | 188 | ILE |
| 2 | Bs | 195 | LEU |
| 2 | Bs | 199 | GLU |
| 2 | Bs | 202 | GLU |
| 2 | Bs | 219 | ILE |
| 2 | Bs | 290 | VAL |
| 2 | Bs | 298 | LYS |
| 2 | Bs | 303 | ASP |
| 2 | Bs | 313 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bs | 344 | LEU |
| 2 | Bs | 383 | LEU |
| 2 | Bs | 390 | GLN |
| 2 | Bs | 417 | ILE |
| 2 | Bs | 450 | ILE |
| 2 | Bs | 455 | LYS |
| 2 | Bs | 536 | TYR |
| 2 | Bs | 576 | ASN |
| 2 | Bs | 598 | LEU |
| 2 | Bs | 606 | VAL |
| 2 | Bt | 8 | ILE |
| 2 | Bt | 14 | THR |
| 2 | Bt | 32 | LYS |
| 2 | Bt | 42 | LYS |
| 2 | Bt | 47 | GLU |
| 2 | Bt | 49 | ASP |
| 2 | Bt | 66 | MET |
| 2 | Bt | 72 | LEU |
| 2 | Bt | 81 | VAL |
| 2 | Bt | 91 | ASN |
| 2 | Bt | 112 | VAL |
| 2 | Bt | 139 | LYS |
| 2 | Bt | 141 | LYS |
| 2 | Bt | 149 | LYS |
| 2 | Bt | 166 | ASN |
| 2 | Bt | 170 | GLU |
| 2 | Bt | 171 | ILE |
| 2 | Bt | 194 | LEU |
| 2 | Bt | 202 | GLU |
| 2 | Bt | 215 | LYS |
| 2 | Bt | 219 | ILE |
| 2 | Bt | 239 | VAL |
| 2 | Bt | 251 | LEU |
| 2 | Bt | 271 | TYR |
| 2 | Bt | 290 | VAL |
| 2 | Bt | 297 | THR |
| 2 | Bt | 298 | LYS |
| 2 | Bt | 303 | ASP |
| 2 | Bt | 344 | LEU |
| 2 | Bt | 383 | LEU |
| 2 | Bt | 404 | LEU |
| 2 | Bt | 417 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bt | 443 | ILE |
| 2 | Bt | 455 | LYS |
| 2 | Bt | 456 | TYR |
| 2 | Bt | 460 | LYS |
| 2 | Bt | 467 | TRP |
| 2 | Bt | 468 | VAL |
| 2 | Bt | 483 | ASN |
| 2 | Bt | 484 | VAL |
| 2 | Bt | 505 | LEU |
| 2 | Bt | 523 | ASN |
| 2 | Bt | 536 | TYR |
| 2 | Bt | 550 | ARG |
| 2 | Bt | 569 | LYS |
| 2 | Bt | 572 | LEU |
| 2 | Bt | 574 | GLU |
| 2 | Bt | 596 | LYS |
| 2 | Bt | 606 | VAL |
| 2 | Bt | 612 | ASN |
| 2 | Bt | 617 | VAL |
| 2 | Bt | 629 | ILE |
| 2 | Bu | 32 | LYS |
| 2 | Bu | 42 | LYS |
| 2 | Bu | 60 | GLU |
| 2 | Bu | 66 | MET |
| 2 | Bu | 88 | THR |
| 2 | Bu | 112 | VAL |
| 2 | Bu | 128 | GLU |
| 2 | Bu | 139 | LYS |
| 2 | Bu | 149 | LYS |
| 2 | Bu | 171 | ILE |
| 2 | Bu | 183 | THR |
| 2 | Bu | 186 | LYS |
| 2 | Bu | 194 | LEU |
| 2 | Bu | 197 | GLU |
| 2 | Bu | 199 | GLU |
| 2 | Bu | 202 | GLU |
| 2 | Bu | 209 | ASP |
| 2 | Bu | 219 | ILE |
| 2 | Bu | 229 | GLU |
| 2 | Bu | 281 | ILE |
| 2 | Bu | 282 | ILE |
| 2 | Bu | 298 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bu | 302 | LYS |
| 2 | Bu | 303 | ASP |
| 2 | Bu | 312 | ASP |
| 2 | Bu | 313 | ASP |
| 2 | Bu | 344 | LEU |
| 2 | Bu | 349 | GLU |
| 2 | Bu | 350 | VAL |
| 2 | Bu | 381 | GLU |
| 2 | Bu | 385 | THR |
| 2 | Bu | 404 | LEU |
| 2 | Bu | 411 | ARG |
| 2 | Bu | 417 | ILE |
| 2 | Bu | 443 | ILE |
| 2 | Bu | 450 | ILE |
| 2 | Bu | 455 | LYS |
| 2 | Bu | 456 | TYR |
| 2 | Bu | 464 | VAL |
| 2 | Bu | 468 | VAL |
| 2 | Bu | 482 | ASP |
| 2 | Bu | 484 | VAL |
| 2 | Bu | 505 | LEU |
| 2 | Bu | 536 | TYR |
| 2 | Bu | 538 | ASP |
| 2 | Bu | 553 | VAL |
| 2 | Bu | 564 | ILE |
| 2 | Bu | 569 | LYS |
| 2 | Bu | 606 | VAL |
| 2 | Bu | 617 | VAL |
| 2 | Bu | 641 | ASN |
| 2 | Bu | 651 | PHE |
| 2 | Bu | 655 | THR |
| 2 | Bv | 14 | THR |
| 2 | Bv | 32 | LYS |
| 2 | Bv | 42 | LYS |
| 2 | Bv | 58 | THR |
| 2 | Bv | 66 | MET |
| 2 | Bv | 72 | LEU |
| 2 | Bv | 81 | VAL |
| 2 | Bv | 84 | VAL |
| 2 | Bv | 88 | THR |
| 2 | Bv | 130 | LYS |
| 2 | Bv | 139 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bv | 141 | LYS |
| 2 | Bv | 149 | LYS |
| 2 | Bv | 166 | ASN |
| 2 | Bv | 194 | LEU |
| 2 | Bv | 195 | LEU |
| 2 | Bv | 199 | GLU |
| 2 | Bv | 202 | GLU |
| 2 | Bv | 205 | MET |
| 2 | Bv | 215 | LYS |
| 2 | Bv | 219 | ILE |
| 2 | Bv | 229 | GLU |
| 2 | Bv | 276 | ASP |
| 2 | Bv | 290 | VAL |
| 2 | Bv | 297 | THR |
| 2 | Bv | 298 | LYS |
| 2 | Bv | 303 | ASP |
| 2 | Bv | 326 | THR |
| 2 | Bv | 344 | LEU |
| 2 | Bv | 378 | CYS |
| 2 | Bv | 382 | SER |
| 2 | Bv | 384 | GLU |
| 2 | Bv | 404 | LEU |
| 2 | Bv | 426 | LEU |
| 2 | Bv | 430 | ARG |
| 2 | Bv | 443 | ILE |
| 2 | Bv | 467 | TRP |
| 2 | Bv | 473 | ASP |
| 2 | Bv | 526 | THR |
| 2 | Bv | 536 | TYR |
| 2 | Bv | 549 | ASP |
| 2 | Bv | 569 | LYS |
| 2 | Bv | 572 | LEU |
| 2 | Bv | 592 | LEU |
| 2 | Bv | 602 | TYR |
| 2 | Bv | 606 | VAL |
| 2 | Bv | 617 | VAL |
| 2 | Bv | 629 | ILE |
| 2 | Bv | 650 | ASP |
| 2 | Bv | 655 | THR |
| 2 | Bw | 32 | LYS |
| 2 | Bw | 49 | ASP |
| 2 | Bw | 66 | MET |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bw | 81 | VAL |
| 2 | Bw | 88 | THR |
| 2 | Bw | 91 | ASN |
| 2 | Bw | 112 | VAL |
| 2 | Bw | 130 | LYS |
| 2 | Bw | 132 | THR |
| 2 | Bw | 139 | LYS |
| 2 | Bw | 149 | LYS |
| 2 | Bw | 171 | ILE |
| 2 | Bw | 178 | LEU |
| 2 | Bw | 186 | LYS |
| 2 | Bw | 195 | LEU |
| 2 | Bw | 199 | GLU |
| 2 | Bw | 202 | GLU |
| 2 | Bw | 205 | MET |
| 2 | Bw | 215 | LYS |
| 2 | Bw | 219 | ILE |
| 2 | Bw | 230 | LEU |
| 2 | Bw | 268 | VAL |
| 2 | Bw | 282 | ILE |
| 2 | Bw | 286 | ASN |
| 2 | Bw | 297 | THR |
| 2 | Bw | 298 | LYS |
| 2 | Bw | 303 | ASP |
| 2 | Bw | 368 | VAL |
| 2 | Bw | 378 | CYS |
| 2 | Bw | 383 | LEU |
| 2 | Bw | 398 | ASP |
| 2 | Bw | 404 | LEU |
| 2 | Bw | 417 | ILE |
| 2 | Bw | 421 | ARG |
| 2 | Bw | 443 | ILE |
| 2 | Bw | 450 | ILE |
| 2 | Bw | 453 | ASN |
| 2 | Bw | 455 | LYS |
| 2 | Bw | 468 | VAL |
| 2 | Bw | 470 | LEU |
| 2 | Bw | 496 | ARG |
| 2 | Bw | 503 | ILE |
| 2 | Bw | 505 | LEU |
| 2 | Bw | 517 | LEU |
| 2 | Bw | 518 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bw | 535 | LEU |
| 2 | Bw | 536 | TYR |
| 2 | Bw | 538 | ASP |
| 2 | Bw | 540 | THR |
| 2 | Bw | 542 | THR |
| 2 | Bw | 552 | ASN |
| 2 | Bw | 553 | VAL |
| 2 | Bw | 564 | ILE |
| 2 | Bw | 606 | VAL |
| 2 | Bw | 650 | ASP |
| 2 | Bw | 653 | GLU |
| 2 | Bx | 32 | LYS |
| 2 | Bx | 47 | GLU |
| 2 | Bx | 66 | MET |
| 2 | Bx | 76 | ASN |
| 2 | Bx | 88 | THR |
| 2 | Bx | 112 | VAL |
| 2 | Bx | 130 | LYS |
| 2 | Bx | 139 | LYS |
| 2 | Bx | 141 | LYS |
| 2 | Bx | 149 | LYS |
| 2 | Bx | 170 | GLU |
| 2 | Bx | 171 | ILE |
| 2 | Bx | 186 | LYS |
| 2 | Bx | 195 | LEU |
| 2 | Bx | 199 | GLU |
| 2 | Bx | 202 | GLU |
| 2 | Bx | 209 | ASP |
| 2 | Bx | 215 | LYS |
| 2 | Bx | 219 | ILE |
| 2 | Bx | 230 | LEU |
| 2 | Bx | 290 | VAL |
| 2 | Bx | 298 | LYS |
| 2 | Bx | 303 | ASP |
| 2 | Bx | 317 | LYS |
| 2 | Bx | 344 | LEU |
| 2 | Bx | 365 | ARG |
| 2 | Bx | 385 | THR |
| 2 | Bx | 398 | ASP |
| 2 | Bx | 404 | LEU |
| 2 | Bx | 415 | VAL |
| 2 | Bx | 417 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bx | 437 | THR |
| 2 | Bx | 453 | ASN |
| 2 | Bx | 456 | TYR |
| 2 | Bx | 495 | ASN |
| 2 | Bx | 523 | ASN |
| 2 | Bx | 536 | TYR |
| 2 | Bx | 542 | THR |
| 2 | Bx | 551 | ILE |
| 2 | Bx | 556 | LEU |
| 2 | Bx | 564 | ILE |
| 2 | Bx | 592 | LEU |
| 2 | Bx | 606 | VAL |
| 2 | Bx | 617 | VAL |
| 2 | Bx | 643 | VAL |
| 2 | By | 14 | THR |
| 2 | By | 32 | LYS |
| 2 | By | 49 | ASP |
| 2 | By | 66 | MET |
| 2 | By | 80 | VAL |
| 2 | By | 81 | VAL |
| 2 | By | 88 | THR |
| 2 | By | 91 | ASN |
| 2 | By | 112 | VAL |
| 2 | By | 130 | LYS |
| 2 | By | 139 | LYS |
| 2 | By | 149 | LYS |
| 2 | By | 171 | ILE |
| 2 | By | 186 | LYS |
| 2 | By | 195 | LEU |
| 2 | By | 215 | LYS |
| 2 | By | 219 | ILE |
| 2 | By | 229 | GLU |
| 2 | By | 282 | ILE |
| 2 | By | 287 | ASP |
| 2 | By | 298 | LYS |
| 2 | By | 302 | LYS |
| 2 | By | 303 | ASP |
| 2 | By | 304 | ILE |
| 2 | By | 344 | LEU |
| 2 | By | 354 | ASP |
| 2 | By | 382 | SER |
| 2 | By | 383 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | By | 398 | ASP |
| 2 | By | 404 | LEU |
| 2 | By | 417 | ILE |
| 2 | By | 426 | LEU |
| 2 | By | 430 | ARG |
| 2 | By | 439 | ASN |
| 2 | By | 467 | TRP |
| 2 | By | 495 | ASN |
| 2 | By | 503 | ILE |
| 2 | By | 526 | THR |
| 2 | By | 536 | TYR |
| 2 | By | 542 | THR |
| 2 | By | 552 | ASN |
| 2 | By | 564 | ILE |
| 2 | By | 573 | PHE |
| 2 | By | 580 | THR |
| 2 | By | 596 | LYS |
| 2 | By | 602 | TYR |
| 2 | By | 606 | VAL |
| 2 | By | 612 | ASN |
| 2 | By | 629 | ILE |
| 2 | By | 655 | THR |
| 2 | Bz | 14 | THR |
| 2 | Bz | 32 | LYS |
| 2 | Bz | 49 | ASP |
| 2 | Bz | 81 | VAL |
| 2 | Bz | 88 | THR |
| 2 | Bz | 112 | VAL |
| 2 | Bz | 128 | GLU |
| 2 | Bz | 130 | LYS |
| 2 | Bz | 139 | LYS |
| 2 | Bz | 149 | LYS |
| 2 | Bz | 166 | ASN |
| 2 | Bz | 171 | ILE |
| 2 | Bz | 178 | LEU |
| 2 | Bz | 186 | LYS |
| 2 | Bz | 202 | GLU |
| 2 | Bz | 219 | ILE |
| 2 | Bz | 298 | LYS |
| 2 | Bz | 303 | ASP |
| 2 | Bz | 344 | LEU |
| 2 | Bz | 368 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bz | 383 | LEU |
| 2 | Bz | 404 | LEU |
| 2 | Bz | 413 | THR |
| 2 | Bz | 417 | ILE |
| 2 | Bz | 443 | ILE |
| 2 | Bz | 453 | ASN |
| 2 | Bz | 455 | LYS |
| 2 | Bz | 467 | TRP |
| 2 | Bz | 473 | ASP |
| 2 | Bz | 477 | LEU |
| 2 | Bz | 487 | THR |
| 2 | Bz | 523 | ASN |
| 2 | Bz | 535 | LEU |
| 2 | Bz | 536 | TYR |
| 2 | Bz | 550 | ARG |
| 2 | Bz | 564 | ILE |
| 2 | Bz | 569 | LYS |
| 2 | Bz | 592 | LEU |
| 2 | Bz | 606 | VAL |
| 2 | Bz | 629 | ILE |
| 2 | Bz | 655 | THR |
| 4 | D | 59 | ASP |
| 4 | D | 77 | LYS |
| 4 | E | 26 | LYS |
| 4 | F | 62 | ILE |
| 4 | K | 3 | ILE |
| 4 | O | 62 | ILE |
| 4 | P | 36 | THR |
| 4 | Q | 2 | ASP |
| 4 | Q | 62 | ILE |
| 4 | S | 76 | ILE |
| 4 | T | 7 | ASP |
| 4 | V | 7 | ASP |
| 4 | V | 60 | LYS |
| 4 | W | 35 | ASP |
| 4 | W | 55 | VAL |
| 4 | X | 59 | ASP |
| 4 | X | 62 | ILE |
| 4 | X | 65 | LEU |
| 4 | Y | 59 | ASP |
| 4 | Y | 65 | LEU |
| 4 | Z | 17 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | c | 36 | THR |
| 4 | f | 36 | THR |
| 4 | f | 65 | LEU |
| 4 | g | 62 | ILE |
| 4 | h | 3 | ILE |
| 4 | h | 59 | ASP |
| 1 | k | 8 | LEU |
| 1 | k | 11 | LYS |
| 1 | k | 13 | GLU |
| 1 | k | 15 | ARG |
| 1 | k | 27 | LEU |
| 1 | k | 51 | ILE |
| 1 | k | 71 | ILE |
| 1 | k | 75 | ASP |
| 1 | k | 78 | ASN |
| 1 | k | 90 | LEU |
| 1 | k | 91 | ASN |
| 1 | k | 110 | VAL |
| 1 | k | 115 | THR |
| 1 | k | 116 | LEU |
| 1 | k | 127 | VAL |
| 1 | k | 128 | ASN |
| 1 | k | 136 | ASP |
| 1 | k | 146 | LEU |
| 1 | k | 169 | ILE |
| 1 | k | 175 | ILE |
| 1 | k | 201 | LEU |
| 1 | k | 202 | ASN |
| 1 | k | 214 | ASN |
| 1 | k | 216 | ASP |
| 1 | k | 232 | VAL |
| 1 | k | 233 | GLU |
| 1 | k | 237 | VAL |
| 1 | k | 245 | PHE |
| 1 | l | 8 | LEU |
| 1 | l | 11 | LYS |
| 1 | l | 15 | ARG |
| 1 | l | 34 | ASN |
| 1 | l | 46 | LEU |
| 1 | l | 75 | ASP |
| 1 | l | 78 | ASN |
| 1 | l | 94 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | l | 110 | VAL |
| 1 | l | 116 | LEU |
| 1 | l | 121 | ASN |
| 1 | l | 127 | VAL |
| 1 | l | 128 | ASN |
| 1 | l | 146 | LEU |
| 1 | l | 158 | PHE |
| 1 | l | 163 | GLN |
| 1 | l | 166 | ILE |
| 1 | l | 169 | ILE |
| 1 | l | 175 | ILE |
| 1 | l | 179 | GLU |
| 1 | l | 213 | ILE |
| 1 | l | 216 | ASP |
| 1 | l | 233 | GLU |
| 1 | l | 239 | ASN |
| 1 | m | 11 | LYS |
| 1 | m | 15 | ARG |
| 1 | m | 27 | LEU |
| 1 | m | 46 | LEU |
| 1 | m | 75 | ASP |
| 1 | m | 90 | LEU |
| 1 | m | 94 | GLU |
| 1 | m | 108 | MET |
| 1 | m | 110 | VAL |
| 1 | m | 115 | THR |
| 1 | m | 118 | ILE |
| 1 | m | 127 | VAL |
| 1 | m | 128 | ASN |
| 1 | m | 146 | LEU |
| 1 | m | 155 | TYR |
| 1 | m | 166 | ILE |
| 1 | m | 169 | ILE |
| 1 | m | 182 | ASN |
| 1 | m | 198 | GLU |
| 1 | m | 213 | ILE |
| 1 | m | 216 | ASP |
| 1 | n | 11 | LYS |
| 1 | n | 13 | GLU |
| 1 | n | 15 | ARG |
| 1 | n | 27 | LEU |
| 1 | n | 46 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | n | 75 | ASP |
| 1 | n | 78 | ASN |
| 1 | n | 90 | LEU |
| 1 | n | 91 | ASN |
| 1 | n | 94 | GLU |
| 1 | n | 110 | VAL |
| 1 | n | 115 | THR |
| 1 | n | 127 | VAL |
| 1 | n | 128 | ASN |
| 1 | n | 134 | GLU |
| 1 | n | 146 | LEU |
| 1 | n | 155 | TYR |
| 1 | n | 163 | GLN |
| 1 | n | 205 | ARG |
| 1 | n | 233 | GLU |
| 1 | n | 245 | PHE |
| 3 | o | 4 | ASP |
| 3 | o | 10 | PHE |
| 3 | o | 23 | VAL |
| 3 | o | 26 | SER |
| 3 | o | 41 | LEU |
| 3 | o | 45 | ILE |
| 3 | o | 48 | LYS |
| 3 | o | 49 | ILE |
| 3 | o | 51 | VAL |
| 3 | o | 55 | ASN |
| 3 | o | 56 | ARG |
| 3 | o | 57 | LYS |
| 3 | o | 58 | ILE |
| 3 | o | 80 | ASP |
| 3 | o | 97 | ASN |
| 3 | o | 112 | ILE |
| 3 | o | 113 | VAL |
| 3 | o | 127 | ILE |
| 3 | o | 137 | VAL |
| 3 | o | 141 | GLN |
| 3 | o | 150 | ILE |
| 1 | p | 11 | LYS |
| 1 | p | 13 | GLU |
| 1 | p | 15 | ARG |
| 1 | p | 26 | ILE |
| 1 | p | 27 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | p | 46 | LEU |
| 1 | p | 51 | ILE |
| 1 | p | 56 | VAL |
| 1 | p | 75 | ASP |
| 1 | p | 90 | LEU |
| 1 | p | 94 | GLU |
| 1 | p | 110 | VAL |
| 1 | p | 118 | ILE |
| 1 | p | 127 | VAL |
| 1 | p | 128 | ASN |
| 1 | p | 136 | ASP |
| 1 | p | 146 | LEU |
| 1 | p | 156 | ASP |
| 1 | p | 166 | ILE |
| 1 | p | 202 | ASN |
| 1 | p | 216 | ASP |
| 1 | p | 245 | PHE |
| 8 | q | 20 | LEU |
| 8 | q | 24 | ILE |
| 8 | q | 26 | ILE |
| 8 | q | 35 | LYS |
| 8 | q | 53 | LEU |
| 8 | q | 62 | GLN |
| 8 | q | 76 | ASN |
| 8 | q | 88 | PHE |
| 8 | q | 98 | LEU |
| 8 | q | 114 | ILE |
| 8 | q | 163 | ILE |
| 8 | q | 164 | LYS |
| 8 | q | 173 | ASP |
| 8 | q | 198 | MET |
| 8 | q | 227 | GLU |
| 8 | q | 229 | VAL |
| 8 | q | 230 | PHE |
| 8 | q | 236 | GLU |
| 8 | q | 238 | VAL |
| 8 | q | 247 | TRP |
| 8 | r | 20 | LEU |
| 8 | r | 35 | LYS |
| 8 | r | 50 | MET |
| 8 | r | 53 | LEU |
| 8 | r | 59 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | r | 60 | ASN |
| 8 | r | 76 | ASN |
| 8 | r | 79 | LEU |
| 8 | r | 98 | LEU |
| 8 | r | 114 | ILE |
| 8 | r | 162 | ASP |
| 8 | r | 163 | ILE |
| 8 | r | 164 | LYS |
| 8 | r | 172 | ILE |
| 8 | r | 179 | ASP |
| 8 | r | 198 | MET |
| 8 | r | 211 | THR |
| 8 | r | 214 | THR |
| 8 | r | 222 | ASP |
| 8 | r | 223 | LEU |
| 8 | r | 227 | GLU |
| 8 | r | 238 | VAL |
| 8 | r | 243 | ASP |
| 8 | r | 263 | THR |
| 8 | s | 7 | ASN |
| 8 | s | 16 | LEU |
| 8 | s | 20 | LEU |
| 8 | s | 50 | MET |
| 8 | s | 72 | LEU |
| 8 | s | 76 | ASN |
| 8 | s | 77 | LEU |
| 8 | s | 93 | LEU |
| 8 | s | 98 | LEU |
| 8 | s | 114 | ILE |
| 8 | s | 120 | LEU |
| 8 | s | 147 | THR |
| 8 | s | 163 | ILE |
| 8 | s | 172 | ILE |
| 8 | s | 198 | MET |
| 8 | s | 204 | ASP |
| 8 | s | 208 | LEU |
| 8 | s | 211 | THR |
| 8 | s | 214 | THR |
| 8 | s | 215 | ASP |
| 8 | s | 222 | ASP |
| 8 | s | 229 | VAL |
| 8 | s | 230 | PHE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | s | 238 | VAL |
| 8 | s | 247 | TRP |
| 8 | s | 256 | THR |
| 8 | s | 258 | ASN |
| 8 | s | 259 | VAL |
| 8 | t | 20 | LEU |
| 8 | t | 30 | LEU |
| 8 | t | 31 | GLU |
| 8 | t | 35 | LYS |
| 8 | t | 50 | MET |
| 8 | t | 62 | GLN |
| 8 | t | 72 | LEU |
| 8 | t | 76 | ASN |
| 8 | t | 93 | LEU |
| 8 | t | 114 | ILE |
| 8 | t | 152 | GLN |
| 8 | t | 163 | ILE |
| 8 | t | 176 | ILE |
| 8 | t | 187 | GLU |
| 8 | t | 208 | LEU |
| 8 | t | 211 | THR |
| 8 | t | 223 | LEU |
| 8 | t | 227 | GLU |
| 8 | t | 229 | VAL |
| 8 | t | 236 | GLU |
| 8 | t | 238 | VAL |
| 8 | t | 241 | ASP |
| 8 | t | 259 | VAL |
| 8 | u | 1 | MET |
| 8 | u | 51 | MET |
| 8 | u | 60 | ASN |
| 8 | u | 62 | GLN |
| 8 | u | 79 | LEU |
| 8 | u | 85 | ASN |
| 8 | u | 93 | LEU |
| 8 | u | 100 | LYS |
| 8 | u | 114 | ILE |
| 8 | u | 116 | MET |
| 8 | u | 121 | SER |
| 8 | u | 127 | GLU |
| 8 | u | 147 | THR |
| 8 | u | 163 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | u | 172 | ILE |
| 8 | u | 198 | MET |
| 8 | u | 208 | LEU |
| 8 | u | 215 | ASP |
| 8 | u | 230 | PHE |
| 8 | u | 236 | GLU |
| 8 | u | 238 | VAL |
| 9 | v | 5 | LEU |
| 9 | v | 47 | THR |
| 9 | v | 64 | VAL |
| 9 | v | 68 | TYR |
| 9 | v | 76 | ILE |
| 9 | v | 94 | THR |
| 9 | v | 156 | THR |
| 9 | v | 167 | GLU |
| 9 | w | 5 | LEU |
| 9 | w | 10 | ASN |
| 9 | w | 19 | VAL |
| 9 | w | 64 | VAL |
| 9 | w | 68 | TYR |
| 9 | w | 114 | LEU |
| 9 | w | 129 | ASN |
| 9 | w | 140 | GLU |
| 9 | w | 175 | GLU |
| 9 | x | 5 | LEU |
| 9 | x | 11 | GLN |
| 9 | x | 19 | VAL |
| 9 | x | 25 | ASN |
| 9 | x | 47 | THR |
| 9 | x | 64 | VAL |
| 9 | x | 68 | TYR |
| 9 | x | 129 | ASN |
| 9 | x | 138 | LEU |
| 9 | x | 156 | THR |
| 9 | x | 172 | ILE |
| 9 | y | 5 | LEU |
| 9 | y | 47 | THR |
| 9 | y | 64 | VAL |
| 9 | y | 65 | THR |
| 9 | y | 66 | PHE |
| 9 | y | 68 | TYR |
| 9 | y | 76 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | y | 79 | GLU |
| 9 | y | 129 | ASN |
| 9 | y | 140 | GLU |
| 9 | y | 156 | THR |
| 9 | y | 167 | GLU |
| 9 | z | 5 | LEU |
| 9 | z | 10 | ASN |
| 9 | z | 23 | HIS |
| 9 | z | 64 | VAL |
| 9 | z | 68 | TYR |
| 9 | z | 77 | VAL |
| 9 | z | 81 | LEU |
| 9 | z | 102 | ASN |
| 9 | z | 129 | ASN |
| 9 | z | 138 | LEU |
| 9 | z | 172 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (468) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 91 | ASN |
| 1 | 0 | 192 | ASN |
| 1 | 0 | 206 | ASN |
| 2 | 1 | 200 | ASN |
| 2 | 1 | 308 | ASN |
| 2 | 1 | 523 | ASN |
| 2 | 1 | 641 | ASN |
| 2 | 2 | 73 | GLN |
| 2 | 2 | 211 | GLN |
| 2 | 2 | 329 | ASN |
| 2 | 2 | 392 | HIS |
| 2 | 2 | 501 | ASN |
| 2 | 2 | 552 | ASN |
| 2 | 2 | 613 | ASN |
| 2 | 3 | 52 | ASN |
| 2 | 3 | 308 | ASN |
| 2 | 3 | 328 | GLN |
| 2 | 3 | 439 | ASN |
| 2 | 3 | 523 | ASN |
| 2 | 3 | 612 | ASN |
| 2 | 4 | 34 | GLN |
| 2 | 4 | 440 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 4 | 511 | GLN |
| 2 | 4 | 523 | ASN |
| 2 | 4 | 590 | GLN |
| 2 | 4 | 641 | ASN |
| 2 | 5 | 16 | GLN |
| 2 | 5 | 22 | ASN |
| 2 | 5 | 56 | GLN |
| 2 | 5 | 76 | ASN |
| 2 | 5 | 286 | ASN |
| 2 | 5 | 453 | ASN |
| 2 | 5 | 486 | GLN |
| 2 | 5 | 523 | ASN |
| 3 | 6 | 31 | ASN |
| 3 | 8 | 59 | ASN |
| 3 | 8 | 75 | ASN |
| 3 | 8 | 151 | GLN |
| 4 | A | 19 | GLN |
| 4 | A | 61 | ASN |
| 5 | A0 | 81 | ASN |
| 5 | A0 | 310 | ASN |
| 5 | A0 | 504 | GLN |
| 5 | A1 | 327 | ASN |
| 5 | A1 | 367 | GLN |
| 5 | A2 | 85 | ASN |
| 5 | A2 | 112 | ASN |
| 5 | A2 | 124 | ASN |
| 5 | A2 | 181 | GLN |
| 5 | A2 | 183 | GLN |
| 5 | A2 | 212 | HIS |
| 5 | A2 | 323 | ASN |
| 5 | A2 | 358 | ASN |
| 5 | A2 | 411 | GLN |
| 5 | A2 | 483 | HIS |
| 5 | A2 | 500 | GLN |
| 5 | A3 | 48 | ASN |
| 5 | A3 | 159 | HIS |
| 5 | A3 | 181 | GLN |
| 5 | A3 | 263 | GLN |
| 5 | A3 | 300 | HIS |
| 6 | A4 | 75 | ASN |
| 6 | A4 | 191 | GLN |
| 6 | A4 | 265 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | A4 | 303 | ASN |
| 6 | A5 | 303 | ASN |
| 7 | A6 | 39 | GLN |
| 7 | A6 | 152 | GLN |
| 7 | A6 | 175 | ASN |
| 6 | A7 | 83 | GLN |
| 6 | A8 | 398 | GLN |
| 6 | A9 | 115 | GLN |
| 6 | A9 | 236 | GLN |
| 6 | A9 | 315 | GLN |
| 6 | A9 | 505 | ASN |
| 3 | AA | 55 | ASN |
| 8 | AB | 95 | GLN |
| 2 | AD | 21 | ASN |
| 2 | AD | 40 | GLN |
| 2 | AD | 453 | ASN |
| 2 | AD | 563 | ASN |
| 2 | AD | 590 | GLN |
| 2 | AD | 613 | ASN |
| 3 | AE | 83 | GLN |
| 3 | AF | 75 | ASN |
| 3 | AG | 22 | GLN |
| 3 | AG | 95 | GLN |
| 3 | AG | 115 | GLN |
| 3 | AH | 89 | GLN |
| 3 | AH | 148 | ASN |
| 3 | AI | 147 | ASN |
| 2 | AK | 98 | ASN |
| 2 | AK | 144 | ASN |
| 2 | AK | 213 | ASN |
| 2 | AK | 274 | GLN |
| 2 | AK | 552 | ASN |
| 2 | AK | 613 | ASN |
| 2 | AL | 274 | GLN |
| 2 | AM | 213 | ASN |
| 2 | AM | 439 | ASN |
| 2 | AM | 552 | ASN |
| 2 | AN | 286 | ASN |
| 2 | AN | 519 | GLN |
| 2 | AN | 523 | ASN |
| 2 | AN | 612 | ASN |
| 2 | AO | 211 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | AO | 329 | ASN |
| 2 | AO | 465 | ASN |
| 2 | AO | 495 | ASN |
| 2 | AO | 621 | ASN |
| 2 | AP | 486 | GLN |
| 2 | AP | 519 | GLN |
| 2 | AP | 523 | ASN |
| 2 | AP | 552 | ASN |
| 10 | AS | 337 | HIS |
| 10 | AT | 299 | HIS |
| 10 | AT | 316 | GLN |
| 10 | AT | 358 | ASN |
| 10 | AU | 342 | GLN |
| 10 | AU | 354 | GLN |
| 6 | AV | 123 | GLN |
| 6 | AV | 157 | GLN |
| 6 | AW | 282 | HIS |
| 6 | AX | 183 | GLN |
| 6 | AX | 257 | GLN |
| 6 | AX | 356 | GLN |
| 6 | AX | 466 | ASN |
| 6 | AX | 497 | GLN |
| 6 | AX | 505 | ASN |
| 7 | AY | 7 | GLN |
| 7 | AY | 200 | ASN |
| 7 | AY | 239 | GLN |
| 6 | AZ | 105 | ASN |
| 6 | AZ | 115 | GLN |
| 6 | AZ | 171 | GLN |
| 7 | Aa | 49 | HIS |
| 7 | Aa | 91 | ASN |
| 7 | Aa | 167 | ASN |
| 7 | Aa | 175 | ASN |
| 7 | Ab | 91 | ASN |
| 7 | Ab | 143 | GLN |
| 7 | Ab | 167 | ASN |
| 7 | Ab | 177 | GLN |
| 6 | Ac | 282 | HIS |
| 6 | Ac | 356 | GLN |
| 6 | Ad | 171 | GLN |
| 6 | Ad | 195 | GLN |
| 6 | Ad | 356 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | Ad | 381 | ASN |
| 6 | Ae | 105 | ASN |
| 6 | Ae | 497 | GLN |
| 6 | Af | 115 | GLN |
| 6 | Af | 240 | ASN |
| 6 | Af | 315 | GLN |
| 6 | Af | 367 | GLN |
| 6 | Ag | 335 | GLN |
| 6 | Ag | 367 | GLN |
| 6 | Ag | 431 | GLN |
| 6 | Ah | 157 | GLN |
| 6 | Ah | 195 | GLN |
| 6 | Ah | 303 | ASN |
| 6 | Ah | 384 | ASN |
| 6 | Ai | 115 | GLN |
| 6 | Ai | 398 | GLN |
| 6 | Ak | 257 | GLN |
| 6 | Ak | 303 | ASN |
| 7 | Al | 221 | ASN |
| 7 | Al | 239 | GLN |
| 6 | Am | 115 | GLN |
| 6 | Am | 398 | GLN |
| 6 | An | 105 | ASN |
| 6 | An | 123 | GLN |
| 6 | An | 265 | GLN |
| 6 | An | 315 | GLN |
| 6 | An | 367 | GLN |
| 6 | Ao | 115 | GLN |
| 6 | Ao | 265 | GLN |
| 6 | Ao | 384 | ASN |
| 6 | Ap | 171 | GLN |
| 6 | Ap | 183 | GLN |
| 6 | Ap | 236 | GLN |
| 6 | Ap | 311 | ASN |
| 6 | Ap | 315 | GLN |
| 6 | Ap | 398 | GLN |
| 7 | Aq | 7 | GLN |
| 7 | Aq | 101 | ASN |
| 7 | Aq | 167 | ASN |
| 7 | Ar | 101 | ASN |
| 7 | Ar | 164 | ASN |
| 7 | Ar | 224 | HIS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | Ar | 239 | GLN |
| 7 | As | 175 | ASN |
| 7 | As | 200 | ASN |
| 7 | As | 220 | ASN |
| 7 | At | 39 | GLN |
| 7 | At | 91 | ASN |
| 6 | Au | 265 | GLN |
| 6 | Au | 356 | GLN |
| 6 | Au | 482 | ASN |
| 6 | Au | 497 | GLN |
| 5 | Av | 112 | ASN |
| 5 | Av | 124 | ASN |
| 5 | Av | 183 | GLN |
| 5 | Av | 382 | GLN |
| 5 | Av | 483 | HIS |
| 6 | Aw | 105 | ASN |
| 6 | Aw | 157 | GLN |
| 6 | Aw | 245 | ASN |
| 6 | Aw | 356 | GLN |
| 6 | Aw | 482 | ASN |
| 5 | Ax | 124 | ASN |
| 5 | Ax | 263 | GLN |
| 5 | Ax | 306 | ASN |
| 5 | Ax | 367 | GLN |
| 5 | Ax | 438 | ASN |
| 5 | Ax | 492 | GLN |
| 6 | Ay | 171 | GLN |
| 6 | Ay | 245 | ASN |
| 6 | Ay | 265 | GLN |
| 6 | Ay | 356 | GLN |
| 6 | Ay | 384 | ASN |
| 6 | Az | 72 | HIS |
| 6 | Az | 171 | GLN |
| 6 | Az | 191 | GLN |
| 6 | Az | 195 | GLN |
| 6 | Az | 240 | ASN |
| 6 | Az | 265 | GLN |
| 6 | Az | 398 | GLN |
| 2 | B1 | 16 | GLN |
| 2 | B1 | 274 | GLN |
| 2 | B1 | 439 | ASN |
| 2 | B1 | 462 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B1 | 511 | GLN |
| 2 | B1 | 513 | GLN |
| 2 | B1 | 576 | ASN |
| 2 | B2 | 52 | ASN |
| 2 | B2 | 98 | ASN |
| 2 | B2 | 211 | GLN |
| 2 | B2 | 329 | ASN |
| 2 | B2 | 453 | ASN |
| 2 | B2 | 498 | GLN |
| 2 | B2 | 511 | GLN |
| 2 | B3 | 286 | ASN |
| 2 | B3 | 347 | ASN |
| 2 | B3 | 453 | ASN |
| 2 | B3 | 462 | ASN |
| 2 | B3 | 511 | GLN |
| 2 | B3 | 621 | ASN |
| 2 | B3 | 636 | ASN |
| 2 | B4 | 328 | GLN |
| 2 | B4 | 576 | ASN |
| 2 | B5 | 34 | GLN |
| 2 | B5 | 70 | ASN |
| 2 | B5 | 211 | GLN |
| 2 | B5 | 213 | ASN |
| 2 | B5 | 286 | ASN |
| 2 | B5 | 329 | ASN |
| 2 | B5 | 486 | GLN |
| 2 | B5 | 513 | GLN |
| 2 | B5 | 552 | ASN |
| 2 | B5 | 576 | ASN |
| 2 | B5 | 612 | ASN |
| 2 | B6 | 21 | ASN |
| 2 | B6 | 465 | ASN |
| 2 | B6 | 486 | GLN |
| 2 | B6 | 519 | GLN |
| 2 | B6 | 593 | GLN |
| 2 | B6 | 641 | ASN |
| 2 | B7 | 98 | ASN |
| 2 | B7 | 144 | ASN |
| 2 | B7 | 213 | ASN |
| 2 | B7 | 523 | ASN |
| 5 | BA | 23 | GLN |
| 5 | BA | 59 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | BA | 438 | ASN |
| 5 | BA | 492 | GLN |
| 5 | BB | 249 | ASN |
| 5 | BB | 263 | GLN |
| 5 | BB | 324 | GLN |
| 5 | BB | 326 | HIS |
| 5 | BB | 382 | GLN |
| 5 | BB | 384 | GLN |
| 5 | BB | 438 | ASN |
| 5 | BB | 442 | ASN |
| 7 | BC | 132 | ASN |
| 7 | BC | 177 | GLN |
| 7 | BC | 239 | GLN |
| 5 | BD | 249 | ASN |
| 5 | BD | 291 | ASN |
| 5 | BD | 326 | HIS |
| 5 | BD | 384 | GLN |
| 7 | BE | 7 | GLN |
| 7 | BE | 167 | ASN |
| 7 | BE | 243 | ASN |
| 5 | BF | 85 | ASN |
| 5 | BF | 310 | ASN |
| 5 | BG | 19 | ASN |
| 5 | BG | 249 | ASN |
| 5 | BG | 382 | GLN |
| 5 | BG | 492 | GLN |
| 5 | BH | 124 | ASN |
| 5 | BH | 135 | ASN |
| 5 | BH | 136 | HIS |
| 5 | BH | 183 | GLN |
| 6 | BI | 115 | GLN |
| 6 | BJ | 90 | GLN |
| 6 | BJ | 236 | GLN |
| 6 | BK | 215 | GLN |
| 6 | BK | 315 | GLN |
| 6 | BK | 482 | ASN |
| 7 | BL | 91 | ASN |
| 7 | BL | 118 | ASN |
| 7 | BL | 167 | ASN |
| 6 | BM | 115 | GLN |
| 6 | BM | 123 | GLN |
| 6 | BM | 356 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | BM | 398 | GLN |
| 11 | BP | 39 | HIS |
| 11 | BP | 47 | GLN |
| 11 | BQ | 15 | GLN |
| 11 | BU | 63 | ASN |
| 11 | BV | 64 | GLN |
| 3 | BY | 22 | GLN |
| 3 | BZ | 55 | ASN |
| 3 | Ba | 22 | GLN |
| 3 | Ba | 83 | GLN |
| 3 | Bb | 22 | GLN |
| 3 | Bb | 35 | GLN |
| 3 | Bb | 147 | ASN |
| 3 | Bc | 31 | ASN |
| 3 | Bc | 83 | GLN |
| 3 | Bf | 136 | ASN |
| 3 | Bf | 147 | ASN |
| 3 | Bg | 59 | ASN |
| 3 | Bg | 136 | ASN |
| 3 | Bh | 95 | GLN |
| 3 | Bh | 141 | GLN |
| 3 | Bi | 147 | ASN |
| 3 | Bo | 148 | ASN |
| 2 | Bp | 166 | ASN |
| 2 | Bp | 211 | GLN |
| 2 | Bp | 347 | ASN |
| 2 | Bp | 371 | GLN |
| 2 | Bp | 523 | ASN |
| 2 | Bp | 630 | GLN |
| 2 | Bq | 34 | GLN |
| 2 | Bq | 98 | ASN |
| 2 | Bq | 144 | ASN |
| 2 | Bq | 211 | GLN |
| 2 | Bq | 286 | ASN |
| 2 | Bq | 329 | ASN |
| 2 | Bq | 390 | GLN |
| 2 | Bq | 593 | GLN |
| 2 | Bq | 630 | GLN |
| 2 | Br | 519 | GLN |
| 2 | Br | 523 | ASN |
| 2 | Bs | 286 | ASN |
| 2 | Bs | 519 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Bs | 552 | ASN |
| 2 | Bs | 593 | GLN |
| 2 | Bt | 286 | ASN |
| 2 | Bt | 428 | ASN |
| 2 | Bt | 523 | ASN |
| 2 | Bt | 621 | ASN |
| 2 | Bu | 428 | ASN |
| 2 | Bu | 513 | GLN |
| 2 | Bu | 523 | ASN |
| 2 | Bv | 76 | ASN |
| 2 | Bv | 274 | GLN |
| 2 | Bv | 511 | GLN |
| 2 | Bv | 519 | GLN |
| 2 | Bw | 98 | ASN |
| 2 | Bw | 211 | GLN |
| 2 | Bw | 329 | ASN |
| 2 | Bw | 425 | ASN |
| 2 | Bw | 439 | ASN |
| 2 | Bw | 495 | ASN |
| 2 | Bw | 576 | ASN |
| 2 | Bx | 70 | ASN |
| 2 | Bx | 200 | ASN |
| 2 | Bx | 211 | GLN |
| 2 | Bx | 523 | ASN |
| 2 | Bx | 552 | ASN |
| 2 | Bx | 563 | ASN |
| 2 | By | 70 | ASN |
| 2 | By | 278 | GLN |
| 2 | By | 291 | GLN |
| 2 | By | 347 | ASN |
| 2 | By | 439 | ASN |
| 2 | By | 457 | GLN |
| 2 | Bz | 52 | ASN |
| 2 | Bz | 98 | ASN |
| 2 | Bz | 144 | ASN |
| 2 | Bz | 211 | GLN |
| 2 | Bz | 390 | GLN |
| 2 | Bz | 401 | GLN |
| 2 | Bz | 576 | ASN |
| 2 | Bz | 641 | ASN |
| 4 | C | 27 | ASN |
| 4 | I | 73 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | J | 19 | GLN |
| 4 | K | 19 | GLN |
| 4 | M | 73 | ASN |
| 4 | P | 45 | ASN |
| 4 | R | 19 | GLN |
| 4 | S | 6 | ASN |
| 4 | S | 61 | ASN |
| 4 | T | 27 | ASN |
| 4 | V | 61 | ASN |
| 4 | V | 73 | ASN |
| 4 | W | 27 | ASN |
| 4 | X | 37 | GLN |
| 4 | X | 73 | ASN |
| 4 | Y | 19 | GLN |
| 4 | a | 45 | ASN |
| 4 | b | 45 | ASN |
| 4 | f | 73 | ASN |
| 4 | h | 6 | ASN |
| 4 | i | 6 | ASN |
| 4 | i | 37 | GLN |
| 4 | j | 45 | ASN |
| 4 | j | 73 | ASN |
| 1 | k | 109 | GLN |
| 1 | k | 188 | ASN |
| 1 | l | 52 | GLN |
| 1 | l | 78 | ASN |
| 1 | l | 109 | GLN |
| 1 | l | 126 | GLN |
| 1 | l | 192 | ASN |
| 1 | l | 206 | ASN |
| 1 | m | 91 | ASN |
| 1 | m | 182 | ASN |
| 1 | m | 211 | HIS |
| 1 | n | 34 | ASN |
| 1 | n | 78 | ASN |
| 1 | n | 91 | ASN |
| 1 | n | 121 | ASN |
| 1 | n | 163 | GLN |
| 1 | n | 182 | ASN |
| 1 | n | 192 | ASN |
| 3 | o | 31 | ASN |
| 3 | o | 95 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | o | 97 | ASN |
| 1 | p | 121 | ASN |
| 1 | p | 160 | GLN |
| 1 | p | 164 | ASN |
| 1 | p | 192 | ASN |
| 1 | p | 202 | ASN |
| 1 | p | 206 | ASN |
| 8 | q | 258 | ASN |
| 8 | r | 144 | HIS |
| 8 | r | 152 | GLN |
| 8 | r | 155 | ASN |
| 8 | s | 152 | GLN |
| 8 | s | 155 | ASN |
| 8 | s | 180 | ASN |
| 8 | s | 219 | ASN |
| 8 | t | 132 | GLN |
| 8 | t | 146 | ASN |
| 8 | t | 152 | GLN |
| 8 | t | 155 | ASN |
| 8 | t | 180 | ASN |
| 8 | u | 76 | ASN |
| 8 | u | 142 | GLN |
| 8 | u | 155 | ASN |
| 9 | w | 35 | GLN |
| 9 | y | 16 | ASN |
| 9 | z | 13 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no 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.

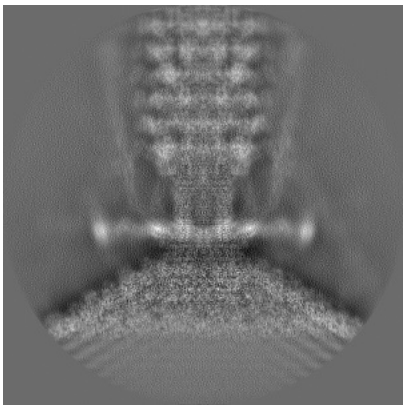
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48458. These allow visual inspection of the internal detail of the map and identification of artifacts.

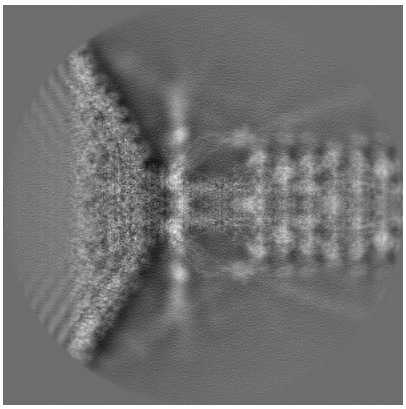
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

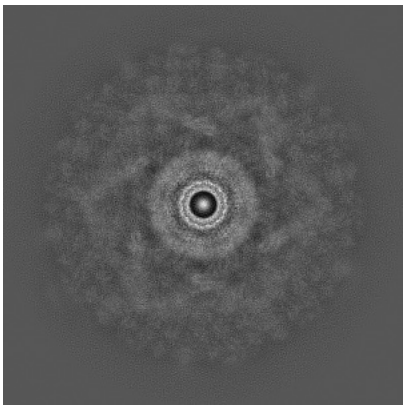
### 6.1.1 Primary map



X

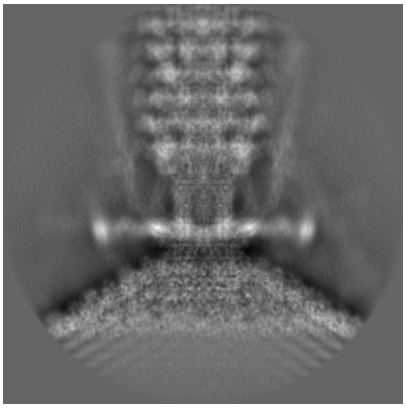


Y

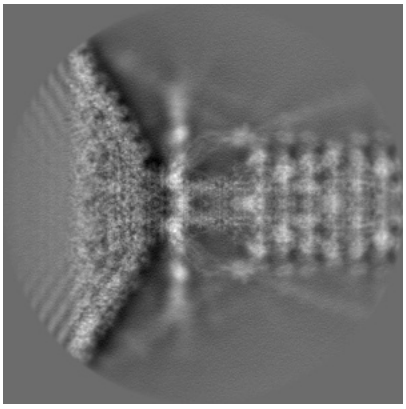


Z

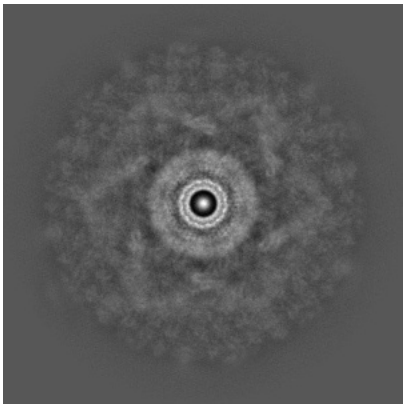
### 6.1.2 Raw map



X



Y

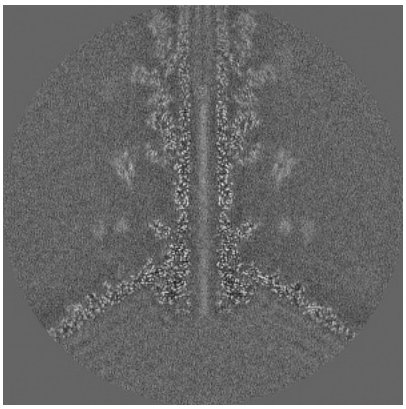


Z

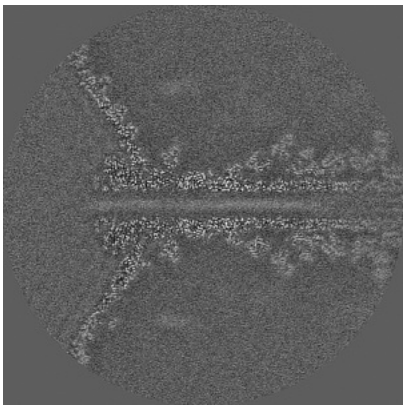
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

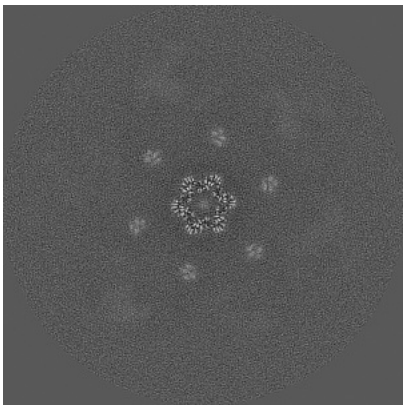
### 6.2.1 Primary map



X Index: 200

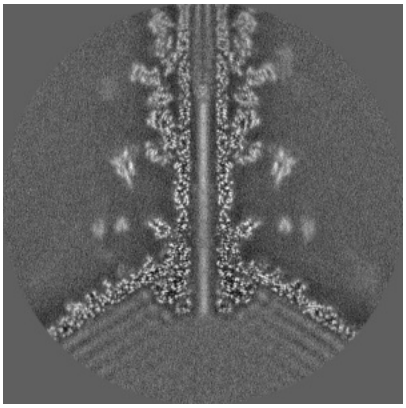


Y Index: 200

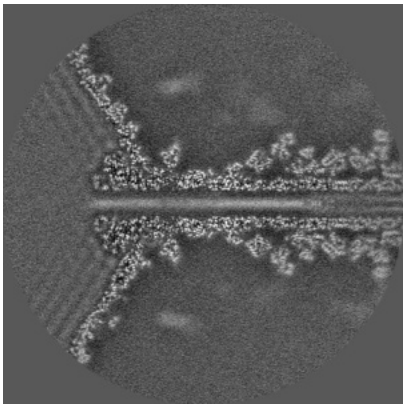


Z Index: 200

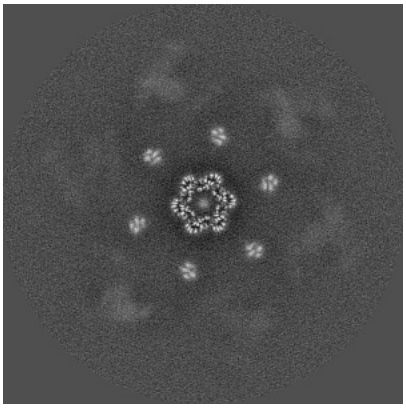
### 6.2.2 Raw map



X Index: 200



Y Index: 200

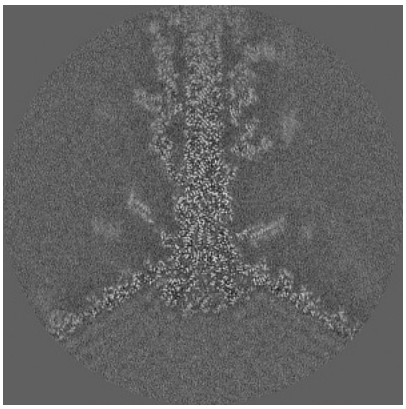


Z Index: 200

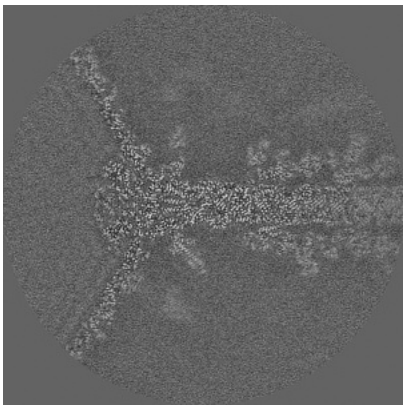
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

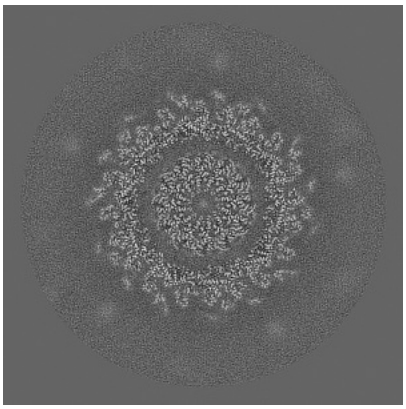
### 6.3.1 Primary map



X Index: 184

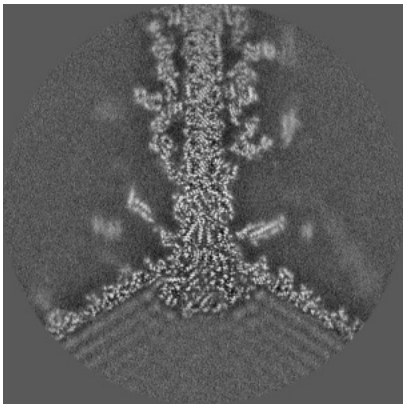


Y Index: 184

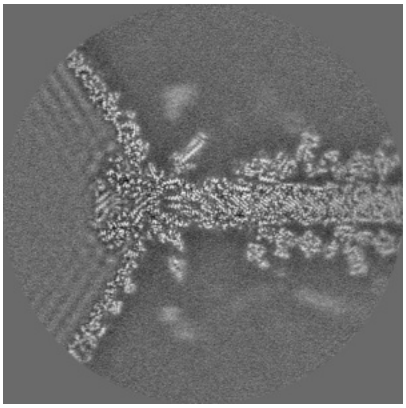


Z Index: 115

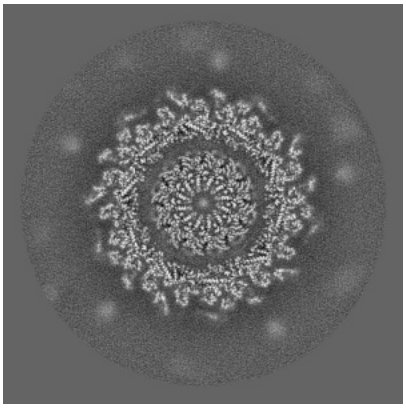
### 6.3.2 Raw map



X Index: 184



Y Index: 215

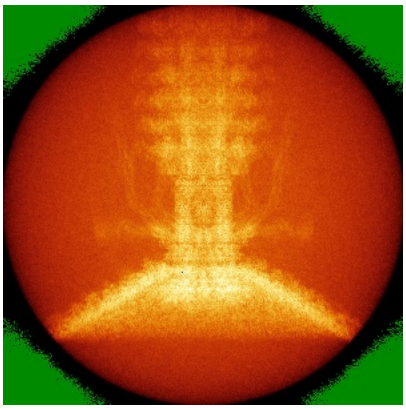


Z Index: 115

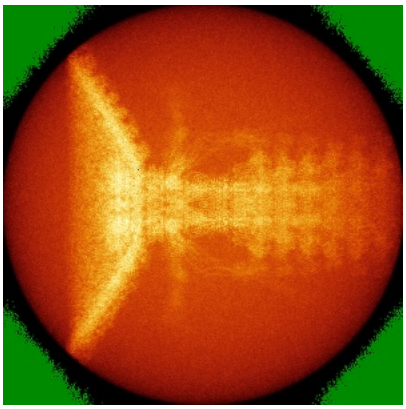
The images above show the largest variance slices of the map in three orthogonal directions.

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

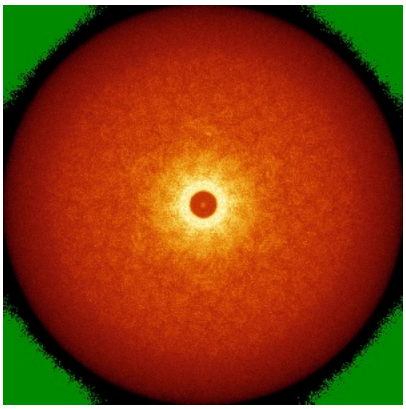
### 6.4.1 Primary map



X

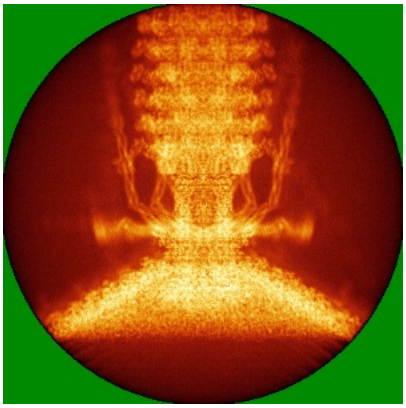


Y

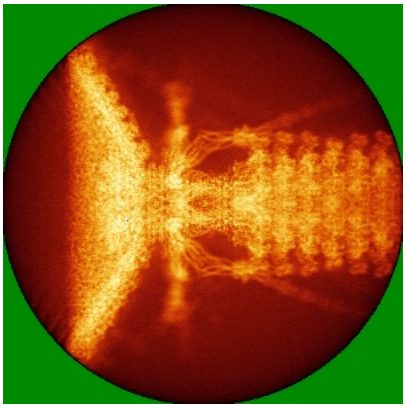


Z

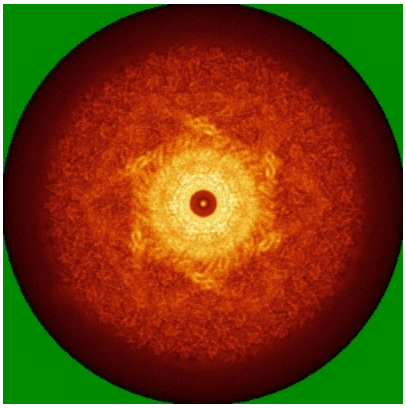
### 6.4.2 Raw map



X



Y

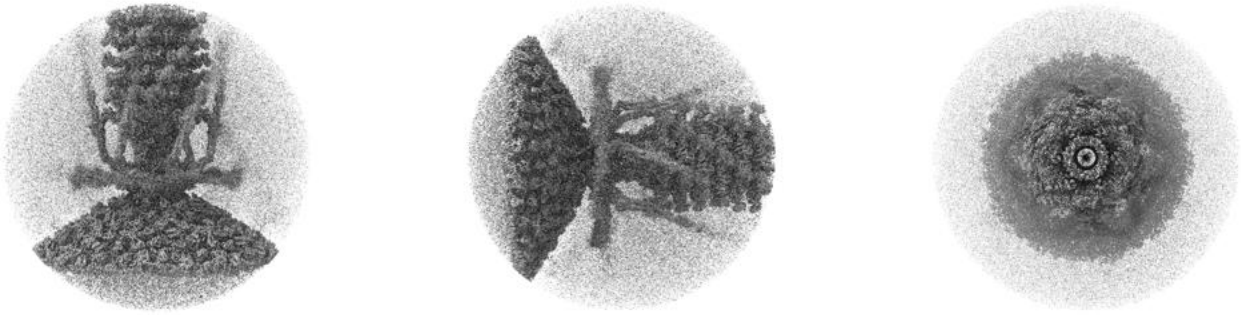


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

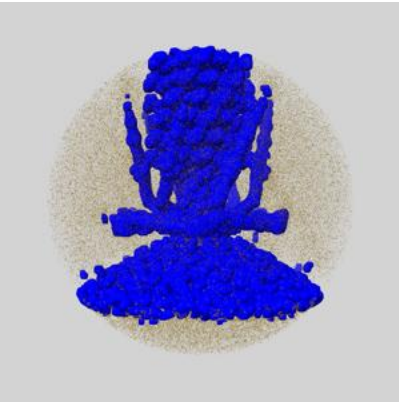
## 6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

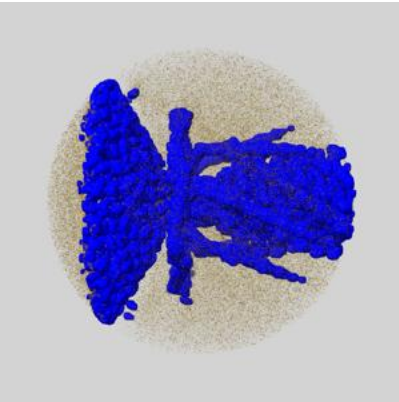
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

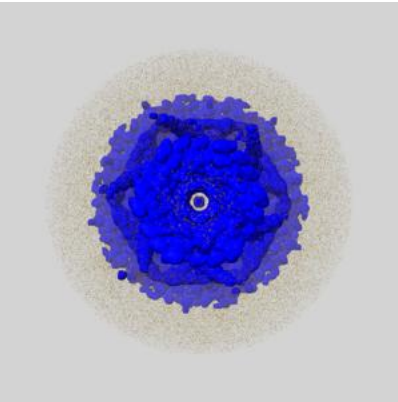
### 6.6.1 emd_48458_msk_1.map (i)



X



Y

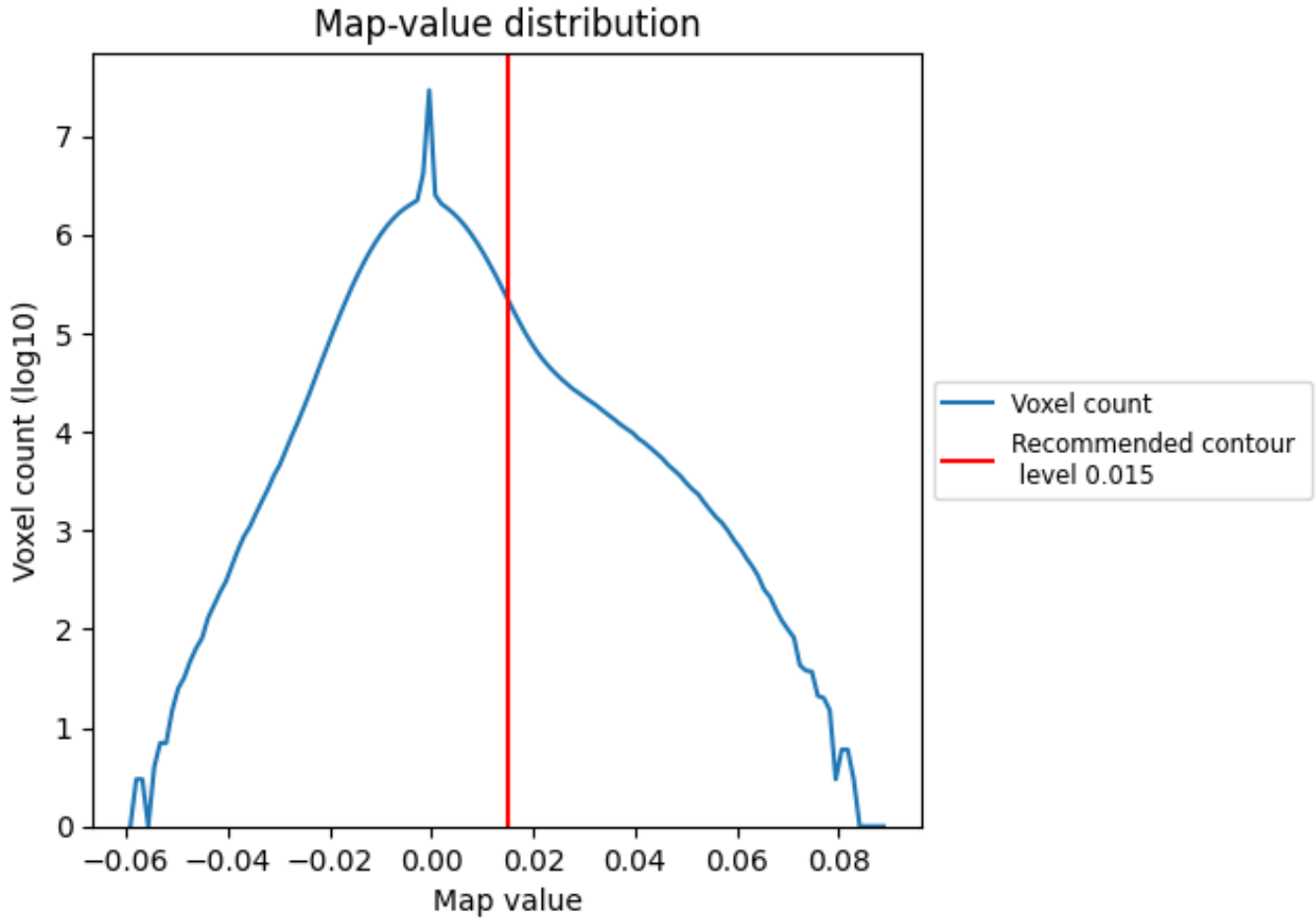


Z

# 7 Map analysis

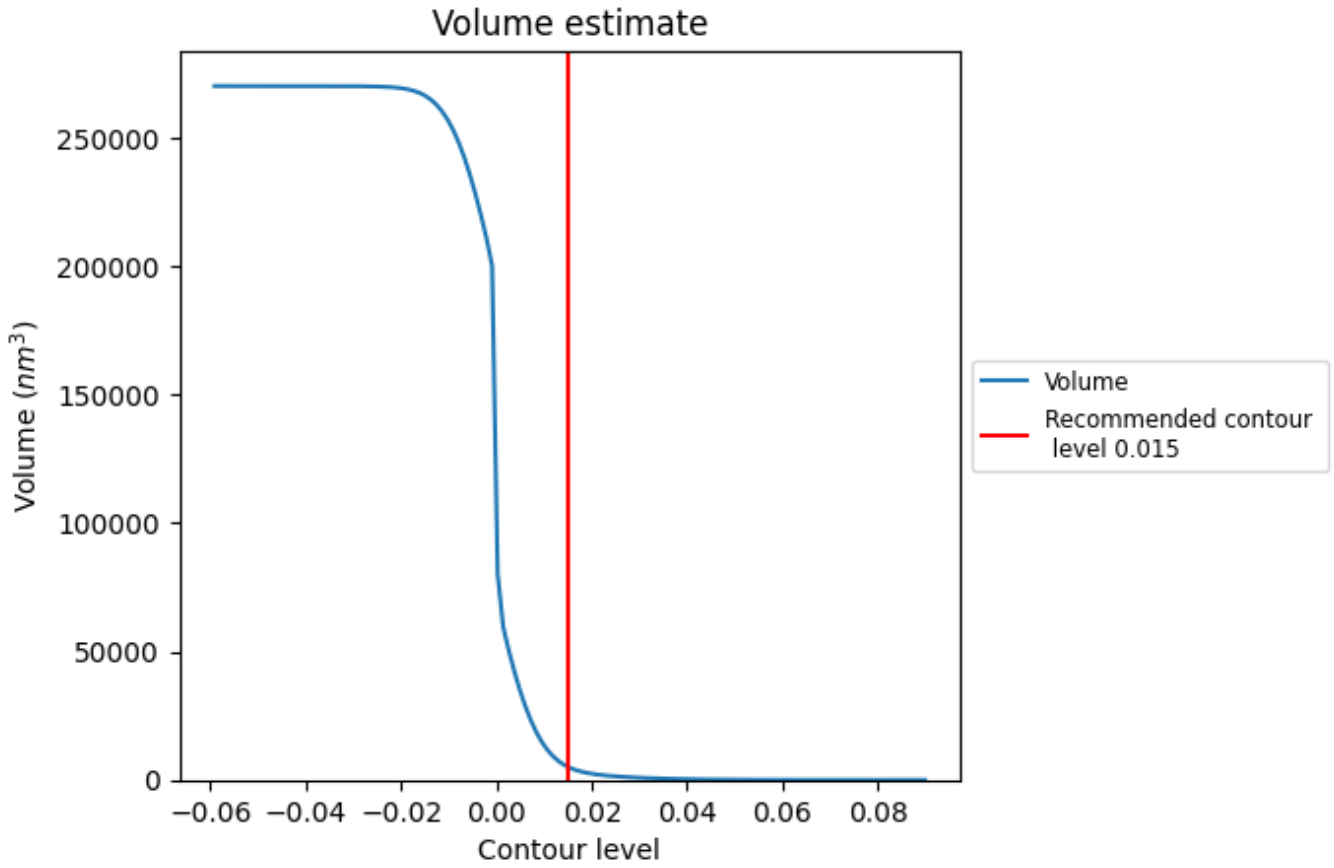
This section contains the results of statistical analysis of the map.

## 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.

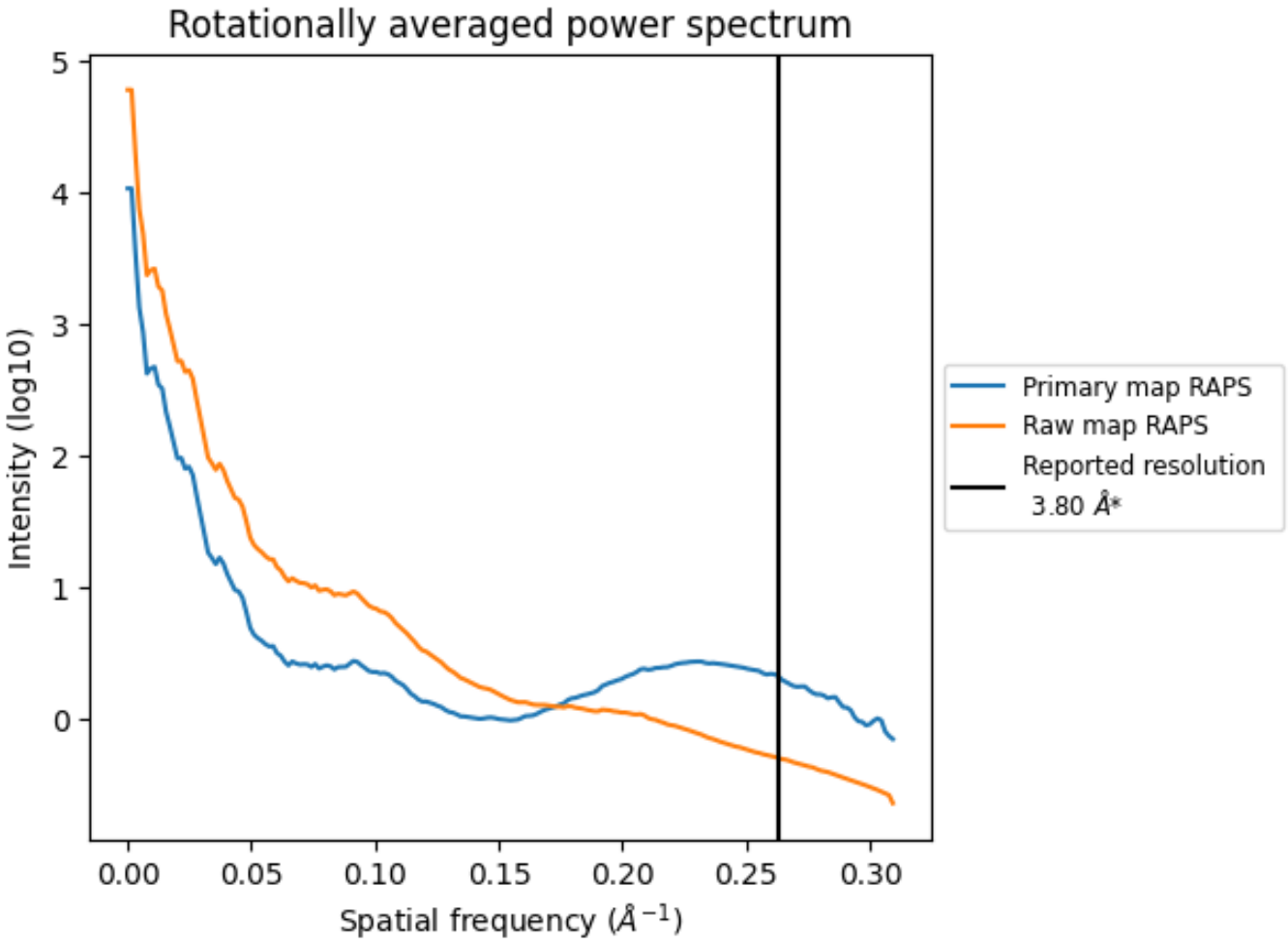
## 7.2 Volume estimate




The volume at the recommended contour level is 5141 $nm^3$; this corresponds to an approximate mass of 4644 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)

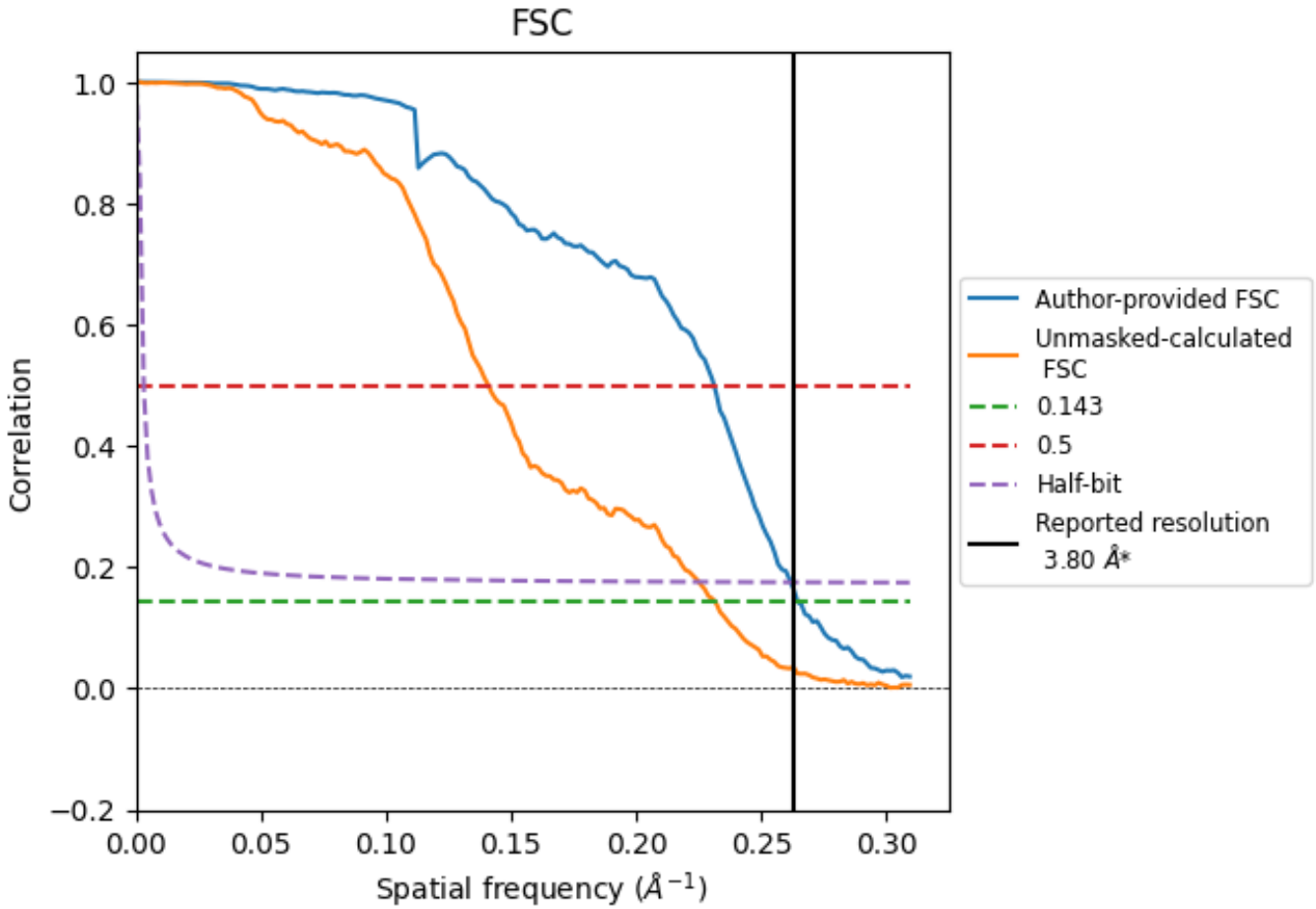



*Reported resolution corresponds to spatial frequency of 0.263 Å$^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.263 Å$^{-1}$

## 8.2 Resolution estimates (i)

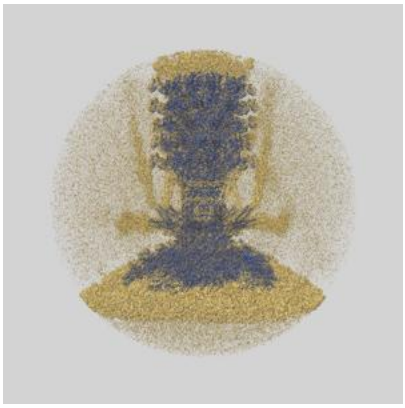
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.80 | - | - |
| Author-provided FSC curve | 3.78 | 4.33 | 3.82 |
| Unmasked-calculated* | 4.32 | 7.10 | 4.44 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.8 by more than 10 %

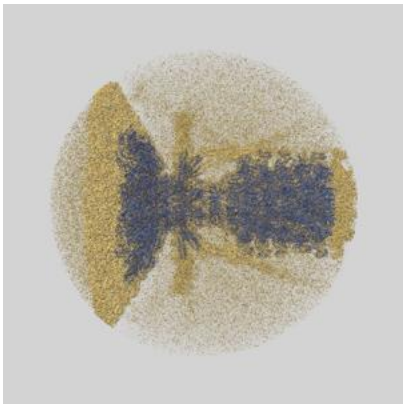
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48458 and PDB model 9MOF. Per-residue inclusion information can be found in section 3 on page 23.

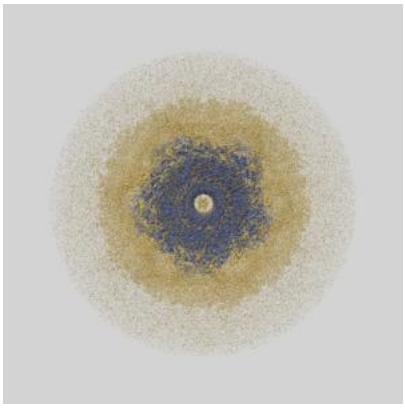
## 9.1 Map-model overlay



X



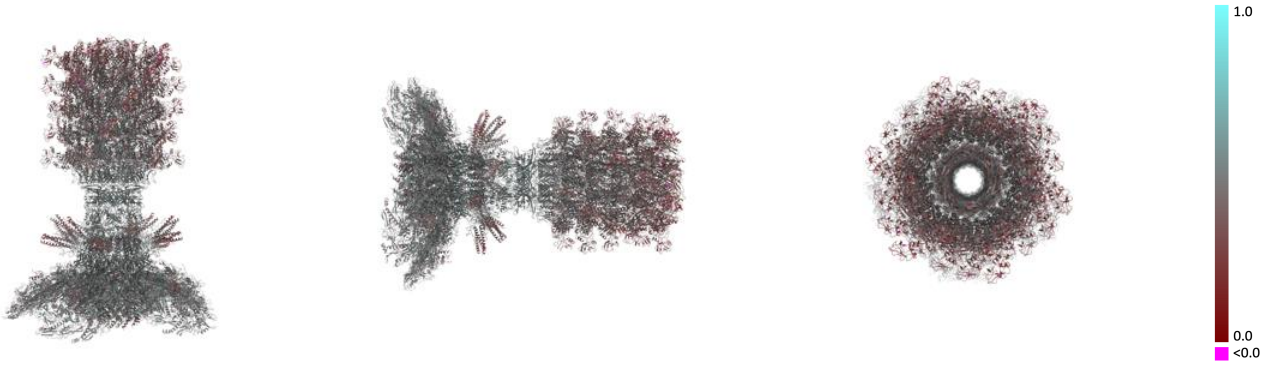
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

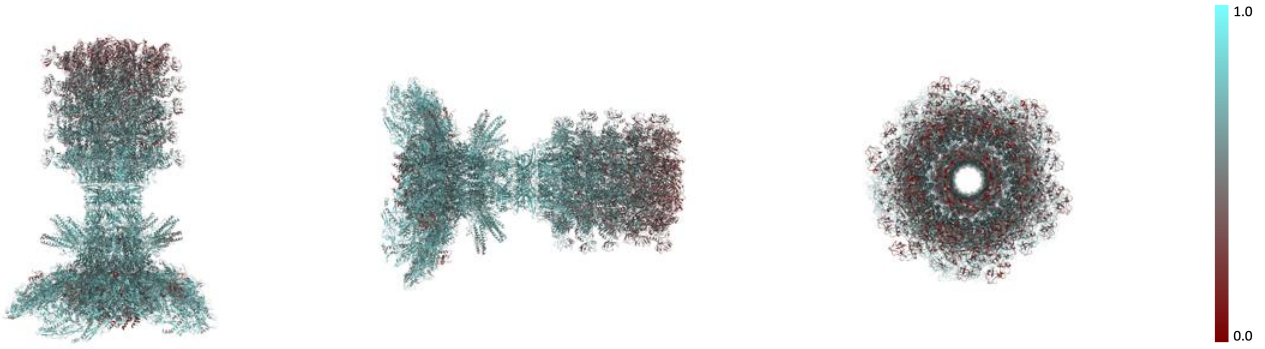
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

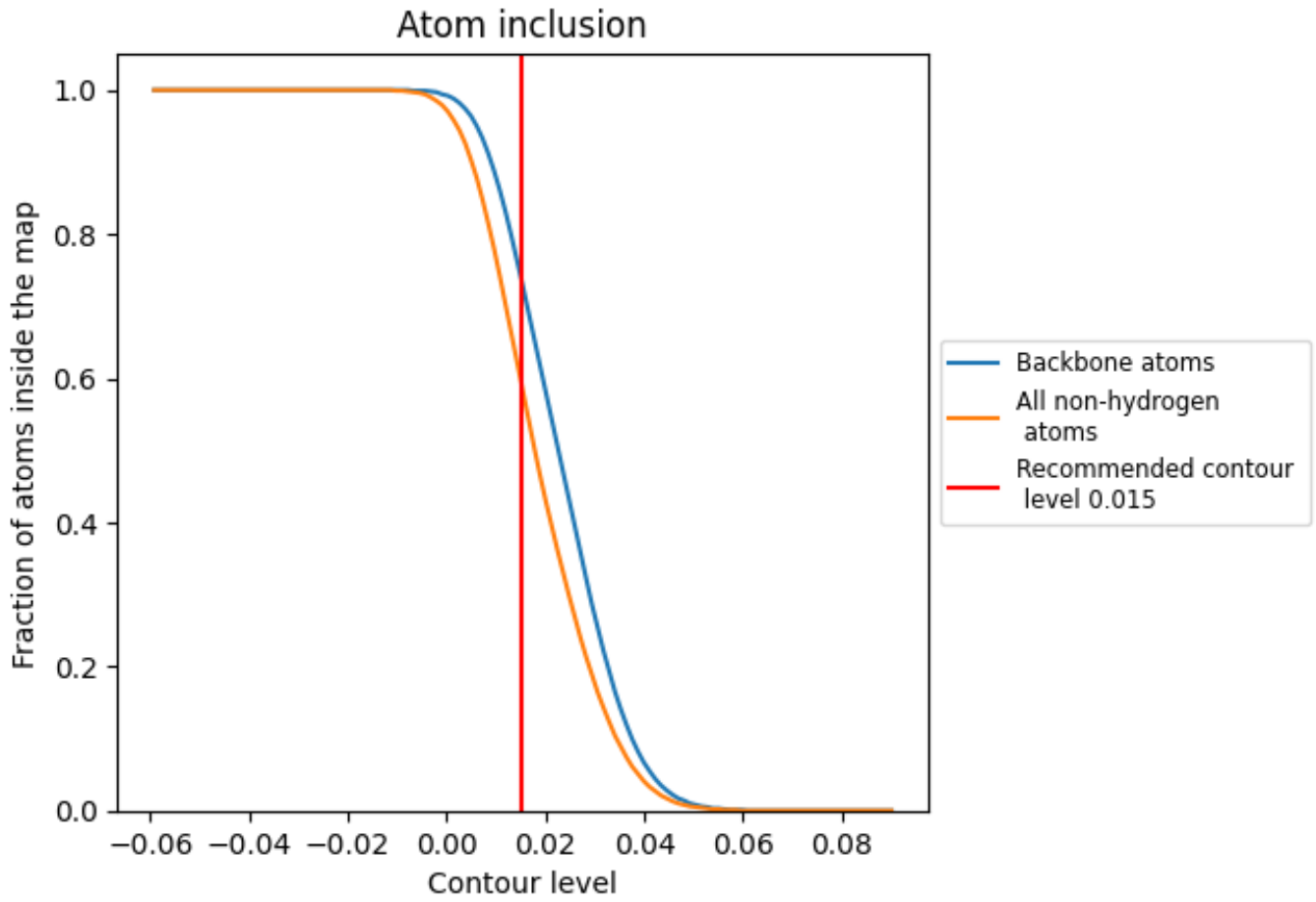
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

## 9.4 Atom inclusion (i)




At the recommended contour level, 74% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5960 | 0.4460 |
| 0 | 0.7510 | 0.5060 |
| 1 | 0.6370 | 0.4330 |
| 2 | 0.6330 | 0.4280 |
| 3 | 0.6410 | 0.4320 |
| 4 | 0.6490 | 0.4340 |
| 5 | 0.6450 | 0.4300 |
| 6 | 0.6820 | 0.4960 |
| 7 | 0.6860 | 0.4970 |
| 8 | 0.7000 | 0.4940 |
| 9 | 0.6980 | 0.5070 |
| A | 0.6740 | 0.4400 |
| A0 | 0.5520 | 0.4700 |
| A1 | 0.5420 | 0.4710 |
| A2 | 0.5400 | 0.4600 |
| A3 | 0.5550 | 0.4680 |
| A4 | 0.6720 | 0.4820 |
| A5 | 0.6670 | 0.4790 |
| A6 | 0.6800 | 0.4920 |
| A7 | 0.6820 | 0.4840 |
| A8 | 0.6870 | 0.4890 |
| A9 | 0.6890 | 0.4910 |
| AA | 0.6970 | 0.5060 |
| AB | 0.7490 | 0.4970 |
| AC | 0.7210 | 0.5090 |
| AD | 0.6360 | 0.4300 |
| AE | 0.6730 | 0.4890 |
| AF | 0.6650 | 0.4960 |
| AG | 0.6550 | 0.4890 |
| AH | 0.6640 | 0.4860 |
| AI | 0.6560 | 0.4900 |
| AJ | 0.6460 | 0.4830 |
| AK | 0.5860 | 0.4210 |
| AL | 0.5830 | 0.4180 |
| AM | 0.5760 | 0.4170 |




*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| AN | 0.5570 | 0.4110 |
| AO | 0.5570 | 0.4090 |
| AP | 0.5690 | 0.4120 |
| AQ | 0.2760 | 0.3540 |
| AR | 0.3000 | 0.3680 |
| AS | 0.3120 | 0.3770 |
| AT | 0.3180 | 0.3670 |
| AU | 0.3330 | 0.3880 |
| AV | 0.6960 | 0.4960 |
| AW | 0.6550 | 0.4700 |
| AX | 0.6850 | 0.4880 |
| AY | 0.6960 | 0.5000 |
| AZ | 0.6840 | 0.4940 |
| Aa | 0.6870 | 0.5030 |
| Ab | 0.6910 | 0.4970 |
| Ac | 0.6690 | 0.4750 |
| Ad | 0.6790 | 0.4800 |
| Ae | 0.6730 | 0.4820 |
| Af | 0.6520 | 0.4660 |
| Ag | 0.6540 | 0.4700 |
| Ah | 0.6700 | 0.4800 |
| Ai | 0.6530 | 0.4710 |
| Aj | 0.6610 | 0.4760 |
| Ak | 0.6730 | 0.4800 |
| Al | 0.6760 | 0.4900 |
| Am | 0.6820 | 0.4880 |
| An | 0.6790 | 0.4850 |
| Ao | 0.6910 | 0.4910 |
| Ap | 0.6900 | 0.4880 |
| Aq | 0.6780 | 0.4940 |
| Ar | 0.7000 | 0.4960 |
| As | 0.6730 | 0.4950 |
| At | 0.6500 | 0.4800 |
| Au | 0.6970 | 0.4940 |
| Av | 0.5470 | 0.4710 |
| Aw | 0.6750 | 0.4860 |
| Ax | 0.5600 | 0.4760 |
| Ay | 0.6840 | 0.4930 |
| Az | 0.6690 | 0.4790 |
| B | 0.6850 | 0.4550 |
| B1 | 0.3570 | 0.3380 |
| B2 | 0.5220 | 0.3920 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| B3 | 0.4490 | 0.3750 |
| B4 | 0.3390 | 0.3300 |
| B5 | 0.5150 | 0.3970 |
| B6 | 0.4460 | 0.3710 |
| B7 | 0.3490 | 0.3440 |
| BA | 0.5610 | 0.4710 |
| BB | 0.5610 | 0.4750 |
| BC | 0.6750 | 0.4940 |
| BD | 0.5440 | 0.4680 |
| BE | 0.6880 | 0.4960 |
| BF | 0.5440 | 0.4640 |
| BG | 0.5640 | 0.4710 |
| BH | 0.5550 | 0.4700 |
| BI | 0.6780 | 0.4860 |
| BJ | 0.6950 | 0.4890 |
| BK | 0.7000 | 0.4920 |
| BL | 0.6830 | 0.4930 |
| BM | 0.6950 | 0.4920 |
| BN | 0.6780 | 0.4890 |
| BO | 0.6850 | 0.4830 |
| BP | 0.6750 | 0.4740 |
| BQ | 0.6720 | 0.4710 |
| BR | 0.6850 | 0.4870 |
| BS | 0.6740 | 0.4720 |
| BT | 0.6830 | 0.4730 |
| BU | 0.6590 | 0.4660 |
| BV | 0.6990 | 0.4950 |
| BW | 0.6820 | 0.4820 |
| BX | 0.5800 | 0.4750 |
| BY | 0.4890 | 0.4440 |
| BZ | 0.3490 | 0.4000 |
| Ba | 0.5980 | 0.4740 |
| Bb | 0.4960 | 0.4430 |
| Bc | 0.3290 | 0.3990 |
| Bd | 0.5960 | 0.4700 |
| Be | 0.4800 | 0.4330 |
| Bf | 0.3290 | 0.4020 |
| Bg | 0.5970 | 0.4800 |
| Bh | 0.4750 | 0.4350 |
| Bi | 0.3450 | 0.3830 |
| Bj | 0.5920 | 0.4690 |
| Bk | 0.4800 | 0.4460 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| Bl | 0.3250 | 0.3940 |
| Bm | 0.5930 | 0.4790 |
| Bn | 0.4710 | 0.4370 |
| Bo | 0.3320 | 0.3980 |
| Bp | 0.5430 | 0.4020 |
| Bq | 0.4620 | 0.3810 |
| Br | 0.3510 | 0.3370 |
| Bs | 0.5480 | 0.4050 |
| Bt | 0.4750 | 0.3800 |
| Bu | 0.3620 | 0.3440 |
| Bv | 0.5520 | 0.4100 |
| Bw | 0.4800 | 0.3830 |
| Bx | 0.3650 | 0.3360 |
| By | 0.5350 | 0.3980 |
| Bz | 0.4580 | 0.3770 |
| C | 0.6730 | 0.4530 |
| D | 0.6800 | 0.4410 |
| E | 0.6800 | 0.4370 |
| F | 0.6850 | 0.4320 |
| G | 0.7270 | 0.4400 |
| H | 0.7020 | 0.4370 |
| I | 0.6970 | 0.4280 |
| J | 0.6880 | 0.4450 |
| K | 0.6980 | 0.4290 |
| L | 0.6710 | 0.4370 |
| M | 0.6320 | 0.3820 |
| N | 0.6190 | 0.3890 |
| O | 0.6390 | 0.4300 |
| P | 0.6530 | 0.4100 |
| Q | 0.6780 | 0.4350 |
| R | 0.6810 | 0.4310 |
| S | 0.6610 | 0.4310 |
| T | 0.6800 | 0.4340 |
| U | 0.6510 | 0.4330 |
| V | 0.6730 | 0.4140 |
| W | 0.6440 | 0.4090 |
| X | 0.6420 | 0.3940 |
| Y | 0.6510 | 0.4250 |
| Z | 0.6590 | 0.4080 |
| a | 0.6220 | 0.3840 |
| b | 0.6290 | 0.4020 |
| c | 0.6120 | 0.3760 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| d | 0.6260 | 0.3850 |
| e | 0.6140 | 0.3820 |
| f | 0.6370 | 0.4130 |
| g | 0.6360 | 0.4150 |
| h | 0.6190 | 0.4280 |
| i | 0.6000 | 0.4120 |
| j | 0.5970 | 0.4130 |
| k | 0.7490 | 0.4990 |
| l | 0.7400 | 0.5020 |
| m | 0.7480 | 0.5010 |
| n | 0.7550 | 0.5020 |
| o | 0.6970 | 0.5070 |
| p | 0.7510 | 0.4980 |
| q | 0.7380 | 0.4950 |
| r | 0.7460 | 0.4980 |
| s | 0.7390 | 0.4910 |
| t | 0.7340 | 0.4960 |
| u | 0.7410 | 0.4940 |
| v | 0.7210 | 0.5080 |
| w | 0.7140 | 0.5030 |
| x | 0.7200 | 0.5080 |
| y | 0.7340 | 0.5070 |
| z | 0.7160 | 0.5050 |