**Supplementary Table 2.** Molecular docking parameters of the interactions between the plant cystatins and SARS-CoV-2 Mpro dimer

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Inhibitor**  **(PDB ID)** | **FRODOCKa** | **Punctuationb** | **ClusProc** | **Punctuationb,d** | **Sume** |
| 2MZV | 3583.961 | 1.000 | -1058.1 | 0.875 | 1.875 |
| 2L4V | 3193.857 | 0.875 | -1122.2 | 1.000 | 1.875 |
| 2GZB | 3150.900 | 0.750 | -829.7 | 0.500 | 1.250 |
| 4TX4 | 3136.427 | 0.625 | -830.1 | 0.625 | 1.000 |
| 2W9Q | 2977.104 | 0.500 | -709.4 | 0.375 | 0.875 |
| 1EQK | 2860.555 | 0.375 | -903.1 | 0.750 | 1.125 |

a Docking score values calculated by FRODOCK v.3.12 server.

b,d Punctuation associated to both FRODOCK score and ClusPro lowest biding energy. A punctuation of 1 was attributed to inhibitor with high docking score or with the lowest biding energy. The subsequent scores were calculated by decreasing 0.125 as the docking score values decrease (or the value of biding energy) when compared to inhibitor that received score 1.

c  Biding free energies (ΔG) calculated by ClusPro server.

e Sum of the punctuation (scores) calculated in b and d.

**Supplementary Table 3.** Quantum description of the multi-point interactions between Pineapple cystatin and SARS-CoV-2 Mpro

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Amino acid residues** | | **Distance** | **Interaction energy** | **Residue charge** | |  | **Residue atom** | |
| MPro | Pineapple cystatin | (Å) | (kcal mol-1) | MPro | Pineapple cystatin |  | MPro | Pineapple cystatin |
| GLU270 (C) | LYS73 | 1.59 | -8.80 | -1 | 1 |  | OE1 | HZ3 |
| ARG279 (C) | GLU15 | 1.66 | -13.86 | 1 | -1 |  | HH11 | OE2 |
| ARG279 (C) | ARG124 | 1.73 | -6.03 | 1 | 1 |  | HH22 | O |
| GLN192 (A) | MET43 | 1.91 | -9.29 | 0 | 0 |  | H | O |
| LYS236 (A) | GLU20 | 2.08 | -11.31 | 1 | -1 |  | HZ3 | OE2 |
| ALA193 (A) | ILE42 | 2.09 | -4.67 | 0 | 0 |  | H | O |
| THR169 (A) | MET94 | 2.29 | -4.02 | 0 | 0 |  | HB | HB1 |
| PRO168 (A) | VAL90 | 2.29 | -4.19 | 0 | 0 |  | HG1 | HG12 |
| LEU220 (C) | VAL10 | 2.33 | -4.10 | 0 | 0 |  | H | O |
| THR280 (C) | MET121 | 2.51 | -3.42 | 0 | 0 |  | H | SD |
| ALA194 (A) | HIS40 | 2.56 | -4.89 | 0 | 0 |  | O | HE1 |
| ARG279 (C) | PHE123 | 2.57 | -6.07 | 1 | 0 |  | HH11 | HD2 |
| ARG217 (C) | PRO9 | 2.64 | -5.09 | 1 | 0 |  | HG2 | HA |
| ARG222 (C) | PRO11 | 2.79 | -3.01 | 1 | 0 |  | HG2 | HG2 |
| ARG279 (C) | MET121 | 2.90 | -7.20 | 1 | 0 |  | HD2 | HE1 |
| ALA191 (A) | MET43 | 3.10 | -5.74 | 0 | 0 |  | HA | O |
| TRP218 (C) | PRO11 | 3.11 | 1.78 | 0 | 0 |  | O | C |
| GLN192 (A) | ILE42 | 3.21 | -4.19 | 0 | 0 |  | H | O |
| ARG279 (C) | GLN125 | 3.34 | -3.76 | 1 | 0 |  | HH22 | HB1 |
| GLU270 (C) | GLU14 | 7.16 | 1.50 | -1 | -1 |  | OE1 | OE2 |

**Supplementary Table 4.** Quantum description of the multi-point interactions between Pineapple cystatin and SARS-CoV-2 Mpro

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Amino acid residues** | | **Distance** | **Interaction energy** | **Residue charge** | |  | **Residue atom** | |
| MPro | Sesame Cystatin | (Å) | (kcal mol-1) | MPro | Sesame Cystatin |  | MPro | Sesame Cystatin |
| ASN142 (C) | HIS117 | 1.70 | -7.00 | 0 | 0 |  | HD22 | O |
| LYS137 (C) | TRP77 | 1.72 | -12.69 | 1 | 0 |  | HA | HE1 |
| LYS236 (C) | ASP15 | 1.83 | -9.19 | 1 | -1 |  | O | HN |
| THR196 (C) | THR3 | 1.83 | -14.49 | 0 | 0 |  | HG1 | O |
| ALA194 (C) | VAL7 | 1.96 | -5.60 | 0 | 0 |  | O | HN |
| THR196 (C) | LEU4 | 1.98 | -5.31 | 0 | 0 |  | HG1 | HA |
| LYS236 (C) | PRO14 | 2.06 | -9.05 | 1 | 0 |  | HA | HA |
| THR196 (C) | HIS8 | 2.13 | -5.59 | 0 | 0 |  | HN | O |
| GLN256 (A) | HIS149 | 2.16 | -7.60 | 0 | 0 |  | HE21 | ND1 |
| MET235 (C) | ASN13 | 2.30 | -7.54 | 0 | 0 |  | O | HD22 |
| LEU220 (A) | TRP111 | 2.32 | -5.40 | 0 | 0 |  | HD13 | HB1 |
| ASP197 (C) | ALA2 | 2.39 | -16.19 | -1 | 0 |  | OD2 | HA |
| GLY195 (C) | HIS8 | 2.41 | -8.74 | 0 | 0 |  | HA2 | HN |
| THR257 (A) | ASN151 | 2.69 | -4.90 | 0 | 0 |  | O | HB1 |
| THR196 (C) | ASP9 | 2.80 | -4.76 | 0 | -1 |  | HB | HA |
| TYR237 (C) | PRO14 | 3.20 | -5.10 | 0 | 0 |  | C | HB1 |
| ARG131 (C) | MET1 | 3.77 | -5.42 | -2 | 1 |  | HH12 | HE2 |
| ARG131 (C) | ALA2 | 4.95 | 7.53 | -2 | 0 |  | HH22 | HB1 |
| ILE200 (C) | ALA2 | 6.39 | 7.50 | 0 | 0 |  | N | HB1 |
| ILE200 (C) | MET1 | 6.59 | 7.33 | 0 | 1 |  | HN | HE2 |

**Supplementary Table 5.** Amino acid residues that participate in the formation of hydrogen bond, hydrophobic, cation-pi, and ionic interactions between Pineapple cystatin and SARS-CoV-2 Mpro

|  |  |  |
| --- | --- | --- |
| **Interaction** | **MPro** | **Pineapple cystatin** |
|  | Residue | Residue |
| Hydrophobic | LEU220 (C) | PRO9 |
| TRP218 (C) | VAL10 |
| PHE219 (C) | ALA12 |
| TRP218 (C) | MET121 |
| LEU50 (A) | ILE46 |
| LEU50 (A) | TYR47 |
| PRO168 (A) | VAL90 |
| VAL171 (A) | VAL119 |
| VAL171 (A) | MET43 |
| ALA191 (A) | MET43 |
| Hydrogen bonds | TRP218 (C) | ALA12 |
| PHE219 (C) | VAL10 |
| LEU220 (C) | VAL10 |
| ASN274 (C) | ALA13 |
| ARG279 (C) | ARG124 |
| THR280 (C) | MET121 |
| GLU270 (C) | LYS73 |
| ARG279 (C) | GLU15 |
| ALA191 (A) | GLY44 |
| GLN192 (A) | MET43 |
| ALA193 (A) | ILE42 |
| THR169 (A) | MET94 |
| THR169 (A) | MET43 |
| LYS236 (A) | GLU20 |
| Ionic | ARG279 (C) | GLU15 |
| GLU270 (C) | LYS73 |
| LYS236 (A) | GLU20 |
| Cation-Pi | ARG279 (C) | PHE123 |

**Supplementary Table 6.** Amino acid residues that participate in the formation of hydrogen bond, hydrophobic, cation-pi, ionic and aromatic-sulphur interactions between Sesame cystatin and SARS-CoV-2 Mpro

|  |  |  |
| --- | --- | --- |
| **Interaction** | **Mpro** | **Sesame  cystatin** |
|  | Residue | Residue |
| Hydrophobic | TYR239 (C) | MET1 |
| LEU287 (C) | MET1 |
| PRO184 (C) | VAL7 |
| ALA193 (C) | VAL7 |
| PRO168 (C) | ALA49 |
| VAL171 (C) | TRP77 |
| LEU286 (C) | MET78 |
| LEU141 (C) | PRO115 |
| LEU141 (C) | VAL116 |
| VAL212 (A) | PRO113 |
| ILE213 (A) | PRO113 |
| LEU220 (A) | TRP111 |
| ILE259 (A) | TRP111 |
| Hydrogen bonds | ALA194 (C) | VAL7 |
| LYS236 (C) | ASP15 |
| THR196 (C) | GLY5 |
| THR196 (C) | HIS8 |
| ASP197 (C) | THR3 |
| MET235 (C) | ASN13 |
| LYS137 (C) | TRP77 |
| ASN142 (C) | HIS117 |
| THR196 (C) | THR3 |
| ASN238 (C) | SER10 |
| ASN238 (C) | ASN13 |
| TYR239 (C) | MET1 |
| ARG217 (A) | GLN107 |
| GLN258 (A) | HIS149 |
| GLY258 (A) | ASN151 |
| ALA255 (A) | ASN151 |
| GLN256 (A) | HIS149 |
|  | ARG217 (A) | GLN107 |
| Ionic | ARG217 (A) | ASP106 |
| Aromatic-Sulphur | TYR239 (C) | MET1 |
| Cation-Pi | TYR279 (A) | PHE80 |

**Supplementary Table 7.** Quantum Biochemistry description of the interactions between Pineapple cystatin and SARS-CoV-2 Mpro.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Amino acid residues** | | **Distance** | **Interaction energy** | **Residue charge** | |  | **Residue atom** | |
| MPro | Pineapple cystatin | (Å) | (kcal mol-1) | Mpro | Pineapple cystatin |  | Mpro | Pineapple cystatin |
| GLU270 (C) | LYS73 | 1.59 | -8.80 | -1 | 1 |  | OE1 | HZ3 |
| ARG279 (C) | GLU15 | 1.66 | -13.86 | 1 | -1 |  | HH11 | OE2 |
| ARG279 (C) | ARG124 | 1.73 | -6.03 | 1 | 1 |  | HH22 | O |
| GLN192 (A) | MET43 | 1.91 | -9.29 | 0 | 0 |  | H | O |
| ALA193 (A) | MET43 | 1.94 | -1.86 | 0 | 0 |  | H | HB2 |
| GLU270 (C) | ALA12 | 2.05 | -0.04 | -1 | 0 |  | HG2 | H |
| LYS236 (A) | GLU20 | 2.08 | -11.31 | 1 | -1 |  | HZ3 | OE2 |
| ALA193 (A) | ILE42 | 2.09 | -4.67 | 0 | 0 |  | H | O |
| THR169 (A) | MET43 | 2.20 | -2.70 | 0 | 0 |  | HG22 | HG2 |
| GLY278 (C) | PHE123 | 2.22 | -1.65 | 0 | 0 |  | HA2 | HZ |
| ASN221 (C) | PRO11 | 2.22 | -1.26 | 0 | 0 |  | HA | HB2 |
| GLY170 (A) | VAL119 | 2.25 | -0.97 | 0 | 0 |  | HA2 | HG22 |
| VAL171 (A) | MET43 | 2.26 | -1.81 | 0 | 0 |  | HG23 | HE1 |
| ALA194 (A) | MET43 | 2.26 | -1.98 | 0 | 0 |  | HB1 | HE1 |
| LEU220 (C) | PRO9 | 2.27 | -2.13 | 0 | 0 |  | HD13 | HB2 |
| THR196 (A) | ARG38 | 2.27 | -1.63 | 0 | 1 |  | HG22 | HH12 |
| THR169 (A) | MET94 | 2.29 | -4.02 | 0 | 0 |  | HB | HB1 |
| PRO168 (A) | VAL90 | 2.29 | -4.19 | 0 | 0 |  | HG1 | HG12 |
| ALA191 (A) | ILE42 | 2.32 | -1.43 | 0 | 0 |  | HA | HG22 |
| LEU220 (C) | VAL10 | 2.33 | -4.10 | 0 | 0 |  | H | O |
| GLU270 (C) | PRO11 | 2.41 | -1.82 | -1 | 0 |  | HG1 | HB1 |
| VAL171 (A) | VAL119 | 2.43 | -2.84 | 0 | 0 |  | HG22 | HG12 |
| TRP218 (C) | VAL10 | 2.45 | -1.10 | 0 | 0 |  | HA | HG23 |
| THR280 (C) | MET121 | 2.51 | -3.42 | 0 | 0 |  | H | SD |
| TRP218 (C) | ALA12 | 2.51 | -2.65 | 0 | 0 |  | O | HA |
| THR169 (A) | GLY93 | 2.52 | -0.05 | 0 | 0 |  | O | HA1 |
| ALA194 (A) | HIS40 | 2.56 | -4.89 | 0 | 0 |  | O | HE1 |
| ARG217 (C) | LYS7 | 2.56 | -1.89 | 1 | 1 |  | HD1 | O |
| ARG279 (C) | PHE123 | 2.57 | -6.07 | 1 | 0 |  | HH11 | HD2 |
| THR190 (A) | GLY44 | 2.61 | -1.90 | 0 | 0 |  | O | HA2 |
| ARG217 (C) | PRO9 | 2.64 | -5.09 | 1 | 0 |  | HG2 | HA |
| THR196 (A) | ASN122 | 2.64 | -1.78 | 0 | 0 |  | HG23 | OD1 |
| LEU50 (A) | TYR47 | 2.66 | -1.59 | 0 | 0 |  | HD11 | HH |
| ALA193 (A) | HIS40 | 2.67 | -1.71 | 0 | 0 |  | O | HE2 |
| THR169 (A) | VAL90 | 2.69 | -1.77 | 0 | 0 |  | HG21 | HG13 |
| GLY195 (A) | HIS40 | 2.78 | -1.61 | 0 | 0 |  | HA1 | HE1 |
| ARG222 (C) | PRO11 | 2.79 | -3.01 | 1 | 0 |  | HG2 | HG2 |
| PHE219 (C) | ALA12 | 2.80 | -1.49 | 0 | 0 |  | HA | HB2 |
| ASP197 (A) | ASN122 | 2.82 | -2.14 | -1 | 0 |  | H | HD22 |
| ALA191 (A) | GLY44 | 2.84 | -2.74 | 0 | 0 |  | HA | O |
| THR280 (C) | TRP120 | 2.86 | -2.56 | 0 | 0 |  | HG1 | HD1 |
| THR190 (A) | ILE46 | 2.86 | -1.05 | 0 | 0 |  | HA | HD3 |
| ARG279 (C) | MET121 | 2.90 | -7.20 | 1 | 0 |  | HD2 | HE1 |
| PHE219 (C) | PRO11 | 2.92 | -0.62 | 0 | 0 |  | HA | HA |
| ASN274 (C) | ALA13 | 2.95 | -0.39 | 0 | 0 |  | HD22 | O |
| THR169 (A) | VAL119 | 2.96 | -0.73 | 0 | 0 |  | O | HG23 |
| ARG217 (C) | VAL10 | 2.98 | -0.69 | 1 | 0 |  | O | H |
| ARG217 (C) | LYS8 | 3.00 | -0.95 | 1 | 1 |  | HD1 | O |
| LEU220 (C) | PRO11 | 3.00 | -2.21 | 0 | 0 |  | H | HA |
| ARG279 (C) | GLN118 | 3.08 | -0.42 | 1 | 0 |  | HH21 | HE22 |
| LEU50 (A) | ILE46 | 3.09 | -1.50 | 0 | 0 |  | HD21 | HD1 |
| ALA191 (A) | MET43 | 3.10 | -5.74 | 0 | 0 |  | HA | O |
| TRP218 (C) | PRO11 | 3.11 | 1.78 | 0 | 0 |  | O | C |
| LYS137 (A) | TRP120 | 3.12 | -2.21 | 1 | 0 |  | HZ2 | O |
| GLN189 (A) | ILE46 | 3.14 | -1.35 | 0 | 0 |  | HB2 | HD3 |
| GLN192 (A) | ILE42 | 3.21 | -4.19 | 0 | 0 |  | H | O |
| PRO168 (A) | GLY93 | 3.31 | -1.36 | 0 | 0 |  | O | H |
| ARG279 (C) | GLN125 | 3.34 | -3.76 | 1 | 0 |  | HH22 | HB1 |
| ASN274 (C) | ALA12 | 3.35 | -1.19 | 0 | 0 |  | CG | HB1 |
| GLY170 (A) | GLY93 | 3.36 | -0.33 | 0 | 0 |  | HA2 | HA1 |
| ASN274 (C) | GLU14 | 3.40 | -0.29 | 0 | -1 |  | OD1 | HA |
| LEU271 (C) | ALA12 | 3.40 | -0.68 | 0 | 0 |  | HA | HB2 |
| GLN192 (A) | GLY44 | 3.44 | -2.16 | 0 | 0 |  | H | HA2 |
| PHE219 (C) | VAL10 | 3.45 | -0.22 | 0 | 0 |  | N | O |
| ASN274 (C) | GLU15 | 3.47 | -1.29 | 0 | -1 |  | HD22 | HB1 |
| GLY278 (C) | MET121 | 3.53 | -0.80 | 0 | 0 |  | O | HB1 |
| VAL171 (A) | MET94 | 3.56 | -0.61 | 0 | 0 |  | HG22 | HE3 |
| THR190 (A) | MET43 | 3.60 | -0.42 | 0 | 0 |  | O | O |
| LYS137 (A) | MET121 | 3.63 | -0.79 | 1 | 0 |  | HZ2 | HA |
| PHE185 (A) | MET43 | 3.71 | -0.92 | 0 | 0 |  | HE1 | SD |
| ASN274 (C) | LYS73 | 3.77 | -1.53 | 0 | 1 |  | OD1 | HZ1 |
| GLY170 (A) | TRP120 | 3.78 | -0.64 | 0 | 0 |  | HA2 | HE3 |
| TRP218 (C) | MET121 | 3.83 | -1.05 | 0 | 0 |  | NE1 | HE2 |
| THR169 (A) | GLY44 | 3.86 | -0.44 | 0 | 0 |  | HG22 | N |
| ALA193 (A) | PRO41 | 3.86 | -0.39 | 0 | 0 |  | HA | O |
| LEU167 (A) | MET43 | 4.07 | -0.94 | 0 | 0 |  | HD13 | HG1 |
| GLY195 (A) | ARG38 | 4.13 | -0.07 | 0 | 1 |  | HA1 | HH12 |
| TRP218 (C) | ALA13 | 4.13 | -0.83 | 0 | 0 |  | HE3 | H |
| ARG279 (C) | ALA13 | 4.13 | -0.91 | 1 | 0 |  | HH21 | HB3 |
| GLY195 (A) | MET43 | 4.20 | -0.43 | 0 | 0 |  | O | HE1 |
| ASP216 (C) | TRP120 | 4.23 | -1.18 | -1 | 0 |  | OD1 | HE1 |
| ASP197 (A) | VAL119 | 4.32 | 0.64 | -1 | 0 |  | HB2 | O |
| PRO168 (A) | MET94 | 4.36 | -0.05 | 0 | 0 |  | O | N |
| THR169 (A) | MET95 | 4.37 | -0.32 | 0 | 0 |  | HG23 | H |
| GLY170 (A) | MET94 | 4.46 | -0.46 | 0 | 0 |  | HA2 | H |
| ALA194 (A) | ILE42 | 4.47 | 0.07 | 0 | 0 |  | H | O |
| PRO168 (A) | SER92 | 4.49 | -2.85 | 0 | 0 |  | O | H |
| ARG222 (C) | VAL10 | 4.49 | -0.07 | 1 | 0 |  | HE | HA |
| ALA191 (A) | GLY45 | 4.50 | -0.23 | 0 | 0 |  | HA | N |
| THR169 (A) | TRP120 | 4.51 | -0.30 | 0 | 0 |  | O | HZ3 |
| ALA194 (A) | PRO41 | 4.56 | 0.59 | 0 | 0 |  | O | HD1 |
| THR169 (A) | GLU88 | 4.57 | -0.35 | 0 | -1 |  | HG22 | OE1 |
| TRP218 (C) | TRP120 | 4.60 | -0.04 | 0 | 0 |  | HE1 | HE1 |
| THR196 (A) | GLU117 | 4.68 | -0.76 | 0 | -1 |  | HG21 | OE2 |
| TRP218 (C) | TRP116 | 4.69 | -0.32 | 0 | 0 |  | HB2 | HZ3 |
| THR169 (A) | GLU117 | 4.70 | -0.10 | 0 | -1 |  | O | O |
| LYS137 (A) | VAL119 | 4.72 | -1.00 | 1 | 0 |  | HE2 | O |
| PRO168 (A) | VAL91 | 4.73 | -1.59 | 0 | 0 |  | O | H |
| GLY138 (A) | TRP120 | 4.78 | -0.26 | 0 | 0 |  | H | HA |
| THR196 (A) | HIS40 | 4.80 | -0.62 | 0 | 0 |  | H | HE1 |
| LEU220 (C) | ALA12 | 4.83 | -0.25 | 0 | 0 |  | N | H |
| THR190 (A) | ILE42 | 4.87 | -0.49 | 0 | 0 |  | C | HG22 |
| ARG279 (C) | ALA16 | 4.90 | -0.27 | 1 | 0 |  | HH11 | H |
| ALA191 (A) | ILE46 | 4.92 | -0.46 | 0 | 0 |  | N | HG12 |
| THR196 (A) | VAL119 | 4.93 | -0.78 | 0 | 0 |  | HG21 | HG13 |
| THR280 (C) | PHE123 | 4.95 | -0.37 | 0 | 0 |  | HG23 | HE1 |
| ALA193 (A) | GLY44 | 4.97 | -0.32 | 0 | 0 |  | H | N |
| THR169 (A) | GLN89 | 4.98 | -0.36 | 0 | 0 |  | HG23 | O |
| TRP218 (C) | GLN125 | 4.99 | -0.36 | 0 | 0 |  | HB1 | OE1 |
| LYS236 (A) | ALA21 | 5.02 | -0.02 | 1 | 0 |  | HZ3 | H |
| LYS137 (A) | ASN122 | 5.02 | 0.43 | 1 | 0 |  | HZ3 | HD21 |
| ASN277 (C) | PHE123 | 5.03 | -0.21 | 0 | 0 |  | OD1 | HZ |
| ASN221 (C) | VAL10 | 5.04 | -0.45 | 0 | 0 |  | N | O |
| ALA194 (A) | ARG38 | 5.05 | -0.95 | 0 | 1 |  | O | HH22 |
| ARG217 (C) | TRP116 | 5.11 | -0.18 | 1 | 0 |  | H | HH2 |
| GLY195 (A) | PRO41 | 5.12 | -0.02 | 0 | 0 |  | HA1 | HD1 |
| TRP218 (C) | PRO9 | 5.12 | -0.94 | 0 | 0 |  | HA | HA |
| ARG279 (C) | GLU14 | 5.13 | -1.27 | 1 | -1 |  | HH12 | O |
| ASN277 (C) | GLU15 | 5.15 | -0.50 | 0 | -1 |  | HD22 | HG1 |
| THR196 (A) | PRO41 | 5.19 | -0.20 | 0 | 0 |  | HG22 | HD1 |
| ASN221 (C) | PRO9 | 5.22 | -0.25 | 0 | 0 |  | N | HB1 |
| ASN221 (C) | LYS73 | 5.27 | 0.13 | 0 | 1 |  | HD21 | HZ3 |
| ASN221 (C) | ALA12 | 5.28 | -0.22 | 0 | 0 |  | HA | H |
| PHE223 (C) | PRO11 | 5.28 | -0.29 | 0 | 0 |  | HE2 | HG2 |
| GLY215 (C) | TRP116 | 5.30 | -0.12 | 0 | 0 |  | O | HH2 |
| ASN238 (A) | ASN122 | 5.30 | -0.37 | 0 | 0 |  | HD21 | O |
| ARG188 (A) | TYR47 | 5.32 | 0.12 | 1 | 0 |  | HH21 | HE1 |
| ARG217 (C) | PRO11 | 5.33 | 0.11 | 1 | 0 |  | O | HA |
| ASP216 (C) | TRP116 | 5.34 | -0.11 | -1 | 0 |  | HA | HH2 |
| VAL171 (A) | GLY93 | 5.37 | -0.06 | 0 | 0 |  | H | HA1 |
| ASP197 (A) | MET121 | 5.37 | 0.18 | -1 | 0 |  | OD1 | HA |
| ARG279 (C) | GLU69 | 5.37 | -2.20 | 1 | -1 |  | HH12 | OE1 |
| ASP197 (A) | TRP120 | 5.37 | -0.12 | -1 | 0 |  | OD1 | O |
| GLY215 (C) | SER92 | 5.38 | -0.23 | 0 | 0 |  | O | HG |
| ALA194 (A) | MET94 | 5.38 | -0.07 | 0 | 0 |  | O | HE2 |
| THR169 (A) | PRO41 | 5.40 | -0.13 | 0 | 0 |  | HG22 | HB1 |
| TRP218 (C) | GLN127 | 5.41 | -0.22 | 0 | 0 |  | HA | HE22 |
| THR169 (A) | VAL91 | 5.43 | -0.48 | 0 | 0 |  | HA | H |
| ARG217 (C) | GLN127 | 5.44 | -0.07 | 1 | 0 |  | HG2 | HE22 |
| SER267 (C) | PRO11 | 5.45 | -0.20 | 0 | 0 |  | HA | HB2 |
| THR198 (A) | ASN122 | 5.45 | -0.56 | 0 | 0 |  | HA | HD21 |
| LEU220 (C) | LYS8 | 5.46 | -0.25 | 0 | 1 |  | HD13 | C |
| THR196 (A) | MET94 | 5.47 | -0.07 | 0 | 0 |  | HG21 | HE2 |
| GLN189 (A) | GLY44 | 5.47 | -0.22 | 0 | 0 |  | HA | HA2 |
| GLY195 (A) | ASN122 | 5.48 | -0.15 | 0 | 0 |  | O | HD22 |
| ASN133 (A) | MET43 | 5.50 | -0.03 | 0 | 0 |  | HD21 | HE1 |
| GLU270 (C) | VAL10 | 5.52 | -0.27 | -1 | 0 |  | HG1 | O |
| ARG217 (C) | SER92 | 5.56 | -0.44 | 1 | 0 |  | HH21 | OG |
| ILE259 (C) | PRO9 | 5.57 | -0.11 | 0 | 0 |  | HD1 | HB2 |
| THR190 (A) | GLY45 | 5.57 | -0.15 | 0 | 0 |  | O | N |
| TRP218 (C) | GLN118 | 5.58 | -0.51 | 0 | 0 |  | HB2 | OE1 |
| GLY170 (A) | VAL90 | 5.59 | -0.04 | 0 | 0 |  | H | HG13 |
| PRO168 (A) | GLY44 | 5.61 | -0.08 | 0 | 0 |  | HG1 | HA1 |
| ARG279 (C) | TRP120 | 5.61 | 0.15 | 1 | 0 |  | HA | HD1 |
| LEU167 (A) | GLY93 | 5.61 | -0.12 | 0 | 0 |  | O | HA1 |
| GLY283 (C) | TRP120 | 5.62 | -0.08 | 0 | 0 |  | HA1 | HB1 |
| ARG188 (A) | ILE46 | 5.62 | 0.05 | 1 | 0 |  | HH21 | HD1 |
| THR169 (A) | ILE42 | 5.63 | 0.14 | 0 | 0 |  | HG22 | C |
| ARG222 (C) | PRO9 | 5.65 | -0.52 | 1 | 0 |  | HE | O |
| THR169 (A) | SER92 | 5.66 | -1.50 | 0 | 0 |  | O | C |
| SER139 (A) | TRP120 | 5.69 | -0.23 | 0 | 0 |  | HB2 | HB2 |
| THR196 (A) | MET43 | 5.69 | -0.10 | 0 | 0 |  | HA | HE1 |
| GLY215 (C) | LYS7 | 5.70 | -0.29 | 0 | 1 |  | HA1 | HD2 |
| PHE219 (C) | ALA13 | 5.75 | -0.17 | 0 | 0 |  | HA | H |
| PRO168 (A) | MET43 | 5.76 | 0.09 | 0 | 0 |  | HD1 | HG1 |
| ARG279 (C) | LEU126 | 5.79 | -0.09 | 1 | 0 |  | HH22 | H |
| ARG279 (C) | ALA12 | 5.80 | 0.06 | 1 | 0 |  | HD1 | HB1 |
| THR135 (A) | MET43 | 5.81 | -0.06 | 0 | 0 |  | HG23 | HE1 |
| SER267 (C) | ALA12 | 5.81 | -0.11 | 0 | 0 |  | HA | H |
| THR169 (A) | GLY45 | 5.83 | -0.01 | 0 | 0 |  | HG22 | H |
| GLY278 (C) | GLU15 | 5.86 | -0.48 | 0 | -1 |  | H | OE1 |
| LEU167 (A) | VAL90 | 5.88 | -0.04 | 0 | 0 |  | C | HG12 |
| ILE281 (C) | MET121 | 5.88 | 0.00 | 0 | 0 |  | HG12 | HE2 |
| ILE281 (C) | ALA12 | 5.89 | -0.05 | 0 | 0 |  | HD1 | HB2 |
| GLN192 (A) | GLY45 | 5.89 | -0.09 | 0 | 0 |  | H | N |
| GLY275 (C) | GLU15 | 5.91 | 0.11 | 0 | -1 |  | O | HB1 |
| PRO168 (A) | GLN89 | 5.92 | -0.43 | 0 | 0 |  | O | O |
| THR190 (A) | TYR47 | 5.93 | -0.06 | 0 | 0 |  | HG1 | HD1 |
| GLY170 (A) | SER92 | 5.95 | -0.25 | 0 | 0 |  | HA2 | C |
| VAL171 (A) | ASN122 | 5.95 | -0.02 | 0 | 0 |  | HG21 | HD22 |
| THR169 (A) | TRP116 | 5.95 | -0.17 | 0 | 0 |  | O | HE1 |
| THR169 (A) | GLN118 | 5.95 | -0.20 | 0 | 0 |  | O | HA |
| ALA191 (A) | GLU88 | 5.97 | -0.18 | 0 | -1 |  | HA | OE1 |
| PHE219 (C) | PRO9 | 5.98 | -0.30 | 0 | 0 |  | H | HA |
| GLU270 (C) | ALA13 | 6.00 | 0.18 | -1 | 0 |  | HG2 | N |
| HIS172 (A) | VAL119 | 6.00 | -0.19 | 0 | 0 |  | H | HG22 |
| GLY275 (C) | ALA12 | 6.01 | -0.07 | 0 | 0 |  | O | HB1 |
| LEU220 (C) | LYS7 | 6.02 | -0.07 | 0 | 1 |  | HD13 | O |
| GLY170 (A) | MET43 | 6.07 | -0.25 | 0 | 0 |  | H | HG2 |
| ILE281 (C) | TRP120 | 6.10 | -0.48 | 0 | 0 |  | HA | HE1 |
| ARG279 (C) | ASN72 | 6.10 | -0.13 | 1 | 0 |  | HH12 | HB2 |
| VAL212 (C) | PRO9 | 6.12 | -0.07 | 0 | 0 |  | HG11 | HB2 |
| ARG217 (C) | PRO6 | 6.13 | 0.02 | 1 | 0 |  | HD1 | O |
| GLY170 (A) | GLU117 | 6.16 | -0.06 | 0 | -1 |  | HA2 | O |
| PRO184 (A) | MET43 | 6.18 | -0.09 | 0 | 0 |  | HG1 | HE3 |
| LEU167 (A) | VAL119 | 6.18 | -0.10 | 0 | 0 |  | O | HG22 |
| GLY195 (A) | MET94 | 6.21 | -0.06 | 0 | 0 |  | O | HE2 |
| VAL171 (A) | TRP120 | 6.21 | -0.38 | 0 | 0 |  | HG21 | N |
| PRO184 (A) | HIS40 | 6.22 | -0.09 | 0 | 0 |  | HG2 | HE1 |
| GLN192 (A) | HIS40 | 6.23 | 0.27 | 0 | 0 |  | C | HE2 |
| GLN189 (A) | TYR47 | 6.24 | -0.25 | 0 | 0 |  | O | HE1 |
| ALA191 (A) | ASP48 | 6.27 | -0.09 | 0 | -1 |  | HB2 | HB2 |
| GLY138 (A) | VAL119 | 6.27 | -0.03 | 0 | 0 |  | H | HG21 |
| LEU167 (A) | GLY44 | 6.28 | -0.06 | 0 | 0 |  | HD21 | HA2 |
| ASP216 (C) | MET121 | 6.28 | -0.36 | -1 | 0 |  | OD1 | HE3 |
| ASN133 (A) | ASN122 | 6.30 | 0.01 | 0 | 0 |  | HD21 | HD22 |
| ARG222 (C) | LYS73 | 6.30 | 1.28 | 1 | 1 |  | HH22 | HG1 |
| PHE219 (C) | LYS73 | 6.31 | -0.20 | 0 | 1 |  | HA | HZ2 |
| VAL186 (A) | MET43 | 6.32 | -0.06 | 0 | 0 |  | HG21 | O |
| THR196 (A) | GLU39 | 6.33 | -0.26 | 0 | -1 |  | HG22 | O |
| TRP218 (C) | LYS8 | 6.33 | -0.15 | 0 | 1 |  | HA | O |
| GLY195 (A) | VAL119 | 6.36 | -0.10 | 0 | 0 |  | O | HG13 |
| GLY170 (A) | GLN118 | 6.37 | -0.03 | 0 | 0 |  | HA2 | HA |
| ASN133 (A) | VAL119 | 6.38 | -0.09 | 0 | 0 |  | HD22 | HB |
| ASN238 (A) | PHE123 | 6.38 | -0.23 | 0 | 0 |  | HD21 | HA |
| GLN273 (C) | LYS73 | 6.39 | 0.12 | 0 | 1 |  | O | HZ1 |
| ARG279 (A) | ASN122 | 6.42 | -0.08 | 1 | 0 |  | HG1 | C |
| GLN192 (A) | MET94 | 6.42 | -0.08 | 0 | 0 |  | HB1 | SD |
| LEU271 (C) | LYS73 | 6.44 | -0.31 | 0 | 1 |  | N | HZ3 |
| PRO168 (A) | MET95 | 6.45 | -0.08 | 0 | 0 |  | O | H |
| GLN273 (C) | GLU14 | 6.46 | 0.23 | 0 | -1 |  | O | OE2 |
| GLN192 (A) | GLU88 | 6.47 | -0.26 | 0 | -1 |  | H | OE1 |
| GLY278 (C) | TRP120 | 6.48 | -0.01 | 0 | 0 |  | O | O |
| TRP218 (C) | LYS73 | 6.52 | -0.28 | 0 | 1 |  | O | HZ2 |
| GLU166 (A) | VAL119 | 6.53 | -0.14 | -1 | 0 |  | HG2 | HG22 |
| VAL171 (A) | PRO41 | 6.56 | -0.05 | 0 | 0 |  | HG23 | HG1 |
| MET276 (C) | GLU15 | 6.59 | -0.46 | 0 | -1 |  | HA | OE1 |
| LEU271 (C) | PRO11 | 6.59 | -0.18 | 0 | 0 |  | H | HA |
| GLN273 (C) | ALA12 | 6.60 | -0.06 | 0 | 0 |  | C | HB3 |
| ALA193 (A) | GLU88 | 6.61 | -0.17 | 0 | -1 |  | H | OE2 |
| SER267 (C) | VAL10 | 6.61 | -0.07 | 0 | 0 |  | HB2 | O |
| ASN238 (A) | ARG124 | 6.61 | -0.03 | 0 | 1 |  | HD22 | HH21 |
| ASP216 (C) | SER92 | 6.62 | 0.12 | -1 | 0 |  | HA | HG |
| ALA191 (A) | PRO41 | 6.63 | -0.09 | 0 | 0 |  | HB1 | O |
| ARG222 (C) | LYS8 | 6.64 | 1.23 | 1 | 1 |  | HH11 | HE2 |
| ARG222 (C) | ASN75 | 6.68 | 0.03 | 1 | 0 |  | HH22 | HB2 |
| MET276 (C) | MET121 | 6.69 | -0.09 | 0 | 0 |  | HE1 | SD |
| VAL171 (A) | GLU117 | 6.71 | -0.05 | 0 | -1 |  | HG22 | HB2 |
| LEU282 (C) | TRP120 | 6.72 | -0.09 | 0 | 0 |  | H | HE1 |
| LEU272 (C) | ALA12 | 6.72 | -0.06 | 0 | 0 |  | N | HB2 |
| ARG188 (A) | GLY44 | 6.74 | -0.20 | 1 | 0 |  | O | HA2 |
| ALA193 (A) | MET94 | 6.75 | -0.04 | 0 | 0 |  | H | SD |
| PRO168 (A) | TRP120 | 6.76 | -0.05 | 0 | 0 |  | O | HZ3 |
| GLN192 (A) | ILE46 | 6.76 | -0.07 | 0 | 0 |  | HE21 | HD3 |
| THR280 (C) | GLN118 | 6.76 | -0.08 | 0 | 0 |  | H | HB2 |
| GLN189 (A) | MET43 | 6.76 | -0.10 | 0 | 0 |  | HA | O |
| ASN214 (C) | SER92 | 6.79 | -0.03 | 0 | 0 |  | O | OG |
| LYS236 (A) | ALA19 | 6.80 | 0.03 | 1 | 0 |  | HE2 | O |
| VAL186 (A) | GLY44 | 6.80 | -0.03 | 0 | 0 |  | HG21 | HA2 |
| ALA194 (A) | VAL119 | 6.81 | -0.06 | 0 | 0 |  | HB1 | HG12 |
| ASN238 (A) | ARG38 | 6.82 | -0.27 | 0 | 1 |  | HD22 | HB1 |
| GLY170 (A) | TRP116 | 6.82 | -0.03 | 0 | 0 |  | HA2 | HE1 |
| LYS269 (C) | LYS73 | 6.83 | 1.16 | 1 | 1 |  | O | HZ3 |
| THR198 (A) | MET121 | 6.83 | -0.10 | 0 | 0 |  | HA | O |
| GLU166 (A) | GLY93 | 6.83 | -0.11 | -1 | 0 |  | HG1 | HA1 |
| ARG217 (C) | ALA12 | 6.84 | 0.00 | 1 | 0 |  | O | HA |
| ARG222 (C) | ASN74 | 6.84 | -0.17 | 1 | 0 |  | HH22 | OD1 |
| LEU167 (A) | MET94 | 6.86 | -0.13 | 0 | 0 |  | O | HB1 |
| GLU270 (C) | ASN74 | 6.86 | -0.35 | -1 | 0 |  | OE1 | HD22 |
| PRO168 (A) | VAL119 | 6.86 | -0.17 | 0 | 0 |  | O | HG23 |
| PHE223 (C) | LYS73 | 6.87 | -0.09 | 0 | 1 |  | HE2 | HE1 |
| ALA285 (C) | MET121 | 6.87 | -0.06 | 0 | 0 |  | HA | HB2 |
| HIS172 (A) | MET43 | 6.88 | -0.08 | 0 | 0 |  | H | HE1 |
| GLY283 (C) | MET121 | 6.89 | -0.05 | 0 | 0 |  | HA1 | HB2 |
| THR196 (A) | MET121 | 6.91 | -0.08 | 0 | 0 |  | HB | C |
| GLY275 (C) | ALA13 | 6.91 | 0.28 | 0 | 0 |  | O | O |
| VAL171 (A) | ARG38 | 6.92 | 0.00 | 0 | 1 |  | HG23 | HH22 |
| THR280 (C) | ASN122 | 6.93 | -0.15 | 0 | 0 |  | HG23 | N |
| LYS269 (C) | ALA12 | 6.94 | 0.06 | 1 | 0 |  | O | HB3 |
| ALA193 (A) | GLY45 | 6.94 | -0.02 | 0 | 0 |  | H | N |
| ALA266 (C) | PRO11 | 6.94 | -0.07 | 0 | 0 |  | O | HB2 |
| ARG222 (C) | ALA12 | 6.94 | -0.31 | 1 | 0 |  | HG2 | H |
| GLN192 (A) | PRO41 | 6.95 | -0.03 | 0 | 0 |  | C | O |
| ASN238 (A) | MET121 | 6.96 | -0.22 | 0 | 0 |  | HD21 | O |
| VAL212 (C) | LYS7 | 6.96 | -0.21 | 0 | 1 |  | O | HB2 |
| PRO168 (A) | TRP116 | 6.97 | -0.05 | 0 | 0 |  | O | HE1 |
| ARG217 (C) | TRP120 | 6.99 | 0.06 | 1 | 0 |  | H | HZ2 |
| ALA285 (C) | PHE123 | 6.99 | -0.03 | 0 | 0 |  | HB2 | HE1 |
| MET49 (A) | ILE46 | 7.00 | -0.06 | 0 | 0 |  | O | HD1 |
| ASN274 (C) | ASN72 | 7.01 | -0.04 | 0 | 0 |  | OD1 | O |
| GLU47 (A) | TYR47 | 7.01 | -0.07 | -1 | 0 |  | OE2 | HH |
| ALA191 (A) | HIS40 | 7.02 | -0.01 | 0 | 0 |  | HB1 | HE2 |
| LYS137 (A) | PHE123 | 7.03 | -0.12 | 1 | 0 |  | HZ2 | HE1 |
| MET276 (C) | ALA12 | 7.08 | -0.03 | 0 | 0 |  | HB1 | HB1 |
| SER46 (A) | ILE46 | 7.09 | -0.04 | 0 | 0 |  | O | HD2 |
| THR190 (A) | GLU88 | 7.09 | 0.10 | 0 | -1 |  | O | OE1 |
| TRP218 (C) | GLU15 | 7.10 | 0.02 | 0 | -1 |  | HH2 | OE1 |
| SER267 (C) | PRO9 | 7.10 | -0.03 | 0 | 0 |  | OG | HB1 |
| ALA194 (A) | GLY44 | 7.10 | -0.04 | 0 | 0 |  | H | N |
| ASP197 (A) | MET43 | 7.11 | -0.02 | -1 | 0 |  | H | HE1 |
| GLY278 (C) | ASN122 | 7.11 | -0.05 | 0 | 0 |  | O | N |
| ARG131 (A) | TRP120 | 7.11 | -0.20 | 1 | 0 |  | HG2 | HA |
| ASN274 (C) | PRO11 | 7.12 | -0.05 | 0 | 0 |  | OD1 | C |
| ARG279 (C) | TRP116 | 7.15 | -0.23 | 1 | 0 |  | HH22 | HB2 |
| GLU270 (C) | GLU14 | 7.16 | 1.50 | -1 | -1 |  | OE1 | OE2 |
| LEU271 (C) | ALA13 | 7.17 | -0.04 | 0 | 0 |  | HD13 | H |
| ILE136 (A) | TRP120 | 7.19 | -0.04 | 0 | 0 |  | O | HA |
| ASN51 (A) | TYR47 | 7.19 | -0.05 | 0 | 0 |  | HB1 | HH |
| VAL171 (A) | GLN118 | 7.20 | -0.06 | 0 | 0 |  | HG21 | C |
| ALA173 (A) | MET43 | 7.22 | -0.05 | 0 | 0 |  | HB1 | SD |
| THR196 (A) | GLN118 | 7.24 | -0.03 | 0 | 0 |  | HG21 | O |
| VAL212 (C) | VAL10 | 7.26 | -0.02 | 0 | 0 |  | HG11 | H |
| LYS137 (A) | GLN118 | 7.27 | -0.05 | 1 | 0 |  | HZ2 | O |
| ASP197 (A) | ARG38 | 7.27 | -1.30 | -1 | 1 |  | H | HH22 |
| ASN238 (A) | GLN35 | 7.27 | -0.01 | 0 | 0 |  | HD22 | HE22 |
| ARG188 (A) | MET43 | 7.27 | -0.11 | 1 | 0 |  | O | O |
| VAL171 (A) | VAL90 | 7.28 | -0.03 | 0 | 0 |  | H | HG13 |
| THR135 (A) | VAL119 | 7.29 | -0.06 | 0 | 0 |  | HG23 | HB |
| LYS236 (A) | GLN35 | 7.29 | -0.24 | 1 | 0 |  | HE2 | OE1 |
| TYR237 (A) | GLU20 | 7.31 | 0.03 | 0 | -1 |  | HE2 | OE2 |
| VAL186 (A) | ILE42 | 7.32 | -0.03 | 0 | 0 |  | HG23 | O |
| ASP216 (C) | VAL10 | 7.34 | -0.14 | -1 | 0 |  | C | HG23 |
| TYR237 (A) | PRO17 | 7.35 | -0.04 | 0 | 0 |  | HH | HB2 |
| ASN214 (C) | LYS7 | 7.36 | -0.25 | 0 | 1 |  | O | HZ1 |
| HIS172 (A) | TRP120 | 7.37 | -0.08 | 0 | 0 |  | HE2 | HB2 |
| ASP216 (C) | PRO9 | 7.39 | 0.02 | -1 | 0 |  | C | HA |
| ALA193 (A) | PRO50 | 7.39 | -0.01 | 0 | 0 |  | HA | HB2 |
| PHE223 (C) | ASN74 | 7.40 | -0.03 | 0 | 0 |  | HE2 | HD22 |
| GLY215 (C) | TRP120 | 7.40 | -0.01 | 0 | 0 |  | O | HZ2 |
| PRO168 (A) | GLU88 | 7.41 | -0.14 | 0 | -1 |  | HG1 | OE1 |
| ARG131 (A) | VAL119 | 7.43 | -0.22 | 1 | 0 |  | HG2 | O |
| ARG217 (C) | MET121 | 7.43 | 0.10 | 1 | 0 |  | H | HE2 |
| PHE219 (C) | MET121 | 7.44 | -0.07 | 0 | 0 |  | HD2 | HE2 |
| ASN274 (C) | ALA16 | 7.44 | 0.00 | 0 | 0 |  | HD22 | N |
| ASP197 (A) | GLN118 | 7.45 | -0.03 | -1 | 0 |  | H | O |
| ALA266 (C) | ALA12 | 7.46 | -0.01 | 0 | 0 |  | O | H |
| PHE185 (A) | MET94 | 7.51 | -0.02 | 0 | 0 |  | HE1 | HE2 |
| ARG131 (A) | ASN122 | 7.51 | 0.14 | 1 | 0 |  | HE | HD21 |
| PHE185 (A) | VAL119 | 7.51 | -0.02 | 0 | 0 |  | HE1 | HG12 |
| GLU166 (A) | TRP120 | 7.52 | -0.05 | -1 | 0 |  | OE2 | HE3 |
| THR196 (A) | PHE123 | 7.55 | -0.10 | 0 | 0 |  | HG23 | N |
| GLY215 (C) | PRO9 | 7.56 | -0.01 | 0 | 0 |  | O | HA |
| THR169 (A) | ARG38 | 7.56 | -0.03 | 0 | 1 |  | HB | HH21 |
| GLN189 (A) | VAL90 | 7.57 | -0.04 | 0 | 0 |  | HG1 | HG12 |
| PRO168 (A) | ILE46 | 7.59 | -0.02 | 0 | 0 |  | HG1 | HG11 |
| THR199 (A) | ASN122 | 7.61 | -0.03 | 0 | 0 |  | H | HB1 |
| THR196 (A) | TRP120 | 7.61 | -0.16 | 0 | 0 |  | HA | N |
| ASN133 (A) | HIS40 | 7.62 | -0.04 | 0 | 0 |  | HD21 | HE1 |
| ALA191 (A) | TYR47 | 7.64 | -0.08 | 0 | 0 |  | H | H |
| MET276 (C) | PHE123 | 7.64 | -0.03 | 0 | 0 |  | HA | HE2 |
| LEU268 (C) | ALA12 | 7.65 | -0.04 | 0 | 0 |  | O | HB2 |
| GLY275 (C) | GLU14 | 7.65 | -0.17 | 0 | -1 |  | O | HA |
| LYS236 (A) | ALA18 | 7.66 | -0.10 | 1 | 0 |  | HE2 | HB1 |
| THR198 (A) | VAL119 | 7.67 | 0.04 | 0 | 0 |  | N | O |
| ILE136 (A) | VAL119 | 7.68 | -0.07 | 0 | 0 |  | O | HB |
| GLY170 (A) | VAL91 | 7.68 | -0.01 | 0 | 0 |  | N | H |
| ARG222 (C) | TYR70 | 7.69 | -0.19 | 1 | 0 |  | HH12 | HE2 |
| SER139 (A) | VAL119 | 7.69 | -0.04 | 0 | 0 |  | HB2 | HG21 |
| GLY215 (C) | LYS8 | 7.70 | -0.03 | 0 | 1 |  | O | O |
| SER267 (C) | LYS73 | 7.71 | -0.19 | 0 | 1 |  | HA | HZ3 |
| LEU50 (A) | GLY44 | 7.72 | 0.00 | 0 | 0 |  | HD21 | O |
| ARG279 (C) | PRO17 | 7.73 | -0.12 | 1 | 0 |  | HH11 | HA |
| ASN238 (A) | PRO37 | 7.76 | -0.10 | 0 | 0 |  | HD22 | HA |
| PRO184 (A) | ILE42 | 7.76 | -0.02 | 0 | 0 |  | HG1 | O |
| PRO168 (A) | GLU117 | 7.77 | 0.00 | 0 | -1 |  | O | O |
| SER284 (C) | MET121 | 7.78 | -0.03 | 0 | 0 |  | O | HB2 |
| LEU220 (C) | ALA13 | 7.78 | -0.02 | 0 | 0 |  | H | H |
| ASP216 (C) | GLN118 | 7.79 | -0.07 | -1 | 0 |  | OD1 | HB2 |
| TRP218 (C) | GLU14 | 7.80 | 0.05 | 0 | -1 |  | HZ3 | HA |
| ASN214 (C) | TRP120 | 7.81 | -0.10 | 0 | 0 |  | OD1 | HE1 |
| ILE213 (C) | LYS7 | 7.82 | -0.21 | 0 | 1 |  | O | HD2 |
| PRO168 (A) | GLY45 | 7.82 | -0.01 | 0 | 0 |  | HG1 | H |
| GLY215 (C) | VAL10 | 7.83 | -0.01 | 0 | 0 |  | O | HG23 |
| ASN277 (C) | MET121 | 7.85 | -0.05 | 0 | 0 |  | O | HB1 |
| ALA285 (C) | TRP120 | 7.85 | -0.05 | 0 | 0 |  | HA | HD1 |
| TRP218 (C) | PHE123 | 7.85 | -0.10 | 0 | 0 |  | HZ2 | HB1 |
| ALA193 (A) | ARG38 | 7.86 | -0.08 | 0 | 1 |  | C | HH22 |
| ASP197 (A) | MET94 | 7.86 | -0.03 | -1 | 0 |  | H | HE2 |
| THR169 (A) | HIS96 | 7.87 | -0.03 | 0 | 0 |  | HG23 | N |
| SER284 (C) | TRP120 | 7.87 | -0.04 | 0 | 0 |  | O | HD1 |
| ARG222 (C) | ASN72 | 7.88 | -0.15 | 1 | 0 |  | HH12 | OD1 |
| GLY138 (A) | MET121 | 7.88 | -0.03 | 0 | 0 |  | H | N |
| TYR237 (A) | PHE123 | 7.90 | -0.07 | 0 | 0 |  | O | HZ |
| THR190 (A) | ASP48 | 7.90 | -0.06 | 0 | -1 |  | HA | H |
| LEU167 (A) | ILE42 | 7.90 | -0.04 | 0 | 0 |  | HD13 | O |
| GLY170 (A) | MET121 | 7.91 | -0.02 | 0 | 0 |  | HA2 | H |
| ASN274 (C) | PHE123 | 7.91 | -0.04 | 0 | 0 |  | HD22 | HE2 |
| GLU166 (A) | SER92 | 7.92 | -0.07 | -1 | 0 |  | OE1 | HA |
| ARG279 (C) | ASN71 | 7.92 | -0.04 | 1 | 0 |  | HH12 | O |
| THR199 (A) | PHE123 | 7.93 | -0.02 | 0 | 0 |  | HG1 | HE1 |
| GLN192 (A) | VAL90 | 7.93 | -0.02 | 0 | 0 |  | HG2 | HG12 |
| PHE185 (A) | ILE42 | 7.94 | -0.04 | 0 | 0 |  | HA | O |
| THR169 (A) | PRO50 | 7.94 | -0.01 | 0 | 0 |  | HG23 | HG2 |
| THR199 (A) | MET121 | 7.94 | -0.05 | 0 | 0 |  | HG1 | O |
| ARG217 (C) | GLN118 | 7.95 | -0.20 | 1 | 0 |  | H | OE1 |
| ASN133 (A) | MET94 | 7.96 | 0.00 | 0 | 0 |  | HD21 | HE2 |
| VAL186 (A) | ILE46 | 7.96 | -0.01 | 0 | 0 |  | HG22 | HD3 |
| GLU47 (A) | ILE46 | 7.96 | -0.16 | -1 | 0 |  | HA | HD2 |
| THR280 (C) | VAL119 | 7.96 | -0.07 | 0 | 0 |  | OG1 | C |
| LYS269 (C) | PRO11 | 7.97 | 0.23 | 1 | 0 |  | C | HB1 |
| ASP263 (C) | PRO9 | 7.97 | -0.08 | -1 | 0 |  | HB2 | HG2 |
| ILE259 (C) | LYS7 | 7.98 | -0.05 | 0 | 1 |  | HD1 | O |
| ALA266 (C) | LYS73 | 7.99 | -0.15 | 0 | 1 |  | O | HZ3 |
| ASN277 (C) | PRO17 | 8.00 | -0.02 | 0 | 0 |  | HD22 | HD2 |

**Supplementary Table 8.** Quantum Biochemistry description of the interactions between Sesame cystatin and SARS-CoV-2 Mpro.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Amino acid residues** | | **Distance** | **Interaction energy** | **Residue charge** | |  | **Residue atom** | |
| Mpro | Sesame cystatin | (Å) | (kcal mol-1) | Mpro | Sesame cystatin |  | Mpro | Sesame cystatin |
| ASN142 (C) | HIS117 | 1.70 | -7.00 | 0 | 0 |  | HD22 | O |
| LYS137 (C) | TRP77 | 1.72 | -12.69 | 1 | 0 |  | HA | HE1 |
| ASP197 (C) | THR3 | 1.82 | -1.48 | -1 | 0 |  | OD2 | HN |
| LYS236 (C) | ASP15 | 1.83 | -9.19 | 1 | -1 |  | O | HN |
| THR196 (C) | THR3 | 1.83 | -14.49 | 0 | 0 |  | HG1 | O |
| LEU286 (C) | MET78 | 1.94 | -1.29 | 0 | 0 |  | HD12 | HG1 |
| ASN238 (C) | ASN13 | 1.94 | 3.63 | 0 | 0 |  | HA | HD22 |
| ALA194 (C) | VAL7 | 1.96 | -5.60 | 0 | 0 |  | O | HN |
| THR196 (C) | LEU4 | 1.98 | -5.31 | 0 | 0 |  | HG1 | HA |
| ALA193 (C) | VAL7 | 1.98 | 0.74 | 0 | 0 |  | HN | HG13 |
| LYS236 (C) | PRO14 | 2.06 | -9.05 | 1 | 0 |  | HA | HA |
| THR196 (C) | SER10 | 2.12 | -1.52 | 0 | 0 |  | HG23 | HB1 |
| THR196 (C) | HIS8 | 2.13 | -5.59 | 0 | 0 |  | HN | O |
| GLY283 (A) | MET78 | 2.14 | -0.71 | 0 | 0 |  | HA2 | HE2 |
| GLN256 (A) | HIS149 | 2.16 | -7.60 | 0 | 0 |  | HE21 | ND1 |
| ASN238 (C) | PRO14 | 2.17 | -2.56 | 0 | 0 |  | HB1 | HB1 |
| THR169 (C) | GLY50 | 2.18 | -0.64 | 0 | 0 |  | HG23 | HN |
| LEU286 (C) | ASP79 | 2.20 | -2.53 | 0 | -1 |  | HD23 | HB2 |
| ARG217 (A) | VAL108 | 2.25 | -3.03 | 1 | 0 |  | HH22 | HG13 |
| ILE213 (A) | PRO113 | 2.26 | -2.66 | 0 | 0 |  | HG11 | HG2 |
| ALA194 (C) | GLY6 | 2.28 | -4.13 | 0 | 0 |  | O | HA1 |
| GLY138 (C) | TRP77 | 2.29 | -1.76 | 0 | 0 |  | O | HZ2 |
| LEU287 (C) | MET1 | 2.29 | -0.15 | 0 | 1 |  | O | HE1 |
| MET235 (C) | ASN13 | 2.30 | -7.54 | 0 | 0 |  | O | HD22 |
| ILE259 (A) | TRP111 | 2.32 | -3.49 | 0 | 0 |  | HD1 | HB1 |
| ASP289 (C) | MET1 | 2.32 | -2.49 | -1 | 1 |  | HB1 | HE3 |
| LEU220 (A) | TRP111 | 2.32 | -5.40 | 0 | 0 |  | HD13 | HB1 |
| PRO168 (C) | ALA49 | 2.33 | -1.60 | 0 | 0 |  | HB1 | HA |
| VAL171 (C) | TRP77 | 2.33 | -1.33 | 0 | 0 |  | HG11 | HE1 |
| ASN214 (A) | TRP77 | 2.34 | -0.99 | 0 | 0 |  | HD22 | HZ3 |
| ASN238 (C) | ALA2 | 2.35 | -1.32 | 0 | 0 |  | HD22 | HB3 |
| THR198 (C) | ALA2 | 2.35 | -0.30 | 0 | 0 |  | HA | HB1 |
| GLY195 (C) | GLY6 | 2.37 | -1.45 | 0 | 0 |  | HA2 | HA1 |
| VAL212 (A) | PRO113 | 2.39 | -2.85 | 0 | 0 |  | HG22 | HG2 |
| ASP197 (C) | ALA2 | 2.39 | -16.19 | -1 | 0 |  | OD2 | HA |
| GLY195 (C) | HIS8 | 2.41 | -8.74 | 0 | 0 |  | HA2 | HN |
| THR199 (C) | MET1 | 2.46 | -2.42 | 0 | 1 |  | HG1 | HB1 |
| GLY195 (C) | VAL7 | 2.46 | -1.15 | 0 | 0 |  | HA1 | HG21 |
| PRO184 (C) | VAL7 | 2.48 | -1.56 | 0 | 0 |  | HG1 | HG23 |
| ALA255 (A) | SER199 | 2.48 | -1.30 | 0 | -1 |  | HB2 | HG |
| ARG217 (A) | ARG112 | 2.49 | -0.80 | 1 | 1 |  | HD2 | HB2 |
| GLY258 (A) | ASN151 | 2.51 | -1.14 | 0 | 0 |  | HA2 | OD1 |
| THR257 (A) | PRO113 | 2.54 | -1.38 | 0 | 0 |  | HA | HB2 |
| MET235 (C) | PRO14 | 2.56 | -1.47 | 0 | 0 |  | O | HA |
| THR199 (C) | ALA2 | 2.61 | -1.66 | 0 | 0 |  | HN | HB1 |
| ASN238 (C) | SER10 | 2.63 | -0.38 | 0 | 0 |  | OD1 | HG |
| ASN221 (A) | TRP111 | 2.63 | -3.02 | 0 | 0 |  | HA | HH2 |
| LEU141 (C) | VAL116 | 2.64 | -3.71 | 0 | 0 |  | HD22 | HG21 |
| ARG217 (A) | TRP111 | 2.67 | -1.74 | 1 | 0 |  | HD1 | O |
| THR257 (A) | ASN151 | 2.69 | -4.90 | 0 | 0 |  | O | HB1 |
| PRO252 (A) | SER199 | 2.69 | -1.46 | 0 | -1 |  | HA | HB2 |
| ARG4 (A) | TRP77 | 2.71 | -1.91 | 1 | 0 |  | HG2 | HH2 |
| ALA255 (A) | HIS149 | 2.74 | -3.83 | 0 | 0 |  | HB3 | NE2 |
| ASN133 (C) | THR3 | 2.75 | -1.41 | 0 | 0 |  | HD22 | OG1 |
| ASN238 (C) | LEU4 | 2.76 | -2.41 | 0 | 0 |  | HD22 | HD21 |
| ALA255 (A) | ASN151 | 2.77 | -2.24 | 0 | 0 |  | O | HD21 |
| ARG222 (A) | TRP111 | 2.78 | -2.52 | 1 | 0 |  | N | HH2 |
| ARG279 (A) | PHE80 | 2.78 | -2.00 | 1 | 0 |  | HH12 | HE1 |
| THR196 (C) | ASP9 | 2.80 | -4.76 | 0 | -1 |  | HB | HA |
| PRO184 (C) | HIS8 | 2.80 | -0.99 | 0 | 0 |  | HG2 | HE2 |
| GLU288 (C) | MET1 | 2.85 | -3.31 | -1 | 1 |  | C | HE3 |
| GLY2 (A) | TRP77 | 2.92 | -2.19 | 0 | 0 |  | HA2 | HH2 |
| ARG217 (A) | GLN107 | 2.93 | -2.69 | 1 | 0 |  | HH21 | O |
| LEU141 (C) | PRO115 | 2.96 | -3.45 | 0 | 0 |  | HD21 | HB1 |
| GLN256 (A) | ASN151 | 2.98 | -1.23 | 0 | 0 |  | O | HB2 |
| ASN238 (C) | THR3 | 3.00 | -1.19 | 0 | 0 |  | HD22 | O |
| LEU282 (A) | MET78 | 3.00 | -1.32 | 0 | 0 |  | O | HE2 |
| VAL297 (A) | HIS149 | 3.02 | -0.67 | 0 | 0 |  | HG11 | HE1 |
| ALA194 (C) | THR3 | 3.04 | -0.56 | 0 | 0 |  | HB2 | HG22 |
| LYS236 (C) | ASN13 | 3.05 | -2.32 | 1 | 0 |  | HA | O |
| GLY195 (C) | THR3 | 3.06 | -1.47 | 0 | 0 |  | O | HB |
| LEU141 (C) | HIS117 | 3.07 | -2.04 | 0 | 0 |  | HB2 | HD2 |
| PRO252 (A) | HIS149 | 3.08 | -1.49 | 0 | 0 |  | HB1 | HE1 |
| ASN142 (C) | PRO119 | 3.11 | -0.26 | 0 | 0 |  | HD22 | HD2 |
| GLY195 (C) | GLY5 | 3.14 | 0.53 | 0 | 0 |  | HA2 | O |
| TYR239 (C) | MET1 | 3.16 | -2.39 | 0 | 1 |  | OH | HB1 |
| GLN192 (C) | VAL7 | 3.17 | 1.59 | 0 | 0 |  | HA | HG13 |
| TYR237 (C) | PRO14 | 3.20 | -5.10 | 0 | 0 |  | C | HB1 |
| TYR237 (C) | SER18 | 3.20 | -1.08 | 0 | 0 |  | HE1 | OG |
| THR169 (C) | THR51 | 3.21 | -1.10 | 0 | 0 |  | HG23 | HG21 |
| THR196 (C) | GLY5 | 3.23 | -1.15 | 0 | 0 |  | HB | HA1 |
| ASN133 (C) | HIS8 | 3.35 | -1.13 | 0 | 0 |  | HA | HE1 |
| ASN142 (C) | ASP118 | 3.35 | -3.58 | 0 | -1 |  | HD22 | HA |
| THR169 (C) | ALA49 | 3.37 | -1.59 | 0 | 0 |  | HA | C |
| GLN256 (A) | VAL148 | 3.42 | -1.28 | 0 | 0 |  | HE22 | O |
| ARG217 (A) | PRO113 | 3.44 | -0.73 | 1 | 0 |  | HD2 | HD1 |
| GLN256 (A) | ALA150 | 3.44 | -0.04 | 0 | 0 |  | O | O |
| PHE3 (A) | TRP77 | 3.51 | -0.55 | 0 | 0 |  | H | HH2 |
| LYS137 (C) | PRO76 | 3.51 | -2.03 | 1 | 0 |  | HZ1 | O |
| TYR118 (C) | HIS117 | 3.53 | -1.22 | 0 | 0 |  | HE2 | HD2 |
| CYS300 (A) | HIS117 | 3.57 | -0.58 | 0 | 0 |  | HB1 | NE2 |
| GLN256 (A) | PRO113 | 3.57 | -0.71 | 0 | 0 |  | O | HB2 |
| TYR237 (C) | ALA2 | 3.58 | -0.60 | 0 | 0 |  | O | HB2 |
| THR169 (C) | GLY6 | 3.65 | -0.35 | 0 | 0 |  | HG22 | HA2 |
| GLY258 (A) | ASP162 | 3.67 | -0.70 | 0 | -1 |  | HA1 | OD1 |
| SER139 (C) | TRP77 | 3.67 | -0.75 | 0 | 0 |  | HB1 | HH2 |
| ARG217 (A) | SER109 | 3.72 | -3.38 | 1 | 0 |  | HE | O |
| GLN256 (A) | VAL116 | 3.72 | -0.52 | 0 | 0 |  | HE22 | HG12 |
| CYS300 (A) | VAL116 | 3.74 | -0.42 | 0 | 0 |  | SG | HG21 |
| VAL204 (C) | MET1 | 3.75 | -0.42 | 0 | 1 |  | HG23 | HE3 |
| ARG131 (C) | MET1 | 3.77 | -5.42 | -2 | 1 |  | HH12 | HE2 |
| ILE136 (C) | TRP77 | 3.80 | 0.58 | 0 | 0 |  | O | HE1 |
| TYR237 (C) | LEU4 | 3.80 | -0.42 | 0 | 0 |  | O | HD22 |
| LYS137 (C) | MET1 | 3.81 | 0.28 | 1 | 1 |  | HZ1 | HG2 |
| LYS137 (C) | MET78 | 3.86 | -2.77 | 1 | 0 |  | HZ3 | HA |
| ASN214 (A) | MET78 | 3.86 | -0.59 | 0 | 0 |  | HD22 | HG1 |
| VAL212 (A) | ARG112 | 3.87 | -0.86 | 0 | 1 |  | HB | HA |
| ASN142 (C) | VAL116 | 3.88 | -1.78 | 0 | 0 |  | HN | O |
| TYR237 (C) | ASP15 | 3.89 | -2.86 | 0 | -1 |  | N | HN |
| PRO168 (C) | GLY50 | 3.93 | -0.06 | 0 | 0 |  | O | N |
| ALA255 (A) | LYS177 | 3.94 | -1.13 | 0 | 1 |  | HA | HZ1 |
| GLY251 (A) | SER199 | 3.97 | -0.26 | 0 | -1 |  | O | HG |
| SER1 (A) | TRP77 | 4.00 | -0.93 | 1 | 0 |  | O | CZ2 |
| THR169 (C) | VAL48 | 4.01 | -0.55 | 0 | 0 |  | HG23 | O |
| TYR239 (C) | ALA2 | 4.07 | -0.50 | 0 | 0 |  | HE1 | HN |
| ASP197 (C) | LEU4 | 4.07 | -0.92 | -1 | 0 |  | HN | N |
| ALA194 (C) | HIS8 | 4.11 | -0.07 | 0 | 0 |  | O | HN |
| ARG217 (A) | ASP106 | 4.14 | -3.83 | 1 | -1 |  | HH22 | OD2 |
| ILE259 (A) | PRO113 | 4.19 | -0.30 | 0 | 0 |  | HD2 | HD2 |
| ILE259 (A) | ARG112 | 4.22 | -0.46 | 0 | 1 |  | HD1 | HA |
| ALA255 (A) | ASP162 | 4.25 | 0.95 | 0 | -1 |  | O | OD1 |
| ALA194 (C) | GLY5 | 4.27 | -1.02 | 0 | 0 |  | O | O |
| THR196 (C) | GLY6 | 4.29 | -0.13 | 0 | 0 |  | HN | HA1 |
| ASP197 (C) | MET1 | 4.29 | -1.81 | -1 | 1 |  | OD2 | O |
| ALA255 (A) | LEU164 | 4.33 | -0.34 | 0 | 0 |  | HB1 | HD23 |
| PRO168 (C) | VAL48 | 4.38 | -0.93 | 0 | 0 |  | HG2 | O |
| ALA193 (C) | GLY6 | 4.38 | -0.14 | 0 | 0 |  | HB2 | HA2 |
| SER254 (A) | ASN151 | 4.39 | -0.19 | 0 | 0 |  | O | HD21 |
| GLN256 (A) | VAL114 | 4.39 | 0.13 | 0 | 0 |  | O | H |
| ASP197 (C) | PRO76 | 4.39 | -0.15 | -1 | 0 |  | OD2 | HB1 |
| ASN142 (C) | PRO115 | 4.41 | -0.01 | 0 | 0 |  | HN | HB1 |
| ARG131 (C) | THR3 | 4.42 | 0.61 | -2 | 0 |  | HD1 | HG1 |
| THR257 (A) | TRP111 | 4.43 | -0.49 | 0 | 0 |  | O | HB2 |
| ARG217 (A) | GLY110 | 4.47 | -0.85 | 1 | 0 |  | HD1 | HA2 |
| THR196 (C) | ALA2 | 4.54 | -0.22 | 0 | 0 |  | HG1 | HB3 |
| ALA234 (C) | ASN13 | 4.56 | -0.52 | 0 | 0 |  | O | HD22 |
| THR257 (A) | ARG112 | 4.56 | -0.46 | 0 | 1 |  | O | O |
| MET235 (C) | ASP15 | 4.58 | 0.40 | 0 | -1 |  | O | HN |
| ARG217 (A) | LYS75 | 4.58 | 2.10 | 1 | 1 |  | HH22 | HZ1 |
| LEU282 (A) | TRP77 | 4.59 | -0.22 | 0 | 0 |  | HD21 | HZ3 |
| LEU286 (C) | PHE80 | 4.59 | -0.61 | 0 | 0 |  | HD11 | HB2 |
| GLU288 (C) | MET78 | 4.59 | -0.76 | -1 | 0 |  | OE2 | HE1 |
| PHE185 (C) | VAL7 | 4.61 | -0.57 | 0 | 0 |  | HE1 | HG22 |
| TYR237 (C) | ASN13 | 4.62 | 0.03 | 0 | 0 |  | C | HD22 |
| THR257 (A) | ALA150 | 4.63 | -0.21 | 0 | 0 |  | HA | O |
| GLY143 (C) | HIS117 | 4.66 | -0.44 | 0 | 0 |  | HA1 | HB2 |
| TYR239 (C) | ASN13 | 4.67 | -0.36 | 0 | 0 |  | HN | HD22 |
| THR169 (C) | THR3 | 4.68 | -0.23 | 0 | 0 |  | HG1 | HG22 |
| GLU290 (C) | MET1 | 4.70 | -0.77 | -1 | 1 |  | HN | HE3 |
| ALA193 (C) | VAL47 | 4.71 | -0.16 | 0 | 0 |  | HB3 | HG13 |
| LYS236 (C) | ARG21 | 4.71 | -3.81 | 1 | -2 |  | HZ2 | HH22 |
| LYS236 (C) | SER18 | 4.73 | -0.69 | 1 | 0 |  | HE1 | HG |
| THR196 (C) | VAL7 | 4.74 | 0.44 | 0 | 0 |  | HN | HG21 |
| ALA191 (C) | VAL47 | 4.77 | -0.15 | 0 | 0 |  | HB1 | HG12 |
| LYS137 (C) | ASP79 | 4.78 | -0.62 | 1 | -1 |  | HZ1 | HN |
| THR169 (C) | VAL7 | 4.78 | -0.21 | 0 | 0 |  | HG22 | HN |
| THR198 (C) | ASN13 | 4.78 | -0.12 | 0 | 0 |  | OG1 | HD21 |
| ALA191 (C) | VAL7 | 4.79 | 0.10 | 0 | 0 |  | O | HG11 |
| THR257 (A) | VAL114 | 4.80 | -0.26 | 0 | 0 |  | HA | H |
| GLY170 (C) | TRP77 | 4.81 | -0.53 | 0 | 0 |  | O | HE1 |
| HIS172 (C) | TRP77 | 4.89 | -0.42 | 0 | 0 |  | HN | HE1 |
| THR257 (A) | ALA152 | 4.89 | 0.36 | 0 | 0 |  | O | H |
| GLY258 (A) | LYS177 | 4.90 | -0.01 | 0 | 1 |  | HA1 | HZ3 |
| VAL212 (A) | TRP111 | 4.92 | -0.33 | 0 | 0 |  | HB | O |
| SER284 (A) | MET78 | 4.94 | -0.19 | 0 | 0 |  | H | HE2 |
| ARG131 (C) | ALA2 | 4.95 | 7.53 | -2 | 0 |  | HH22 | HB1 |
| PHE223 (A) | TRP111 | 4.96 | -0.60 | 0 | 0 |  | H | HH2 |
| LEU287 (C) | ASP79 | 4.97 | -0.88 | 0 | -1 |  | HN | HB2 |
| ALA255 (A) | ALA150 | 4.98 | -0.26 | 0 | 0 |  | O | H |
| LEU220 (A) | ARG112 | 5.00 | 0.06 | 0 | 1 |  | HD11 | HA |
| LEU286 (C) | MET1 | 5.05 | -1.53 | 0 | 1 |  | HB1 | HE1 |
| TYR237 (C) | MET1 | 5.06 | -1.17 | 0 | 1 |  | HB2 | HT1 |
| PRO241 (C) | ASN13 | 5.06 | -0.23 | 0 | 0 |  | HD1 | HD21 |
| LEU253 (A) | HIS149 | 5.10 | 0.08 | 0 | 0 |  | HA | HE1 |
| THR169 (C) | TRP73 | 5.11 | -0.22 | 0 | 0 |  | HA | HZ2 |
| GLY170 (C) | GLY50 | 5.11 | -0.21 | 0 | 0 |  | N | HA1 |
| ILE259 (A) | ASN151 | 5.11 | -0.40 | 0 | 0 |  | H | HD21 |
| THR169 (C) | TRP77 | 5.13 | -0.37 | 0 | 0 |  | O | HB1 |
| ASP197 (C) | HIS8 | 5.13 | 0.49 | -1 | 0 |  | HA | HE1 |
| GLY258 (A) | TRP111 | 5.14 | -0.38 | 0 | 0 |  | O | HD1 |
| ASN238 (C) | ASP15 | 5.15 | -0.20 | 0 | -1 |  | HN | HN |
| PHE134 (C) | HIS8 | 5.16 | -0.75 | 0 | 0 |  | HD1 | HE1 |
| PRO132 (C) | HIS8 | 5.19 | 0.00 | 0 | 0 |  | O | HE1 |
| SER46 (C) | PRO119 | 5.19 | -0.17 | 0 | 0 |  | HG | HB1 |
| ASP197 (C) | SER10 | 5.20 | -0.11 | -1 | 0 |  | HN | HB2 |
| THR257 (A) | HIS149 | 5.20 | -0.61 | 0 | 0 |  | N | HB2 |
| SER284 (C) | MET78 | 5.23 | -0.07 | 0 | 0 |  | HB2 | HE2 |
| THR198 (C) | THR3 | 5.24 | 0.43 | 0 | 0 |  | HA | O |
| TYR209 (A) | PRO113 | 5.24 | -0.20 | 0 | 0 |  | O | HG2 |
| LEU287 (C) | MET78 | 5.25 | -1.28 | 0 | 0 |  | O | HE2 |
| GLY215 (A) | LYS75 | 5.27 | -0.59 | 0 | 1 |  | O | HZ3 |
| ARG131 (C) | TRP77 | 5.28 | -0.25 | -2 | 0 |  | HD2 | HA |
| ASN214 (A) | PRO113 | 5.29 | -0.16 | 0 | 0 |  | H | HG2 |
| ALA194 (C) | THR51 | 5.30 | -0.18 | 0 | 0 |  | O | HG21 |
| LEU220 (A) | GLY110 | 5.31 | -0.66 | 0 | 0 |  | HD12 | HA2 |
| THR135 (A) | TRP77 | 5.31 | -0.07 | 0 | 0 |  | HG1 | HD1 |
| THR280 (A) | MET78 | 5.32 | -0.25 | 0 | 0 |  | HG22 | HG2 |
| ALA193 (A) | GLY50 | 5.32 | -0.10 | 0 | 0 |  | HB2 | HN |
| VAL171 (C) | THR3 | 5.35 | -0.18 | 0 | 0 |  | HG21 | HG22 |
| ASP216 (A) | MET78 | 5.36 | -0.07 | -1 | 0 |  | OD2 | HG1 |
| GLY258 (A) | GLU153 | 5.37 | 0.17 | 0 | -1 |  | HA2 | HB1 |
| GLN256 (A) | PRO115 | 5.38 | -0.36 | 0 | 0 |  | OE1 | HA |
| TYR237 (C) | ARG21 | 5.39 | 0.54 | 0 | -2 |  | OH | NH2 |
| TYR239 (C) | PRO14 | 5.40 | -0.30 | 0 | 0 |  | HN | HB1 |
| ASP197 (C) | GLY5 | 5.42 | 0.02 | -1 | 0 |  | HN | O |
| THR198 (C) | LEU4 | 5.43 | -0.02 | 0 | 0 |  | HA | HD21 |
| ILE213 (A) | VAL114 | 5.43 | -0.27 | 0 | 0 |  | HG11 | H |
| LEU220 (A) | PRO113 | 5.43 | -0.09 | 0 | 0 |  | HD11 | HD2 |
| ALA285 (C) | MET78 | 5.43 | 0.17 | 0 | 0 |  | HN | HE2 |
| THR196 (C) | GLU45 | 5.45 | -0.11 | 0 | -1 |  | HB | HG1 |
| GLY215 (A) | PRO113 | 5.45 | -0.06 | 0 | 0 |  | HA1 | HD1 |
| ALA193 (C) | ALA49 | 5.48 | -0.03 | 0 | 0 |  | HB1 | HA |
| GLY195 (C) | ASP9 | 5.49 | -4.63 | 0 | -1 |  | HA2 | N |
| GLU240 (C) | ASN13 | 5.49 | -0.18 | -1 | 0 |  | HA | HD21 |
| ALA255 (A) | HIS198 | 5.50 | -0.11 | 0 | 0 |  | HB2 | O |
| THR169 (C) | PRO76 | 5.54 | -0.42 | 0 | 0 |  | O | HD1 |
| ASN133 (C) | GLY5 | 5.55 | -0.09 | 0 | 0 |  | HD22 | O |
| GLY195 (C) | THR51 | 5.56 | -0.06 | 0 | 0 |  | HA2 | HG23 |
| GLY183 (C) | HIS8 | 5.59 | 0.38 | 0 | 0 |  | HA2 | HE2 |
| ALA193 (C) | VAL48 | 5.60 | 0.00 | 0 | 0 |  | HB1 | O |
| GLN256 (A) | SER199 | 5.61 | -0.18 | 0 | -1 |  | H | HB2 |
| ALA193 (C) | HIS8 | 5.62 | -0.30 | 0 | 0 |  | O | HE2 |
| ARG279 (A) | LYS75 | 5.63 | 1.51 | 1 | 1 |  | HH12 | HZ2 |
| GLY258 (A) | HIS149 | 5.63 | -0.09 | 0 | 0 |  | H | HB2 |
| TYR239 (C) | ASP79 | 5.63 | -0.17 | 0 | -1 |  | HE1 | OD1 |
| THR196 (C) | THR51 | 5.64 | -0.11 | 0 | 0 |  | HA | HG23 |
| VAL171 (C) | PRO76 | 5.67 | -0.17 | 0 | 0 |  | HG13 | HG1 |
| ILE213 (A) | PRO115 | 5.67 | -0.14 | 0 | 0 |  | HG23 | HA |
| GLY251 (A) | HIS198 | 5.67 | -0.15 | 0 | 0 |  | HA1 | O |
| THR135 (C) | THR3 | 5.67 | -0.15 | 0 | 0 |  | HG1 | OG1 |
| PRO168 (C) | TRP73 | 5.68 | -0.09 | 0 | 0 |  | O | HZ2 |
| SER254 (A) | SER199 | 5.68 | -0.27 | 0 | -1 |  | HB2 | HG |
| THR196 (C) | PRO14 | 5.68 | -0.07 | 0 | 0 |  | HG1 | HG1 |
| LEU167 (C) | VAL7 | 5.68 | -0.12 | 0 | 0 |  | HD21 | HG13 |
| GLY258 (A) | ALA152 | 5.69 | -0.18 | 0 | 0 |  | HA2 | O |
| SER144 (C) | HIS117 | 5.70 | -0.13 | 0 | 0 |  | HN | HD2 |
| ARG131 (C) | PRO76 | 5.72 | 2.65 | -2 | 0 |  | HD1 | HB1 |
| GLY258 (A) | PRO113 | 5.74 | -0.04 | 0 | 0 |  | N | HA |
| LEU141 (C) | ASP118 | 5.76 | -0.47 | 0 | -1 |  | HD21 | HB2 |
| ALA193 (C) | THR51 | 5.77 | -0.06 | 0 | 0 |  | HB2 | HG21 |
| ARG279 (A) | GLN82 | 5.77 | -0.37 | 1 | 0 |  | HH12 | OE1 |
| PHE185 (C) | HIS8 | 5.77 | -0.15 | 0 | 0 |  | HZ | HE2 |
| ASN238 (C) | MET1 | 5.80 | -0.48 | 0 | 1 |  | HB2 | HT3 |
| ALA234 (C) | PRO14 | 5.81 | -0.25 | 0 | 0 |  | O | HB1 |
| MET276 (C) | ASP79 | 5.81 | -0.04 | 0 | -1 |  | HB2 | HB2 |
| ASN133 (C) | VAL7 | 5.81 | -0.15 | 0 | 0 |  | HB1 | HG21 |
| PRO132 (C) | ALA2 | 5.81 | 0.02 | 0 | 0 |  | HG2 | HB1 |
| SER254 (A) | ASP162 | 5.82 | 0.11 | 0 | -1 |  | O | OD1 |
| ASN238 (C) | ASN11 | 5.82 | -0.17 | 0 | 0 |  | HB1 | HA |
| THR169 (C) | GLY5 | 5.85 | -0.06 | 0 | 0 |  | HG22 | O |
| ALA211 (A) | PRO113 | 5.85 | 0.02 | 0 | 0 |  | C | HG2 |
| ILE259 (A) | GLU153 | 5.86 | -0.23 | 0 | -1 |  | HG11 | HG2 |
| THR257 (A) | ASP162 | 5.87 | -0.31 | 0 | -1 |  | O | HB2 |
| TYR126 (C) | TRP77 | 5.88 | -0.09 | 0 | 0 |  | HE1 | HZ2 |
| ALA255 (A) | MET163 | 5.90 | -0.06 | 0 | 0 |  | O | HA |
| ALA255 (A) | VAL148 | 5.92 | -0.35 | 0 | 0 |  | HB3 | HG13 |
| PRO168 (C) | VAL7 | 5.93 | -0.08 | 0 | 0 |  | HD1 | HG13 |
| LEU141 (C) | VAL114 | 5.93 | 0.13 | 0 | 0 |  | HD23 | O |
| ASN142 (C) | GLN122 | 5.94 | -0.04 | 0 | 0 |  | HD22 | HB2 |
| PRO168 (C) | VAL47 | 5.96 | -0.09 | 0 | 0 |  | HG2 | HG13 |
| ASN119 (C) | HIS117 | 5.96 | -0.18 | 0 | 0 |  | HB2 | HE1 |
| ASP263 (A) | TRP111 | 5.97 | -0.36 | -1 | 0 |  | OD1 | HZ2 |
| GLY251 (A) | HIS149 | 5.99 | -0.17 | 0 | 0 |  | O | NE2 |
| LYS236 (C) | THR16 | 5.99 | 0.04 | 1 | 0 |  | O | N |
| TYR118 (C) | VAL116 | 6.00 | -0.22 | 0 | 0 |  | HE2 | HG22 |
| ARG217 (A) | GLN82 | 6.00 | -0.10 | 1 | 0 |  | HH22 | HE22 |
| GLY195 (C) | LEU4 | 6.00 | -0.54 | 0 | 0 |  | O | N |
| LEU253 (A) | SER199 | 6.00 | -0.14 | 0 | -1 |  | N | HB2 |
| GLU240 (C) | ALA2 | 6.03 | 0.46 | -1 | 0 |  | HN | HB1 |
| TYR237 (C) | LYS81 | 6.04 | -0.10 | 0 | 1 |  | HE1 | HZ3 |
| GLY170 (C) | ALA49 | 6.04 | -0.13 | 0 | 0 |  | N | O |
| SER254 (A) | LYS177 | 6.05 | -0.16 | 0 | 1 |  | O | HZ1 |
| THR257 (A) | GLU153 | 6.05 | 0.18 | 0 | -1 |  | O | HB1 |
| LEU272 (C) | MET1 | 6.07 | -0.17 | 0 | 1 |  | HD21 | HB1 |
| GLY258 (A) | ARG112 | 6.08 | -0.04 | 0 | 1 |  | HA2 | H |
| LEU286 (C) | TRP77 | 6.10 | -0.02 | 0 | 0 |  | HD12 | O |
| ARG222 (A) | GLU153 | 6.10 | -1.94 | 1 | -1 |  | HH21 | OE1 |
| THR169 (C) | VAL47 | 6.11 | -0.07 | 0 | 0 |  | HG21 | HG13 |
| LYS236 (C) | LEU4 | 6.12 | -0.13 | 1 | 0 |  | O | HD22 |
| PRO252 (A) | VAL148 | 6.12 | -0.12 | 0 | 0 |  | HB1 | HG13 |
| ASN133 (C) | GLY6 | 6.12 | -0.06 | 0 | 0 |  | HD22 | HA1 |
| MET235 (C) | SER12 | 6.13 | -0.36 | 0 | 0 |  | HB1 | O |
| ALA210 (A) | PRO113 | 6.13 | -0.08 | 0 | 0 |  | O | HG2 |
| LEU253 (A) | ASN151 | 6.15 | -0.10 | 0 | 0 |  | O | HD21 |
| SER254 (A) | HIS149 | 6.17 | -0.36 | 0 | 0 |  | O | HB2 |
| PRO252 (A) | LEU164 | 6.17 | -0.06 | 0 | 0 |  | HA | HD23 |
| LYS137 (C) | THR3 | 6.19 | -0.08 | 1 | 0 |  | HE1 | HG1 |
| THR280 (A) | PHE80 | 6.21 | -0.25 | 0 | 0 |  | HG1 | HB1 |
| MET235 (C) | SER10 | 6.22 | -0.04 | 0 | 0 |  | O | HG |
| THR198 (C) | MET1 | 6.22 | -0.29 | 0 | 1 |  | HA | C |
| VAL296 (A) | HIS149 | 6.23 | -0.07 | 0 | 0 |  | HG12 | HE1 |
| THR199 (C) | THR3 | 6.23 | -0.01 | 0 | 0 |  | OG1 | HN |
| TYR237 (C) | LEU19 | 6.24 | -0.17 | 0 | 0 |  | HD1 | HD11 |
| ALA260 (A) | TRP111 | 6.25 | -0.20 | 0 | 0 |  | H | HD1 |
| LYS236 (C) | SER12 | 6.27 | -0.15 | 1 | 0 |  | HA | O |
| ASN133 (C) | PRO76 | 6.27 | -0.07 | 0 | 0 |  | HD22 | HG1 |
| ILE259 (A) | ALA152 | 6.28 | -0.19 | 0 | 0 |  | HG12 | O |
| GLY258 (A) | LYS160 | 6.29 | -0.22 | 0 | 1 |  | HA2 | HE1 |
| ASN238 (C) | SER12 | 6.30 | -0.21 | 0 | 0 |  | OD1 | HN |
| PHE219 (A) | TRP111 | 6.31 | -0.28 | 0 | 0 |  | C | HZ3 |
| TRP207 (C) | MET1 | 6.34 | -0.14 | 0 | 1 |  | HE3 | HE3 |
| LEU167 (C) | ALA49 | 6.34 | -0.04 | 0 | 0 |  | C | HA |
| GLY258 (A) | ALA150 | 6.34 | -0.14 | 0 | 0 |  | N | O |
| ASN133 (C) | ALA2 | 6.35 | 0.14 | 0 | 0 |  | HD22 | HA |
| GLN189 (C) | PRO119 | 6.35 | -0.06 | 0 | 0 |  | OE1 | HG1 |
| GLN256 (A) | ARG112 | 6.36 | -0.27 | 0 | 1 |  | O | O |
| LYS137 (C) | ALA2 | 6.37 | -0.52 | 1 | 0 |  | HZ1 | HA |
| ILE259 (A) | GLY110 | 6.37 | 0.05 | 0 | 0 |  | HD1 | C |
| THR196 (C) | ASN11 | 6.38 | -0.19 | 0 | 0 |  | HG23 | N |
| TYR239 (C) | LEU4 | 6.38 | -0.18 | 0 | 0 |  | HD1 | HD22 |
| ILE200 (C) | ALA2 | 6.39 | 7.50 | 0 | 0 |  | N | HB1 |
| ASN133 (C) | LEU4 | 6.39 | -0.08 | 0 | 0 |  | HD22 | N |
| GLN299 (A) | VAL116 | 6.39 | -0.14 | 0 | 0 |  | HB2 | HG22 |
| THR196 (C) | PRO76 | 6.40 | -0.06 | 0 | 0 |  | HA | HG2 |
| THR280 (A) | ASP79 | 6.42 | -0.22 | 0 | -1 |  | HG1 | O |
| ILE281 (A) | MET78 | 6.42 | -0.09 | 0 | 0 |  | C | HE2 |
| ALA194 (C) | PRO76 | 6.43 | -0.04 | 0 | 0 |  | HB2 | HG1 |
| LEU220 (A) | GLU153 | 6.43 | -0.13 | 0 | -1 |  | HD13 | HG2 |
| PHE140 (C) | TRP77 | 6.43 | -0.10 | 0 | 0 |  | HN | HZ2 |
| ASN238 (C) | GLY5 | 6.44 | -0.09 | 0 | 0 |  | HD22 | N |
| PRO252 (A) | HIS198 | 6.44 | 0.00 | 0 | 0 |  | HA | O |
| GLN256 (A) | ASP162 | 6.45 | 0.25 | 0 | -1 |  | N | OD1 |
| GLU166 (C) | PRO115 | 6.46 | -0.12 | -1 | 0 |  | OE2 | HG1 |
| ASN142 (C) | GLU146 | 6.46 | -0.11 | 0 | -1 |  | HD22 | OE2 |
| ILE213 (A) | ARG112 | 6.46 | -0.27 | 0 | 1 |  | HA | HA |
| LEU286 (C) | LYS75 | 6.47 | -0.05 | 0 | 1 |  | HD11 | O |
| LYS236 (C) | LEU19 | 6.47 | -0.15 | 1 | 0 |  | O | HD11 |
| THR199 (C) | LEU4 | 6.47 | -0.04 | 0 | 0 |  | HN | HD21 |
| ALA194 (C) | GLY50 | 6.48 | -0.04 | 0 | 0 |  | O | O |
| PRO132 (C) | THR3 | 6.49 | -0.13 | 0 | 0 |  | HD1 | HN |
| THR198 (C) | SER10 | 6.50 | -0.07 | 0 | 0 |  | HB | OG |
| GLN256 (A) | LEU164 | 6.51 | -0.08 | 0 | 0 |  | HA | HB2 |
| SER1 (A) | PRO115 | 6.55 | 0.04 | 1 | 0 |  | HA | HB2 |
| LEU253 (A) | PRO113 | 6.55 | -0.08 | 0 | 0 |  | O | HB2 |
| LEU232 (C) | ASP15 | 6.55 | 0.07 | 0 | -1 |  | O | HB2 |
| ASN133 (C) | THR51 | 6.56 | -0.03 | 0 | 0 |  | HD22 | HG23 |
| PHE3 (A) | PRO113 | 6.56 | -0.07 | 0 | 0 |  | HB1 | HG2 |
| LEU220 (A) | SER109 | 6.58 | -0.06 | 0 | 0 |  | HD12 | O |
| ILE200 (C) | MET1 | 6.59 | 7.33 | 0 | 1 |  | HN | HE2 |
| GLN256 (A) | ALA152 | 6.59 | -0.08 | 0 | 0 |  | O | H |
| PHE140 (C) | PRO115 | 6.59 | -0.06 | 0 | 0 |  | O | HB2 |
| ASP216 (A) | PRO113 | 6.60 | -0.07 | -1 | 0 |  | O | HD1 |
| ASP197 (C) | ASN13 | 6.60 | -0.23 | -1 | 0 |  | O | HD21 |
| GLY215 (A) | ARG112 | 6.60 | 0.02 | 0 | 1 |  | HA1 | HB1 |
| MET235 (C) | LEU4 | 6.61 | -0.02 | 0 | 0 |  | O | HD22 |
| ILE213 (A) | ALA150 | 6.61 | -0.05 | 0 | 0 |  | HG11 | O |
| THR169 (C) | LYS75 | 6.61 | -0.34 | 0 | 1 |  | O | HA |
| ASN203 (C) | MET1 | 6.62 | 0.03 | 0 | 1 |  | HB1 | HE3 |
| VAL297 (A) | VAL148 | 6.65 | -0.09 | 0 | 0 |  | HG11 | HG13 |
| GLY215 (A) | TRP77 | 6.66 | -0.08 | 0 | 0 |  | N | HZ3 |
| GLY215 (A) | VAL108 | 6.66 | -0.06 | 0 | 0 |  | O | HG13 |
| LEU232 (C) | PRO14 | 6.66 | -0.04 | 0 | 0 |  | O | HA |
| GLN273 (C) | ARG21 | 6.67 | 1.55 | 0 | -2 |  | HE22 | HH22 |
| GLN256 (A) | VAL147 | 6.67 | -0.04 | 0 | 0 |  | HE22 | O |
| THR135 (C) | HIS8 | 6.69 | -0.05 | 0 | 0 |  | HG21 | HE2 |
| GLY2 (A) | MET78 | 6.70 | -0.09 | 0 | 0 |  | HA1 | HB1 |
| GLN256 (A) | LYS177 | 6.71 | -0.27 | 0 | 1 |  | N | HZ1 |
| PHE291 (C) | MET1 | 6.72 | -0.11 | 0 | 1 |  | HN | HE3 |
| TRP218 (A) | PHE80 | 6.72 | -0.11 | 0 | 0 |  | HB2 | HE1 |
| ASN231 (C) | ASN13 | 6.72 | -0.04 | 0 | 0 |  | O | OD1 |
| LEU232 (C) | ASN13 | 6.72 | -0.04 | 0 | 0 |  | O | O |
| VAL233 (C) | PRO14 | 6.73 | -0.06 | 0 | 0 |  | O | HA |
| GLN256 (A) | MET163 | 6.74 | -0.07 | 0 | 0 |  | HA | HA |
| PRO252 (A) | LYS175 | 6.74 | -0.01 | 0 | 1 |  | HB2 | HZ2 |
| THR169 (C) | LEU52 | 6.75 | -0.07 | 0 | 0 |  | HG23 | HN |
| CYS300 (A) | VAL148 | 6.76 | -0.07 | 0 | 0 |  | SG | O |
| THR199 (C) | ASP79 | 6.76 | -0.65 | 0 | -1 |  | HG1 | HB1 |
| ASP197 (C) | ASP9 | 6.76 | 0.97 | -1 | -1 |  | HN | HA |
| VAL297 (A) | SER199 | 6.77 | -0.04 | 0 | -1 |  | HG11 | HB2 |
| ASN142 (C) | VAL120 | 6.78 | -0.02 | 0 | 0 |  | HD22 | HN |
| ALA255 (A) | ASP197 | 6.78 | -0.07 | 0 | -1 |  | HB1 | HA |
| VAL212 (A) | ASN151 | 6.78 | -0.07 | 0 | 0 |  | HG23 | HB2 |
| GLY183 (C) | VAL7 | 6.79 | 0.03 | 0 | 0 |  | C | HG23 |
| PRO168 (C) | GLY6 | 6.80 | 0.01 | 0 | 0 |  | HG2 | HA2 |
| THR135 (C) | VAL7 | 6.80 | -0.03 | 0 | 0 |  | HG21 | HG22 |
| ILE213 (A) | ASN151 | 6.81 | -0.05 | 0 | 0 |  | HG11 | HB2 |
| ILE259 (A) | ASP162 | 6.82 | 0.11 | 0 | -1 |  | N | OD1 |
| MET264 (A) | TRP111 | 6.82 | -0.10 | 0 | 0 |  | HE2 | HB1 |
| THR24 (C) | GLU143 | 6.84 | -0.05 | 0 | -1 |  | HG22 | OE1 |
| PRO252 (A) | ASN151 | 6.85 | -0.04 | 0 | 0 |  | O | HD21 |
| PHE140 (C) | HIS117 | 6.85 | -0.14 | 0 | 0 |  | C | HD2 |
| ASN119 (C) | GLU146 | 6.86 | -0.01 | 0 | -1 |  | HB2 | HG2 |
| ASP289 (C) | ALA2 | 6.87 | -0.14 | -1 | 0 |  | OD2 | HB1 |
| THR196 (C) | ASN13 | 6.89 | -0.08 | 0 | 0 |  | HG23 | HB1 |
| LYS5 (A) | TRP77 | 6.89 | -0.11 | 1 | 0 |  | H | HH2 |
| ALA285 (C) | ASP79 | 6.89 | -0.03 | 0 | -1 |  | O | HB2 |
| ALA193 (C) | THR3 | 6.89 | 0.00 | 0 | 0 |  | HB2 | HG22 |
| ASN142 (C) | VAL121 | 6.90 | -0.02 | 0 | 0 |  | HD22 | HB |
| THR198 (C) | PRO14 | 6.90 | -0.04 | 0 | 0 |  | HG1 | HD1 |
| ALA234 (C) | ALA2 | 6.90 | -0.03 | 0 | 0 |  | O | HB2 |
| ASP248 (A) | SER199 | 6.91 | 1.19 | -1 | -1 |  | O | HA |
| ARG279 (A) | LYS81 | 6.93 | 0.70 | 1 | 1 |  | HH12 | O |
| LYS236 (C) | HIS17 | 6.93 | -0.02 | 1 | 0 |  | HB2 | HN |
| ASN238 (C) | ASP9 | 6.93 | -0.08 | 0 | -1 |  | HD21 | C |
| ALA193 (C) | GLY5 | 6.94 | 0.00 | 0 | 0 |  | HB2 | O |
| VAL171 (C) | GLY50 | 6.94 | -0.03 | 0 | 0 |  | HN | HA1 |
| ASP216 (A) | LYS75 | 6.96 | -1.59 | -1 | 1 |  | HA | HZ2 |
| VAL212 (A) | VAL114 | 6.96 | -0.08 | 0 | 0 |  | HG22 | H |
| LEU287 (C) | TRP77 | 6.97 | -0.01 | 0 | 0 |  | O | O |
| GLN299 (A) | HIS117 | 6.97 | -0.22 | 0 | 0 |  | O | HD2 |
| LEU141 (C) | PRO113 | 6.98 | -0.03 | 0 | 0 |  | HD23 | HB1 |
| ASP216 (A) | PHE80 | 7.00 | -0.25 | -1 | 0 |  | OD1 | HB1 |
| GLN192 (C) | VAL47 | 7.00 | -0.05 | 0 | 0 |  | HA | HG13 |
| VAL296 (A) | PRO113 | 7.00 | -0.06 | 0 | 0 |  | HG13 | HB2 |
| GLY195 (C) | PRO76 | 7.01 | -0.03 | 0 | 0 |  | O | HG2 |
| ASP197 (C) | TRP77 | 7.01 | 0.13 | -1 | 0 |  | OD2 | HA |
| ASP197 (C) | THR51 | 7.02 | 0.06 | -1 | 0 |  | HN | HG23 |
| ARG4 (A) | MET78 | 7.02 | -0.17 | 1 | 0 |  | HG1 | HE1 |
| TYR237 (C) | SER10 | 7.03 | -0.08 | 0 | 0 |  | C | HG |
| TRP218 (A) | TRP111 | 7.04 | -0.13 | 0 | 0 |  | HA | HZ3 |
| THR199 (C) | PRO76 | 7.06 | -0.04 | 0 | 0 |  | HG1 | HB1 |
| CYS300 (A) | GLU146 | 7.08 | 0.02 | 0 | -1 |  | SG | HG1 |
| ASP197 (C) | PRO14 | 7.08 | -0.10 | -1 | 0 |  | O | HG1 |
| LEU167 (C) | GLY50 | 7.09 | -0.08 | 0 | 0 |  | C | HN |
| THR135 (C) | PRO76 | 7.09 | -0.02 | 0 | 0 |  | HG1 | HG1 |
| ILE213 (A) | TRP77 | 7.09 | -0.10 | 0 | 0 |  | O | HZ3 |
| GLU290 (C) | TRP77 | 7.10 | 0.01 | -1 | 0 |  | OE1 | HZ2 |
| GLY283 (A) | ASP79 | 7.11 | -0.04 | 0 | -1 |  | HA1 | H |
| VAL233 (C) | ASP15 | 7.11 | 0.11 | 0 | -1 |  | O | HN |
| SER139 (C) | PRO115 | 7.12 | -0.04 | 0 | 0 |  | O | HB2 |
| GLY283 (A) | TRP77 | 7.13 | -0.06 | 0 | 0 |  | N | HZ3 |
| GLU288 (C) | TRP77 | 7.13 | 0.30 | -1 | 0 |  | OE1 | O |
| THR169 (C) | HIS8 | 7.13 | -0.06 | 0 | 0 |  | HG22 | HN |
| THR199 (C) | ASN13 | 7.14 | -0.04 | 0 | 0 |  | HN | HD21 |
| MET264 (A) | PRO113 | 7.16 | -0.02 | 0 | 0 |  | HE2 | HD2 |
| CYS300 (A) | VAL147 | 7.16 | -0.04 | 0 | 0 |  | SG | O |
| VAL233 (C) | ASN13 | 7.17 | -0.04 | 0 | 0 |  | O | HD22 |
| GLY215 (A) | PHE80 | 7.19 | -0.07 | 0 | 0 |  | O | HD1 |
| ASP216 (A) | ARG112 | 7.19 | -0.81 | -1 | 1 |  | O | HA |
| THR196 (C) | SER12 | 7.19 | -0.04 | 0 | 0 |  | HG23 | HN |
| ALA194 (C) | VAL47 | 7.19 | -0.08 | 0 | 0 |  | O | HG13 |
| ARG217 (A) | ALA152 | 7.19 | -0.10 | 1 | 0 |  | HD2 | O |
| LEU286 (C) | PRO76 | 7.21 | -0.06 | 0 | 0 |  | HD11 | HA |
| TYR118 (C) | GLU146 | 7.21 | -0.05 | 0 | -1 |  | HB1 | HG2 |
| ASP216 (A) | TRP111 | 7.22 | 0.07 | -1 | 0 |  | O | O |
| ALA234 (C) | ASP15 | 7.22 | 0.05 | 0 | -1 |  | O | HN |
| TYR237 (C) | ASP79 | 7.22 | 0.02 | 0 | -1 |  | HB2 | OD1 |
| ALA255 (A) | PRO113 | 7.22 | -0.04 | 0 | 0 |  | O | HA |
| PRO168 (C) | THR51 | 7.24 | -0.26 | 0 | 0 |  | O | N |
| GLY195 (C) | GLU45 | 7.25 | 0.10 | 0 | -1 |  | HA2 | HG1 |
| GLU288 (C) | ASP79 | 7.25 | 0.80 | -1 | -1 |  | HA | HN |
| GLY143 (C) | VAL116 | 7.25 | -0.08 | 0 | 0 |  | N | O |
| GLY258 (A) | VAL114 | 7.25 | -0.04 | 0 | 0 |  | N | H |
| GLY170 (C) | PRO76 | 7.26 | -0.16 | 0 | 0 |  | HA2 | HD1 |
| ASN238 (C) | PRO76 | 7.26 | -0.03 | 0 | 0 |  | HD22 | HB2 |
| THR169 (C) | GLN46 | 7.27 | -0.03 | 0 | 0 |  | HG23 | O |
| GLY195 (C) | SER10 | 7.27 | -0.12 | 0 | 0 |  | C | HB2 |
| LEU208 (A) | PRO113 | 7.27 | -0.03 | 0 | 0 |  | O | HG2 |
| LEU167 (C) | THR3 | 7.28 | -0.02 | 0 | 0 |  | HD11 | HG22 |
| GLY215 (A) | MET78 | 7.29 | -0.08 | 0 | 0 |  | HA2 | HB2 |
| LEU141 (C) | VAL121 | 7.30 | -0.02 | 0 | 0 |  | HD21 | HG21 |
| TYR237 (C) | THR3 | 7.30 | 0.00 | 0 | 0 |  | O | N |
| GLY195 (C) | ALA2 | 7.31 | -0.47 | 0 | 0 |  | O | C |
| ILE213 (A) | VAL116 | 7.31 | -0.07 | 0 | 0 |  | HG23 | H |
| ASP197 (C) | GLY6 | 7.33 | 0.05 | -1 | 0 |  | HN | HA1 |
| ASN221 (A) | GLY110 | 7.35 | -0.09 | 0 | 0 |  | HA | HA1 |
| GLY2 (A) | PRO113 | 7.36 | -0.02 | 0 | 0 |  | H | HG1 |
| LEU268 (C) | MET1 | 7.36 | -0.07 | 0 | 1 |  | HD11 | SD |
| THR169 (C) | VAL74 | 7.37 | -0.11 | 0 | 0 |  | HG23 | O |
| LEU250 (A) | SER199 | 7.37 | -0.03 | 0 | -1 |  | O | HG |
| ALA194 (C) | TRP77 | 7.37 | -0.03 | 0 | 0 |  | HB1 | HD1 |
| SER301 (A) | HIS117 | 7.38 | 0.01 | 0 | 0 |  | N | NE2 |
| GLU290 (C) | MET78 | 7.39 | 0.01 | -1 | 0 |  | HB2 | HE1 |
| ASN133 (C) | TRP77 | 7.42 | -0.04 | 0 | 0 |  | HD21 | HD1 |
| ASP289 (C) | MET78 | 7.44 | -0.07 | -1 | 0 |  | HN | HE1 |
| ASN214 (A) | LYS75 | 7.44 | -0.06 | 0 | 1 |  | O | HZ3 |
| GLY143 (C) | PRO119 | 7.44 | -0.04 | 0 | 0 |  | HN | HD2 |
| GLY215 (A) | ASP106 | 7.44 | 0.12 | 0 | -1 |  | HA2 | OD2 |
| LYS137 (C) | LYS75 | 7.44 | 0.79 | 1 | 1 |  | HZ1 | O |
| MET235 (C) | ASN11 | 7.44 | -0.03 | 0 | 0 |  | O | HA |
| THR201 (C) | MET1 | 7.44 | -0.07 | 0 | 1 |  | HA | HE3 |
| GLY251 (A) | LYS177 | 7.44 | -0.18 | 0 | 1 |  | O | HZ1 |
| GLU166 (C) | TRP77 | 7.45 | -0.05 | -1 | 0 |  | HG2 | HE1 |
| GLY143 (C) | ASP118 | 7.45 | -0.01 | 0 | -1 |  | N | HA |
| ALA260 (A) | GLU153 | 7.47 | -0.06 | 0 | -1 |  | H | OE2 |
| ARG217 (A) | GLU153 | 7.49 | -0.75 | 1 | -1 |  | HD1 | HA |
| ALA211 (A) | TRP77 | 7.49 | -0.02 | 0 | 0 |  | HA | HZ3 |
| LYS236 (C) | ASN11 | 7.49 | -0.10 | 1 | 0 |  | HA | HA |
| SER301 (A) | VAL116 | 7.49 | -0.01 | 0 | 0 |  | H | HG21 |
| MET276 (C) | MET1 | 7.51 | -0.12 | 0 | 1 |  | HB2 | HB2 |
| TYR239 (C) | ASP15 | 7.52 | 0.03 | 0 | -1 |  | HN | HN |
| PRO252 (A) | LYS177 | 7.53 | -0.15 | 0 | 1 |  | HA | HZ1 |
| GLY143 (C) | GLU146 | 7.53 | 0.04 | 0 | -1 |  | HA1 | OE2 |
| LEU286 (C) | LYS81 | 7.54 | -0.01 | 0 | 1 |  | HD23 | HN |
| PRO252 (A) | ALA150 | 7.55 | 0.01 | 0 | 0 |  | O | H |
| SER254 (A) | PRO113 | 7.56 | -0.03 | 0 | 0 |  | O | HB2 |
| TYR237 (C) | HIS17 | 7.57 | -0.07 | 0 | 0 |  | HE1 | C |
| SER284 (C) | MET1 | 7.57 | 0.06 | 0 | 1 |  | HB2 | HE1 |
| THR198 (C) | HIS8 | 7.58 | -0.03 | 0 | 0 |  | HN | HE1 |
| ASP289 (C) | TRP77 | 7.58 | 0.19 | -1 | 0 |  | OD1 | O |
| SER46 (C) | VAL120 | 7.58 | -0.02 | 0 | 0 |  | HG | HG21 |
| ALA194 (C) | LEU4 | 7.58 | -0.10 | 0 | 0 |  | HB2 | HN |
| ALA255 (A) | VAL114 | 7.58 | -0.05 | 0 | 0 |  | O | H |
| CYS128 (C) | TRP77 | 7.58 | -0.04 | 0 | 0 |  | HB1 | HZ2 |
| GLY170 (C) | TRP73 | 7.58 | -0.04 | 0 | 0 |  | N | HZ2 |
| SER267 (A) | TRP111 | 7.59 | -0.04 | 0 | 0 |  | HG | HZ3 |
| ALA194 (C) | ASP9 | 7.59 | -0.15 | 0 | -1 |  | O | N |
| SER1 (A) | GLY50 | 7.59 | -0.02 | 1 | 0 |  | OG | HA1 |
| MET235 (C) | ALA2 | 7.60 | -0.02 | 0 | 0 |  | O | HB2 |
| ASP289 (C) | PRO76 | 7.60 | 0.07 | -1 | 0 |  | OD1 | O |
| PHE3 (A) | MET78 | 7.60 | -0.06 | 0 | 0 |  | H | SD |
| GLY258 (A) | MET163 | 7.61 | -0.03 | 0 | 0 |  | HA1 | N |
| PHE3 (A) | PRO115 | 7.61 | -0.02 | 0 | 0 |  | HD2 | HA |
| GLN299 (A) | PRO115 | 7.61 | -0.01 | 0 | 0 |  | HG1 | HA |
| LEU220 (A) | ALA152 | 7.65 | -0.02 | 0 | 0 |  | HD13 | O |
| PHE219 (A) | PRO113 | 7.65 | -0.02 | 0 | 0 |  | HZ | HD2 |
| ALA194 (C) | ALA49 | 7.66 | -0.03 | 0 | 0 |  | HN | HA |
| GLN192 (C) | ALA49 | 7.66 | -0.02 | 0 | 0 |  | O | HA |
| VAL171 (C) | THR51 | 7.66 | -0.03 | 0 | 0 |  | HG21 | HG21 |
| TYR209 (A) | TRP111 | 7.67 | -0.03 | 0 | 0 |  | HE1 | HB2 |
| TYR237 (C) | THR16 | 7.67 | 0.00 | 0 | 0 |  | HA | N |
| VAL297 (A) | VAL116 | 7.68 | -0.05 | 0 | 0 |  | HA | HG13 |
| SER1 (A) | LYS75 | 7.68 | 0.98 | 1 | 1 |  | HB1 | HZ3 |
| PRO132 (C) | MET1 | 7.68 | -0.03 | 0 | 1 |  | HD1 | O |
| PHE3 (A) | VAL116 | 7.69 | -0.03 | 0 | 0 |  | HE2 | HG22 |
| PRO184 (C) | GLY6 | 7.70 | -0.04 | 0 | 0 |  | HG1 | C |
| SER254 (A) | HIS198 | 7.70 | 0.01 | 0 | 0 |  | HB2 | O |
| SER1 (A) | ALA49 | 7.72 | -0.11 | 1 | 0 |  | OG | O |
| LEU272 (C) | ALA2 | 7.72 | -0.01 | 0 | 0 |  | HD23 | HN |
| GLU166 (C) | ASP118 | 7.72 | 1.17 | -1 | -1 |  | OE2 | HB2 |
| ILE213 (A) | HIS149 | 7.74 | -0.04 | 0 | 0 |  | HD3 | ND1 |
| PHE140 (C) | VAL116 | 7.74 | -0.17 | 0 | 0 |  | C | O |
| THR257 (A) | LYS177 | 7.76 | 0.14 | 0 | 1 |  | C | HZ3 |
| GLY195 (C) | GLY50 | 7.77 | -0.01 | 0 | 0 |  | HA2 | O |
| GLY275 (C) | ASP79 | 7.77 | -0.16 | 0 | -1 |  | HA2 | OD2 |
| MET165 (C) | VAL7 | 7.78 | 0.00 | 0 | 0 |  | HE2 | HG13 |
| LYS236 (C) | SER10 | 7.78 | -0.05 | 1 | 0 |  | HA | HG |
| ARG222 (A) | GLY110 | 7.78 | 0.07 | 1 | 0 |  | HB1 | HA1 |
| THR196 (C) | VAL74 | 7.78 | -0.01 | 0 | 0 |  | HG1 | HG12 |
| TYR118 (C) | PRO115 | 7.79 | -0.02 | 0 | 0 |  | HE2 | HB1 |
| ALA194 (C) | VAL48 | 7.79 | 0.02 | 0 | 0 |  | HN | O |
| VAL212 (A) | VAL108 | 7.79 | -0.05 | 0 | 0 |  | O | HB |
| TYR239 (C) | SER10 | 7.80 | -0.02 | 0 | 0 |  | N | HG |
| GLY170 (C) | THR51 | 7.81 | 0.03 | 0 | 0 |  | N | HG21 |
| ARG217 (A) | VAL154 | 7.82 | -0.03 | 1 | 0 |  | HE | HG11 |
| LEU141 (C) | VAL148 | 7.83 | -0.02 | 0 | 0 |  | HD22 | O |
| THR198 (C) | PRO76 | 7.83 | 0.00 | 0 | 0 |  | HA | HB1 |
| GLY2 (A) | PRO115 | 7.84 | -0.05 | 0 | 0 |  | O | HB2 |
| PRO252 (A) | ASP197 | 7.84 | -0.04 | 0 | -1 |  | HB2 | OD1 |
| SER1 (A) | PRO113 | 7.84 | -0.06 | 1 | 0 |  | HA | HG1 |
| GLN192 (C) | GLY6 | 7.84 | 0.34 | 0 | 0 |  | HA | C |
| ASP248 (A) | HIS198 | 7.85 | 0.07 | -1 | 0 |  | O | O |
| LEU141 (C) | PRO119 | 7.86 | 0.06 | 0 | 0 |  | C | HD2 |
| TRP207 (A) | MET78 | 7.87 | -0.01 | 0 | 0 |  | HE1 | HE2 |
| ALA234 (C) | LEU4 | 7.88 | -0.01 | 0 | 0 |  | O | HD22 |
| LEU167 (C) | TRP77 | 7.88 | -0.05 | 0 | 0 |  | HB1 | HD1 |
| SER123 (C) | HIS117 | 7.88 | -0.03 | 0 | 0 |  | HG | NE2 |
| ASN133 (C) | MET1 | 7.88 | 0.05 | 0 | 1 |  | HD22 | O |
| SER254 (A) | ALA150 | 7.88 | -0.05 | 0 | 0 |  | O | H |
| ARG279 (A) | ASP106 | 7.90 | -1.13 | 1 | -1 |  | HH12 | OD1 |
| TYR209 (A) | ASN151 | 7.90 | -0.04 | 0 | 0 |  | HE1 | HD21 |
| LEU272 (C) | ASP79 | 7.90 | 0.10 | 0 | -1 |  | HD22 | OD2 |
| ARG298 (A) | HIS149 | 7.91 | -0.08 | 1 | 0 |  | N | HE1 |
| ARG279 (A) | ASP79 | 7.92 | -1.20 | 1 | -1 |  | HG2 | O |
| THR190 (C) | VAL7 | 7.92 | -0.03 | 0 | 0 |  | HG21 | HG11 |
| THR257 (A) | LYS160 | 7.92 | -0.10 | 0 | 1 |  | O | HE1 |
| ILE259 (A) | LYS177 | 7.92 | -0.21 | 0 | 1 |  | N | HZ3 |
| PHE291 (A) | TRP77 | 7.93 | -0.02 | 0 | 0 |  | HZ | HH2 |
| GLY215 (A) | GLN107 | 7.94 | -0.01 | 0 | 0 |  | O | O |
| TYR237 (C) | PHE22 | 7.94 | 0.12 | 0 | 0 |  | HE1 | HB2 |
| ASP216 (A) | TRP77 | 7.94 | -0.05 | -1 | 0 |  | OD2 | HZ3 |
| GLY195 (C) | VAL47 | 7.95 | -0.03 | 0 | 0 |  | HA2 | HG22 |
| GLY258 (A) | PHE161 | 7.95 | -0.01 | 0 | 0 |  | HA2 | HA |
| GLN299 (A) | TRP77 | 7.95 | -0.02 | 0 | 0 |  | HE22 | HH2 |
| ASN238 (C) | LEU19 | 7.95 | -0.02 | 0 | 0 |  | HB1 | HD11 |
| CYS117 (C) | HIS117 | 7.96 | -0.05 | 0 | 0 |  | O | HD2 |
| GLU240 (C) | MET1 | 7.96 | -0.90 | -1 | 1 |  | HN | HB1 |
| SER1 (A) | VAL108 | 7.97 | -0.03 | 1 | 0 |  | HB2 | HG12 |
| SER1 (A) | MET78 | 7.97 | -0.14 | 1 | 0 |  | HG | HB1 |
| VAL212 (A) | ALA150 | 7.97 | -0.02 | 0 | 0 |  | HG22 | O |
| VAL171 (C) | MET78 | 7.97 | -0.05 | 0 | 0 |  | HG13 | HN |
| GLY258 (A) | SER199 | 7.98 | -0.02 | 0 | -1 |  | HA1 | HG |
| ALA211 (A) | ARG112 | 7.98 | 0.03 | 0 | 1 |  | O | HA |
| ALA210 (A) | TRP77 | 7.99 | -0.01 | 0 | 0 |  | O | HZ3 |
| LEU141 (C) | ALA150 | 7.99 | -0.03 | 0 | 0 |  | HD22 | HN |
| PHE134 (C) | THR3 | 7.99 | -0.05 | 0 | 0 |  | HN | OG1 |
| LEU141 (C) | HIS149 | 7.99 | -0.02 | 0 | 0 |  | HD22 | HA |
| LEU287 (C) | ALA2 | 7.99 | 0.00 | 0 | 0 |  | HD12 | HN |
| THR135 (C) | GLY6 | 8.00 | 0.00 | 0 | 0 |  | HG21 | HA1 |
| TRP207 (C) | MET78 | 8.00 | -0.03 | 0 | 0 |  | HZ2 | HE2 |