Supporting Information for Quantum Biochemical Analysis of the TtgR Regulator and Effectors

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Table S1: Description of TtgR residues interacting with the quercetin effector (QUE) identified in the radius of the binding pocket ranging from 2.0 to 13.0Å. We also expose the regions and groups where there is interaction between TtgR residues and the energetic values (in kcal/mol) for ε=10 and ε=40 calculated by the B97D functional combined with the base set 6-311+G(d,p)

| Residue  | Atomic Group | Radius (Å) | Energy (ε=10) | Energy (ε=40) |
|----------|--------------|------------|---------------|---------------|
| ASP172   | i(O4)H       | 2.0        | 6.00          | 4.23          |
| MET89    | i(C6)O       | 2.5        | -0.72         | -0.62         |
| LEU93    | i(C4)H       | 2.5        | -3.16         | -2.82         |
| ILE141   | i(C2)O       | 2.5        | -4.35         | -2.83         |
| VAL171   | i(C5)H       | 2.5        | -4.53         | -3.92         |
| ILE175   | iii(C18)H    | 2.5        | -1.34         | -1.16         |
| LEU92    | i(O30)H      | 3.0        | -2.09         | -1.78         |
| VAL96    | iii(C19)H    | 3.0        | -2.38         | -2.09         |
| HIS114   | iii(C17)O    | 3.0        | -0.03         | -0.21         |
| MET167   | i(C6)O       | 3.0        | -3.33         | -2.51         |
| PHE168   | iii(O4)H     | 3.0        | -4.72         | -4.65         |
| ASN110   | iii(C18)H    | 3.5        | -0.95         | -0.89         |
| HIS70    | ii(O27)H     | 4.0        | -0.41         | -0.44         |
| LEU100   | iii(C18)H    | 4.0        | -0.57         | -0.46         |
| CYS137   | i(C2)O       | 4.0        | -1.53         | -1.85         |
| LEU199   | i(C6)O       | 4.0        | -0.36         | -0.38         |
| ARG176   | iii(O4)H     | 4.5        | -2.54         | -0.85         |
| LEU202   | i(C6)O       | 4.5        | -0.39         | -0.25         |
| HIS67    | ii(O27)H     | 5.0        | 0.14          | -0.09         |
| SER77    | i(O30)H      | 5.0        | -0.14         | -0.10         |
| VAL134   | iii(O4)H     | 5.0        | -0.02         | -0.23         |
| TYR170   | ii(C5)H      | 5.0        | -1.05         | -0.61         |
| LEU66    | iii(C18)H    | 5.5        | -0.19         | -0.19         |
| ALA74    | i(O30)H      | 5.5        | -0.09         | -0.12         |
| ALA144   | i(C1)H       | 5.5        | -0.59         | -0.25         |
| LEU145   | i(C6)O       | 5.5        | -0.35         | -0.22         |
| ALA169   | i(C5)H       | 5.5        | -0.22         | -0.21         |
| GLY173   | iii(O4)H     | 5.5        | -0.42         | -0.28         |
| GLU78    | i(O30)H      | 6.0        | 3.42          | 0.79          |
| PHE97    | iii(C19)H    | 6.0        | -0.48         | -0.41         |
| LEU113   | iii(C17)O    | 6.0        | -0.29         | -0.20         |
| ARG130   | iii(O24)H    | 6.0        | -2.09         | -0.62         |
| GLY140   | i(C2)O       | 6.0        | -0.72         | -0.39         |
| ALA164   | i(C5)H       | 6.0        | 0.41          | -0.03         |
| LEU86    | i(C1)H       | 6.5        | 0.19          | 0.00          |
| ALA166   | i(C5)H       | 6.5        | -0.45         | -0.29         |
| LEU179   | iii(C17)O    | 6.5        | -0.17         | -0.10         |
| Residue | Atom | i | j | k | Value 1 | Value 2 | Value 3 |
|---------|------|---|---|---|--------|--------|--------|
| GLY198  | i(C6)O | 6.5 | -0.25 | -0.11 |
| CYS88   | i(O30)H | 7.0 | -0.24 | -0.13 |
| ARG90   | i(C1)H | 7.0 | -2.32 | -0.62 |
| THR106  | iii(C18)H | 7.0 | -0.06 | -0.04 |
| HIS138  | i(C2)O | 7.0 | -0.02 | -0.10 |
| ALA163  | i(C6)O | 7.0 | 0.18 | 0.01  |
| LEU174  | iii(O4)H | 7.0 | -0.47 | -0.25 |
| VAL195  | i(C6)O | 7.0 | 0.26 | 0.00  |
| LEU63   | iii(O24)H | 7.5 | 0.05 | -0.04 |
| LEU73   | i(O30)H | 7.5 | -0.15 | -0.08 |
| THR142  | i(C1)H | 7.5 | 0.16 | 0.07  |
| VAL165  | i(C5)H | 7.5 | 0.22 | 0.00  |
| MET201  | i(C6)O | 8.0 | -0.45 | -0.14 |
| ASP71   | ii(C9)O | 8.5 | 2.27 | 0.55  |
| ARG75   | i(O30)H | 8.5 | -2.12 | -0.54 |
| PRO85   | i(C1)H | 8.5 | 0.13 | 0.02  |
| LYS91   | i(O30)H | 8.5 | -2.45 | -0.66 |
| LEU94   | i(C6)O | 8.5 | 0.04 | 0.01  |
| GLN95   | iii(C19)H | 8.5 | -0.21 | -0.11 |
| GLU99   | iii(C19)H | 8.5 | 2.30 | 0.55  |
| ARG107  | iii(C18)H | 8.5 | -1.57 | -0.40 |
| ILE109  | iii(C18)H | 8.5 | -0.13 | -0.07 |
| GLU111  | iii(O24)H | 8.5 | 1.68 | 0.40  |
| ALA133  | iii(O24)H | 8.5 | 0.10 | -0.01 |
| ASP136  | i(O30)H | 8.5 | 2.14 | 0.46  |
| LYS139  | i(O30)H | 8.5 | -2.39 | -0.63 |
| LEU143  | i(O30)H | 8.5 | -0.22 | -0.08 |
| ARG177  | iii(O24)H | 8.5 | -1.88 | -0.49 |
| LEU187  | iii(C19)H | 8.5 | 0.03 | -0.01 |
| LEU154  | i(C1)H | 9 | -0.05 | -0.02 |
| TRP178  | iii(C18)H | 9 | -0.12 | -0.06 |
| TRP194  | i(C5)H | 9 | 0.03 | -0.01 |
| GLU68   | ii(O27)H | 9.5 | 1.73 | 0.42  |
| THR69   | ii(O27)H | 9.5 | -0.18 | -0.06 |
| ALA76   | i(O30)H | 9.5 | -0.14 | -0.04 |
| ASN98   | iii(C19)H | 9.5 | -0.09 | -0.02 |
| HIS115  | iii(O24)H | 9.5 | -0.01 | -0.01 |
| PHE119  | iii(O24)H | 9.5 | 0.00 | -0.01 |
| LEU135  | iii(O4)H | 9.5 | 0.10 | 0.00  |
| ALA148  | i(C1)H | 9.5 | -0.16 | -0.05 |
| ASP196  | i(C6)O | 9.5 | 1.34 | 0.66  |
| ASP200  | i(C6)O | 9.5 | 1.12 | 0.58  |
| HIS72   | i(O30)H | 10 | -0.11 | -0.04 |
| GLY87   | i(C1)H | 10 | 0.07 | 0.01  |
| Residue | Atom   | Type | Residue Number | Type |
|---------|--------|------|----------------|------|
| VAL101  | iii(C18)H | 10   | -0.11         | -0.04|
| ILE112  | iii(O24)H | 10   | -0.08         | -0.03|
| GLN131  | iii(O4)H  | 10   | 0.10          | 0.02 |
| ALA146  | i(C1)H    | 10   | -0.05         | -0.02|
| ALA160  | i(C1)H    | 10   | 0.25          | 0.06 |
| THR197  | i(C6)O    | 10   | -0.23         | -0.07|
| LEU208  | i(C6)O    | 10   | 0.03          | 0.00 |
| ASP64   | iii(O27)H | 10.5 | 0.99          | 0.54 |
| SER65   | iii(O27)H | 10.5 | -0.13         | -0.04|
| ARG162  | i(O29)    | 10.5 | -1.88         | -0.48|
| LEU62   | iii(C18)H | 11   | 0.03          | 0.00 |
| SER79   | i(O30)H   | 11   | 0.13          | 0.03 |
| ARG108  | iii(C18)H | 11   | -1.37         | -0.35|
| LYS116  | iii(O4)H  | 11   | -1.54         | -0.39|
| CYS117  | iii(O4)H  | 11   | 0.02          | 0.00 |
| LEU158  | i(O29)    | 11   | -0.06         | -0.02|
| GLU161  | i(O29)    | 11   | 2.46          | 0.61 |
| LEU180  | iii(O24)H | 11   | -0.06         | -0.02|
| VAL191  | iii(C19)H | 11   | 0.15          | 0.03 |
| ARG203  | i(O29)    | 11   | -2.21         | -0.56|
| ASP84   | i(C1)H    | 11.5 | 2.20          | 0.55 |
| ARG105  | iii(C18)H | 12   | -1.51         | -0.38|
| GLN129  | iii(O4)H  | 12   | 0.09          | 0.02 |
| SER132  | iii(O4)H  | 12   | 0.04          | 0.00 |
| ASN147  | i(C1)H    | 12   | -0.11         | -0.03|
| VAL59   | iii(O24)H | 12   | 0.06          | 0.01 |
| GLU82   | i(O30)H   | 12   | 1.95          | 0.49 |
| LEU102  | iii(C18)H | 12   | -0.10         | -0.03|
| ASP103  | iii(C18)H | 12   | 1.71          | 0.42 |
| VAL149  | i(C1)H    | 12   | -0.08         | -0.02|
| GLN153  | i(C1)H    | 12   | 0.10          | 0.02 |
| VAL185  | iii(C18)H | 12   | -0.10         | -0.03|
| GLU192  | i(C6)O    | 12   | 2.09          | 0.52 |
| LYS193  | i(C6)O    | 12   | -1.71         | -0.43|
| ILE126  | iii(O24)H | 12.5 | 0.08          | 0.02 |
| ARG127  | iii(O24)H | 12.5 | -139          | -0.35|
| ASP159  | i(O29)    | 12.5 | 2.07          | 0.52 |
| GLN60   | iii(O27)H | 13   | 0.21          | 0.05 |
| ALA104  | iii(C18)H | 13   | 0.06          | 0.01 |
| PRO155  | i(O29)    | 13   | 0.13          | 0.03 |
| SER205  | i(O29)    | 13   | 0.03          | 0.01 |
Table S2: Description of TtgR residues interacting with the tetracycline effector (TAC) identified in the radius of the binding pocket ranging from 2.0 to 13.0Å. We also expose the regions and groups where there is interaction between TtgR residues and the energetic values (in kcal/mol) for ε=10 and ε=40 calculated by the B97D functional combined with the base set 6-311+G(d,p).

| Residue | Atomic Group | Radius (Å) | Energy (ε=10) | Energy (ε=40) |
|---------|--------------|------------|---------------|---------------|
| ASN110  | iii(C43)H    | 2.0        | -1.85         | -0.57         |
| LEU86   | iii(N4)H     | 2.5        | -1.24         | -0.60         |
| HIS70   | i(C62)H      | 2.5        | -3.17         | -3.13         |
| LEU92   | i(C62)H      | 2.5        | -2.53         | -2.51         |
| LEU93   | i(C9)H       | 2.5        | -3.18         | -2.02         |
| VAL96   | ii(C51)H     | 2.5        | -4.78         | -3.14         |
| PHE168  | iii(C1)O     | 2.5        | 0.45          | 0.33          |
| VAL171  | i(C10)OH     | 2.5        | -3.34         | -2.91         |
| HIS67   | iii(C4)H     | 3.0        | 1.68          | 1.58          |
| MET89   | i(C8)H       | 3.0        | -1.16         | -1.29         |
| ARG130  | iii(N21)H    | 3.0        | -4.41         | -1.75         |
| CYS137  | i(C6)OH      | 3.0        | -0.64         | -0.53         |
| MET167  | ii(C10)OH    | 3.5        | -1.72         | -1.82         |
| THR106  | iii(C42)H    | 3.5        | -0.70         | -0.82         |
| ALA133  | iii(N21)H    | 3.5        | -1.16         | -1.12         |
| ILE141  | i(C6)OH      | 4.0        | -2.44         | -2.31         |
| LEU63   | iii(N21)H    | 4.0        | -0.28         | -0.86         |
| LEU100  | iii(C42)H    | 4.0        | -0.54         | -0.52         |
| LEU113  | iii(N21)H    | 4.0        | -3.61         | -1.81         |
| HIS114  | iii(C43)H    | 4.0        | -0.33         | -0.68         |
| VAL134  | iii(N21)H    | 4.0        | -0.56         | -0.73         |
| ASP172  | ii(C12)O     | 4.0        | 1.90          | -0.47         |
| ILE175  | iii(C43)H    | 4.0        | -1.73         | -1.44         |
| ALA74   | i(C62)H      | 4.5        | 0.35          | -0.32         |
| GLU99   | iii(C42)H    | 4.5        | 2.26          | 0.15          |
| ASP64   | iii(N21)H    | 5.5        | 2.55          | 0.88          |
| THR89   | iii(C42)H    | 5.5        | -0.45         | -0.28         |
| ILE109  | iii(C43)H    | 5.5        | -0.52         | -0.41         |
| LEU199  | i(C9)H       | 5.5        | -0.09         | -0.11         |
| CYS88   | i(C8)H       | 6.0        | -0.09         | -0.08         |
| ARG90   | i(C8)H       | 6.0        | -1.59         | -0.47         |
| GLN95   | i(C62)H      | 6.0        | -0.19         | -0.21         |
| PHE97   | ii(C10)OH    | 6.0        | -0.51         | -0.52         |
| ALA164  | i(C10)OH     | 6.0        | 0.13          | -0.04         |
| ALA169  | i(C10)OH     | 6.0        | 0.19          | -0.01         |
| LEU202  | i(C9)H       | 6.0        | -0.11         | -0.08         |
| Residue | Type | Position | pKa | q | r | s |
|---------|------|----------|-----|---|---|---|
| LEU62  | iii(C3) | 6.5 | -0.04 | -0.07 |
| SER65  | iii(C42) | 6.5 | -0.87 | -0.6 |
| SER77  | i(C7) | 6.5 | -0.15 | -0.09 |
| ARG107 | iii(C43) | 6.5 | -1.77 | -0.50 |
| GLN129 | iii(N21) | 6.5 | 0.02 | -0.04 |
| LEU145 | i(C9) | 6.5 | -0.16 | -0.09 |
| TYR170 | i(C10) | 6.5 | -0.61 | -0.45 |
| GLU68  | iii(C42) | 7.0 | 2.41 | 0.60 |
| ASP71  | i(C62) | 7.0 | 0.02 | 0.49 |
| LEU73  | i(C7) | 7.0 | -0.23 | -0.15 |
| LYS91  | i(C8) | 7.0 | -1.63 | -0.46 |
| LEU94  | i(C8) | 7.0 | -0.03 | -0.08 |
| GLU111 | iii(C43) | 7.0 | 2.65 | 0.71 |
| HIS138 | i(C6) | 7.0 | -0.47 | -0.26 |
| GLY140 | i(C6) | 7.0 | -0.38 | -0.18 |
| ALA144 | i(C8) | 7.0 | -0.22 | -0.10 |
| LEU179 | iii(C43) | 7.0 | -0.20 | -0.11 |
| VAL195 | i(C9) | 7.0 | 0.05 | -0.04 |
| VAL101 | iii(C42) | 7.5 | -0.05 | -0.04 |
| ARG105 | iii(C43) | 7.5 | -2.17 | -0.58 |
| GLN131 | iii(N21) | 7.5 | 0.12 | -0.01 |
| SER132 | iii(N21) | 7.5 | -0.20 | -0.10 |
| ASP136 | i(C6) | 7.5 | 2.46 | 0.52 |
| VAL165 | i(C10) | 7.5 | 0.20 | 0.01 |
| ALA166 | i(C10) | 7.5 | 0.03 | -0.01 |
| GLY173 | ii(C12) | 7.5 | -0.05 | -0.05 |
| ARG176 | iii(C21) | 7.5 | -3.16 | -0.87 |
| GLY198 | i(C10) | 7.5 | -0.10 | -0.04 |
| GLN60  | iii(N21) | 8.0 | 0.56 | 0.12 |
| ARG75  | i(C62) | 8.0 | -2.41 | -0.65 |
| GLU78  | i(C62) | 8.0 | 2.4 | 0.56 |
| LEU86  | i(C8) | 8.0 | 0.06 | -0.01 |
| ASN98  | iii(C42) | 8.0 | -0.14 | -0.07 |
| ARG108 | iii(C43) | 8.0 | -2.02 | -0.53 |
| PHE119 | iii(N21) | 8.0 | -0.01 | -0.02 |
| LEU135 | iii(N21) | 8.0 | -0.03 | -0.05 |
| ALA163 | i(C10) | 8.0 | 0.07 | 0.00 |
| LEU187 | iii(C43) | 8.0 | -0.06 | -0.04 |
| VAL59  | iii(N21) | 8.5 | 0.18 | 0.03 |
| PRO85  | i(C8) | 8.5 | 0.05 | 0.00 |
| ASP103 | iii(C42) | 8.5 | 0.02 | 0.49 |
| LEU174 | ii(C12) | 8.5 | -0.37 | -0.17 |
| HIS72  | i(C62) | 9.0 | -0.09 | -0.05 |
| GLY87  | i(C8) | 9.0 | 0.02 | 0.00 |
| Residue | Sidechain | pKa | Charge 1 | Charge 2 |
|---------|-----------|-----|----------|----------|
| ILE112  | iii(C43)H | 9.0 | -0.26    | -0.11    |
| ILE126  | iii(N21)H | 9.0 | 0.18     | 0.04     |
| LYS139  | i(C6)OH   | 9.0 | -2.71    | -0.72    |
| THR142  | i(C6)OH   | 9.0 | -0.17    | -0.08    |
| TRP178  | iii(C43)H | 9.0 | -0.15    | -0.07    |
| MET201  | i(C10)OH  | 9.0 | -0.16    | -0.06    |
| ALA61   | iii(C3)O  | 9.5 | 0.12     | 0.02     |
| ALA76   | i(C62)H   | 9.5 | -0.08    | -0.03    |
| LEU102  | iii(C42)H | 9.5 | -0.1     | -0.04    |
| ALA104  | iii(C43)H | 9.5 | 0.07     | 0.01     |
| ARG127  | iii(N21)H | 9.5 | -1.82    | -0.46    |
| GLN128  | iii(N21)H | 9.5 | 0.08     | 0.01     |
| CYS117  | iii(N21)H | 10.0| 0.03     | 0.00     |
| LEU154  | i(C9)H    | 10.0| -0.05    | -0.02    |
| ARG177  | ii(C12)O  | 10.0| -1.87    | -0.48    |
| TRP194  | i(C10)OH  | 10.0| 0.02     | -0.01    |
| ASP196  | i(C9)H    | 10.0| 1.7      | 0.41     |
| HIS115  | iii(C43)H | 10.5| -0.06    | -0.03    |
| ALA148  | i(C8)H    | 10.5| -0.07    | -0.02    |
| ARG162  | ii(C10)OH | 10.5| -1.4     | -0.35    |
| GLU21   | iii(C42)H | 11.0| 2.14     | 0.53     |
| ASP84   | i(C8)H    | 11.0| 1.45     | 0.36     |
| GLU125  | iii(N21)H | 11.0| 1.80     | 0.45     |
| LEU143  | i(C8)H    | 11.0| -0.14    | 1.53     |
| GLU161  | ii(C10)OH | 11.0| 2.20     | 0.55     |
| VAL191  | i(C9)H    | 11.0| 0.06     | 0.00     |
| THR197  | i(C9)H    | 11.0| -0.12    | -0.04    |
| ASP200  | i(C9)H    | 11.0| 1.45     | 0.35     |
| TYR25   | iii(C43)H | 11.5| -0.04    | -0.01    |
| LEU58   | iii(N21)H | 11.5| 0.10     | 0.02     |
| ALA146  | i(C8)H    | 11.5| -0.06    | -0.02    |
| ASN147  | i(C8)H    | 11.5| -0.16    | -0.05    |
| ALA160  | i(C9)H    | 11.5| 0.05     | 0.01     |
| LEU208  | i(C9)H    | 11.5| 0.01     | 0.00     |
| VAL29   | iii(N21)H | 12.0| -0.09    | -0.03    |
| ALA56   | iii(N21)H | 12.0| 0.14     | 0.04     |
| SER79   | i(C7)H    | 12.0| 0.08     | 0.02     |
| GLU82   | i(C8)H    | 12.0| 1.39     | 0.34     |
| LYS116  | iii(N21)H | 12.0| -2.11    | -0.54    |
| VAL185  | iii(C12)O | 12.0| 0.01     | 0.00     |
| LEU188  | iii(C42)H | 12.0| 0.04     | 0.00     |
| ARG203  | i(C9)H    | 12.0| -1.39    | -0.35    |
| ILE17   | iii(N4)H  | 12.5| 0.03     | 0.00     |
| PHE24   | iii(C3)O  | 12.5| -0.07    | -0.02    |
Table S3: Description of TtgR residues interacting with the chloramphenicol (CLM) effector identified in the radius of the binding pocket ranging from 2.0 to 13.0Å. We also expose the regions and groups where there is interaction between TtgR residues and the energetic values (in kcal/mol) for ε=10 and ε=40 calculated by the B97D functional combined with the base set 6-311+G(d,p).

| Residue | Atomic Group | Radius (Å) | Energy (ε=10) | Energy (ε=40) |
|---------|--------------|------------|---------------|---------------|
| LEU92   | i(C11)H      | 2.5        | -2.47         | -2.43         |
| LEU93   | i(C5)H       | 2.5        | -2.07         | -2.05         |
| VAL96   | i(C4)H       | 2.5        | -2.20         | -1.62         |
| CYS137  | i(C8)H       | 2.5        | 2.66          | 2.80          |
| GLY140  | i(N9)O       | 2.5        | -1.47         | -1.38         |
| ILE141  | i(C8)H       | 2.5        | -3.11         | -3.06         |
| VAL171  | i(O4)H       | 2.5        | -1.86         | -1.79         |
| HIS70   | iii(C2)O     | 3.0        | -2.03         | -1.86         |
| GLU78   | i(N9)O       | 3.0        | 1.12          | 1.31          |
| PHE168  | i(C7)H       | 3.0        | -2.64         | -2.61         |
| ILE175  | i(C4)H       | 3.0        | -0.96         | -0.93         |
| HIS67   | iii(C1)Cl    | 3.5        | -2.08         | -1.94         |
| ALA74   | i(N9)O       | 3.5        | -0.97         | -0.91         |
| MET89   | i(C11)H      | 3.5        | -1.99         | -1.74         |
| PHE97   | ii(C4)H      | 4.0        | -0.52         | -0.52         |
| SER77   | i(C10)H      | 4.5        | -0.40         | -0.37         |
| ASP136  | i(N9)O       | 4.5        | 0.07          | -0.27         |
| HIS138  | i(C8)H       | 4.5        | 0.26          | 0.28          |
| ASP172  | ii(O4)H      | 4.5        | -0.91         | -0.63         |
| LEU66   | iii(C1)H     | 5.0        | -0.56         | -0.58         |
| LYS139  | i(N9)O       | 5.0        | -0.92         | -0.58         |
| ALA144  | i(N9)O       | 5.0        | -0.30         | -0.27         |
| ALA133  | iii(C1)Cl    | 5.5        | -0.27         | -0.23         |
| VAL134  | iii(C1)Cl    | 5.5        | -0.34         | -0.34         |
| MET167  | ii(O5)H      | 5.5        | -0.58         | -0.55         |
| ARG75   | i(N9)O       | 6.0        | -0.53         | -0.26         |
| Residue | Type     | Position | Energy 1 | Energy 2 | Energy 3 |
|---------|----------|----------|----------|----------|----------|
| THR142  | i(N9)O   | 6.0      | -0.10    | -0.05    |
| GLU68   | iii(C1)Cl| 6.5      | 0.13     | -1.00    |
| LEU73   | i(C10)H  | 6.5      | -0.21    | -0.16    |
| LEU143  | i(N9)O   | 6.5      | -0.23    | -0.16    |
| LEU63   | iii(C1)Cl| 7.0      | -0.19    | -0.16    |
| ASP71   | iii(C1)Cl| 7.0      | 0.29     | 0.03     |
| CYS88   | i(C10)H  | 7.0      | -0.06    | -0.05    |
| LEU100  | ii(C4)H  | 7.0      | -0.06    | -0.03    |
| ASN110  | ii(C4)H  | 7.0      | -0.24    | -0.19    |
| LEU135  | i(N9)O   | 7.0      | -0.12    | -0.11    |
| ALA164  | i(C8)H   | 7.0      | -0.14    | -0.13    |
| ALA169  | ii(O5)H  | 7.0      | -0.12    | -0.10    |
| TYR170  | ii(O5)H  | 7.0      | -0.13    | -0.13    |
| ASP64   | iii(C1)Cl| 7.5      | 0.02     | -0.04    |
| ARG90   | i(C11)H  | 7.5      | -1.00    | -0.02    |
| LEU94   | ii(C5)H  | 7.5      | -0.12    | -0.08    |
| GLN95   | ii(C2)O  | 7.5      | -0.08    | -0.03    |
| LEU113  | ii(C1)H  | 7.5      | -0.05    | -0.03    |
| LEU145  | i(N9)O   | 7.5      | -0.10    | -0.10    |
| GLY173  | ii(O4)H  | 7.5      | -0.03    | -0.03    |
| LEU174  | ii(C4)H  | 7.5      | -0.01    | -0.04    |
| LEU199  | i(C11)H  | 7.5      | -0.03    | -0.04    |
| THR69   | iii(C1)Cl| 8.0      | -0.20    | -0.13    |
| ALA76   | i(N9)O   | 8.0      | -0.03    | -0.03    |
| LYS91   | i(C11)H  | 8.0      | -0.17    | -0.10    |
| GLU99   | iii(C1)H | 8.0      | -0.18    | -0.09    |
| THR106  | ii(C4)H  | 8.0      | -0.04    | -0.04    |
| HIS114  | ii(C4)O  | 8.0      | -0.07    | -0.05    |
| ARG130  | iii(C1)Cl| 8.0      | 0.15     | -0.01    |
| VAL195  | ii(C5)H  | 8.0      | -0.05    | -0.05    |
| SER65   | i(C1)Cl  | 8.5      | -0.01    | -0.04    |
| SER79   | i(N9)O   | 8.5      | 0.06     | 0.04     |
| PRO85   | i(C10)H  | 8.5      | -0.02    | -0.02    |
| SER132  | iii(C1)Cl| 8.5      | -0.01    | -0.03    |
| VAL165  | ii(C7)H  | 8.5      | -0.07    | -0.06    |
| ALA166  | ii(O5)H  | 8.5      | -0.06    | -0.04    |
| ARG176  | ii(O4)H  | 8.5      | 0.18     | 0.02     |
| LEU187  | ii(C4)H  | 8.5      | -0.01    | -0.01    |
| LEU202  | i(C11)H  | 8.5      | -0.03    | -0.03    |
| HIS72   | i(N9)O   | 9.0      | -0.02    | -0.03    |
| LEU86   | i(C10)H  | 9.0      | -0.03    | -0.02    |
| ASN98   | ii(C4)H  | 9.0      | -0.02    | -0.02    |
| ASN147  | i(N9)O   | 9.0      | -0.06    | -0.03    |
| GLY198  | ii(O5)H  | 9.0      | 0.01     | -0.01    |
| Residue | Atom Type | Charge | Delta Charge | Value |
|---------|-----------|--------|--------------|-------|
| LEU62  | iii(C1)H  | 9.5    | -0.01        | -0.01 |
| ILE109 | iii(C1)H  | 9.5    | 0.00         | -0.01 |
| ALA163 | ii(C5)O   | 9.5    | -0.04        | -0.03 |
| LEU179 | ii(C4)H   | 9.5    | 0.00         | -0.01 |
| GLN129 | iii(C1)Cl | 10.0   | -0.04        | -0.02 |
| GLN131 | iii(C1)Cl | 10.0   | -0.04        | -0.02 |
| ALA146 | i(N9)O    | 10.0   | 0.00         | -0.01 |
| MET201 | ii(O5)H   | 10.0   | 0.00         | -0.01 |
| GLY87  | i(C10)H   | 10.0   | -0.04        | -0.02 |
| VAL101 | ii(C4)H   | 10.5   | -0.01        | -0.01 |
| ALA148 | i(C10)H   | 10.5   | -0.01        | -0.01 |
| TRP178 | ii(C4)H   | 10.5   | 0.00         | -0.01 |
| TRP194 | ii(C4)H   | 10.5   | 0.00         | -0.01 |
| GLU82  | i(C10)H   | 11.0   | 0.10         | 0.02  |
| ARG107 | ii(C4)H   | 11.0   | 0.09         | 0.02  |
| LEU154 | i(C10)H   | 11.0   | 0.00         | -0.01 |
| ALA160 | i(C8)H    | 11.0   | -0.02        | -0.01 |
| GLU161 | i(C8)H    | 11.0   | 0.10         | 0.02  |
| ARG177 | ii(C4)O   | 11.0   | 0.13         | 0.03  |
| VAL191 | ii(C4)H   | 11.0   | -0.03        | -0.01 |
| GLN60  | iii(C1)H  | 11.5   | -0.03        | -0.02 |
| ASP84  | i(C10)H   | 11.5   | 0.01         | 0.00  |
| ASP196 | ii(C5)H   | 11.5   | -0.12        | -0.03 |
| ALA61  | iii(C1)H  | 12.0   | 0.01         | 0.00  |
| ASP103 | ii(C4)H   | 12.0   | -0.11        | -0.03 |
| GLU111 | ii(C4)H   | 12.0   | -0.17        | -0.05 |
| ARG162 | ii(C5)O   | 12.0   | -0.01        | -0.01 |
| THR197 | ii(O5)H   | 12.0   | 0.02         | 0.00  |
| VAL59  | iii(C1)H  | 12.5   | 0.00         | -0.01 |
| GLU80  | i(N9)O    | 12.5   | 0.13         | 0.03  |
| ARG150 | i(N9)O    | 12.5   | -0.16        | -0.04 |
| VAL185 | ii(C4)H   | 12.5   | -0.01        | 0.00  |
| LEU102 | ii(C4)H   | 13.0   | 0.00         | 0.00  |
| ARG105 | iii(C1)H  | 13.0   | 0.00         | 0.00  |
| PHE119 | iii(C1)Cl | 13.0   | 0.00         | 0.00  |
| GLN128 | iii(C1)Cl | 13.0   | 0.00         | 0.00  |
| VAL149 | i(C10)H   | 13.0   | 0.00         | 0.00  |
| GLN153 | i(C10)H   | 13.0   | 0.00         | 0.00  |
| LEU158 | i(C10)H   | 13.0   | 0.00         | 0.00  |
| ASP200 | ii(O5)H   | 13.0   | 0.00         | 0.00  |
| LEU208 | ii(C5)O   | 13.0   | 0.00         | 0.00  |
