**Table S3. Hydrogen bonding partners prevalent during the simulation (common pairs are highlighted in bold)**

|  |  |
| --- | --- |
| **Simulation** | **H-bonding pair occupancy during simulation (%)** |
| **Control (25 °C)** | VAL171-VAL211 (85.8), **MET72-VAL55-Main** (85), **ARG170-THR163** (83), LYS56-THR94 (82.2), ILE213-LEU169 (81.6), LEU212-ARG205 (81) |
| **Temp 45 °C** | **MET72-VAL55** (87), **ARG170-THR163** (80.8), LEU212-ARG205 (80.6), VAL171-VAL211 (80), ALA61-ARG65 (80) |
| **Temp 65 °C** | **VAL171-VAL211** (82.8)**,** MET72-VAL55 (81.6) |