Additional file 4: Table S2

|  |  |
| --- | --- |
| WT residue (normalized) | FOLD X (kcal/mol\*Å2) |
| I368 (t=0) | I368 (t>100 ns) | N368 mutant (t=0)$ ∆∆$G | N368 mutant (t>100 ns) $∆∆$G  | Overall Stability |
| 0 | <0.3 | 1.37 | 1.56 – 2.1 | Less stable pocket |