| *Enzyme* | *Energy terms (kcal.mol* -1*)* | | | | | |
| --- | --- | --- | --- | --- | --- | --- |
| *E. coli* dimer | *∆HMM* | -297.8 (49.5) | *∆Gsolv* | 83.3 (26.1) | *∆Gbind* | -214.5 (68.3) |
| *∆HCoulomb* | -191.1 (53.3) | *∆Gsolv-pol* | 98.5 (26.6) |  |  |
| *∆HvdW* | -106.7 (11.3) | *∆Gsolv-np* | -15.2 (1.1) |  |  |
|  |  |  |  |  |  |  |
| MR*SA* | *∆HMM* | -556.3 (97.3) | *∆Gsolv* | 80.5 (23.5) | *∆Gbind* | -475.9 (106.5) |
| *∆HCoulomb* | -455.8 (97.7) | *∆Gsolv-pol* | 96.1 (23.9) |  |  |
| *∆HvdW* | -100.6 (12.5) | *∆Gsolv-np* | -15.6 (1.3) |  |  |

**Table S2.** Binding energies and their components at the end of the simulations. Values are averaged over two simulations for each enzyme. Standard deviations are given in brackets.