

| | N_{res} | N_s | <i>Time</i> μs | N_f | N_u | T K | ΔG_f kcal mol^{-1} | ΔH_f kcal mol^{-1} | ΔCv_f kcal mol^{-1} K^{-1} | T_m K | τ_f μs | τ_u μs | τ_{tp} μs |
|----------------------|-----------|-------|------------------------|-------|-------|----------|------------------------------------|------------------------------------|---|------------------------|---------------------|---------------------|------------------------|
| Chignolin | 10 | 1 | 106 | 39 | 38 | 340 | -0.9 | -6.1(1) | -0.1(2) | 381.0 (361.0–393.0) | 0.6(1) | 2.2(4) | 0.04(1) |
| Trp-cage | 20 | 1 | 208 | 12 | 12 | 290 | 0.8 | -2.1(2) | 0.0(1) | 206.0 (0.0–233.0) | 14(4) | 3(1) | 0.22(5) |
| BBA | 28 | 2 | 325 | 14 | 14 | 325 | 0.7 | -2.9(2) | -0.2(2) | undefined | 18(5) | 5(1) | 0.7(1) |
| Villin | 35 | 1 | 125 | 34 | 34 | 360 | 0.8 | -15(1) | 0.2(3) | 343.0 (339.0–346.0) | 2.8(5) | 0.9(2) | 0.27(3) |
| WW domain | 35 | 2 | 1137 | 12 | 11 | 360 | -0.9 | -26(3) | -0.1(2) | 373.0 (365.0–376.0) | 21(6) | 80(24) | 0.5(1) |
| NTL9 | 39 | 4 | 2936 | 17 | 14 | 355 | -1.3 | -26.3(3) | -0.5(1) | 370.0 (367.0–371.0) | 29(7) | 175(47) | 0.9(1) |
| BBL | 47 | 2 | 429 | 12 | 11 | 298 | 0.8 | -2(1) | 0.1(5) | 251.0 (0.0–267.0) | 29(8) | 7(2) | 3.1(6) |
| Protein B | 47 | 1 | 104 | 19 | 19 | 340 | 0.6 | -8(1) | 0.0(2) | 317.0 (311.0–328.0) | 3.9(9) | 1.6(4) | 0.7(1) |
| Homeodomain | 52 | 2 | 327 | 27 | 28 | 360 | -0.7 | -7.2(8) | 0.2(3) | > 360 | 3.1(6) | 9(1) | 1.1(1) |
| Protein G | 56 | 4 | 1155 | 12 | 13 | 350 | 0.3 | -22(1) | -0.5(1) | 345.0 (339.0–348.0) | 56(16) | 37(10) | 1.8(3) |
| $\alpha 3D$ | 73 | 2 | 707 | 12 | 12 | 370 | -0.1 | -38(1) | -0.6(2) | 370.0 (367.0–372.0) | 27(8) | 31(9) | 0.9(2) |
| λ -repressor | 80 | 4 | 643 | 10 | 12 | 350 | 0.9 | -11(1) | -0.7(2) | undefined | 49(15) | 13(4) | 3.1(7) |

Table S1. Summary of the thermodynamic and kinetic parameters of 12 proteins, calculated from simulations of reversible folding. N_{res} is the number of amino acid residues; N_s is the number of independent simulations performed; *Time* is the total simulation time; N_f and N_u are the total number of folding and unfolding events observed in the simulations; T is the simulation temperature; ΔG_f is the free energy for the folding reaction at the simulation temperature, calculated from the folding and unfolding rates; ΔH_f is the enthalpy of the folding reaction at the simulation temperature, calculated as the difference in potential energy between the unfolded and the folded state; ΔCv_f is the heat capacity change for the folding reaction, calculated from the difference in the potential energy fluctuations in the folded and unfolded states; T_m is the melting temperature (and 68% confidence interval) when it can be extrapolated from the calculated ΔG_f , ΔH_f , and ΔCv_f values; τ_f and τ_u are the mean folding and unfolding times; τ_{tp} is the mean transition path time. Times are in μs , temperatures are in K and energies are in $kcal\ mol^{-1}$. Standard errors are reported in parentheses. A comparison of some of these quantities with the experimental data is presented below in the sections describing the individual proteins.