String method for calculation of minimum free-energy paths in Cartesian space in freely-tumbling systems

Supporting Information

Davide Branduardi* and José D. Faraldo-Gómez*

Theoretical Molecular Biophysics Group, Max Planck Institute of Biophysics,
Max-von-Laue Strasse 3, DE-60438, Frankfurt-am-Main, Germany

E-mail: davide.branduardi@biophys.mpg.de; jose.faraldo@biophys.mpg.de

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*To whom correspondence should be addressed

1 Errors on the free-energy estimates

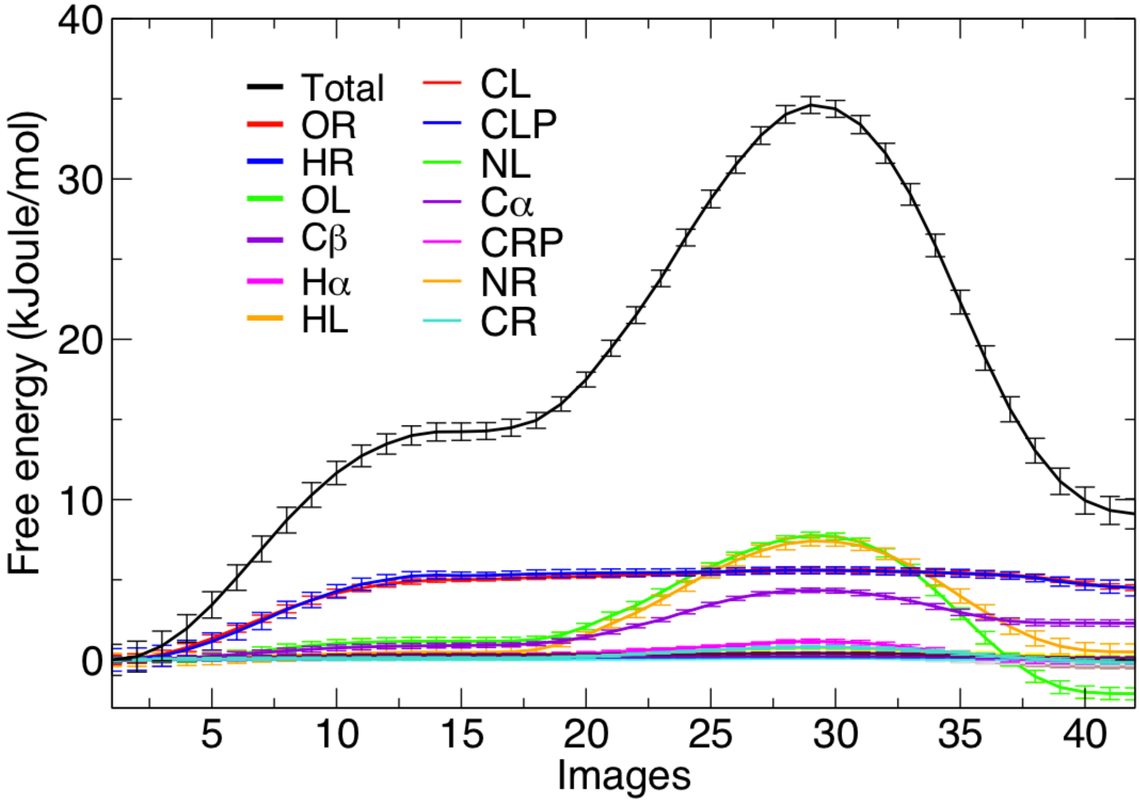

Figure 1: **Total free energy and per atom decomposition for alanine dipeptide.** The average free energy profile calculated over the last 30 iterations of string optimization together with per-atom decomposition. Error bars are associated to the variation in free energy in these last 30 steps. The error on the total free energy amounts to 1.4 kJoule/mol maximum.

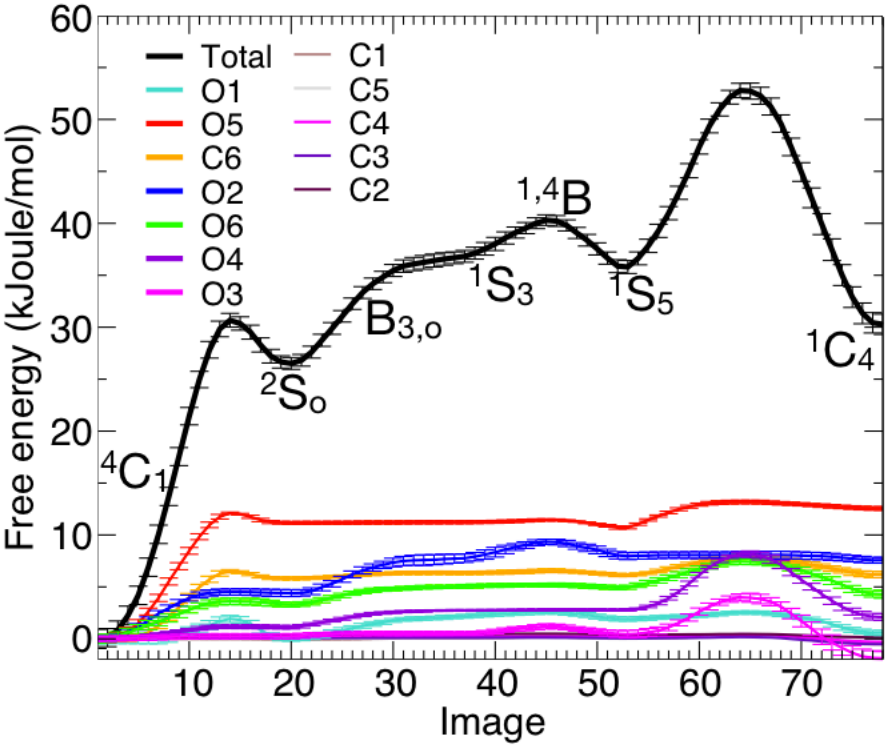

Figure 2: **Total free energy and per atom decomposition for β-D mannose in water** The average free energy profile calculated over the last 30 iterations of string optimisation together with per-atom decomposition. Error bars are associated to the variation in free energy in these last 30 steps. The error on the total free energy amounts to 1.4 kJoule/mol maximum.

2 Committor distributions

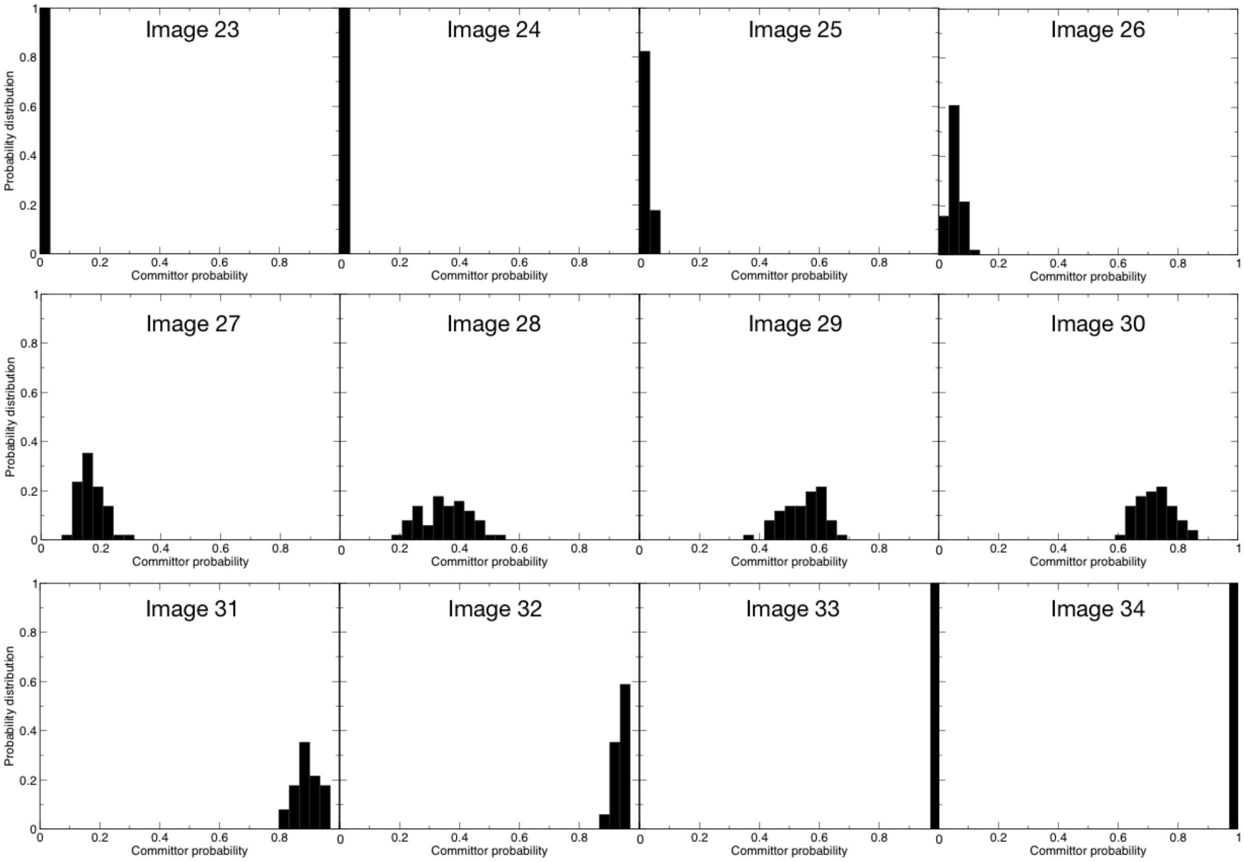

Figure 3: **Committor distributions for the optimized string for alanine dipeptide using all the atoms but methyl hydrogens.** This figure is an expanded version of Fig. 5A (main text).

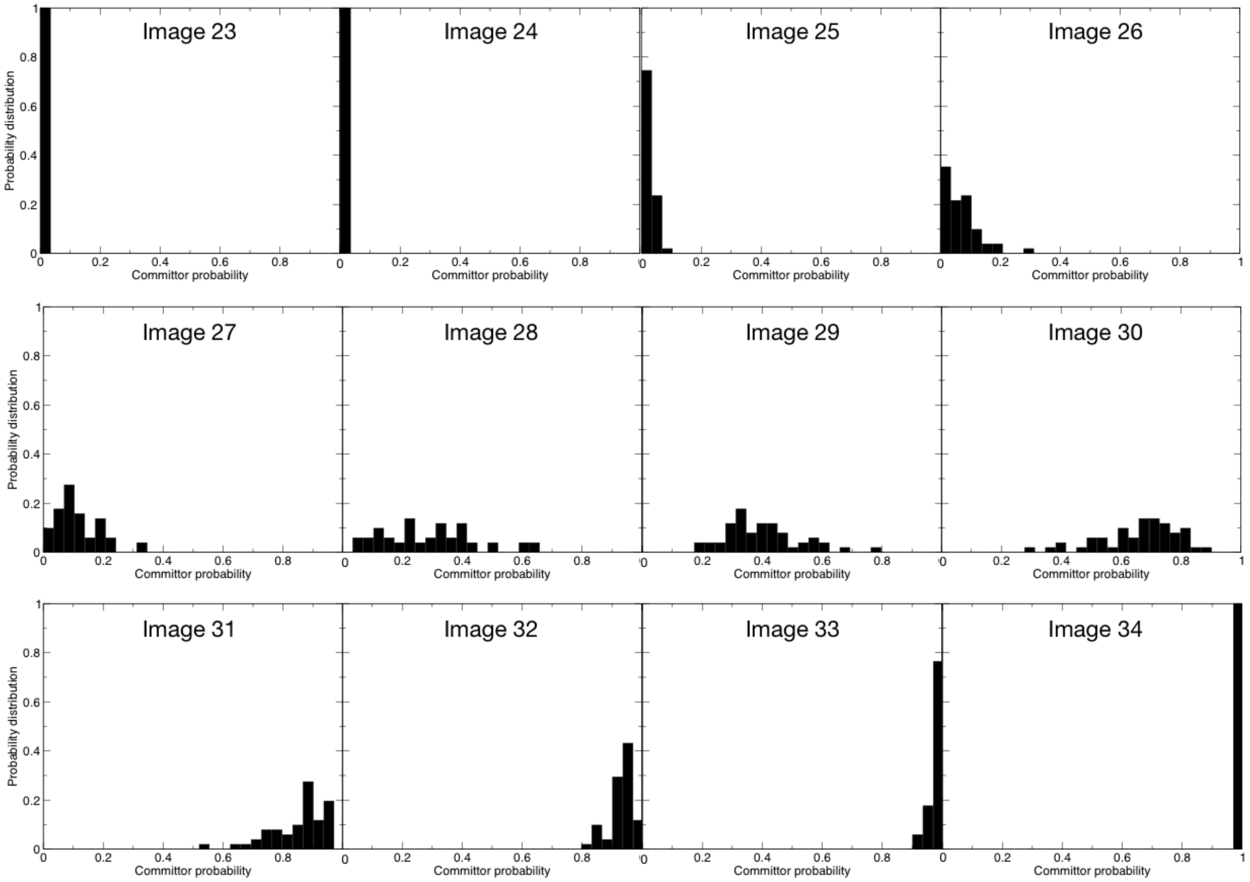

Figure 4: **Committor distributions for the optimized string for alanine dipeptide using only the atoms that carry substantial free energy contributions.** This figure is an expanded version of Fig. 9A (main text).