

Supporting Information

Are coarse-grained models apt to detect protein thermal stability? The case of OPEP force field.

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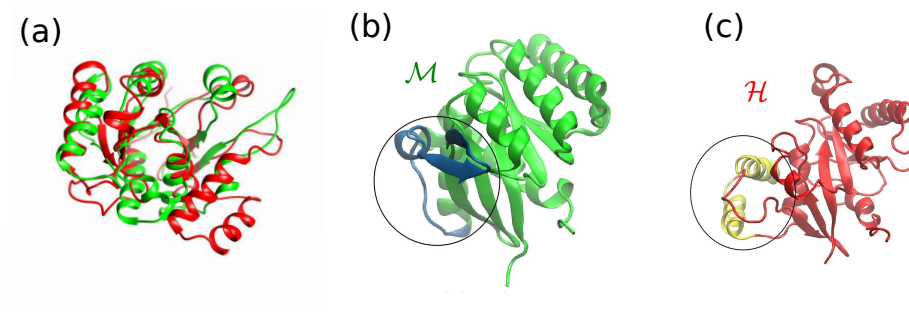


Figure 1: G-domains of Ef-Tu and -1a. (a) Overlap of the two homologues, \mathcal{M} in green and \mathcal{H} in red, (b) mesophilic homologue with the switch I region highlighted in blue and (c) hyperthermophilic homologue with the switch I region highlighted in yellow.

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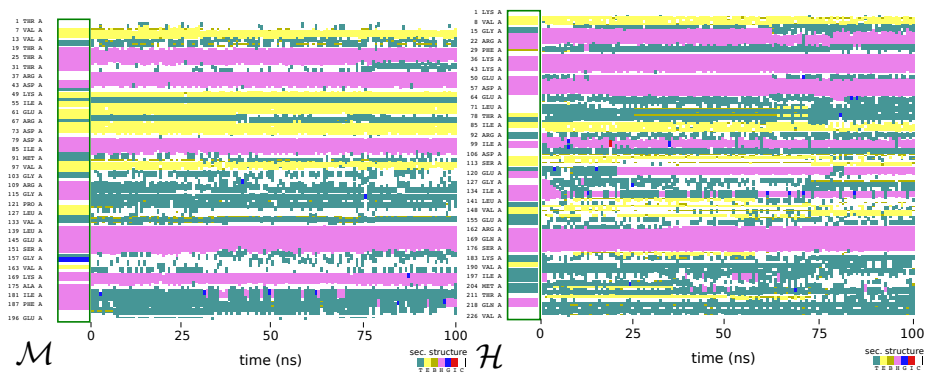


Figure 2: Secondary structure timeline for the 100ns OPEP simulation at ambient temperatures. The mesophilic system is on the left and the thermophilic one on the right. At the beginning of each timeline, in a green-bordered box the secondary structure of the crystal structure is also reported.

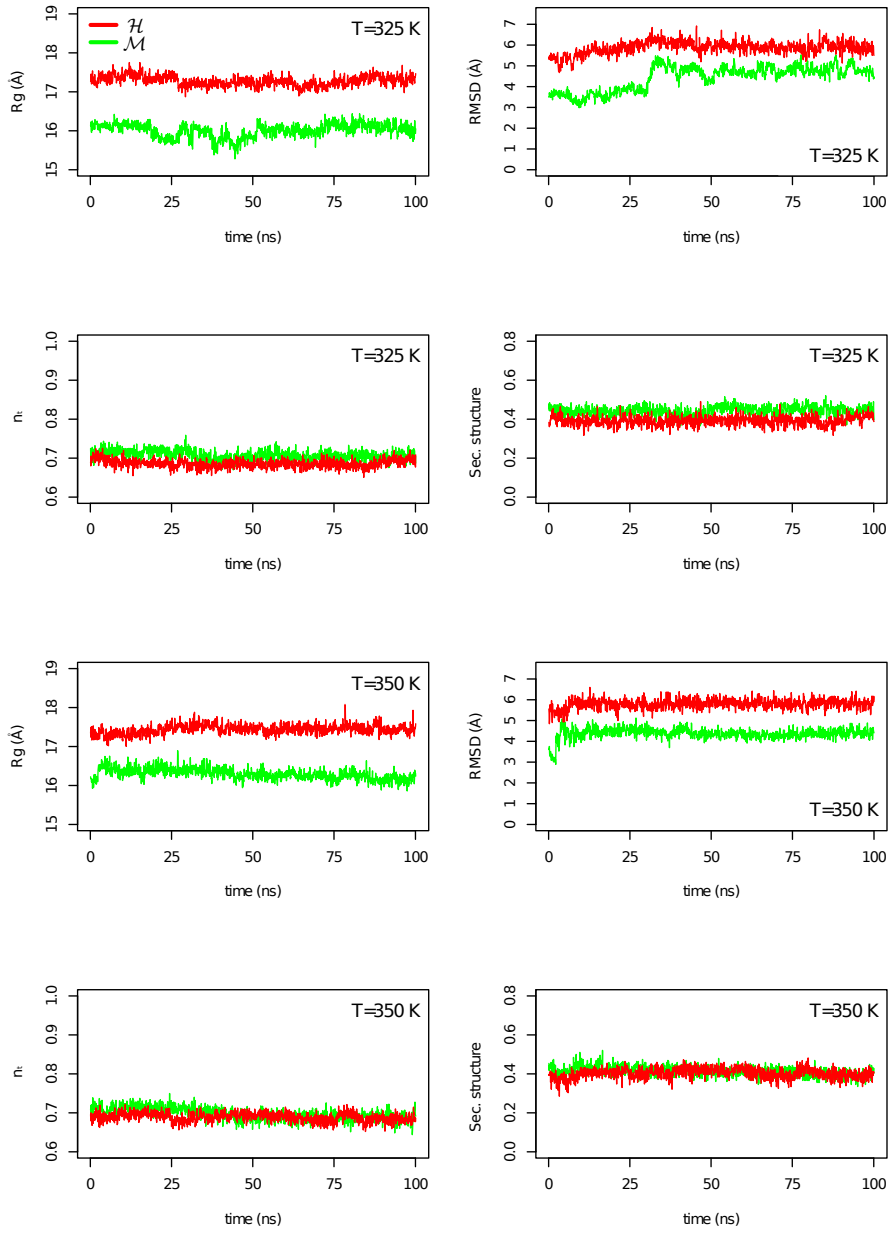


Figure 3: Timeline of radius of gyration R_g , rigid-core C_α RMSD, fraction of native torsion angles n_t and fraction of secondary structure for the two independent OPEP simulations at 325 K (top) and 350 K (bottom).