SUPPLEMENTARY INFORMATION

Structural and thermodynamic characterization of the allosteric transitions in human serum albumin with meta dynamics simulations

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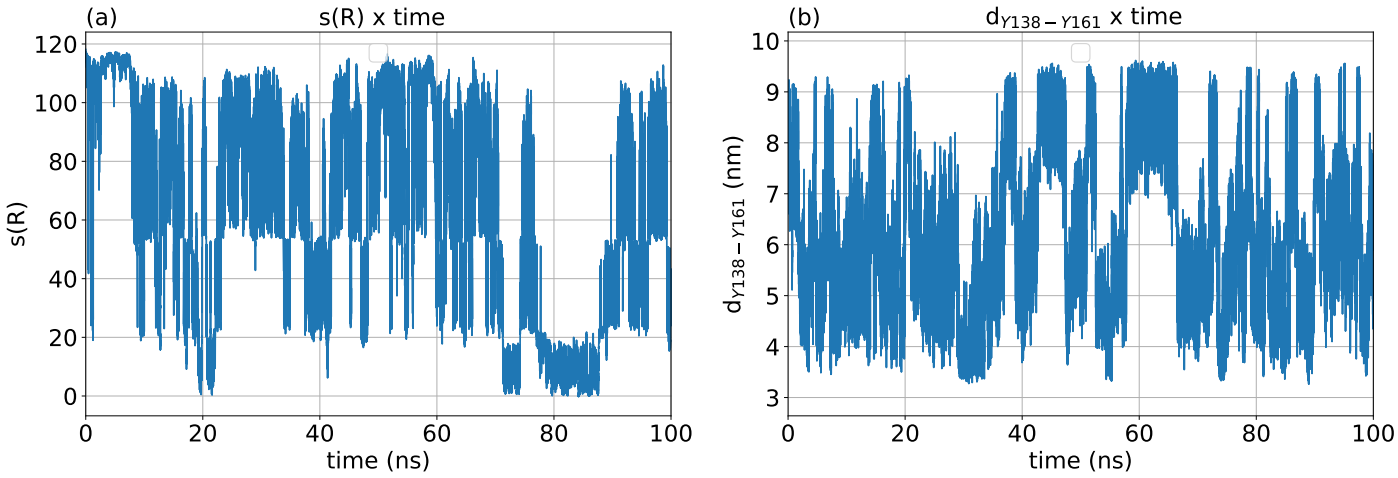

Figure 1 Time series of path CV (a) $s(R)$ combined with (b) $d_{Y138-168}$. Wt-metad simulation were started at B state, near $s(R) = 120$ and $d_{Y138-168} = 8.4$ nm, and explored the whole CVs space, recrossing the main barrier several times.

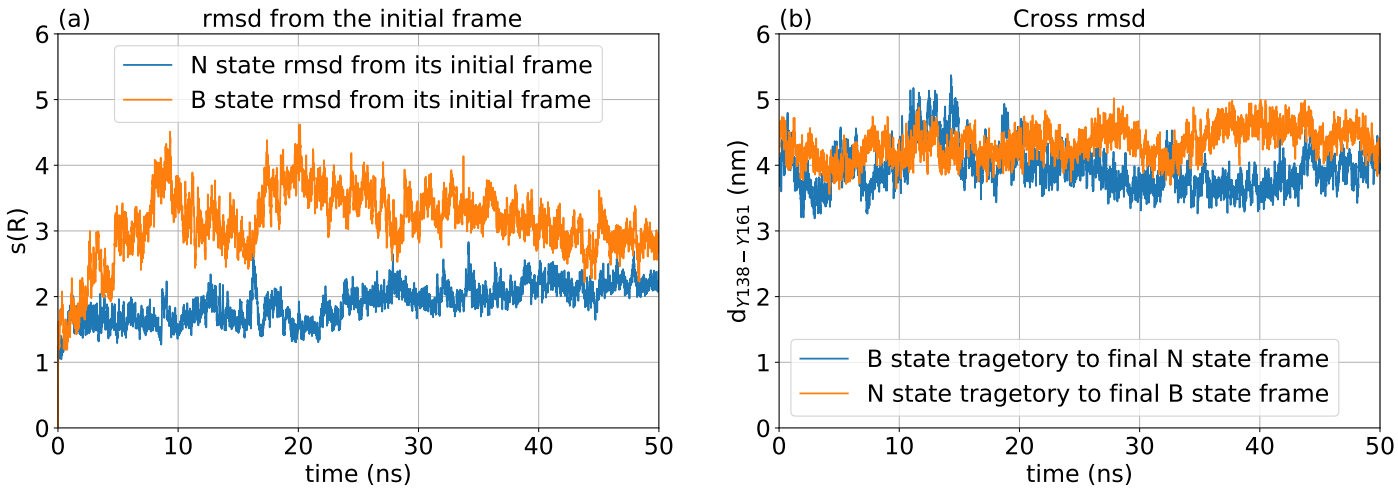

Figure 2 Time series of rmsd for the non-biased MD production stage, prior to wt-metad simulation (a) relative to its initial frame, showing the stabilization of each state used for wt-metad, and (b) the final frame of each trajectory compared to the other, showing that the structure remained far from each other through the whole MD, and were therefore stable at the respective N and B states.