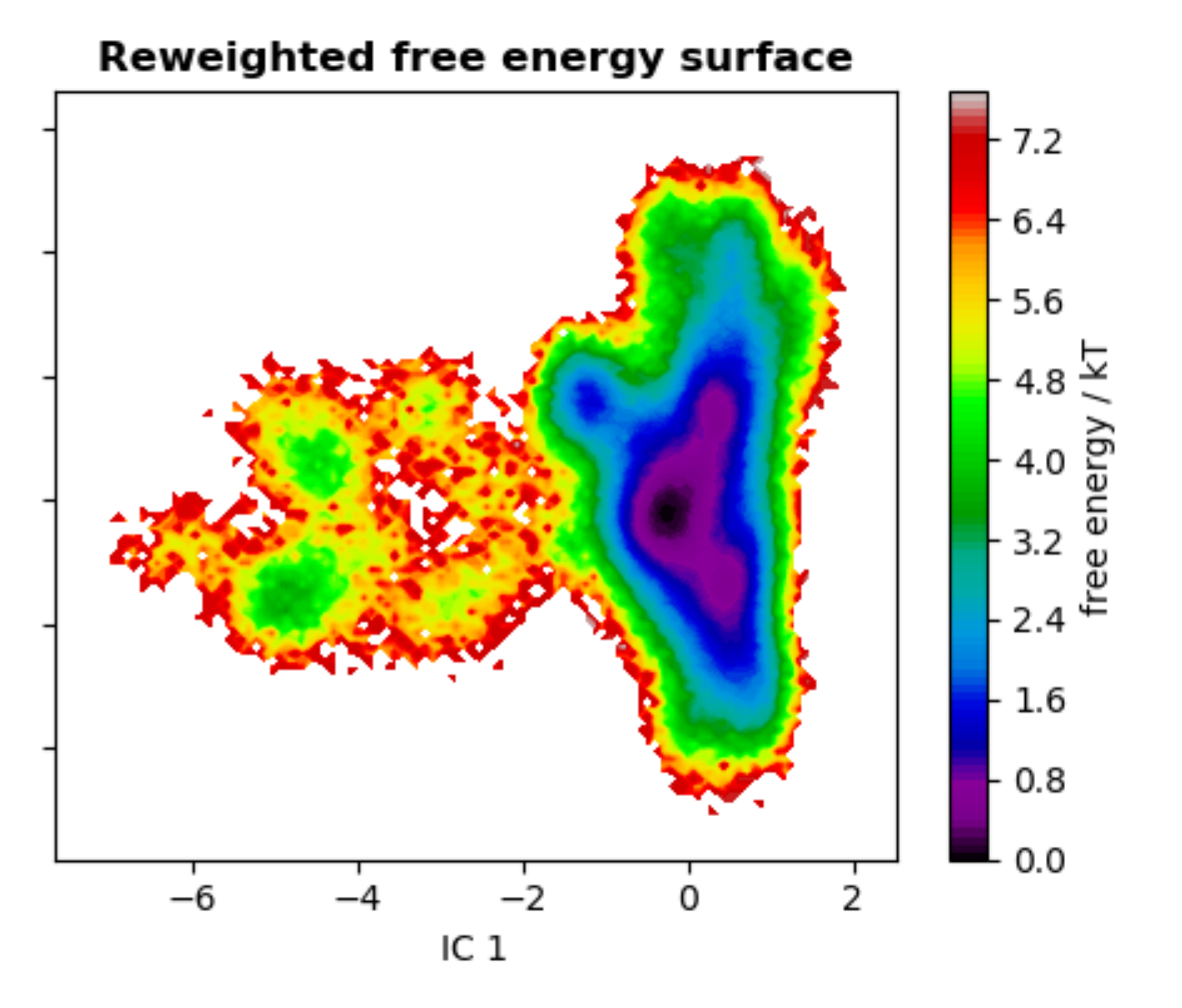
MSM of T4 lysozyme

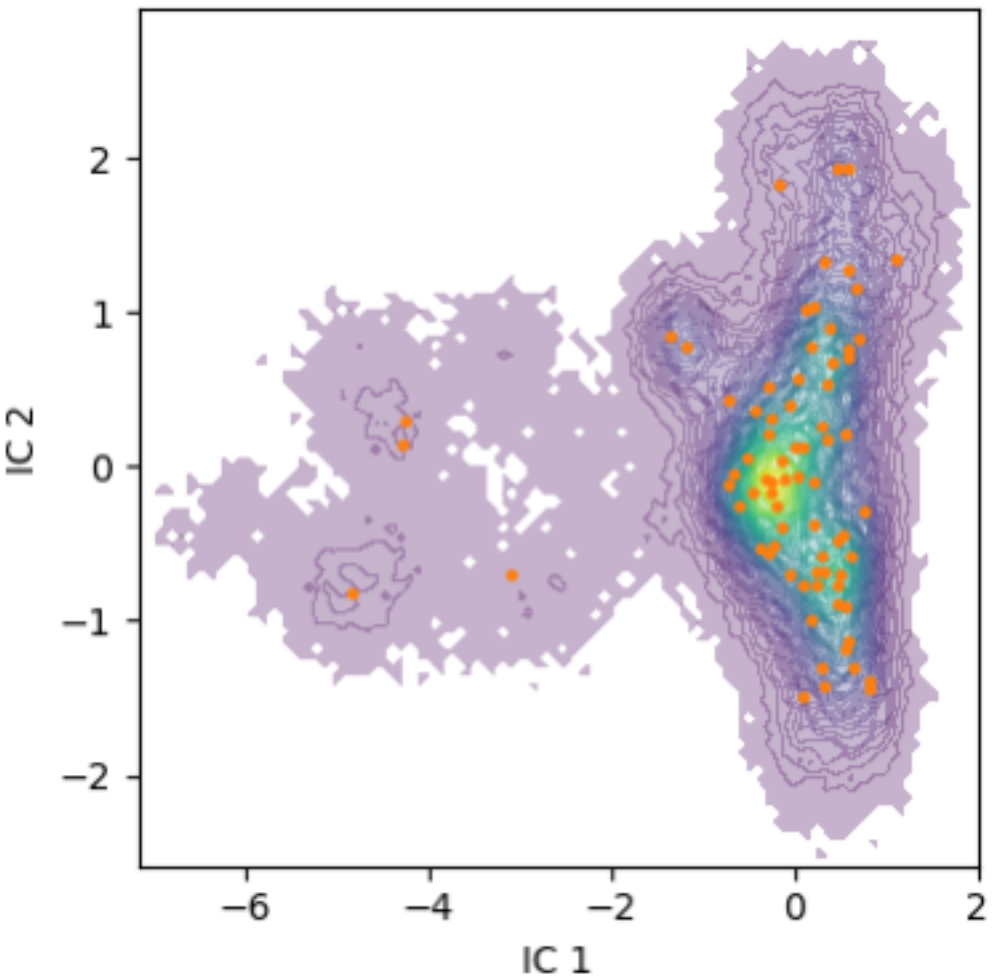
- 1 μs MD trajectories initiated from 4 crystal structures: open, 1qud (blue); closed, 2otz (pink); intermediate, 183l (gold); intermediate, 3dn3 (green)

- Clustering using TICA of protein backbone (from folding)

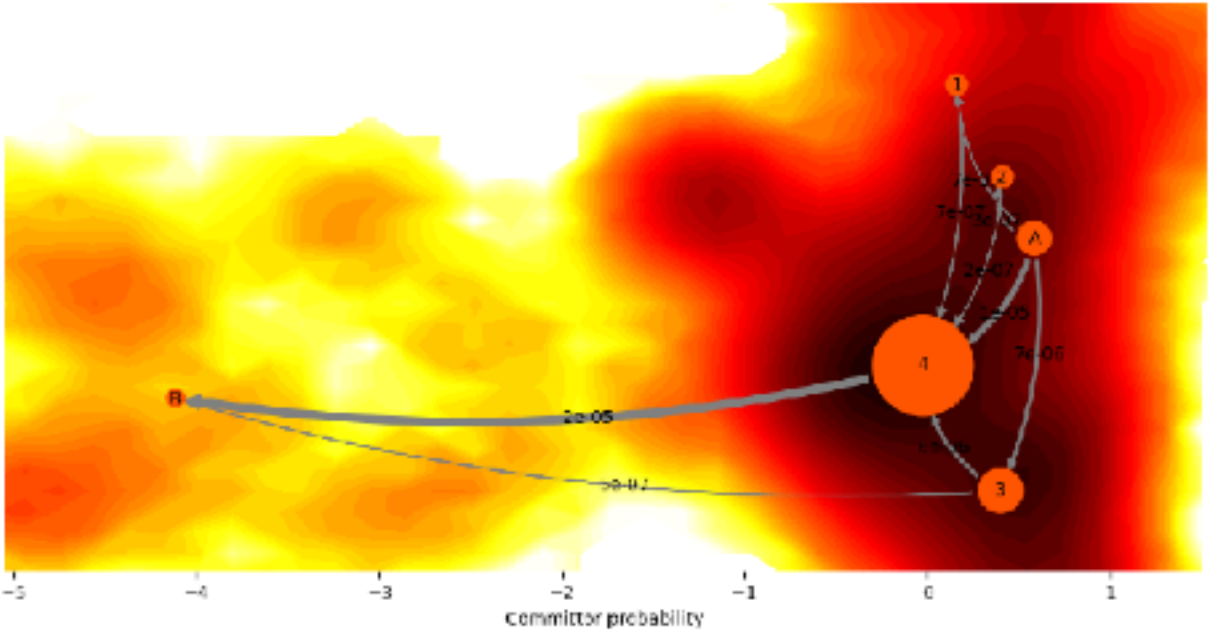
15


Reweighted free energy surface
7.2
6.4
5.6
4.8
4.0
3.2
2.4
1.6
0.8
0.0
free energy / kT
−6
−4
−2
0
2
IC 1

Cluster centers



Kinetic description



15

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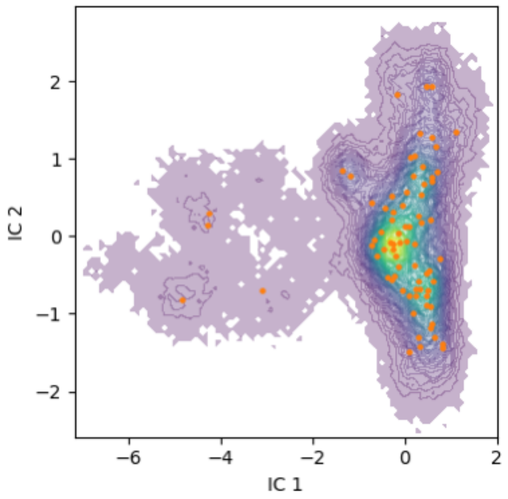
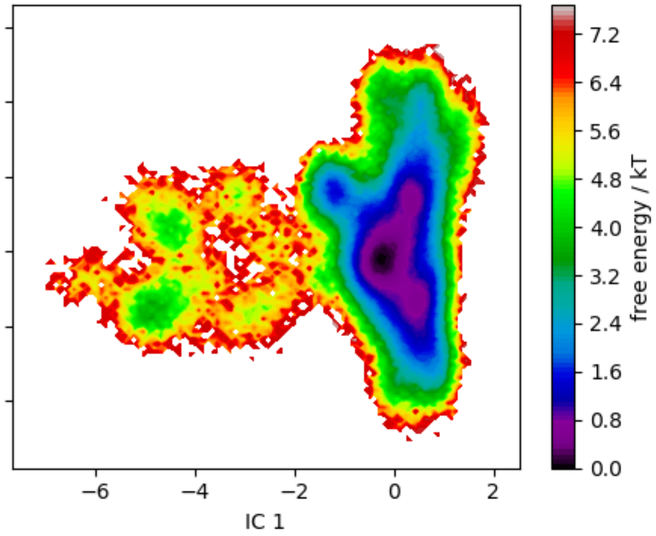
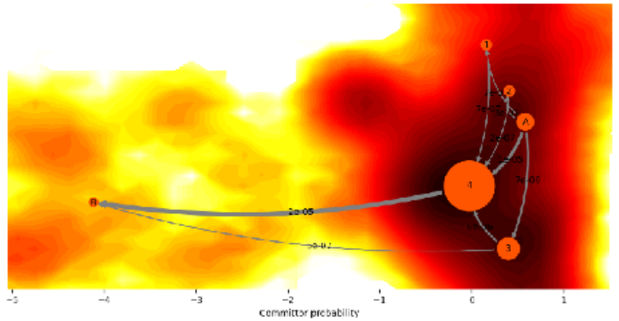


Reweighted free energy surface



Kinetic description



References

- [1] Pande, V. S.; Beauchamp, K. A.; Bowman, G. R. Everything You Wanted to Know about Markov State Models but Were Afraid to Ask. Methods (San Diego, Calif.) 2010, 52 (1), 99–105. https://doi.org/10.1016/j.ymeth.2010.06.002.
- [2] Chodera, J. D.; Noé, F. Markov State Models of Biomolecular Conformational Dynamics. Current Opinion in Structural Biology 2014, 25, 135–144. https://doi.org/10.1016/j.sbi.2014.04.002.
- [3] Xie, B.; Clark, J. D.; Minh, D. D. L. Efficiency of Stratification for Ensemble Docking Using Reduced Ensembles. Journal of Chemical Information and Modeling 2018, 58 (9), 1915–1925. https://doi.org/10.1021/acs.jcim.8b00314.