

Supplemental Information (High resolution approach to the native state ensemble kinetics and thermodynamics)

Sangwook Wu,Pavel I. Zhuravlev,Garegin A. Papoian¹

¹Correspondence should be addressed to GAP. Email: gpapoian@unc.edu

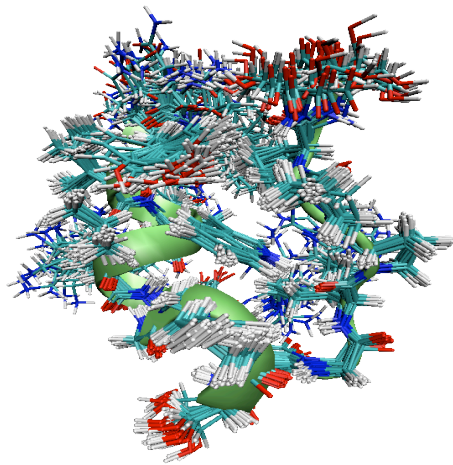


Figure 7: 38 NMR structures for Trp-cage superimposed.

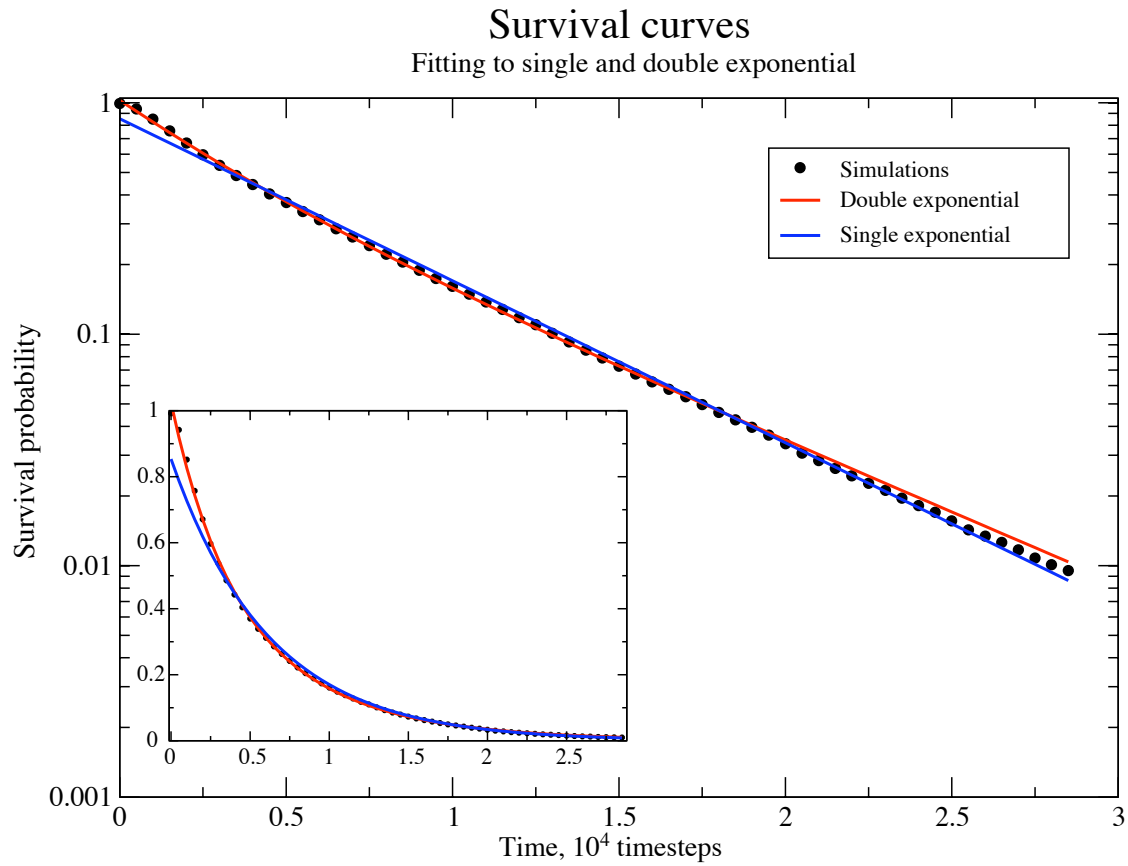


Figure 8: The survival curve (the probability that the "37" to "1" has not yet occurred after time t) fitted by a single (blue) and double (red) exponential. Inset shows the same plot on linear scale.

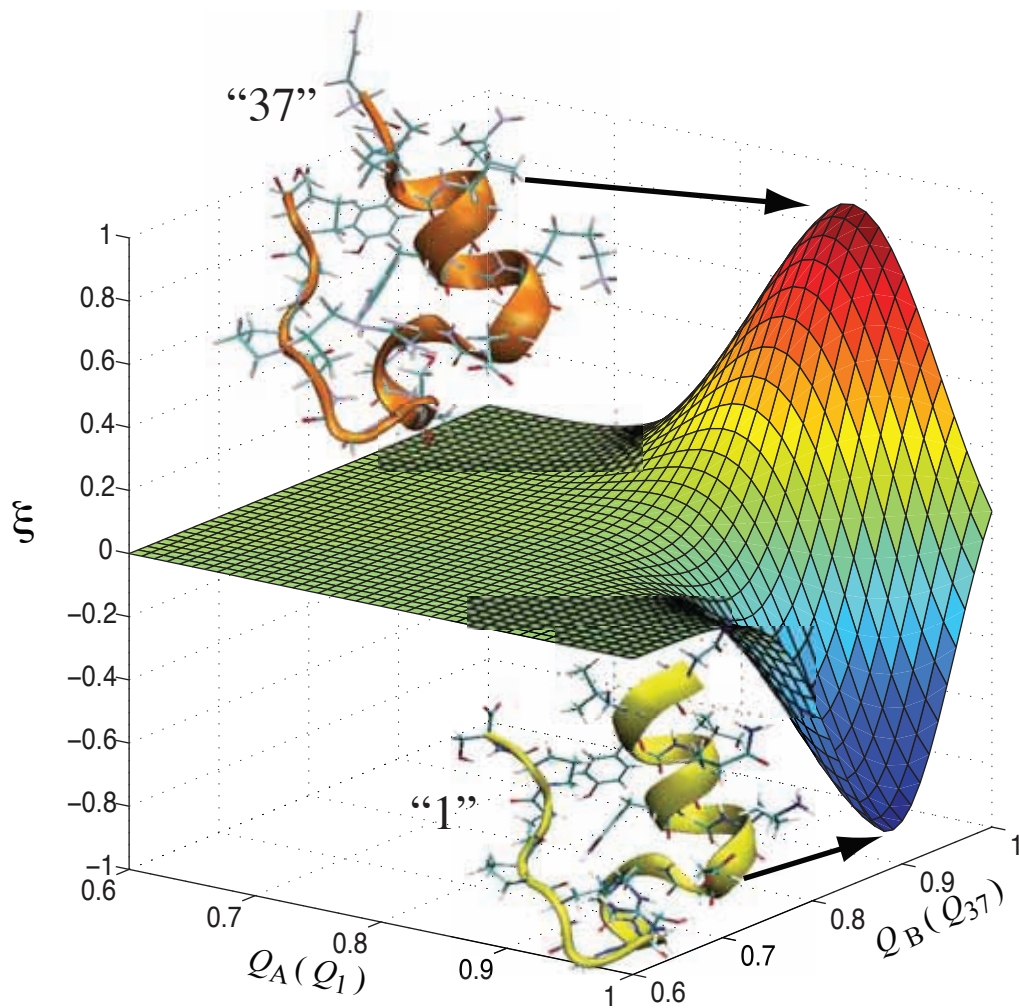


Figure 9: 1D order parameter, the sum of positive and negative gaussians centered on models 37 and 1 respectively.

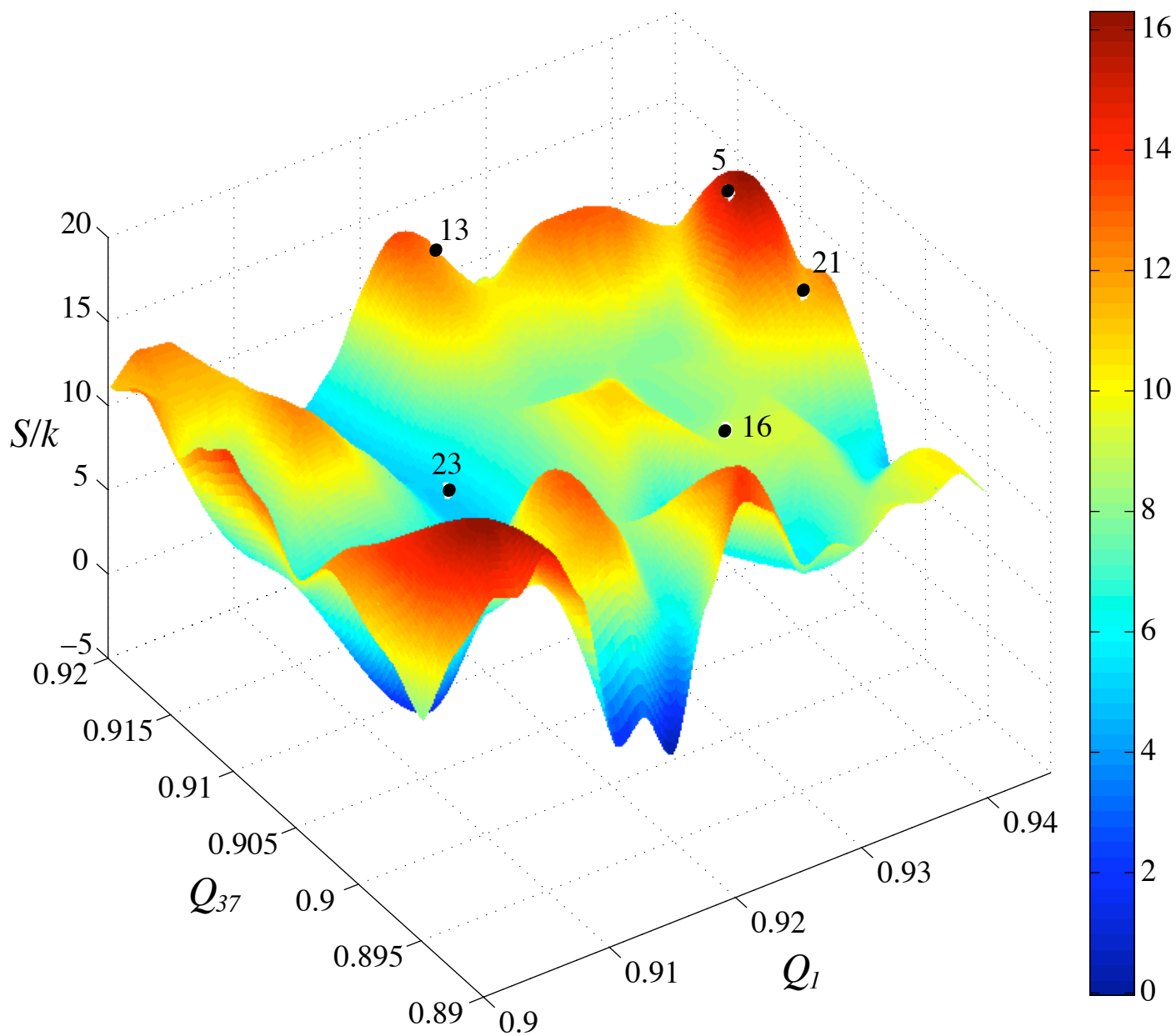


Figure 10: Rugged entropy landscape around model 16 location spans 16 entropy units. The average energy landscape is very similar. Corresponding contributions to free energy is 10 times larger than change in free energy itself.

(Q_1, Q_{37})	SASA of HP core	SASA of the whole protein
Model 1	955	1888
Hydrophobically favorable region		
(0.907, 0.807)	975	1943
(0.905, 0.809)	975	1952
(0.901, 0.802)	969	1931
(0.900, 0.808)	964	1901
Hydrophobically unfavorable region		
(0.774, 0.762)	1089	1936
(0.772, 0.763)	1120	1932
(0.773, 0.764)	1092	1920
(0.773, 0.761)	1038	2027

Table 1: Solvent Accesible Surface Areas for several structures (\AA^2) indicated on Fig. 6.