Supporting information for: pH Induced Stability Switching of the Bacteriophage HK97 Maturation Pathway

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Supporting Information Available

Pathway Analysis

We performed additional analyses on our pathway to support the feasibility of the path. We examined the normal mode contributions to the displacements in the pathway and observed a good balance between low frequency (modes 1-500) and high frequency displacements throughout the path, Figure 1.

In Figure 2, we compare the initial pathway with the string refined pathway in ΔRMSD space, to illustrate the non-linearity in the displacements introduced by refinement to a low-energy path.

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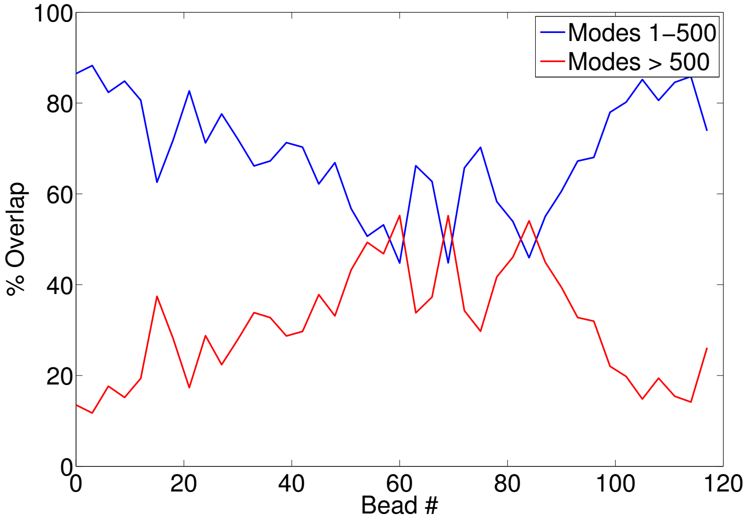

Figure S1: Normal Mode projections onto displacements between beads in string converged pathway. The modes were computed for the initial (prohead 2) state using the an elastic network model with the RTB method[1] in which blocking was based upon secondary structural elements. Displacments were computed between bead i and bead $i+2$. The percent overlap is the square of the normalized dot product between the normal mode and the displacement vector.

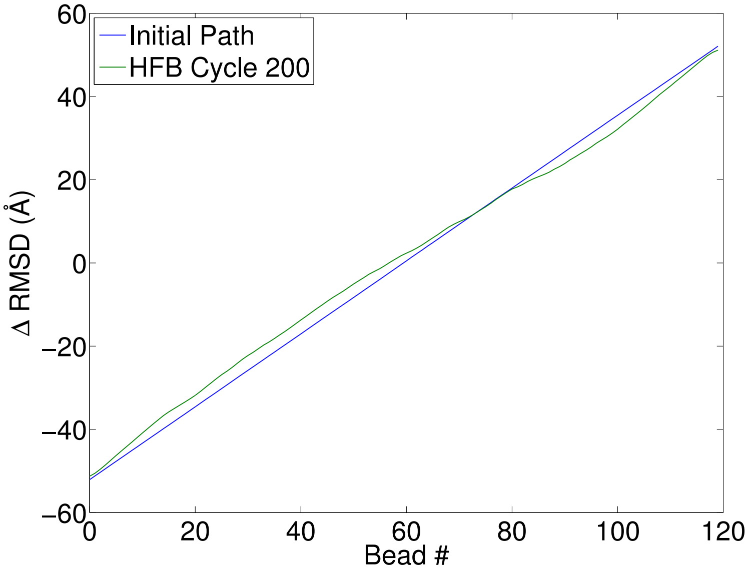

Figure S2: Comparision of ΔRMSD ($RMSD_{initialstate} - RMSD_{finalstate}$), computed over all heavy atoms, between the initial pathway and string converged pathway.

References

(1) Tama, F.; Gadea, F. X.; Marques, O.; Sanejouand, Y. H. *Proteins: Structure, Function, and Bioinformatics* **2000**, *41*, 1–7.