# Supporting Information

## Pfaendtner et al. 10.1073/pnas.0911675107

### SI Text

**Details of DB loop flexibility.** The observed increase in mobility of SD2 in our simulations could potentially account for the disorder observed in the maps of cofilactin obtained by electron microscopy (EM) (1). Although it is possible to calculate theoretical EM density maps from individual protein structures as well as ensembles of protein structures, prediction of disorder in EM maps is more difficult. Theoretical EM prediction methods permit a cutoff based on a threshold for the crystallographic β-factor (which is directly proportional to the mean-squared fluctuation of atoms in the protein crystal), and atoms with β-factors above the threshold are not included in the calculation. Therefore, we calculated the mean-squared fluctuations (the MSF is directly proportional to a crystallographic β-factor) of the actin subunits in the cofilactin and bare actin filaments. The MSF values for each residue were then averaged over the number of filament subunits in order to obtain relative flexibilities of the various parts of the protein as determined via MD simulation (Fig. 1). Note that the numerical scale used for presentation (Fig. 1) is a relative one (i.e., the MSF values in each system were divided by the minimum observed value). In the cofilactin subunit (Fig. 2*B*) the DB loop region is distinctly more flexible than the other actin residues as indicated by the red coloring.

1. Galkin VE, Orlova A, Cherepanova O, Lebart MC, Egelman EH (2008) High-resolution cryo-EM structure of the F-actin-fimbrin/plastin ABD2 complex. *Proc Natl Acad Sci USA* 105:1494–1498.

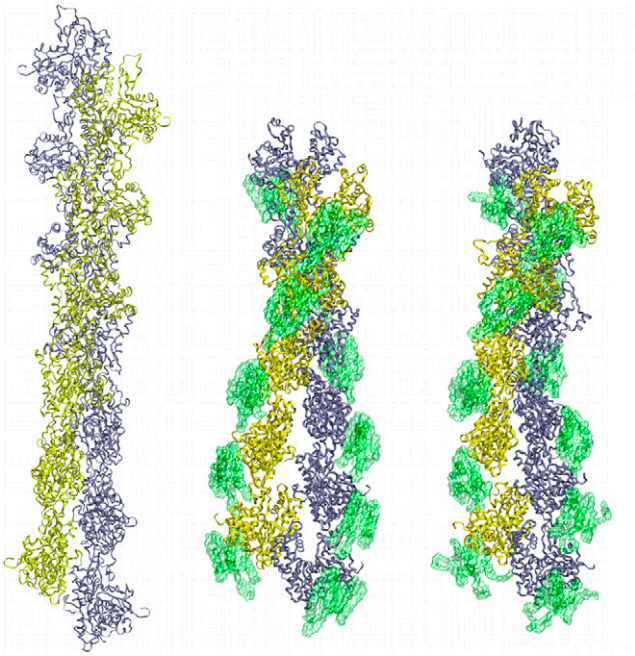

**Fig. S1.** Snapshot of initial bare actin (*Left*), initial cofilactin (*Middle*), and at 50 ns of MD simulation (*Right*) of cofilactin filament. The two helical strands are colored blue and yellow, and the bound ADF/cofilin is shown in transparent surface representation.

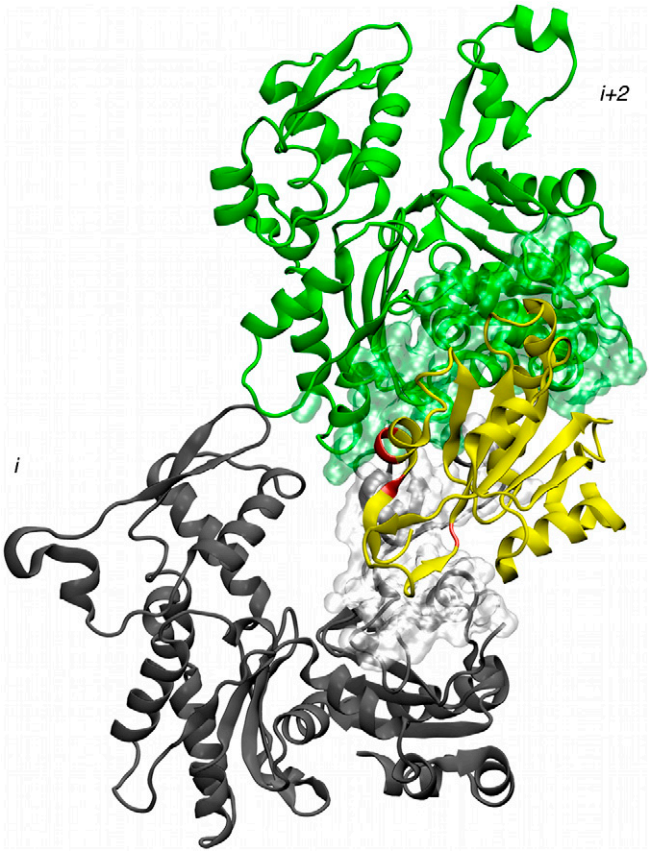


**Fig. S2.** Representative ADF/cofilin binding surface taken from MD snapshot. Two long-pitch actin subunits (*Gray/Green*) are shown with a bound cofilin (*Yellow*). The red residues on the cofilin subunit are K82/E134/R135/R138, which have been shown to be important for cofilactin binding (see main text). The regions of the actin subunits drawn in surface representation are within 8.0 Å of ADF/cofilin.

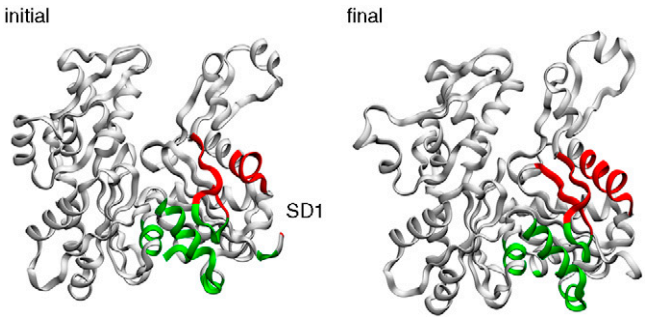


**Fig. S3.** Neighbor effects in ADF/cofilin-induced actin filament remodeling. A single actin subunit from a cofilactin simulation is shown in initial and final forms. Bound ADF/cofilin proteins are omitted for clarity. Contacts between subdomain 1 and the bound ADF/cofilin (*Green*) as well as subdomain 1 and the next adjacent ADF/cofilin (*Red*) are labeled. Two residues are in contact if $C^{\alpha}$ atoms are within 10.0 Å.