Supporting Information

Tsuge *et al*. 10.1073/pnas.0801215105

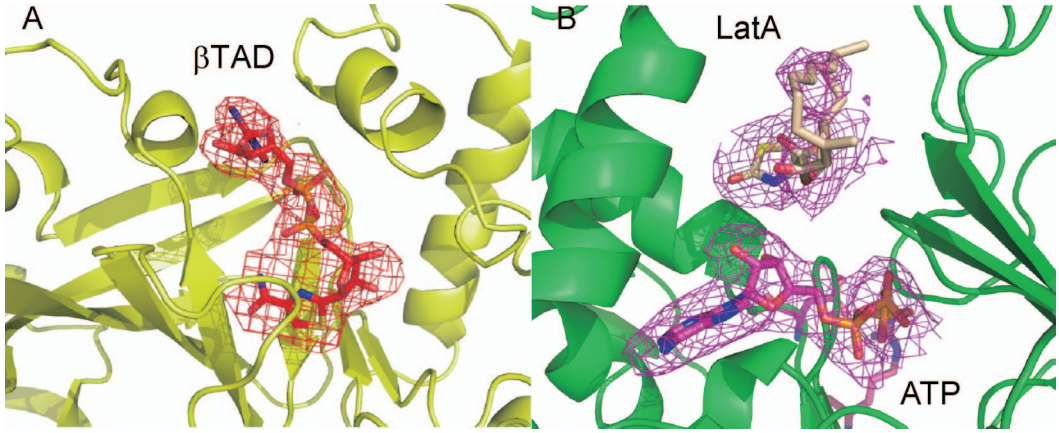

Fig. S1. The electron densitiy of βTAD, ATP, and latrunculin A. (*A*) Omit $2F_o - F_c$ maps around βTAD at 2σ. (*B*) Omit $2F_o - F_c$ maps around ATP and latrunculin A at 2σ.

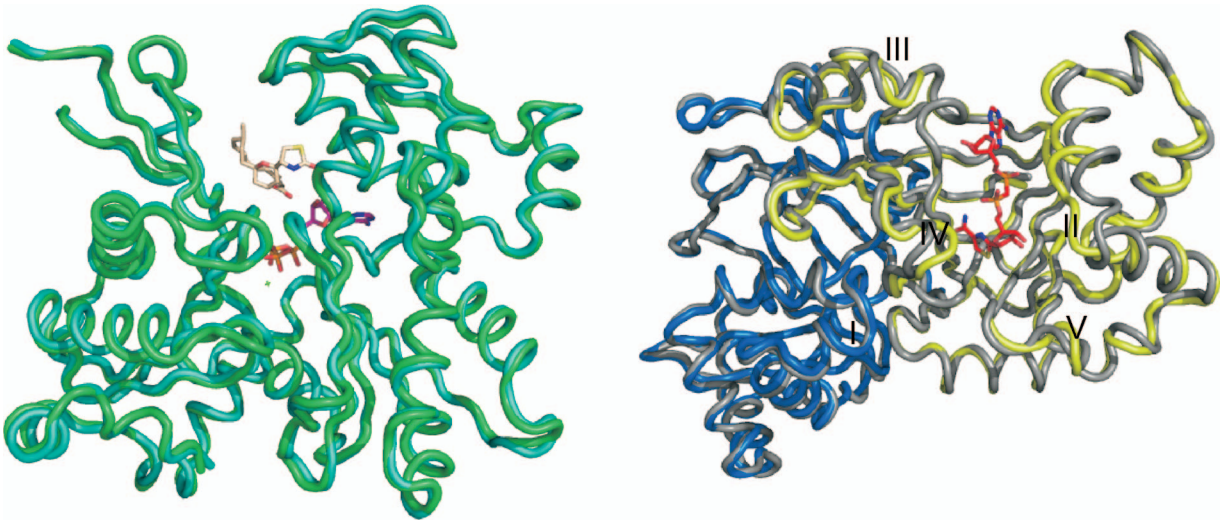

Fig. S2. Structural comparisons of Ia or actin in complex and as a monomer. (*A*) Structural comparison of actin in complex (green) and as a monomer (cyan). (*B*) Structural comparison of Ia in complex (N-term:marine, C-term:yellow) and as a monomer (gray). Roman numerals (I–V) show the five binding loops in Ia.

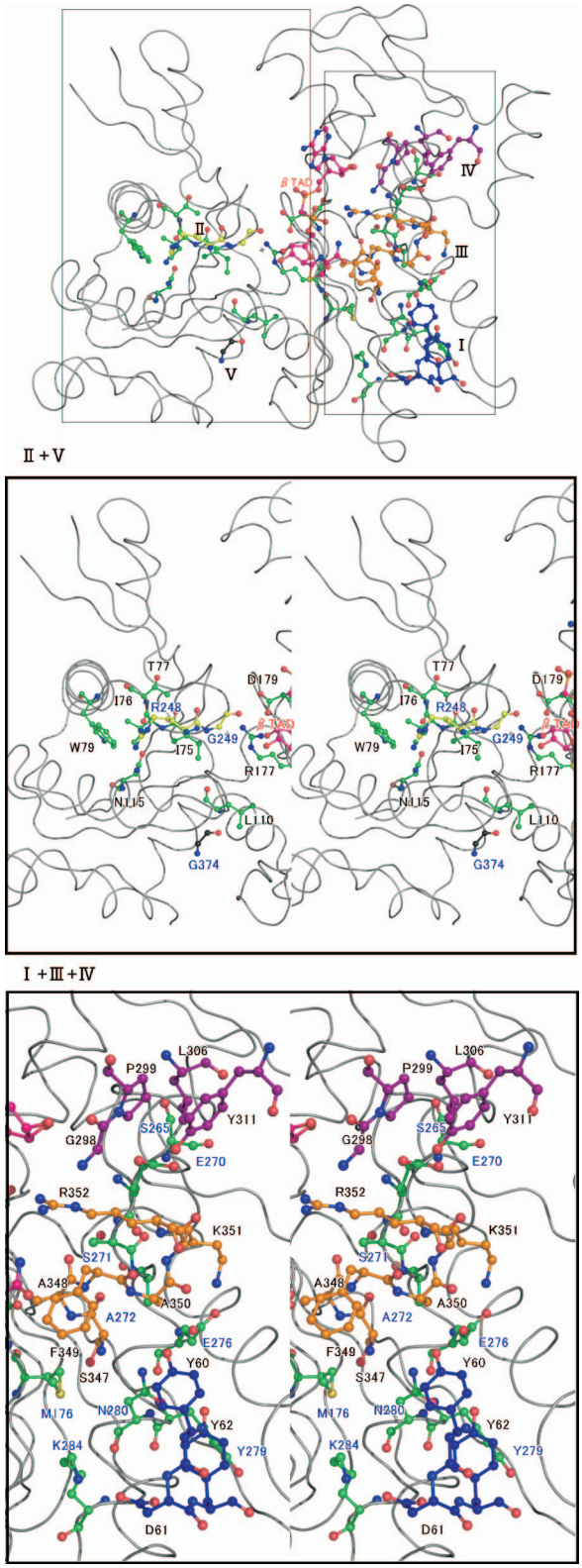

Fig. S3. The recoginition residues between Ia and actin. (*Upper*) The actin-recognition residues on five loops of Ia are shown against actin (main chain:gray and side chain: green). The side chain of Ia are shown as follows; loop I, blue; loop II, yellow; loop III, purple; loop IV, orange; loop V, black. (*Lower*) Stereo close-up of two regions.

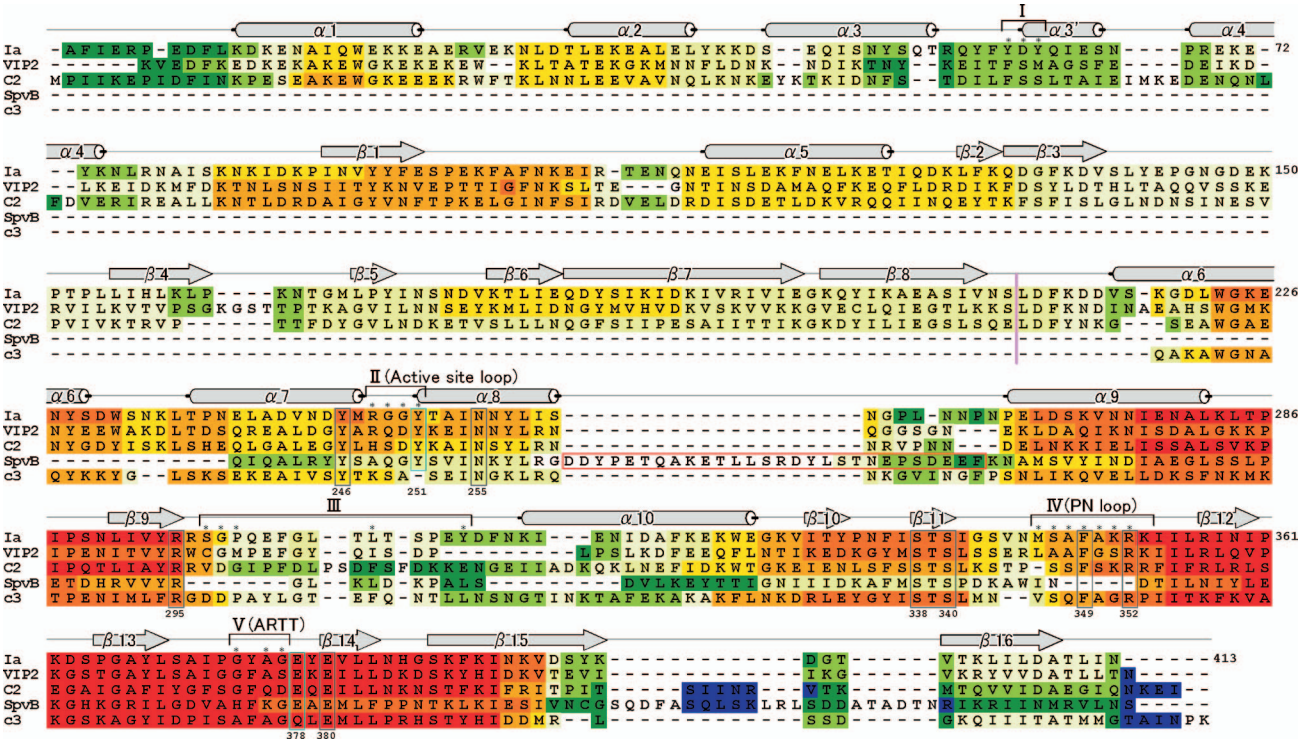

Fig. S4. Sequence alignment of actin-binding ADPRTs and C3 ADPRT by TCOFFEE. Residue similarity is indicated by color, where red is high, purple is low, and green is in the middle. Black-boxed residues are involved in NAD binding or catalysis. Asterisks show the actin-binding residues. The red box shows the helical insertion of SpvB. Roman numbers (I–V) show the actin-binding loops. Two key residues (Y251 and E378) are boxed in blue. The purple line shows the interface between the N and C domains.

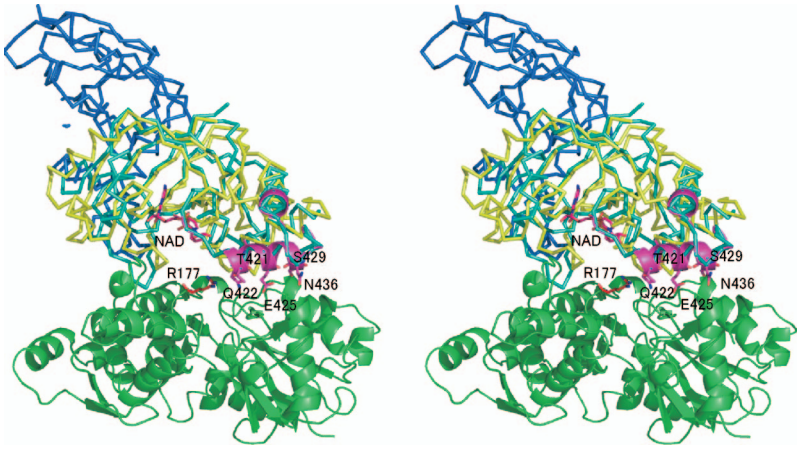

Fig. S5. Stereo of the model structure of actin(green)–SpvB(cyan) complex. Ia is shown in the same color as Fig. 1. The helical insertion of SpvB (residues 415–445) is shown in purple. The actin-binding residues on the helical insertion, Arg-177 of actin, and NAD are labeled.

Table S1. Data collection and structure refinement statistics

Unit cell/space group	a = 57.0 Å, b = 126.3 Å, c = 147.1 Å/*P212121*
Beamline	PF-AR NW12
Wavelength	1.0 Å
Temperature	100 K
Resolution	50–2.8 Å
Number of reflections	26,445 (2,580)
Completeness	99.4 (99.7)
R_{sym}	0.070 (0.337)
I/σ	15.3
Redundancy	6.4
Solvent content	58.3%
Matthews coefficient	2.2
Proteins	One actin [5–374 (40–49 missing)] and one Ia (1–413)
Ligand/ion	βTAD, ATP, latrunculin A, calcium, 79 waters
R_{work}/R_{free}	0.223/0.296
rmsd	
Bond length, Å/ bond angle, °	0.023/2.198
Mean B value (all)	49.6
Mean B value (Ia)	48.9
Mean B value (actin)	50.3
Mean B value (water)	38.8

*Values in parentheses are for the last resolution shell.

†$R_{sym} = \Sigma_h \Sigma_i |I_i(h) - <I(h)>| / \Sigma_h \Sigma_i I_i(h)|$, where $I_i(h)$ is the intensity measurement for a reflection h, and $<I(h)>$ is the mean intensity for this reflection.

‡$R_{work} = \Sigma_h ||F_{obs}| - |F_{calc}|| / \Sigma_h |F_{obs}|$.

§R_{free} was calculated with randomly selected reflections (5%).