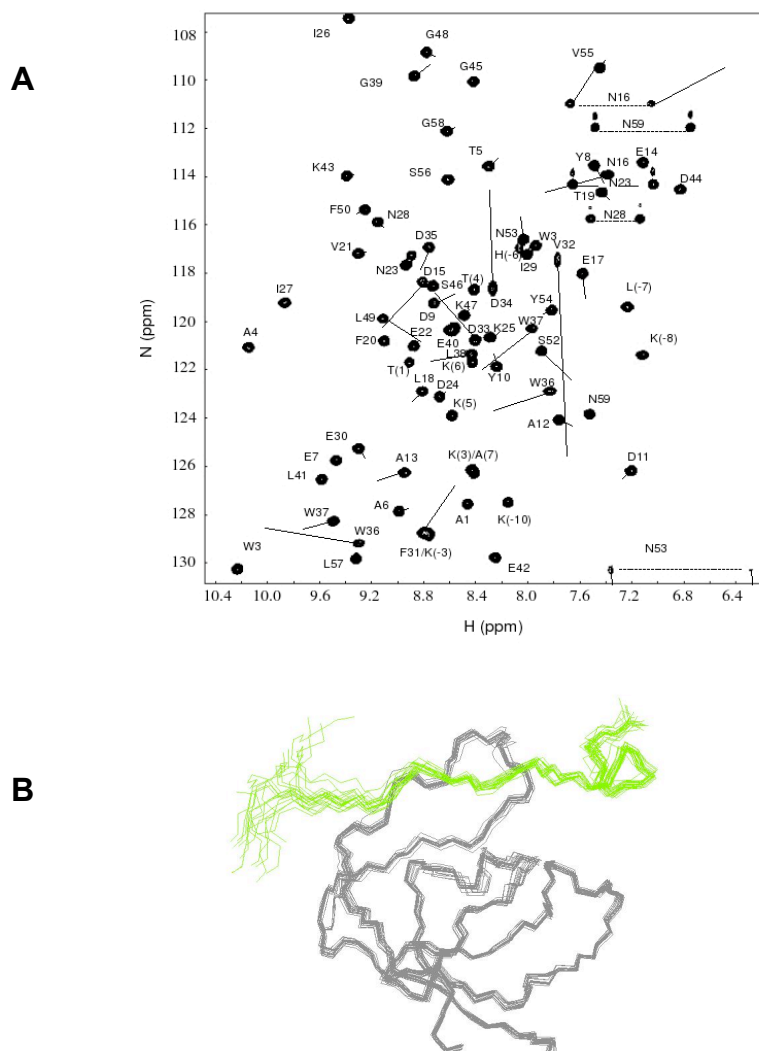


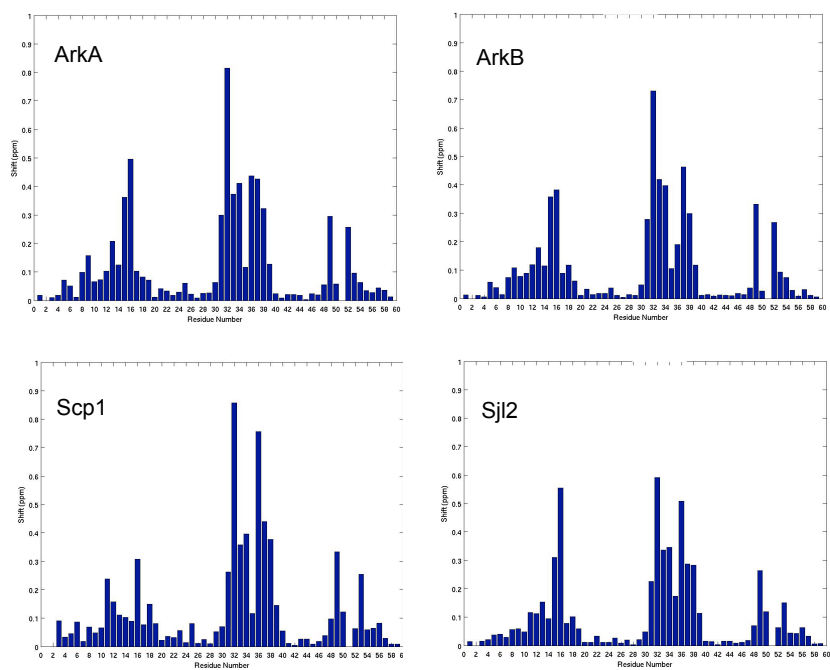
# SUPPLEMENTAL DATA

Supplementary Figure 1. Stollar et al



**(A)** The  $^1\text{H}$ - $^{15}\text{N}$  HSQC of the AbpSH3:ArkA complex. The end of the solid line indicates the position of the peak in the unbound state. The dashed lines indicate pairs of sidechain amide protons. **(B)** Superimposition of 20 lowest energy structures of the AbpSH3-ArkA complex. The SH3 domain is in silver with the peptide in green.

## Supplementary Figure 2. Stollar et al



Chemical shift differences between unbound and peptide bound AbpSH3 complexes.

## Supplementary table 1. Stollar et al

### NOEs

Intermolecular NOEs	248
Intramolecular NOEs (AbpSH3)	1930
Intramolecular NOEs (ArkA)	317

### Dipolar coupling restraints (Q factor)

HN-N	67 (0.15 ± 0.013)
CA-CB	62 (0.16 ± 0.013)
CA-HA	53 (0.14 ± 0.010)
CA-CO	66 (0.24 ± 0.017)
N-CO	60 (0.30 ± 0.022)

### RMSD from ideal distances (Å)

Bonds	0.0038 ± 0.0002
NOEs	0.0280 ± 0.0050

### RMSD from ideal angles (degrees)

Bond angles (°)	0.59 ± 0.013
Improper (°)	0.57 ± 0.036

### RMSD from mean structure (Å)

	<u>Backbone</u>	<u>Heavy Atoms</u>
AbpSH3 (1 to 59)	0.30 ± 0.1	0.90 ± 0.1
Ark1 (3 to -10)	0.41 ± 0.3	1.41 ± 0.5
Complex (1 to 59, 3 to -10)	0.37 ± 0.2	1.05 ± 0.2

### Procheck ramachandran analysis for complex (1 to 59, 3 to -10)

Residues in most favored regions	77.9%
Residues in additional allowed regions	17.9%
Residues in generously allowed regions	2.2%*
Residues in disallowed regions	1.9%*

\* D15 is the major residue in the disallowed region. CPMG relaxation-dispersion experiments in the bound complex revealed the presence of millisecond to microsecond timescale exchange with a minor state for the D15 amide only (data not shown), suggesting that NOEs arising from these two states are constraining this position.

## Supplementary Table 2. Stollar et al

Strain	Genotype	Source
BY263 <sup>a</sup>	MATa trp1Δ63 ura3-52 lys2-801 ade2-107 his3Δ200 leu2-Δ1	Measday et al (1994) Science 266:1391-5.
BY4741 <sup>b</sup>	MATa ura3Δ0 leu2Δ0 his3Δ1 met15Δ0	Brachmann et al (1998) Yeast 14:115-32.
<i>ark1Δ::kan</i>	BY4741 <i>ark1Δ::kan</i>	Deletion consortium
BY4075 <sup>b</sup>	MATa ura3 leu2 his3 ark1-Δ608-626- 3xMyc::Hph prk1Δ::kan	Haynes et al (2007) Genetics 176: 193-208.

<sup>a</sup> S288C derivative.

<sup>b</sup> Strains from the deletion consortium are isogenic to the parent strain, BY4741, also an S288C derivative.

### Supplementary Table 3. Stollar et al

Plasmid	Description
pARK1 WT	Contains a 2.8-kb fragment including 0.9-kb promoter region, and the 1.9-kb <i>ARK1</i> coding sequence (codons 1-638), fused to the N terminus of GFP
pΔArkB	pARK1 WT derivative containing <i>ARK1</i> with the 622-629 amino acid deletion
pArkA_P(2)A	pARK1 WT derivative containing <i>ARK1</i> with the P <sub>609</sub> A substitution and 622-629 amino acid deletion
pArkA_P(2)V	pARK1 WT derivative containing <i>ARK1</i> with the P <sub>609</sub> V substitution and 622-629 amino acid deletion
pArkA_P(0)A	pARK1 WT derivative containing <i>ARK1</i> with the P <sub>611</sub> A substitution and 622-629 amino acid deletion
pArkA_P(-1)A	pARK1 WT derivative containing <i>ARK1</i> with the P <sub>612</sub> A substitution and 622-629 amino acid deletion
pArkA_K(-3)A	pARK1 WT derivative containing <i>ARK1</i> with the K <sub>614</sub> A substitution and 622-629 amino acid deletion
pArkA_K(-3)R	pARK1 WT derivative containing <i>ARK1</i> with the K <sub>614</sub> R substitution and 622-629 amino acid deletion
pArkA_H(-6)A	pARK1 WT derivative containing <i>ARK1</i> with the H <sub>617</sub> A substitution and 622-629 amino acid deletion
pArkA_L(-7)A	pARK1 WT derivative containing <i>ARK1</i> with the L <sub>618</sub> A substitution and 622-629 amino acid deletion
pArkB	pARK1 WT derivative containing <i>ARK1</i> with the 605-615 amino acid deletion
pPrk	pARK1 WT derivative containing <i>ARK1</i> with the 605-629 amino acid replacement for residues 746-762 from Prk1p
pScp	pARK1 WT derivative containing <i>ARK1</i> with the 605-629 amino acid replacement for residues 154-170 from Scp1p
pSrv	pARK1 WT derivative containing <i>ARK1</i> with the 605-629 amino acid replacement for residues 350-367 from Srv2p
pSjl	pARK1 WT derivative containing <i>ARK1</i> with the 605-629 amino acid replacement for residues 1111-1127 from Sjl2p