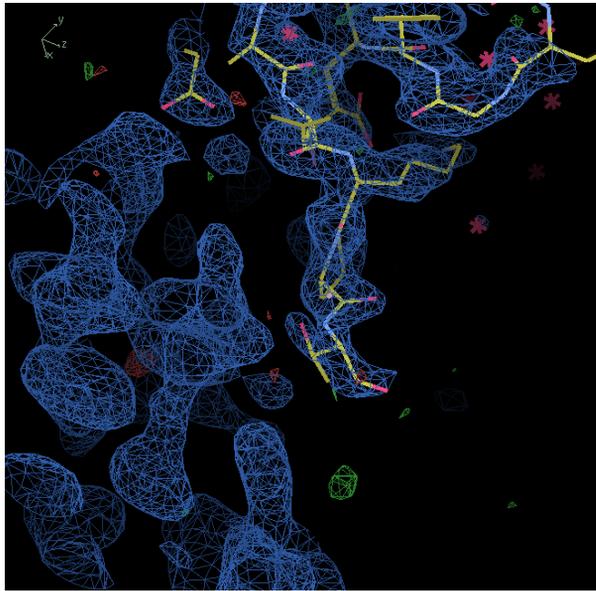
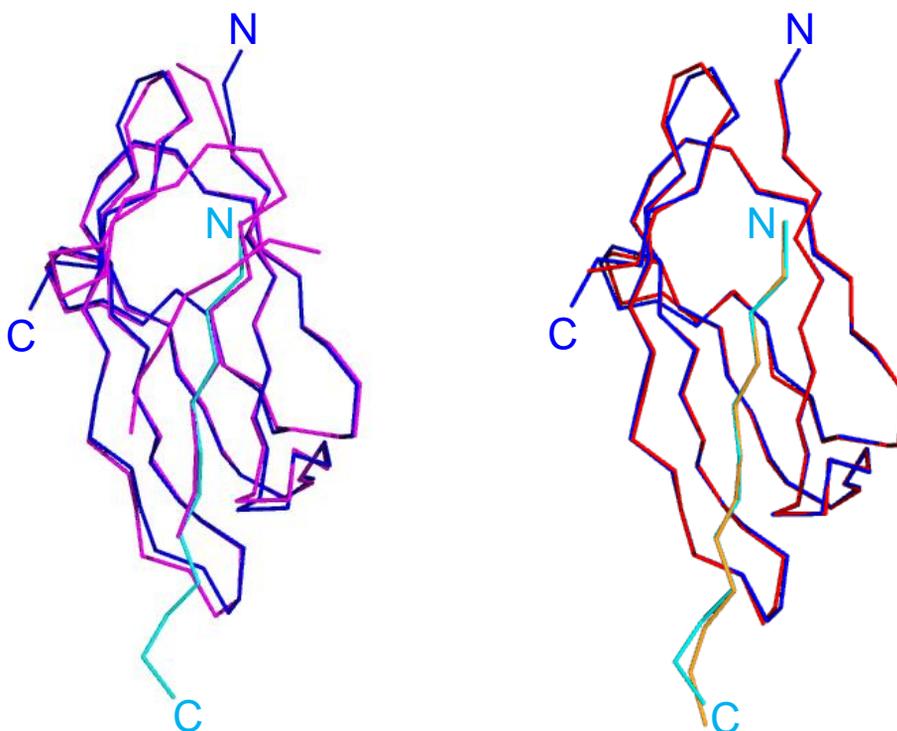


# SI Figure 1



**Supplemental Fig. 1.** Electron density map showing the interaction between the tail of the SpyTag/SpyCatcher complex (backbone carbons in yellow) with the adjacent protein (only electron density shown) in the crystal packing. Electron density is shown as blue mesh at  $1 \sigma$ , with water molecules labeled as red asterisks.

# SI Figure 2



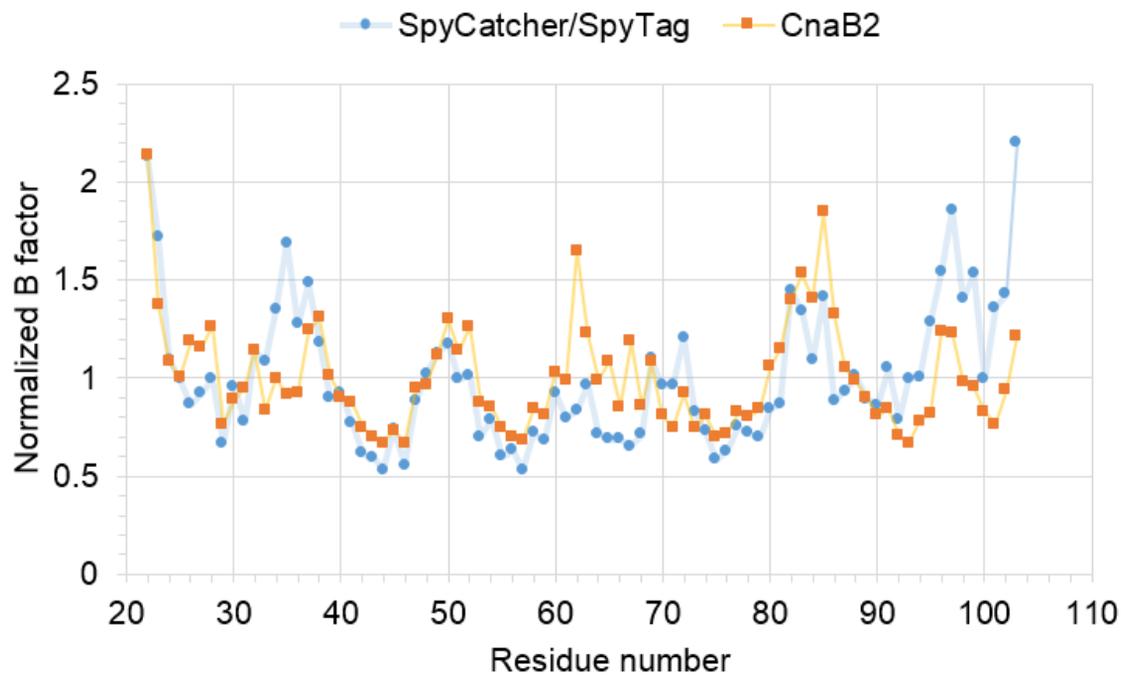
Ribbon diagram overlay

CnaB2  
SpyTag/SpyCatcher

SpyTag/SpyCatcherΔN1  
SpyTag/SpyCatcher

**Supplemental Fig. 2.** Superimposition of crystal structures. The left panel shows CnaB2 (magenta) overlaid with SpyTag/SpyCatcher (cyan/navy). An internal disordered stretch of CnaB2 is shown as a dashed line. The right panel shows SpyTag/SpyCatcherΔN1 (orange/red) overlaid with SpyTag/SpyCatcher. The structures show the backbone in ribbon representation, with N- and C-termini from the SpyTag/SpyCatcher structure marked.

# SI Figure 3



**Supplemental Fig. 3.** Comparison of Normalized B factors between SpyCatcher and CnaB2. Normalized B factor was calculated by dividing the mean main-chain B factor for each residue by the mean main-chain B factor for residues 22-103 of that chain (using the Baverage tool in CCP4 software). 22-103 are the only SpyCatcher residues resolved in the structure. Comparison is made to Chain A in the SpyCatcher/SpyTag structure.