SUPPLEMENTAL FIGURE 1:

Electron density. (A) Experimental and (B) 2Fo-Fc simulated annealed composite omit maps of a representative view of the $TnpA_{Dra2}$/LE27/T5 complex, both contoured at the 1 sigma level.

SUPPLEMENTAL FIGURE 2:

Ramachandran plots of the IS*200*/IS*605* transposases represented by PDB code 2fyx and two complexes of the IS*Dra2* transposase with DNA. For 2fyx, its two αD helices are in cis and two residues (H115, T116) in the loop that precedes helix αD are in a most favored region (in green) of the phi/psi plot. For the TnpA/LE27/T5 and TnpA/Cd structures, the structurally equivalent residues are N124 and T125; they are found in a different most favored region, and the phi/psi space connecting the regions (in dark yellow) represents "allowed" protein conformations. The conformational change represented by this tunneling between the two regions is permitted, as population analysis suggests that the phi/psi region that connects the two regions is populated in protein structures (Lovell at al, 2003). The double-headed red arrows show how the critical residues move between different regions of the plots. These results indicate that cis-to-trans transitions of helix αD, proposed to be mechanistically important, are structurally reasonable.

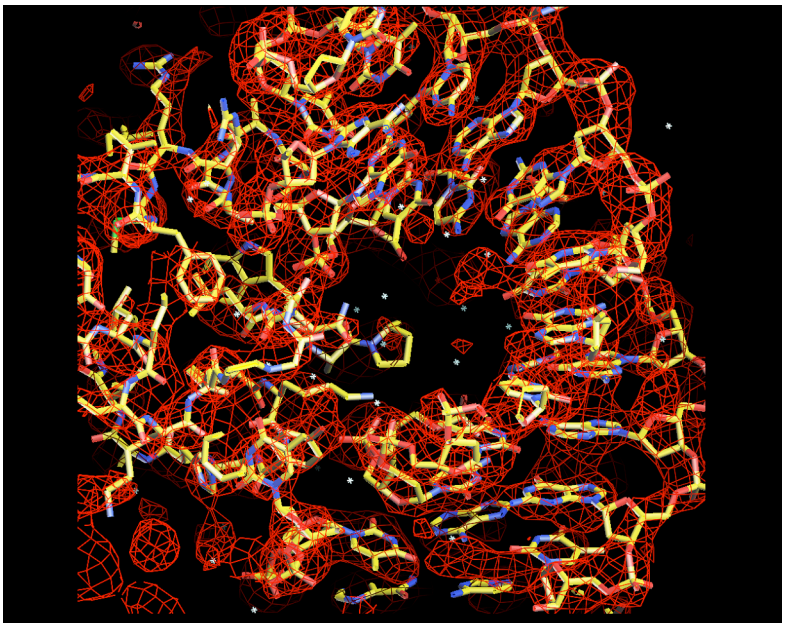
Lovell SC, Davis IW, Adrendall WB, de Bakker PIW, Word JM, Prisant MG, Richardson JS, Richardson DC (2003) Structure Validation by Cα Geometry: ϕ,φ and Cβ Deviation. *Proteins* **50**: 437-450

SUPPLEMENTAL FIGURE 3:

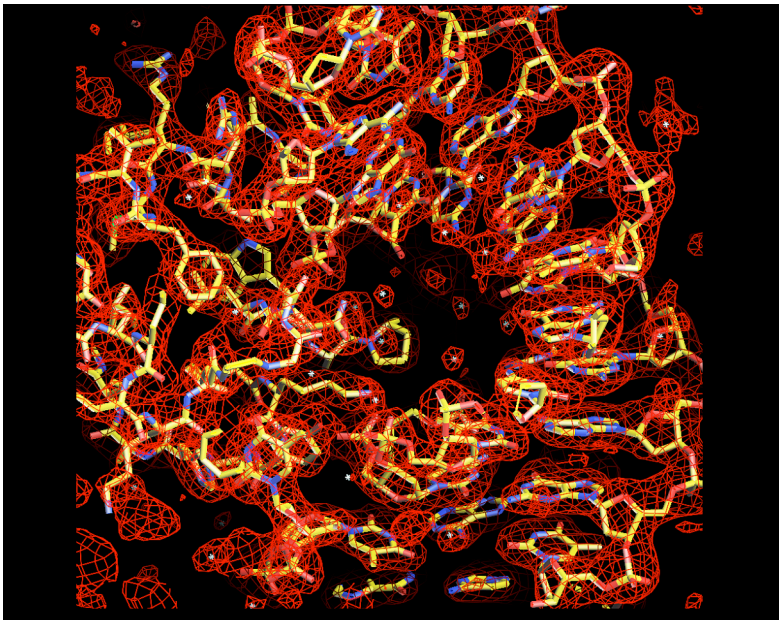
Helix αD which contains the nucleophilic tyrosine is a mobile structural element. (A) Cartoon representation of the three TnpA/LE27/T5 complexes (designated A-B, C-D, and E-F) related to each other by a pseudo-translational relationship in the crystallographic asymmetric unit. As noted in "The first view of a fully assembled active site" section of the main text, the positions of the C-terminal αD helices vary substantially.
(B) Superposition of the three complexes in (A). The A-B dimer is in green, the C-D dimer in blue, and the E-F dimer is in red. While most of the transposase and the bound DNA molecules are essentially identical, helix αD occupies various positions in the three different dimers, suggesting that crystal packing forces are sufficient to reposition them relative to the rest of the complex.

SUPPLEMENTAL FIGURE 1 - Hickman et al.

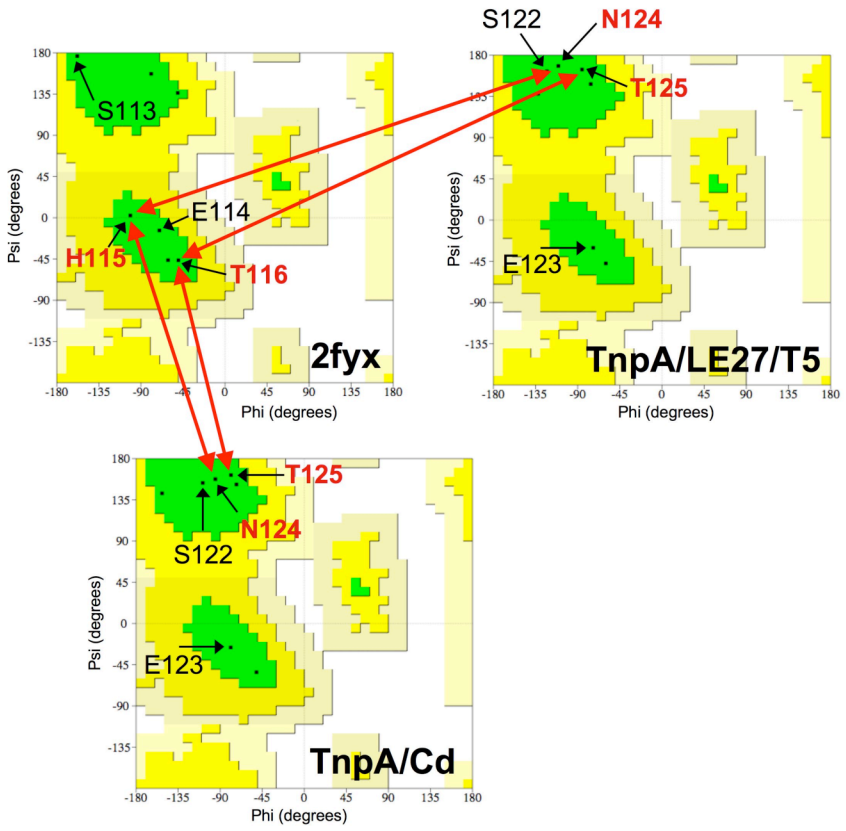
A



B

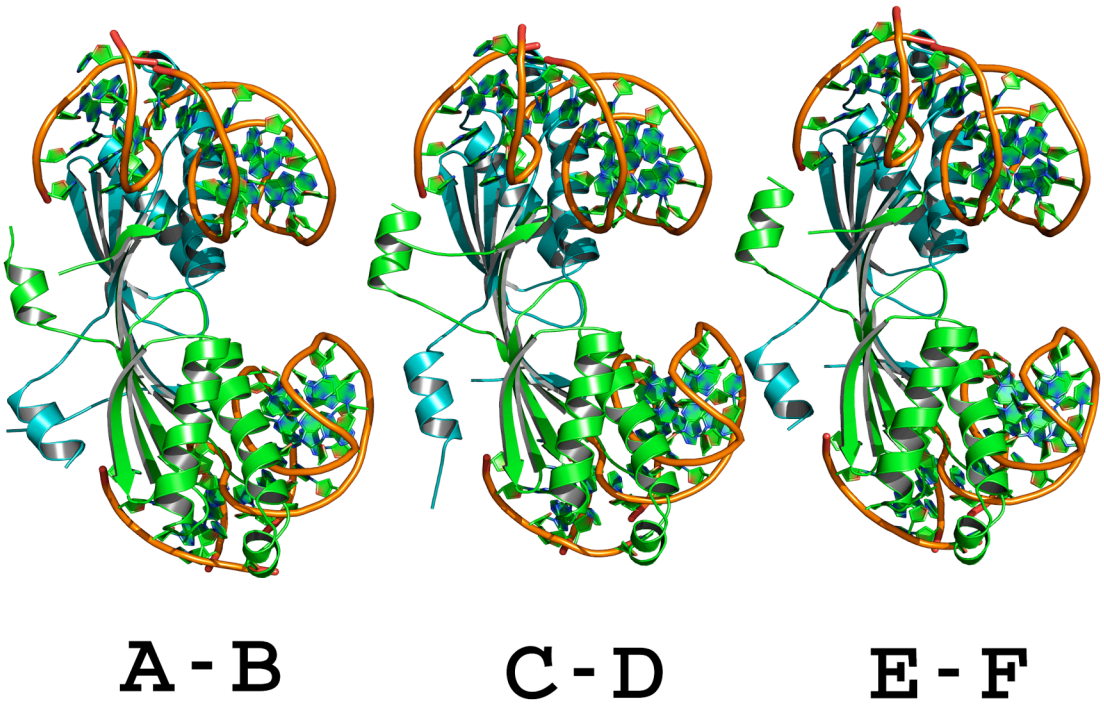


SUPPLEMENTAL FIGURE 2 - Hickman et al.



SUPPLEMENTAL FIGURE 3 - Hickman et al.

A



B