Supporting Information

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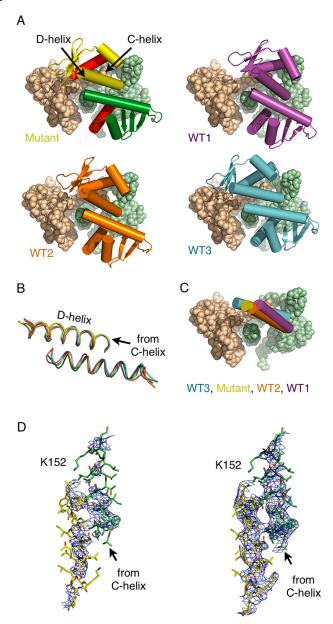
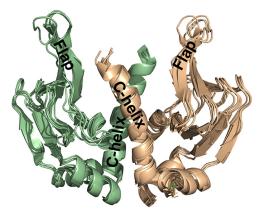


Fig. S1. Unliganded WT catabolite gene activator protein (CAP) structures. (*A*) "Top view" of the protein is shown. The DNA binding domains of each molecule are colored magenta, orange, and cyan. A similar view of the mutant is shown as reference using the previous color scheme. (*B*) Superposition of the pair of D-helices, represented as diagram loops, of the mutant and the three WT molecules. (*C*) Superposition of the cAMP binding domains of the mutant and the three WT molecules. One D-helix of each molecule is shown to emphasize the different orientations DNA binding domains. (*D*) Unbiased electron density (i.e., the DNA binding domains were not included in model phases) shown at 3.6-Å resolution of the D-helices before (*Left*) and after (*Right*) 6-fold averaging contoured at



 $\textbf{Fig. S2.} \quad \text{Superposition of the cAMP binding domains. All 3 nt binding domain dimers of the WT and the only dimer of the D138L mutant CAP were superimposed.}$

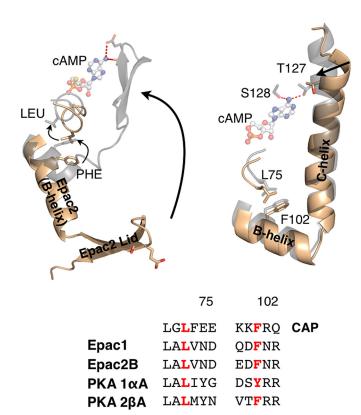
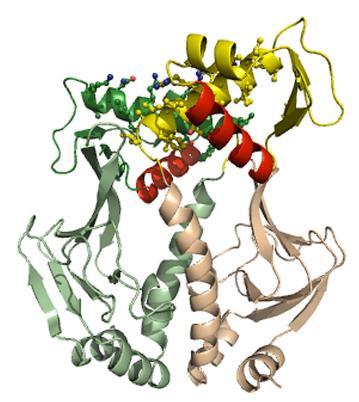


Fig. 53. Comparison of cAMP induced conformational changes between CAP and other cAMP binding proteins. The cAMP binding domains of the liganded and the unliganded structures of Epac2 (*Left*) and CAP (*Right*) were superimposed showing two different mechanisms of cAMP induced changes.



Movie S1. Movie showing the rigid-body-like movements of the dimerized DNA binding domains of the apo-CAP and the conformational changes associated with cAMP binding leading to the activation of CAP for site specific DNA recognition. Previously determined active structures, 1G6N.pdb and 1CGP.pdb, were used to complete the movie.

Movie S1 (AVI)