Transmembrane prolines mediate signal sensing and decoding in *Bacillus subtilis* DesK histidine kinase

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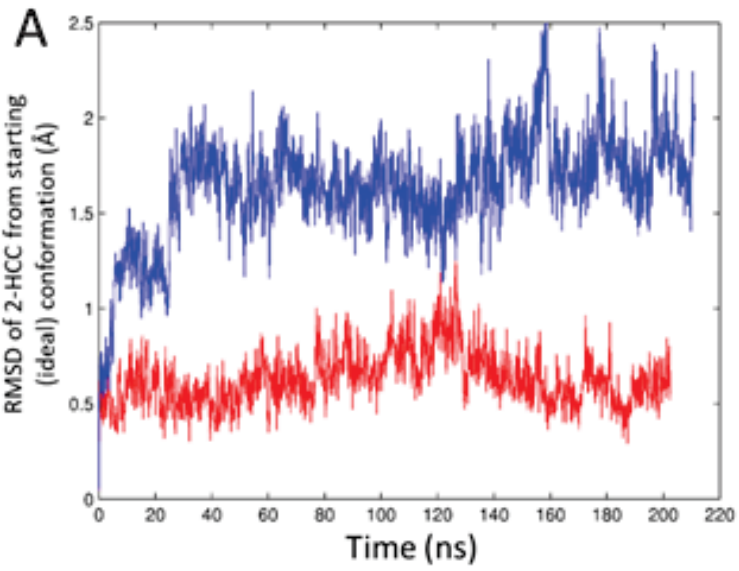
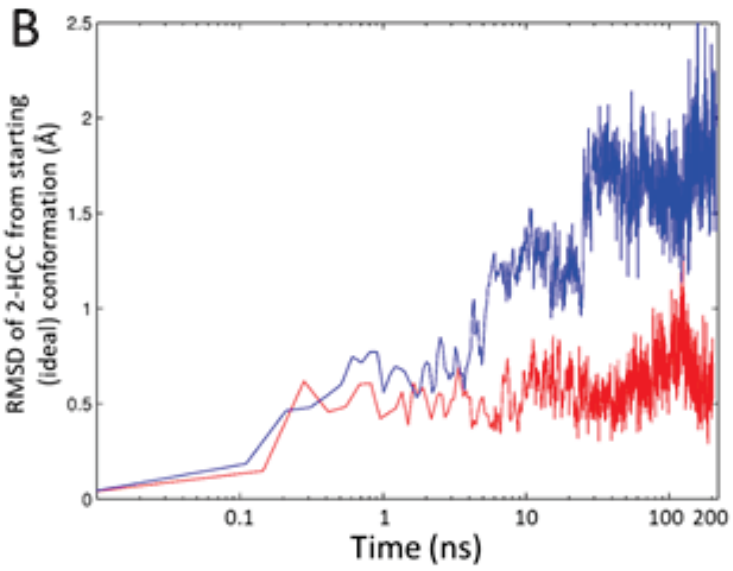
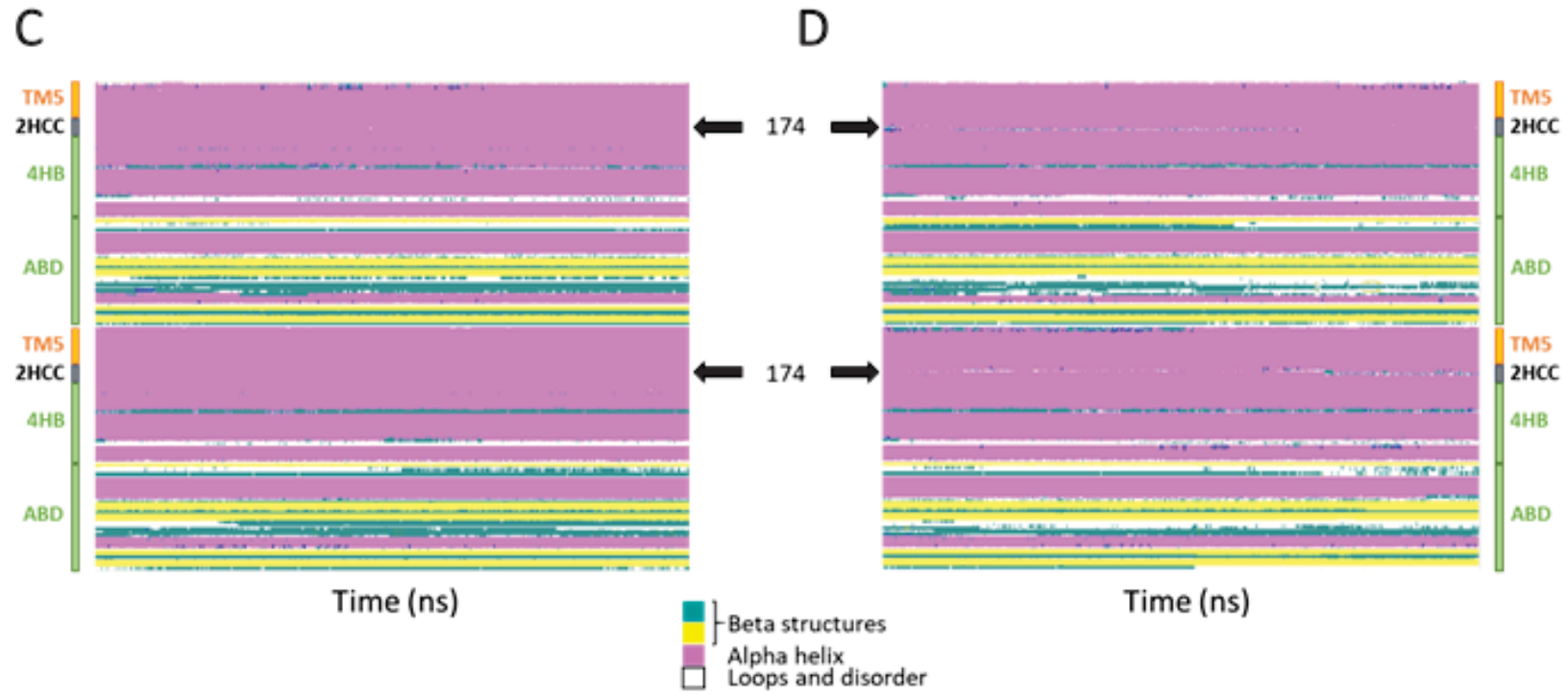
Supplemental material legends

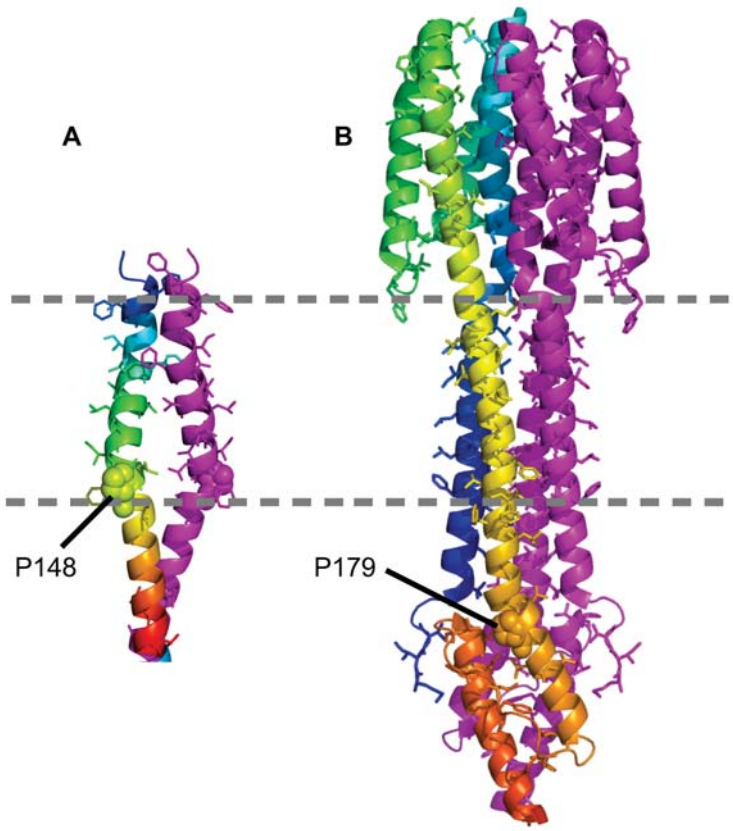
Figure S1. Effect of L174P on the structure of the 2-HCC. Panels **A** and **B** show the RMSD of the core of the 2-HCC element (residues L160 through to L177) relative to its starting conformation, which corresponds to an ideal coiled coil geometry, for TM5-DesKC P148A (red) and P148A/L174P (blue). (Panel **B** shows a logarithmic scale to better make the point of immediate destabilization.). Panels **C** and **D** show the time dependence of secondary structures, to stress that the helical conformation is readily lost around Pro174 in the double mutant, but retained around Leu174 in the single mutant.

Figure S2. Comparison of DesK's Pro148 and NarQ's Pro179. A. DesK's TM5 and beginning of 2-HCC as modeled in Saita et al. (17). B. NarQ's cytosolic, transmembrane and HAMP domains plus the beginning of its 2-HCC, from PDB ID 5JEQ (5). In both panels, one monomer is colored magenta and the other is colored from blue at the N-terminus to red at the C-terminus.


A
RMSD of 2-HCC from starting (ideal) conformation (Å)
Time (ns)


B
RMSD of 2-HCC from starting (ideal) conformation (Å)
Time (ns)


C
D
TM5
2HCC
4HB
ABD
174
Time (ns)
Beta structures
Alpha helix
Loops and disorder


A
B
P148
P179