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

Pilar Fernández\(^a,\)\(^1\), Lucia Porrini\(^{a,b,}\)\(^1\), Daniela Albanesi\(^{a,b,}\)\(^#\), Luciano A. Abriata\(^{c,d}\), Matteo Dal Peraro\(^{c,d}\), Diego de Mendoza\(^{a,b}\), María C. Mansilla\(^{a,b,}\)\(^#\)

\(^a\)Instituto de Biología Molecular y Celular de Rosario (IBR-CONICET), Rosario, Argentina
\(^b\)Departamento de Microbiología Facultad de Ciencias Bioquímicas y Farmacéuticas, Universidad Nacional de Rosario, Rosario, Argentina
\(^c\)Institute of Bioengineering, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
\(^d\)Swiss Institute of Bioinformatics, Lausanne, Switzerland
\(^1\)These authors contributed equally to this work.

# Address correspondence to:
Daniela Albanesi albanesi@ibr-conicet.gov.ar
María C. Mansilla mansilla@ibr-conicet.gov.ar

**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.
