

Supplemental Data

Crystal Structures of C₄-Dicarboxylate Ligand Complexes with Sensor Domains of Histidine Kinases DcuS and DctB Jonah Cheung and Wayne A. Hendrickson

Figure 1.

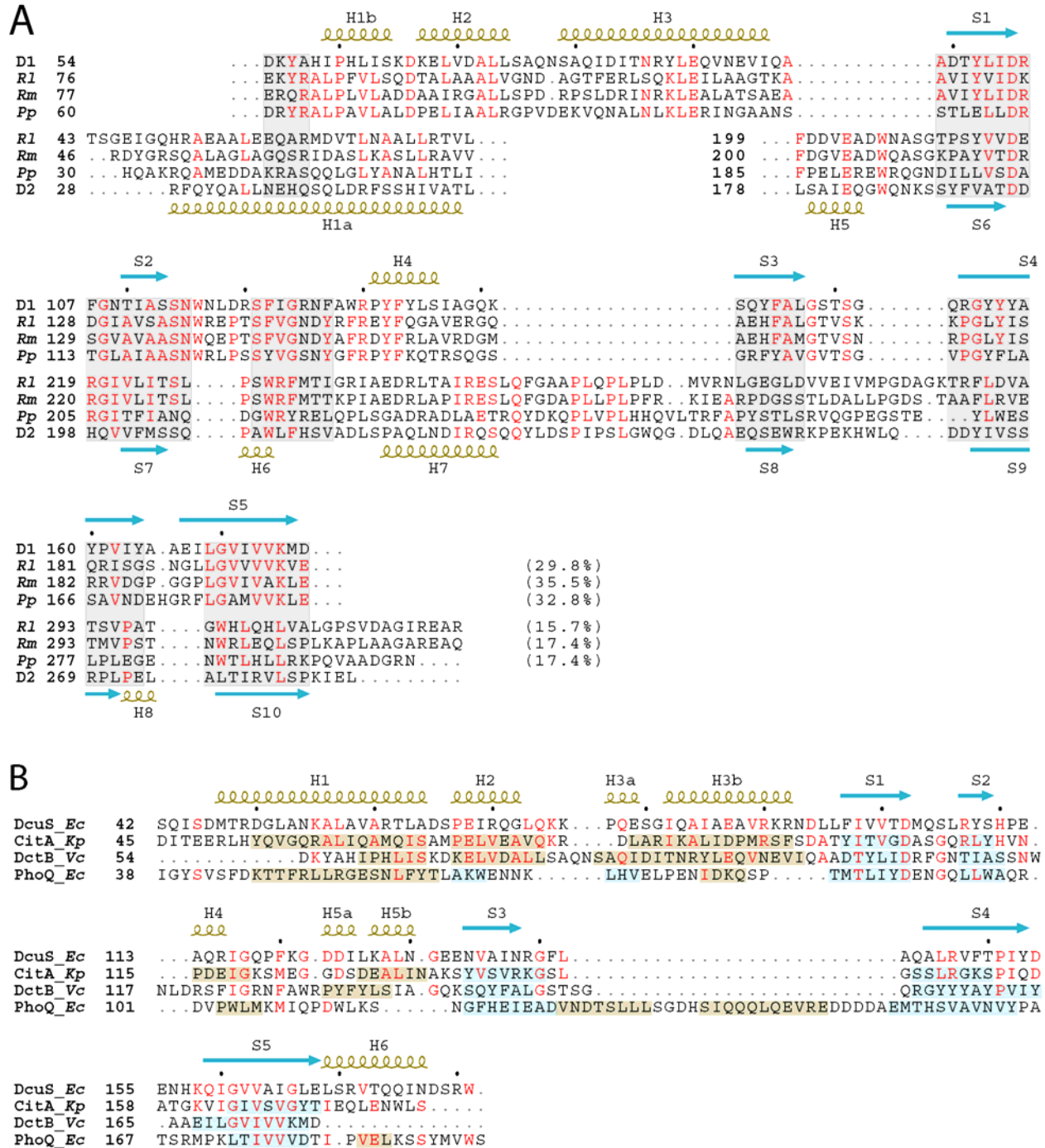


Fig.1. Structure-based sequenced alignments. A. Structure-based sequence alignment between the two subdomains of the *V. cholerae* DctB periplasmic sensor domain. Secondary structure elements for the distal subdomain 1 (D1) and the proximal subdomain 2 (D2) are labeled above and below the sequences, respectively, and are colored olive (helices) and light blue (strands). Organism names for DctB from other species are abbreviated in italics (*Rl* for *Rhizobium leguminosarum*, *Rm* for *Rhizobium meliloti*, and *Pp* for *Pseudomonas putida*). Conserved residues are shown in red. The shaded regions represent aligned regions. Percent sequence identity values between the DctB homologues to *V. cholerae* DctB are shown at the end of the alignment, in each respective subdomain. B. Structure-based sequence alignment of DcuS 42-181 and DctB 28-286 distal subdomain 1 (D1) to each other and to the sensor domains of CitA and PhoQ. Conserved residues are shown in red. The secondary structure elements of DcuS 42-181 are labeled above the alignment, while that for the other structures are shown as shaded regions that overlay the sequences themselves. Secondary structure elements are colored olive (helices) and light blue (strands). Organism names are abbreviated in italics (*Ec* for *Escherichia coli*, *Kp* for *Klebsiella pneumoniae*, and *Vc* for *Vibrio cholerae*).

Figure 2.

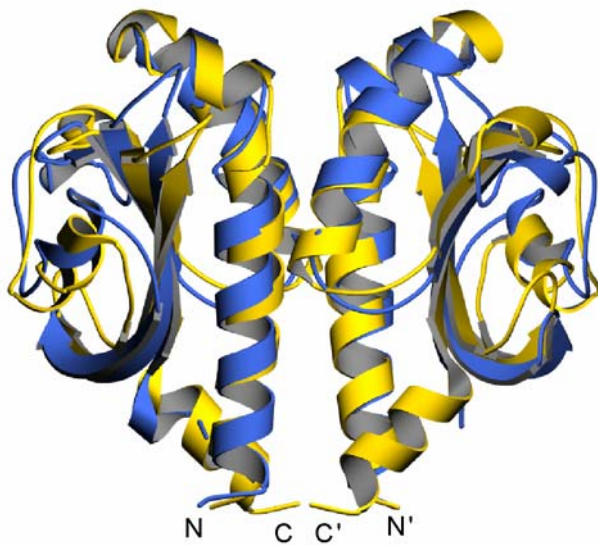


Fig. 2. Superimposition of dimeric PDC sensor domains of DcuS and CitA. The dimeric malate:DcuS 42-181 and citrate:CitAP (1) ligand complexes are shown superimposed. Overall structures are shown as ribbon diagrams with DcuS 42-181 in yellow and CitAP in blue. Ligands have been omitted for greater clarity. A root mean square deviation of 3.1Å is obtained by the superimposition of 229 C $^{\alpha}$ positions. The diagram was created using MolScript (2).

References

1. Sevvana, M., Vijayan, V., Zweckstetter, M., Reinelt, S., Madden, D. R., Herbst-Irmer, R., Sheldrick, G. M., Bott, M., Griesinger, C., and Becker, S. (2008) *J. Mol. Biol.* **377**, 512-523
2. Kraulis, P. J. (1991) *J. Appl. Crystallogr.* **24**, 946-950