Supplementary Tables to

Brüderlin et al., Intermediaries in phosphotransfer: structural features discriminating Rec domains of hybrid histidine kinases from response regulator homologs

Supplementary Table 1. Crystallographic data collection and refinement statistics

Data collection	
Synchrotron source	SLS, PXI
Wavelength (Å)	1.00004
Space group	I 1 2 1
a, b, c (Å)	37.4, 42.9, 65.0
α, β, γ (°)	90.0, 94.4, 90.0
Resolution (Å)	28.2-1.25 (1.29-1.25)
No. of unique reflections	28065 (2818)
No of reflections used for R_{free}	1372 (136)
Completeness (%)	98.37 (99.58)
I/σ (I)	17.24 (4.96)
Redundancy	2.0 (2.0)
R_{merge} (%)	1.7 (12.9)
R_{pim} (%)	1.7 (12.9)
CC (1/2) (%)	99.9 (94.0)
Refinement	
R_{work}/R_{free} (%)	20.6/22.7
RMSD from ideal values	
-- Bond length (Å)	0.0123
-- Bond angles (°)	1.7
Molecules/asymmetric unit	1
No. of atoms	
-- Protein	839
-- Water	93
Average B-factor (Å^2)	18.9
-- Protein (Å^2)	17.5
-- Water (Å^2)	31.7
Ramachandran statistics	
-- Favored regions (%)	100.0
-- Allowed regions (%)	0.0
-- Disallowed regions (%)	0.0
PDB Code	6TNE

*) The values recorded in parentheses are those for the highest resolution shell.

Supplementary Table 2. Amide proton linewidth of $CckA^{Rec}$ residues in the inactive and active state.

Residue	Linewidth of amide proton (Hz)	
	native $CckA^{Rec}$	BeF_3^- modified $CckA^{Rec}$
L574	22.3	20.6
V576	24.9	21.4
V582	24.8	18.4
V585	19.9	15.4
G603	24.0	23.4
I608	18.6	16.8

Supplementary Table 3. Primers used to obtain the recombinant plasmids used in this study .

ID	Name	Sequence (5'>3')	Length	Tm* (°C)	Exp Ta** (°C)
1	Q5SDM_$CckA^{Rec}$_F	CACCATCACCATCACGGTTCTGGTTCTGG CGCCGGCCGCATCCT	44	75.3	72.0
2	Q5SDM_$CckA^{Rec}$_R	TCAATGGTGATGATGGTGGTGCTACG CCGCCTGCAGCTGCTGCTT	45	76.3	72.0
3	Q5SDM_$CckA^{Rec}$_N-histag_F	AAGGAGATATACCATATGGGCCATCAC CATCACCATCACGGT	42	68.0	72.0
4	Q5SDM_$CckA^{Rec}$_ N-histag_R	TCAATGGTGATGATGGTGGTGCTA CGCCGCCTGCAGCTGCTGCTT	45	76.3	72.0

* Tm = calculated melting temperature ** Exp Ta = annealing temperature used experimentally