S2 Table. Average and standard deviation of RMSD for the C1 and C2 domains of AC5, α-helix angles for both domains and characterization of the C1/C2 interface: gap volume, change in accessible surface area (ΔASA) and gap index, for the systems studied with molecular dynamics simulation. To compute the RMSD we used the average structure as the reference state.

Data	**AC5+FOK**	**AC5+ATP+FOK**
RMSD C1 (Å)	0.8 ± 0.1	0.8 ± 0.1
RMSD C2 (Å)	0.8 ± 0.1	0.9 ± 0.2
α_{C1} (°)	23 ± 4	44 ± 5
α_{C2} (°)	46 ± 4	40 ± 3
Gap Volume ($Å^3$)	7500 ± 464	6256 ± 385
ΔASA ($Å^2$)	2354 ± 88	2308 ± 77
Gap index (Å)	3.2 ± 0.2	2.7 ± 0.2