

**S4 Table.** Average and standard deviation of the gap volume,  $\Delta$ ASA and the gap index of the AC5/Gs $\alpha$  interface in presence and in the absence of ATP.

<b>Data</b>	<b>AC5+ATP+Gs<math>\alpha</math></b>	<b>AC5+Gs<math>\alpha</math></b>
Gap Volume ( $\text{\AA}^3$ )	$3286 \pm 333$	$3424 \pm 361$
$\Delta$ ASA ( $\text{\AA}^2$ )	$1244 \pm 123$	$1067 \pm 63$
Gap index ( $\text{\AA}$ )	$2.7 \pm 0.5$	$3.2 \pm 0.4$