Table S2. Different transient states of the AdeB protomers.

Protomer	Cleft State	Exit site distance, Q125 to Y749	Hydrogen-bonded distance, K931 to				Protomer Assignment
			D407 (Å)	D408 (Å)	N932 (Å)	T968 (Å)	
AdeB-I, A	Closed	13.04	-	-	3.00	3.15	Extrusion
AdeB-I, B	Closed	13.04	-	-	3.00	3.15	Extrusion
AdeB-I, C	Closed	13.04	-	-	3.00	3.15	Extrusion
AdeB-II, A	Closed	13.53	-	-	3.12	3.17	Extrusion
AdeB-II, B	Closed	14.89	-	-	3.03	3.04	Extrusion
AdeB-II, C	Closed	13.99	-	-	3.15	3.00	Extrusion
AdeB-III, A	Closed	14.24	-	-	3.20	3.01	Extrusion
AdeB-III, B	Closed	14.24	-	-	3.20	3.01	Extrusion
AdeB-III, C	Closed	14.24	-	-	3.20	3.01	Extrusion
AdeB-Et-I, A	Closed	13.87	-	-	3.17	2.86	Extrusion
AdeB-Et-I, B	Closed	14.01	-	-	3.03	3.18	Extrusion
AdeB-Et-I, C	Open	9.40	2.75	2.85	-	-	Binding
AdeB-Et-II, A	Closed	9.19	-	-	3.08	2.82	Resting
AdeB-Et-II, B	Closed	15.25	-	-	2.79	2.71	Extrusion
AdeB-Et-II, C	Open	9.01	3.12	2.67	-	-	Binding
AdeB-Et-III, A	Open	9.38	2.95	-	-	-	Access*
AdeB-Et-III, B	Closed	14.71	-	-	2.62	2.99	Extrusion
AdeB-Et-III, C	Open	8.50	2.93	2.97	-	-	Binding

Protomer states were defined using three criteria. (1) State of the periplasmic cleft between PC1 and PC2. (2) Size of the extrusion tunnel measured by the distance between the $C\alpha$ atoms of Q125 and Y749, which form the substrate exit site. (3) Hydrogen-bonded distance between the "proton sweeper" K931 and other residues within the proton-relay network (D407, D408, N932 or T968). Only distances of 3.20 Å and under are noted.