

Table S5 Bottleneck residues of the top ranked tunnels of DhaA identified by CAVER 3.0 in molecular dynamics trajectory using the probe radius of 0.9 Å and the clustering threshold of 3.5.

Pathway	p1a	p1a'	p1b	p2a	p2b	p2c	p3
Bottleneck residues^a	F149 (71 %),	A172 (91 %),	V245 (98%),	L246 (93 %),	W141 (82 %),	P210 (73 %),	I211 (72 %),
	C176 (59 %),	F152 (90%),	F144 (85%),	L209 (57 %),	V245 (78 %),	I135 (47 %),	I135 (56 %),
	A172 (50 %),	F168 (82 %),	P142 (79 %),	W141 (54 %),	L246 (69 %),	R133 (41 %),	W138 (56 %),
	A145 (38 %),	A167 (20 %)	A145 (30 %)	I135 (36 %),	P142 (59 %)	P134 (37 %),	W141 (41 %),
	K175 (27 %),			I132 (34 %)			T137 (20 %)
	T148 (23 %)						

^athree residues closest to the pathway bottleneck were considered in each snapshot; only the most frequent bottleneck residues are listed together with the percentage of snapshots in which they formed the bottleneck.