

Table S3 Characteristics of the pathways identified in DhaA crystal structures using the probe radius of 0.8 Å

Rank	PDB-ID 1BN6 ^a			PDB-ID 1BN7 ^a			PDB-ID 1CQW ^a		
	Pathway	Bottleneck radius [Å]	Average Throughput	Pathway	Bottleneck radius [Å]	Average Throughput	Pathway	Bottleneck radius [Å]	Average Throughput
1	p1	1.5	0.713	p1a	1.2	0.722	p1a	1.6	0.709
2	p2a	1.4	0.607	p2ab	0.9	0.500	p2ab	1.0	0.492
3	p2b	1.1	0.602	p1b	0.8	0.422	p1a'	0.9	0.422
4	-	0.9	0.301	-	0.8	0.325	-	0.9	0.272
5	-	0.8	0.221	-	0.9	0.265	p3	0.8	0.241
6	-	0.8	0.125	p3	0.9	0.236	-	0.8	0.099
7	-	0.9	0.100	-	0.8	0.216	-	0.9	0.083
8	-	0.9	0.090	-	0.8	0.097	-	0.8	0.032
9	-	0.8	0.042	-	0.8	0.091	-	0.8	0.028
10	-	0.8	0.038	-	0.8	0.085	-	0.8	0.018
11	-	0.8	0.030	-	0.8	0.051	-	0.8	0.005
12	-	0.8	0.026	-	0.8	0.036	n.a. ^b	-	-
13	-	0.8	0.004	-	0.8	0.034	n.a. ^b	-	-
14	-	0.8	0.0004	n.a. ^b	-	-	n.a. ^b	-	-

^aDhaA crystal structures with introduced substitutions V172A, I209L and G292A (see Protocol S4), without hydrogen atoms; ^bpathway not identified (n.a. - not applicable).