Table S4 Comparison of characteristics of the DhaA p1 tunnel obtained by the analysis of the molecular dynamics trajectory and crystal structures

	Molecular dynamics trajectory	**PDB-ID 1CQW**[a]	**PDB-ID 1BN7**[a]	**PDB-ID 1BN6**[a]
Mean bottleneck radius[Å]	1.4	1.3	1.2	1.2
Maximum bottleneck radius [Å]	2.3	1.3	1.2	1.2
Bottleneck residues[b]	F149 (71 %), C176 (59 %), A172 (50 %), A145 (38 %), K175 (26 %), T148 (23 %)	A145, F149, C176	A145, F149, C176	A145, F149, C176

[a]crystal structures with introduced substitutions V172A, I209L and G292A and added hydrogen atoms (see Protocol S4); [b]three residues closest to the tunnel bottleneck; for molecular dynamics, only the most frequent bottleneck residues are listed, together with the percentage of snapshots in which they formed the bottleneck of the p1 tunnel.