

Table 1. Estimated rates for the processes discussed in the text

process	base	direction	\mathbf{V}_R		\mathbf{V}		\mathbf{D}		\mathbf{e}	Δ	k
unstacking	mGua	forward	12.4	0.8	-10.8	4.8	0.4	0	$0.997d_1 - 0.074d_2$	2.6	3.0×10^{-3}
			0.8	2.3	4.8	20.8	0	1.0			
unstacking	mGua	backward	20.7	1.6	-10.8	4.8	0.4	0	$0.997d_1 - 0.074d_2$	8.4	6.3×10^{-7}
			1.6	1.7	4.8	20.8	0	1.0			
unstacking	Gua	forward	14.5	1.7	-15.5	2.7	0.4	0	$0.991d_1 - 0.131d_2$	2.2	2.5×10^{-2}
			1.7	4.7	2.7	1.7	0	0.9			
unstacking	Gua	backward	18.2	0.2	-15.5	2.7	0.4	0	$0.991d_1 - 0.131d_2$	8.5	7.2×10^{-7}
			0.2	1.9	2.7	1.7	0	0.9			
insertion	mGua	forward	4.4	0.1	-14.0	-0.3	0.4	0	$0.999d_5 + 0.015d_4$	1.1	1.4×10^{-1}
			0.1	4.8	-0.3	3.0	0	0.4			
insertion	mGua	backward	10.6	1.3	-14.0	-0.3	0.4	0	$0.999d_5 + 0.015d_4$	16.3	1.2×10^{-12}
			1.3	3.3	-0.3	3.0	0	0.4			
insertion	Gua	forward	4.4	0.5	-14.5	0.1	0.1	0	$0.999d_5 - 0.002d_4$	7.0	1.1×10^{-6}
			0.5	3.6	0.1	4.3	0	1.0			
insertion	Gua	backward	7.6	1.1	-14.5	0.1	0.1	0	$0.999d_5 - 0.002d_4$	17.0	7.6×10^{-14}
			1.1	3.2	0.1	4.3	0	1.0			

\mathbf{V}_R and \mathbf{V} are in \AA^{-2} , \mathbf{D} is in $\text{\AA}^2 \text{ps}^{-1}$, Δ is in kcal mol^{-1} , and k is in ps^{-1} . For the active-site ‘‘insertion’’ steps, the ordering of coordinates in the matrices is d_5 first and d_4 second since d_5 substitutes for d_3 identified for mGua (see main text).