

Table 4. Bias annealing for the unstacking step

k_{a_1}	k_{a_2}	k_s	L	n	a
1000.0	1000.0	100.0	15	10	0.60
400.0	400.0	50.0	20	20	0.60
200.0	200.0	20.0	25	20	0.40
100.0	100.0	15.0	30	20	0.40
50.0	50.0	10.0	40	20	0.30
0.0	0.0	0.0	60	30	0.10

Trajectories of L ps were generated with biasing force constants k_{a_1} , k_{a_2} in kcal mol⁻¹ rad⁻², and k_s in kcal mol⁻¹ Å⁻². n is the total number of paths shot and a is the acceptance rate.