

Supplementary Information

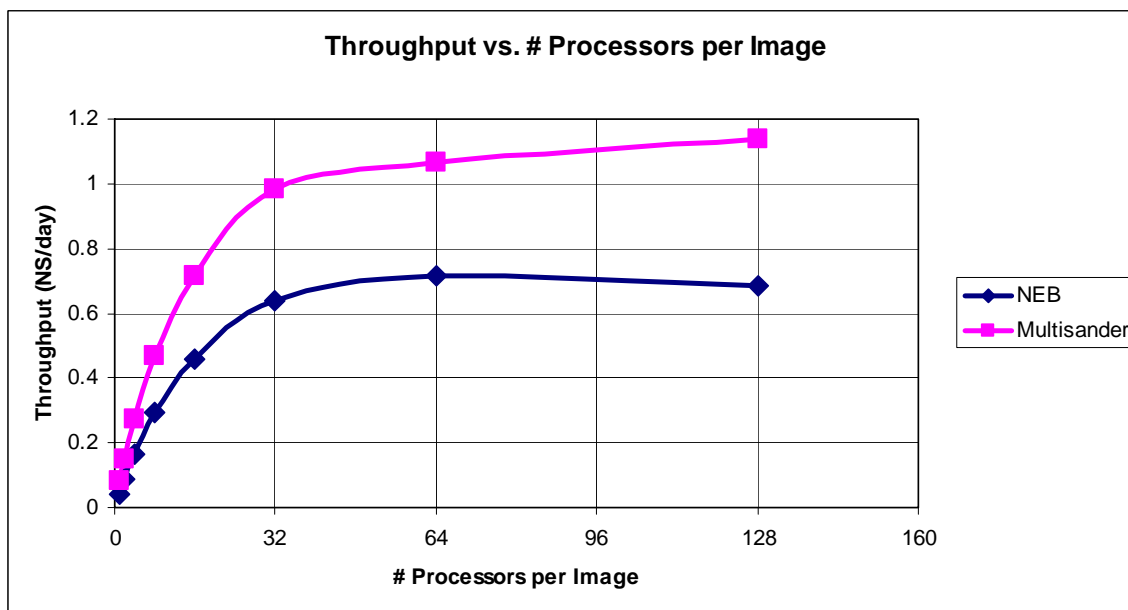


Figure 1S Throughput vs. Processors per image for PNEB vs. Multisander

Table 1S Benchmark Data for NEB vs. Multisander, Amber 11. 60,000 atom system, 1000 steps MD, dt=0.001, 30 images total

NEB	# Processors per image	Time (seconds)	Speedup (vs. 1 proc)	Efficiency (speedup/# proc)	% efficiency	Steps/Sec	NS/sec	NS/day
	1	2137	1.00	1.00	100.00	0.47	4.68E-07	0.04
	2	982	2.18	1.09	108.81	1.02	1.02E-06	0.09
	4	530	4.03	1.01	100.80	1.89	1.89E-06	0.16
	8	295	7.24	0.91	90.55	3.39	3.39E-06	0.29
	16	188	11.37	0.71	71.04	5.32	5.32E-06	0.46
	32	135	15.83	0.49	49.47	7.41	7.41E-06	0.64
	64	121	17.66	0.28	27.60	8.26	8.26E-06	0.71
	128	126	16.96	0.13	13.25	7.94	7.94E-06	0.69

Multisander	# Processors per image	Time (seconds)	Speedup (vs. 1 proc)	Efficiency (speedup/# proc)	% efficiency	Steps/Sec	NS/sec	NS/day
	1	1058	1.00	1.00	100.00	0.95	9.45E-07	0.08
	2	582	1.82	0.91	90.89	1.72	1.72E-06	0.15
	4	316	3.35	0.84	83.70	3.16	3.16E-06	0.27
	8	184	5.75	0.72	71.88	5.43	5.43E-06	0.47
	16	121	8.74	0.55	54.65	8.26	8.26E-06	0.71
	32	88	12.02	0.38	37.57	11.36	1.14E-05	0.98
	64	81	13.06	0.20	20.41	12.35	1.23E-05	1.07
	128	76	13.92	0.11	10.88	13.16	1.32E-05	1.14

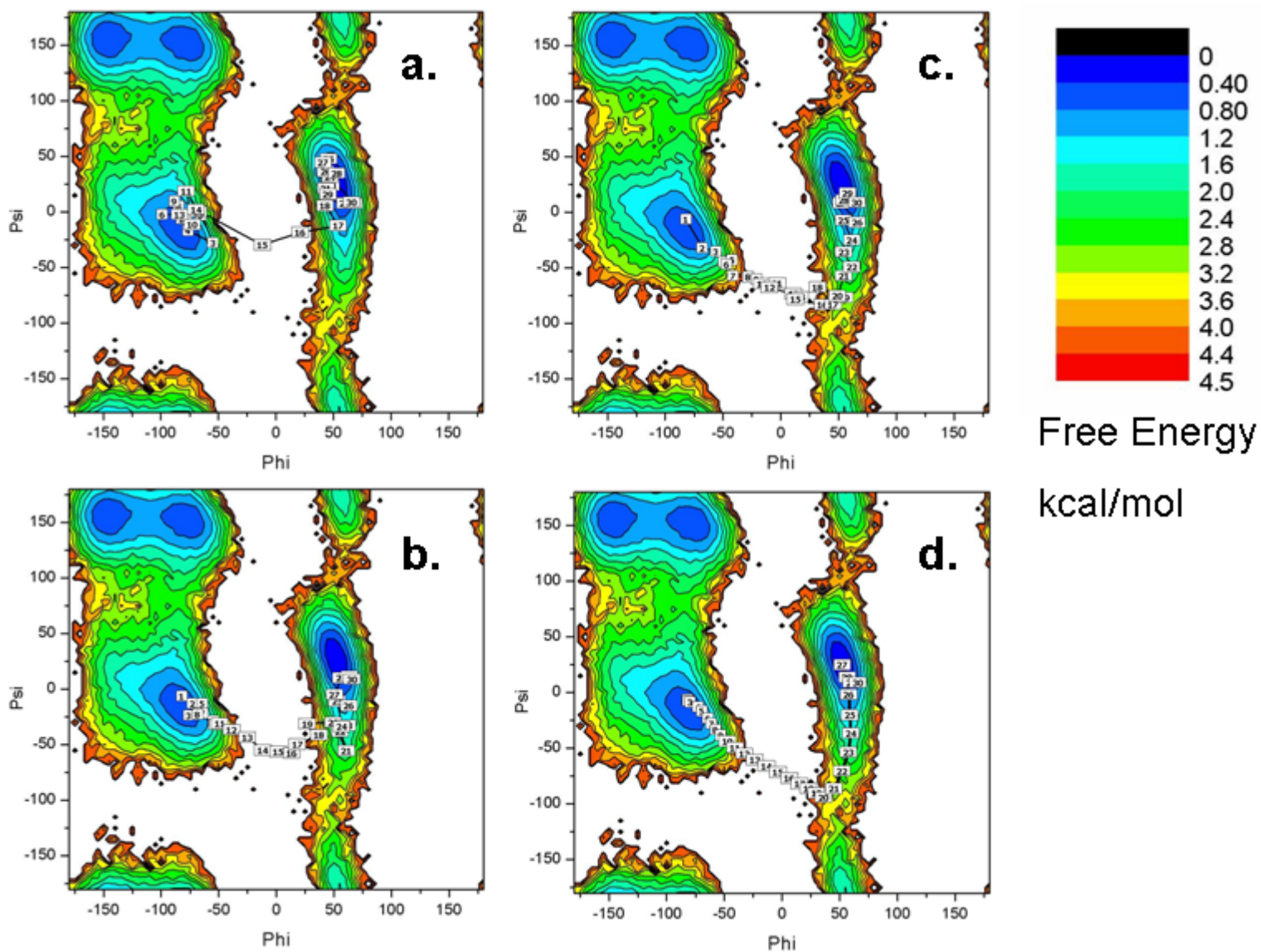


Figure 2S Structure distribution along path at different levels of optimization in PNEB simulated annealing protocol. a) Initial interpolating path between left handed helix and right handed helix minima, b) After equilibration of initial path, c) Images after simulated annealing step, d) Images in final path distribution.

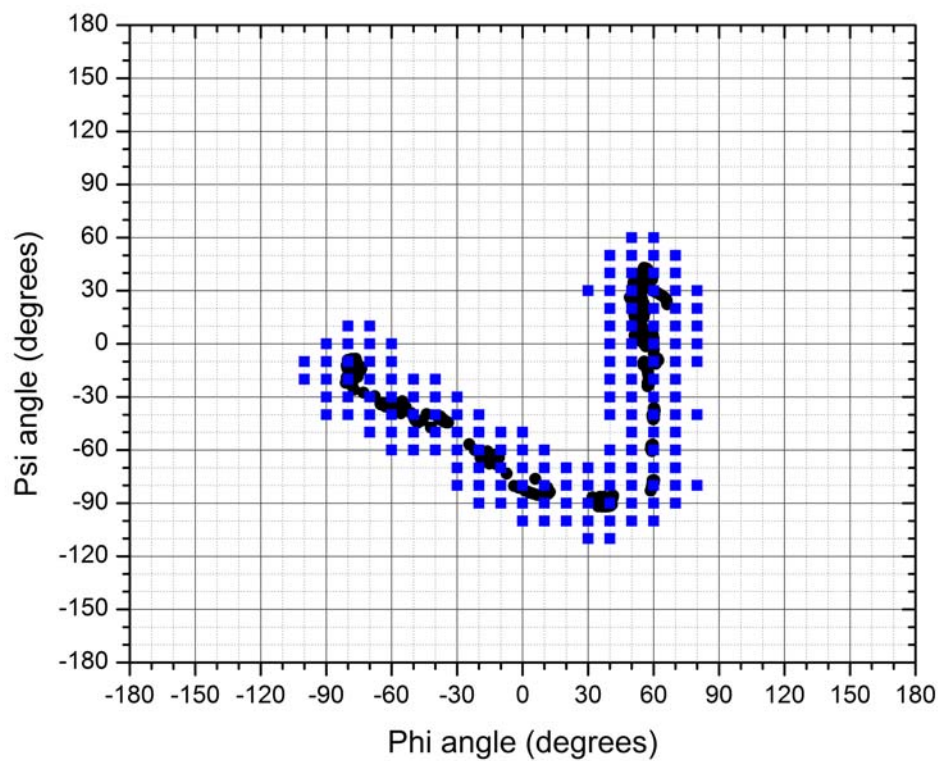


Figure 3S Initial distribution (shown in blue squares) of umbrella sampling starting structures from PNEB path (shown in black dots).

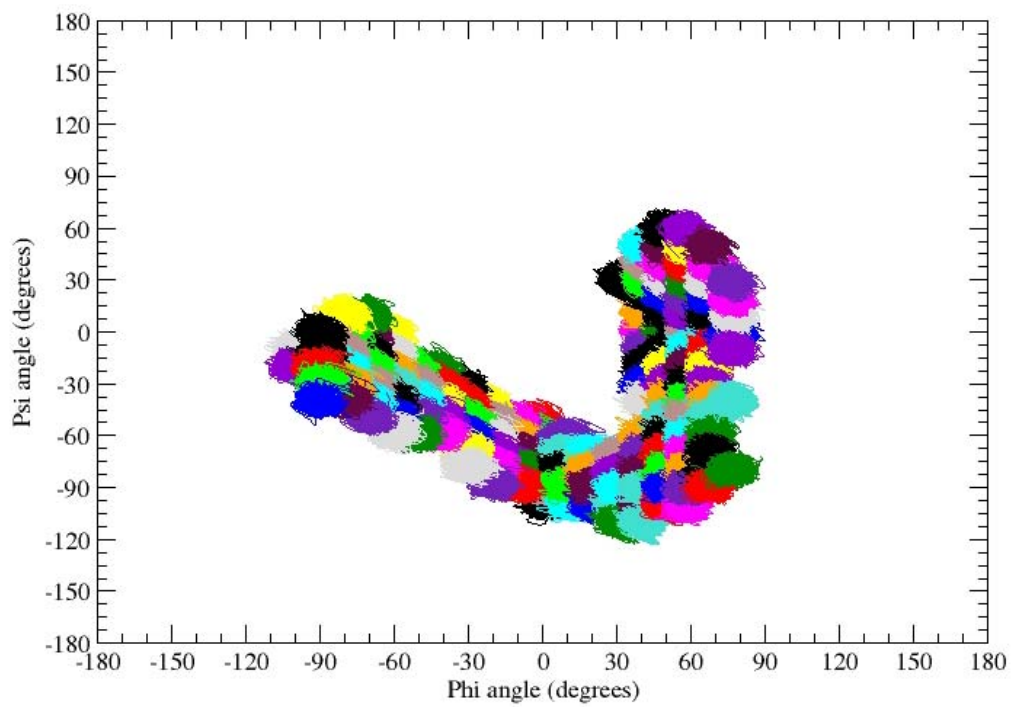


Figure 4S Population distribution of each umbrella sampling window run for 2D WHAM analysis.