

	RMSD (Å)				
	(Snapshot time /Total simulation time)				
Simulated System MD Run	Akt2/GSK3-pept · ATP/MG	Akt2/LBR-S78 · ATP/MG	Akt2/LBR-S80 · ATP/MG	Akt2/LBR-S82 · ATP/MG	Akt2/LBR-S84 · ATP/MG
MD1	1.35 (42.53 /50ns)	1.28 (43.86 /50ns)	1.27 (42.49 /50ns)	1.29 (43.66 /50ns)	1.89 (45.70 /50ns)
MD2	1.25 (46.78 ns)	1.53 (45.39 ns)	1.67 (47.43 ns)	1.69 (46.01 ns)	1.77 (45.09 ns)
MD3	1.61 (47.72 ns)	1.37 (49.43 ns)	1.33 (41.99 ns)	1.37 (47.42 ns)	1.44 (48.46 ns)
MD4					1.51 (45.76 ns)