	MD	REPLICAS	TIME (ns)	ANALYSIS
APO	Loop-IN (PDB ID: 1sgz)	100	(100) X 100	**Principal Component Analysis** 1st: 23%, 2nd: 13%, 3d: 8% **Clustering** Loop-IN: 13 clusters, with pocket sizes from 40 to 125 Å^{3} Loop-OUT: 50 clusters; pocket sizes from 490 to 1,250 Å^{3} **Druggability** Cluster 13 (population of 1.5%): 0,35 (catalytic site), 0.17 (secondary site) Cluster 21 (population of 1.0%): 0.70
	Loop-OUT (PDB ID: 2p4j)	100	(100) X 100	
HOLO	(+)-1 [conformer A]	3	(3) X 50	**Binding mode** Catalytic site: Asp32, Asp228 Leu30, Tyr71, Phe108, Trp115, and Ile118, Tyr198, Ile226 Secondary site: Arg307-Glu339 Lys 9, Ser10,Glu310 Phe159, Leu161, Leu 167, Pro308, Val309
	(−)-1 [conformer A]	3	(3) X 50	
	3 [conformer A]	3	(3) X 50	
	(+)-1 [conformer B]	3	(3) X 50	
	(−)-1 [conformer B]	3	(3) X 50	
	3 [conformer B]	3	(3) X 50	