S4 Table. P-value statistics testing the hypothesis that simulation metrics have the same distribution as the unmodified control simulations started from the same ZAP-70 crystal structure. Using the medians of each simulation as the data.

Data are medians of each simulation	K377-ubiq	K476-ubiq	K377-acet	K476-acet	K377-Ig domain
Active state F349 Cα - D379 Cβ distance	3.787×10^{-8}	0.1616	0.8992		0.1460
Inactive state F349 Cα - D379 Cβ distance	0.4192	9.967×10^{-13}		5.277×10^{-4}	
Active state helicity	4.394×10^{-6}*	0.09151*	0.04873*		0.1703*
Inactive state helicity	0.3879*	0.09907*		0.8886*	
Active state N348 Cα - W501 Cα distance	5.479×10^{-3}	0.6647	0.5616		0.3327
Inactive state N348 Cα - W501 Cα distance	3.141×10^{-11}	1.902×10^{-5}		0.8614*	

*indicates p-values that could not be computed exactly with the Wilcoxon test in R because there were duplicate values.