

S3 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 means of each simulation as the data.

Data are means of each simulation	K377-ubiq	K476-ubiq	K377-acet	K476-acet	K377-Ig domain
Active state F349 Cα - D379 Cβ distance	1.422x10 ⁻¹⁰	0.1060	0.6744		0.1031
Inactive state F349 Cα - D379 Cβ distance	0.3394	3.124x10 ⁻¹⁴		3.026x10 ⁻⁴	
Active state helicity	2.219x10 ⁻⁶	0.03266	5.277x10 ⁻⁴		0.04564
Inactive state helicity	0.3463	0.1031		0.9098	
Active state N348 Cα - W501 Cα distance	7.084x10 ⁻³	0.7338	0.5798		0.3673
Inactive state N348 Cα - W501 Cα distance	6.334x10 ⁻¹¹	1.081x10 ⁻⁵		0.7138	