A

trajectory termination distance threshold (250 Å)

B

ZAP-70 + LAT Tyr 127
ZAP-70 + LAT Tyr 226
ZAP-70 + LAT Tyr 171
ZAP-70 + LAT Tyr 110
ZAP-70 + LAT Tyr 191
Lck + LAT Tyr 127

C

N-lobe quadrant distal to active site
N-lobe quadrant proximal to active site
C-lobe quadrant distal to active site
C-lobe quadrant proximal to active site
activation loop
G helix

percent occupancy within 70 Å of kinase

kinase substrate net charge
domain tyrosine charge

ZAP-70 Tyr 127 -6
ZAP-70 Tyr 226 -6
ZAP-70 Tyr 171 -4
ZAP-70 Tyr 110 -3
ZAP-70 Tyr 191 -2
Lck Tyr 127 -6