

**S1 Table.** Details of simulation solvent box for ZAP-70 constructs.

<b>Construct</b>	<b># of water molecules in box</b>	<b>Box dimensions (Å)</b>		
Active-state control	12,588	72	78	75
Active-state K377-ubiquitinated	35,867	102	104	108
Active-state K476-ubiquitinated	15,996	88	82	76
Active-state K377-acetylated	12,581	73	79	77
Active-state K377-Ig domain	75,547	130	134	136
Inactive-state control	13,029	75	77	75
Inactive-state K377-ubiquitinated	38,834	106	109	107
Inactive-state K476-ubiquitinated	15,691	87	82	76
Inactive-state K476-acetylated	13,027	77	79	77