

**Supplementary Data 1.**

PDB file of best model of the IKK $\beta$ /I $\kappa$ B $\alpha$  pep complex.

**Supplementary Data 2.**

Matches for the YDD $\Phi$ x $\Phi$  motif. Results from SLIMSearch<sup>35</sup> using the motif consensus (YDD[MILVCF].[MILVCF]).

**Supplementary Data 3.** List of reagents.

**Supplementary Data 4.**

HADDOCK parameter file for docking calculations.

**Supplementary Data 5.**

Unambiguous distance restraints used for the docking calculations. During the calculations, residues of protomer B of the IKK $\beta$  dimer were renumbered from 1008-1664.