SUPPLEMENTS

Supplement 1: Data and refinement statistics for X-ray crystal structure determination.

Values for the determination of the X-ray crystal structure of human hepsin with the KQLR-chloromethyletone (KQLR-cmk) peptide inhibitor.

Data (Hepsin / KQLR-cmk Complex)	
Space group	P2$_1$
Unit cell	a = 55.7 Å, b = 47.6 Å, c = 67.8 Å, β = 108.2°
Resolution range (Å) (outer shell)	24-1.55 (1.61-1.55)
Number of observations	163831
Number of unique reflections	46843
Completeness (%) (outer shell)	95.0 (59.2)
R$_{sym}$ (%) (outer shell)	5.6 (32.7)
I/σI (outer shell)	21.6 (2.1)

Model (Hepsin / KQLR-cmk Complex)	
Molecules in the asymmetric unit	1
R$_{cryst}$/R$_{free}$ (all data)	0.198/0.217
RMS deviations from ideal geometry	
Bonds (Å)	0.004
Angles (°)	1.343

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