Supplementary Table S1. CDK9/cyclin T - (S)-CR8 co-crystal structure. Statistics of the dataset used and of the refined structures.

Data collection	**CDK9/cyclin T1/ (S)-CR-8**
Beam line	Diamond I-02
Space group & unit cell (Å)	H3 a=b=173.25 ; c=99.24 α=β=90°; γ=120°
Resolution (highest resolution shell) (Å)	50.01-3.00 (3.14-3.00)
Total observations	76157 (11267)
Unique	21867 (3222)
R_{merge}	0.074 (0.542)
Multiplicity	3.5 (3.5)
Mean I/ σ(I)	9.7 (2.1)
Completeness	98.4% (99.3%)
Refinement Statistics (highest resolution shell) (Å)	 (3.14-3.00)
Total number of atoms	4589
Number of waters	9
R	16.23 (26.99)
R_{free} (highest resolution shell)	21.47 (33.57)
Rms bonds	0.009
Rms angles	1.153
Coordinates, pdb file #	3LQ5