

Figure 1S. C-alpha rmsd matrix (right panel) and structural cluster analysis (left panel) from Cdc34 MD ensemble. The RMSD values are ordered on a color scale which ranges from blue (values close to 0) to red (high values). In the right panel the red boxes indicates structures belonging to different clusters or that revisited the same cluster in the ensemble.

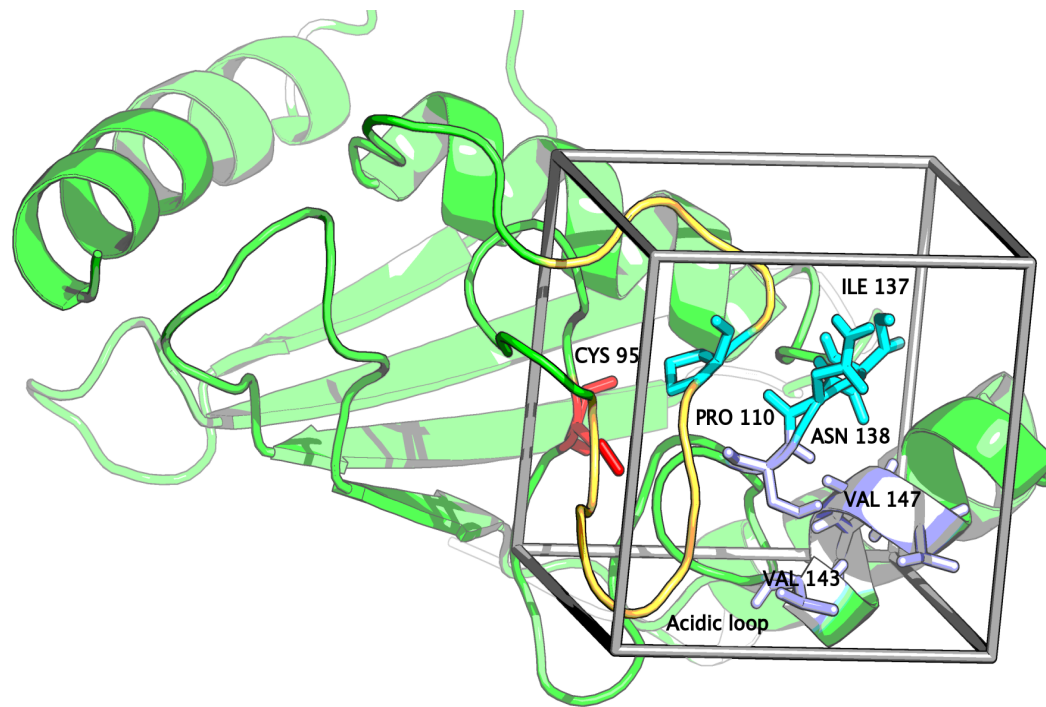


Figure 2S. The grid describing the Autodock search space was drawn using the Autodock tools (MGL-tools).

Sc_Cdc34MSSRKSTASSLLLRQYRELTPDKKAIPSFHIELEDDSNIFTWNIGVMVLNEDSIYH	60
Hs_Cdc34	. . .MARPLVPSSQKALLLELKLQEE.PVEG.FRVTLVDEGDLYNWEVAIFGP.PNTYYE	
Sc_Cdc34	GG.FFKAQMRFPEDFPFSPQFRFTPAIYHPNVYRDGRLCISILHQSG.DPMTDEPDAET	120
Hs_Cdc34	GG.YFKARLKFPIDYPYSPPAFRFLTKMWHPNYETGDVCISILHPPVDDPQSGELPSER	
Sc_Cdc34	WSPVQTVESVLISIVSLLLEDPNINSPANVDAADVDRK.NPEQYKQRVKMEEVERS	180
Hs_Cdc34	WNPTQNVRTILLSVISLLNEPNTFSPANVDASVMYRKWKESKGGKDR.EYTDIIRKQVLGT	
Sc_Cdc34	KQD	183
Hs_Cdc34	KVD	

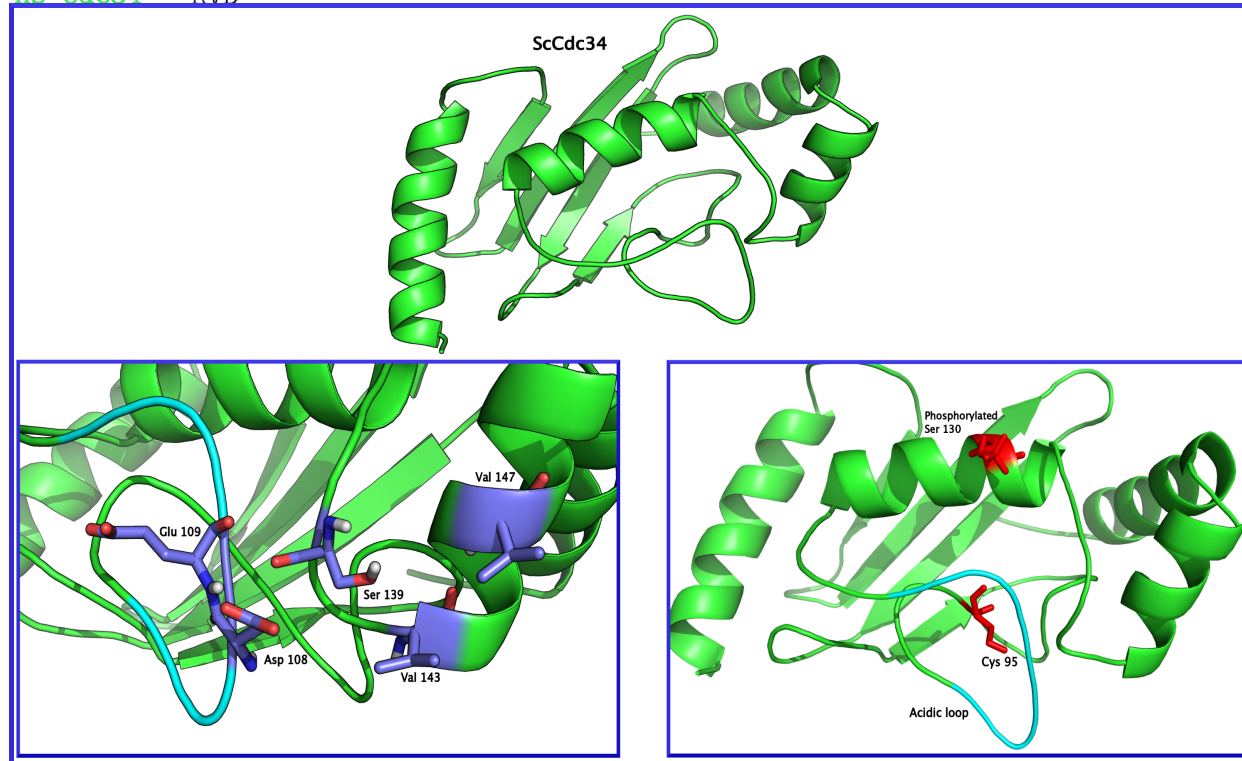


Figure 3S. Sequence conservation between ScCdc34 and HsCdc34: conserved residues implicated in inhibitors binding are coloured in violet, the catalytic cysteine and serine 139 are reported in red.