

Figure SM1A

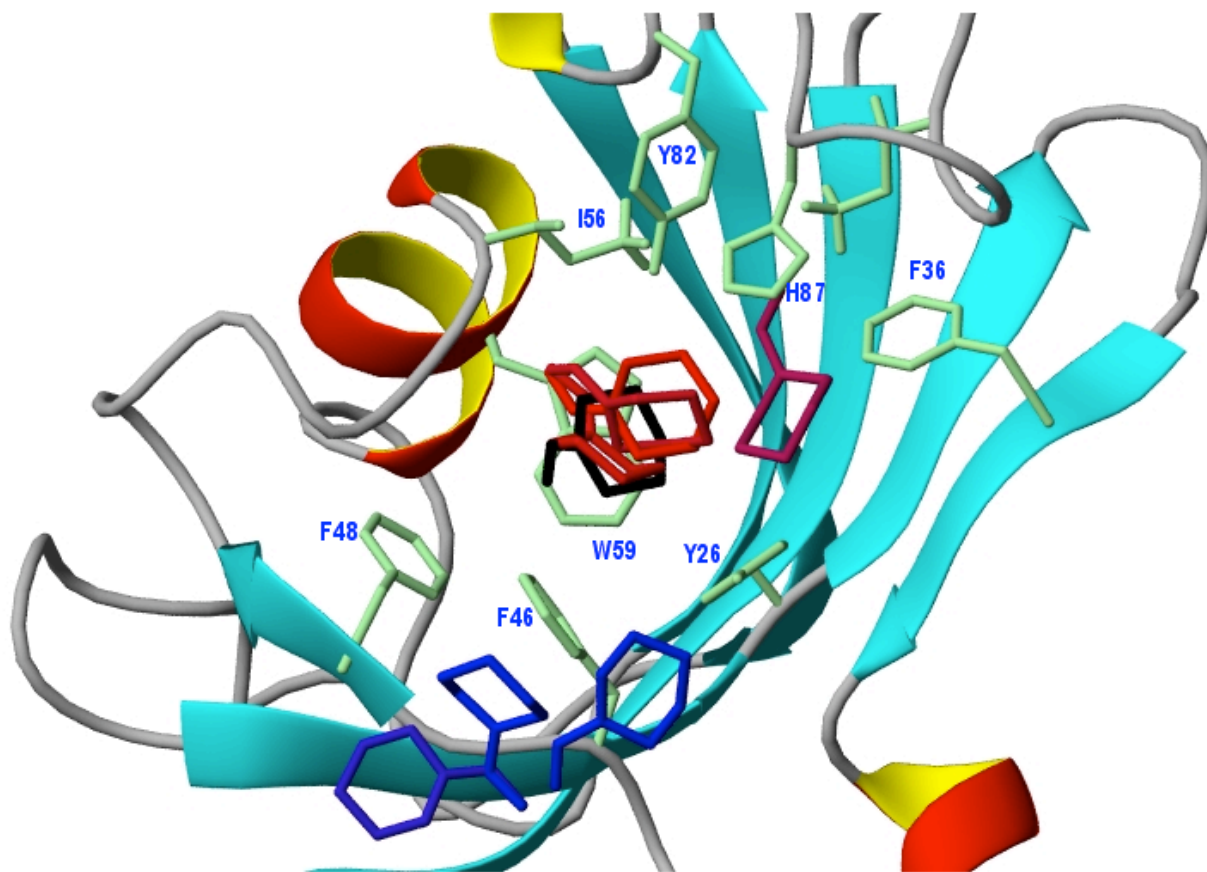


Figure SM1B

Figure Supplementary Material 1: Distribution of formyl piperidine minima in the binding pocket of FKBP12. The minima are grouped in clusters based on their van der Waals interactions with the protein (cf. Method section). Each cluster is represented by its minimum with the most favorable binding to the protein. The NMR position with the smallest NOE violations is shown in black for comparison. A) The minima are colored from red (tight binding) to blue (weak binding) using the ranking based on the force field interaction energy plus ligand deformation. B) The minima are colored from red (tight binding) to blue (weak binding) using the ranking based on Eq. 1.