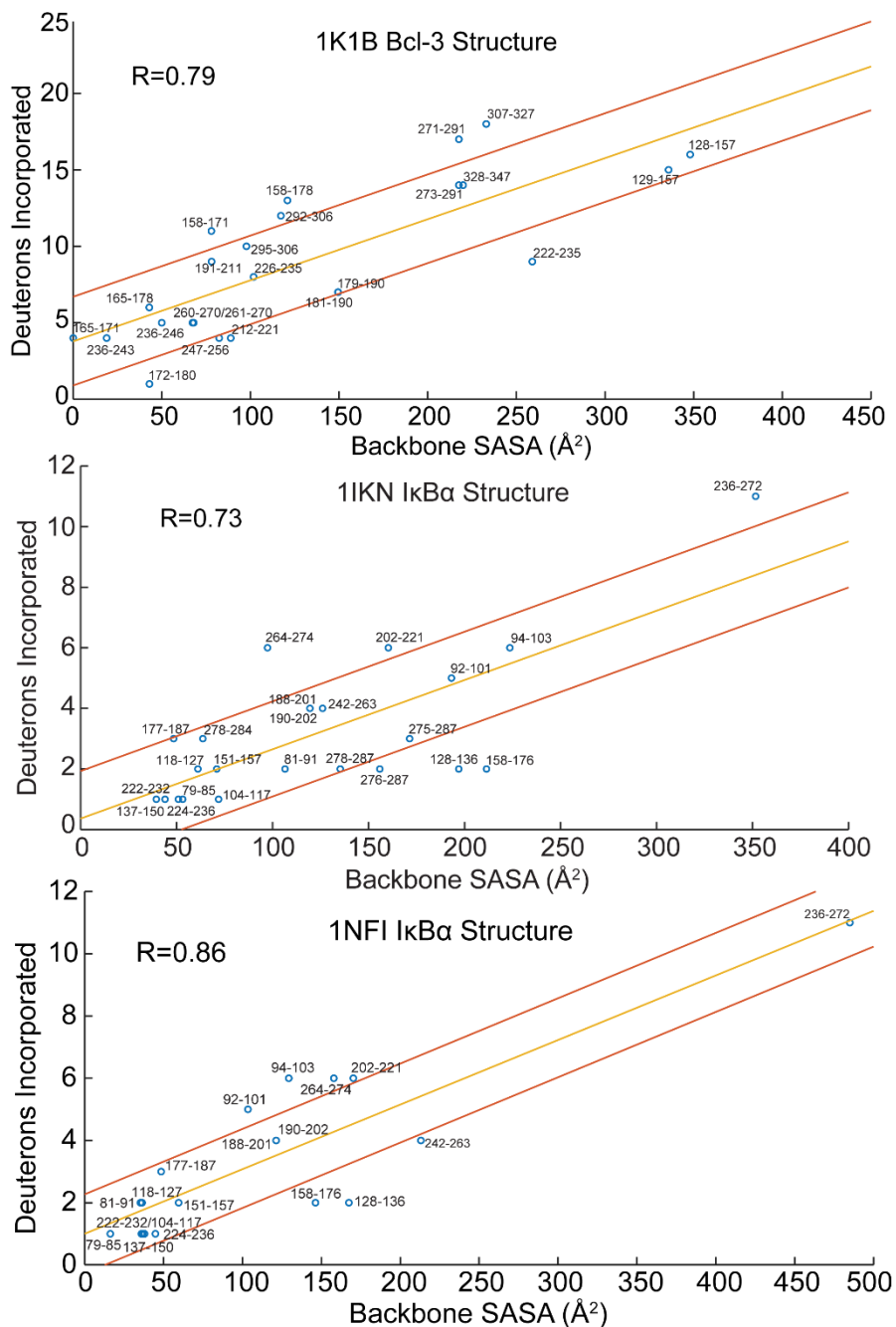


Supplementary Information for Ramsey et al



Supplementary Figure 1. Backbone solvent accessible surface area (SASA) correlates strongly with deuterium uptake from HDXMS. The GetArea server was used to calculate the backbone SASA for each residue in the crystal structures of Bcl-3 (PDB 1K1B) and IκBα (PDB codes 1NFI, 11KN). HDXMS was performed on each of these proteins and the deuterium uptake for each peptide was plotted (y axis) as a function of backbone SASA (x axis). The upper panel shows the

correlation for Bcl-3, for which the correlation coefficient (R) was 0.79. The middle panel shows the correlation for I κ B α (PDB 1IKN), for which the correlation coefficient (R) was 0.73. The lower plot shows the correlation for I κ B α (PDB 1NFI), for which the correlation coefficient (R) was 0.86. The plots show the correlation line from regression analysis in yellow with lines above and below in red indicating the region within one standard deviation of the regression line. The majority of HDXMS peptides fall within one standard deviation of the correlation line. These data were used to ascertain the goodness of fit for the correlation plots of the homology models.