



S7_Fig. Distribution of dihedral angles for two cases. In the folded case (filled areas) all angles populate a single state. In an unfolded case (framed areas) especially the ϕ -angle of GLY shows a broad variation. The ψ -angle of GLY is slightly shifted. The ϕ -angle of PRO does not change due to its ring structure, whereas the ψ -angle shows a second state around 330° .