



Figure S6. Exposed surface area of the A3G C-CDA. Comparison of the exposed surface area of starting structures with the representative structures from the clustering analysis of MD simulations. Residues indicated in purple have a SASA value greater than 90 Å² and those indicated in green have a SASA value lower than 40 Å². SASA values were calculated with the POPS program. (A) NMR1-2K3A; (B) NMR2; (C) NMR3-2K3A; (D) XRAY1 and (E) XRAY2-2K3A.