

Supporting information

Identifying the key residues instrumental in imparting stability to amyloid beta protofibrils – a comparative study using MD simulations of 17-42 residues

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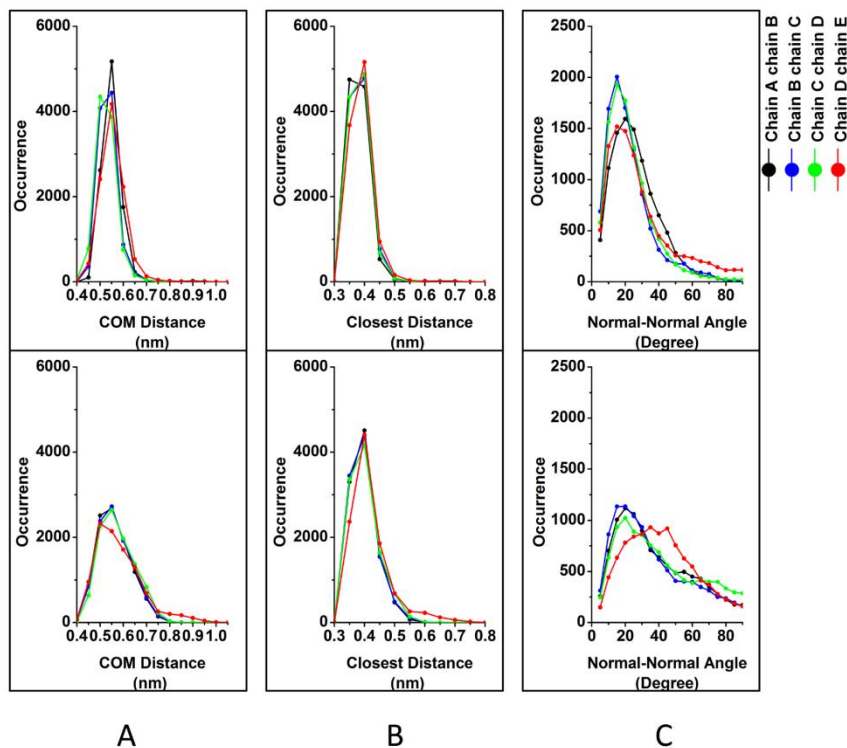


Figure S1. For WT Aβ protofibril (A) occurrence versus COM distance between two phenyl rings of F19 of two consecutive chains (upper panel) and F20 of two consecutive chains (lower panel). (B) Occurrence versus closest distance between two phenyl rings of F19 of two consecutive chains (upper panel) and F20 of two consecutive chains (lower panel). (C) Occurrence versus normal-normal angle between two phenyl rings of F19 of two consecutive chains (upper panel) and F20 of two consecutive chains (lower panel).

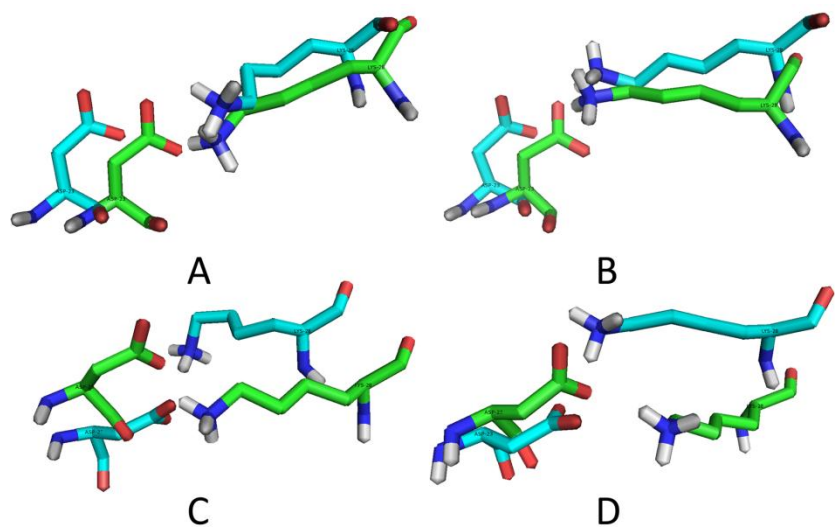


Figure S2. Relative position of the side chain of D23 and K28 upon alignment of final (cyan) and corresponding energy minimized (green) structure. (A) Chain-B of L34G (B) Chain-C of L34G (C) Chain-B of I32G/L34G (D) Chain-C of I32G/L34G.