Supplementary Information

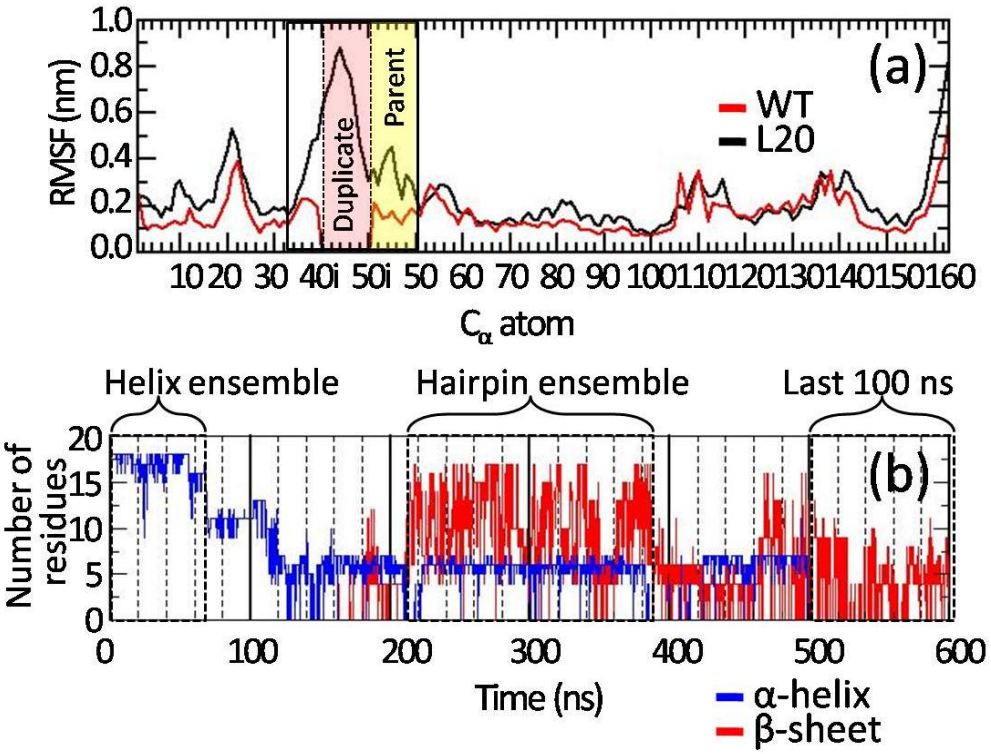

Figure S1 Root mean square fluctuation (RMSF) of the Cα atoms of the L20 and WT protein indicates similar fluctuations in two proteins, except for the segment of residues 33 to 50, indicated by bold lines in (a). This segment was found to be region of maximum fluctuation for L20. Trajectory (600 ns) of L20 protein was distributed into 3 conformational ensembles (b) based on the secondary structural analysis (DSSP) of the segment of residues 33 to 50: *helix* ensemble – here, most of the residues adopted native α-helical conformation (initial 70 ns), *hairpin* ensemble – here, most of the residues adopted β-hairpin conformation (210-380 ns) and in the *last 100ns* the parent region of the full helix in L20 (Figure 1b) uncoils to adopt bend/turn conformation in the last 100 ns.

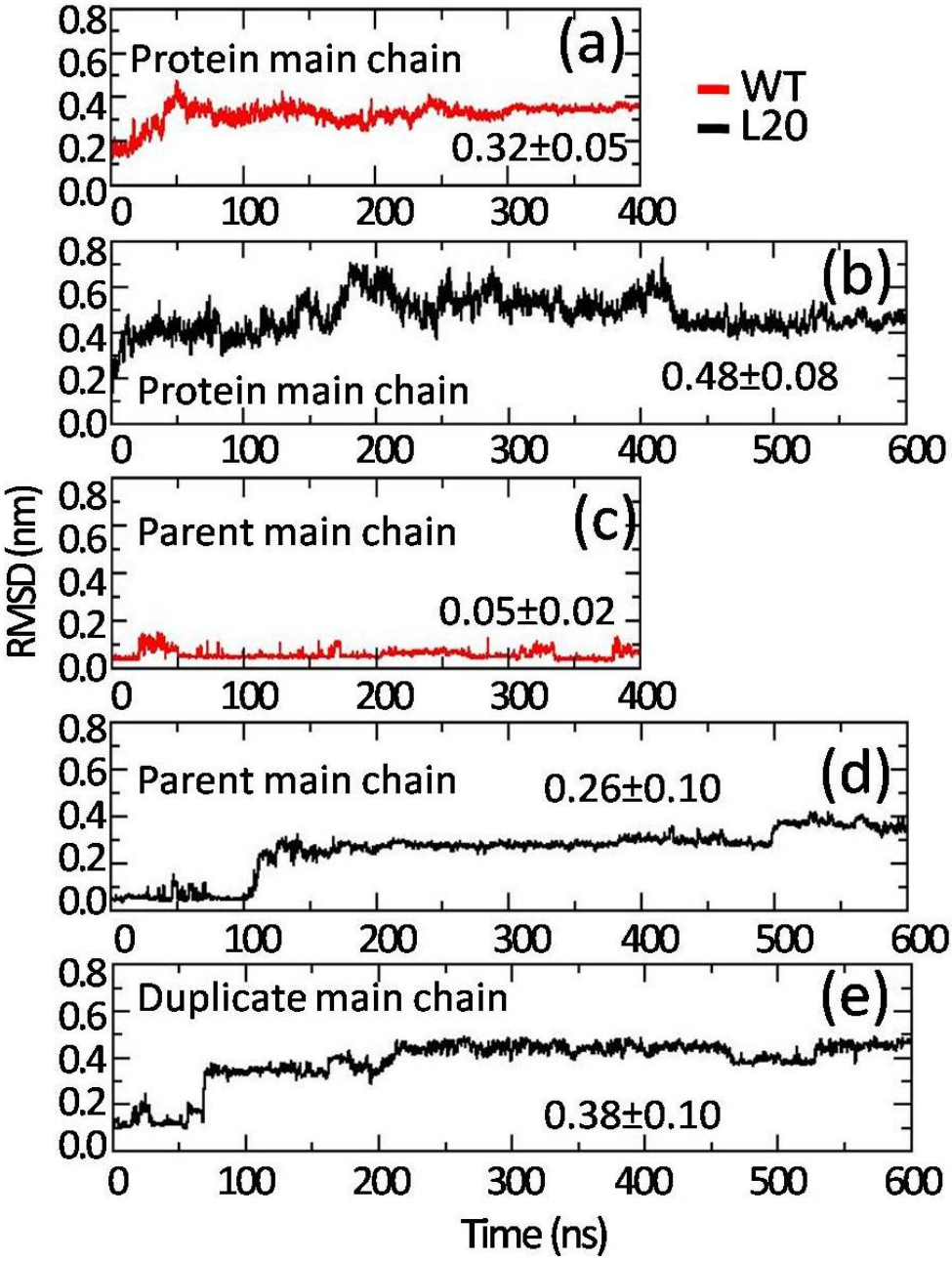

Figure S2 Root mean square deviation of main chain atoms, with respect to respective crystal structure, for complete protein chain (a and b) and parent region (residue 40 to 50, c and d) in WT and L20 protein, respectively and (e) duplicate region in L20 (residue 40i to 50i) displayed greater deviations for L20 in comparison to WT protein. Average RMSD values along with

standard deviation are also shown (in nm). Time is shown in units of nano seconds along all the axes.

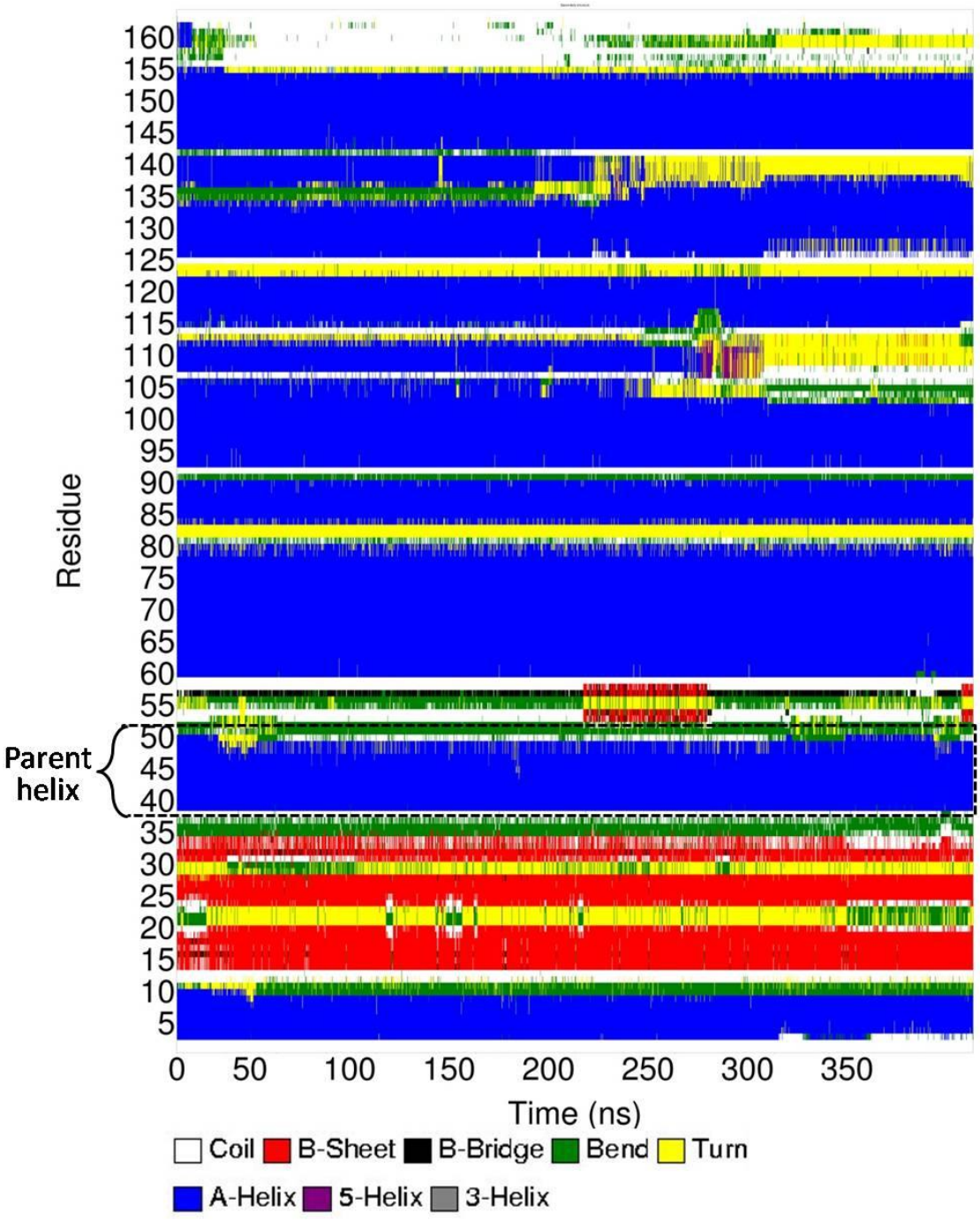

Figure S3 DSSP plots for WT protein.

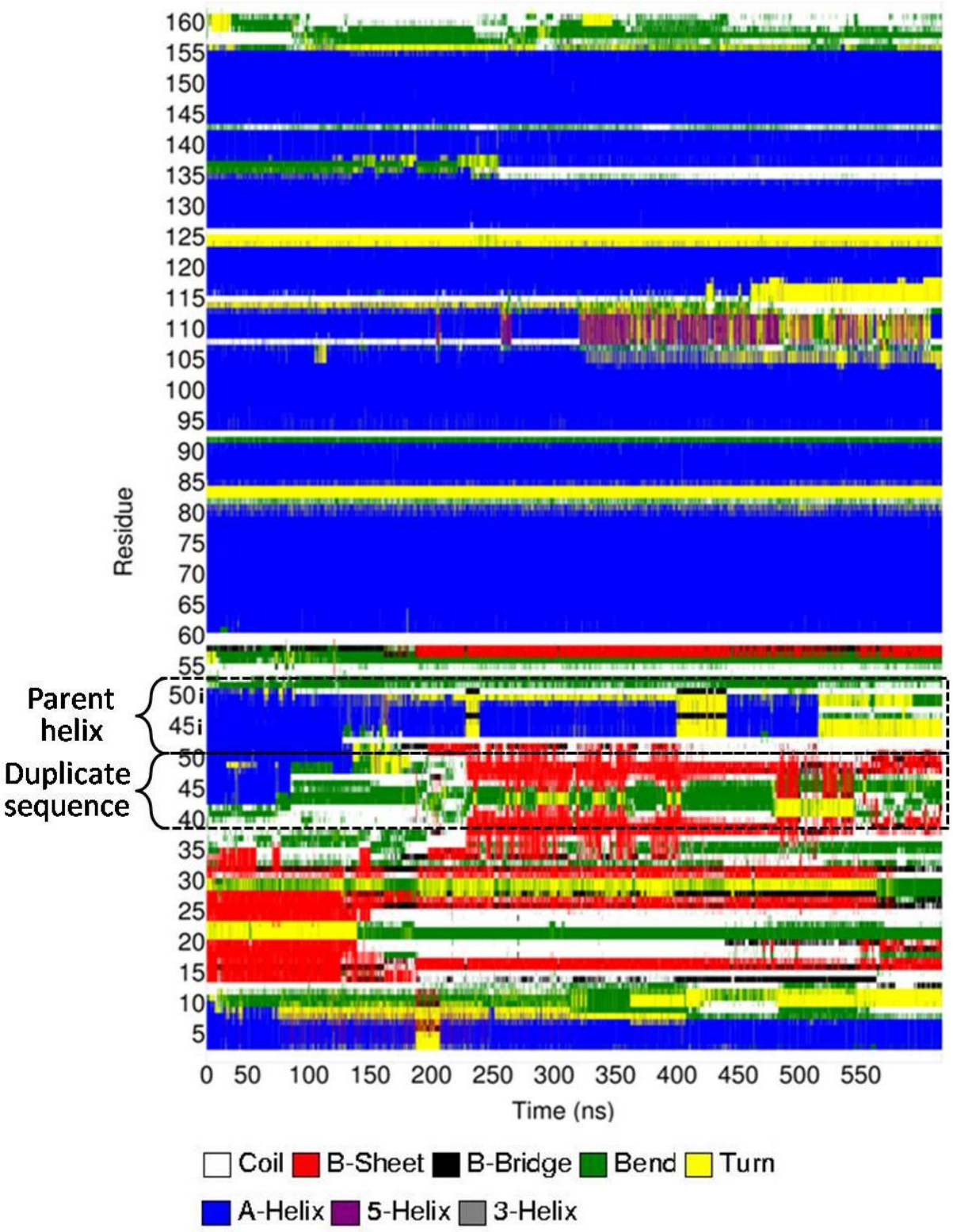

Figure S4 DSSP for L20 protein.

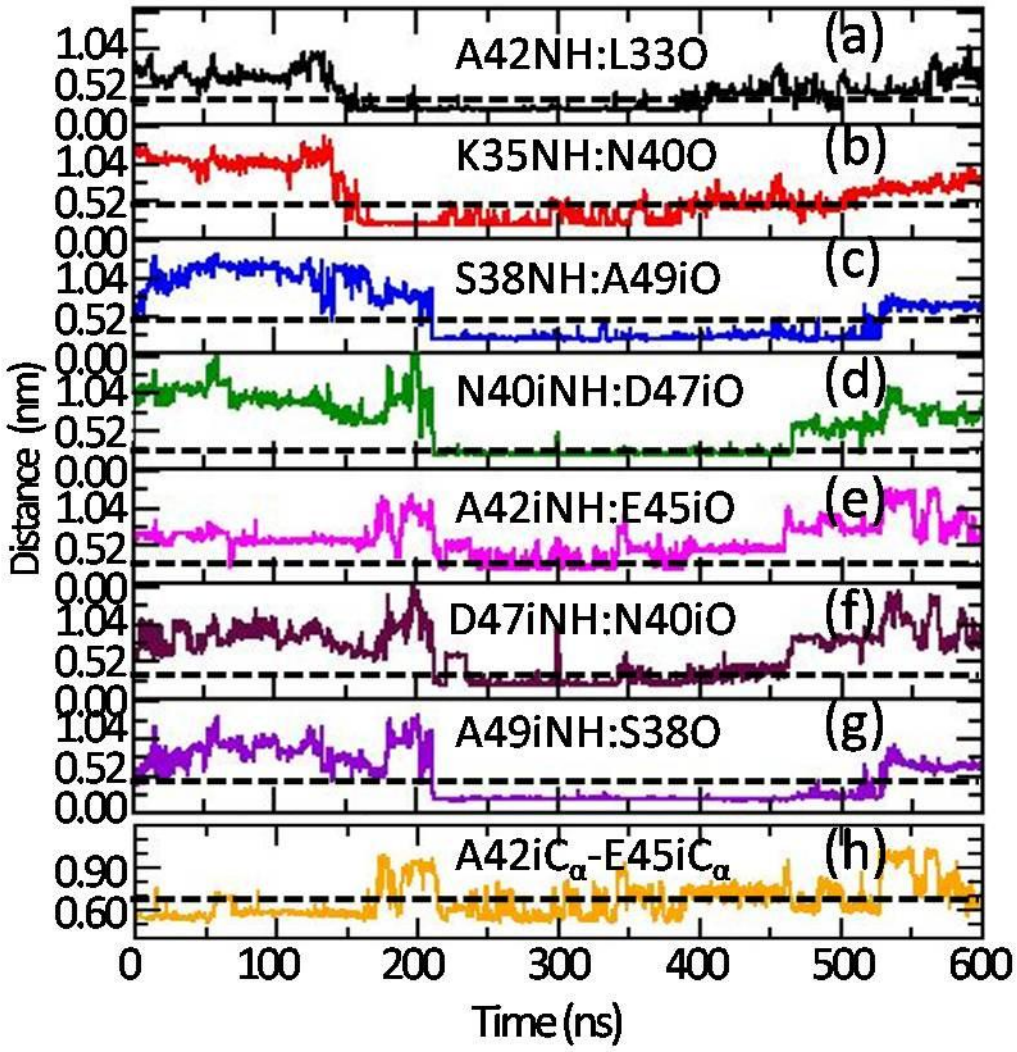

Figure S5 Variation of amide hydrogen and acceptor (carbonyl oxygen) distance for intra-strand backbone hydrogen bonds for β-hairpin forming residues (33 to 42, Figure1c) in L20 (a to g) and distance between C_α atoms of the turn forming residues Ala42i and Glu45i (h). More stable terminal and middle hydrogen bonds (see Figure 4) were observed to be playing a significant role in β-hairpin formation, while the turn hydrogen bonds (Ala42iNH:Glu45iO and Glu45iNH:Ala42iO) displayed relatively lesser stability. Dotted lines indicate ideal hydrogen-acceptor distance (0.26 nm, see Methods section 2.3) for formation of a hydrogen bond.

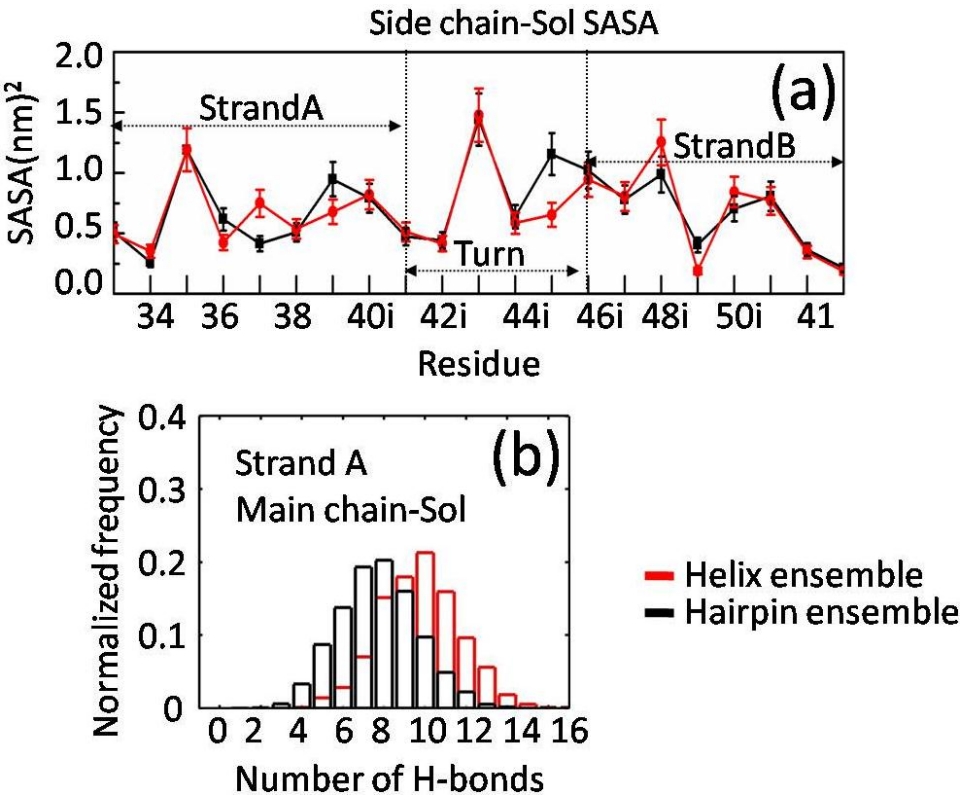

Figure S6 (a) Side chain solvent accessible surface area (SASA), in *helix* and *hairpin* ensembles (Figure S1b), for the residues involved in β-hairpin formation (33 to 42, Figure 1c) showed no significant change in the two ensembles, (b) number of main chain-solvent hydrogen bonds for strand A (33 to 41i, Figure 1c). The standard deviations in observed SASA are shown as error bars in (a).

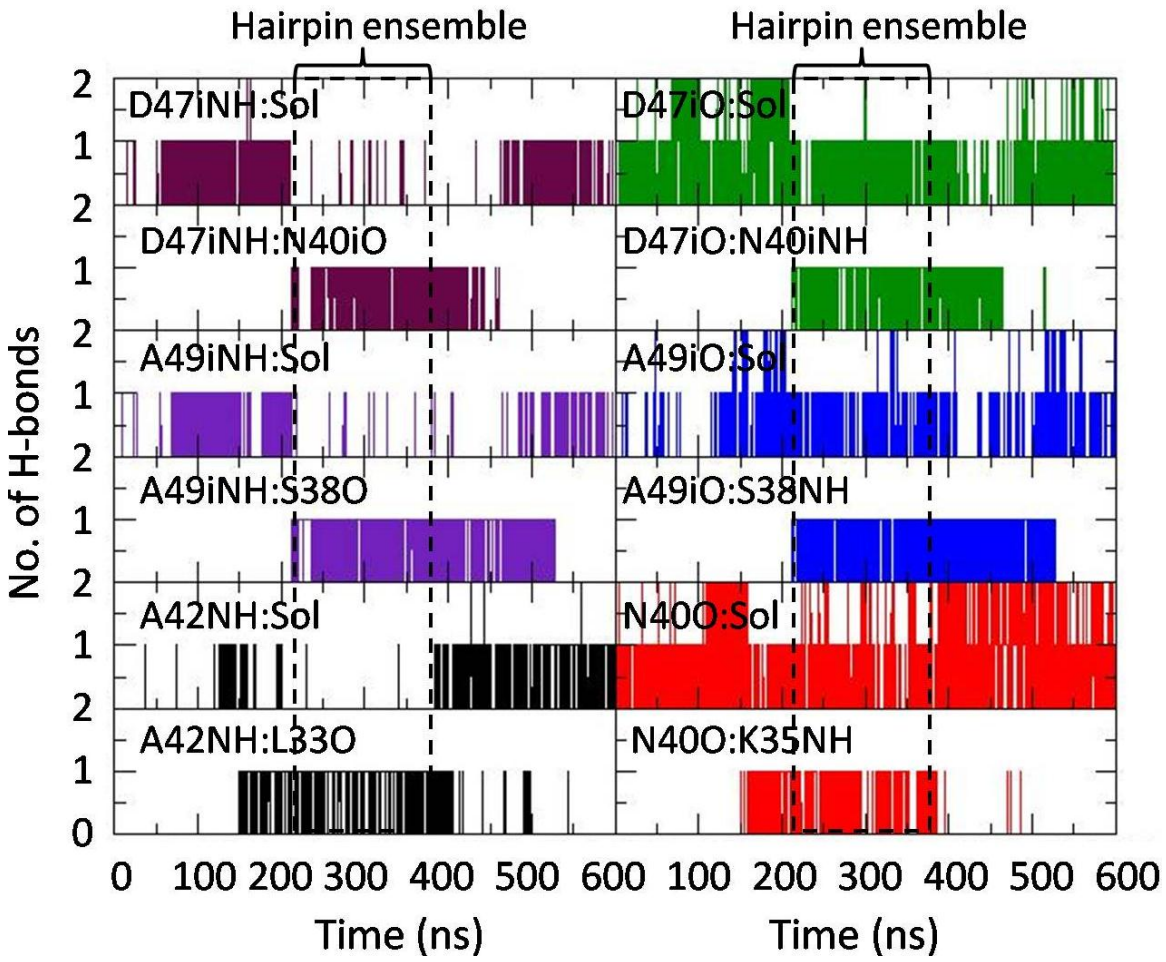

Figure S7 Comparison of inter-strand backbone hydrogen bonds, formed by residues D47i, A49i, N40 and A42, with the main chain-solvent hydrogen bond formed by same residues as a function of time. It can be seen that the amide hydrogen of D47i, A49i and A42 were well protected from solvent in the *hairpin* ensemble (210-380 ns, also see Figure 7b), as no solvent hydrogen bonds were seen. The carbonyl oxygen of D47i, A49i and N40 were found to be involved in both inter-strand and protein-solvent hydrogen bond formation, in the β-hairpin conformation.

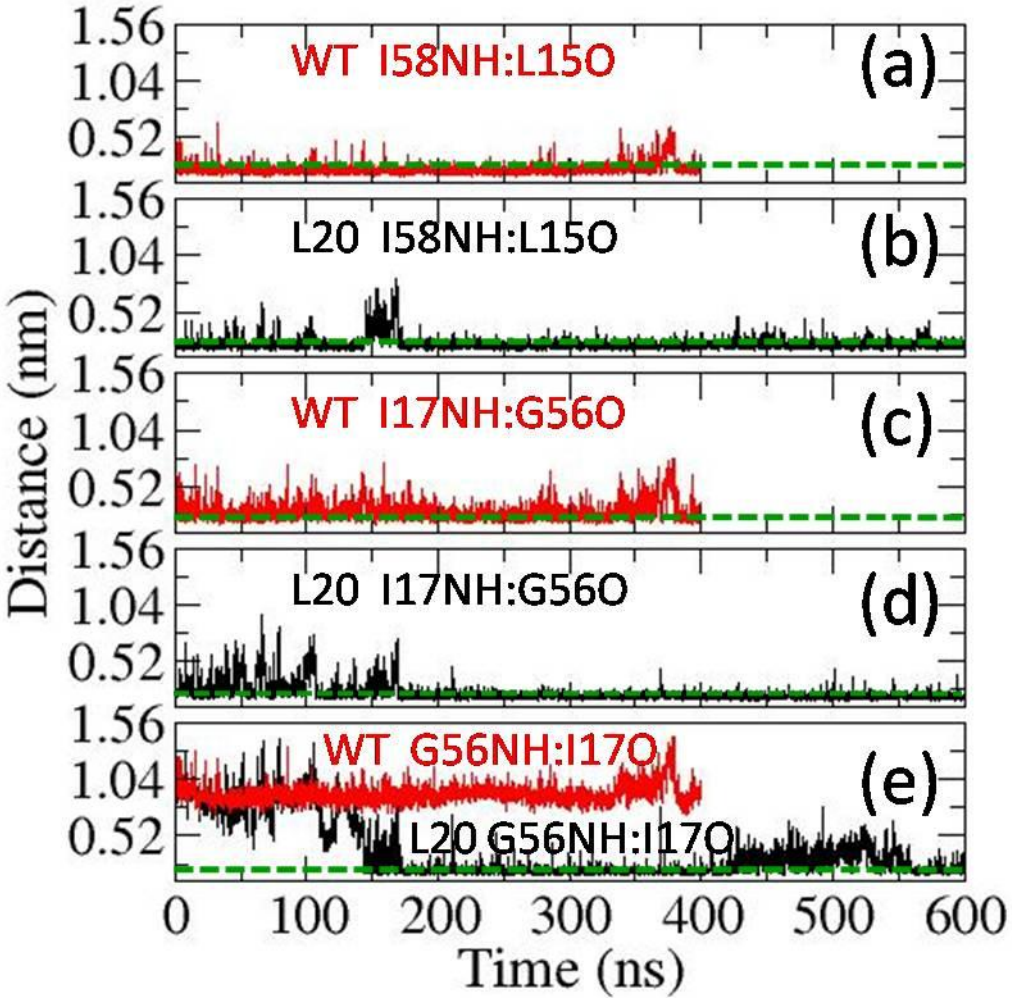

Figure S8 Variation of amide hydrogen and acceptor (carbonyl oxygen) distance for I58NH:L15O (a, b), I17NH:G56O (c, d) and G56NH:I17O hydrogen bonds in WT and L20, respectively. These inter-strand hydrogen bonds were seen to stabilize a β-sheet (formed by strand1 and strand4, Figure 1) in the C-terminal region of the parent helix, in both WT and L20. Formation of G56NH:I17O bond was seen (around ~ 150 ns) only in case of L20 mutant; it was absent in WT.

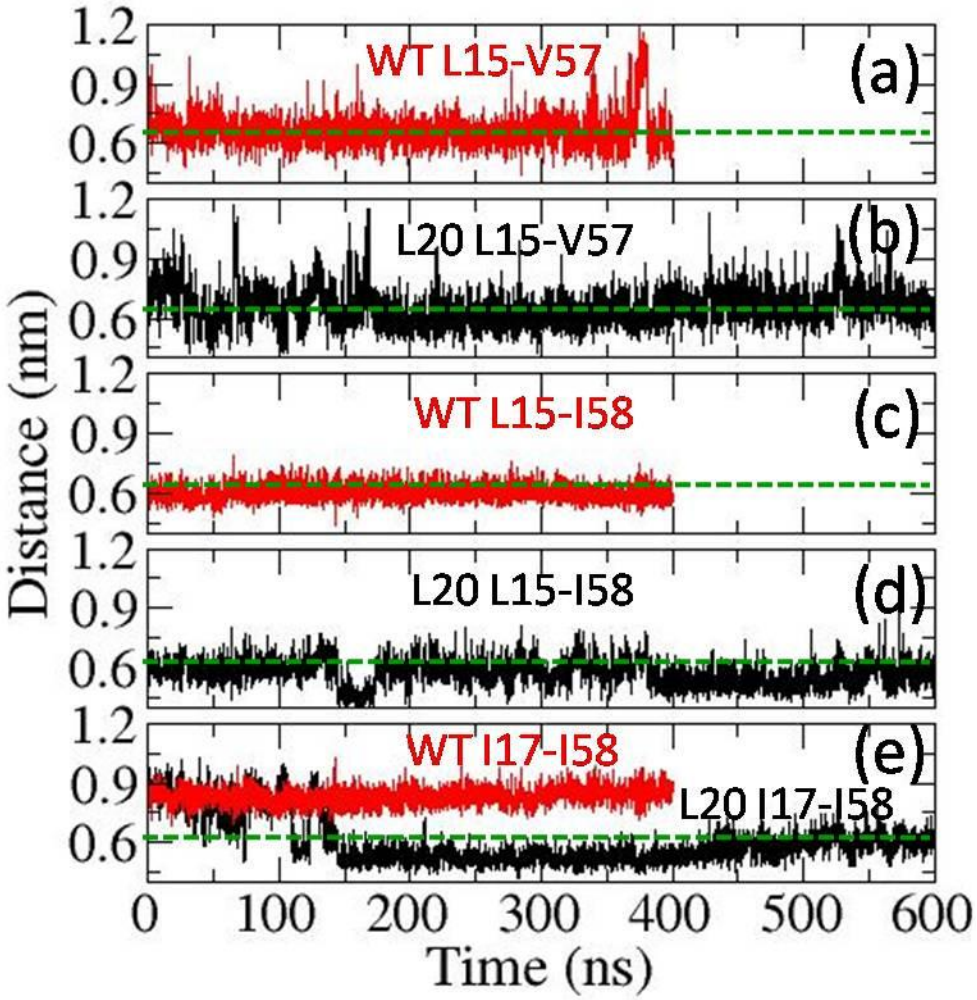

Figure S9 Variation of distance between side chains of pairs of hydrophobic residues for (a) L15-V57 (b) L15-I58 and (c) I17-I58 in WT and L20. These hydrophobic residues were seen to stabilize a β-sheet (formed by strand1 and strand4, Figure 1) in the C-terminal region of the parent helix, in both WT and L20. L15-V57 and L15-I58 pair displayed a value ≤ 0.6 nm (a distance cut-off for side chain packing interaction, see Methods), in both WT and L20, indicating hydrophobic association between inter-strand residues in the β-sheet. Hydrophobic interaction between I17-I58 was seen to appear (around ~ 150 ns) only in case of L20 mutant; it was absent in WT.

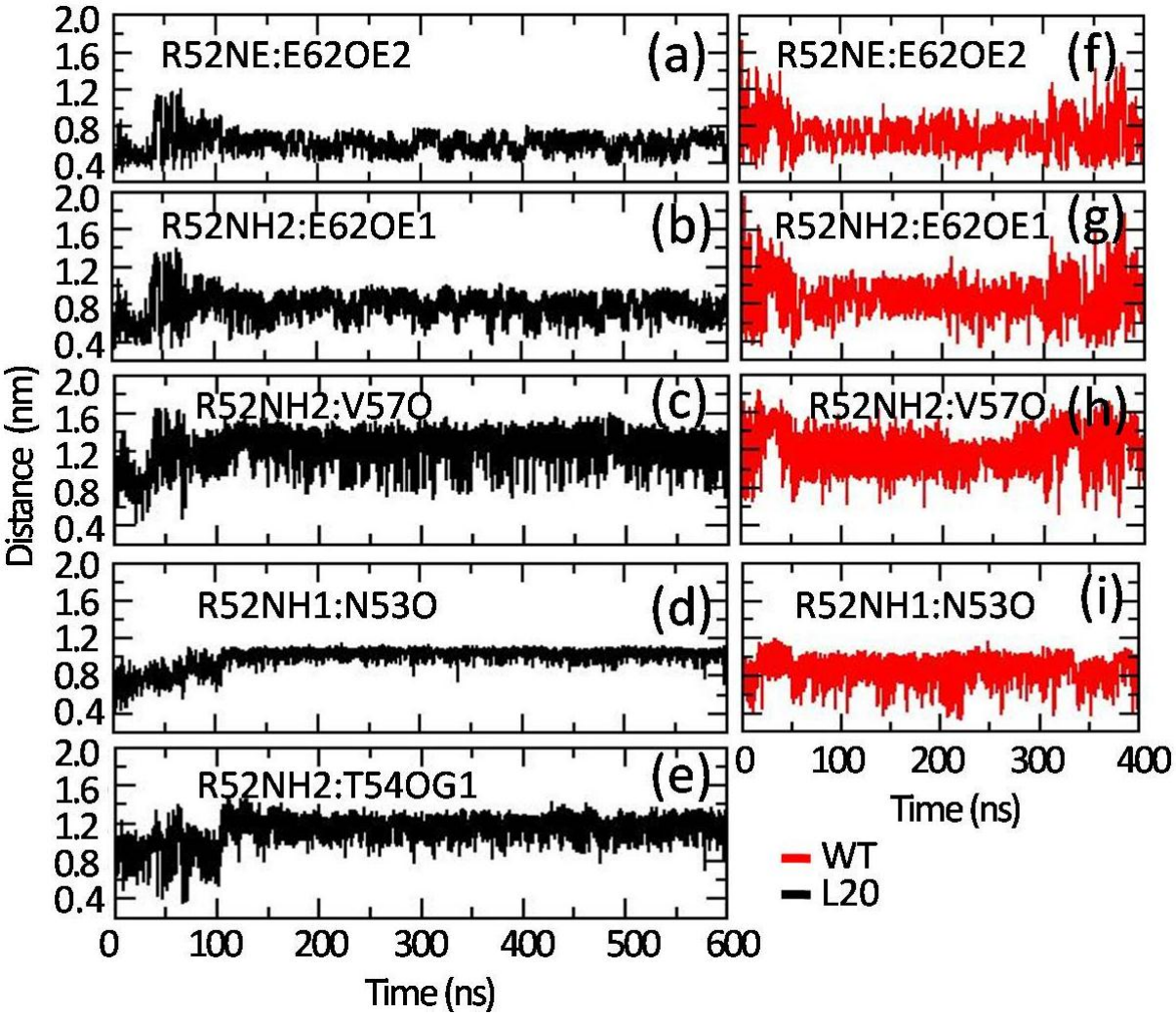

Figure S10 Variation of distance between pair of interacting atoms for Arg52 interactions with the residues present in the C-terminal loop of the parent helix in L20 (a to e) and WT protein (f to i), during respective simulation time. These interactions were found to be absent during both the simulations.