

Computational investigation on the impact of point mutations on the N-terminal domain of SHANK3, indicating distinct synaptopathies in Autism Spectrum Disorder

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Supplementary Data

Table S1 — The interface statistics of the SHANK3 WT protein with α CaMKII protein

Chain	No. of interface residues	Interface area (Å ²)	No. of salt bridges	No. of disulphide bonds	No. of hydrogen bonds	No. of non-bonded contacts
A (WT)	27	1471	4	-	15	203
B (α CaMKII)	30	1450				

Table S2 — The interface statistics of the SHANK3 P141A mutant with α CaMKII protein

Chain	No. of interface residues	Interface area (Å ²)	No. of salt bridges	No. of disulphide bonds	No. of hydrogen bonds	No. of non-bonded contacts
A (P141A)	23	1238	2	-	12	146
B (α CaMKII)	26	1189				

Table S3 — The interface statistics of the SHANK3 L270M mutant with α CaMKII protein

Chain	No. of interface residues	Interface area (Å ²)	No. of salt bridges	No. of disulphide bonds	No. of hydrogen bonds	No. of non-bonded contacts
A (L270M)	15	872	3	-	11	116
B (α CaMKII)	18	850				

Table S4 — Secondary structure content of the SHANK3 WT protein and two mutant forms, SHANK3 L270M and SHANK3 P141A, showing the secondary contents of α -helix, β -sheets, Turns, 3_{10} -helix, Coils, and Pi

Complex	α -helix %	β -sheet %	Turn %	Pi-helix %	3_{10} helix %	Coil %
SHANK3WT	40.8	6.9	17.3	0	0	35
SHANK3L270M	43.4	7.8	19.4	0	0	29.5
SHANK3P141A	43.1	10	16.8	0	0	30.1

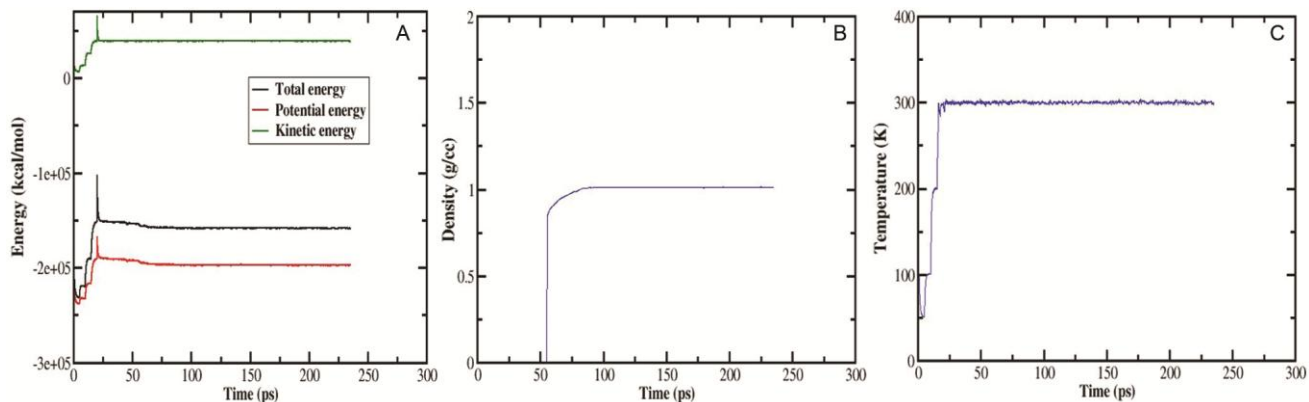


Fig. S1 — The visualization of SHANK3 WT of (A) Energy; (B) Density; and (C) Temperature to ensure correct equilibration

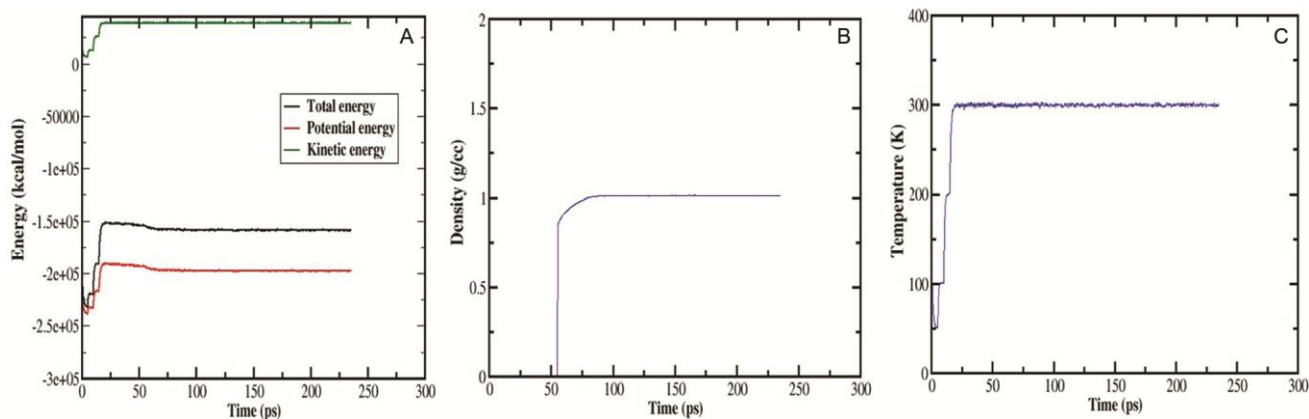


Fig. S2 — The visualization of SHANK3 L270M of (A) Energy; (B) Density; and (C) Temperature to ensure correct equilibration

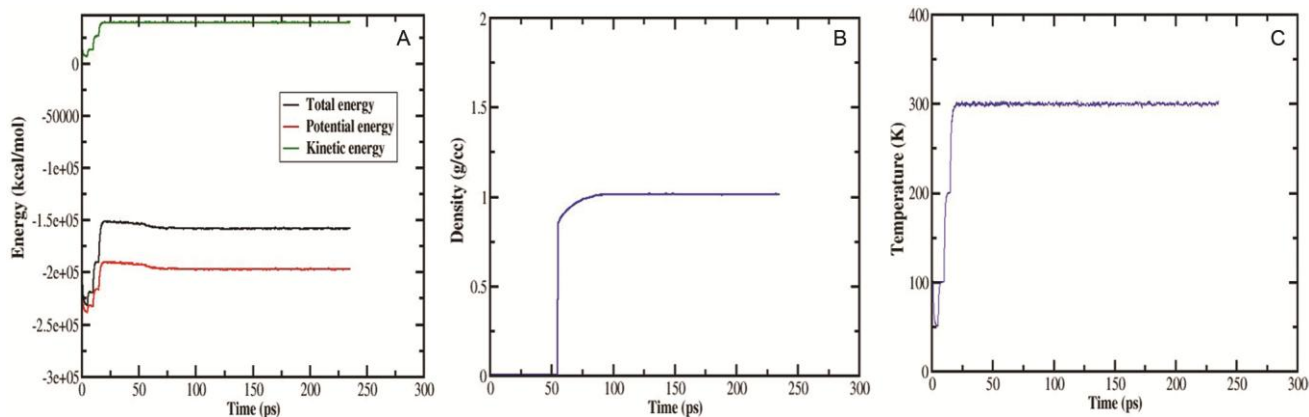


Fig. S3 — The visualization of SHANK3 P141A of (A) Energy; (B) Density; and (C) Temperature to ensure correct equilibration

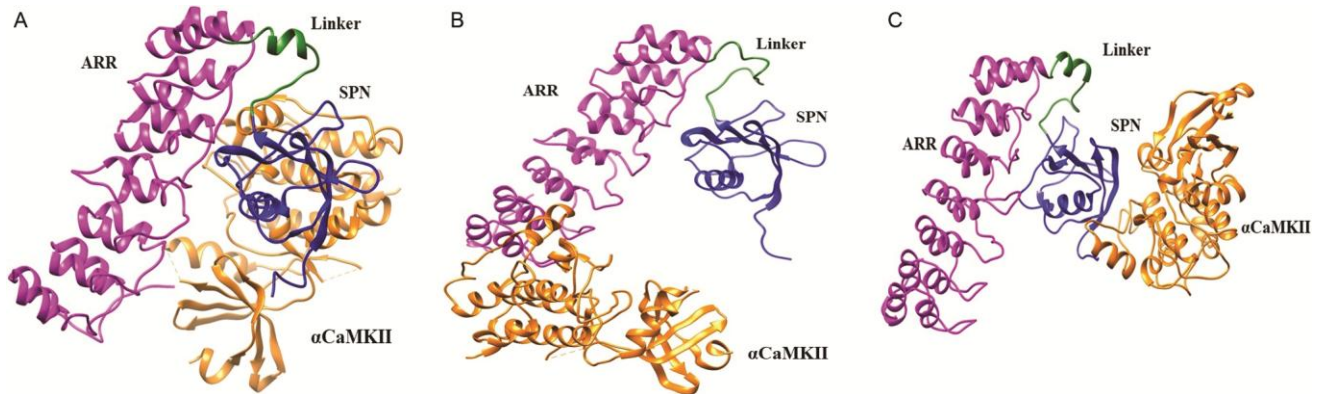


Fig. S4 — The docking interaction between (A) SHANK3 WT protein and α CaMKII; (B) SHANK3 P141A mutant and α CaMKII; and (C) SHANK3 L270M protein and α CaMKII

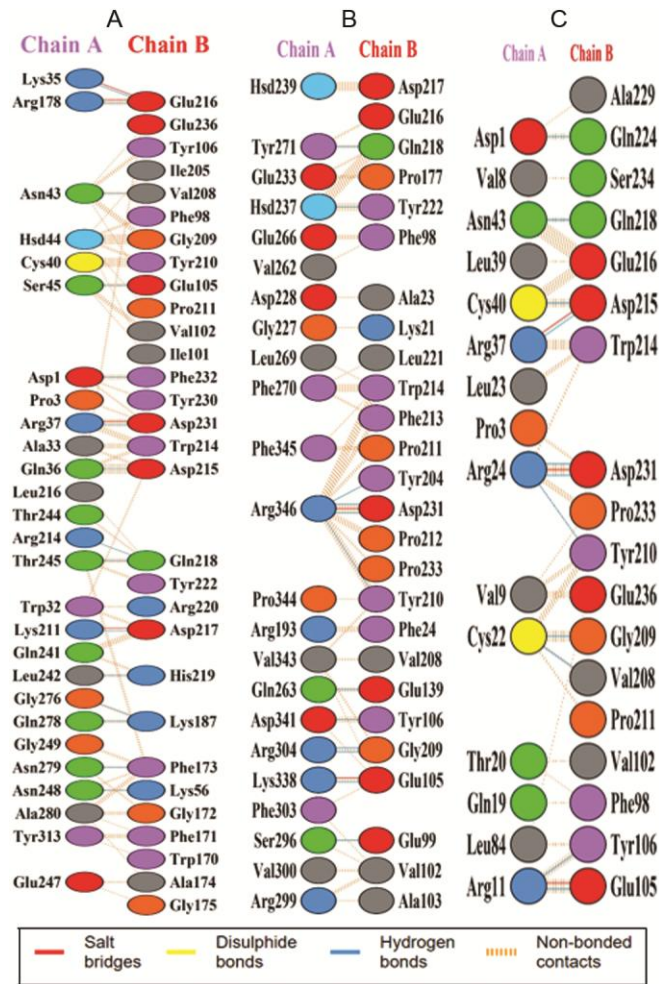


Fig. S5 — The interactions between (A) SHANK3 WT protein (chain A) and α CaMKII (chain B); (B) SHANK3 P141A mutant (chain A) with α CaMKII (chain B); and (C) SHANK3 L270M mutant (chain A) with α CaMKII (chain B)

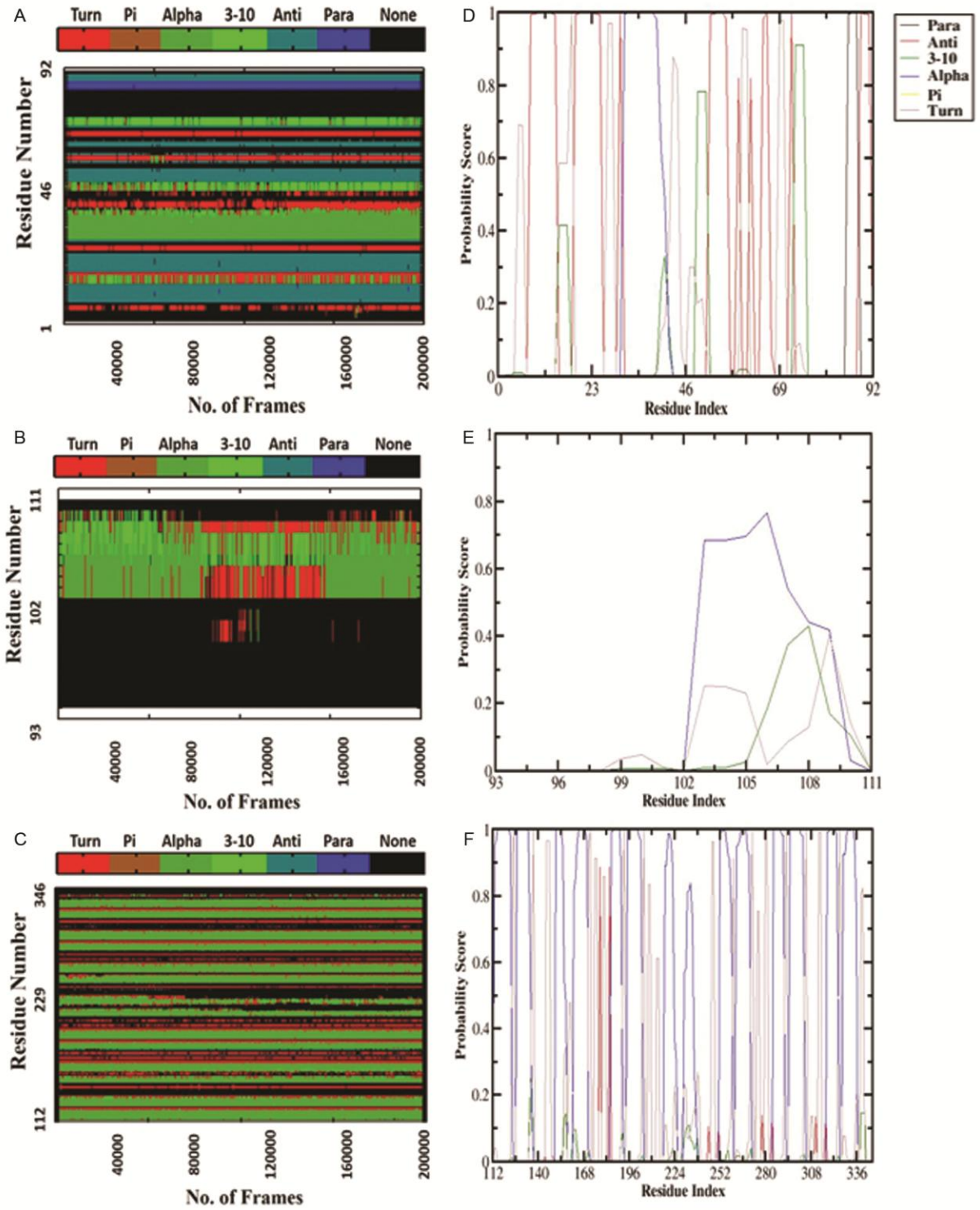


Fig. S6 — Secondary structure analysis of SHANK3 WT protein; (A) SHANK3 SPN domain; (B) Linker domain; (C) (ARR) domain. Secondary structure probability score of residue index; (D) SPN domain; (E) Linker domain; and (F) (ARR) domain

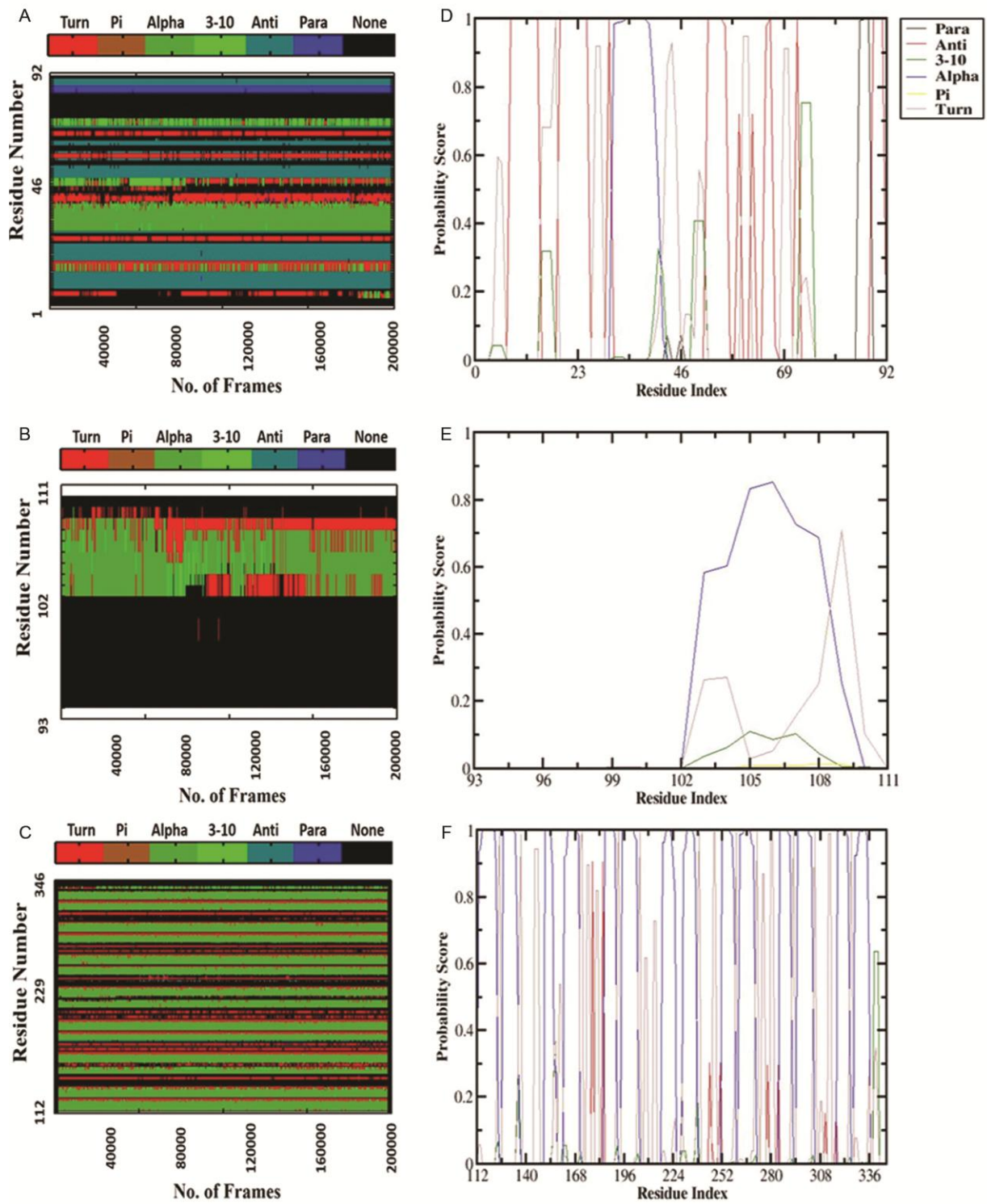


Fig. S7 — Secondary structure analysis of SHANK3 L270M mutant; (A) SHANK3 SPN domain; (B) Linker domain; (C) (ARR) domain. Secondary structure probability score of residue index; (D) SPN domain; (E) Linker domain; and (F) (ARR) domain

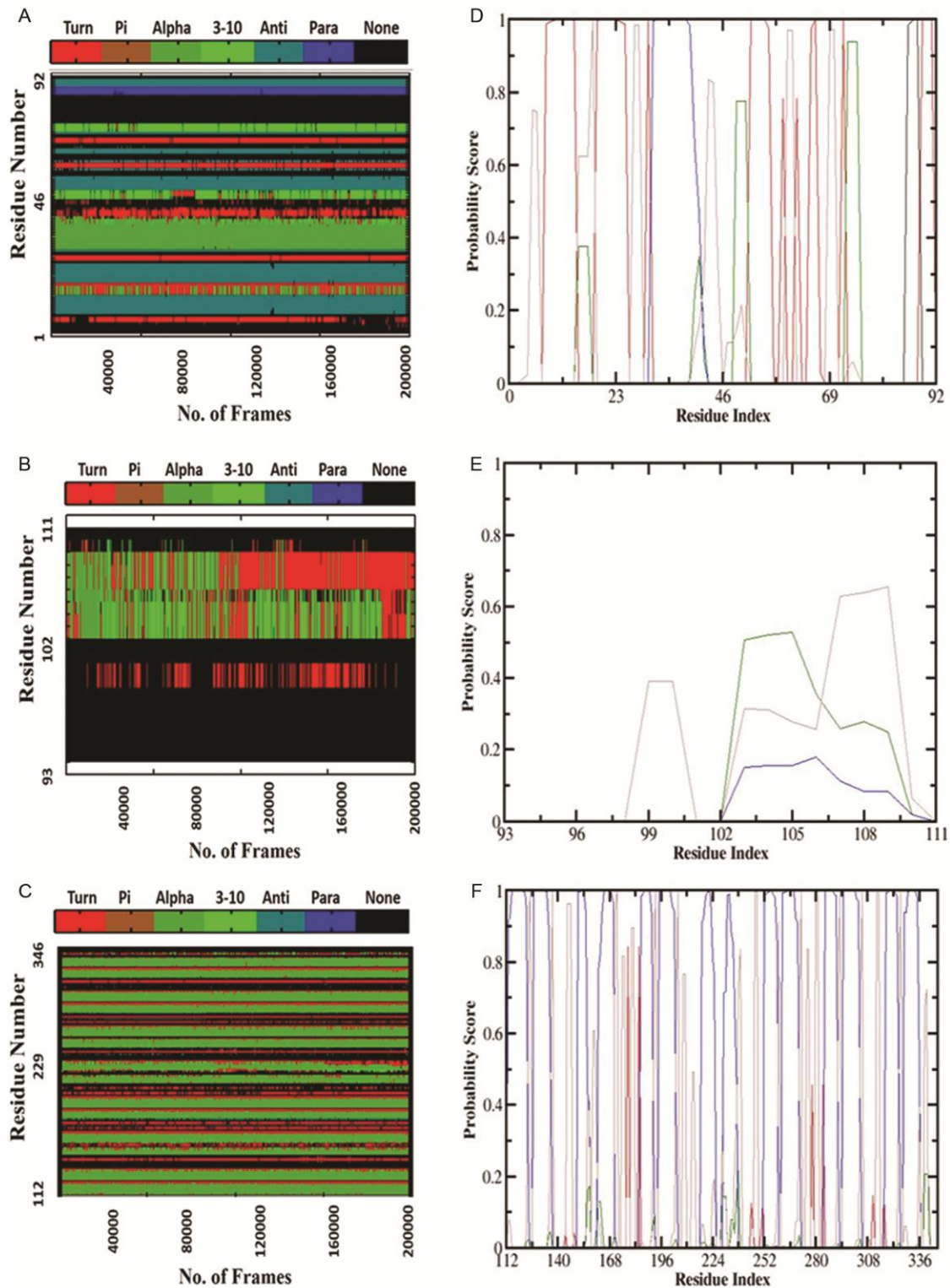


Fig. S8 — Secondary structure analysis of SHANK3 P141A mutant, (A) SHANK3 SPN domain; (B) Linker domain; (C) (ARR) domain. Secondary structure probability score of residue index; (D) SPN domain; (E) Linker domain; and (F) (ARR) domain