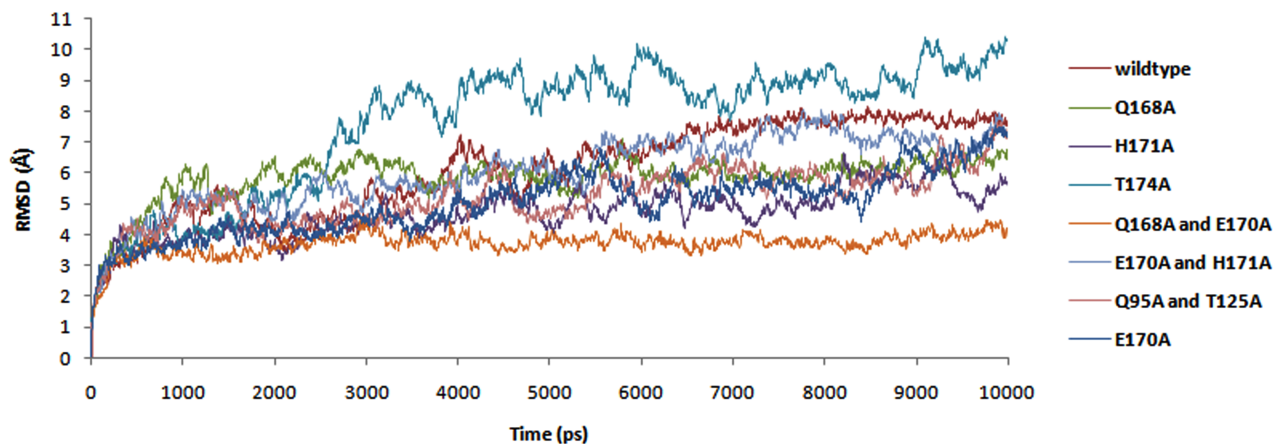**Figure S1**. RMSD of side chains of wild type and mutant forms during the simulation. (A) RMSD of wild type and mutant forms of IN-LEDGF/p75 complexes. (B) RMSD of only LEDGF/p75 in wild type and mutant forms of IN-LEDGF/p75 complexes through 10 ns MD simulations.



**Table S1**. Summary of model systems for MD simulations.

| IN-LEDGF/p75 complex models | No. of Atoms | Time |
|---|---|---|
| Wild type | 70,729 | 10 ns |
| Single mutant form (Q168A) | 70,797 | 10 ns |
| Single mutant form (E170A) | 70,339 | 10 ns |
| Single mutant form (H171A) | 70,764 | 10 ns |
| Single mutant form (T174A) | 70,348 | 10 ns |
| Double mutant form (Q168A and E170A) | 70,785 | 10 ns |
| Double mutant form (E170A and H171A) | 70,775 | 10 ns |
| Double mutant form (Q95A and T125A) | 70,724 | 10 ns |