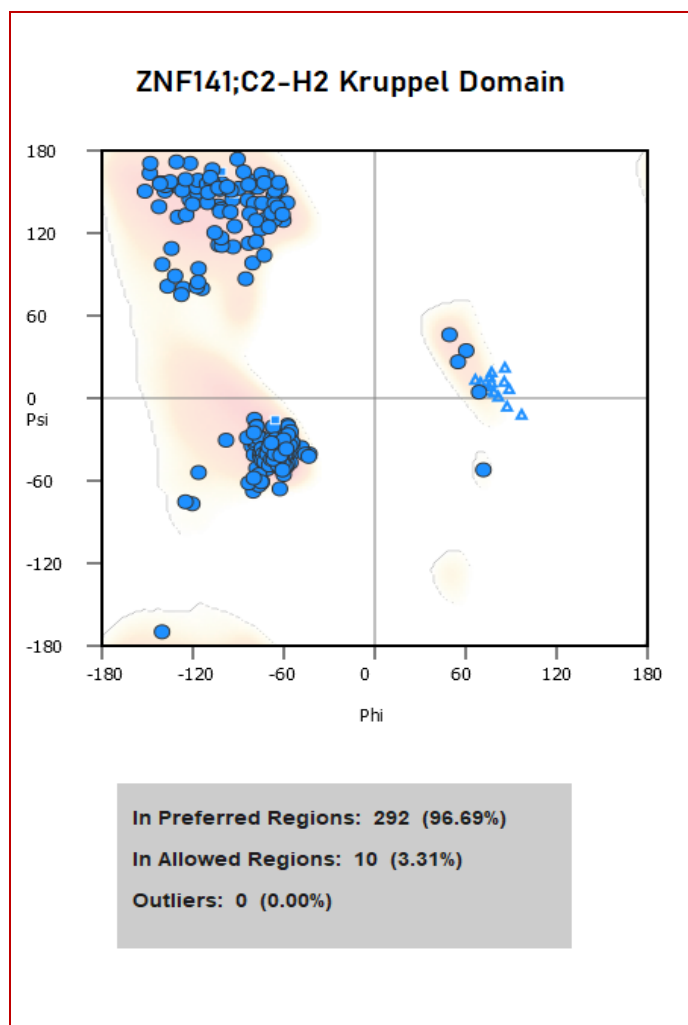


***Decoding the molecular basis of Postaxial polydactyly type-A promoted by  
ZNF141 gene; an eScience view***

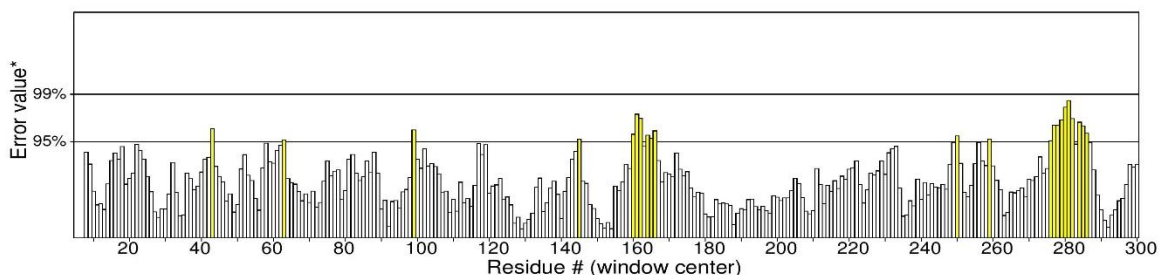


***Supplementary Figure S1: InterPro server annotation of the ZNF141 protein showing C2-H2; IPR013087 domain from residue 171-474 with ten Zinc finger motifs.***



**Supplementary Figure S2:** Ramachandran plot of ZNF141; C2-H2 domain (Res 171-474) with all the residues in Preferred and allowed regions and no residue in the disallowed region.

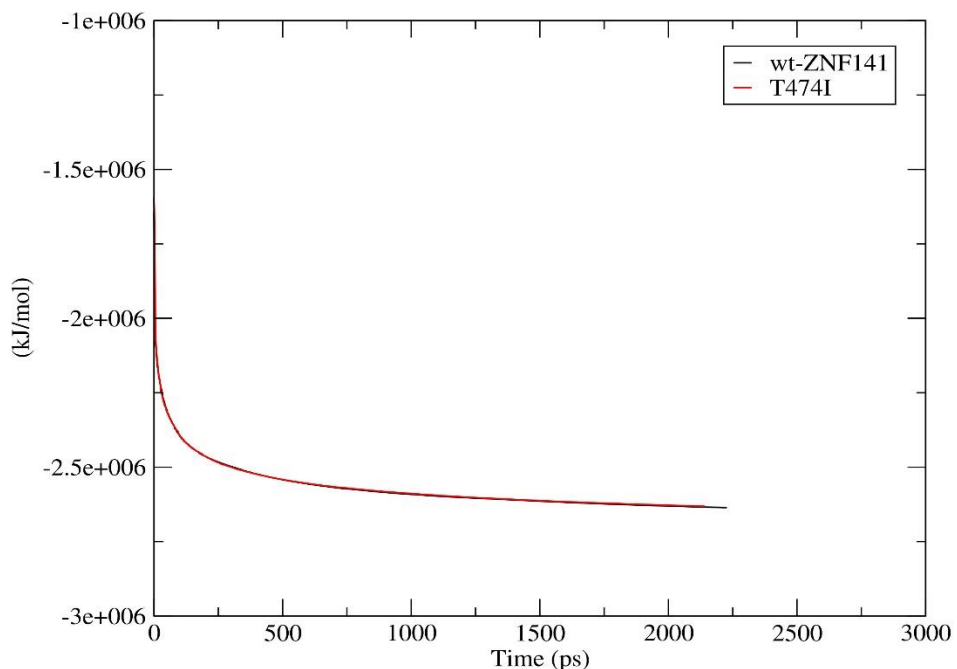
Program: ERRAT2  
 File: compiled-coot-minim.pdb  
 Chain#:A  
 Overall quality factor\*\*: 92.491



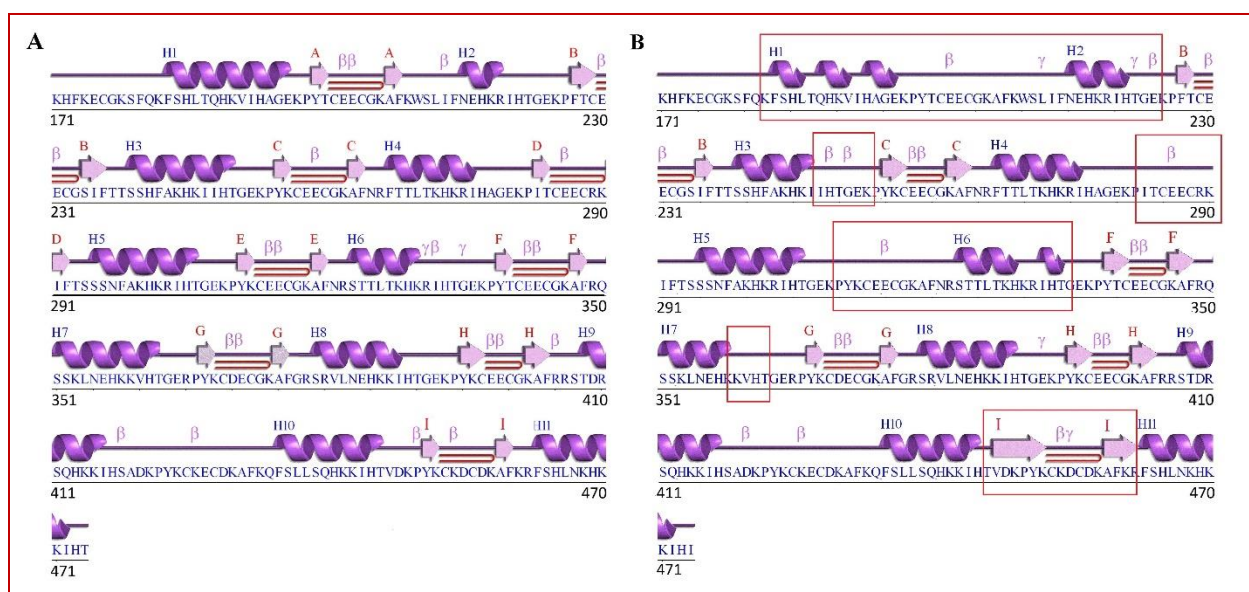
\*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.  
 \*\*Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

**Supplementary Figure S3:** ERRAT validation graph showing an overall quality score of the structure as 92.491 with the low relatively low confidence score of the error for the rest of the residues.

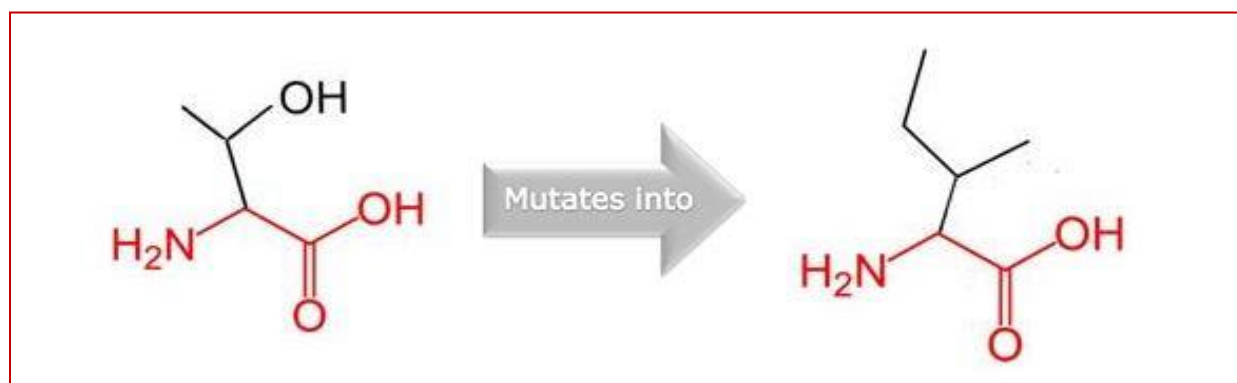
### Potential Energy



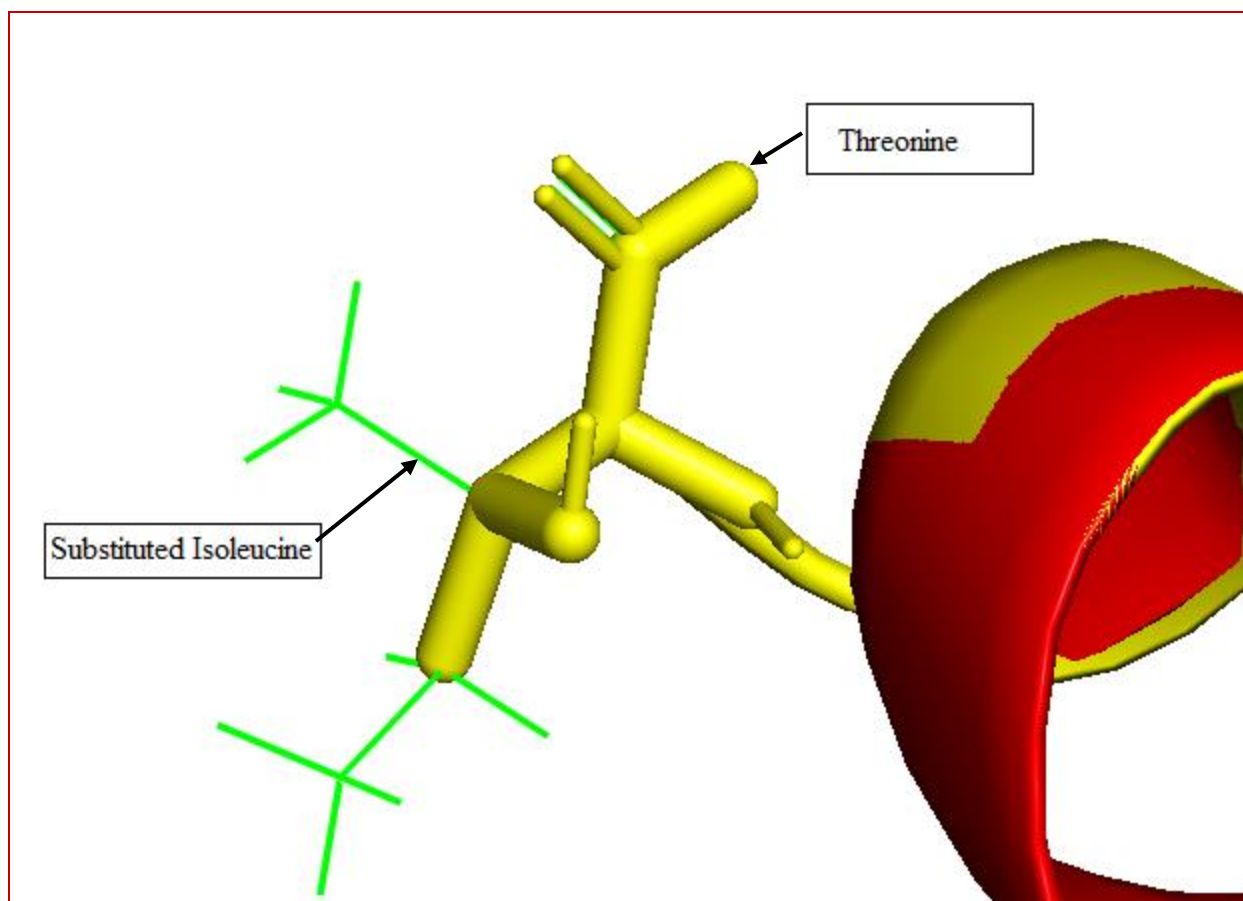
**Supplementary Figure S4:** The potential energy of both wt-ZNF141 and T474I models after energy minimization.



**Supplementary Figure S5.** Secondary structure analysis of (A) wt-ZNF141 and (B) mutant T474I protein after 100ns molecular dynamics simulations.



**Supplementary Figure S6 (a):** The figure shows the schematic structures of the original (left; threonine) and the mutant (right; isoleucine) amino acid. The backbone, which is the same for each amino acid, is colored red. The side chain, unique for each amino acid, is colored black.



**Supplementary Figure S6 (b):** Superimposition of wild-type and mutant-type residues at 474<sup>th</sup> position. The wild type of threonine is shown in sticks while mutant Isoleucine is shown in Lines.

**Supplementary Table S1:** Functional impact of ZNF141 T474I mutation predicted by different tools

Variant ID	Genomic substitution	A.A.	Location	SIFT	Polyphon	Revel	CADD	MetaLR
rs587776959	C>T	T>I	474	0.01	0.998	0.119	17	0.046