Supplementary Informations

Insights on the structural perturbations in Human MTHFR Ala222Val mutant by protein modeling and molecular dynamics

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The Human MTHFR was subjected to PSI-BLAST to recognize the ideal templates to perform homology modeling. The top BLAST hits were MTHFR protein structures from *E. coli* (3FSU, 3FST and 1B5T) and *Thermus thermophilus* Hb8 (1V93, 3APT). All these proteins showed an identity of 40-45% each and with query coverage of > 90% in the amino acid region 42-338.

Template Protein	Organism	Query Coverage	E value	Identity
<u>1V93_A</u>	<i>Thermus thermophilus</i> Hb8	42%	1e-57	39%
<u>3APT_A</u>	<i>Thermus thermophilus</i> Hb8	42%	2e-57	39%
<u>3FST_A</u>	<i>E. coli</i>	45%	9e-42	34%
<u>3FSU_A</u>	<i>E. coli</i>	45%	2e-41	33%
<u>1B5T_A</u>	<i>E. coli</i>	42%	2e-41	34%