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Structural model of tRNA(guanine-N1)-methyltransferase by a computational method

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In this research, we have modeled a three-dimensional structure of tRNA(guanine-N1-)-methyltransferase which consists of 232 amino acids. This enzyme belongs to the family of transferases that catalyzes the reaction of methylating guanosine (G) at position 37 of tRNA to N1-methylguanine (1-methylguanosine (m1G)) via *S-adenosyl-L-methionine*. The presence of m1G improves the cellular growth rate and polypeptide step-time and also prevents the tRNA from shifting the reading frame. Computer software (O, SOD, and MOLEMAN) from Uppsala Software Factory (USF) has been used as main tools for modeling, and NCBI, PDB, BLAST and CLUSTALW databases were used for sequence comparison and alignment. The model was evaluated by PROCHECK. The crystal structure of a putative tRNA (guanine-7)-methyltransferase (PDB ID: 3ky7) which was shown 53% sequence identity with the target protein was used as the template. The region 229-232 in the C-terminus in the target protein was not modeled. The gap between residues 41-42 found in a loop region was inserted using O program. The other gap found between residues 68-69 in a helical region was not inserted. This model consists of two domains. The domain I contains five parallel β-strands forming a β-sheet and five α-helices. The α-helices are wrapped around both sides of the beta sheet similar to the other methyltransferases. The domain II contains two α-helices. The PROCHECK analysis showed only Asn44 and Trp71 found in the disallowed region of the Ramachandran plot. Therefore, it suggests that the model is of good quality. For the best of our knowledge, this is the first structural model of tRNA (guanine-N1-)-methyltransferase and will be much more useful for further studies of this protein.

Key words: 3D-structural model, homology modelling, methyltransferase, tRNA (guanine-N1)-methyltransferase

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