

Supplementary data

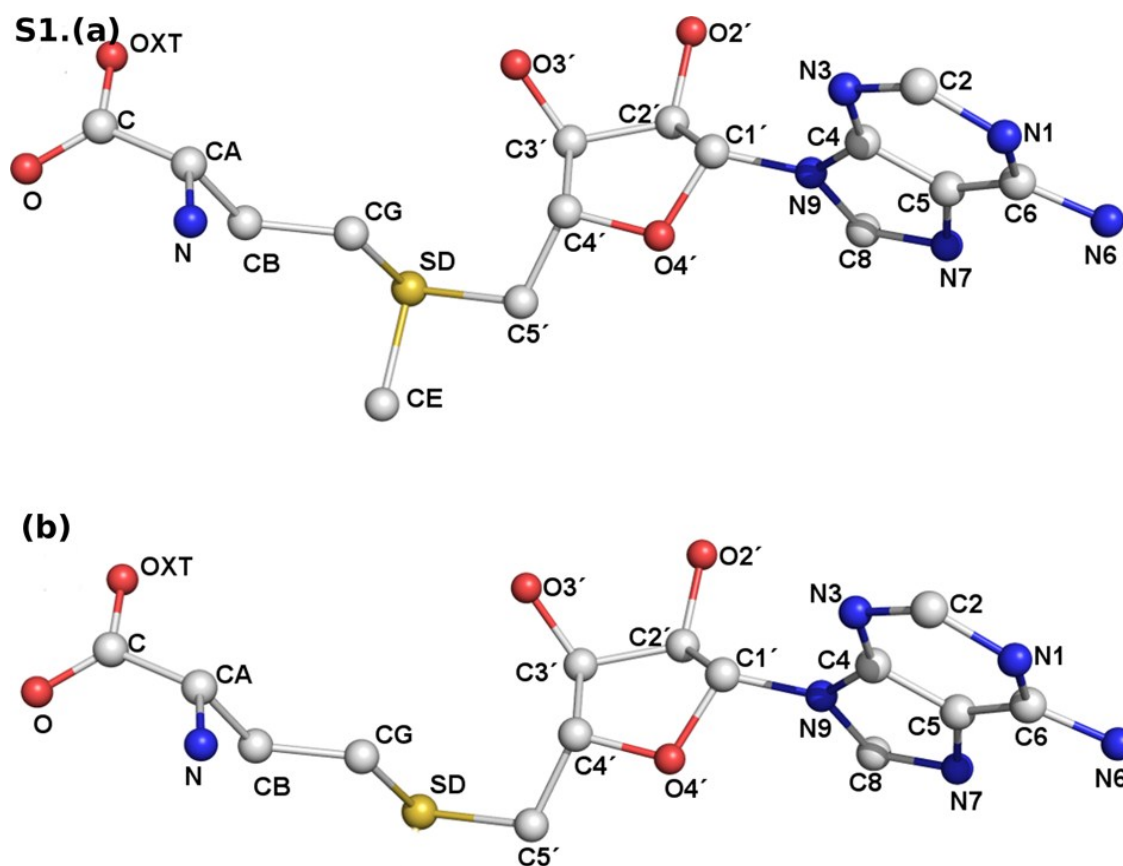


Figure S1. Structure of (a) S-Adenosyl-L- methionine (SAM or AdoMet) (b) S-Adenosyl-L- homocysteine (SAH or AdoHcy).

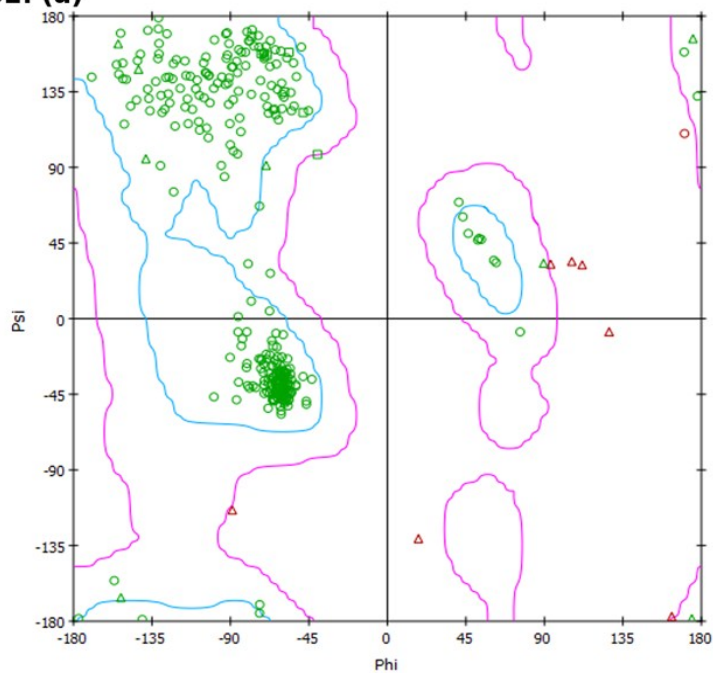
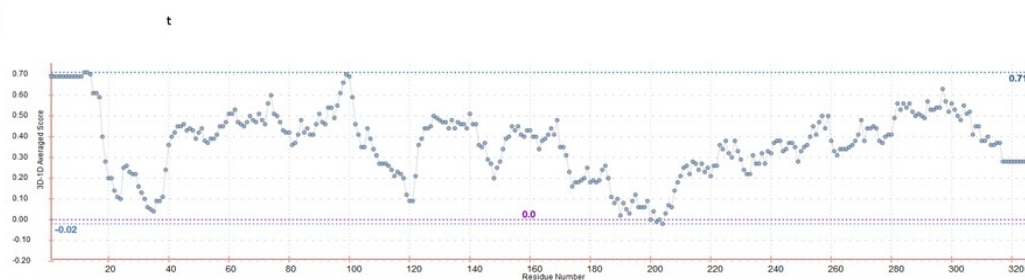
S2. (a)**(b)**

Figure S2. Quality assessment of M. Hpy C5mC model using (a) PROCHECK and (b) Verify_3D.

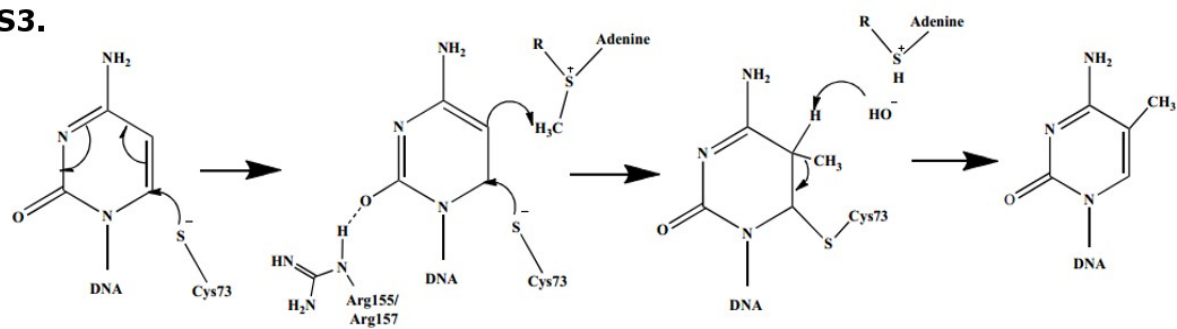
S3.

Figure S3. Mechanism of methyl-group transfer from AdoMet to DNA in M. Hpy C5mC.

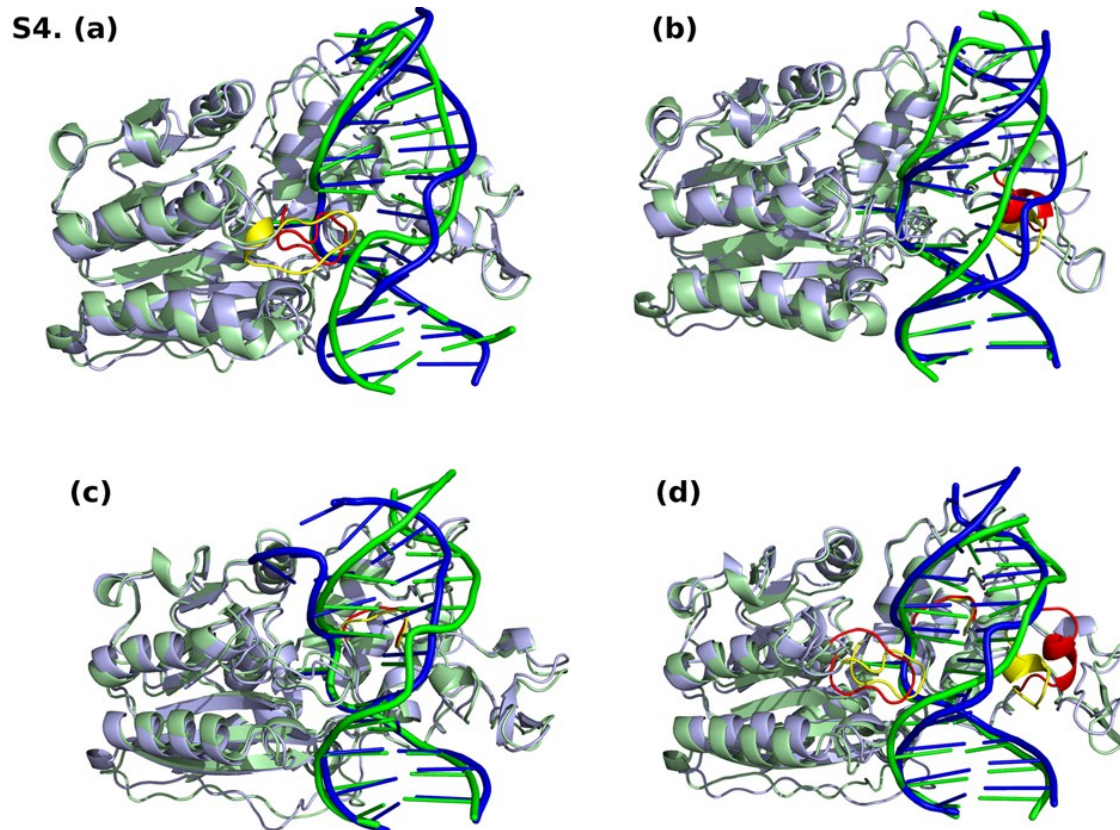


Figure S4. Superimposition of native (protein shown in light blue and DNA is represented in dark blue) and mutant protein (protein shown in light green and DNA is represented in dark green) structure having mutations in the region (a) 75-83 (b) 221-229 (c) 243-246 and (d) structure accommodating mutations in all the three loops. Specific mutated region are represented in yellow (native) and red (mutant) in all the superimposed structure.