

Supplementary Material for the manuscript:

**Deciphering the Flexibility and Dynamics of *Geobacillus*
zalihae strain T1 Lipase at High Temperature by
Molecular Dynamics Simulation**

By:

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Donald Jacobs, Mahiran Basri, Adam Leow Thean Chor, Habibah Abdul Wahab,
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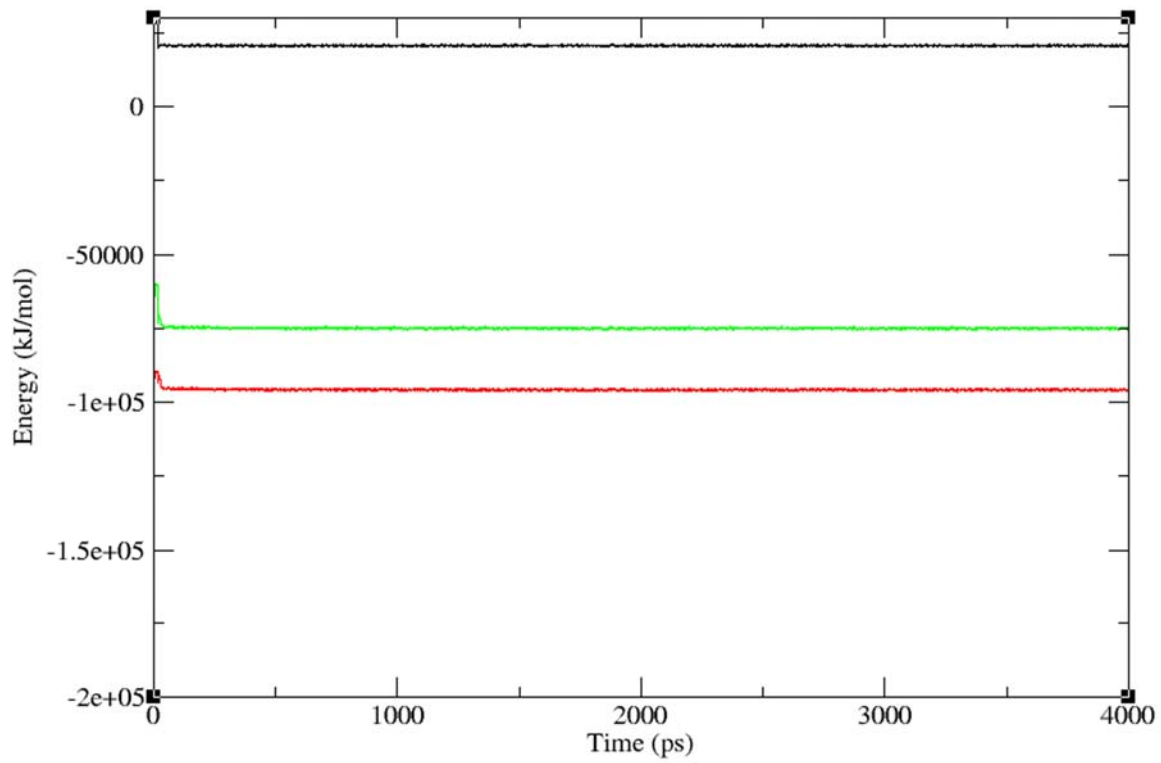


Fig. 1. T1 lipase energy fluctuation as a function of time at 300 K; kinetic energy (black), potential energy (red), total energy (green).

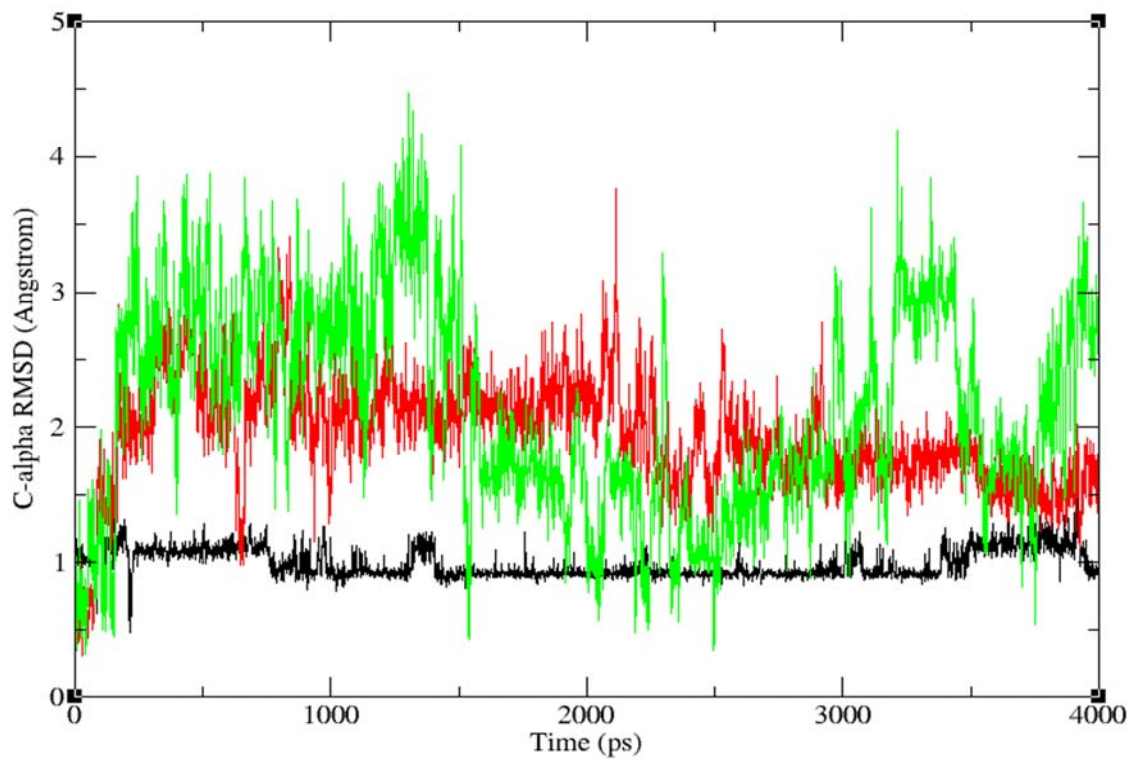


Fig. 2. T1 lipase backbone atoms root mean square deviations of His-81 and His-87 from the small domain of the enzyme towards time at 300 K (black), 400 K (red), and 500 K (green).

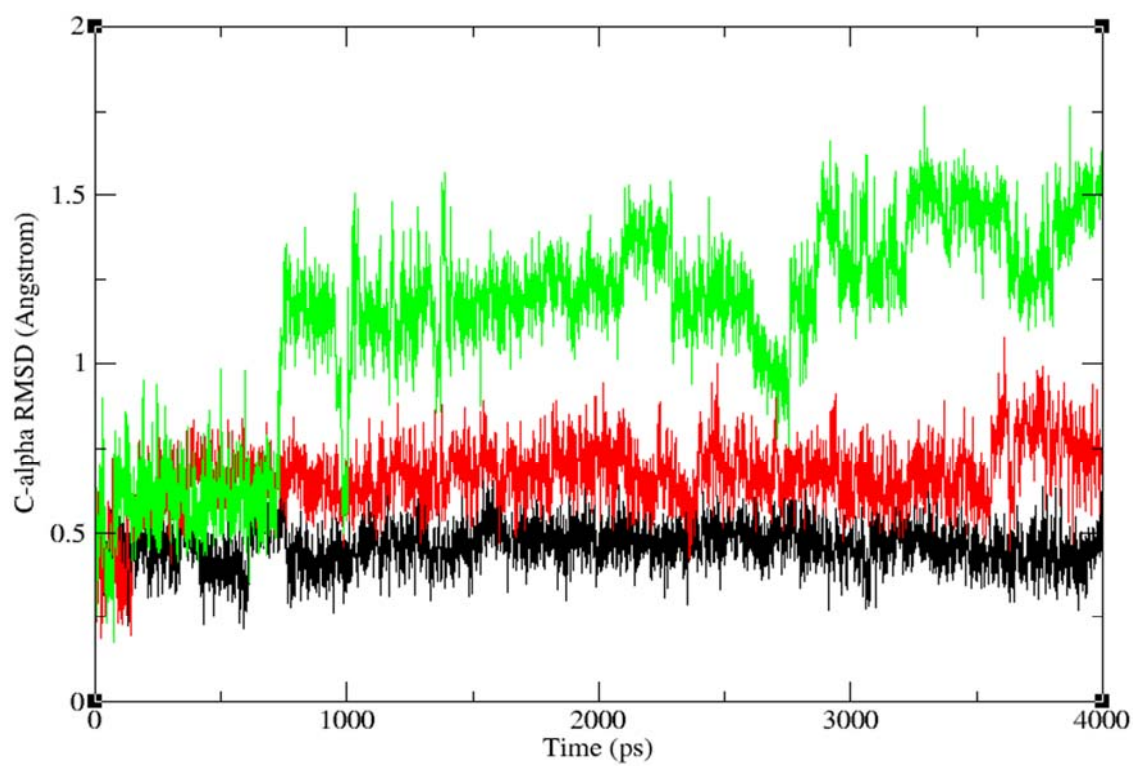


Fig. 2. T1 lipase backbone atoms root mean square deviations of Asp-611 and Asp-238 from the main catalytic domain of the enzyme towards time at 300 K (black), 400 K (red), and 500 K (green).

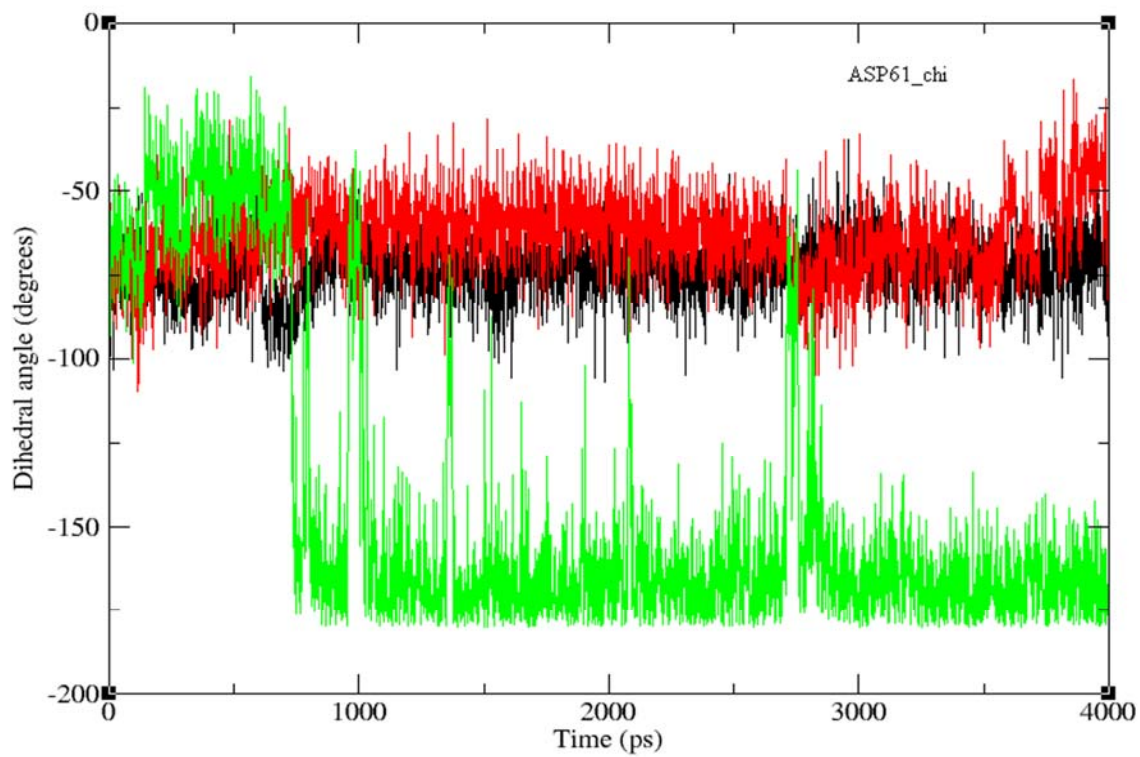


Fig. 4. T1 lipase side chain dihedral angles distributions of zinc chelating residues as a function of time for Asp-61 and Asp-238 from the core domain and His-81 and His-87 from the small domain of the enzyme at 300 K (black), 400 K (red), and 500 K (green).

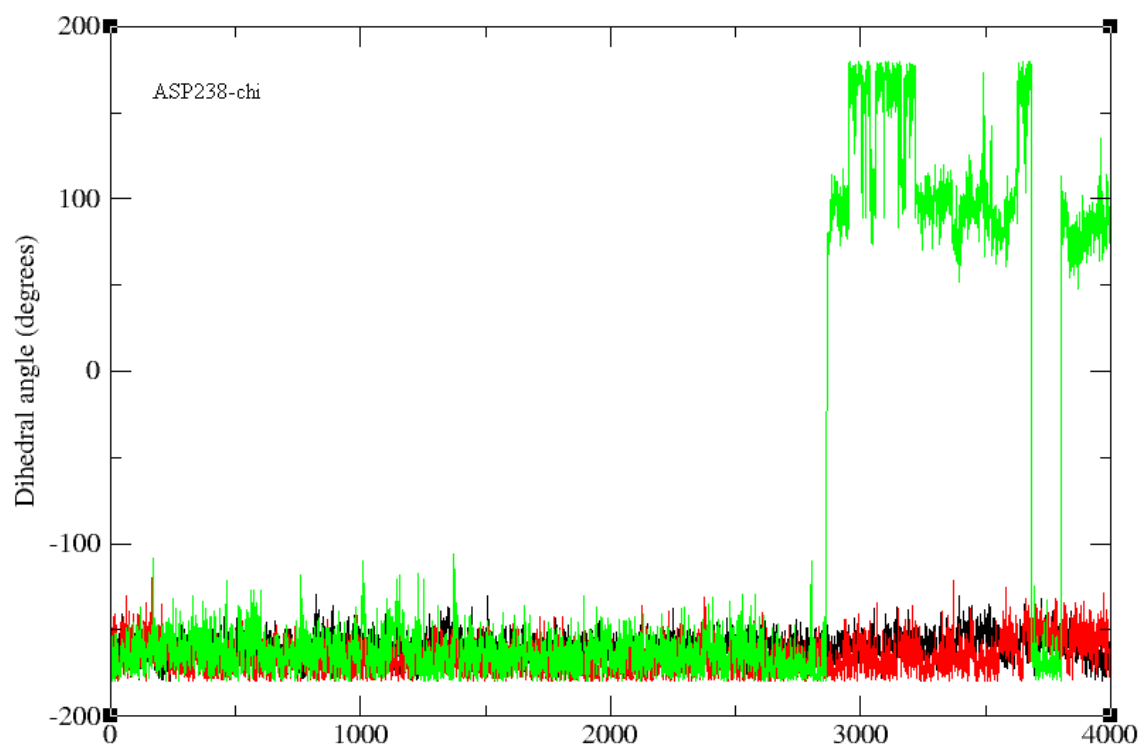


Fig. 4 (b)

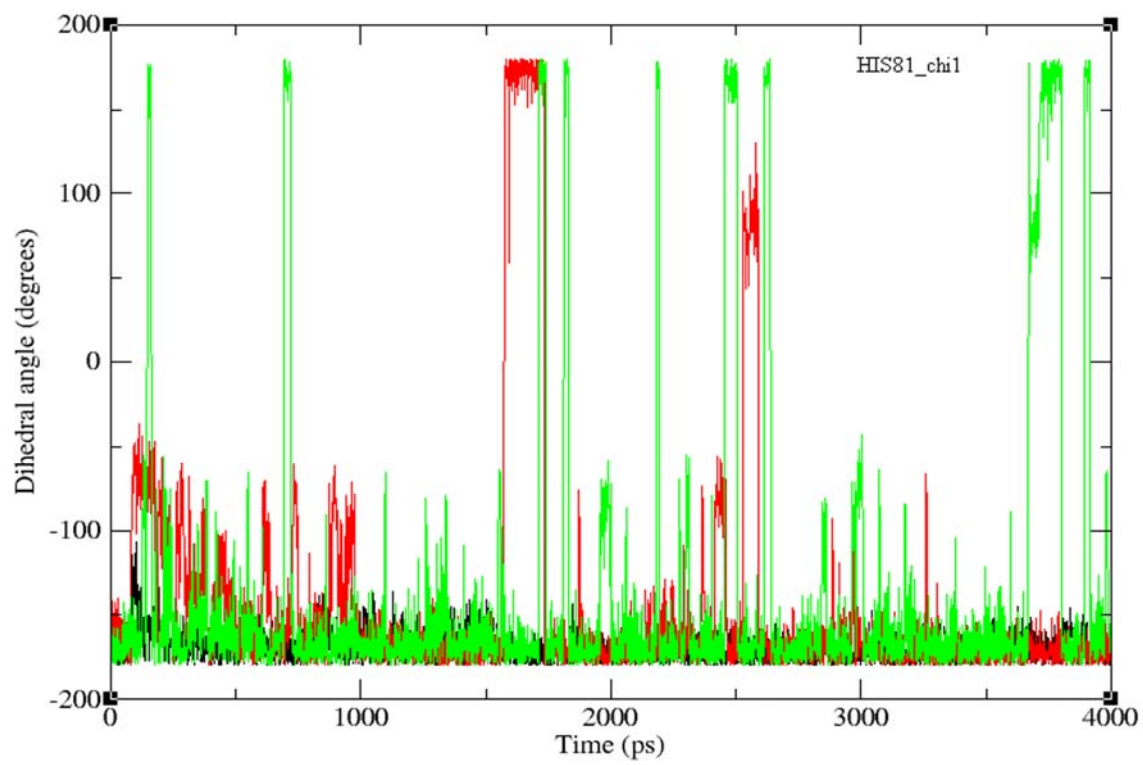


Fig. 4 (c)

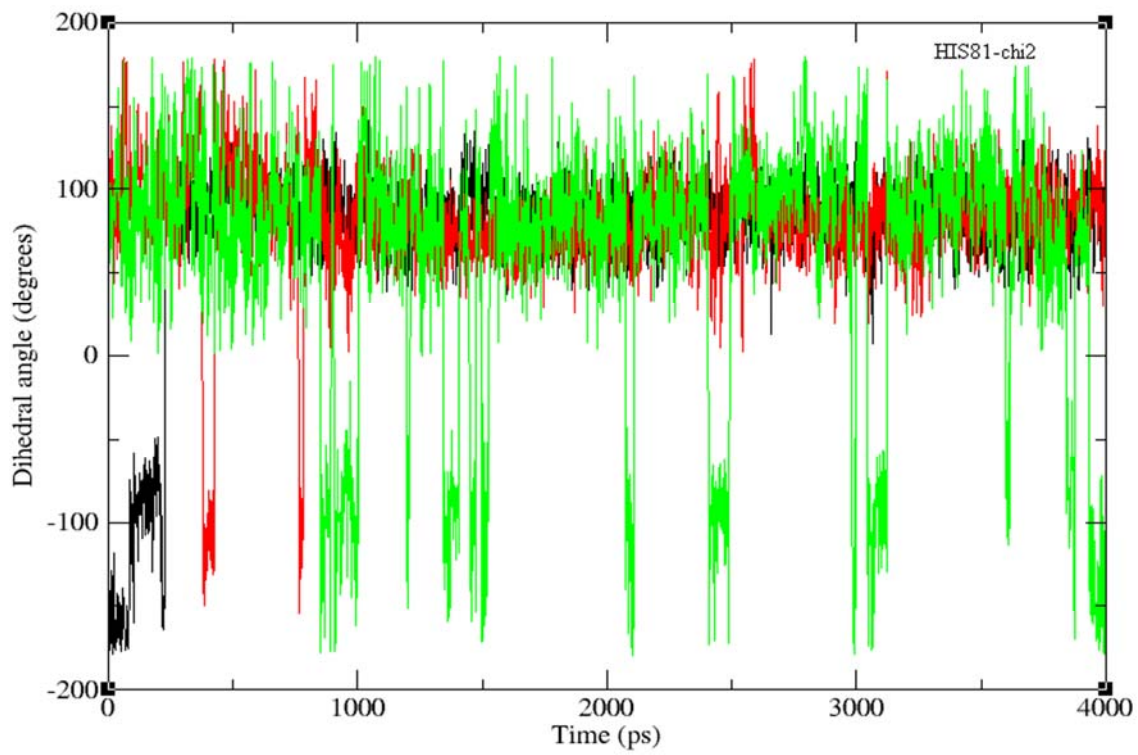


Fig. 4 (d)

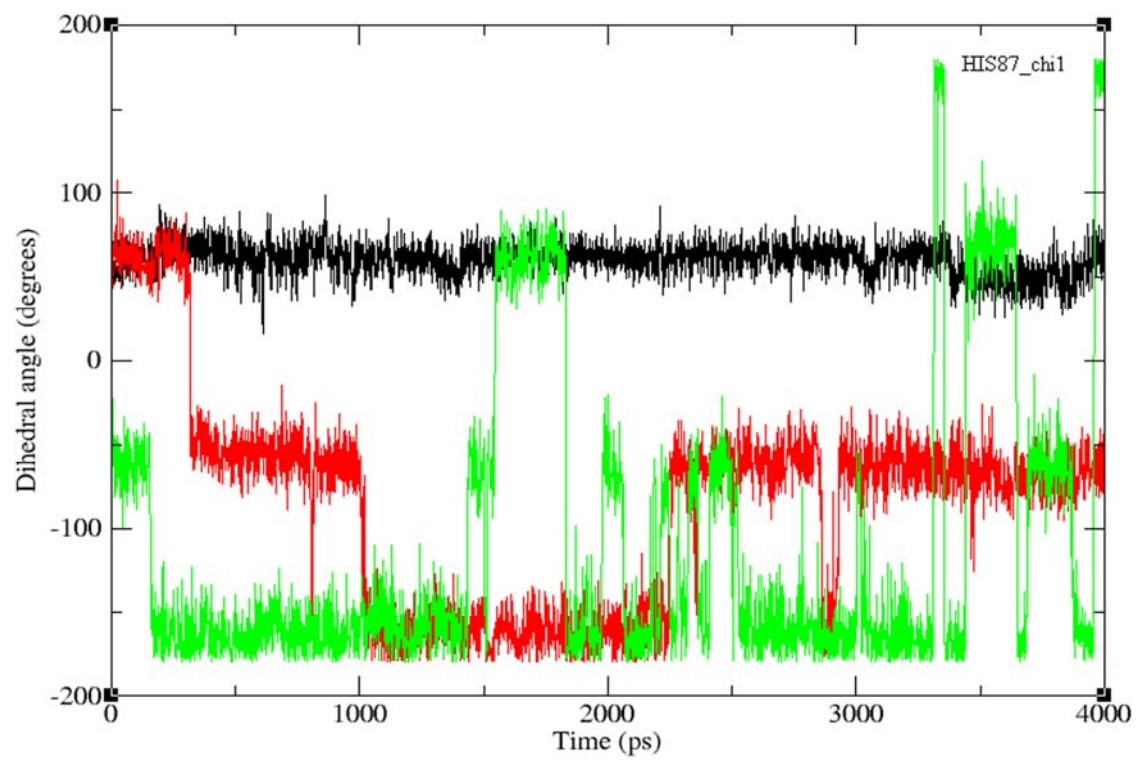


Fig. 4 (e)

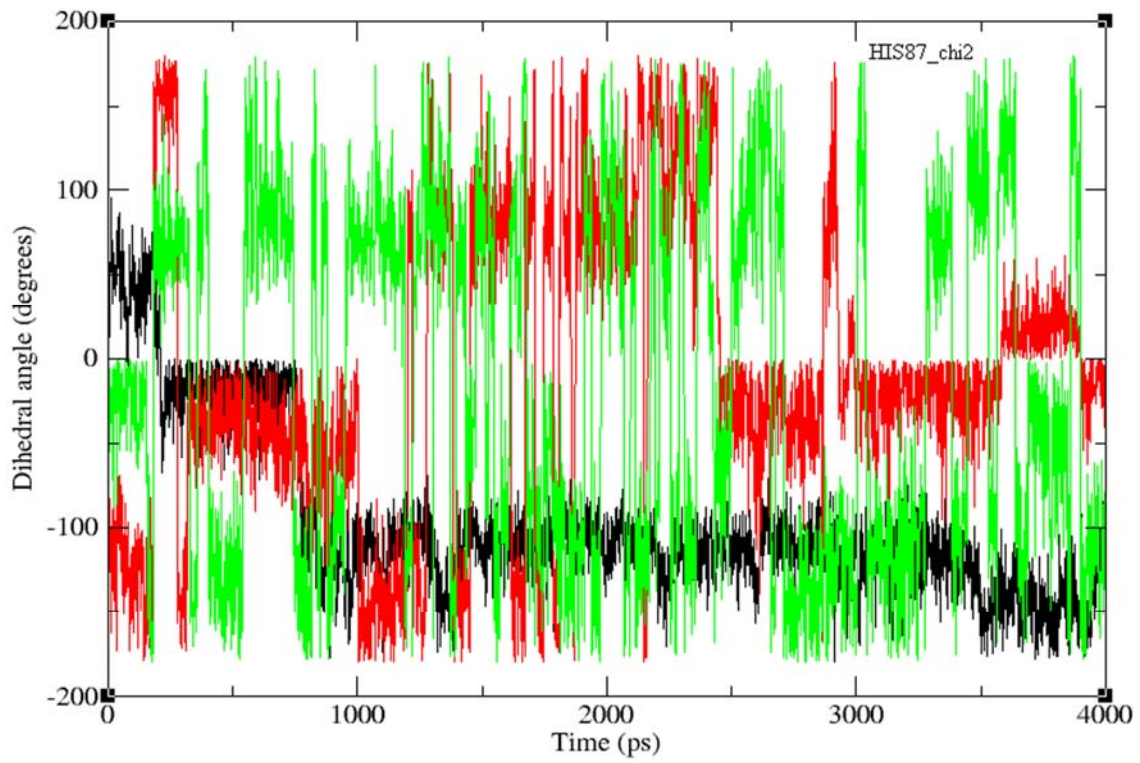


Fig. 4 (f)