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Electronic supplementary material for

Molecular Dynamics Simulation of Thermal Unfolding of Thermatoga maritima DHFR

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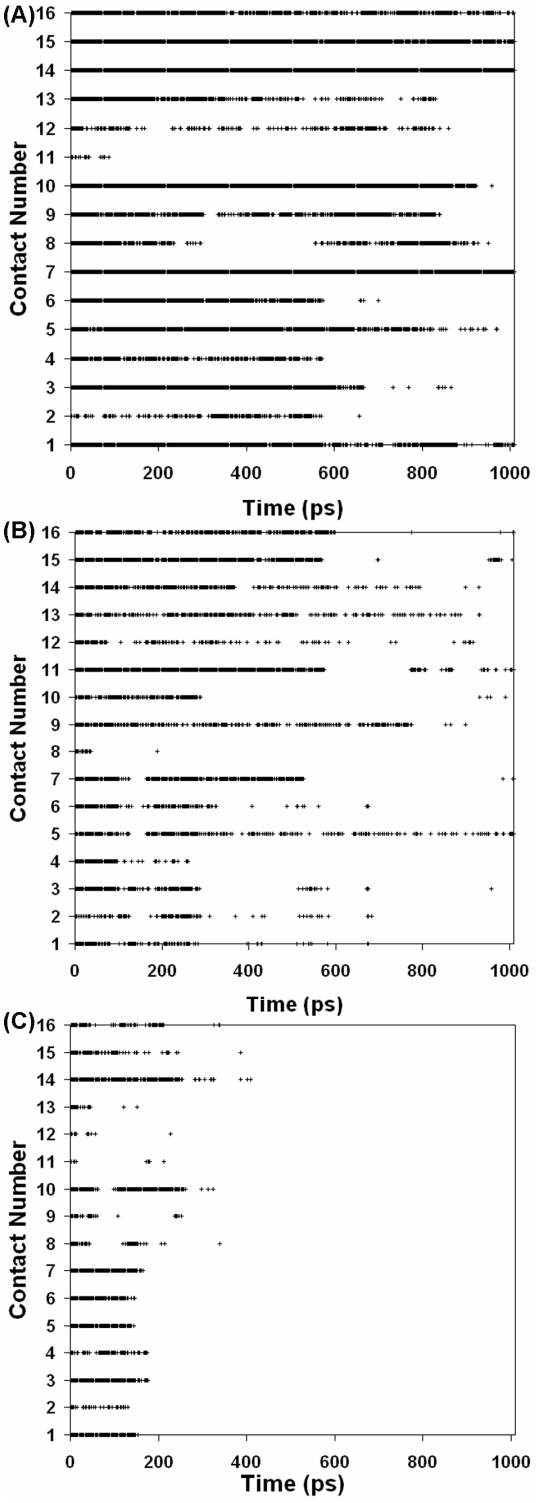

Figure S1: Existence of the contacts in the intermolecular anti-parallel β-sheets in the simulations of the dimer of TmDHFR at 400 K (A), 450 K (B) and 500 K (C). Each Figure is the average over the total number of simulations at one temperature. The Table below

lists the contacts which are defined as the distance between the two Cα atoms in the two strands of the β-sheet less than 6 Å in the crystal structure of TmDHFR (1D1G.pdb).

Contact No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Residue in Subunit A	124	125	125	125	126	126	127	128	140	140	140	141	141	142	143	143
Residue in Subunit B	143	141	142	143	140	141	140	140	126	127	128	125	126	125	124	125

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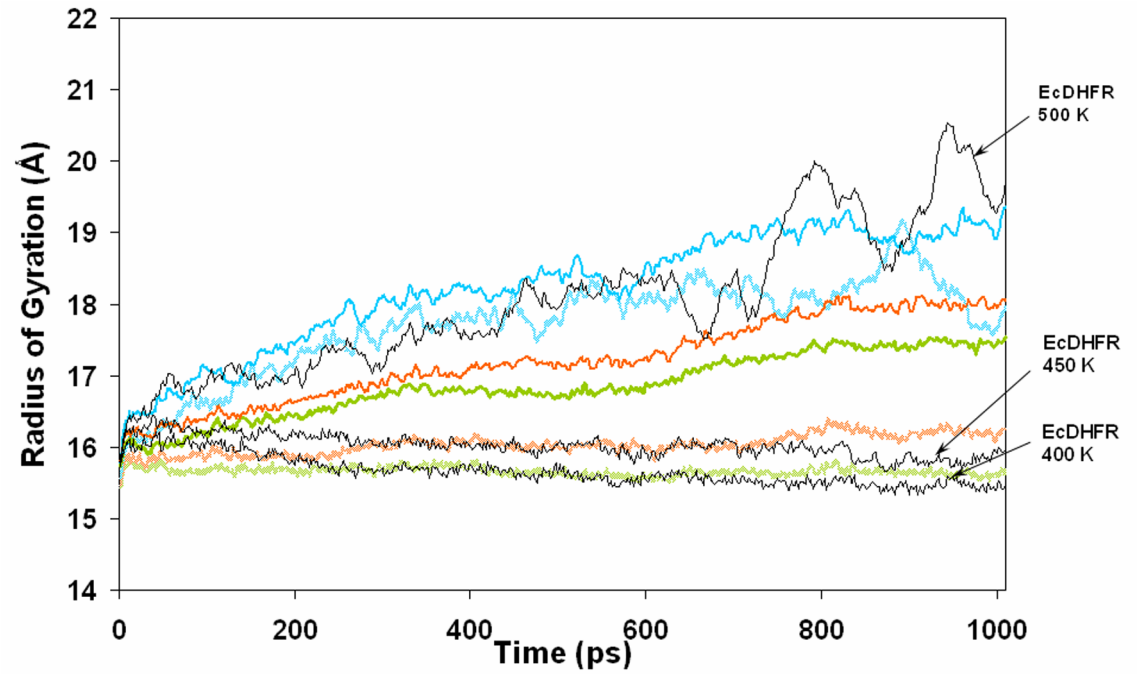

Figure S2: The radius of gyration of the dimer (solid line) and monomer (dashed line) of TmDHFR. Simulations at 400 K are coloured in green, 450 K in orange and 500 K in light blue. The plot of the dimer corresponds to a single subunit of the dimer for comparison with the monomer of TmDHFR. The results of EcDHFR are shown in black for comparison with those of TmDHFR.

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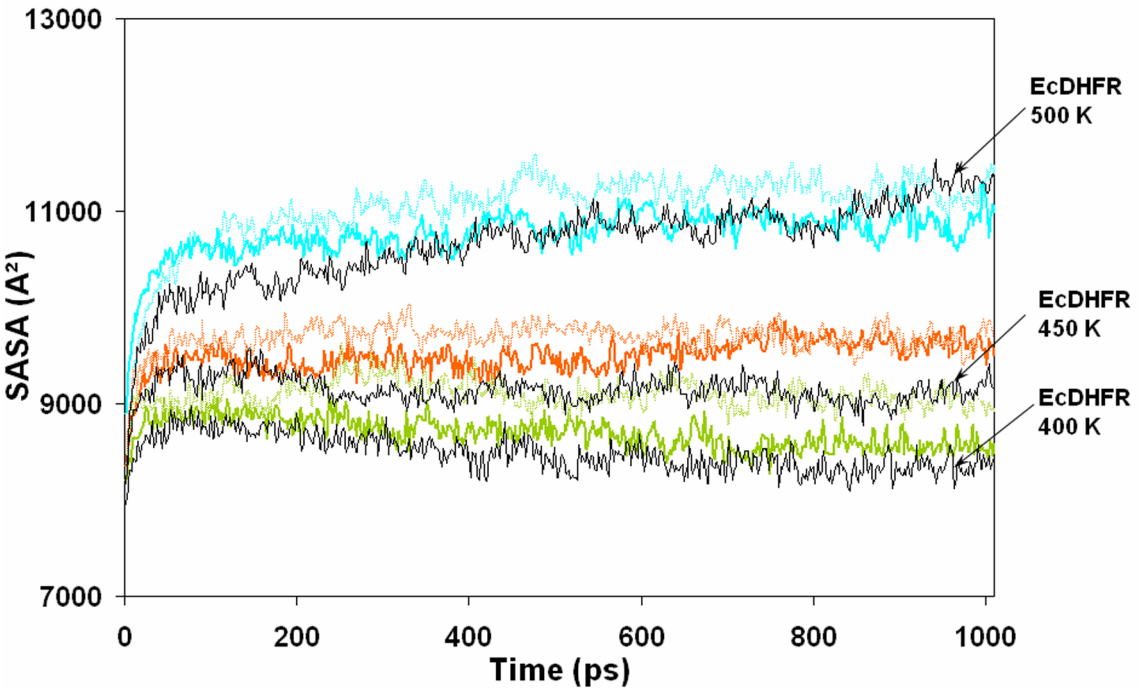

Figure S3: The SASA of the dimer (solid line) and monomer (dashed line) of TmDHFR. Simulations at 400 K are coloured in green, 450 K in orange and 500 K in light blue. The plot of the dimer corresponds to a single subunit of the dimer for comparison with the monomer of TmDHFR. The results of EcDHFR are shown in black for comparison with those of TmDHFR.

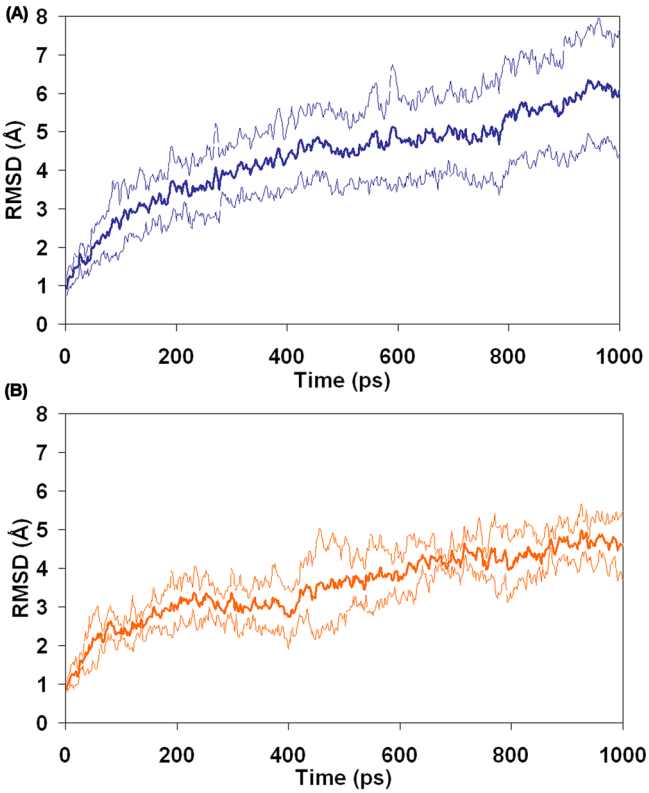

Figure S4: The RMSDs of the Cα atoms of the NDLD in the monomer (A) and in the dimer (B) of TmDHFR in the 450 K simulations. Their respective standard deviations of the RMSDs are shown in thinner lines. They were calculated based on 10 trajectories from dimer and monomer simulations, respectively. The plot of the dimer corresponds to a single subunit of the dimer for comparison with the monomer of TmDHFR.