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Supporting Information

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Supporting Information

for

Understanding the Plasticity of the a/ß Hydrolase Fold: Lid Swapping on the *Candida antarctica* Lipase B Results in Chimeras with Interesting Biocatalytic Properties

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This supporting infromation aims to present a more detailed analysis of the MD simulation described in the text. We first report here (Figure S1) the time dependence of the temperature and the pressure of the system.

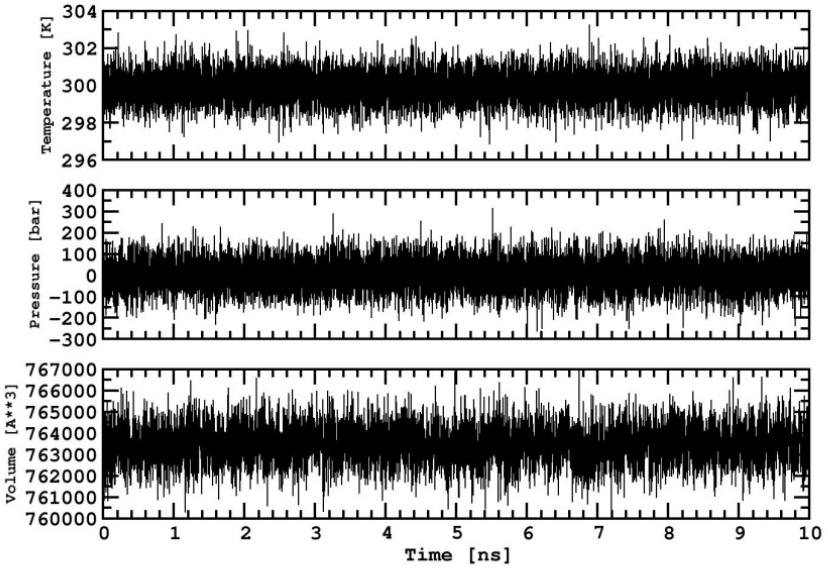

Figure S1. Time dependence of key simulation parameters. In the upper/middle/lower panel the temperature/pressure/volume of the system are followed as a function of the simulation time.

In Figure S2 the time dependence of key CALB properties is reported.

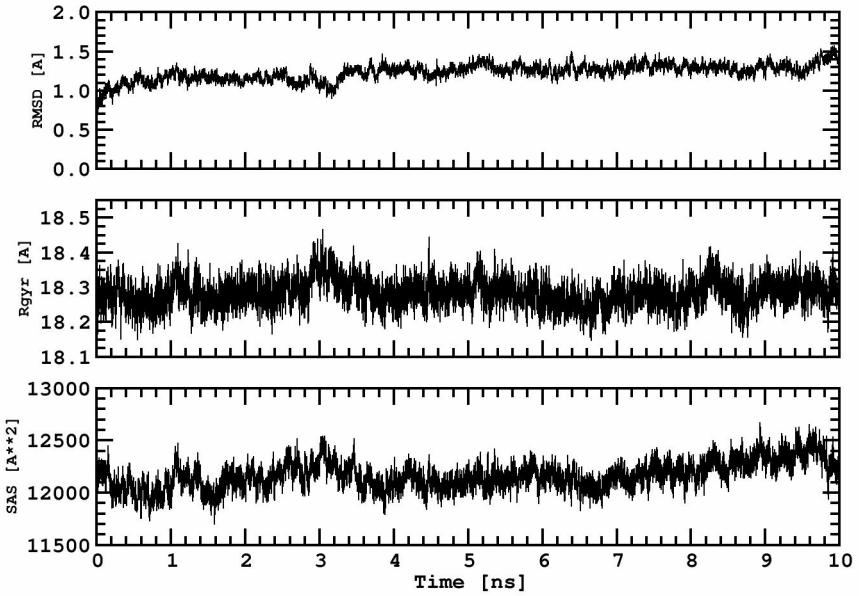

Figure S2. Time dependence of key protein properties. In the upper/middle/lower panel the RMSD/RGYR/SAS of CALB are followed as a function of the simulation time. The RMSD is calculated for the Cα atoms after superimposing every snapshot to the starting crystal structure 1TCA. The radius of gyration is referred as RGYR and the solvent accessible surface (SAS) of the enzyme was calculated using a probe with a radius of 1.4 Å.

Principal component analysis (also referred as essential dynamics, see A. Amadei, A. B. M. Linssen, H. J. C. Berendsen, *Proteins* **1993**, *17*, 412–425) was performed on the coordinates of the Cα atoms originating from each saved snapshot. Overall translation and rotation were removed by optimal superimposition. Figure C shows the projection of the motion along the first six modes, accounting in total for 38% of the total fluctuations.

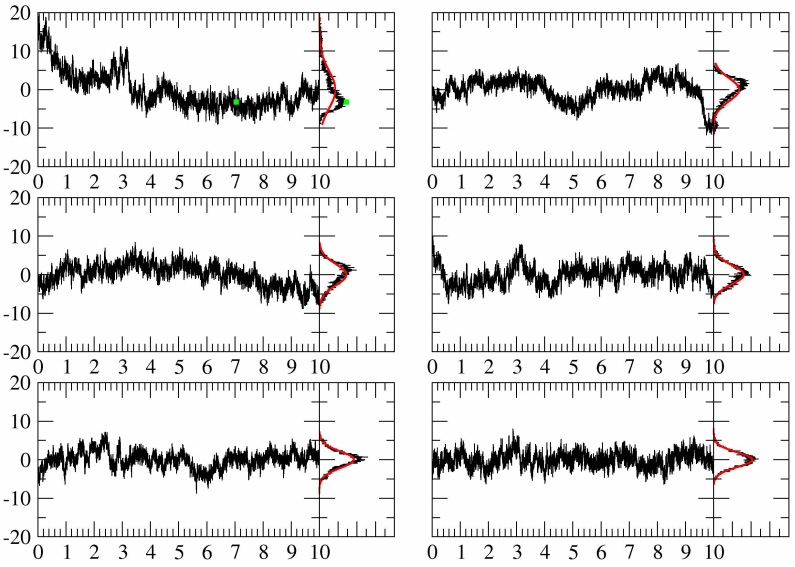

Figure S3. Projection of the CALB motion generated in the simulation along each of the first six principal components. The upper row shows the first and second component, the middle row shows the third and the fourth component, whereas the lower row shows the fifth and sixth component. For each panel the figure on the left shows the simulation time in ns on the *x*-axis and the value of the projection on the *y*-axis in Å. The small diagram on the right of every panel shows a histogram of the *y*-axis projection values. The red curves correspond to Gaussians having the same average value (zero for all cases) and fluctuations as the projected distribution. The more different from the Gaussian a distribution is, the more inharmonic (i.e. as opposite to harmonic thermal fluctuations) in nature the motion along the projection.

The structure shown in Figure 1 (right) in the paper corresponds to the most represented when considering the projection of the motion of the enzyme along the first principal component. It is indicated with a green square in Figure C. In this case it corresponded to the snapshot arising after 7044 ps.

An animated gif file is also provided showing the motion of the enzyme along the first principal component.