(at the conditions of measurement of simulations (e.g. biological in normal case $T \approx 300$ K, PH ≈ 7, etc, etc) are averages. The dynamics as a function of the distance from the geometric center of the protein is characterized by defining interior (int) Lindemann parameter

$$\Delta_L^{int}(r_{cut}) = \frac{\sqrt{\sum_{i,r_i<r_{cut}} \langle \Delta r_i^2 \rangle / N}}{a'},$$

which is obtained by averaging over the atoms that are within a chosen cutoff distance, r_{cut}, from the center of mass of the protein.

Simulations and experimental data for a number of proteins, in particular Barnase, Myoglobin, Crambin and Ribonuclease A indicate ≈ 0.14 as the critical value distinguishing between solid-like and liquid-like behaviour and $r_{cut} \approx 6$ Å. As can be seen from Table 1, the interior of a protein is solid-like ($\Delta_L^{int} < 0.14$), while its surface is liquid-like ($\Delta_L > 0.14$) under physiological conditions. The beginning of thermal denaturation in the simulations appears to be related to the melting of its interior (i.e. $\Delta_L^{int} > 0.14$), so that the entire protein becomes liquid-like

	Δ_L (Δ_L^{int}(6Å)) (300K)			
	MD simulations			X-ray data
Proteins	Barnase	Myoglobin	Crambin	Ribonuclease A
all atoms	0.21 (0.12)	0.16 (0.11)	0.16 (0.09)	0.16 (0.12)
backbone atoms only	0.16 (0.10)	0.12 (0.09)	0.12 (0.08)	0.13 (0.10)
side-chain atoms only	0.25 (0.14)	0.18 (0.12)	0.19 (0.10)	0.19 (0.13)

Table 1. The heavy-atom Δ_L (Δ_L^{int}) value, for four proteins at 300K; After Zhou et al (1999)