Alanine dipeptide

Molecular dynamics simulation

The terminally blocked alanine peptide Ace-Ala-Nme has been modeled by the OPLS force field [1] with the program Gromacs 3.3.1 [2] and solvated with TIP4P waters [3]. A Langevin MD simulation has been performed at 400K with a friction coefficient of 5 ps^{-1}. In order to set up the CMN, a single trajectory of 250 ns has been analyzed with conformations saved every 0.01 ps (5 MD steps).

Direct inter-basins transitions

An extension of Table 2 of main text is shown in Table S2 with the whole data for the direct transitions.

Table S2. Characteristic times for direct transition inter-basins.

$a \rightarrow b$	$1/k_{ba}$ (ps)		
$C_{7eq} \rightarrow C_5$	0.66	$\alpha' \rightarrow C_5$	1.35
$C_{7eq} \rightarrow \alpha_R$	3.32	$\alpha' \rightarrow C_{7eq}$	3.48
$C_{7eq} \rightarrow \alpha'$	10.80	$\alpha' \rightarrow \alpha_R$	0.30
$C_{7eq} \rightarrow \alpha_L$	1968.34	$\alpha' \rightarrow \alpha_L$	400.57
$C_5 \rightarrow C_{7eq}$	0.33	$C_{7ax} \rightarrow C_5$	6.63
$C_5 \rightarrow \alpha_R$	98.25	$C_{7ax} \rightarrow \alpha_R$	815.87
$C_5 \rightarrow \alpha'$	2.11	$C_{7ax} \rightarrow \alpha_L$	0.78
$C_5 \rightarrow C_{7ax}$	393.75	$\alpha_L \rightarrow C_5$	1213.40
$C_5 \rightarrow \alpha_L$	51187.87	$\alpha_L \rightarrow C_{7eq}$	88.24
$\alpha_R \rightarrow C_5$	110.28	$\alpha_L \rightarrow \alpha'$	58.47
$\alpha_R \rightarrow C_{7eq}$	1.88	$\alpha_L \rightarrow C_{7ax}$	4.80
$\alpha_R \rightarrow \alpha'$	0.54		
$\alpha_R \rightarrow C_{7ax}$	58011.74		

References

1. Jorgensen WL, Maxwell DS, Tirado-Rives J (1996) Development and testing of the opls all-atom force field on conformational energetics and properties of organic liquids. J Am Chem Soc 118: 11225–11236.

2. Van Der Spoel D, Lindahl E, Hess B, Groenhof G, Mark AE, et al. (2005) Gromacs: fast, flexible, and free. J Comput Chem 26: 1701–1718.

3. Jorgensen WL, Chandrasekhar J, Madura JD, Impey RW, Klein ML (1983) Comparison of simple potential functions for simulating liquid water. J Chem Phys 79: 926–935.