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# Chain length, temperature and solvent effects on the structural properties of α-aminoisobutyric acid homooligopeptides

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# Content

**Table S1**. Averaged intramolecular hydrogen bonds[a] (in Å) as issuing from MD simulations of Aib homopeptides.

| helix | solvent | H1 | H2 | H3 | H4 | H5 | H6 | H7 | H8 | H9 |
|---|---|---|---|---|---|---|---|---|---|---|
| Ac-$(Aib)_{10}$-NMe | | | | | | | | | | |
| $3_{10}$ | water | 3.25 | 3.27 | 3.27 | 2.29 | 3.29 | 3.27 | 3.28 | 3.27 | 3.19 |
| α | water | 3.15 | 3.25 | 3.25 | 3.25 | 3.25 | 3.25 | 3.25 | 3.25 | |
| Ac-$(Aib)_7$-NMe | | | | | | | | | | |
| $3_{10}$ | water | 3.27 | 3.26 | 3.24 | 3.27 | 3.20 | 3.28 | | | |
| α | water | 3.25 | 3.24 | 3.25 | 3.10 | 3.25 | | | | |
| Ac-$(Aib)_7$-NMe | | | | | | | | | | |
| $3_{10}$ | DMSO | 3.20 | 3.23 | 3.23 | 3.21 | 3.15 | 3.23 | | | |
| α | DMSO | 3.22 | 3.20 | 3.23 | 3.11 | 3.22 | | | | |
| Ac-$(Aib)_6$-NMe | | | | | | | | | | |
| $3_{10}$ | water | 3.26 | 3.27 | 3.27 | 3.27 | 3.27 | | | | |
| α | water | 3.16 | 3.24 | 3.25 | 2.92 | | | | | |
| Ac-$(Aib)_5$-NMe | | | | | | | | | | |
| $3_{10}$ | water | 3.35 | 3.39 | 3.37 | 3.31 | | | | | |
| α | water | 3.11 | 3.15 | 2.91 | | | | | | |

[a] Distances are between the donor nitrogen and the acceptor oxygen (N…O)

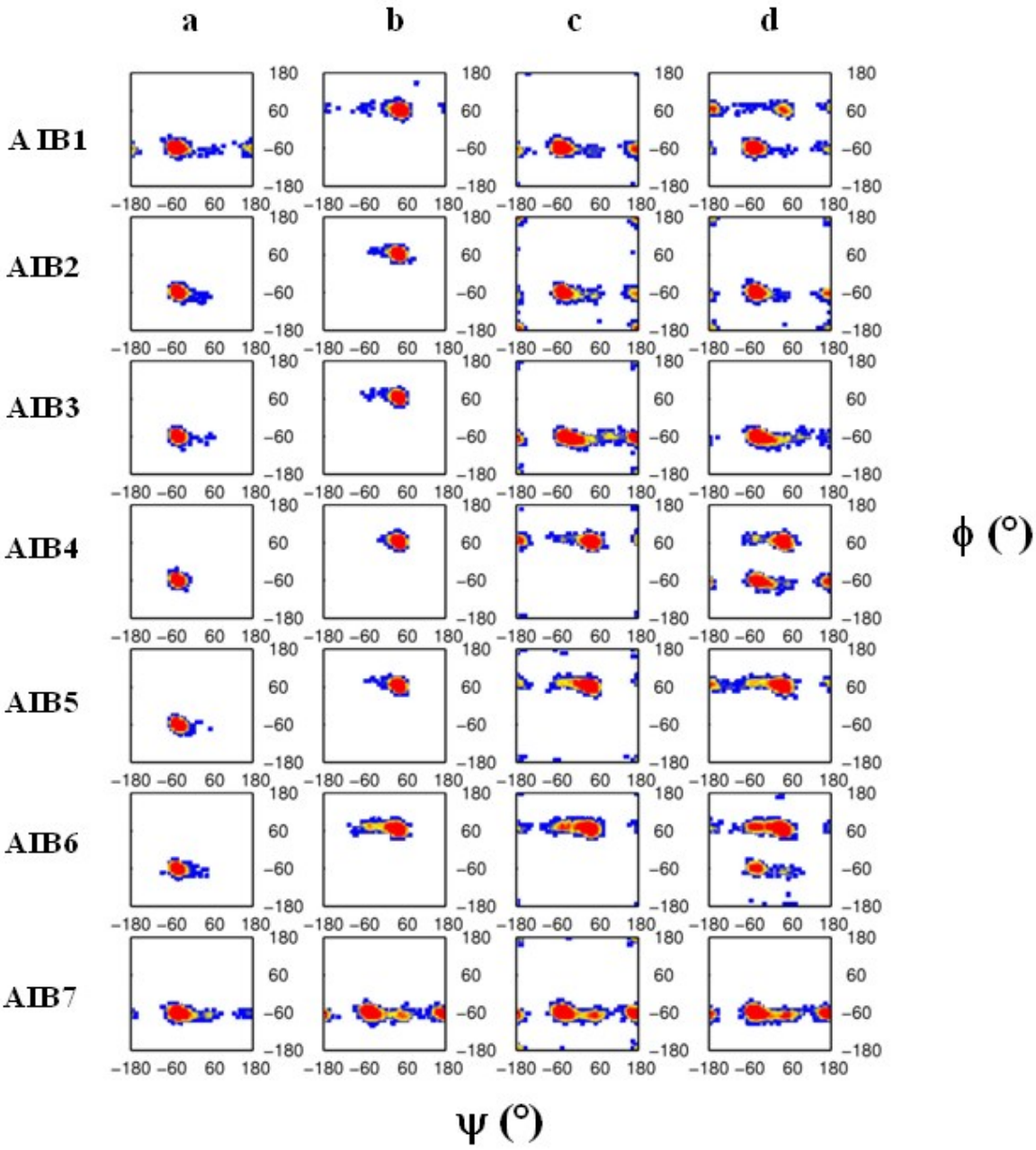


**Figure S1.** Ramachandran plots of all residues (from base up) for the 1-100ns simulations at 300 K with four different initial configurations: (a) random coil, (b) right-handed α-helix, (c) fully-extended conformation and (d) right-handed semi-extended conformation. Red and blue regions correspond to the highest and lowest population density, respectively.

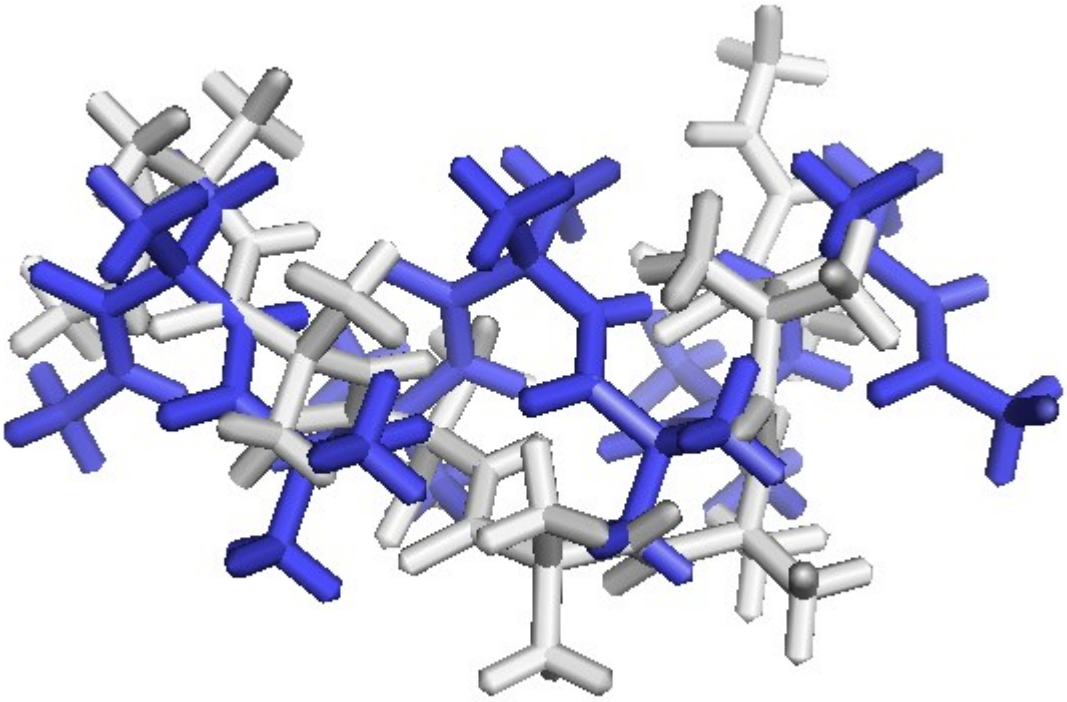

**Figure S2.** Superposition of the initial $3_{10}$ structure (blue) and the representative unfolded structure (grey) taken at 60 ns of the 400 K MD simulation in water.

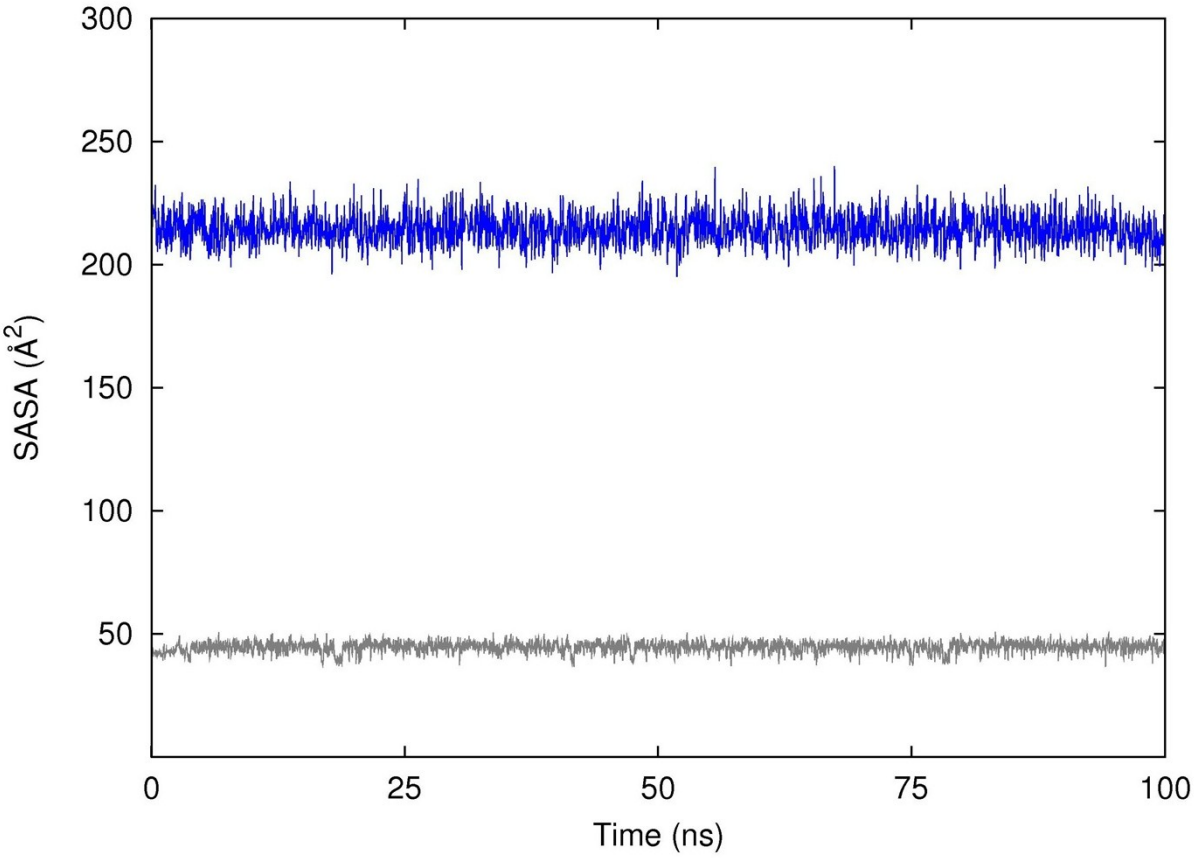


**Figure S3.** Solvent accessible surface areas (SASA's) of the Aib heptapeptide as issuing from the MD simulation at room temperature (grey line, water; blue line, DMSO).

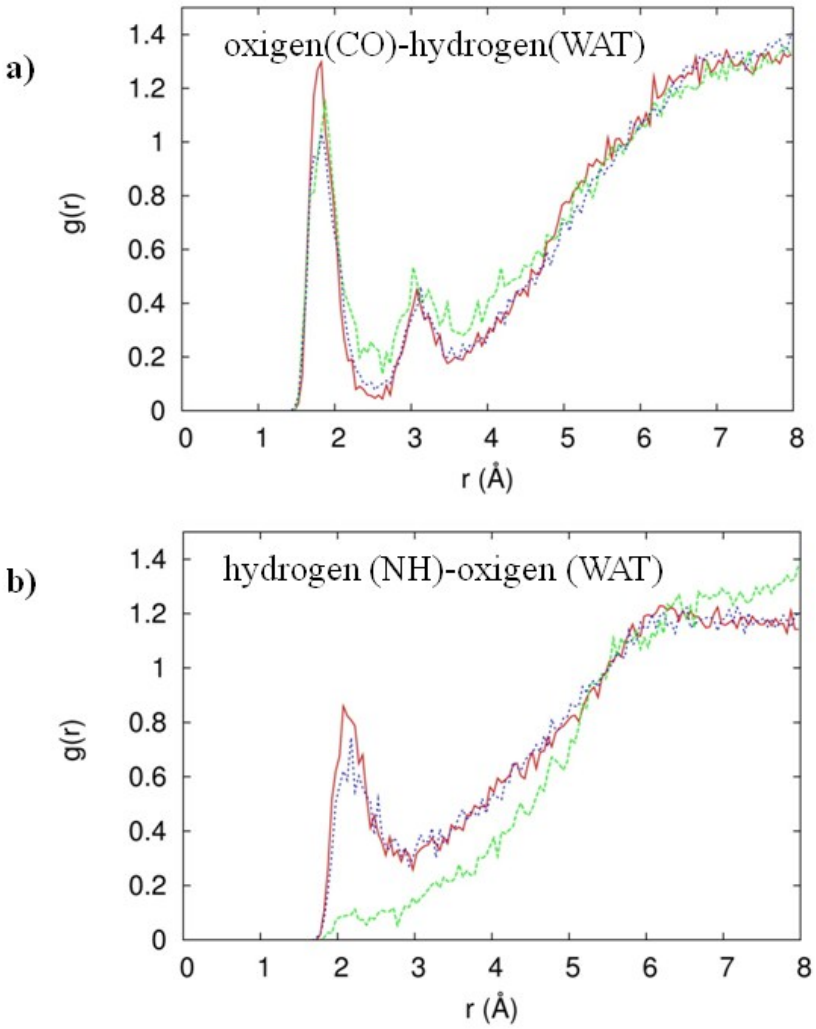


**Figure S4.** Radial distribution functions of the hydrogen and oxigen atoms of water around the selected CO (a) and NH (b) groups of the Aib heptapeptide as issuing from the 1-100ns MD simulation at 300 K (red curves), 350 K (blue curves) and 400 K (green curves) .

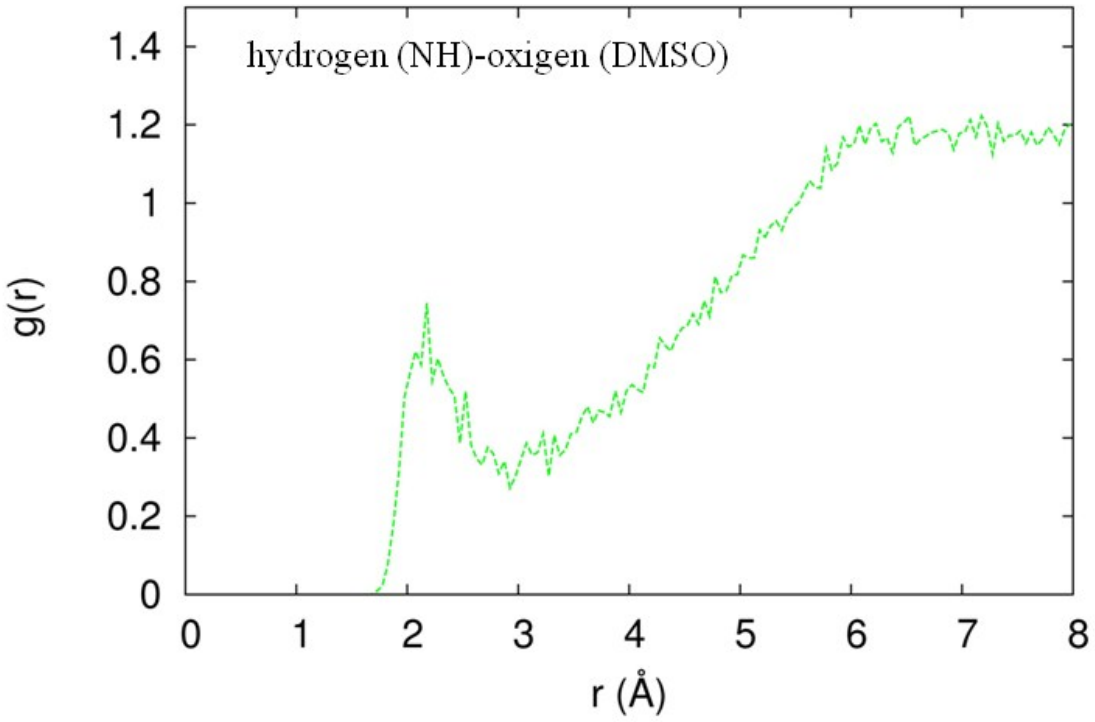


**Figure S5.** Radial distribution function of the oxigen atom of DMSO around the selected NH group of the Aib heptapeptide as issuing from the 1-100ns MD simulation at 300 K.