An easy way to include weak alignment constraints into NMR structure calculations

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We have recently shown that an energy penalty for the incorporation of residual tensorial constraints into molecular structure calculations can be formulated without the explicit knowledge of the Saupe orientation tensor (Moltke and Grzesiek. J. Biomol. NMR, 1999, 15, 77-82). Here we report the implementation of such an algorithm into the program X-PLOR. The new algorithm is easy to use and has good convergence properties. The algorithm is used for the structure refinement of the HIV-1 Nef protein using 252 dipolar coupling restraints. The approach is compared to the conventional penalty function with explicit knowledge of the orientation tensor's amplitude and rhombicity. No significant differences are found with respect to speed, Ramachandran core quality or coordinate precision.
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