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Improved B-factor Restraint Models for Macromolecular Structure Refinement. Mark White, HBC&G, UTMB, 301 University, Galveston, TX 77555-0647 USA.

Improved models of B-factor restraints are described with specific application to several structures shown. An empirically derived variable sigma model for isotropic B-factor restraints has been used to refine several macromolecular structures. This model has been optimized to be independent of data resolution or quality. The model of restraint used for non-crystallographic symmetry (NCS) related atoms was similarly modified to permit each group's average B-factor to float, while restraining deviations from the average to be similar for all groups. In each case optimization of these restraints lead to a significant decrease in the free R factor, indicating that previously the refinement was over restrained. These restraint models have been implemented in the refinement program CNS {Brunger, 1997}, and are easily applicable to any protein structure refinement.