

## Publication

## Analysis of alpha-helical coiled coils with the program TWISTER reveals a structural mechanism for stutter compensation

**JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)****ID** 155488**Author(s)** Strelkov, Sergei V; Burkhard, Peter**Author(s) at UniBasel** [Burkhard, Peter](#) ;**Year** 2002**Title** Analysis of alpha-helical coiled coils with the program TWISTER reveals a structural mechanism for stutter compensation**Journal** Journal of structural biology**Volume** 137**Number** 1-2**Pages / Article-Number** 54-64**Keywords** coiled coil, computer program, Crick parameters, heptad repeat, protein conformation, skips, stutters

Alpha-helical coiled coils represent a widespread protein structure motif distinguished by a seven-residue periodicity of apolar residues in the primary sequence. A characteristic "knobs-into-holes" packing of these residues into a hydrophobic core results in a superhelical, usually left-handed, rope of two or more alpha-helices. Such a geometry can be parameterized. For this purpose, a new computer program, TWISTER, was developed. With the three-dimensional coordinates as input, TWISTER uses an original algorithm to determine the local coiled-coil parameters as a function of residue number. In addition, heptad positions are assigned based on structural criteria. It is known that frequently encountered discontinuities in the heptad repeat, such as stutters and skips, can be tolerated within a continuous coiled coil but result in a local distortion of its geometry. This was explored in detail with the help of TWISTER for several two- and three-stranded coiled coils. Depending on the particular protein, stutters were found to be compensated locally by an unwinding of the superhelix, alpha-helical unwinding, or both. In the first case, there is often a local switch from a left-handed to a right-handed superhelix. In general, the geometrical distortion is confined to about two alpha-helical turns at either side of the stutter. Furthermore, stutters result in a local increase of the coiled-coil radius.

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