

BetaPrec Instructions

- for calculating the precession of the modeled ideal β -helices

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BetaPrec is an m-file script written to be run in Matlab™. It is designed for calculating the precession of modeled ideal β -helices.

It consists of a main function named betaprec, and 10 other functions, each in their own file with the same name as the function and with the extension “.m”.

The syntax for running the script from within Matlab is:

`betaprec(skip, number, length, source, results)`

where:

`skip` = number of half creps to skip at the start
`number` = number of creps used to calculate precession
`length` = number of residue units in each length (equivalent to number of inward pointing hydrophobic residues along the length (uses the two C^α 's on either side))
`source` = PDB file (including path) of protein
`results` = file (including path) to which the results will be appended

The program outputs the coordinates of the C^α atoms in each β -strand; it then displays the equations describing the line that has been fitted to these coordinates. That is, the line in the XY plane and the line in the ZY plane - which completely describes the line in 3D. It then shows a vector derived from this line, and finally, the angles between the vectors.

The lines are in the form:

$$c + n_1x + n_2y = 0$$

$$d + m_1z + m_2y = 0$$

In the output file, the angle between the first and last line is calculated and displayed as TotalB and TotalT for the bottom and top respectively.

Note: A β -strand is defined as *length* residue units following a Glycine residue. This can be easily modified to any other residue in the file `getLength.m`.