

## Helixator Instructions

The program will enable you to create helices of C $\alpha$  atoms. The helices can be made up of any number of repeated units where one repeated unit comprises a  $\beta$  strand of variable length and a turn of variable number of C $\alpha$  atoms. The user is required to enter a number of parameters such as length of strand, relative angle between strands, number of atoms in a turn etc.

When entering parameters, it is important to understand how the script is implemented:

The script will implement right handed coils to have strands that rotate clockwise about z (looking down from +ve z), and vice versa for left handed. For consistency, choose turn parameters that cause the helix to grow in the negative z direction. I.e. the helical axis is meant to be in the -ve z direction. Although a right handed helix may not come out right handed due to the turn parameters entered, these are general rules which must be kept in mind when creating helices to retain consistency.

The local coordinates changes per strand. The turns are measured relative to the co-ordinate system of the preceding strand.

For a turn following a strand:

- The strand is in the +ve y direction
- The helical axis is in the negative z direction
- x is inferred from these

## Parameters

The parameters are entered within braces, with a comma in between.

Terminology

$T_n$	=	Turn number n
$P_n$	=	Point number n
$S_n$	=	Strand number n

### **Turn Parameters**

#### Alpha

- $-90 < \text{Alpha} < 90$
- angle in XY plane
- Measured from +ve y axis
- +ve btwn x and y, -ve btwn y and -ve x

$T\text{AlphaDEG} = \{\{T_1\}, \{T_2\}, \dots, \{T_n\}\};$

#### ThetaZX

- $0 < \text{ThetaZX} < 180$
- angle in ZX plane :

- measured from +ve z axis
- $T_{\theta ZXDEG} = \{\{T_1\}, \{T_2\}, \dots, \{T_n\}\};$

#### pTsLength

- Length of turn
- Used when one wants to approximate a turn quickly, without putting in every  $\alpha$ .
- If using a real bond, should be a distance of 3.79

$pTsLength = \{\{T_1P_1, T_1P_2, \dots, T_1P_n\}, \{T_2P_1, T_2P_2, \dots, T_2P_n\}, \dots, \{T_nP_1, T_nP_2, \dots, T_nP_n\}\};$

### **Strand Paramters**

#### SpsiDEG

- angle of elevation of strand in degrees
- -ve is toward helical axis

$SpsiDEG = \{S_1, S_2, \dots, S_n\}$

#### SAngleDEG

- Angle of strand relative to preceding strand in degree
- Should be between 0 and 180
- The sign is ignored

$SAngleDEG = \{S_1, S_2, \dots, S_n\}$

#### k

- Indicates which direction the segments ( $\alpha$ - $\alpha$  bonds) of a strand will rotate
- 1 = First segment rotates towards centre
- -1 = First segment rotates outwards

$k = \{S_1, S_2, \dots, S_n\}$

#### ruNumS

- Number of residue units for repeated strand
- Consists of three  $\alpha$ s in a triangle ( two segments)
- can ONLY be multiples of 1/2
- each unit = 6.6 Å

$ruNumS = \{S_1, S_2, \dots, S_n\}$

### **General**

#### L

- Indicates left handed or right handed helix
- -1 = right handed
- 1 = left handed

#### Converting

- If the parameters have been entered for a handedness, and then the complimentary opposite handed helix is desired, this is set to 1 (TRUE), and then the turns do not have to be re-entered differently. Otherwise just leave as -1 (FALSE).

#### Resid

- The sequence of amino acids

### Repeat

- Number of iterations of the repeating units

### Improvements

- Add the option of estimating a turn, or putting in every point.