**ZAŁOŻENIA:**

**Zaimplementowanie następujących funkcji z biblioteki FR3D w pythonie:**

**xDiscrepancyFast**

xDiscrepancy(Model,Cand) calculates the discrepancy between Model and Cand, which is an array of NT's.

One must take the square root and divide by the number of nucleotides after.

As soon as the discrepancy exceeds Model.RelCutoff, the calculation stops.   
 The current sum is returned as a negative discrepancy, shifted to record when the calculation stopped.

# zAnalyzePair

zAnalyzePair(N1,N2,CL) computes distances, angles, and classification codes.

**zAngle**

zAngle(A,B,C) computes the angle at B made by vectors BA and BC

# zAngleOfRotation

zAngleOfRotation calculates the angle of rotation from a rotation matrix R

A good online reference is:

http://www.mathworks.com/access/helpdesk/help/toolbox/physmod/mech/mech\_review7.html

# zAxisAngle

zAxisAngle(R) computes the axis and angle of rotation in an orthogonal matrix R, then makes the axis point up and the angle be between -90 and 270 degrees

# zAxisAngleRadians

zAxisAngleRadians computes the axis and angle of rotation in an orthogonal matrix R

# zBestRotation

zBestRotation(X,Y) finds the least squares rotation of points X onto points Y

X and Y are n by 3 matrices containing the locations of corresponding points   
 What is returned is the best fit to Y = X\*R'

R is the 3x3 rotation matrix

# zCheckCutoffs

zCheckCutoffs(D,Normal,Ang,Gap,B) finds the categories whose cutoffs include the given displacement D, Normal, angle Ang, and Gap, according to the cutoffs in matrix B

# zCheckHydrogen

This program is generated by zGenerateCheckHydrogen.m based on the Excel file H\_bonding\_Atoms\_from\_Isostericity\_Table.xls created by Jesse Stombaugh.

zCheckHydrogen(NT1,NT2,Class) computes the angles and distances in the hydrogen bonds between two nucleotides assuming their interaction is Class

The program calls the base that should be at the origin N1, the other N2

# zClassLimits

zClassLimits stores the cutoffs for the computer classification of pairs according to displacement, normal vector, and angle of rotation. As such, it is the repository of expert knowledge of pair classifications.

# zClassifyPair

zClassifyPair(N1,N2) calculates the rotation matrix, axis, angle, and shift between bases in File that are close enough to possibly be interacting, then classifies the interaction

# zClassifyPairs

zClassifyPairs(File) calculates the rotation matrix, axis, angle, and shift between bases in File that are close enough to possibly be interacting, then classifies the interaction

# zDistance

zDistance(A,B) finds the Euclidean distances between the rows of A and of B

# zDistanceToExemplars

zDistanceToExemplars(Exemplar,Pair) computes the distance to each exemplar for the given pair of nucleotides

# zEdgeText

zEdgeText converts internal codes for pair interactions into text

# zStackingOverlap

zStackingOverlap(N1,N2) computes a measure of overlap between nucleotides N1 and N2, by projecting N2 onto the plane of N1.

do unikalnych funkcji dla matlaba zastosowanie biblioteki NumPy