**rotamer2.h**

**rotate**

1) move atom j to origin2) execute rotations around axes until atom l is at (xl,yl,0), atom k is at (xk,0,0)3) compute coords of i in this frame4) transform i back to original frame; j no longer at origin**Inputs**

**(int iatom, int jatom, int katom, int latom, double r, double theta, double phi)**

iatom, jatom, katom and latom are the index used to represent 4 atoms.

r – bond length.

theta – Bond angle.

Phi – phi angle (torisional).

**Defined Variables:**

Nil

**Undefined Variables:**

cart\_pdb – Cartesian co-ordinates of the atoms.

**Function calling:**

Nil.

**Int2xyz\_one**

It takes the input of z matrix, ith atom and gives the output of Cartesian co-ordinate of the ith atom.

**Inputs:**

(DMT & zmat, int iatom)

zmat – zmatrix

iatom – atom index to represent ith atom and based on this index other three atoms will be fixed.

**Outputs:**

DMT & cart\_pdb

Cart\_pdb – Cartesian co-ordinates.

**Defined Variables:**

int jatom, katom, latom;

jatom, katom and latom – are atom indexes that has been used to refer the atom from parent.

**Undefined Variables:**

parent

**Function calling:**

rotate

**rotamatrix.h**

It creates the rotation matrix for a given angle theta and the reference axis.

**Inputs:**

(DVC axis, double theta)

axis – reference axis.

theta – rotation angle.

**Outputs:**

rotation

**Defined Variables:**

DMT rotation(3,3)

**Undefined Variables:**

NIL

**Function calling:**

NIL

**get\_side\_atoms**

**Inputs:**

(int ires, int & ilo, int & ihi, IVC &irank)

Ires – ith residue.

ilo and ihi – lower and upper limit for the atoms and their reference.

Irank -

**Outputs:**

nil

**Defined Variables:**

unsigned int ilo\_res, iatom;

unsigned int ihi\_res;

**Undefined Variables:**

NIL

**Function calling:**

NIL

**get rotatable bonds**

* It gets the input of ilow, ihigh and ires and calculated the chi angle for all the atoms from ilow to ihigh.
* Once it calculates the chi angles, then, it creates torsion angle lists using Z matrix. ( z matrix is not originally inputted in this function).

**Inputs:**

(int ires, unsigned int ilo, unsigned int ihi)

ires – ith residue,

ilo and ihi – lower and upper limit for the atoms and their reference.

**Outputs:**

tor\_list\_res

**Defined Variables:**

int iatom,iang,itype,rtype;

iatom – ith atom

iang – ith angle

itype – type of the residue

rtype -

**Undefined Variables:**

iatom\_chi

mtype

rotamer\_libs

rname\_pdb

aname\_pdb, aname\_chi1, aname\_chi2, aname\_chi3, aname\_chi4, iang

tor\_list\_res

rotamer\_libs

**Function calling:**

NIL

int2xyz\_update\_simple

* It uses get rotatable bonds and get sides atoms functions.
* This function is not used anywhere.
* Seems, it is not completed.
* Don’t know how it finds the new rotation co-ordinates.

Int2xyx

* It gets the z matrix and lists of atom
* Tries to calculate the Cartesian co-ordinates of each atom using the function int2xyz\_one.
* It is not completed.

Load\_lib

* It deals with reading the rotamer library.

add\_side\_rot

* It reads the torsion angle list from the rotamer library.
* It uses get rotatable bonds and get sides atoms functions.