**Input file for the rotamer2.h**

This file calculates the Cartesian co-ordinates (cart\_pdb) for a given protein sequence (side chain) with its internal co-ordinates or z-matrix (zmat) such as bond length (rij), bond angle (theta) and torsional angles (phi, psi, chi).

The internal co-ordinates of the side chain (ires) are sampled from the rotamer library (rotamer\_lib). Rotamer library will have all possible torsional angles (tor\_list\_res – we will generate this from the rotamer library). Essentially protein design problem is to find an optimal side chain that maximizes the binding affinity. For an assumed side chain, rotamer library will give the internal co-ordinates (zmat) and rotamer2.h file will convert them in to Cartesian co-ordinates.

**The flow of the algorithm is as follows.**

Load the rotamer libraries using a single .lib file.

This file should have different types of rotamer library and each rotamer library has an array with name, nrot, nang, ilo, gridres, igraph.

get\_side\_atoms

This file should be supplied with the residue number which needs to be considered for the conversion of internal to Cartesian co-ordinates.

get\_rotatable\_bonds

Loop iatom from ilo to ihi (returned from get\_side\_atoms); for each iatom loop over ichi; check iatom's unique name, if matches atom name assigned to chi angle, assign iatom to ichi

For a given atom name, it gets the possible torsional angles from the rotamer library.

add\_side\_rot

int2xyz\_update\_simple

This file will creat the Z matrix from the get\_side\_atoms and get\_rotatable\_bonds and converts them in to internal co-ordinates.

int2xyz\_one

For a given Z matrix of main chain (bond angle, bond length and torsional angle) this file converts internal co-ordinates of 1 residue in to Cartesian co-ordinates. This file also calls the rotate which rotate the atom to the fixed reference co-ordinates.

Int2xyz

This file calls int2xyz\_one for each residue and converts their internal co-ordinates in to Cartesian co-ordinates.

rotate

This file rotates the given atoms to the reference co-ordinate so that the calculation for the conversion of internal to Cartesian co-ordinates is easy.