**bond\_angle (DVC &carti, DVC &cartj, DVC &cartk)**

For a given 3 atom with it's coordinates, bond\_angle function calculates the angle between two bonds with respect to the centre atom.

**Inputs:**

(DVC &carti, DVC &cartj, DVC &cartk)

carti, cartj and cartk - Co-ordinates of the three different atoms in cartesian co-ordinates.

Atom's coordinates has been taken as input in vector forms. carti, cartj and cartk are the co-ordinates of the atoms or the position vectors.

**Defined Variables:**

dij = difference between i and j co-ordinates - vector

dik = difference between i and k co-ordinates - vector.

dotrprod = dot product between two vectors.

rij = length between two points that has been represented by cartesian co-ordinates.

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**tors\_angle (DVC &carti, DVC &cartj, DVC &cartk, DVC &cartl)**

For a given 4 atom, dihedral\_angle calculates the dihedral angle.

**Inputs:**

**(DVC &carti, DVC &cartj, DVC &cartk, DVC &cartl)**

carti, cartj, cartk and cartl - Co-ordinates of the 4 different atoms in cartesian co-ordinates.

**Defined Variables:**

dij = difference between i and j co-ordinates - vector

djk = difference between i and k co-ordinates - vector.

djl = difference between j and l co-ordinates - vector.

cross\_prod\_1 - Cross product between two vectors - vector

cross\_prod\_2 - corss product between two vectors - vector

rijk - dot product between cross\_prod\_1 - scalar

rjkl - dot product between cross\_prod\_2 - scalar

dotprod - dot product between cross\_prod\_1 and corss\_prod\_2 - scalar

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**zmat\_atom (int iatom, int jatom, int katom, int latom, double & rij, double & theta, double & phi)**

For a given i, j, k and l atom, zmat\_atom function read their cartesian co-ordinates from the pdb file and calaculates their bond length, bond angle and torsional angle.

**Inputs:**

**int iatom, int jatom, int katom, int latom**

iatom, jatom, katom, latom - Number assigned to atoms. This will be useful to locate a particular atom from the pdb file.

**Outputs:**

**double & rij, double & theta, double & phi**

**Defined Variables:**

cart\_i, cart\_j, cart\_l and cart\_k are the cartesian co-ordinates of i,j,k and lth atom and they have been read from the cart\_pdb file using cart\_pbd.slice command.

**Function calling:**

bond\_angle and tors\_angle

================================================================================

**build\_atom(char rname[], int & nbuild, int natom\_res)**

For a given residue name, number of atom in residue and nbuild(I don't know what it is), build\_atom produces parent\_atom and hence parent as well.

**Inputs:**

**(char rname[], int & nbuild, int natom\_res)**

rname - residue name.

nbuild -

natom\_res - number of atom in residue.

**Defined Variables:**

int iatom, iatom\_res, parent\_atom

iatom - ith atom

iatom\_res - ith atom in the residue

parernt\_atom -

**Undefined Variables**

parent -

zmat - zmatrix

zmat\_residue -

**Function calling:**

Nil.

**xyz2int\_atom (int iatom)**

For a given ith atom, this function calculates it's z matrix co-ordinates.

**Inputs:**

**iatom**

iatom - ith atom for which z matrix co-ordinates should be calculated.

**Defined Variables:**

int jatom,katom,latom; double rij,theta,phi;

for a given ith atom, jatom, katom and latom are calculated from the parent.

rij, theta and phi are bond length, bond angle and torisonal angle.

**Undefined Variables**

parent -

zmat - zmatrix

**Function calling:**

zmat\_atom.

**xyz2int (DMT & cart\_pdb, DMT & zmat)**

For a given pdb file, this function calculates the zmatrix of all the atoms.

**Inputs:**

**(DMT & cart\_pdb, DMT & zmat)**

cart\_pdb - pdb file.

zmat - zmatrix.

**Defined Variables:**

int iatom, jatom, katom, latom;

ith atom, jatom, katom and latom are intergers that are used to represent 4 atoms at a time.

**Undefined Variables**

parent -

zmat - zmatrix

**Function calling:**

xyy2int\_atom.

================================================================================

**get\_zmat\_rank (IVC irank\_zmat)**

For a given irank\_zmat, this function calculates the zmatrix rank.

**Inputs:**

**(IVC irank\_zmat)**

irank\_zmat

**Defined Variables:**

num, jatom, katom;

num -

jatom

katom -

**Undefined Variables**

natom -

parent -

**Function calling:**

nil

================================================================================

**backbone\_dihedral (int ires, char rname[])**

For a given ith residue and it's name, this function calcualtes the backbone dihedral angle.

**Inputs:**

**(int ires, char rname)**

ires - ith residue

rname - residue name

**Defined Variables:**

Nil-

**Undefined Variables**

phi - phi angle

psi - psi angle

chi - chi angle

omega - omega angle.

rname\_pdb

**Function calling:**

strcmp

================================================================================

**backbone\_zmat (int ires, char rname[], int sidecnt)**

For a given ith residue and it's name, side chain index this function calcualtes the zmatrix of backbone.

**Inputs:**

**(int ires, char rname, int sidecnt)**

ires - ith residue

rname - residue name

sidecnt - Side chain index.

**Defined Variables:**

Nil-

**Undefined Variables**

zmat\_residue

parent\_residue

**Function calling:**

Nil

================================================================================

**readres(const char \* filename, int ires)**

This reads atom info; also need to read bond, angle, torsion

Necessary even if reading seq from file to assign parents and initialize zmatrix

**Inputs:**

**(const char \* filename, int ires)**

filename - pdb file na,e

ires - ith residue in the pdb file.

**Defined Variables:**

int iatom\_res, iatom\_side;

char atom\_name[6], atom\_type[6], itree\_res[6];

char line[255]

int nbond\_res , iatom\_res, iatom\_side, num, atomnum

double chg;

char dummy[10], dummy2[10];

double ri, phii, psii;

iatom\_res - reference atom in the ith residue.

iatom\_side - reference atom in the corresponding side chain.

atom\_name - atom name that should be represented by 6 letters.

atom\_type - type of the atom - don't know

itree\_res -

line[255] = line 255 in the pdb file.

nbond\_res - number of bonds in the ith residue.

chg -

num -

atomnum - atom number.

ri - ith bond length

phii - ith phi angle

psii - ith psi angle.

**Undefined Variables**

natom\_res

zmat\_res

parent\_residue

rname\_pdb

sidecnt

**Function calling:**

sscanf, strcmp, fgets, fopen

backbone\_dihedral, backbone\_zmat , readres,build\_atom

================================================================================

**get\_atom\_ranks (IVC &irank, IVC &first\_atom\_res)**

This function calculates the atom rank for all the atoms.

**Inputs:**

**(IVC &irank, IVC &first\_atom\_res)**

irank

first\_atom\_res - First atom in the residue

**Defined Variables:**

unsigned int ilo\_res, ihi\_res;

unsigned int iatom,jatom,rank;

ilo\_res - Residue number from one end.

ihi\_res - residue number another end.

iatom, jatom and katom - reference atoms.

**Undefined Variables**

aname\_pdb

parent\_residue

**Function calling:**

strcmp

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