

structure.h

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

zmat\_atom  
bond\_angle.h, tors\_angle.h  
cart\_pdb.slice  
(int iatom, int jatom, int katom, int latom)  
(double &rij, double &theta, double &phi)

xyz2int\_atom  
zmat\_atom  
cart\_pdb.slice  
(int iatom)  
int jatom, katom, latom;  
double rij, theta, phi;  
zmat

xyz2int  
xyz2int\_atom  
zmat.resize  
cart\_pdb.slice  
(DMT & cart\_pdb, DMT & zmat)  
int iatom, jatom, katom, latom;  
parent

get\_zmat\_rank  
irank\_zmat.resize  
(IVC irank\_zmat)  
int num=0, iatom, jatom=-1, katom;  
parent

backbone\_dihedral  
strcmp  
(int ires, char rname[])  
int num=0, iatom, jatom=-1, katom;  
phi, psi, chi, omega, ires, rname\_pdb

backbone\_zmat  
strcmp  
(int ires, char rname[], int sidecnt)  
int num=0, iatom, jatom=-1, katom;  
zmat\_res, parent\_res, phi, psi, omega

build\_atom  
(char rname[], int &nbuild, int natom\_res)  
(double &rij, double &theta, double &phi)  
int iatom, iatom\_res, parent\_atom  
parent\_res, parent, zmat, zmat\_res

readres  
sscanf, fgets, fopen, strcmp,  
(const char \* filename, int ires)  
int iatom\_res, iatom\_side;  
char atom\_name[6], atom\_type[6], char line[255],  
itree\_res[6], int nbond\_res; double chg; int num,  
atomnum=0, double ri, phii, psii;  
natom\_res  
zmat\_res, parent\_res

buildres  
backbone\_dihedral.h,  
backbone\_zmat, readres, build\_atom,  
(const char \* filename, int ires)  
int ires, iatom, sidecnt=0;  
string filename;  
phi, psi, omega, chi, zmat, ires, nres, sidecnt,  
nbuild, natom\_res, rname\_pdb, sidecnt, filename

get\_atom\_ranks  
(IVC &irank, IVC &first\_atom\_res)  
unsigned int ilo\_res, ihi\_res  
unsigned int iatom, jatom, rank;  
phi, psi, omega, chi, zmat, ires, nres, sidecnt,  
nbuild, natom\_res, rname\_pdb, sidecnt, filename

Red color - function that has been defined in the same header file is used.  
Brown color - function that has been defined in the some other header file is used.  
Blue color - Input variables.  
Gree color - Output variables.  
Pink color - Variable that has been defined within the function.  
Purple color - Variable that has been defined in some other function.