

Build res file is the main file.

Input : rname_pdb. This has the sequence information(the order of residue).

A for loop in this file reads the i^{th} residue. For each residue backbone_dihedral function initializes phi, psi and omega array based on the index ires. This update action is only for the back bone. The size of phi, psi and omega is equal to the num of residues. nres is equal to the number of residues. Before backbone_dihedral is being called based on the amino acid Sequence letter, the corresponding template file name is updated which is then called when the readres file is called.

After backbone_dihedral is called, backbone Zmat is called. Here, based on the ires(residue number), Zmat_res matrix is initialized and also parent_res array is updated. parent_res is updated based on the number of atoms in the previous side chain(sidecnt). For 1st residue sidecnt is assigned to be zero.

readres file opens the template and updates the zmat_res array (Z-matrix for the residues) and also updates parent_res. Template has bond length, bond angle, phi, psi, number of atoms in a residue.

The size of the parent_res array is 4 plus the number of atoms in the residues. This is because 4 atoms correspond to the backbone. It also calculates the number of atoms in a residue.

Finally build_atom function is called. The input for this function is the number of atoms in the residues(nbuild and ires). nbuild will take zero for the first residue, the value for the nbuild is updated in build_atom. After 1st residue, the value of the nbuild is equal to number of atom in the first residue + 4. Essentially this is equal to the number of atom in side chain and backbone. For each residue it keeps on increasing.

Parent atom is created in build_atom. This array updates all the atoms. At any point on the protein sequence Parent_atom will be given the current position of the atom.

Also here Zmat is created and updated from Zmat_res which was updated based on the template file.

From Parent_atom array, parent array is created and updated for each residue.

Once Parent is updated, then xyz2int_atom gets the zmat using xyz2int, bind_angle, tors_angle functions.