

buildres (function in structure.h)

Inputs:

rname\_pdb (type ??)

nres, number of residues

.tmp, template files for the different amino acids

buildres pseudo code

for i = 1:nres

    call rname\_pdb(i) → *Identify i<sup>th</sup> residue.*

    call filename.tmp → *call i<sup>th</sup> residue's template file.*

    call backbone\_dihedral → *For each residue, their backbone z-coordinates are initiated*

    call backbone\_zmat → *For each residue, zmatrix for residue (zmat\_res) and parent\_res are initialized*

    call readres → *This will update zmat\_res and parent\_res.*

    call build\_atom → *This creates parent\_atom zmat. From parent\_atom, it creates parent.*

end

For a given parent and zmat from buildres, xyzint → calls cart\_pdb (Cartesian coordinates) and updates the z-matrix.