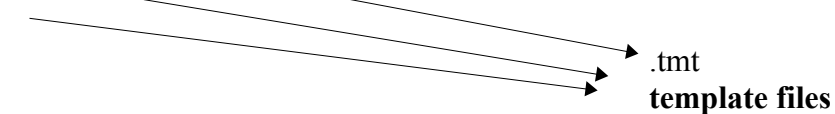


ALA ASP LEU PRO ALA PRO ..... .... LYS PRO  
1 2 3 n-1 n



n = nres

(It has bond angles, bond lengths , Phi, Chi values for a residue)

cart\_pdb

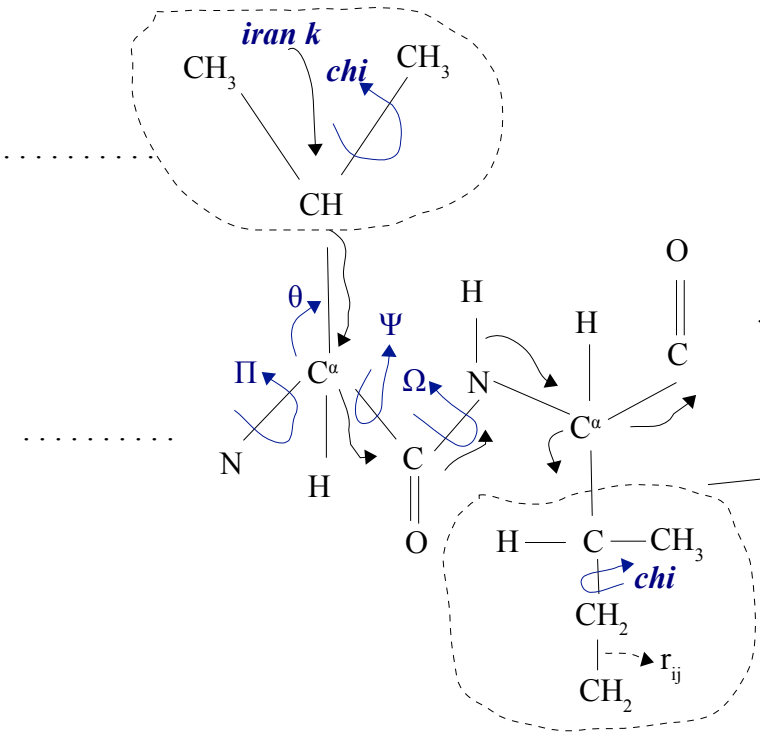
atom

i	x	y	z	cart-i
j				cart-j
k				cart-k
l				cart-l

conversion

Zmat (initialization)

zmat\_backbone  
(r<sub>ij</sub>, phi, theta)

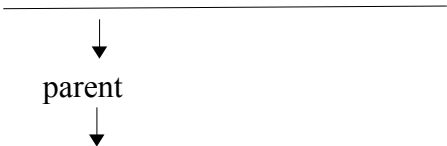


zmat\_res(chi, r, θ)

chi\_res

Parent\_res -----> residue alone

Parent\_atom -----> both residue and back bone



This serves as a reference to update molecules