readPDB.py calculates the contact maps of the protein specified in line 5(pdb structure is needed).

compile and run:

/bin/python3 /home/…/readPDB.py

On output:

1DPX.map: Mapa de contactos a partir de una distancia de corte r\_cut definida en la línea 6.0: i,j,deltaij

1DPX\_elec.map: Mapa de los contactos eléctricos: i,j,q\_ai,q\_aj,r\_aiaj

WSME\_genTden.f90 calculates the thermodynamics of the protein specified in the input file.

compile:

make -f Makefile\_WSME\_genTden

run:

./WSME\_genTden < templateinput\_modified.in

On output:

"thermo" file:

T, M\_avg, (Mavg-M(T=infinity)/(M(T=0)-M(T=infinity)), fractionfolded, F , <E>, S, Cv

where Mavg=<\sum\_i m\_i>,

F=free energy

<E> average energy

S entropy

Cv specific heat

"profile" file:

T, M, F(M)

where M is the number of native residues, F(M) the free energy associated with the sector of the space with M natives

"native strings" file:

T i j mu\_ij nu ij

where mu\_ij=<\prod\_{k=i}^j m\_k >, nu\_ij=<(1-m\_{i-1}) \prod\_{k=i}^j m\_k (1-m\_{j+1}) >