CNS MidSem 2

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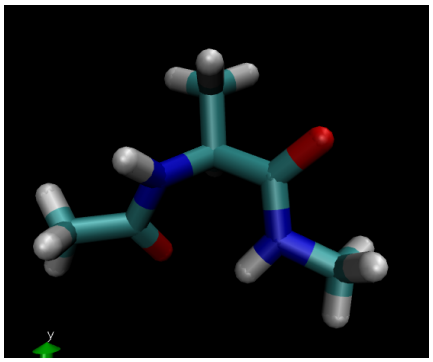
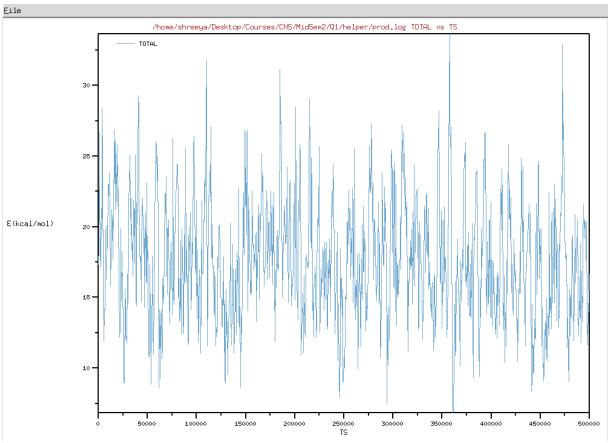
1 MD simulation on Alanine Dipeptide

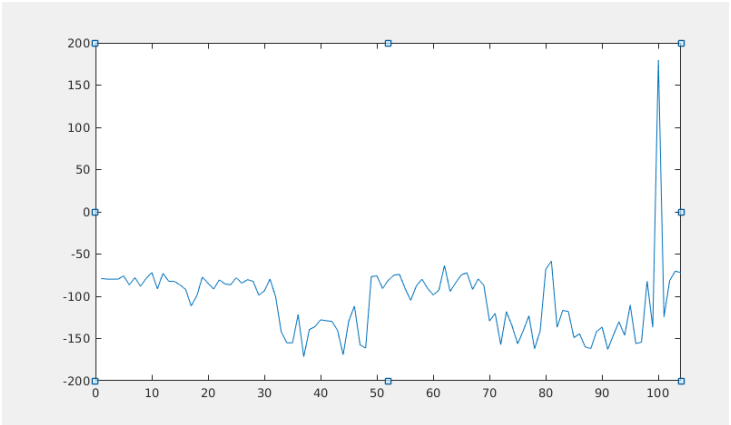
MD simulation was run on Alanine Dipeptide:



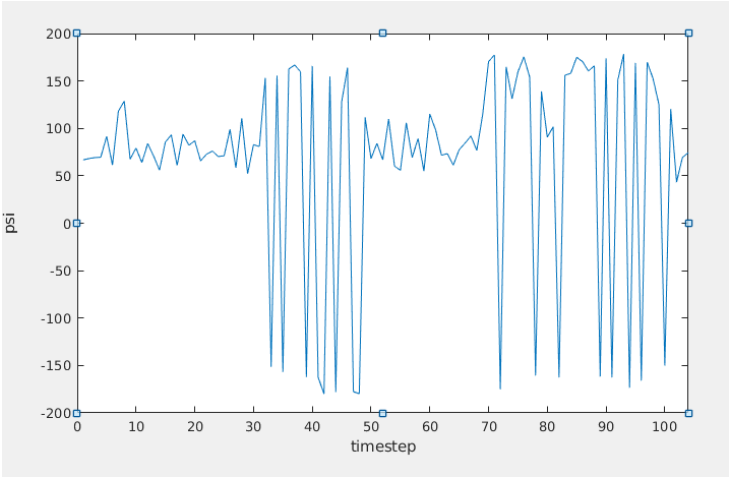
- Energy vs. time



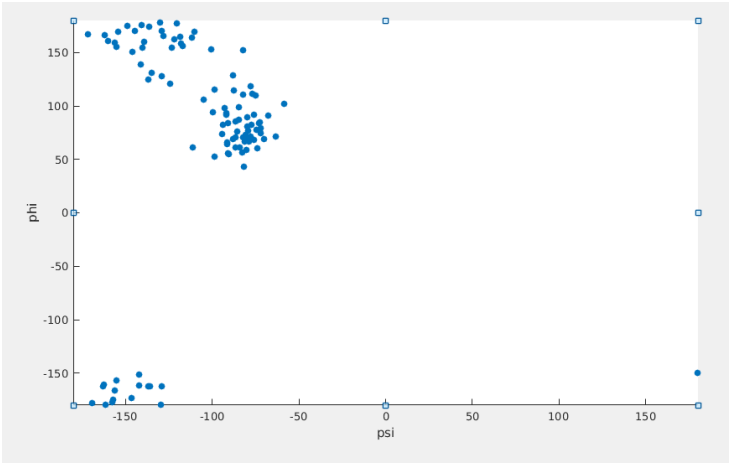
- phi angle vs. time



- psi angle vs. time

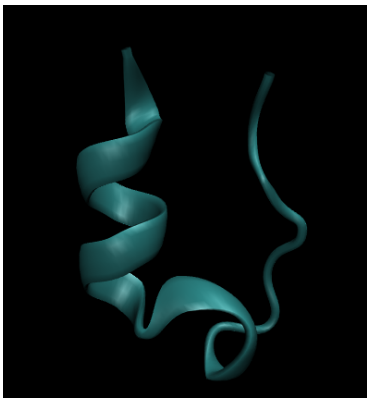


- Ramachandran Plot (using phi and psi values from (b) and (c))



2 Non-bonded Interactions in 1L2Y

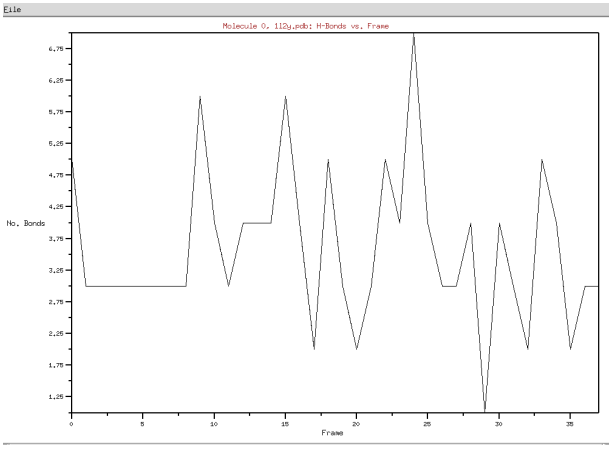
MD simulation was run on given protein 1L2Y:



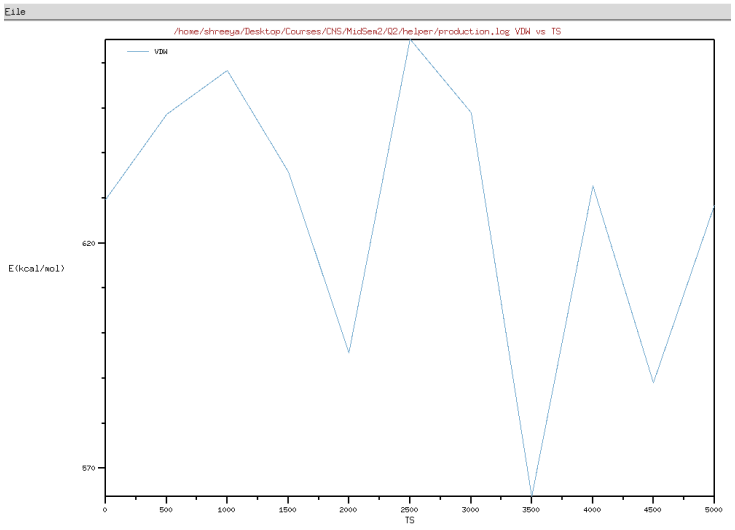
The non-bonded interactions identified were:

- Hydrogen Bonding

  Hydrogen Bond: 2.0 to 3.5 Angstrom (average 3 A)



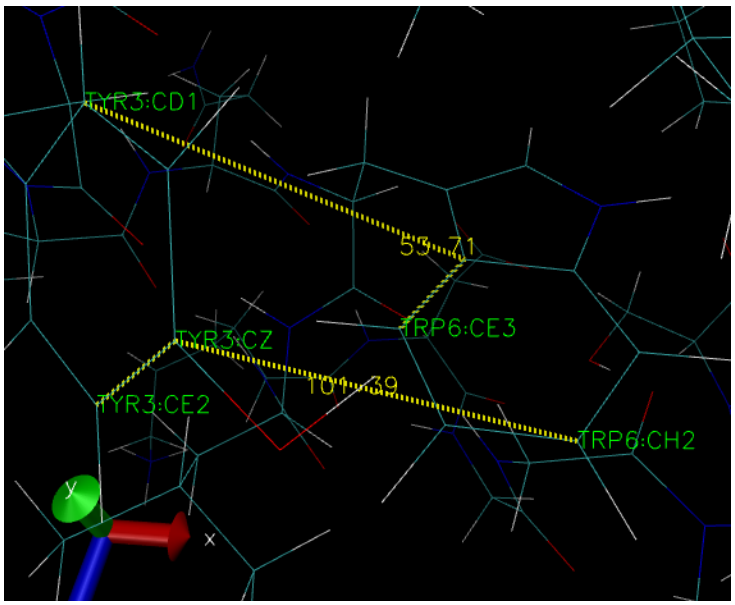
- Vanderwaal Forces



- pi-stacking

  These interactions are included when the maximum distance between ring centers is 5.5 A. The maximum offset of ring centers is 2.0 A (about the radius of benzene plus 0.5 A), the maximum deviation from optimal angle (0 for parallel, 90 for t-shaped) is 30 degree.

  pi-pi stacking exists due to the presence of benzene rings.


TYR3:CD1
5.71
TRP6:CE3
TYR3:CZ
10.39
TYR3:CE2
TRP6:CH2
y
x