BT305 LAB 7

Name: Aditya Jindal
Roll No.: 210106004

1)
1PGB
Initial:
phi & psi angles of 4th residue : -129.838 126.485
phi & psi angles of 8th residue : -86.0263 179.722
Deviation After EM:
phi & psi angles of 4th residue : 7.438 6.42
phi & psi angles of 8th residue : -41.5487 -11.122
Deviation After MD:
phi & psi angles of 4th residue : 19.884 11.112
phi & psi angles of 8th residue : -56.2887 21.131

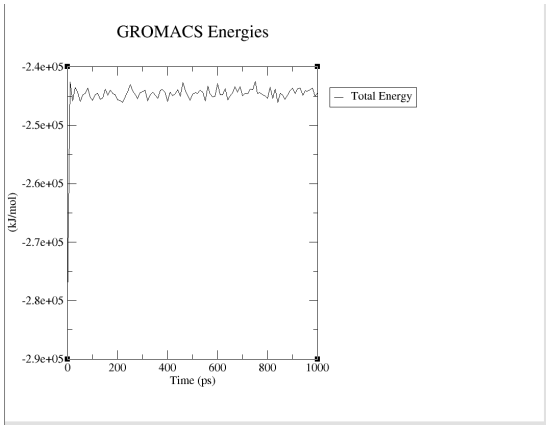
TRP Cage
Initial:
phi & psi angles of 4th residue : -61.5746 -42.7245
phi & psi angles of 8th residue : -73.2076 -18.7175
Deviation After EM:
phi & psi angles of 4th residue : 7.3421 8.5531
phi & psi angles of 8th residue : 3.9723 -9.5835
Deviation After MD:
phi & psi angles of 4th residue : -4.7935 11.4069
phi & psi angles of 8th residue : -96.2384 128.3735

Alpha-Helix
Initial:
phi & psi angles of 4th residue : -64.6311 -34.1108
phi & psi angles of 8th residue : -61.6178 -42.1426
Deviation After EM:
phi & psi angles of 4th residue : 11.6488 -7.0309
phi & psi angles of 8th residue : 3.2649 -13.0852
Deviation After MD:
phi & psi angles of 4th residue : 18.9604 -41.948
phi & psi angles of 8th residue :8.5922 -2.2798

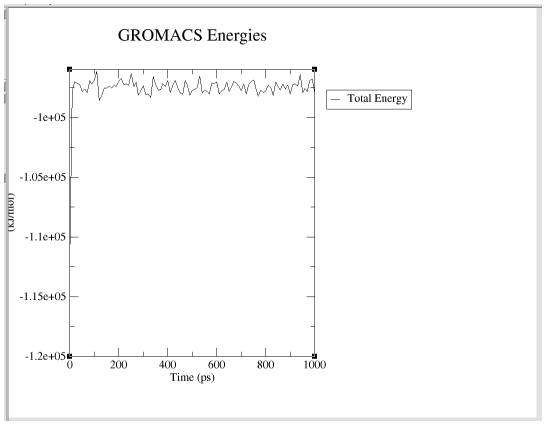
Beta-Sheet

Initial:
phi & psi angles of 4th residue : -103.326 122.067
phi & psi angles of 8th residue : -72.7477 -36.7
Deviation After EM:
phi & psi angles of 4th residue : 17.3887 5.357
phi & psi angles of 8th residue : 5.4159 3.3185
Deviation After MD:
phi & psi angles of 4th residue : 1.763 -78.5052
phi & psi angles of 8th residue : 132.75 -38.07

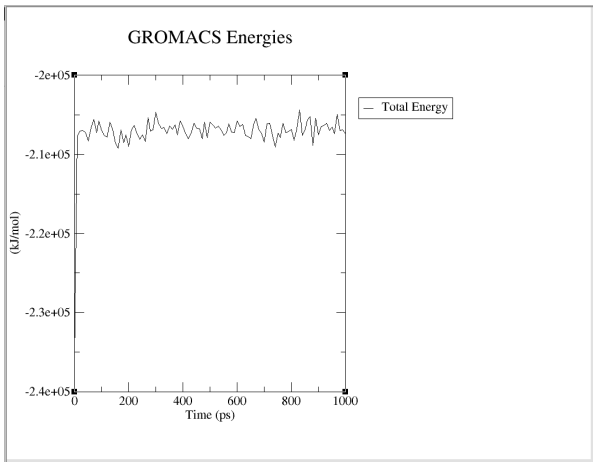
2)
A) Total Energy:
Beta sheet:



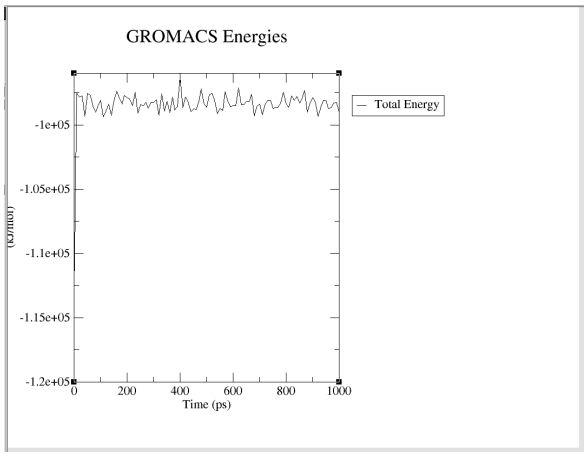
Helix:



PGB:

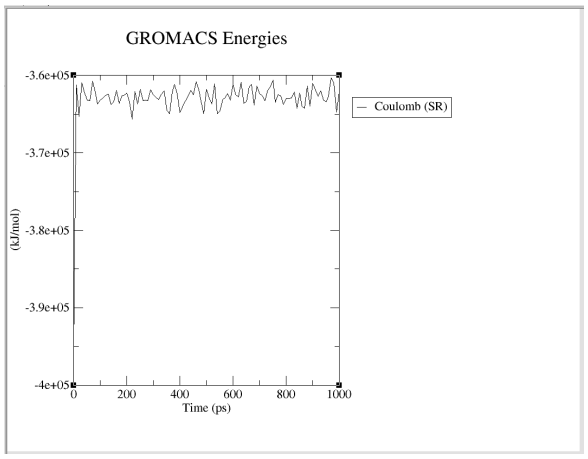


TRP:



B) Coul-SR:

Beta sheet:



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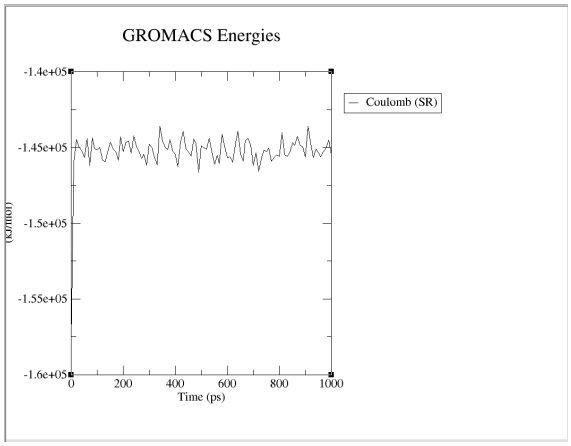
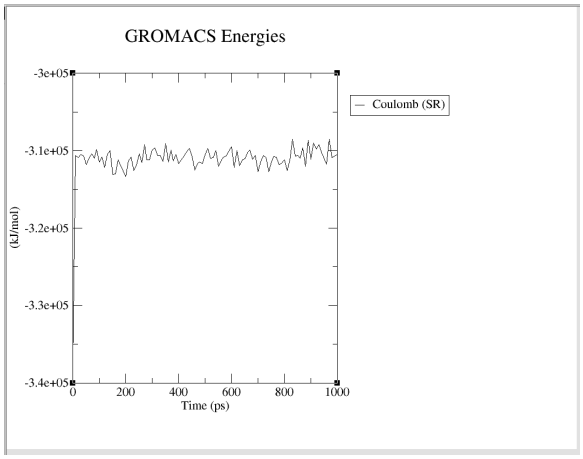
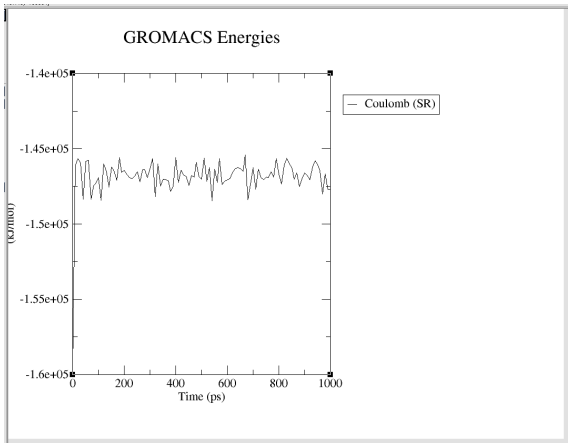


PGB:

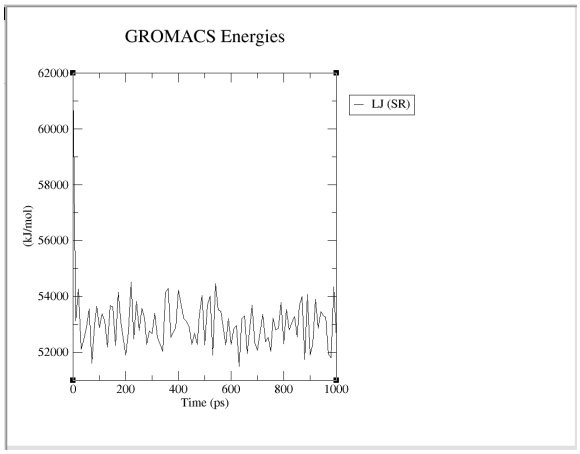


TRP:

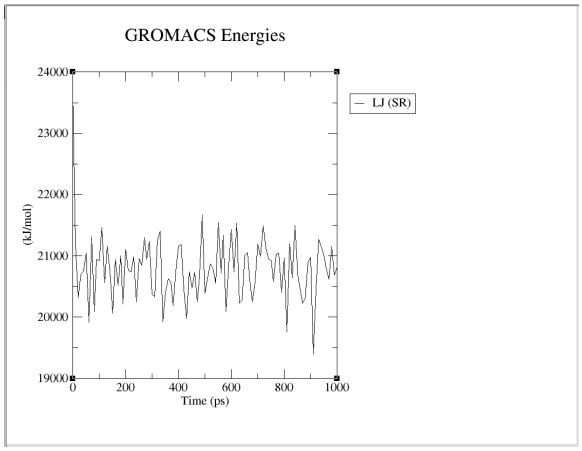


C) LJ-SR:

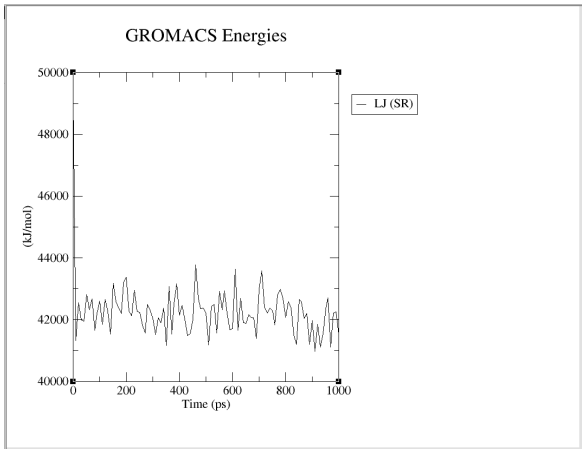
Beta sheet:



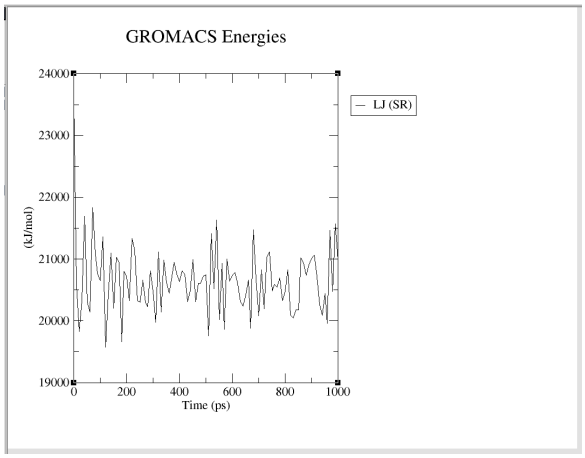
Helix:



PGB:



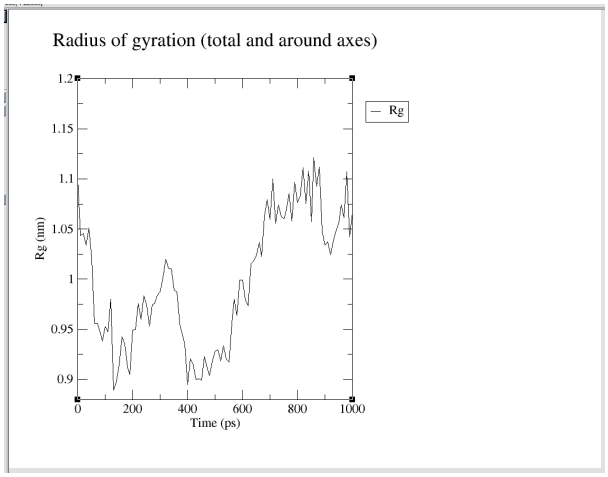
TRP:



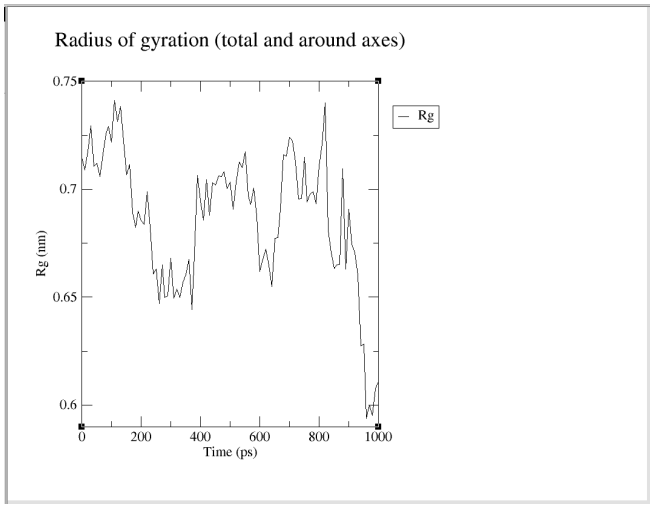
4) Radius of Gyration

The radius of Gyration of TRP: 0.538806
The radius of Gyration of PGB: 0.70167
The radius of Gyration of Helix: 0.382169
The radius of Gyration of BetaSheet: 0.938183

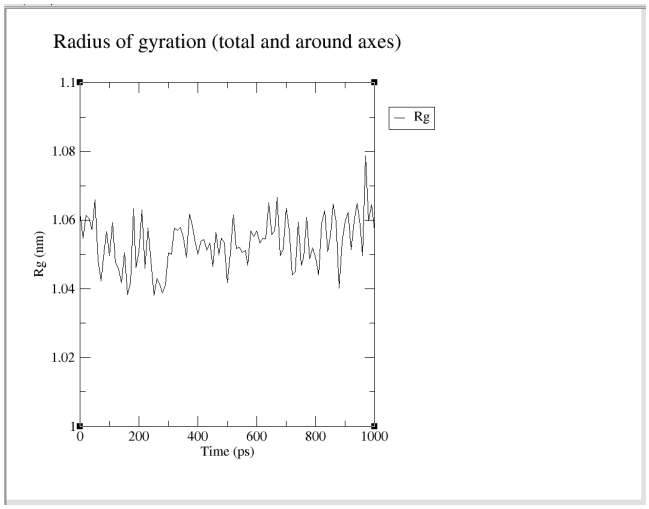
Beta sheet:



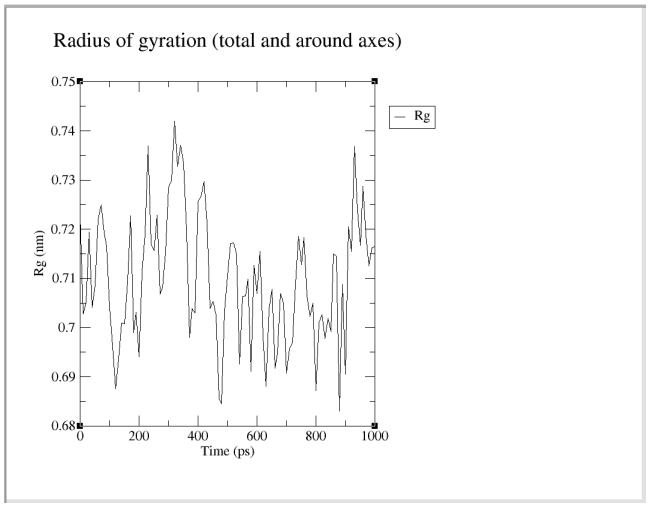
Helix:


Radius of gyration (total and around axes)
Rg
Rg (nm)
Time (ps)
0.75
0.7
0.65
0.6
0
200
400
600
800
1000

PGB:


Radius of gyration (total and around axes)
Rg
Rg (nm)
Time (ps)
1.1
1.08
1.06
1.04
1.02
1
0
200
400
600
800
1000

TRP:


Radius of gyration (total and around axes)
Rg
Rg (nm)
Time (ps)
0.75
0.74
0.73
0.72
0.71
0.7
0.69
0.68
0
200
400
600
800
1000

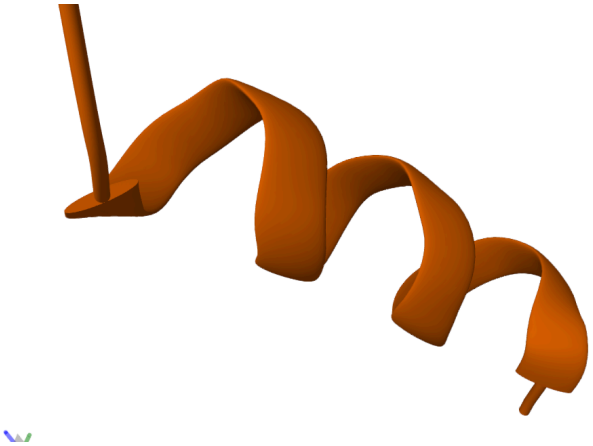
5)

Beta Sheet:
Number of clusters for cutoff 0.15=17

Number of clusters for cutoff 0.1=57

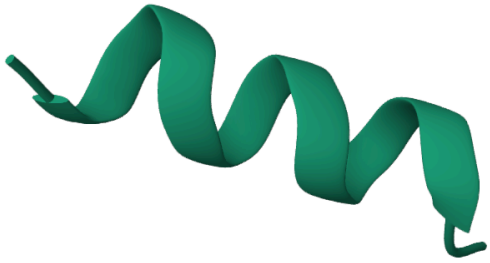
Number of clusters for cutoff 0.30=3

Helix:
Number of clusters for cutoff 0.15=6



Number of clusters for cutoff 0.1=15

Number of clusters for cutoff 0.30=1

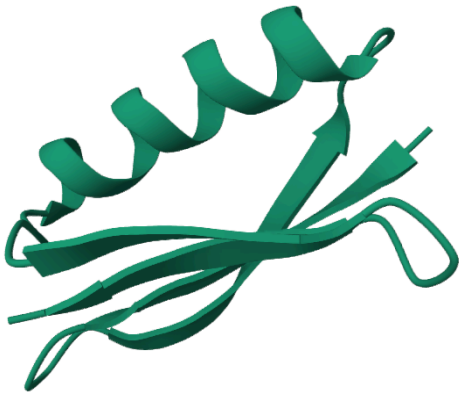


PDB:

Number of clusters for cutoff 0.15=3

Number of clusters for cutoff 0.1=19

Number of clusters for cutoff 0.30=1



TRP:

Number of clusters for cutoff 0.15=10

Number of clusters for cutoff 0.1=40

Number of clusters for cutoff 0.30=1