Ans01: Net Deviation :

Alpha Helix – 300K

4th residue	Vaccuum	EM	MD	8th residue	Vaccuum	EM	MD
phi	-63.9129	-53.3147	-52.8268	phi	-61.1334	-61.4148	-61.4868
psi	-36.9095	-48.0476	-48.0484	psi	-39.8801	-38.8765	-38.5847
RMSD		**15.37463**	**15.71549**	**RMSD**		**1.04230**	**2.94826**

Alpha Helix – 363K

4th residue	Vaccuum	EM	MD	8th residue	Vaccuum	EM	MD
phi	-63.9129	-53.3147	-52.8268	phi	-61.1334	-61.4148	-61.4868
psi	-36.9095	-48.0476	-48.0484	psi	-39.8801	-38.8765	-38.5847
RMSD		**15.37463**	**15.71549**	**RMSD**		**1.04230**	**1.34274**

Beta Sheet – 300K

4th residue	Vaccuum	EM	MD	8th residue	Vaccuum	EM	MD
phi	-117.08	-120.265	-120.554	phi	-131.054	-123.124	-123.567
psi	150.139	154.456	154.38	psi	56.9586	72.3843	71.9429
RMSD		**5.36477**	**5.48222**	**RMSD**		**17.34466**	**16.75065**

Beta Sheet – 363K

4th residue	Vaccuum	EM	MD	8th residue	Vaccuum	EM	MD
phi	-117.08	-120.265	-120.554	phi	-131.054	-123.124	-123.567
psi	150.139	154.456	154.38	psi	56.9586	72.3843	71.9429
RMSD		**5.36477**	**5.48222**	**RMSD**		**17.34466**	**16.75065**

Trp Cage – 300K

4th residue	Vaccuum	EM	MD	8th residue	Vaccuum	EM	MD
phi	-62.0196	-54.322	-54.5711	phi	-58.3622	-56.9538	-56.6273
psi	-52.7863	-61.3736	-61.4498	psi	-29.9879	-29.6602	-29.7111
RMSD		**11.53234**	**11.42525**	**RMSD**		**1.44602**	**1.75684**

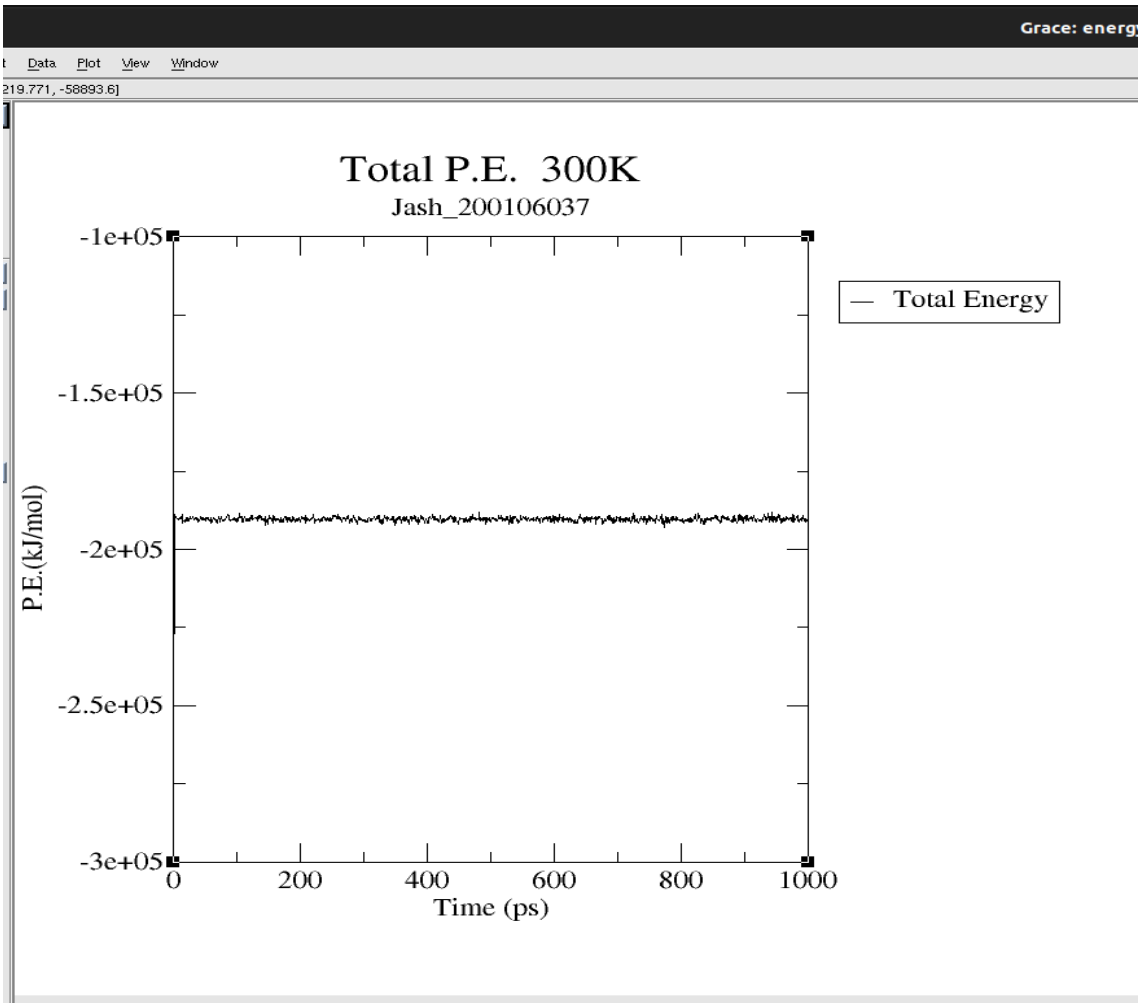
Trp Cage – 363K

4th residue	Vaccuum	EM	MD	8th residue	Vaccuum	EM	MD
phi	-62.0196	-54.322	-54.5711	phi	-58.3622	-56.9538	-56.6273
psi	-52.7863	-61.3736	-61.4498	psi	-29.9879	-29.6602	-29.7111
RMSD		**11.53234**	**11.42525**	**RMSD**		**1.44602**	**1.75684**

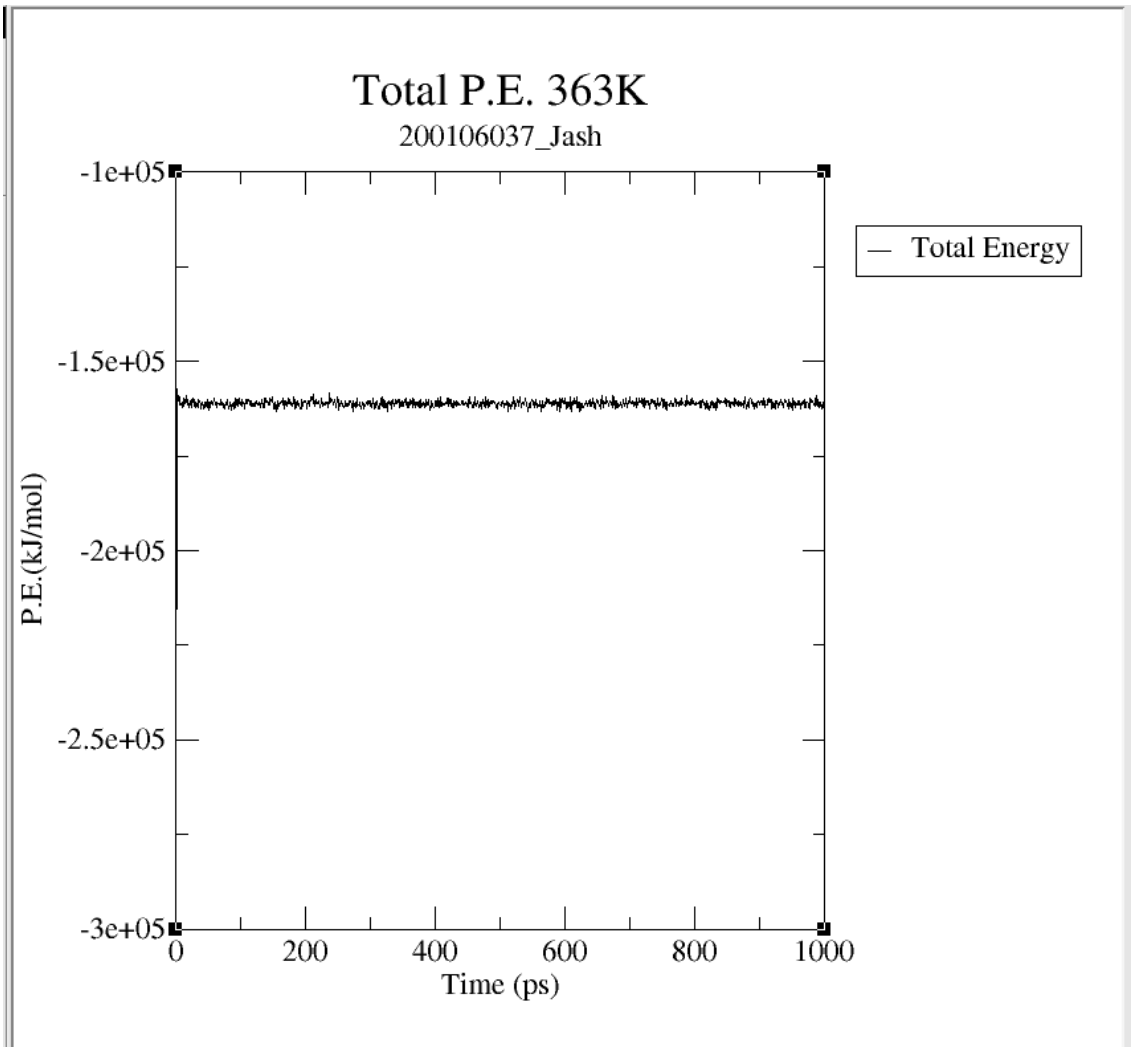
Ans02:

1PGB

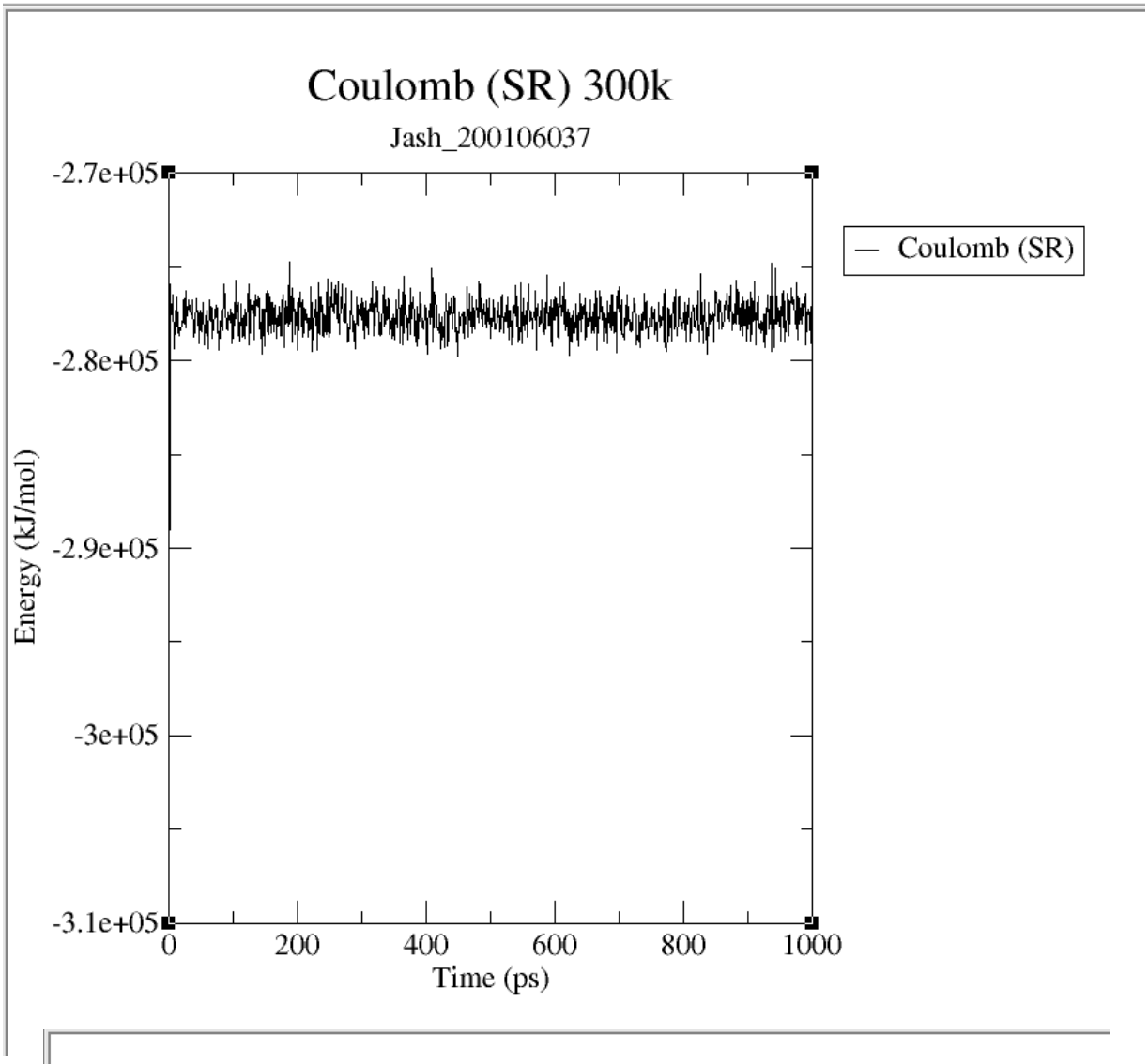
Total Energy – 300K



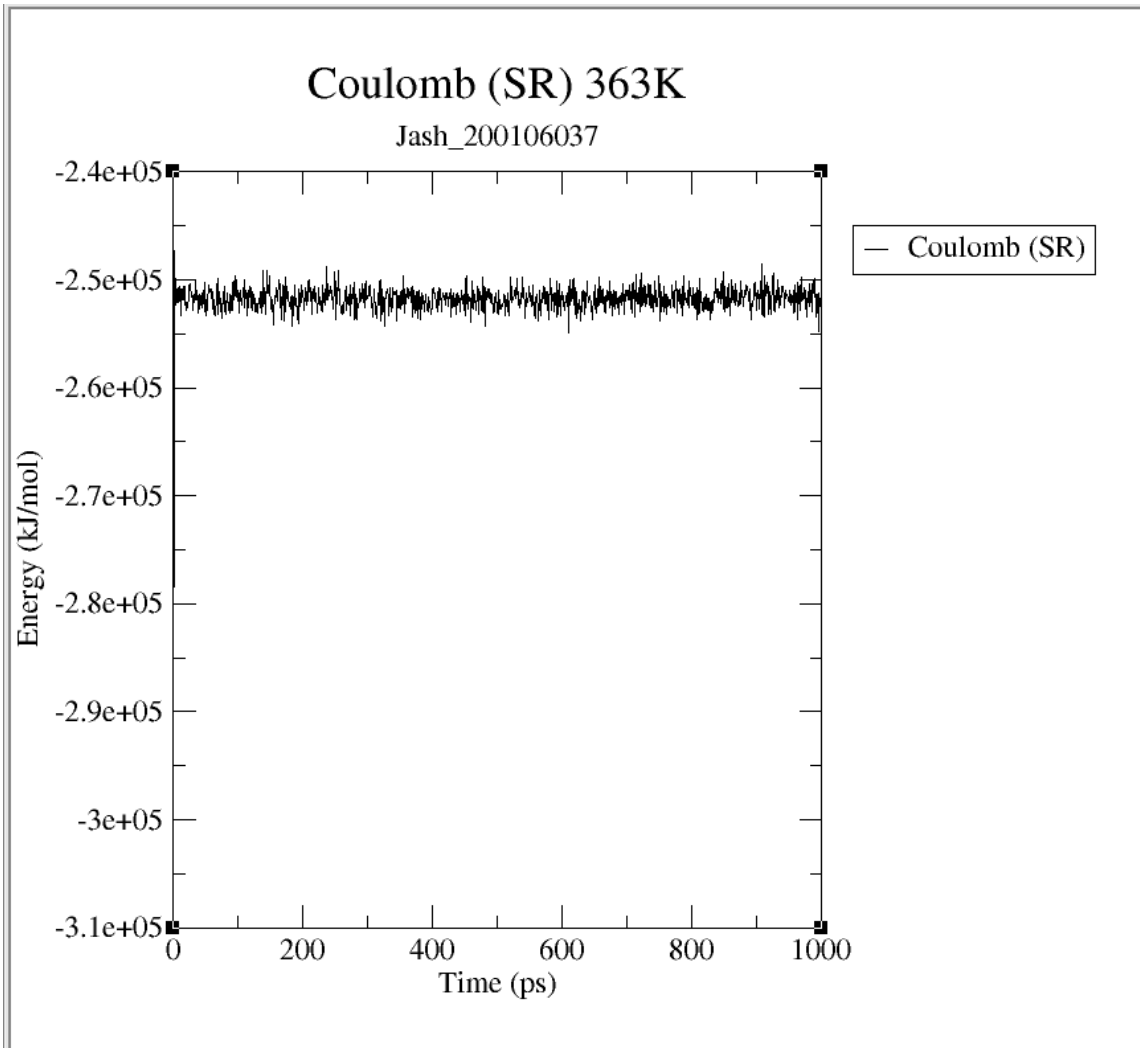
Total Energy – 363K



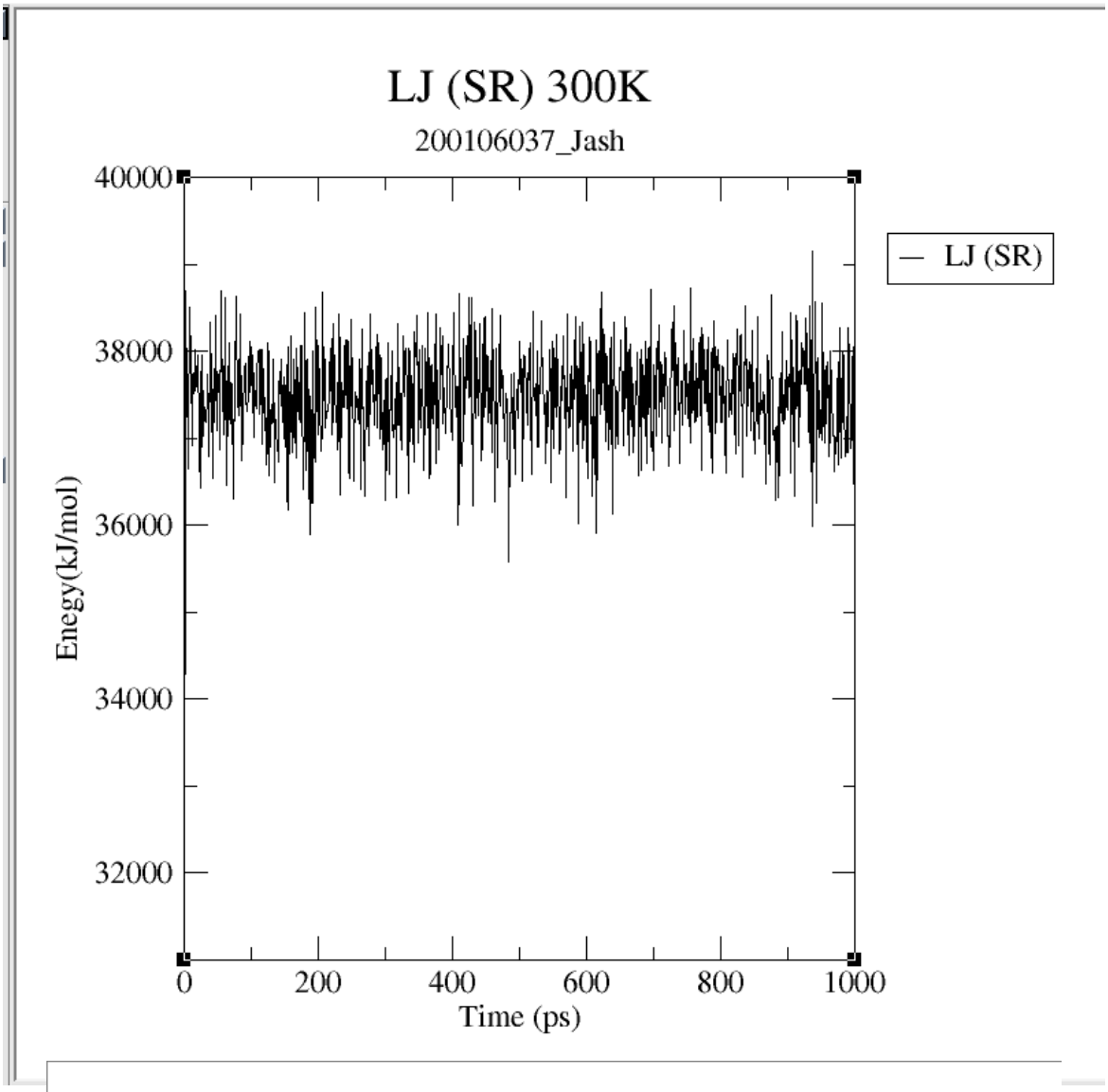
Coul-SR -- 300K



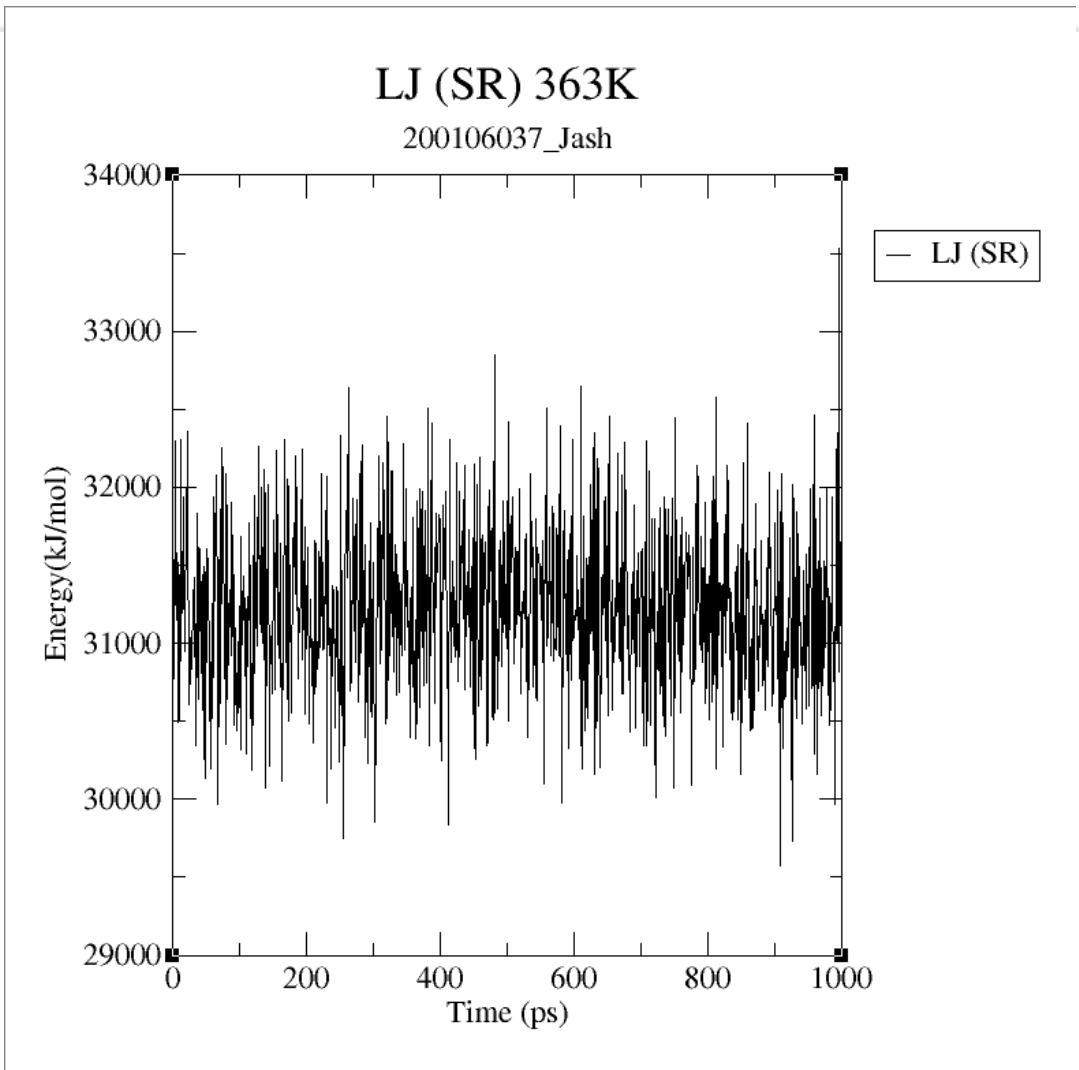
Coul-SR -- 363K



LJ-SR -- 300K

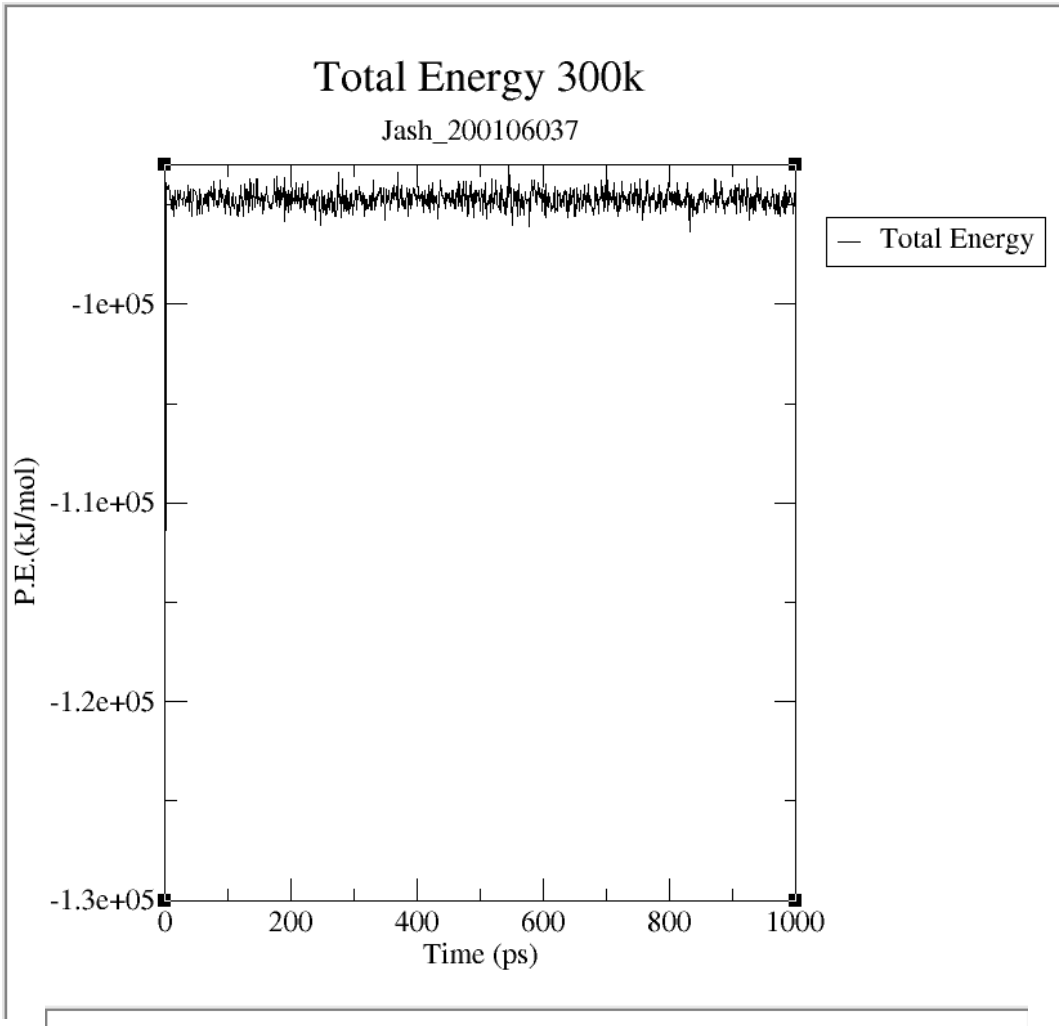


LJ-SR -- 363K

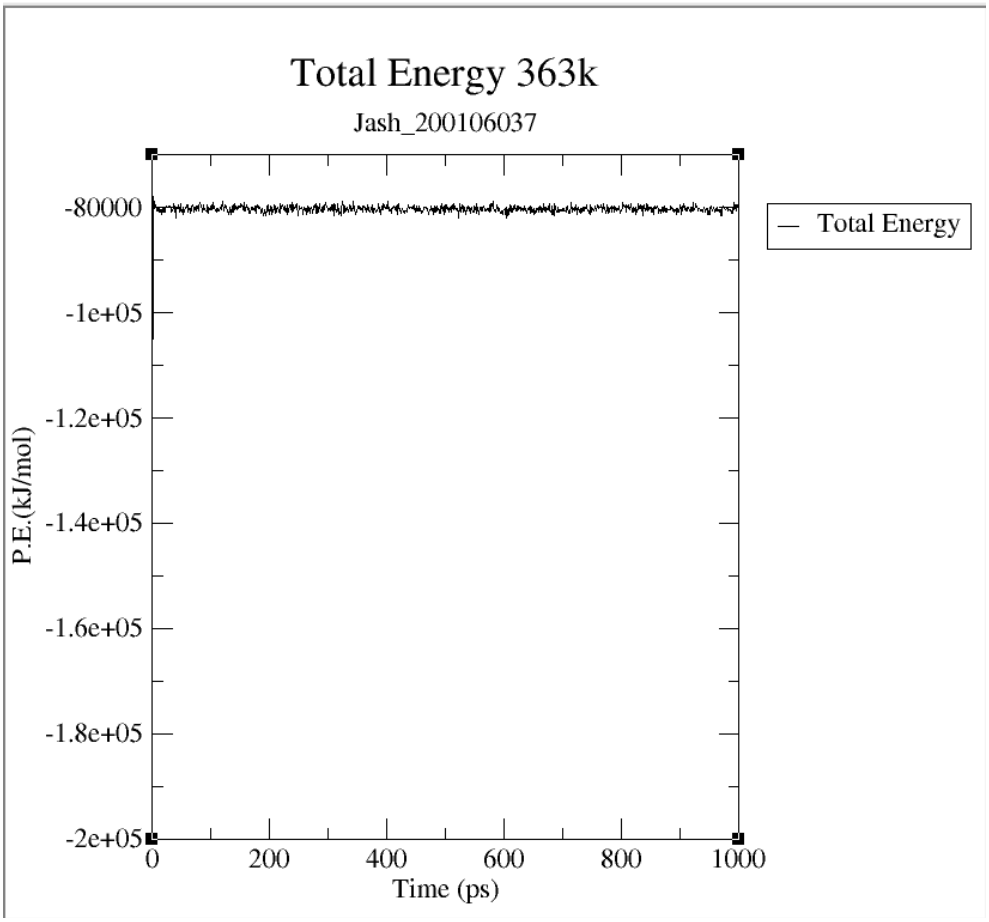


Alpha Helix

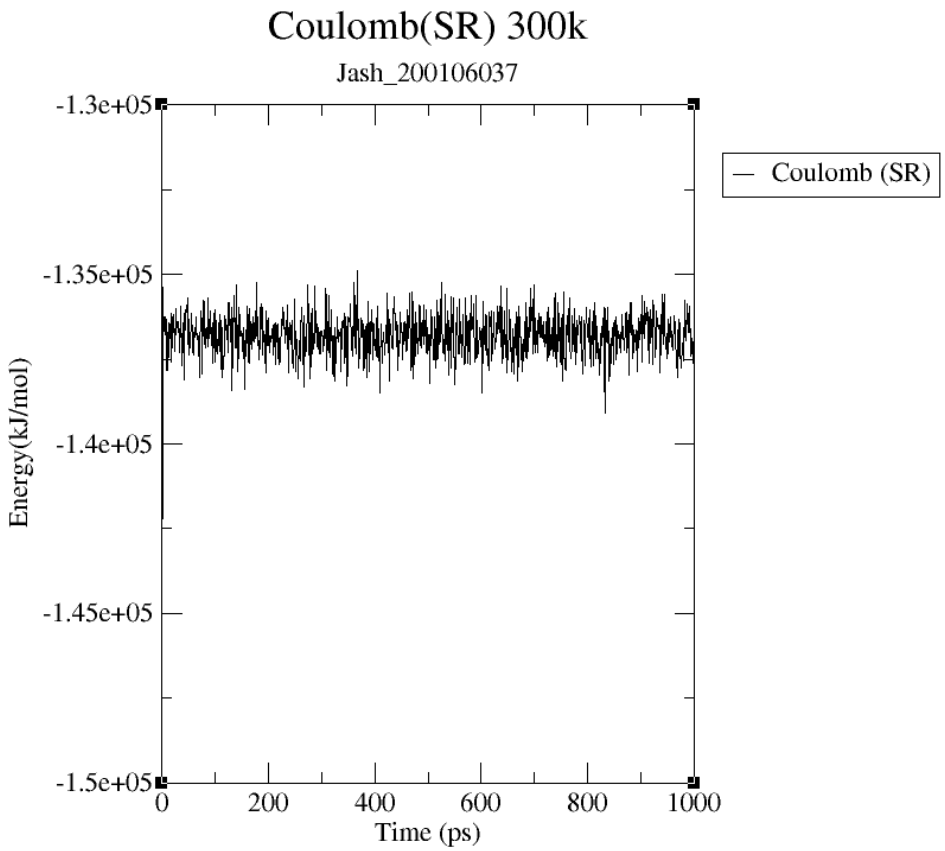
Total Energy – 300K



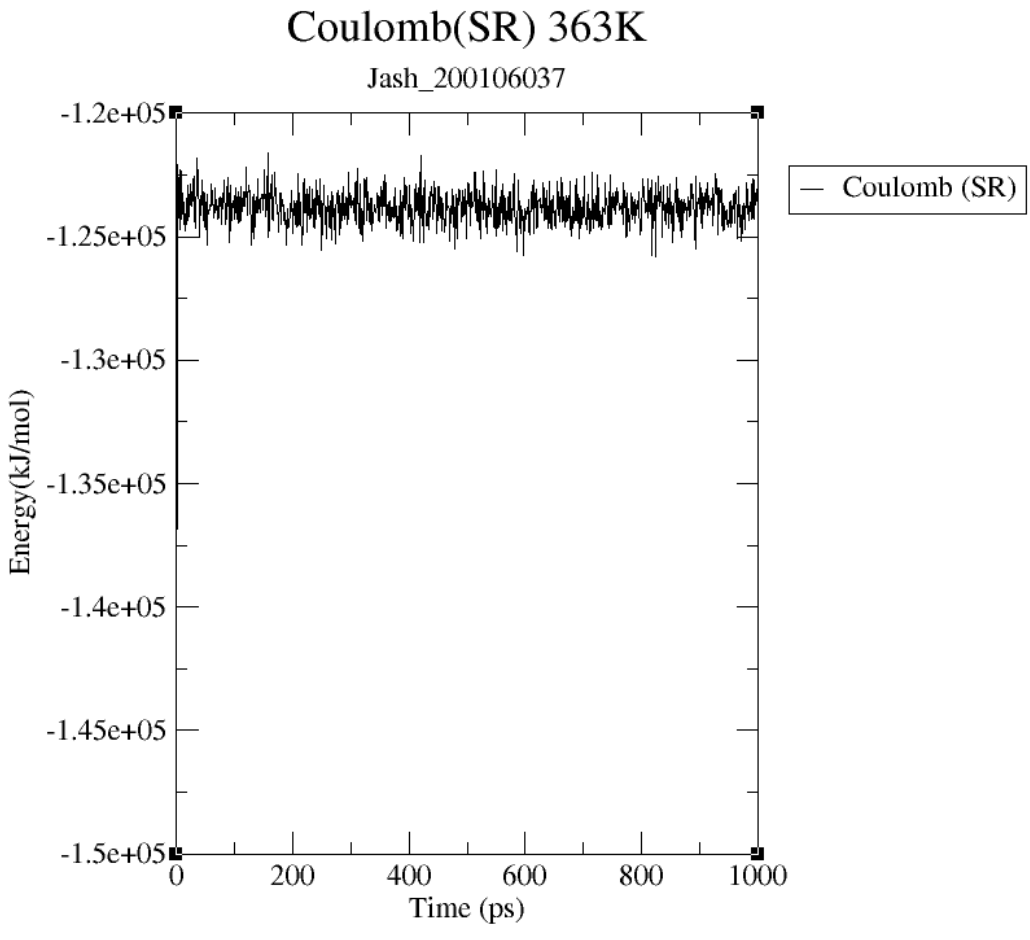
Total Energy – 363K



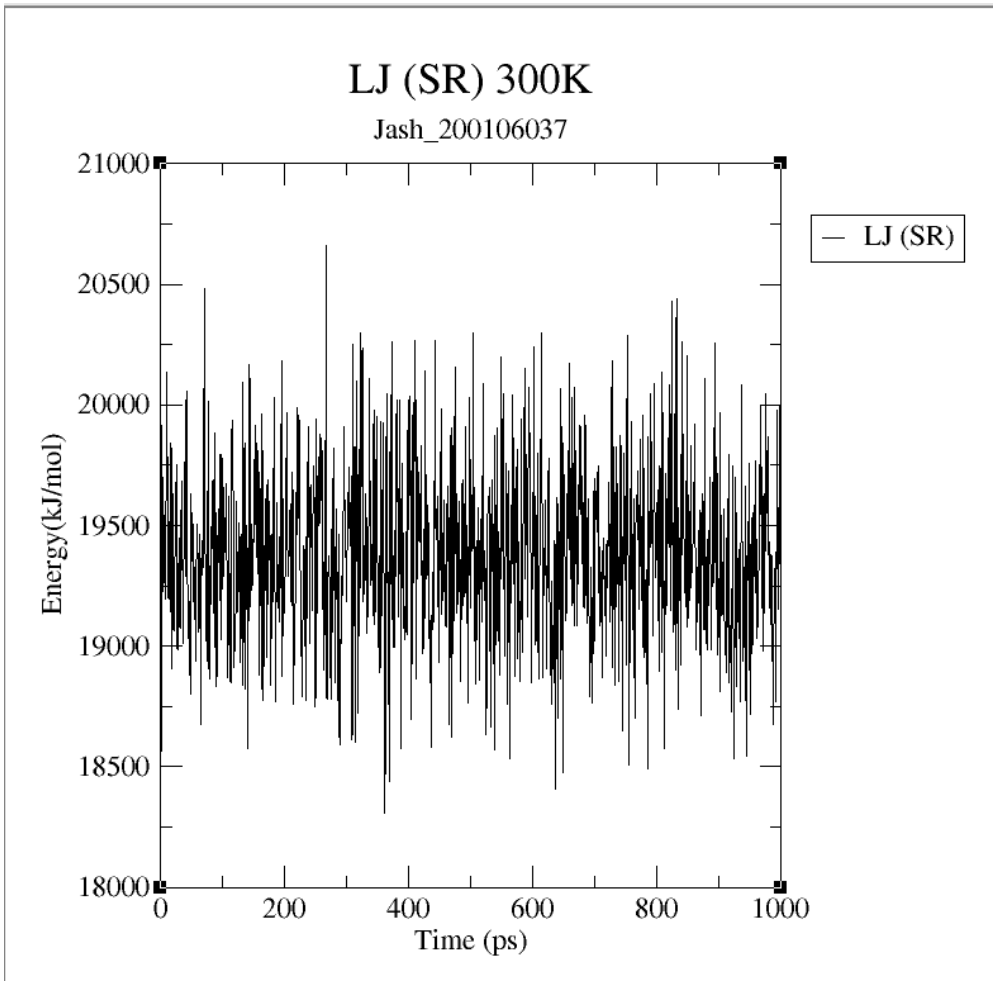
Coul-SR -- 300K



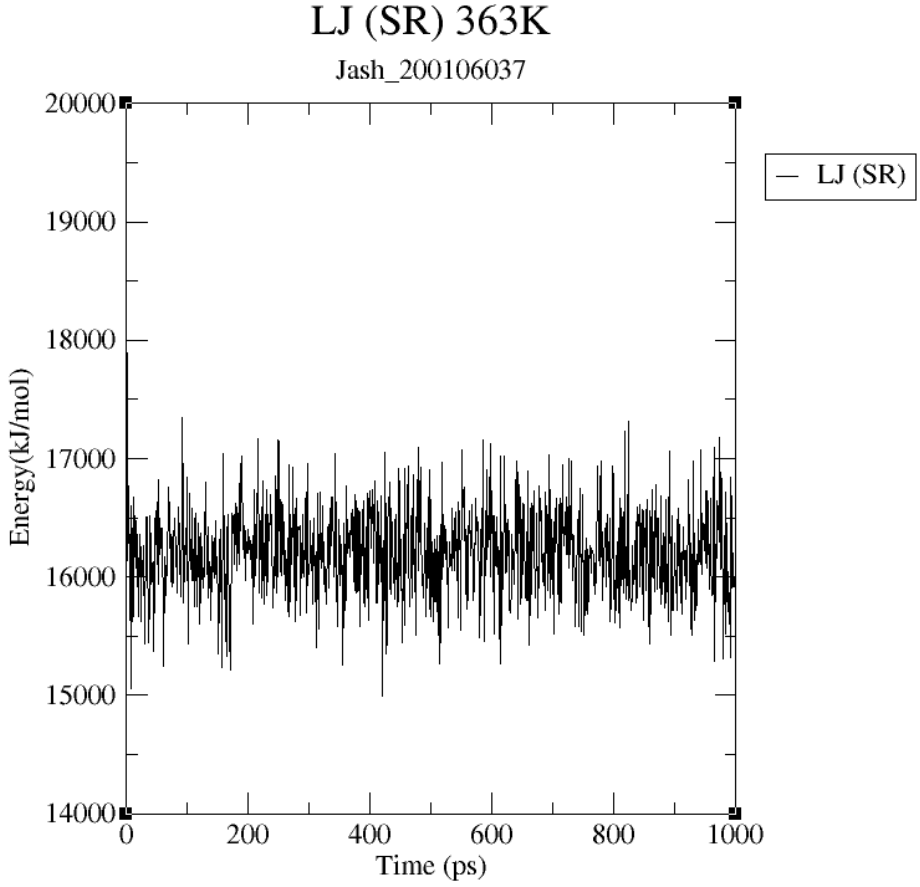
Coul-SR -- 363K



LJ-SR --
300K

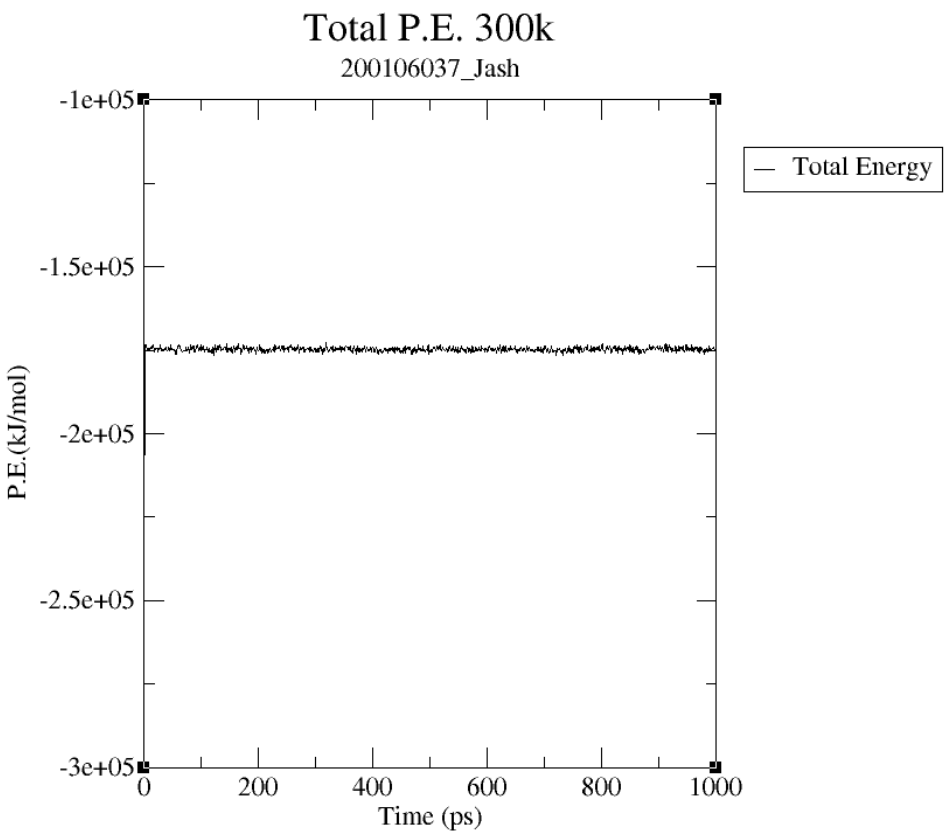


LJ-SR--
363K

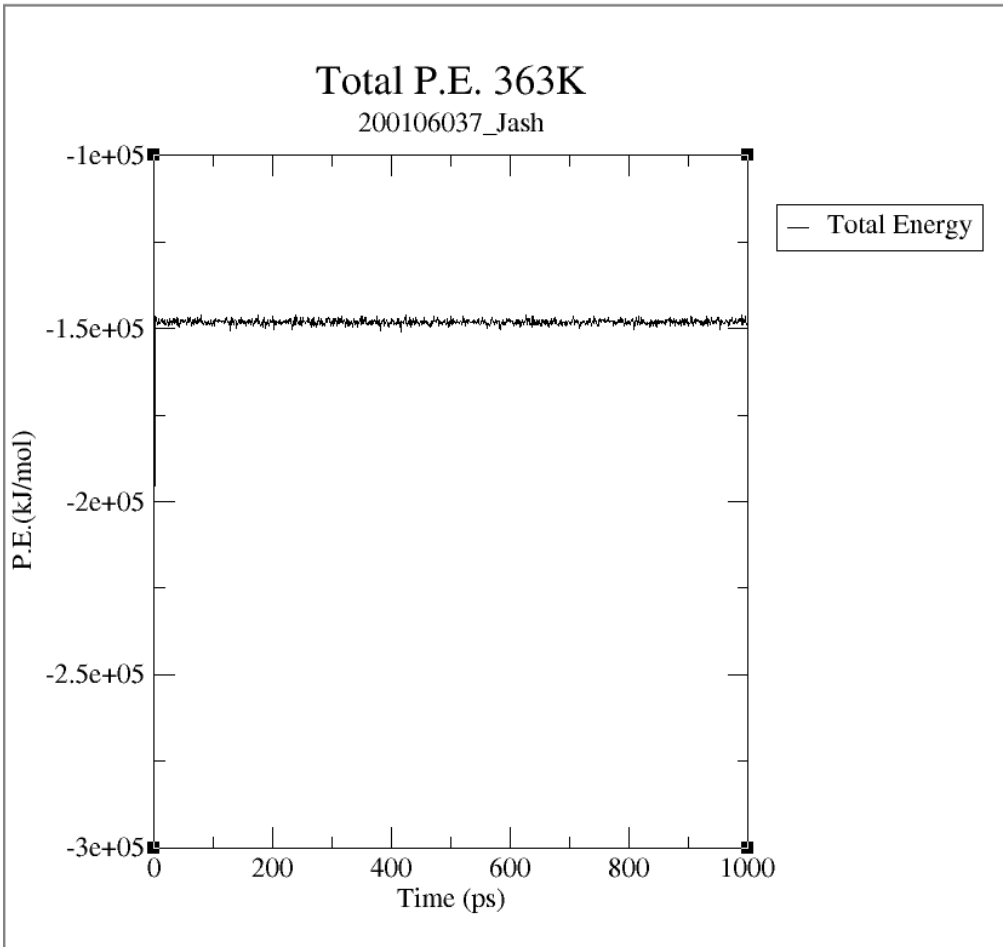


Beta Sheet

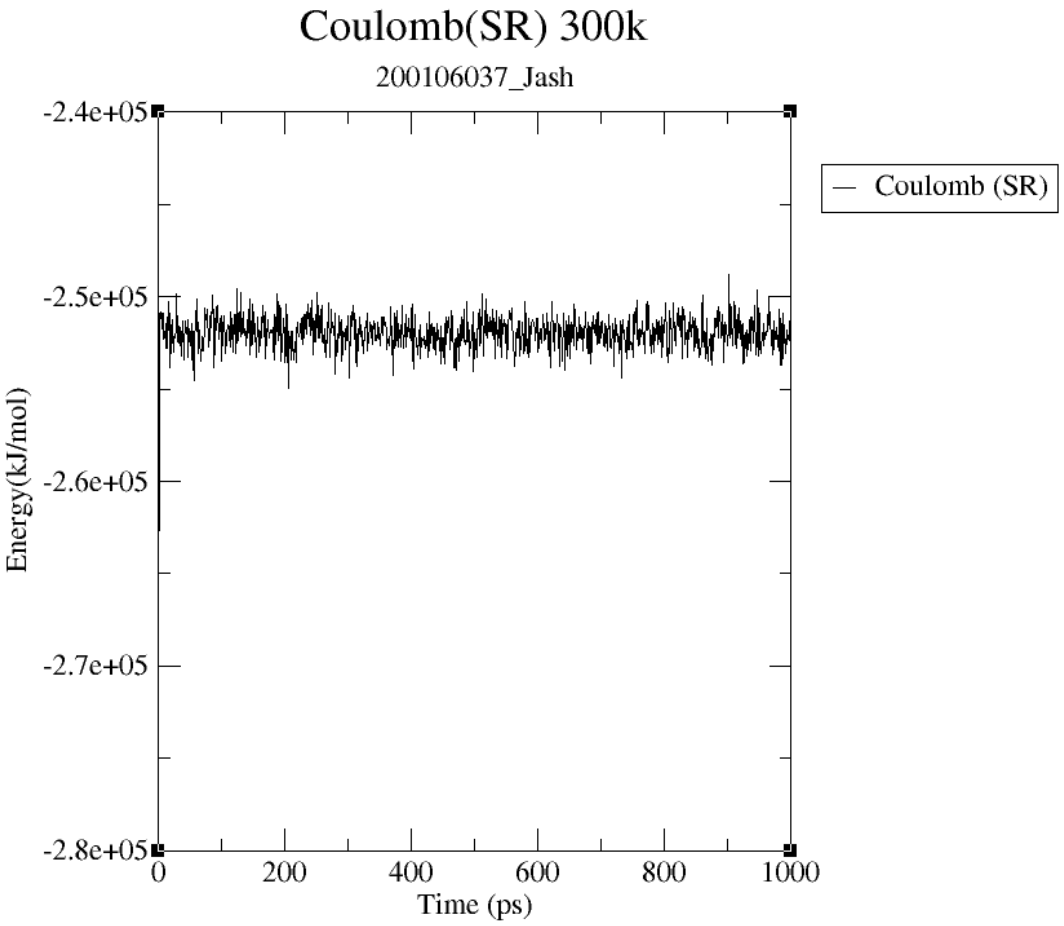
Total Energy – 300K



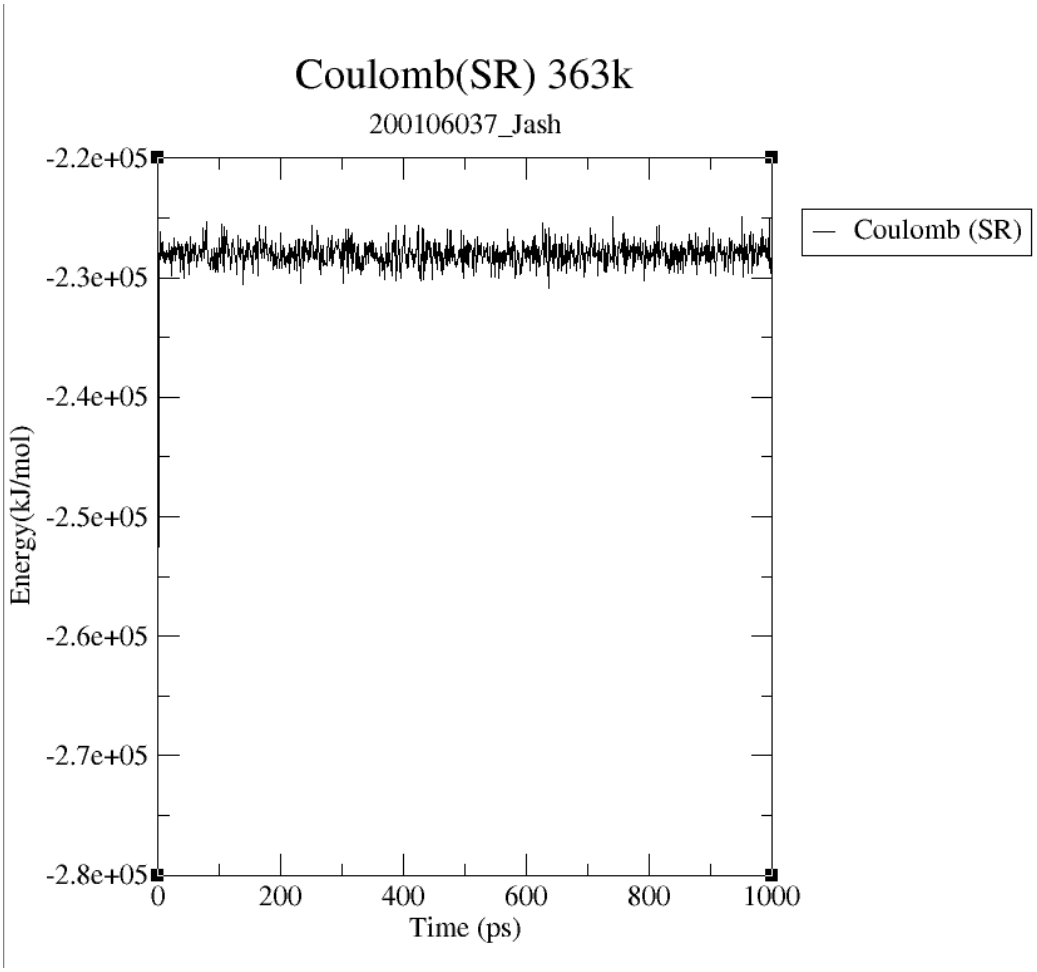
Total Energy – 363K



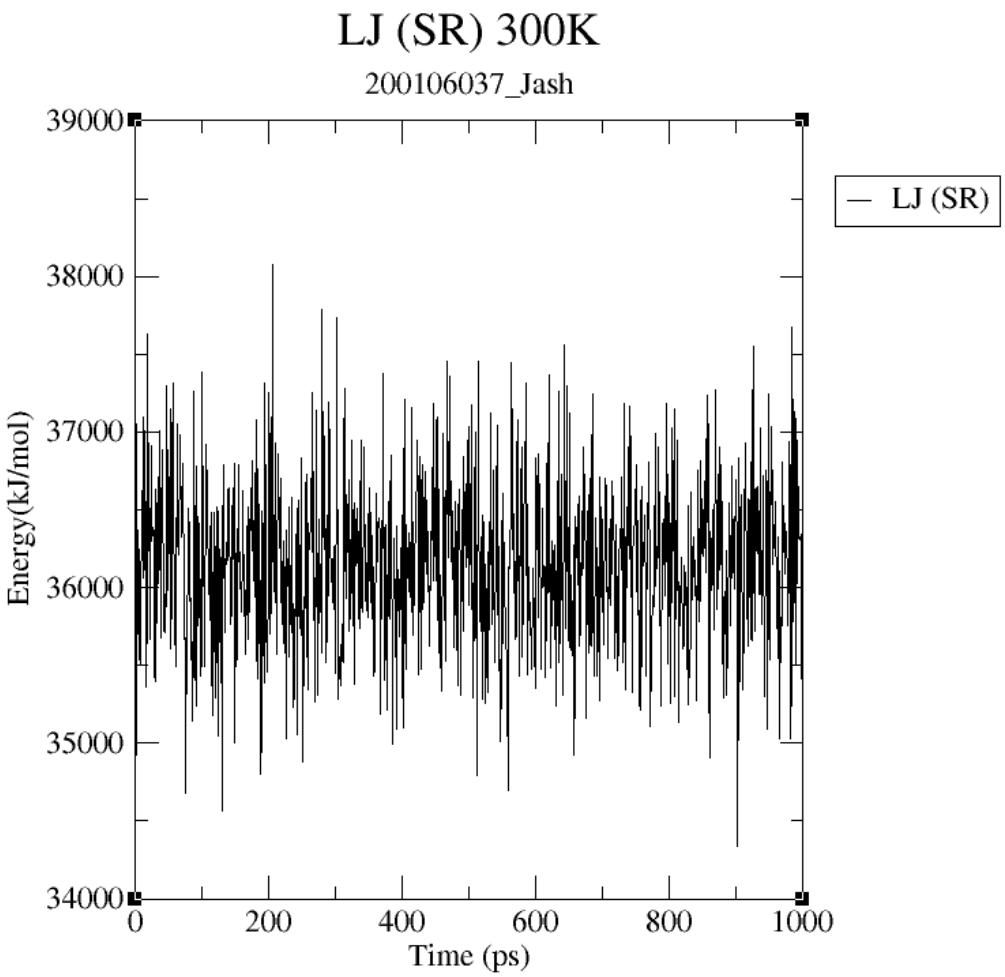
Coul-SR -- 300K



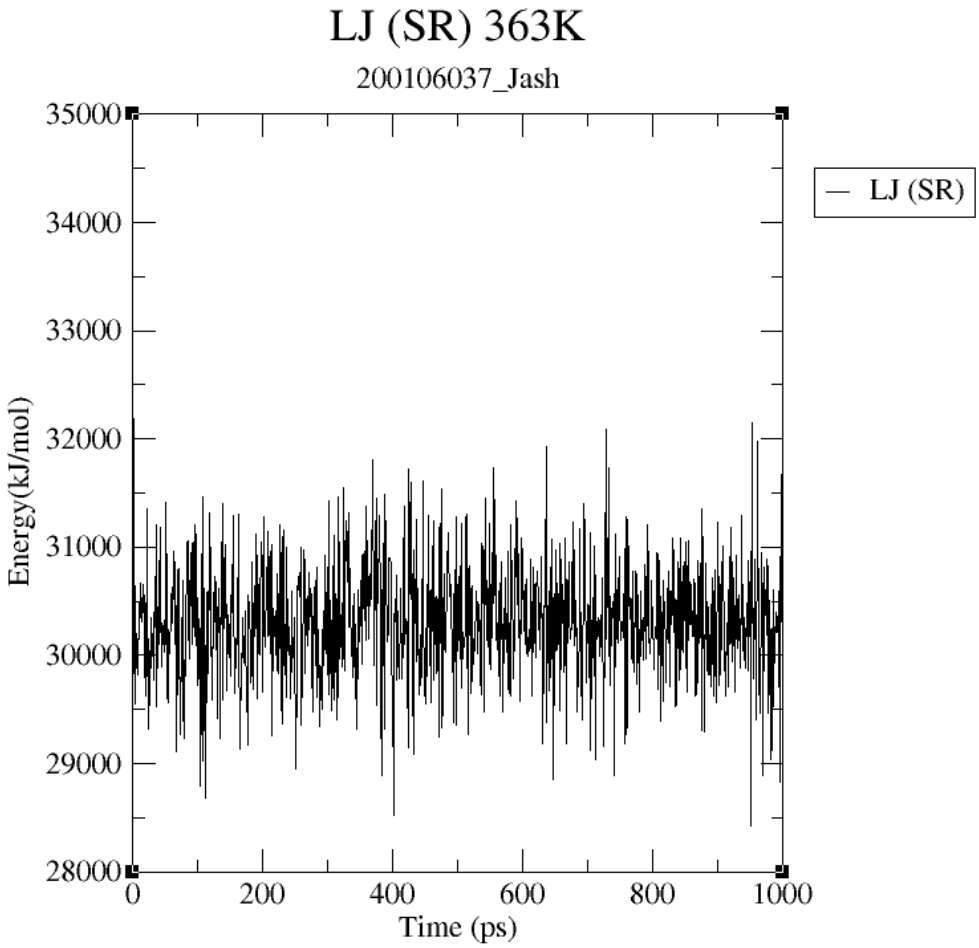
Coul-SR -- 363K



LJ – SR -- 300K

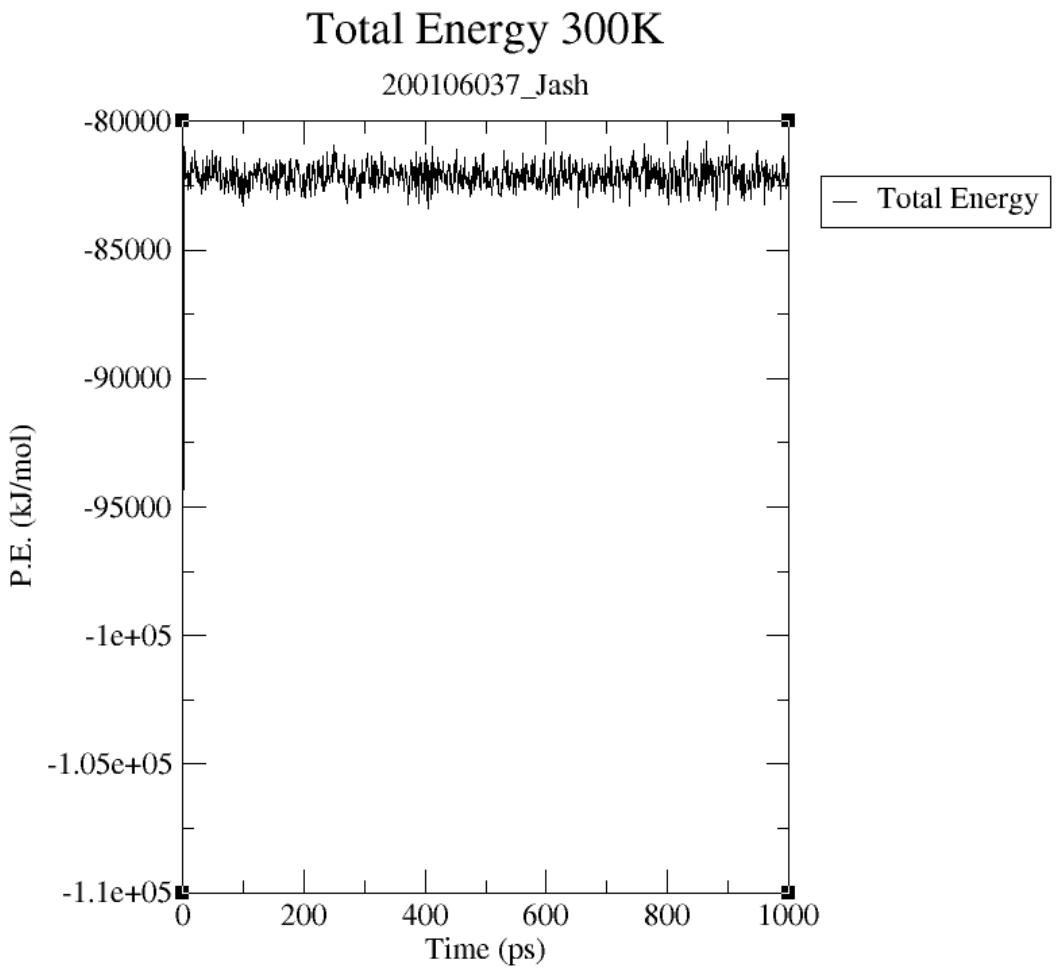


LJ – SR -- 363K

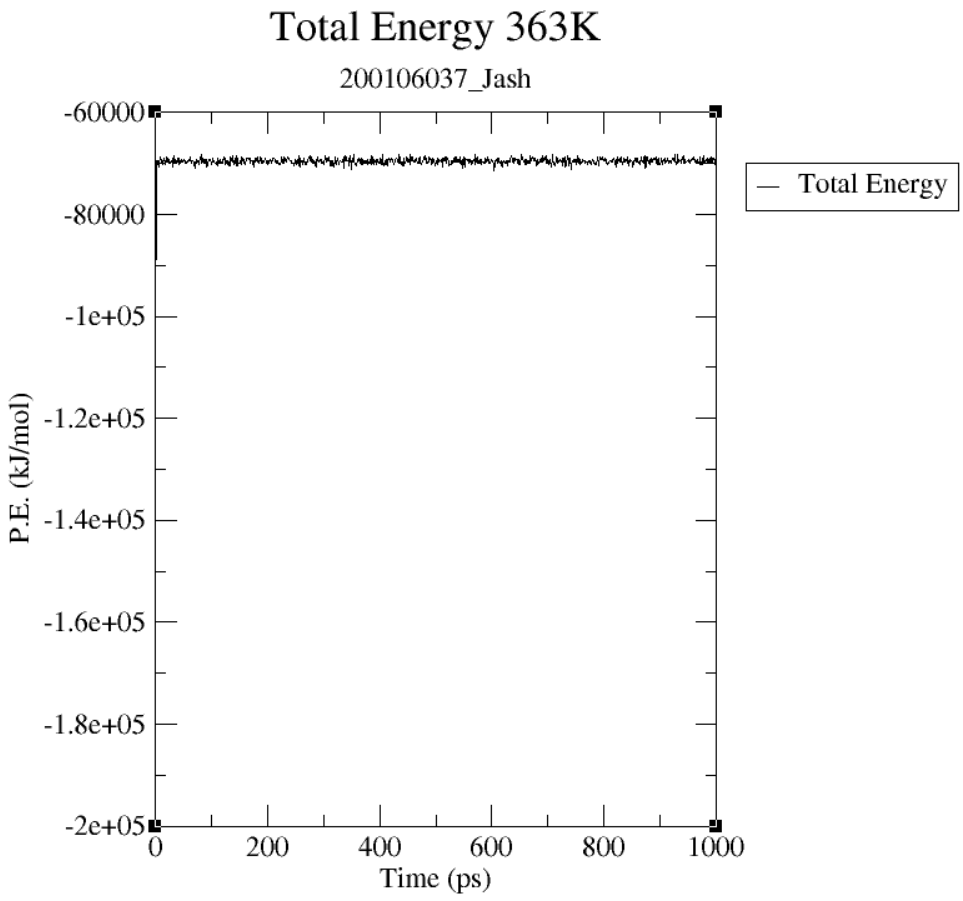


1L2Y

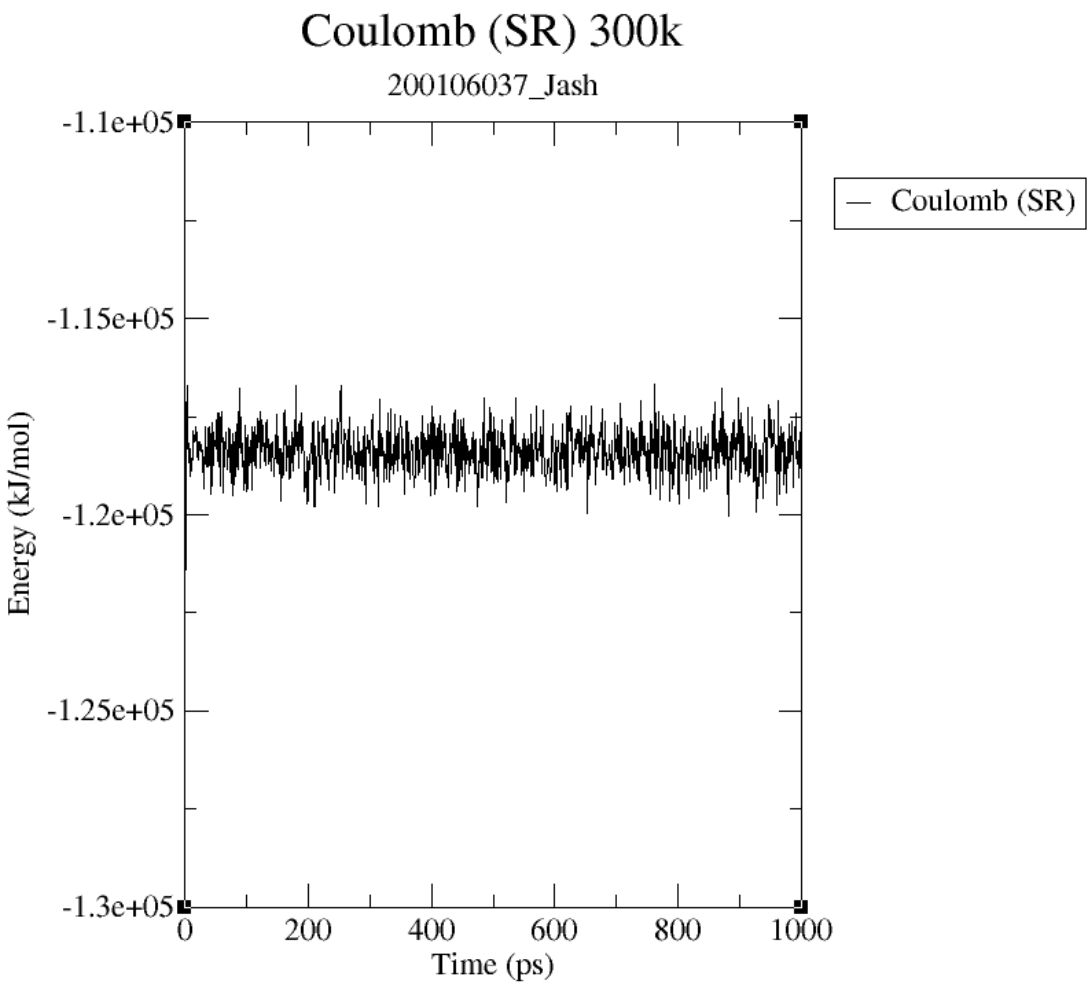
Total Energy -- 300K



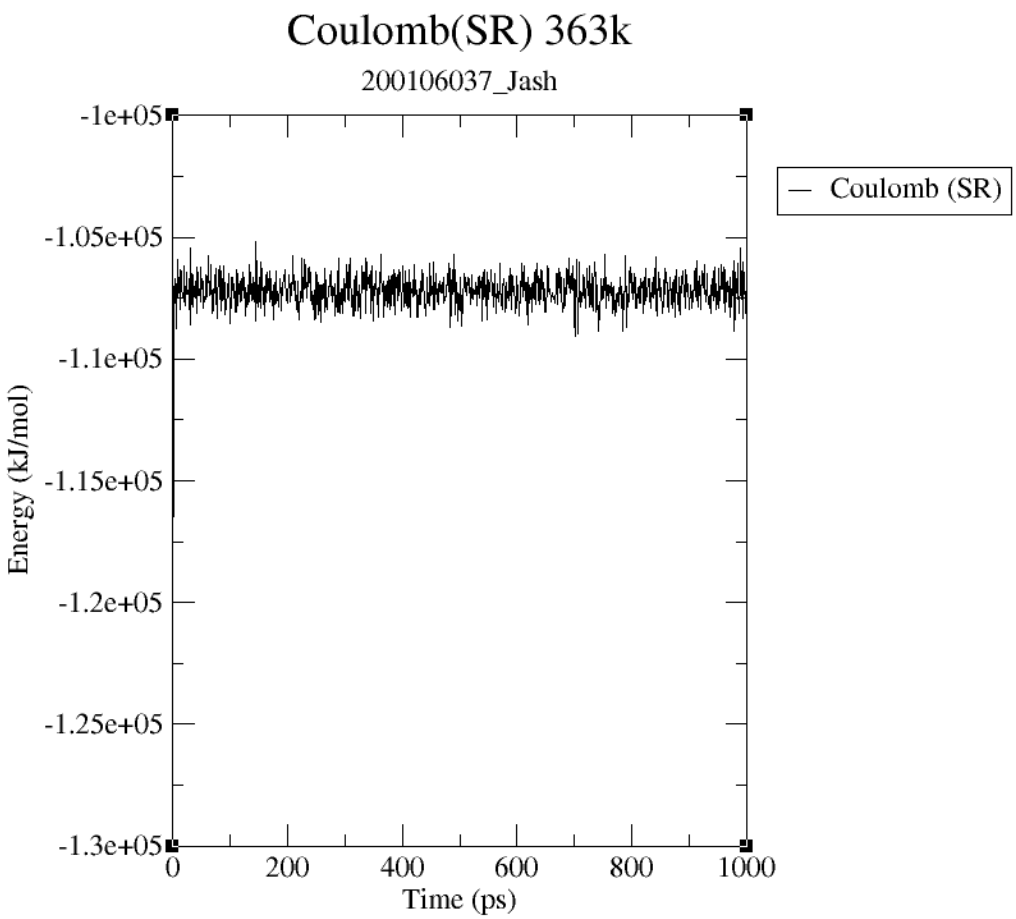
Total Energy -- 363K



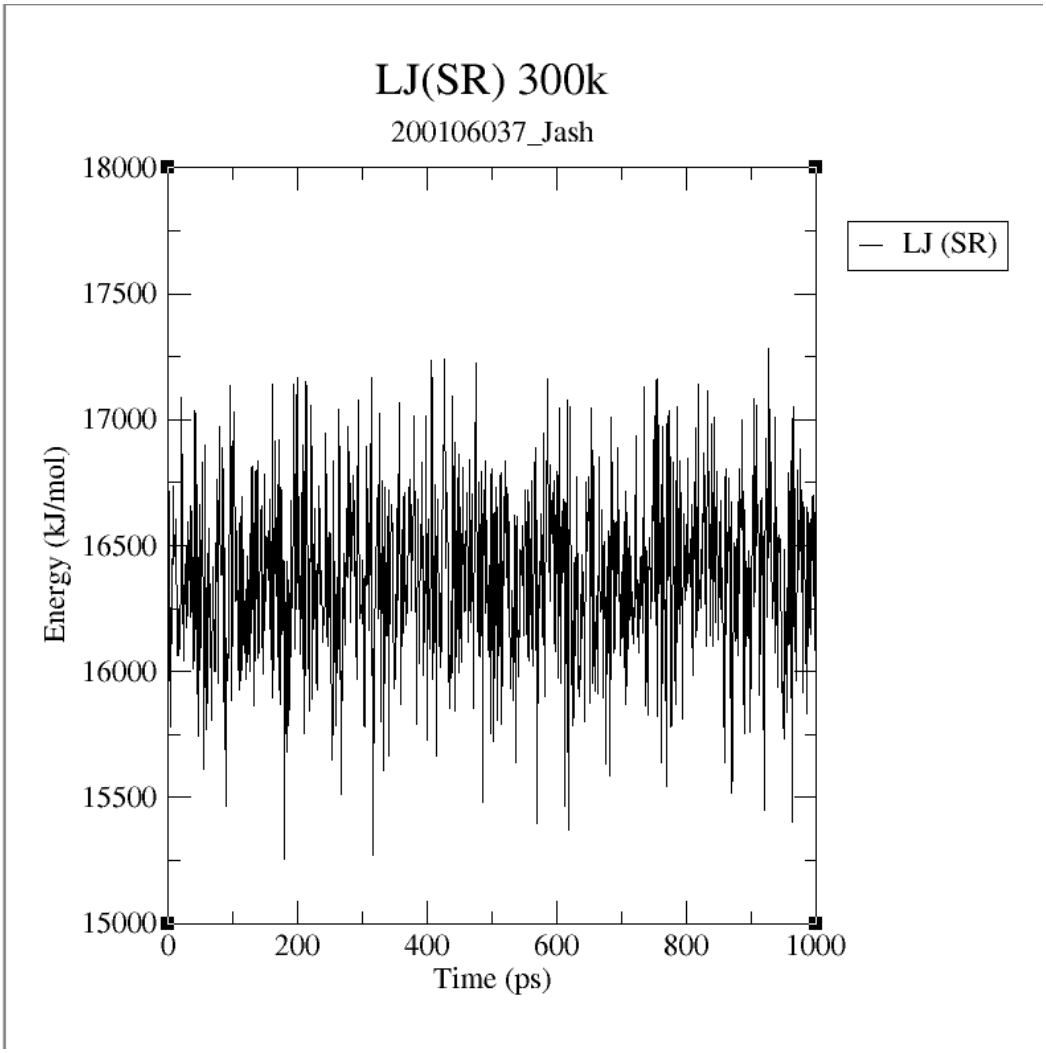
Coul-SR -- 300K



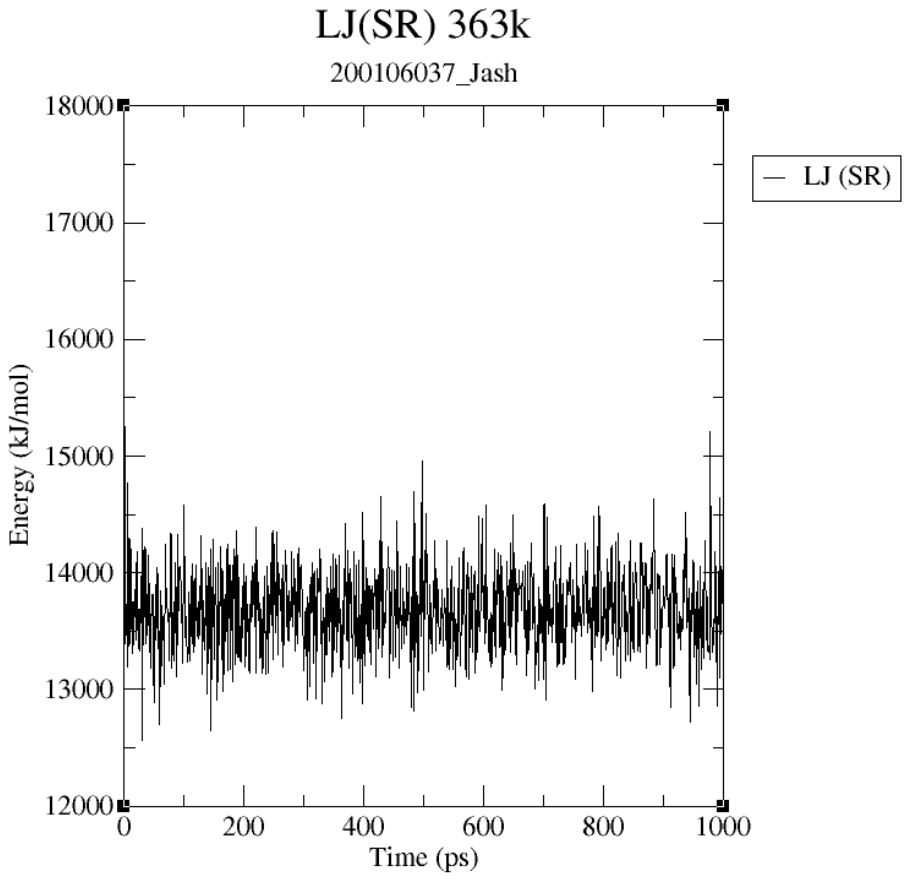
Coul – SR -- 363K



LJ – SR -- 300K

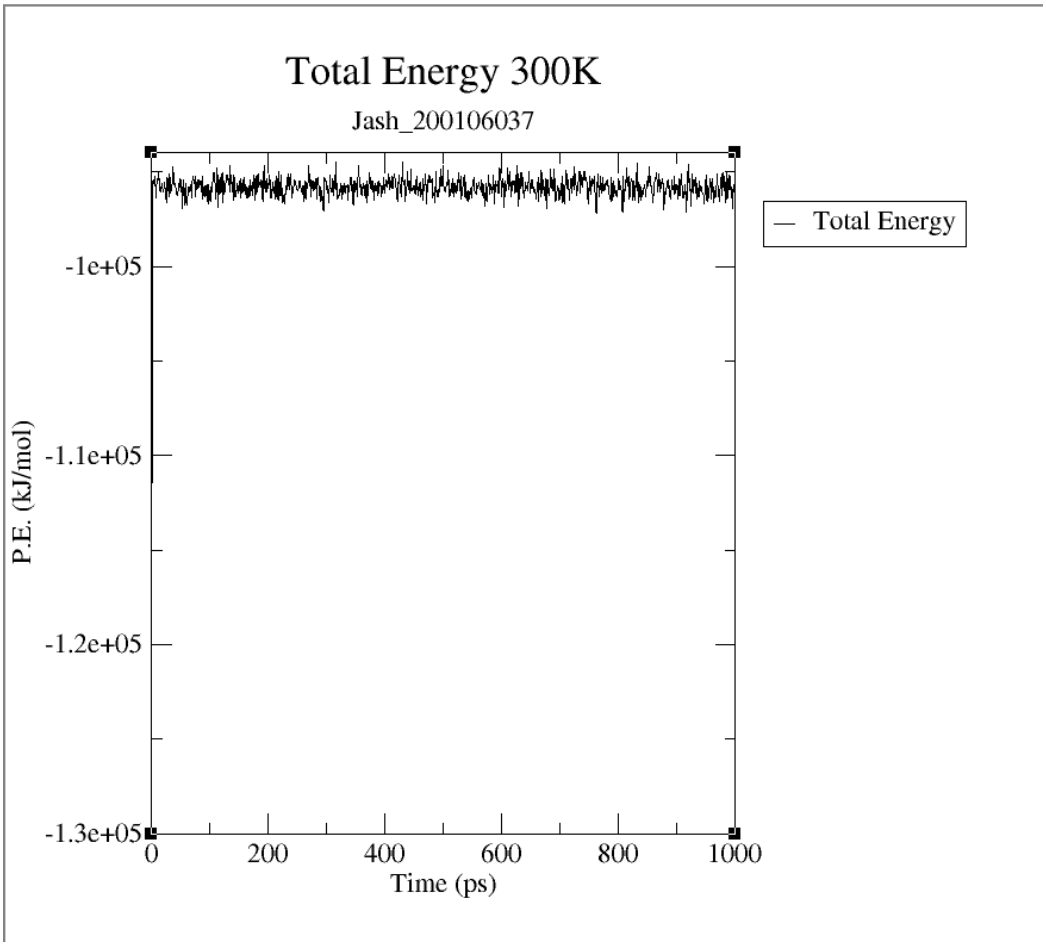


LJ – SR -- 363K

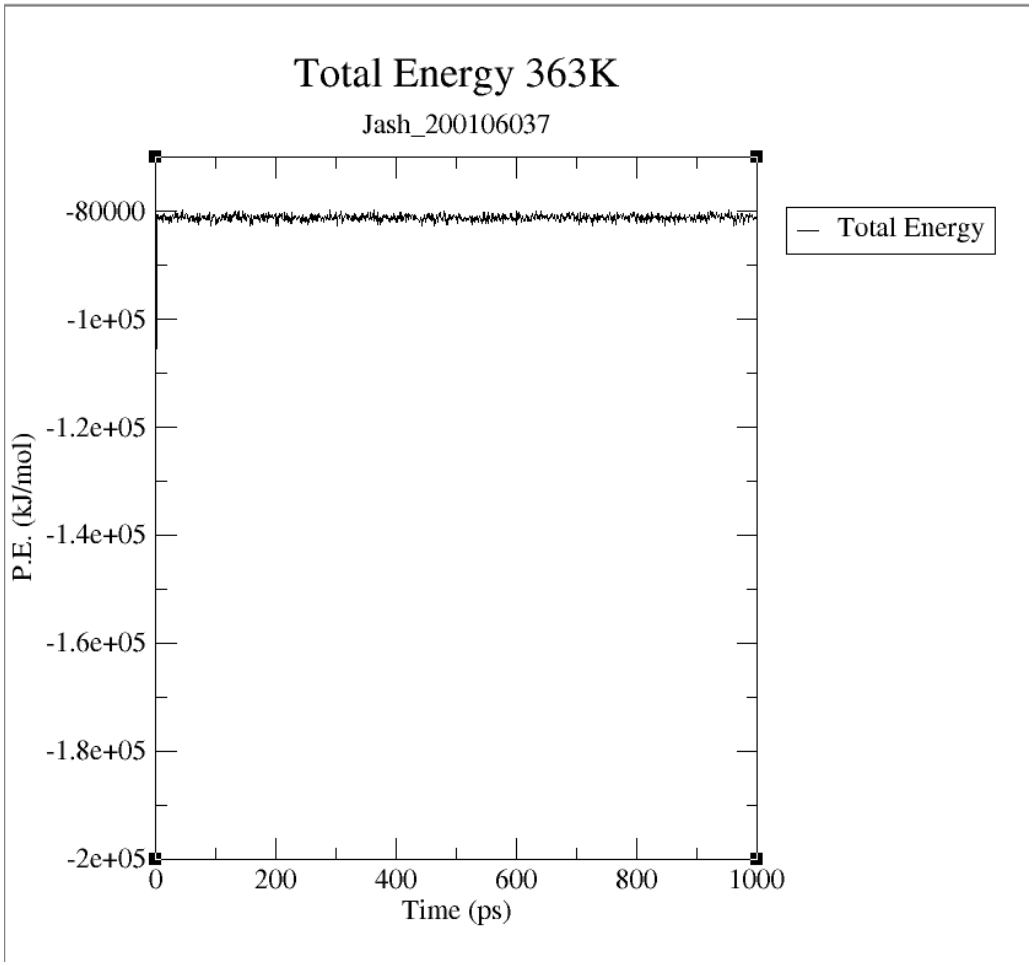


TRP Cage

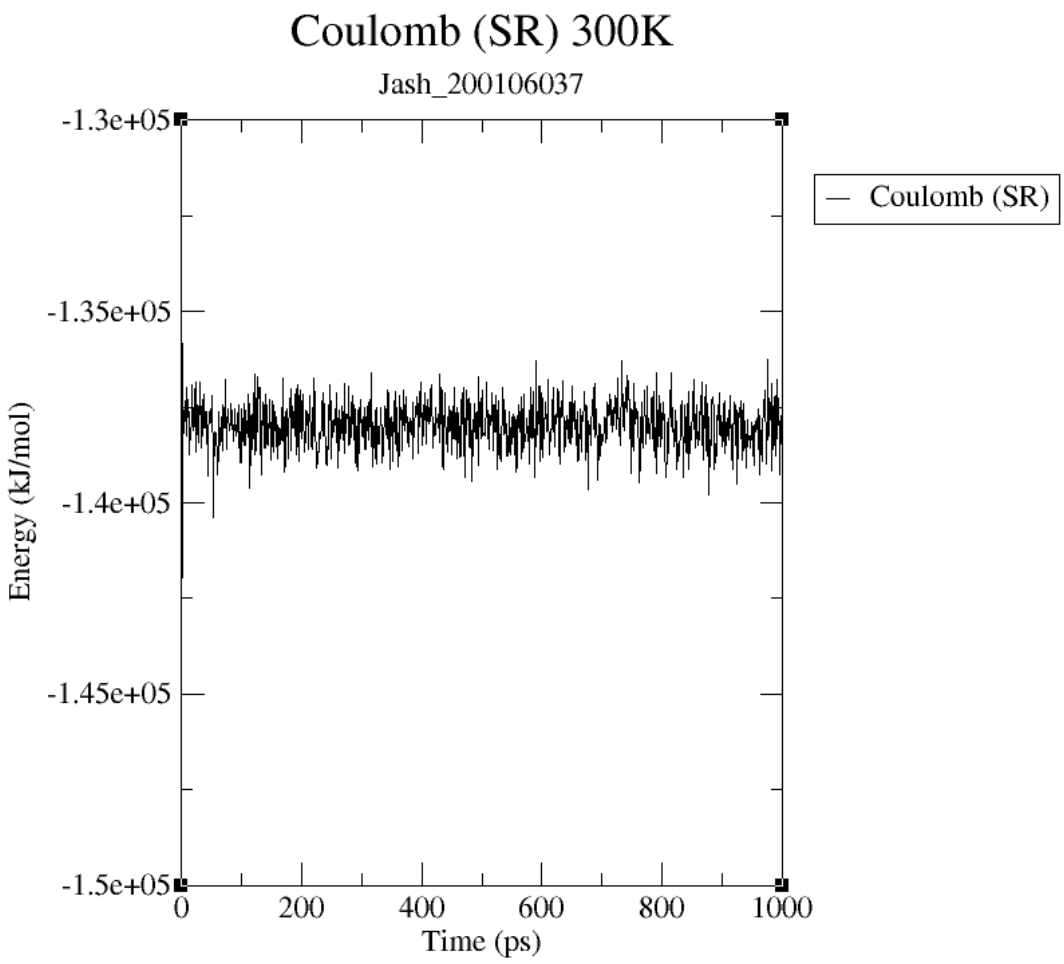
Total Energy -- 300K



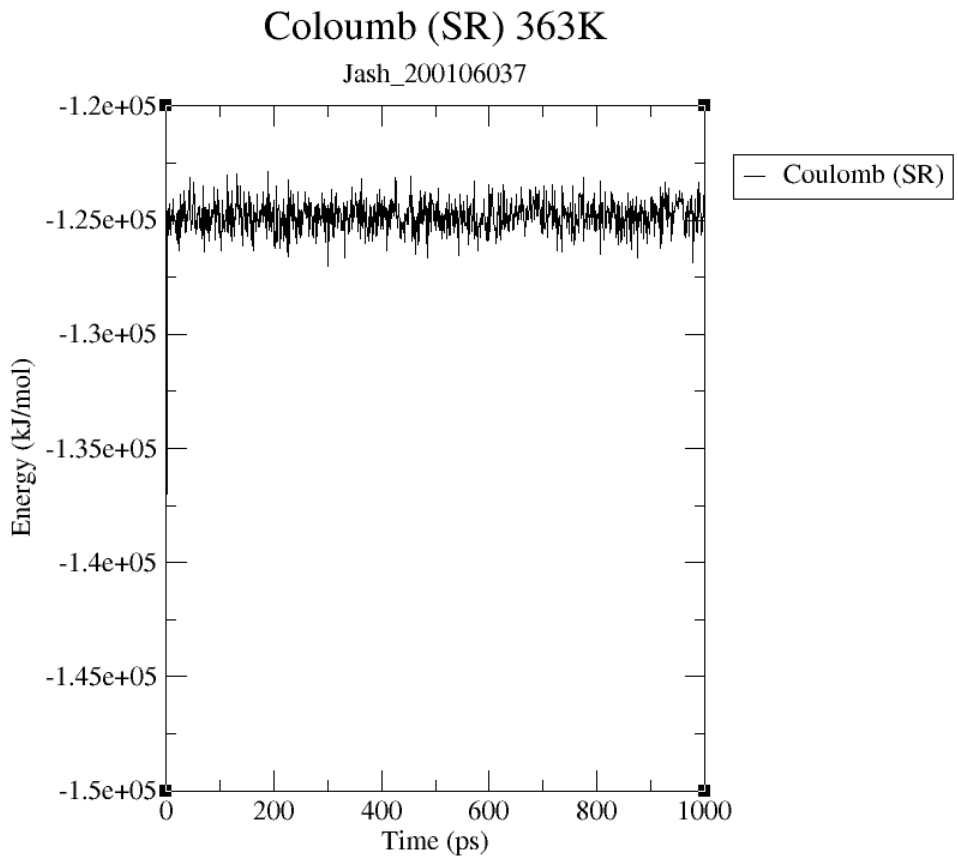
Total Energy -- 363K



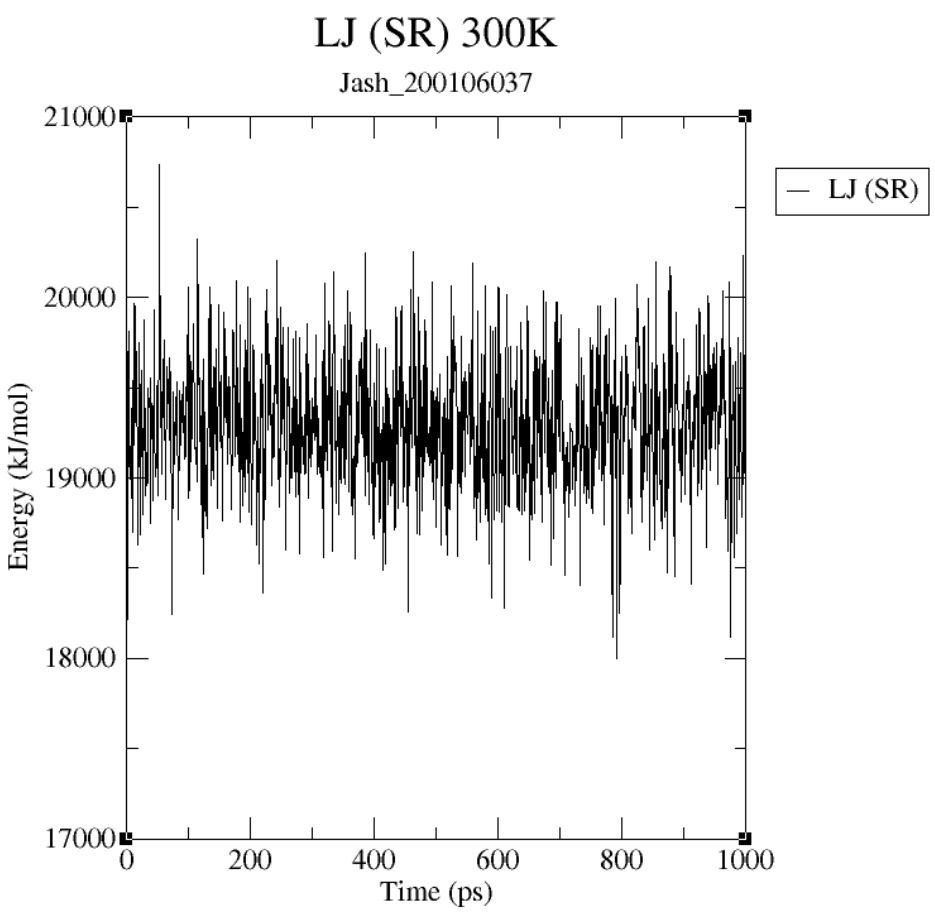
Coul SR -- 300K



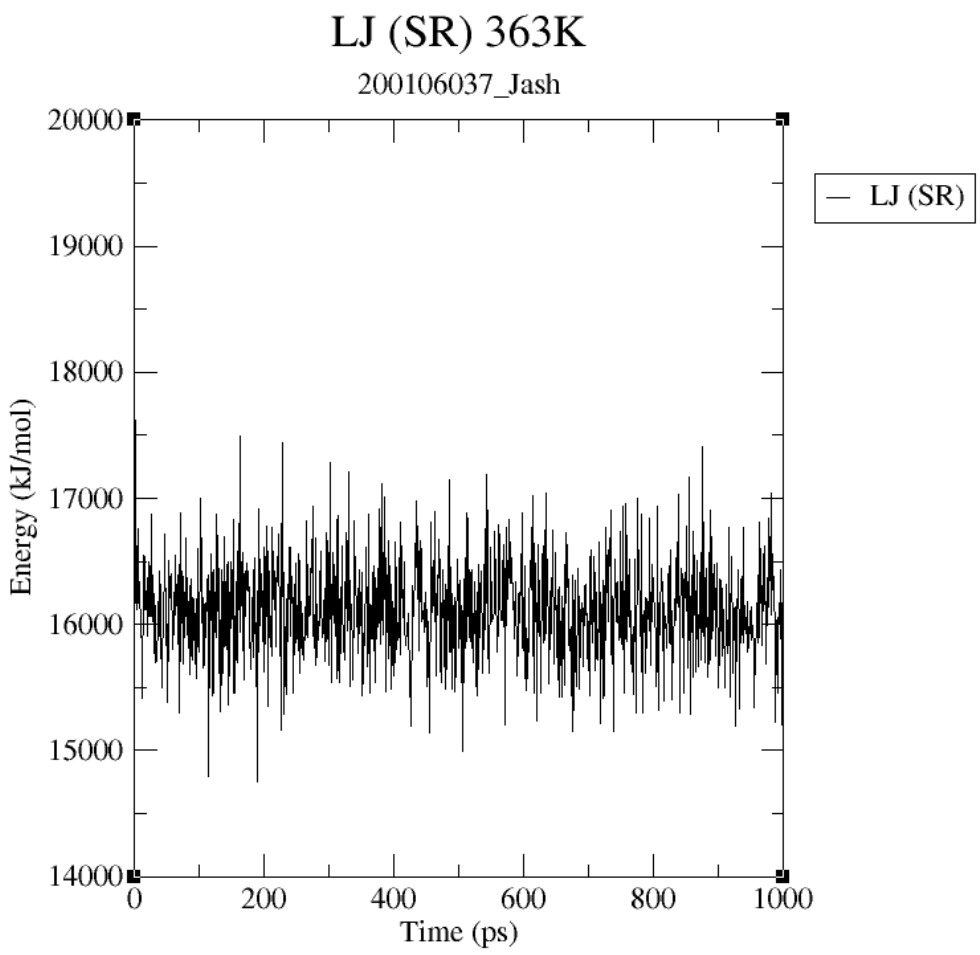
Coul SR -- 363K



LJ-SR --
300K

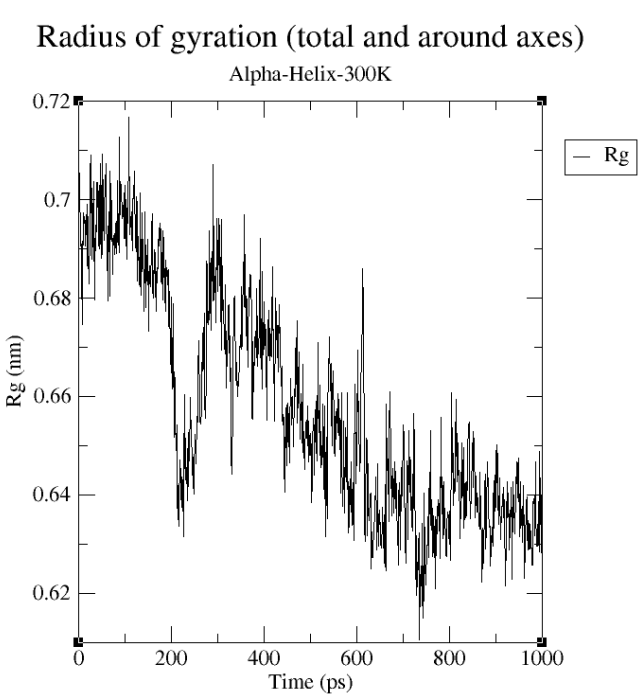


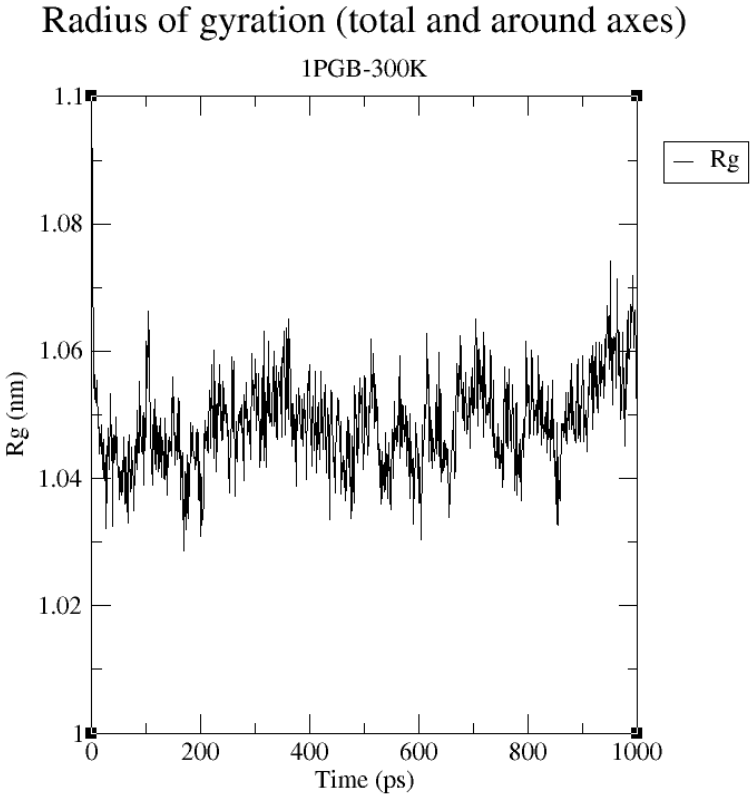
LJ-SR --
363K

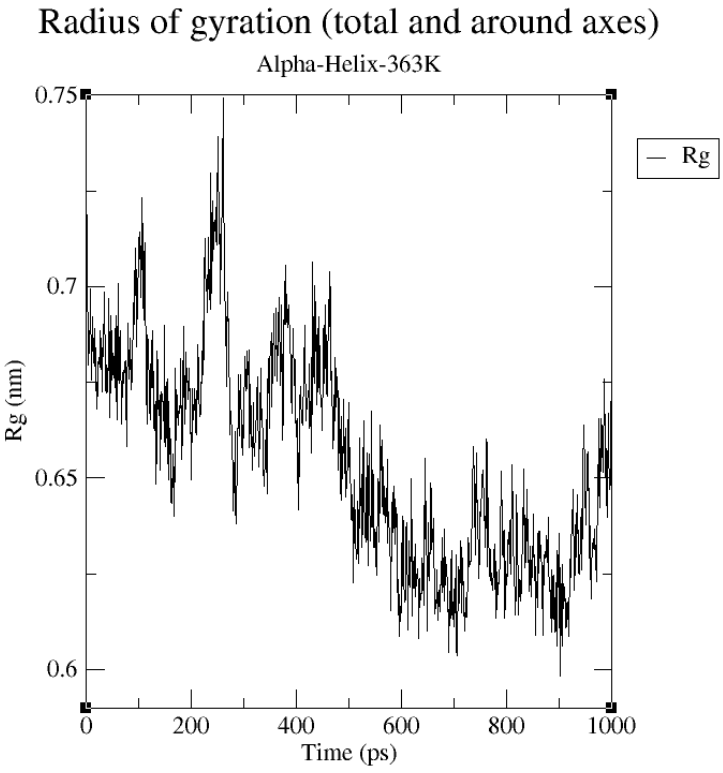


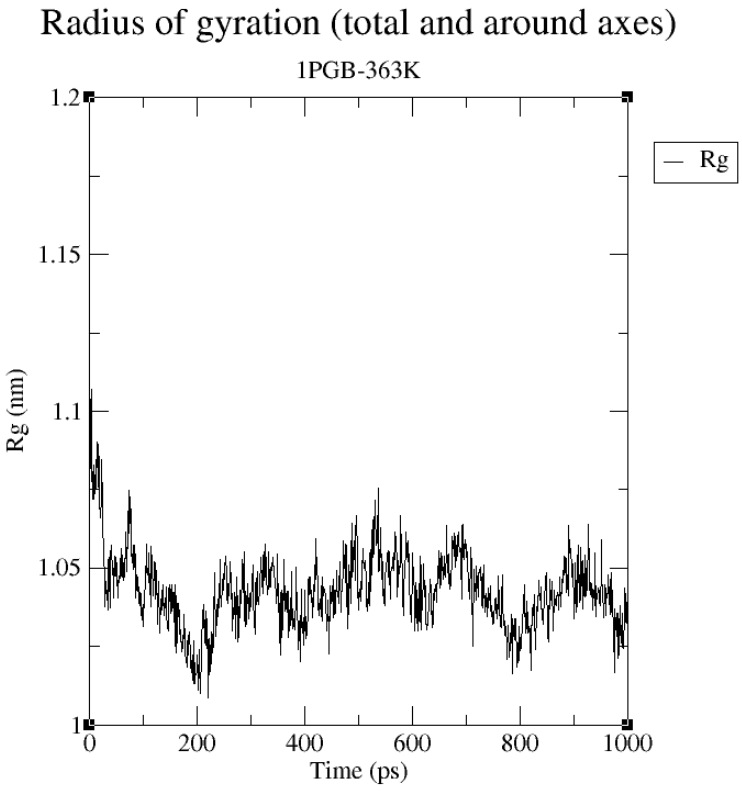
03. Radius of Gyration of all Molecular Structures :

Alpha Helix



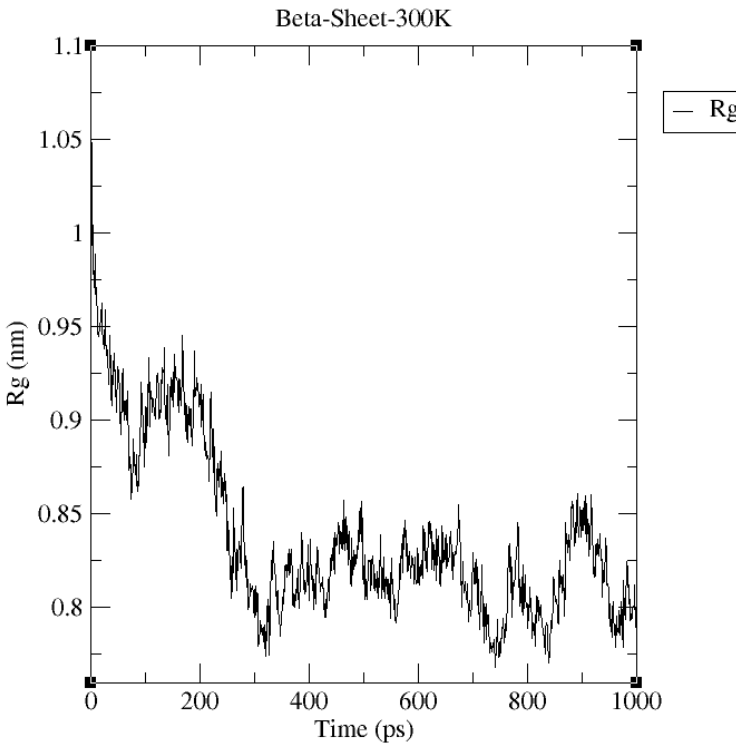




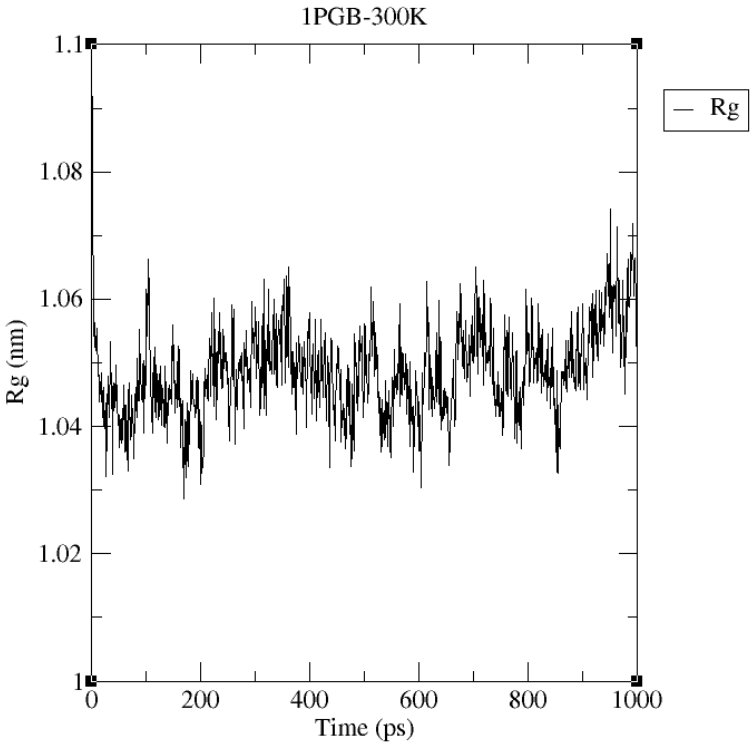


Beta Sheet

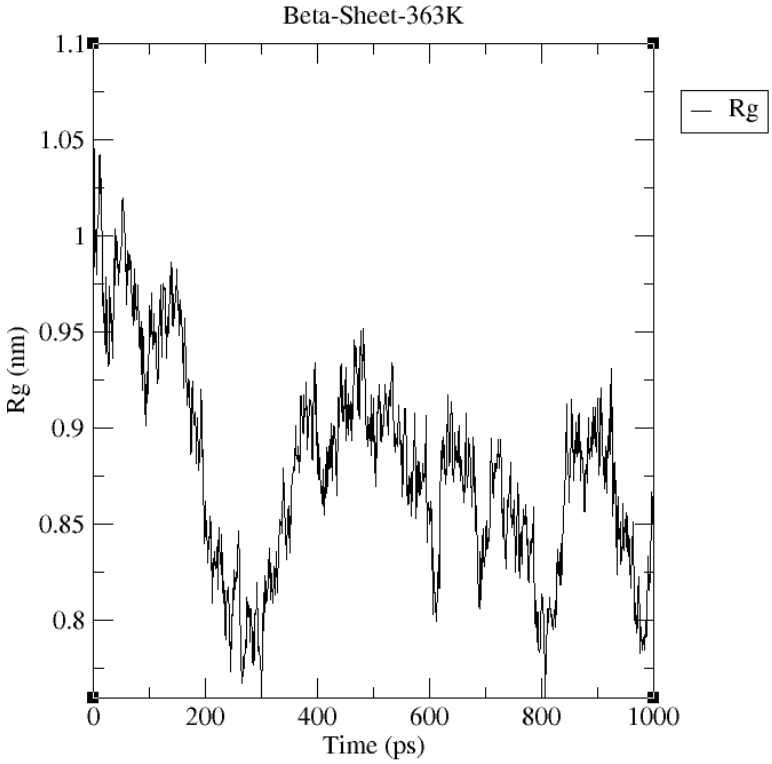
Radius of gyration (total and around axes)



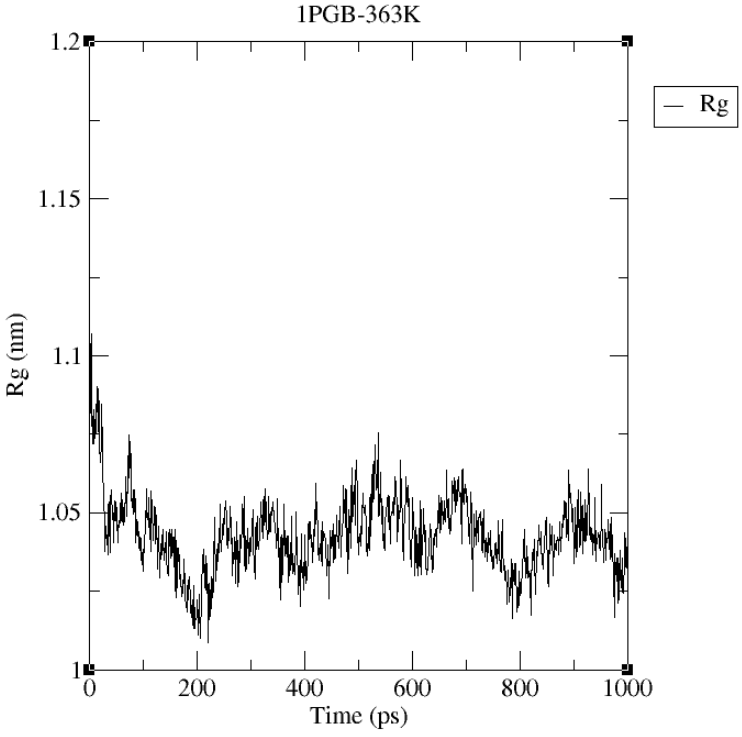
Radius of gyration (total and around axes)



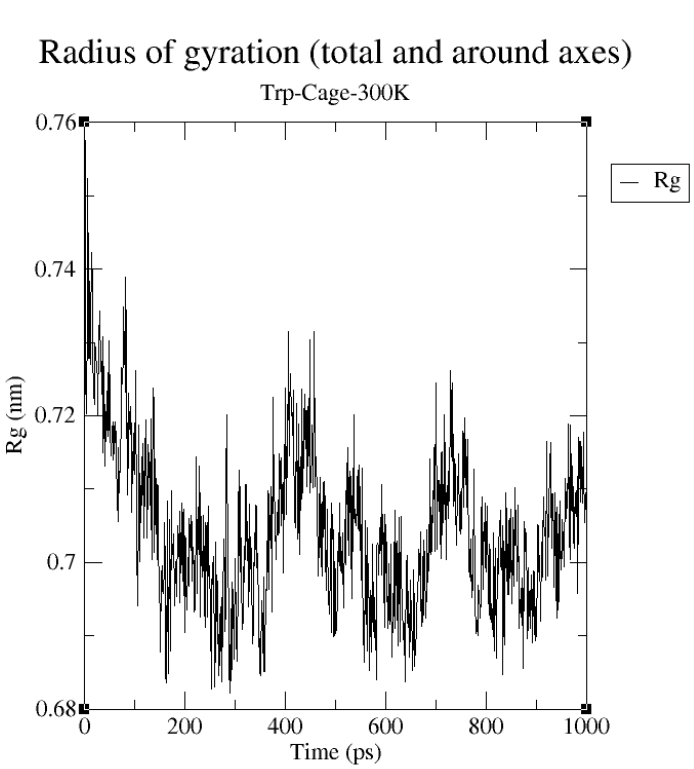
Radius of gyration (total and around axes)

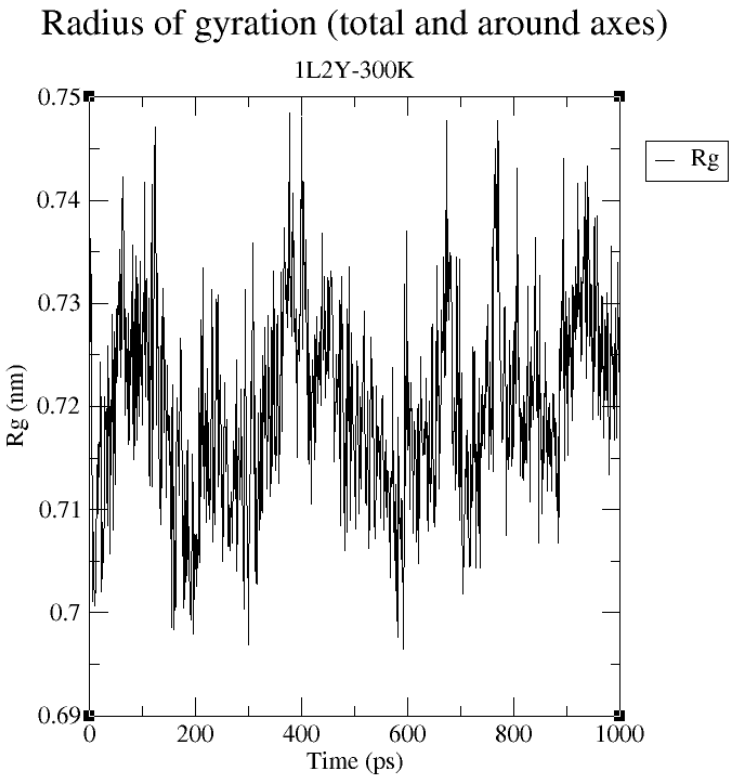


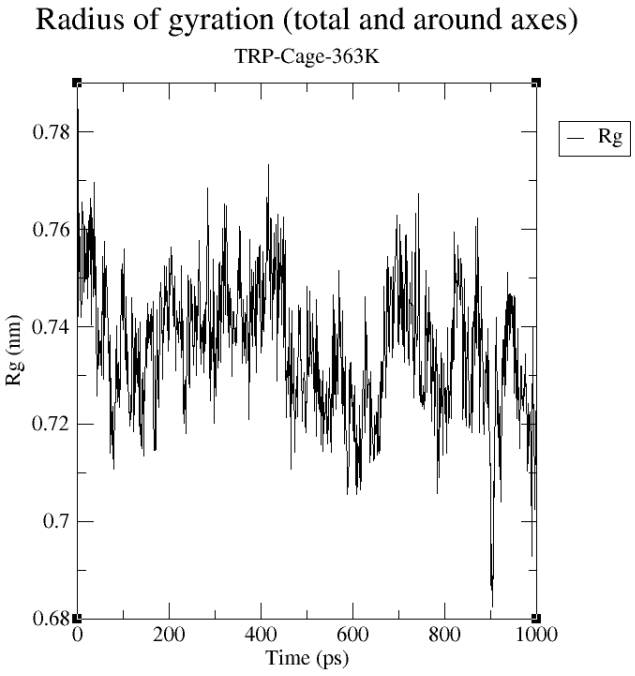
Radius of gyration (total and around axes)

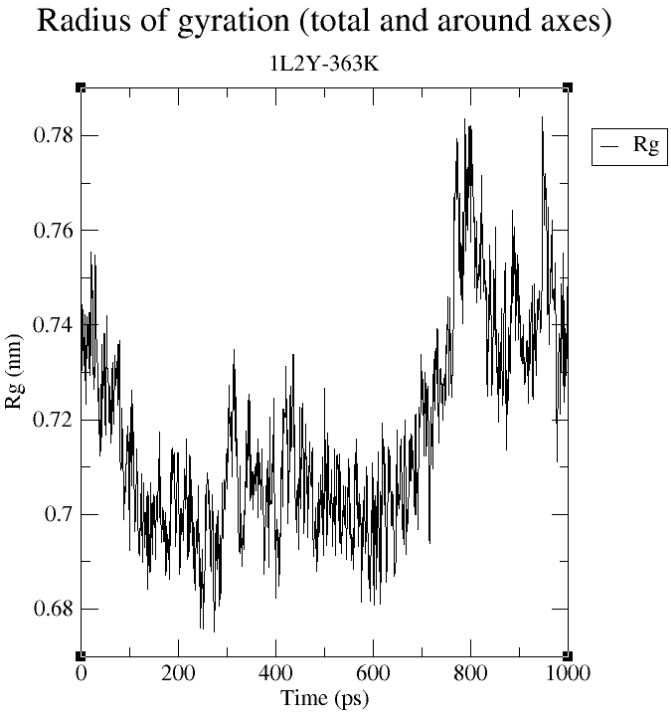


TRP Cage







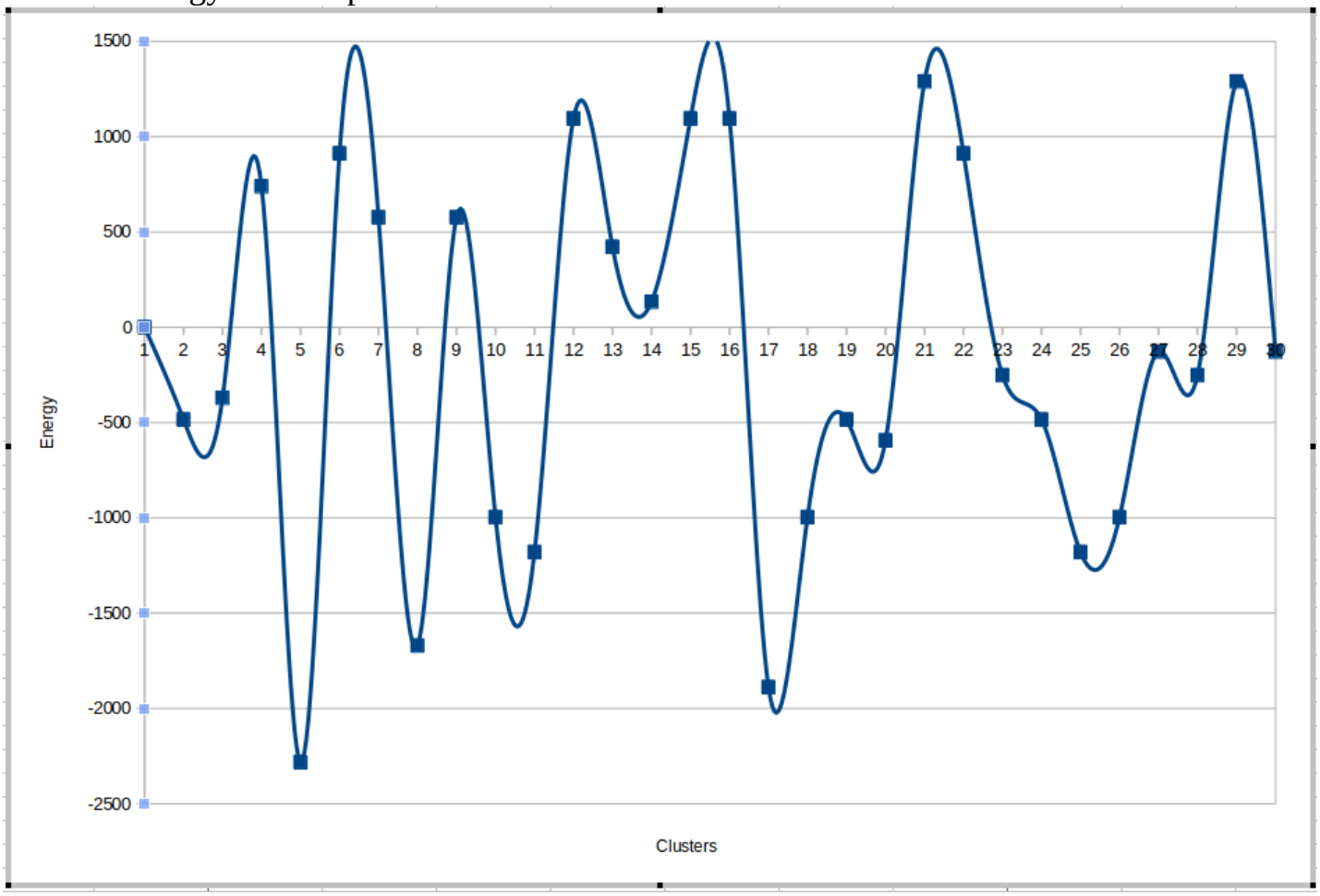


As we know, natural proteins (1PGB and TRP Cage) have a more complex 3-dimensional structure compared to that of designed peptides. Also, as out designed peptides are selective thus they are more specific and particular in terms of shape and size. For e.g. - Alpha Helix has a a defined spiral shape. Thus, we can observe that their Radius of Gyration values are low compared to those of natural proteins. Also, since natural proteins have more random shape and structure, their Rg values are also higher.

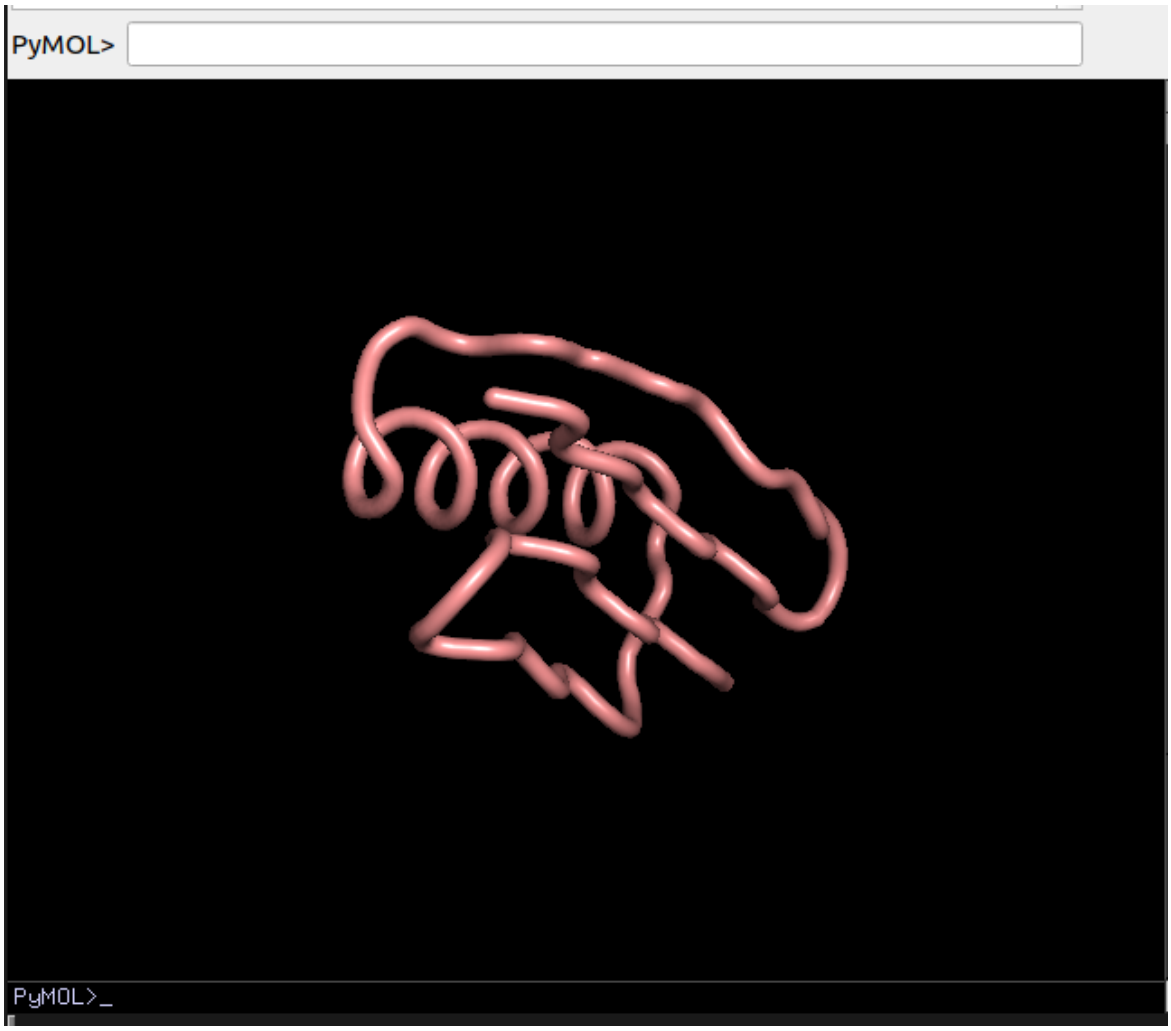
04.

1PGB :	300K	: Found 4 clusters
	363K	: Found 85 clusters
Alpha-Helix :	300K	: Found 2 clusters
	363K	: Found 58 clusters
Beta-Sheet :	300K	: Found 3 clusters
	363K	: Found 272 clusters
1L2Y :	300K	: Found 3 clusters
	363K	: Found 101 clusters
TRP-Cage :	300K	: Found 3 clsuters
	363K	: Found 150 clusters

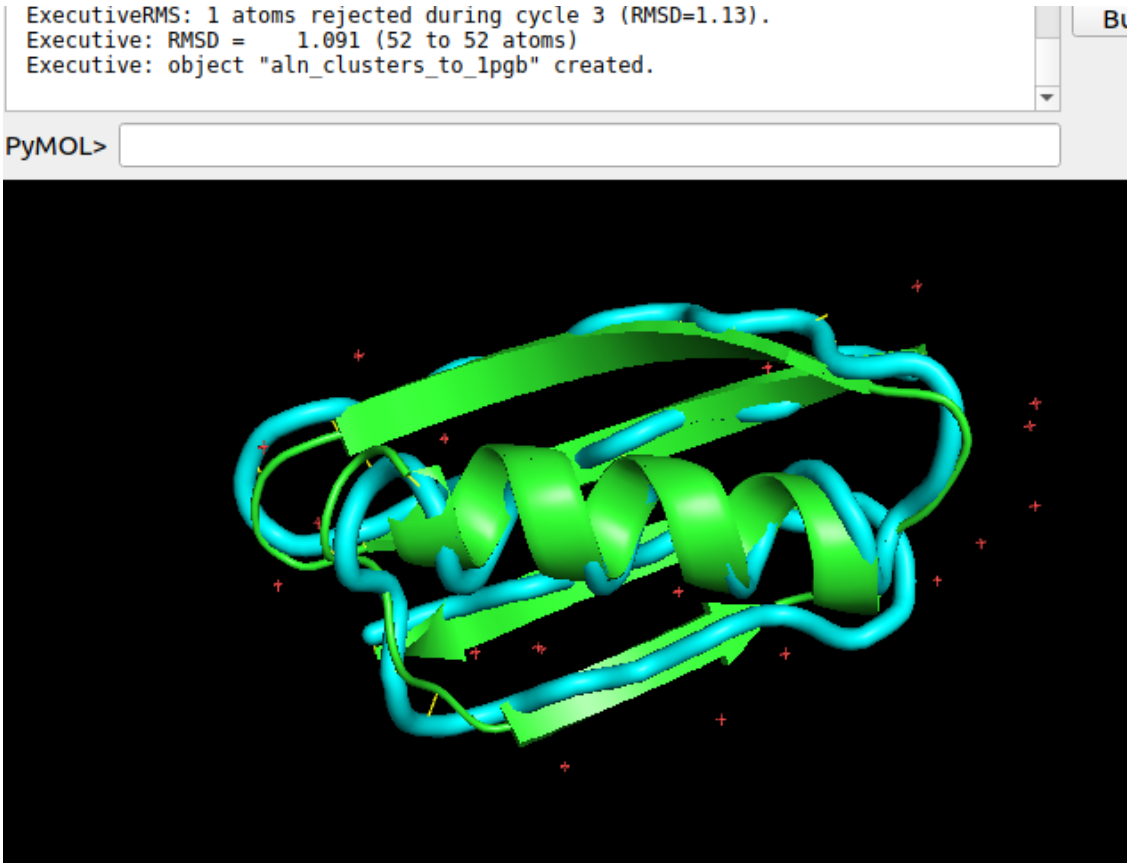
05. Free Energy Landscape of 1PGB at 363K



Average structure of 1PGB.pdb at 363K (cluster.pdb)



Average structure aligned with 1PGB.pdb original structure along with RMSD value :



Inference :

The analysis allows deduction of the key conformational states of 1PGB and their inerconversion. The free energy landscapes exhibits the energy barriers and pathways between these different states. The average structures of each cluster can give an idea about the changes in protein conformation and how it associates with it’s function. This explains the relation of the molecule’s structure with it’s function.