Molecular Dynamics Insights into the Structural Behavior of VAR_C2_8_CTX-M_1
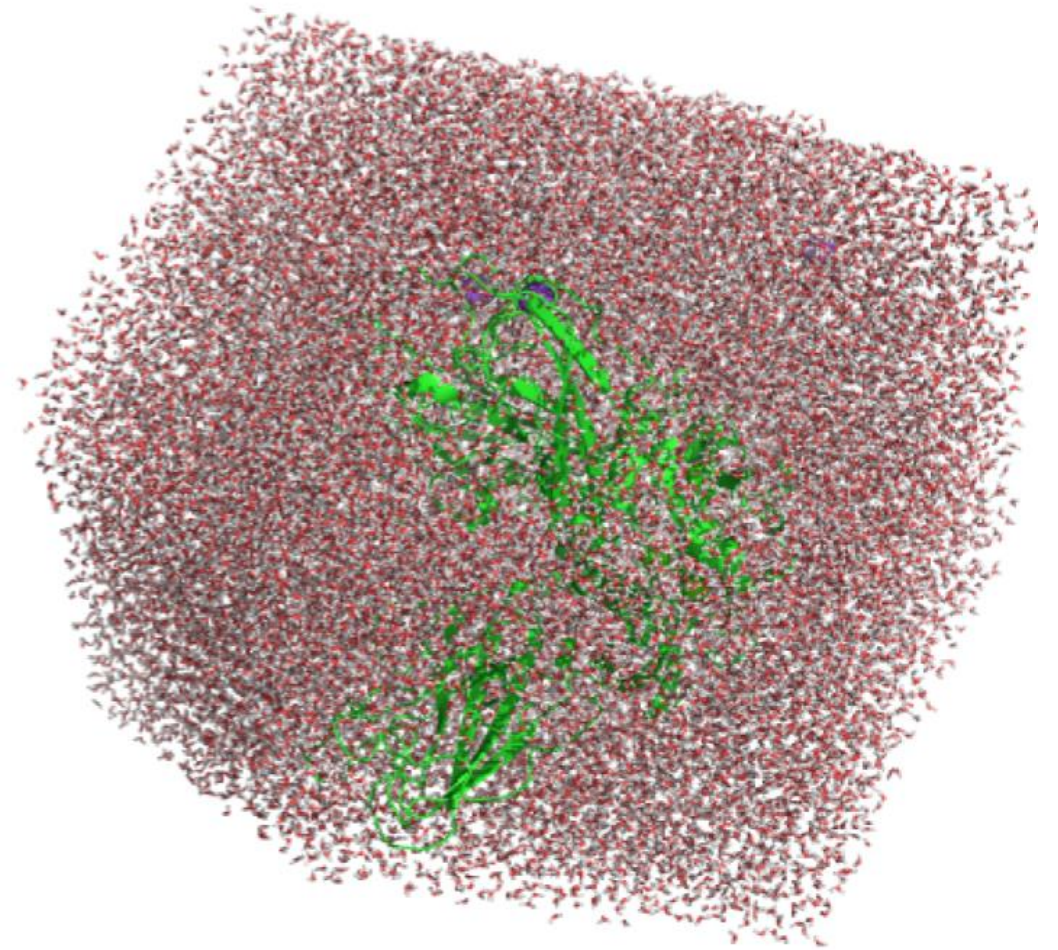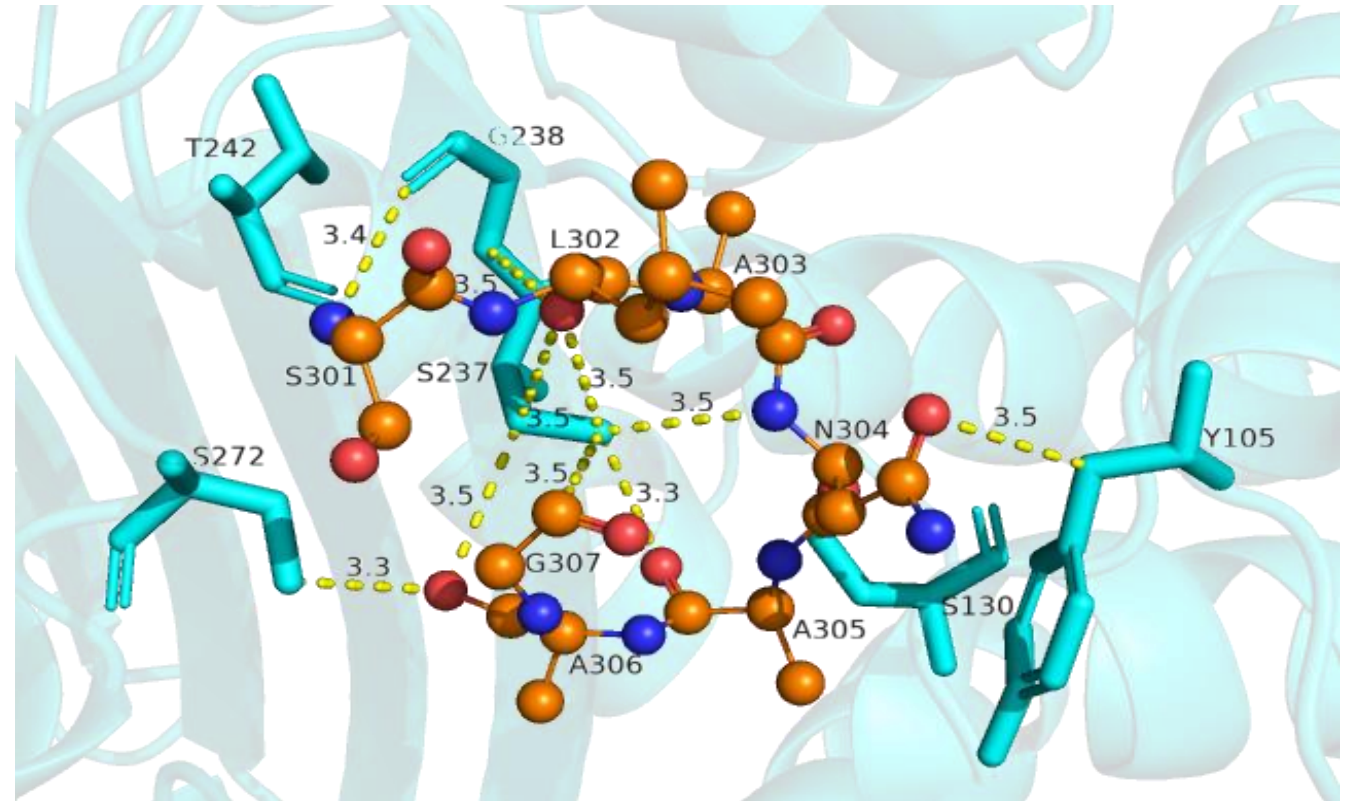
Binding Energy (KJ/Mol)

Predicted Peptide	KPC-2	CTX-M-1	SME-1	TEM-1	SHV-1
VAR_C2_8.pdb	-6	-5.5	-5.4	-1.7	-6

VAR_C2_CTX_M_1.pdb

Ref. peptide sequence	Backbone generation	Length of generated peptide	Generated AA sequence	Generate 3D structure
DERF	C2_8.pdb	7	SLANAAG	VAR_C2_8.pdb

Running Simulation on HPC

full_simulation_for_VAR_C2_8_CTX_M_1

Script_name: run_sim_full.sh

Input_directory:
/home/hazra.lab_bt.iitr/Pakhi/CTX_M_1
/VAR_C2_8_CTX_M_1

Output_directory:
/home/hazra.lab_bt.iitr/Pakhi/CTX_M_1
/VAR_C2_8_CTX_M_1

Submission job id: 379482

```
[hazra.lab_bt.iitr@login09 ~]$ sinfo -p gpu
PARTITION AVAIL  TIMELIMIT   NODES  STATE NODELIST
gpu           up 1-00:00:00     10     mix gpu[003,005,007-008,010-015]
gpu           up 1-00:00:00      8   alloc gpu[001-002,004,006,009,016-018]
gpu           up 1-00:00:00      2    idle gpu[019-020]
```

```
/home/hazra.lab_bt.iitr/Pakhi/All_docked_structure/CTX_M_1/Output/
├── protein_peptide_1_sim/
│   ├── fnl_processed.gro
│   ├── fnl_newbox.gro
│   ├── fnl_solv.gro
│   ├── fnl_solv_ions.gro
│   ├── em.gro
│   ├── nvt.gro
│   ├── npt.gro
│   ├── md.gro
│   ├── protein_peptide_1_sim_rmsd_plot.xvg
│   ├── protein_peptide_1_sim_rmsf_plot.xvg
│   ├── protein_peptide_1_sim_sasa_plot.xvg
│   ├── protein_peptide_1_sim_rg_plot.xvg
│   ├── protein_peptide_1_sim_rmsd_plot.png
│   ├── protein_peptide_1_sim_rmsf_plot.png
│   ├── protein_peptide_1_sim_sasa_plot.png
│   ├── protein_peptide_1_sim_rg_plot.png
│   └── ...
├── protein_peptide_2_sim/
└── ...
```
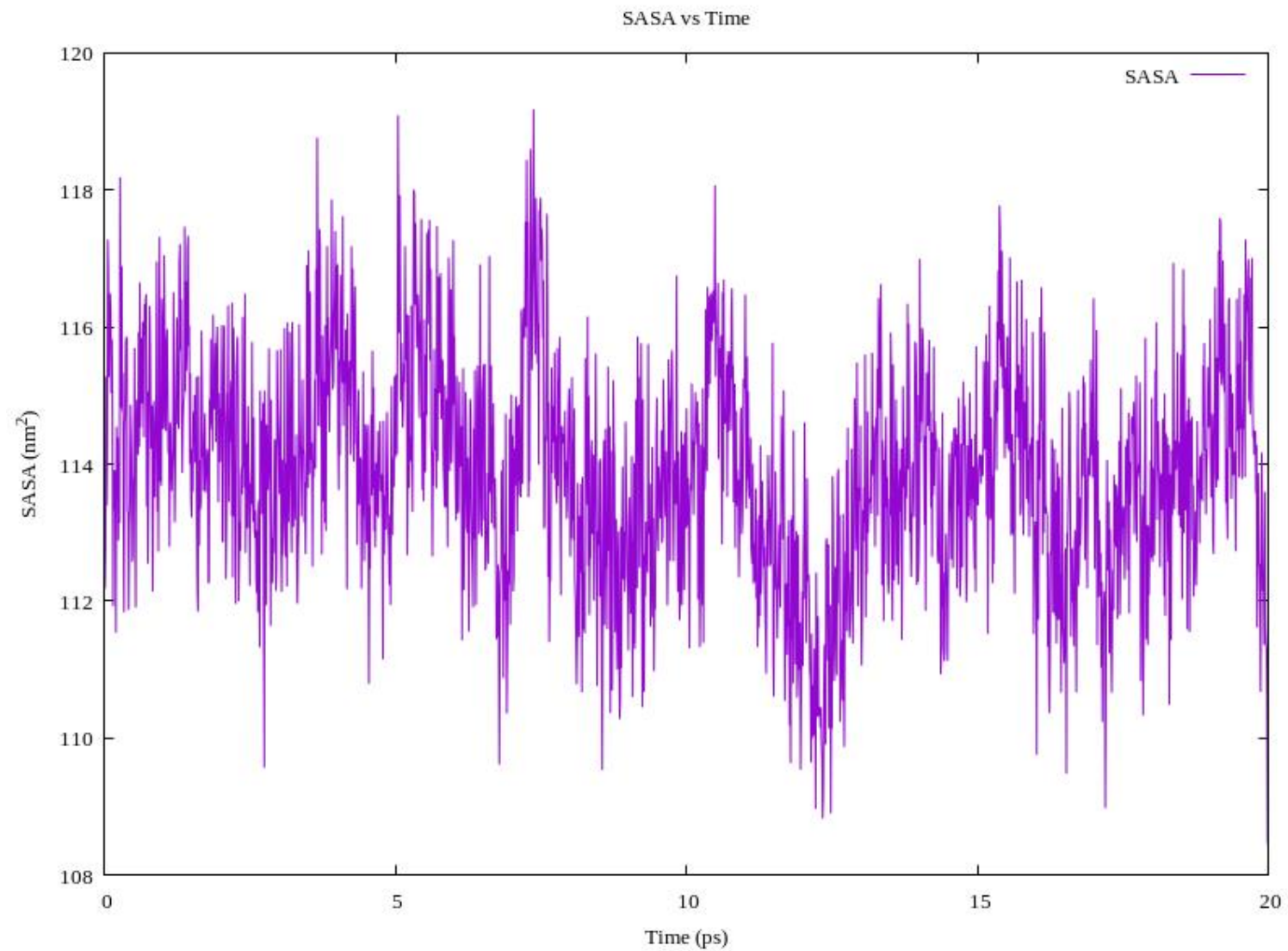
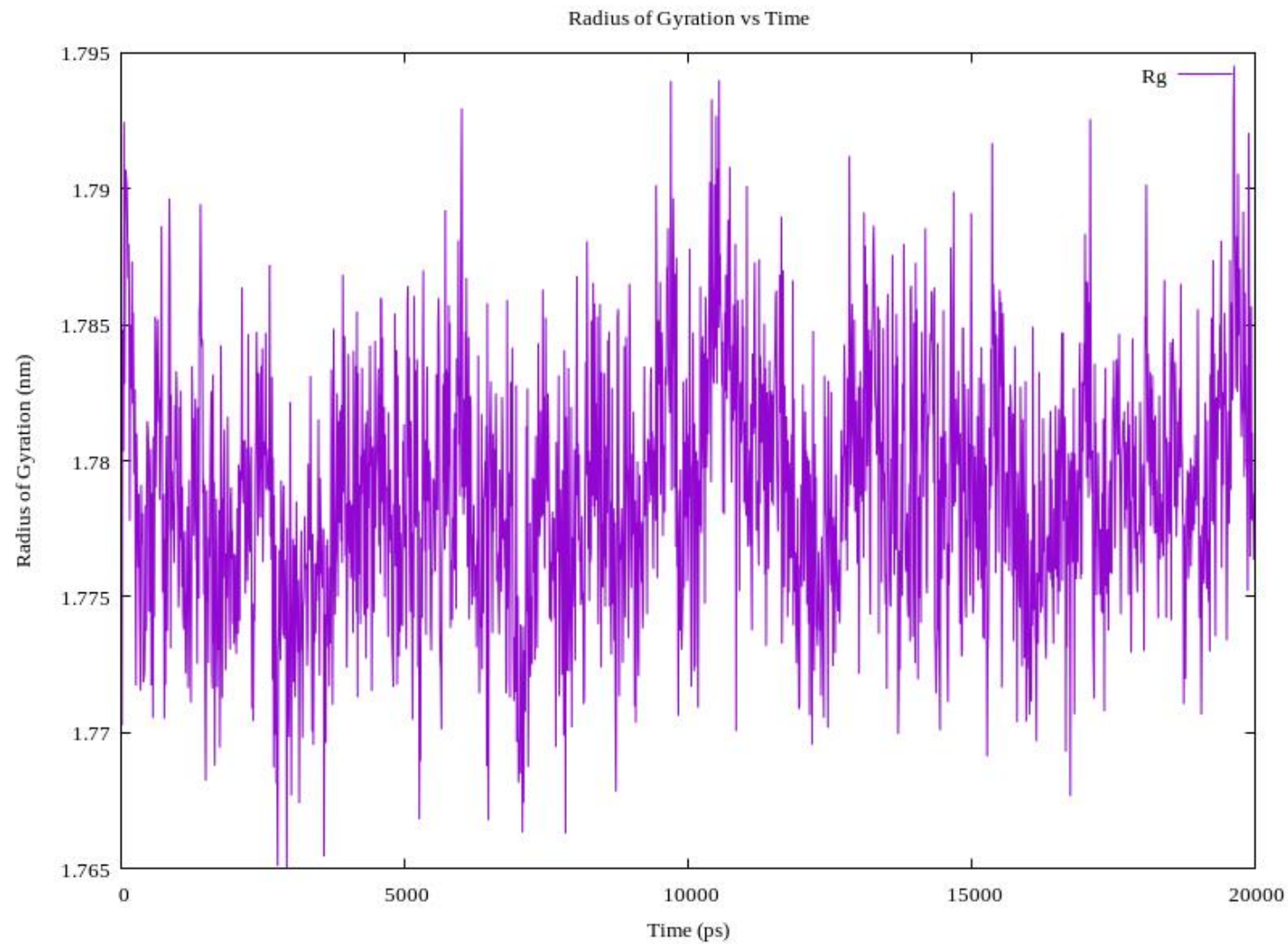Fig. File structure on running Simulation

RMSD plot

RMSD vs Time
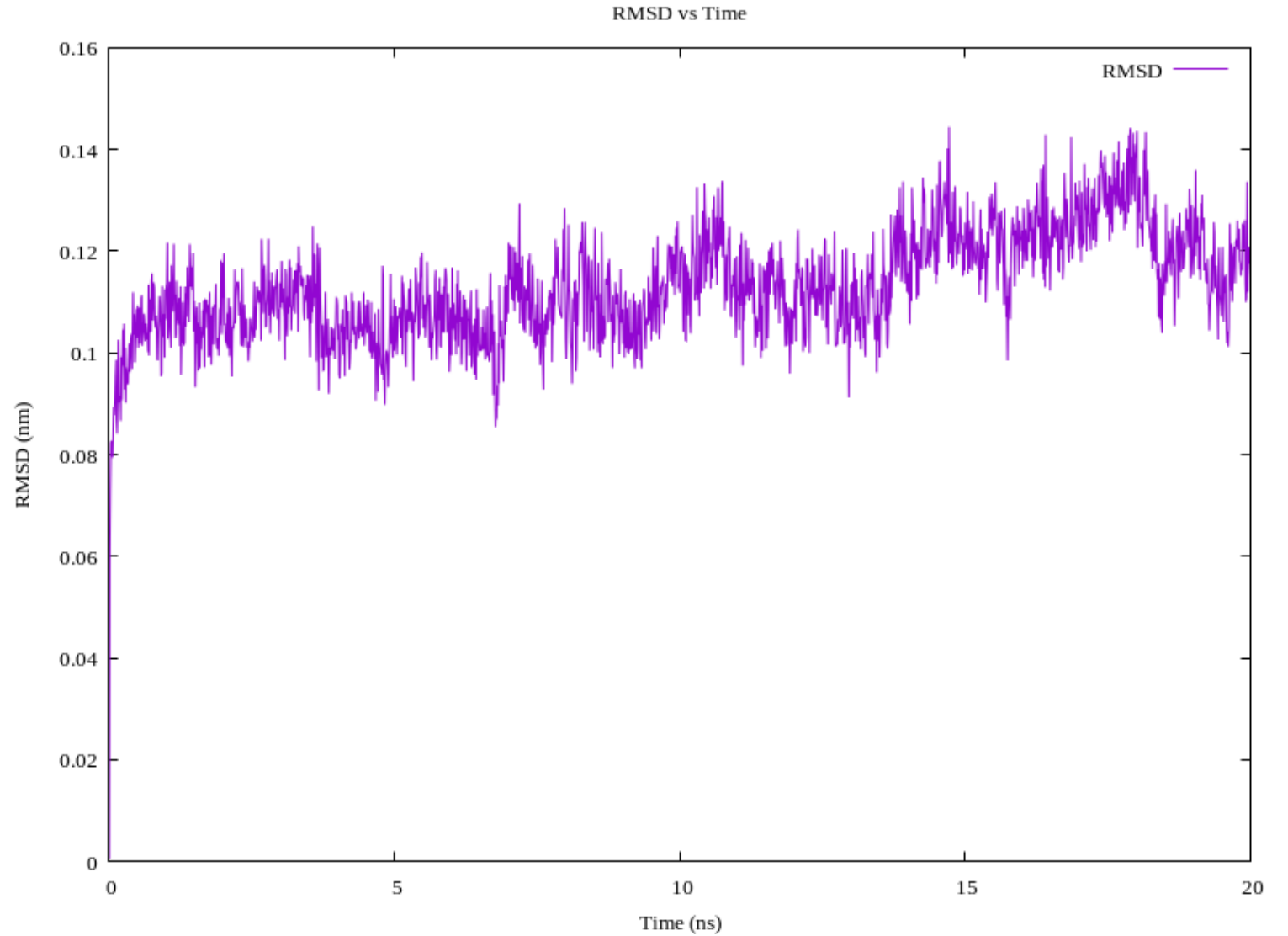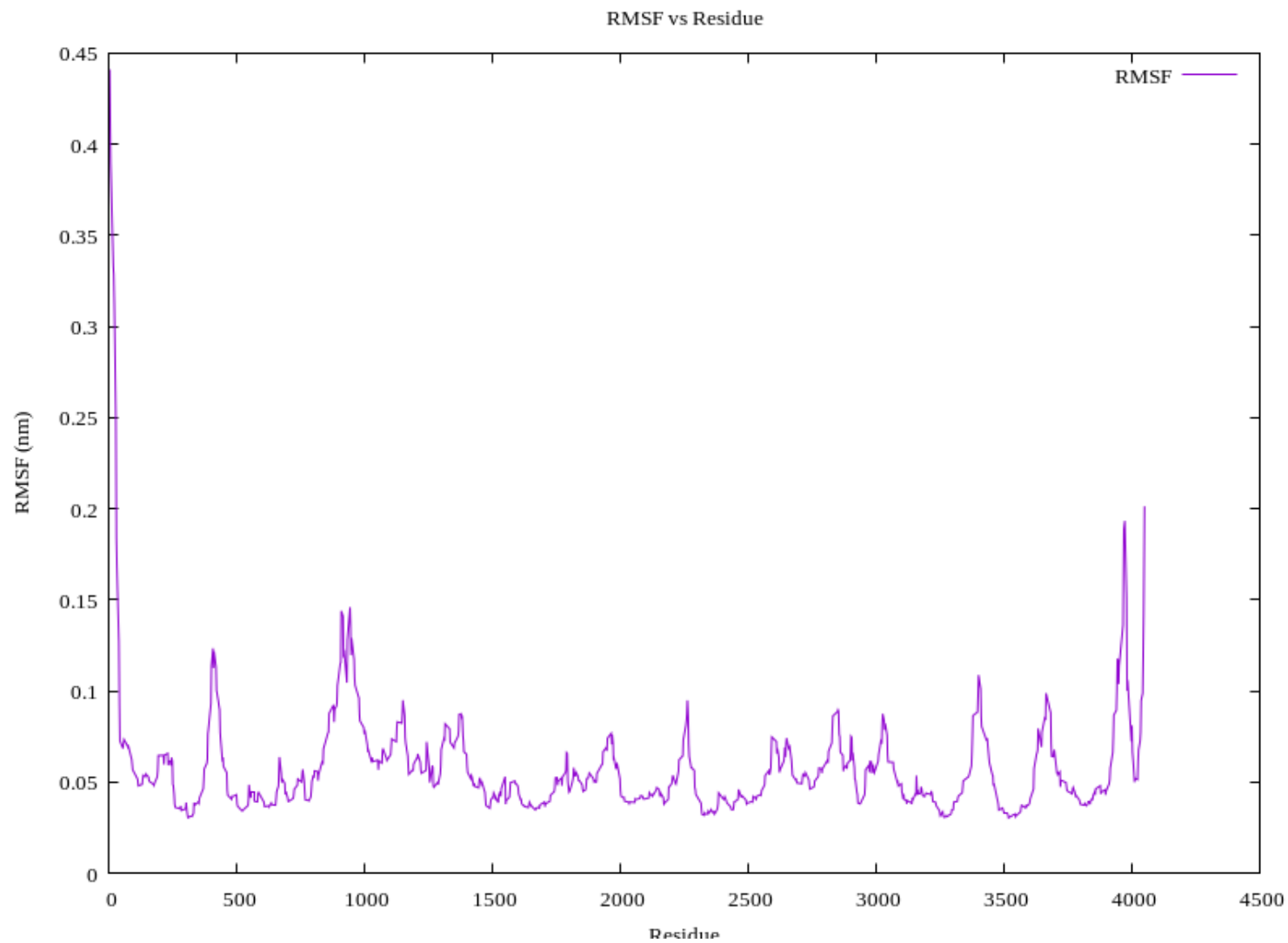
RMSF plot

SASA plot

Radius of Gyration plot

Conclusion

- The RMSD plot indicated complex stabilization after **~5 ns**, maintaining values between **0.12–0.14 nm**.

- RMSF analysis showed minimal residue fluctuations **(<0.1 nm**), with higher flexibility **(~0.35 nm**) in loop and terminal regions.

- SASA remained stable (**110–125 nm²**), and

- Rg ranged from **1.775–1.790 nm**, indicating sustained structural compactness.