Files and Folder Structure for GitHub Repository: DNMT1_Tunneling_2026

Below is a complete list of recommended files and folders to upload into your GitHub repository to satisfy Biophysical Journal's reproducibility standards and Reviewer 2's transparency request.

📁 Root Directory

- `README.md` – Full project overview and usage instructions
- `LICENSE` – MIT License or equivalent
- `environment.yml` – Conda environment file with versions of Python, NumPy, matplotlib, etc.
- `.gitignore` – (optional) to exclude large raw trajectory files

📁 /qm_mm_inputs/

- `dnmt1_qmmm.inp` – TeraChem or Gaussian QM/MM input
- `dnmt1.top` and `dnmt1.crd` – Amber topology and coordinate files
- `qmmm_partition.png` – Figure showing QM/MM boundary (as used in Figure S2)
- `active_site_alignment.pdb` – PDB with SAM, cytosine, and key residues

📁 /rpi_scripts/

- `run_rpi.sh` – Instanton driver script
- `metadata.json` – Defines bead counts, temperature, and convergence settings
- `bead_ladder/` – Subfolder with:
- `P16.out`, `P32.out`, ..., `P128.out` – Action (S/ħ) and tunneling rate files
- `convergence_plot.py` – Script to plot ΔS/ħ vs P (used for Figure S6)

📁 /barrier_fitting/

- `scan_coords.dat` – 1D or 2D reaction coordinate scans
- `fit_morse.py` – Python script to fit Morse or spline potential
- `2D_surface_plot.py` – Code used to generate Figure S7

📁 /kie_analysis/

- `rate_ch3.dat`, `rate_cd3.dat` – Raw tunneling rates
- `bootstrap_kie.py` – Script to compute 95% confidence interval
- `Figure4c_plot.py` – Reproduces Figure 4c with error bars

📁/env/

- `env_info.txt` – Output of `conda list` or `pip freeze`
- `software_versions.md` – List of GROMACS, TeraChem, Python, and system info

📁/docs/

- `workflow.md` – Step-by-step guide to reproduce simulation pipeline
- `Figure_S2_QMMM.png` – QM/MM partition figure
- `Figure_S6_BeadLadder.png`, `Figure_S7_2D_Surface.png` – Supplementary figures

(Optional) 📁/notebooks/

- `instanton_workflow.ipynb` – Interactive Jupyter notebook to re-run the tunneling rate and KIE workflow end-to-end.

Let me know if you'd like help generating placeholder files or creating the environment file for upload.