In [22]: `pip install mdtraj`

```
Defaulting to user installation because normal site-packages is not write
able
Requirement already satisfied: mdtraj in /home/ac7407/.local/lib/python3.
8/site-packages (1.9.7)
Requirement already satisfied: scipy in /share/apps/python/3.8.6/intel/li
b/python3.8/site-packages/scipy-1.5.2-py3.8-linux-x86_64.egg (from mdtra
j) (1.5.2)
Requirement already satisfied: numpy>=1.6 in /share/apps/python/3.8.6/int
el/lib/python3.8/site-packages/numpy-1.19.2-py3.8-linux-x86_64.egg (from
mdtraj) (1.19.2)
Requirement already satisfied: astunparse in /home/ac7407/.local/lib/pyth
on3.8/site-packages (from mdtraj) (1.6.3)
Requirement already satisfied: pyparsing in /share/apps/python/3.8.6/inte
l/lib/python3.8/site-packages (from mdtraj) (2.4.7)
Requirement already satisfied: wheel<1.0,>=0.23.0 in /share/apps/python/
3.8.6/intel/lib/python3.8/site-packages (from astunparse->mdtraj) (0.35.
1)
Requirement already satisfied: six<2.0,>=1.6.1 in /share/apps/python/3.8.
6/intel/lib/python3.8/site-packages (from astunparse->mdtraj) (1.15.0)
WARNING: You are using pip version 20.2.3; however, version 22.2.2 is ava
ilable.
You should consider upgrading via the '/share/apps/python/3.8.6/intel/bi
n/python -m pip install --upgrade pip' command.
Note: you may need to restart the kernel to use updated packages.
```

In [2]:
```python
# import mdtraj as md
import mdtraj as md
import mdtraj.testing
import matplotlib.pyplot as plt

# Load 1hz3_T310.stepid25000000.every100ps.nowater.xtc file using mdtraj
traj = md.load('1hz3_T310.stepid25000000.every100ps.nowater.xtc', top= '1hz

# calculate end-to-end distance at each frame
end_to_end = md.compute_distances(traj, [[0, traj.n_atoms - 1]])

# calculate radius of gyration at each frame
radius_of_gyration = md.compute_rg(traj)

# plot end-to-end distance at left axis and radius of gyration at right axi
# title graph as 'End-to-end distance and radius of gyration as a function
fig, ax1 = plt.subplots()
ax1.plot(end_to_end, 'b-')
ax1.set_xlabel('time (ps)')
ax1.set_ylabel('end-to-end distance (nm)', color='b')
ax1.tick_params('y', colors='b')
ax2 = ax1.twinx()
ax2.plot(radius_of_gyration, 'r-')
ax2.set_ylabel('radius of gyration (nm)', color='r')
ax2.tick_params('y', colors='r')
fig.tight_layout()
plt.title('End-to-end distance and radius of gyration as a function of time
plt.show()
```
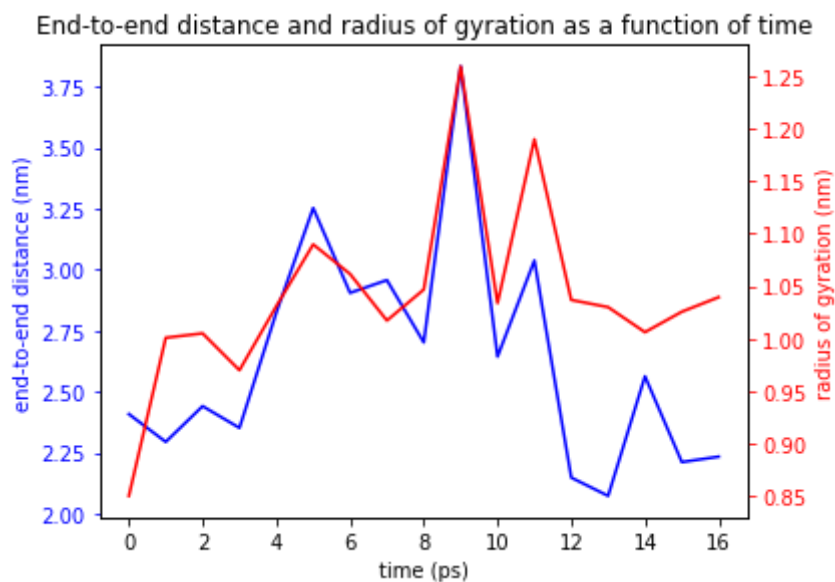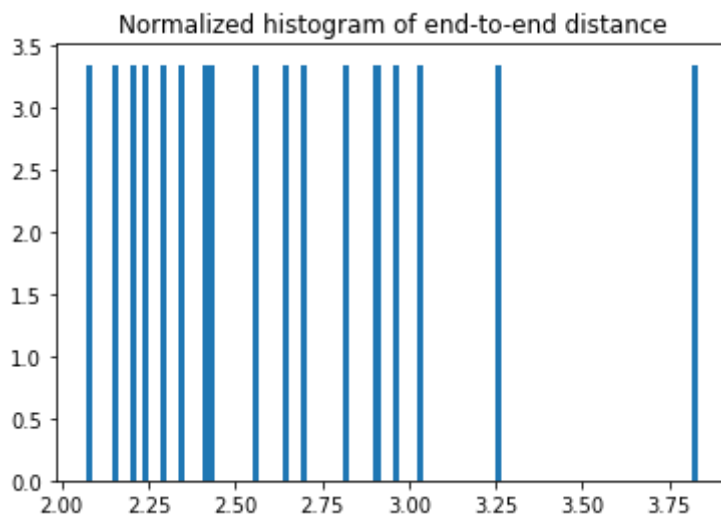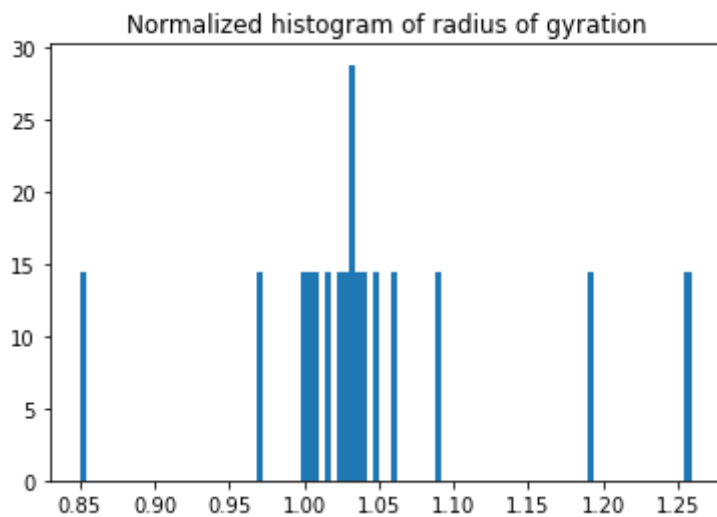
In [3]:
```python
# plot normalized histogram of end-to-end distance
plt.hist(end_to_end, bins=100, density=True)
plt.title('Normalized histogram of end-to-end distance')
plt.show()
```



Normalized histogram of end-to-end distance

In [4]:
```python
# plot normalized histogram of radius of gyration
plt.hist(radius_of_gyration, bins=100, density=True)
plt.title('Normalized histogram of radius of gyration')
plt.show()
```



Normalized histogram of radius of gyration

In [ ]: