

CA_distance_run2

April 21, 2016

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In [9]: import mdtraj as md
import os
import numpy as np
import sys
import matplotlib.pyplot as plt
%matplotlib inline
import time
import seaborn as sns
import pandas as pd

In [10]: def _dist_atom_selection(topology, atom1, atom2, verbose, unpythonize):
    """
    Function takes a topology file and residue selection and verifies if
    the latter is possible. It also returns the C-alpha atom selection
    Input:
        topology:
            mdtraj.Topology or string
            Either mdtraj.Topology object or path to trajectory
            to be loaded
        residue_selection:
            string or list with integers
            String will be interpreted with the Mdtraj atom
            selection language. The list will be treated as
            atom number
        selection (by default True):
            boolean
            if true the function will try to return the residue/
            atom selection
    Output:
        atom_subset
            numpy.array
            array with all the atom numbers corresponding to selection
        md_topology
            mdtraj.core.topology.Topology object of protein
    """
    ## First have to load all the inputs if they are defined by a path
    if isinstance(topology, str):
        if os.path.exists(topology):
            try:
                md_topology = md.load_topology(topology)
            except:
                sys.exit('Make sure you have provided a valid path to topology file!')
        else:
            if verbose > 0:
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        print 'The following topology file was successfully loaded: \n %s \n' %(md_-

elif isinstance(topology, md.core.topology.Topology):
    md_topology = topology
    if verbose > 0:
        print 'The following topology file was successfully loaded: \n %s \n' %(md_topology)
else:
    sys.exit('Invalid input! Must be a valid path to topology file or mdtraj.Topology object')

## check chosen atoms
if isinstance(atom1, str):
    #try:
    atom_subset1 = md_topology.select(atom1)
    #except:
    #    sys.exit('Invalid atom selection!')
    #else:
    #    if verbose > 0:
    #        print 'Atom1 number: %s' %(atom_subset1[0] + 1)

elif isinstance(atom1, int):
    atom1 = atom1 - 1
    try:
        atom_subset1 = []
        if atom1 < md_topology.n_atoms:
            atom_subset1.append(atom1)
    except:
        sys.exit('Atom selection invalid for given topology!')
    else:
        if verbose > 0:
            print 'Atom1 number: %s' %(atom_subset1[0] + 1)

else:
    sys.exit('Invalid atom selection, you need to provide a string or an integer')

if isinstance(atom2, str):
    #try:
    atom_subset2 = md_topology.select(atom2)
    #except:
    #    sys.exit('Invalid atom selection!')
    #else:
    #if verbose > 0:
    #    print 'Atom2 number: %s' %(atom_subset2[0] + 1)

elif isinstance(atom2, int):
    atom2 = atom2 - 1
    try:
        atom_subset2 = []
        if atom2 < md_topology.n_atoms:
            atom_subset2.append(atom2)
    except:
        sys.exit('Invalid atom selection!')
    else:
        if verbose > 0:

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        print 'Atom2 number: %s' %(atom_subset2[0] + 1)

    else:
        sys.exit('Invalid atom selection, you need to provide a string or an integer')

pair = np.append(atom_subset1, atom_subset2).reshape(1,2)

# should work until 1109
if unpythonize:
    # rename residues (still testing)
    final_resid_name = []
    for i in md_topology.subset(pair).atoms:
        residues = str(i)
        # position to substitute
        pos = []
        num = []
        for i in range(len(residues)):
            # skip first three letters
            if i<6 and residues[i].isdigit():
                pos.append(i)
                num.append(int(residues[i]))
        if len(pos) == 1:
            if num[-1] < 9:
                num[-1] += 1
            else:
                num[-1] = 10
        if len(pos) == 2:
            if num[-1] < 9:
                num[-1] += 1
            else:
                num[-1] = 0
                num[0] += 1
        if len(pos) == 3:
            if num[-1] < 9:
                num[-1] += 1
            else:
                num[1] += 1
                num[-1] = 0
        z = 0
        residues = list(residues)
        for j in pos:
            residues[j] = str(num[z])
            z+=1
        final_resid_name.append("".join(residues))
    final_resid = " - ".join(final_resid_name)

    if verbose > 0:
        print 'Calculating distance between following atoms: %s \n' %(final_resid)

return md_topology, pair, final_resid

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In [11]: def _dist_atom_load(md_topology, trajectory, pair, verbose, chunk):

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# first create a list with all the paths that are needed
try:
    trajectory_path = os.listdir(trajectory)
except:
    sys.exit('Make sure you have provided a string for a valid path to a trajectory file!')
else:
    if verbose > 0:
        print 'Loading trajectories from the following files: '
        for trajectory_i in trajectory_path:
            print trajectory_i

all_distances = []
sim_time = []

#try:
for file_i in trajectory_path:
    for chunk_i in md.iterload(trajectory + file_i, chunk, top=md_topology):

        sim_time.append(chunk_i.time)

        if verbose > 1:
            print 'Successfully loaded trajectory: \n %s' %(chunk_i)

        all_distances.append(md.compute_distances(chunk_i, pair))

all_distances_np = np.concatenate(all_distances) * 10
#except:
#    sys.exit('Make sure you provided a valid path to a folder with trajectory files!')
#else:
#    print '\nSuccessfully calculated atom distances in %s frames!' %(all_distances_np.shape[0])

sim_time = np.concatenate(sim_time) / 1000

return all_distances_np.reshape(all_distances_np.shape[0]), sim_time

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In [12]: def main(topology, trajectory, atom1, atom2, verbose = 1, chunk = 100, unpythonize = True, plot_dist = False):
    """
    Function to calculate distance between two atoms and plot pdf
    """

    if verbose > 0:
        # timer for the whole function
        start = time.time()

        # now load topology and verify selection by calling _dist_atom_selection()
        md_topology, pair, final_residues = _dist_atom_selection(topology, atom1, atom2, verbose, chunk)

        # load trajectories and calculate distances
        distance, sim_time = _dist_atom_load(md_topology, trajectory, pair, verbose, chunk)

    if plot_dist:
        # plots:

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# distance as a function of time:
plt.figure(figsize=(12,12))
plt.plot(sim_time, distance, c='k', label = 'Distance')
plt.plot(sim_time, pd.rolling_mean(pd.DataFrame(distance), 50), c='red', label = '50 f')
plt.legend(loc='best', prop={'size':12})
plt.title('Distance between %s' % final_residues, size = 24)
plt.xlabel('Time (ns)', size = 14)
plt.ylabel('Distance (${\AA}$)', size = 14)
plt.show()

# distance density plot
plt.figure(figsize = (12,12))
ax = sns.distplot(distance, hist=False, rug=False)
ax.set_xlabel('Distance (${\AA}$)', size = 16)
ax.set_ylabel('Density', size = 16)
ax.set_title('Distance between %s' % final_residues, size = 24)
plt.show()

total_trajectory_time = sim_time[-1] - sim_time[0] + 0.02

if verbose > 0:
    print 'Total execution time: %.2f seconds \n' %(time.time() - start)
    print 'Total simulation time of all frames: %.2f nanoseconds' %(total_trajectory_time)

return distance, final_residues, total_trajectory_time

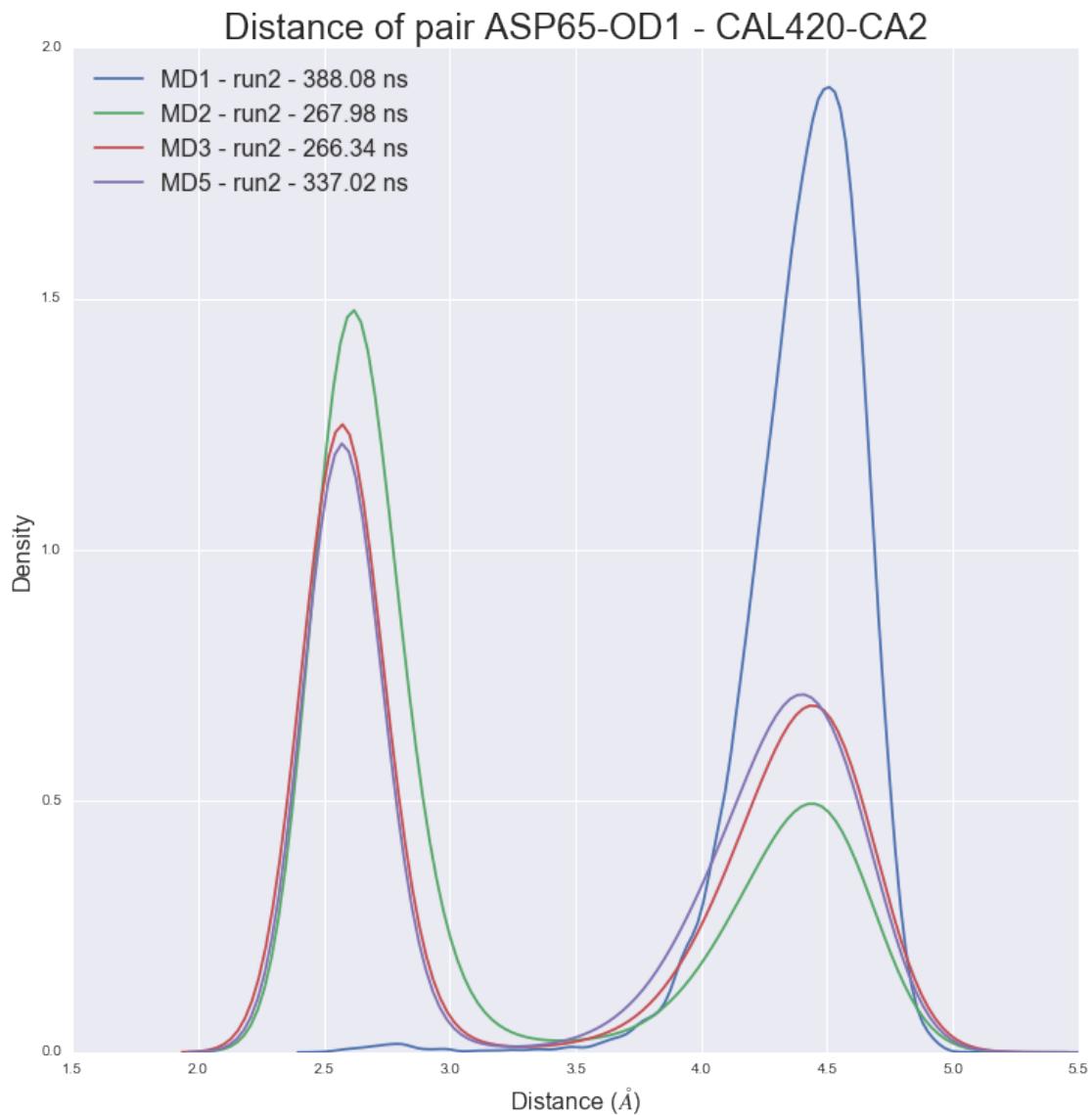
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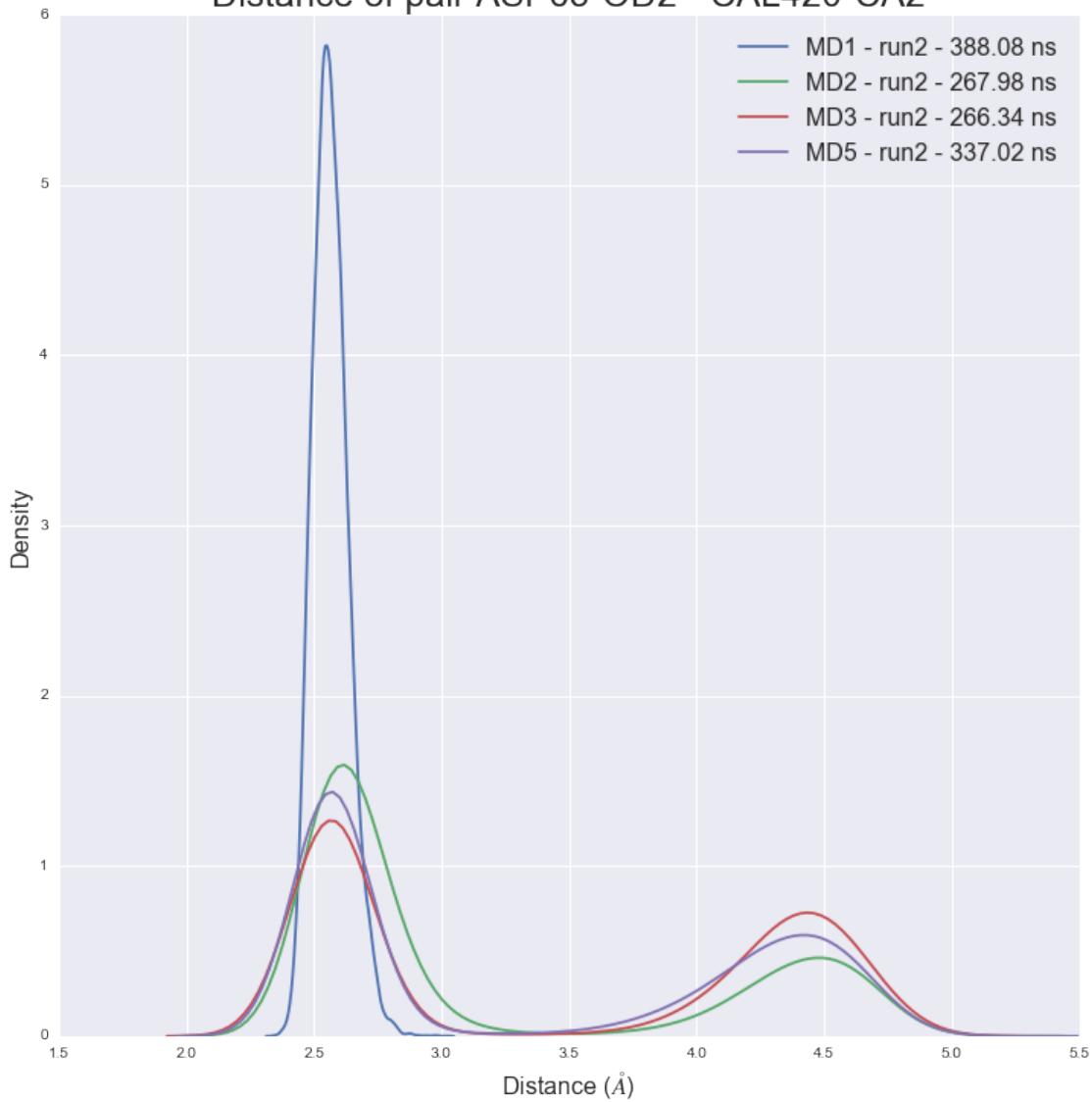
In [13]: traj_list = ['/Users/gil_f.hoben/Troponin_md_processed/MD1/run2/Trajectories/',
                  '/Users/gil_f.hoben/Troponin_md_processed/MD2/run2/Trajectories/',
                  '/Users/gil_f.hoben/Troponin_md_processed/MD3/run2/Trajectories/',
                  '/Users/gil_f.hoben/Troponin_md_processed/MD5/run2/Trajectories',]
top_list = ['/Users/gil_f.hoben/Troponin_md_processed/MD1/run2/troponin_egcg_MD1_nowater.prmto',
            '/Users/gil_f.hoben/Troponin_md_processed/MD2/run2/troponin_egcg_MD2_nowater.prmto',
            '/Users/gil_f.hoben/Troponin_md_processed/MD3/run2/troponin_egcg_MD3_nowater.prmto',
            '/Users/gil_f.hoben/Troponin_md_processed/MD5/run2/troponin_egcg_MD5_nowater.prmto']
complex_names= ['MD1 - run2', 'MD2 - run2', 'MD3 - run2', 'MD5 - run2']
atom1_list = ['name OD1 and resid 64', 'name OD2 and resid 64', 'name OE1 and resid 65',
              'name OE2 and resid 65', 'name OD1 and resid 66',
              'name OD2 and resid 66', 'name OG and resid 68', 'name OG1 and resid 70',
              'name OD1 and resid 72', 'name OD2 and resid 72', 'name OD1 and resid 74',
              'name OD2 and resid 74', 'name OE1 and resid 75', 'name OE2 and resid 75']

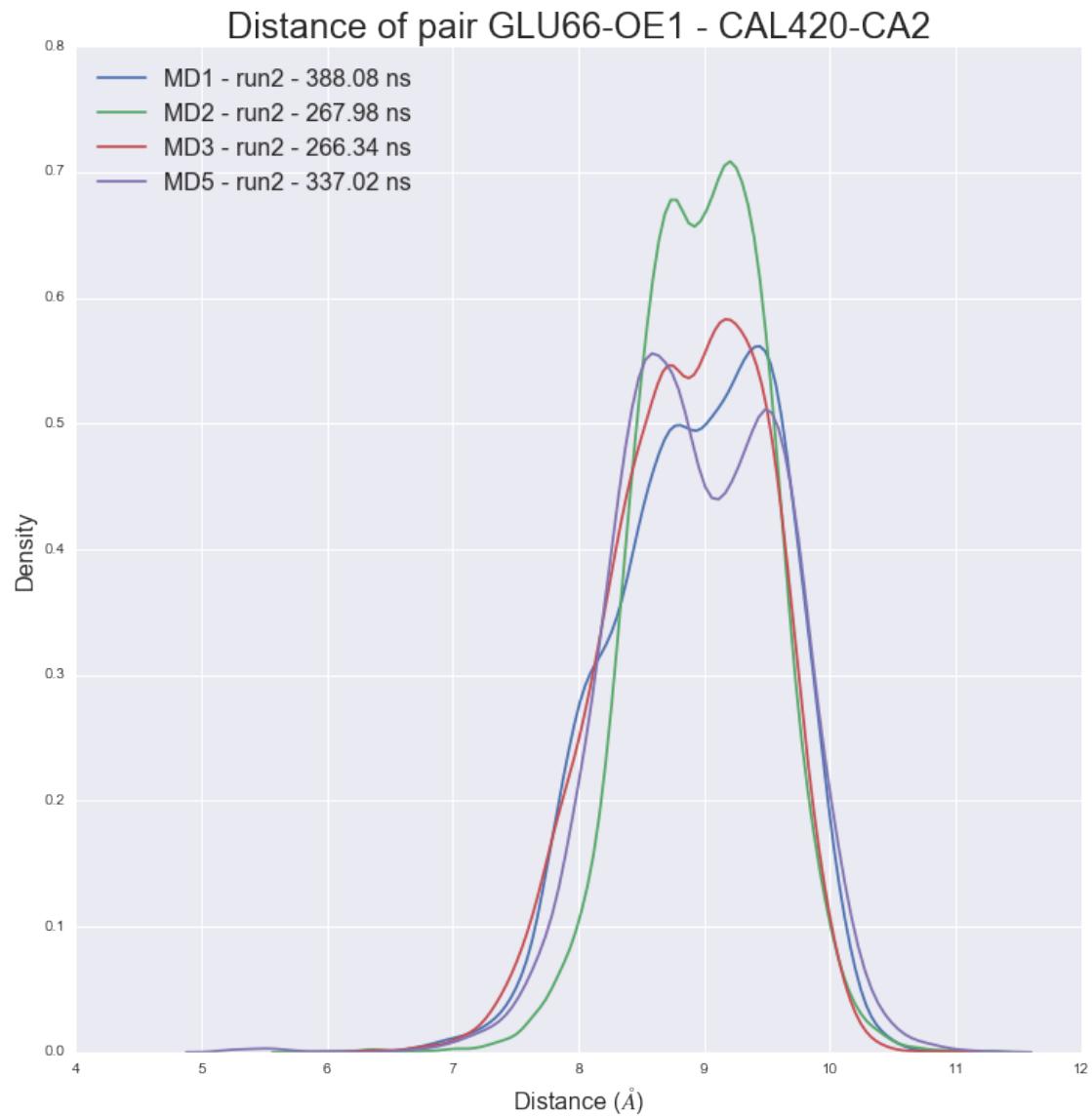
In [14]: atom2 = 'resid 419'
for atom1 in atom1_list:
    plt.figure(figsize = (12,12))
    for traj_i, top_i, name in zip(traj_list, top_list, complex_names):
        distance, pair, sim_time = main(top_i, traj_i, atom1, atom2, verbose = 0, plot_dist = 1)
        ax = sns.distplot(distance, hist=False, label= '%s - %.2f ns' %(name, sim_time))
        ax.set_xlabel('Distance (${\AA}$)', size = 16)
        ax.set_ylabel('Density', size = 16)
        ax.set_title('Distance of pair %s' %(pair) , size = 24)
        ax.legend(loc = 'best', prop={'size':16})
    plt.show()

```

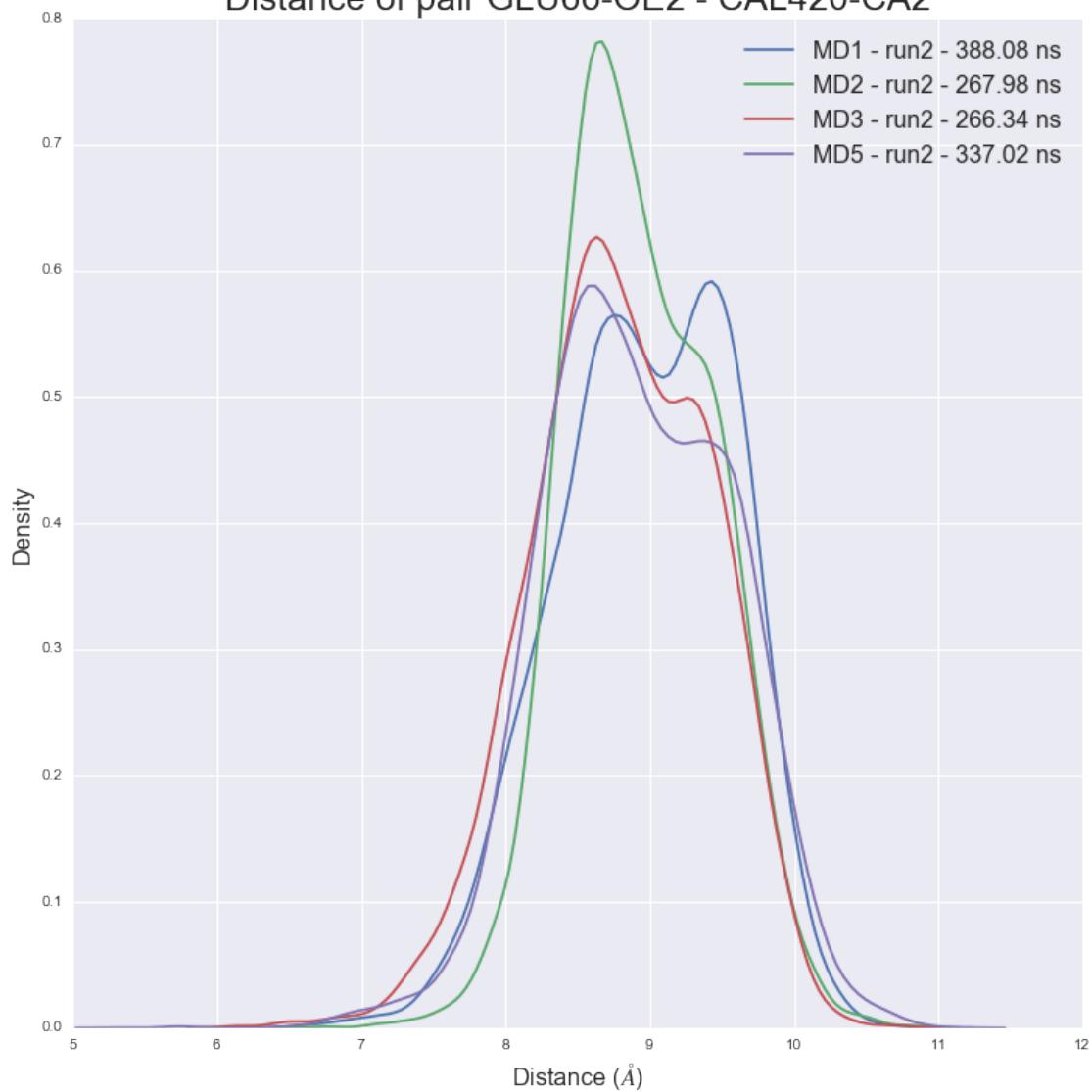


Distance of pair ASP65-OD2 - CAL420-CA2

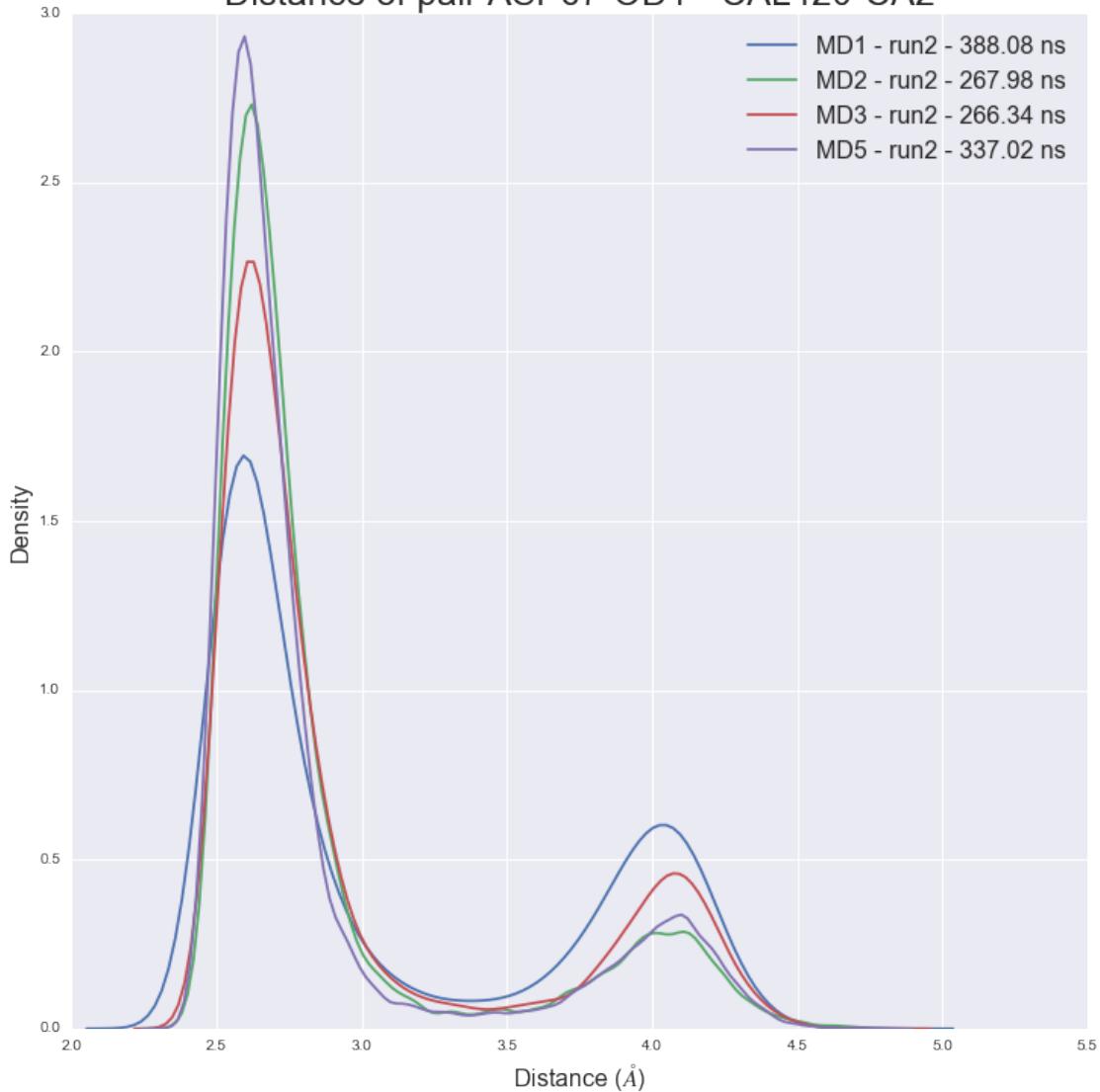




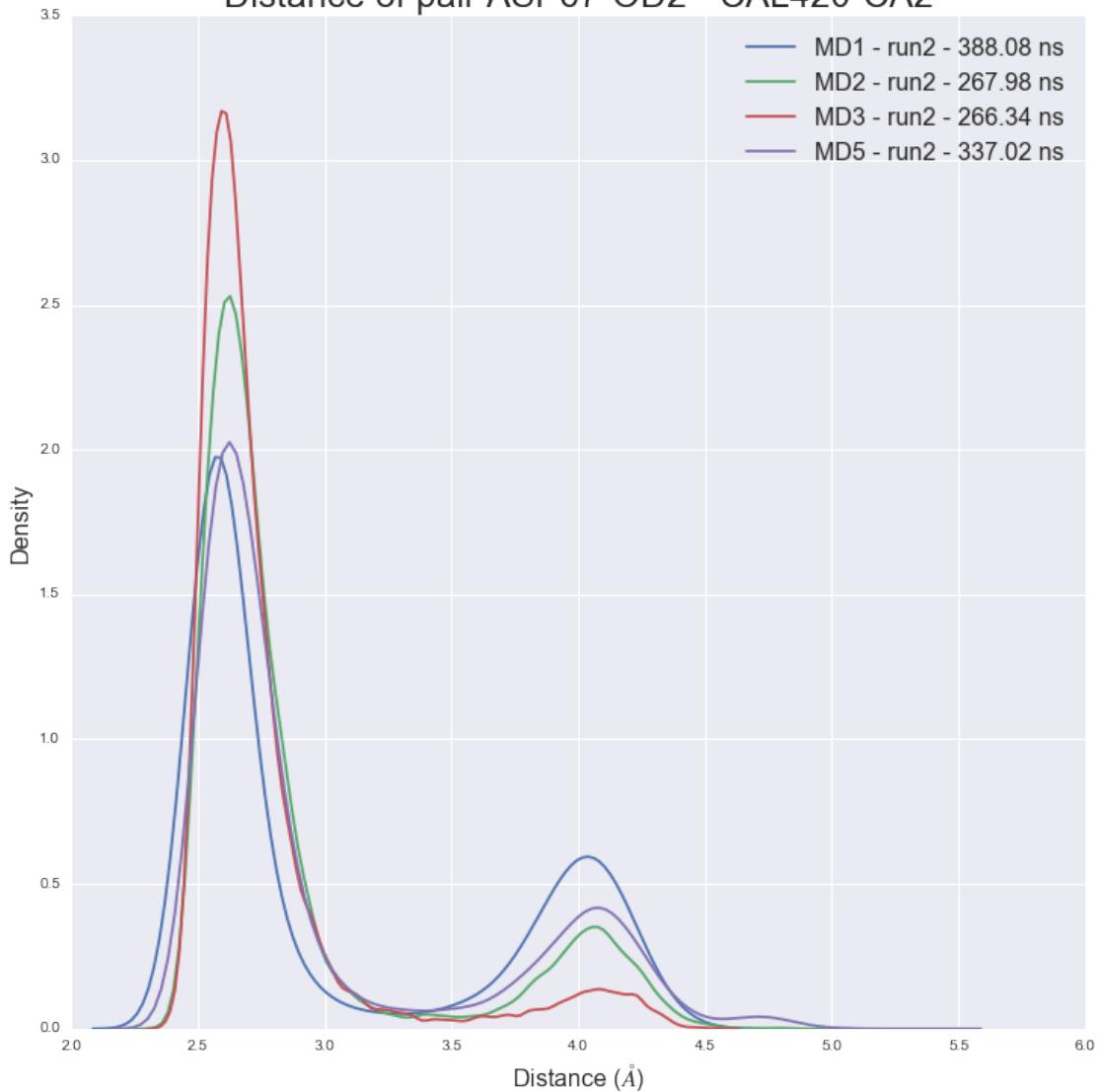
Distance of pair GLU66-OE2 - CAL420-CA2



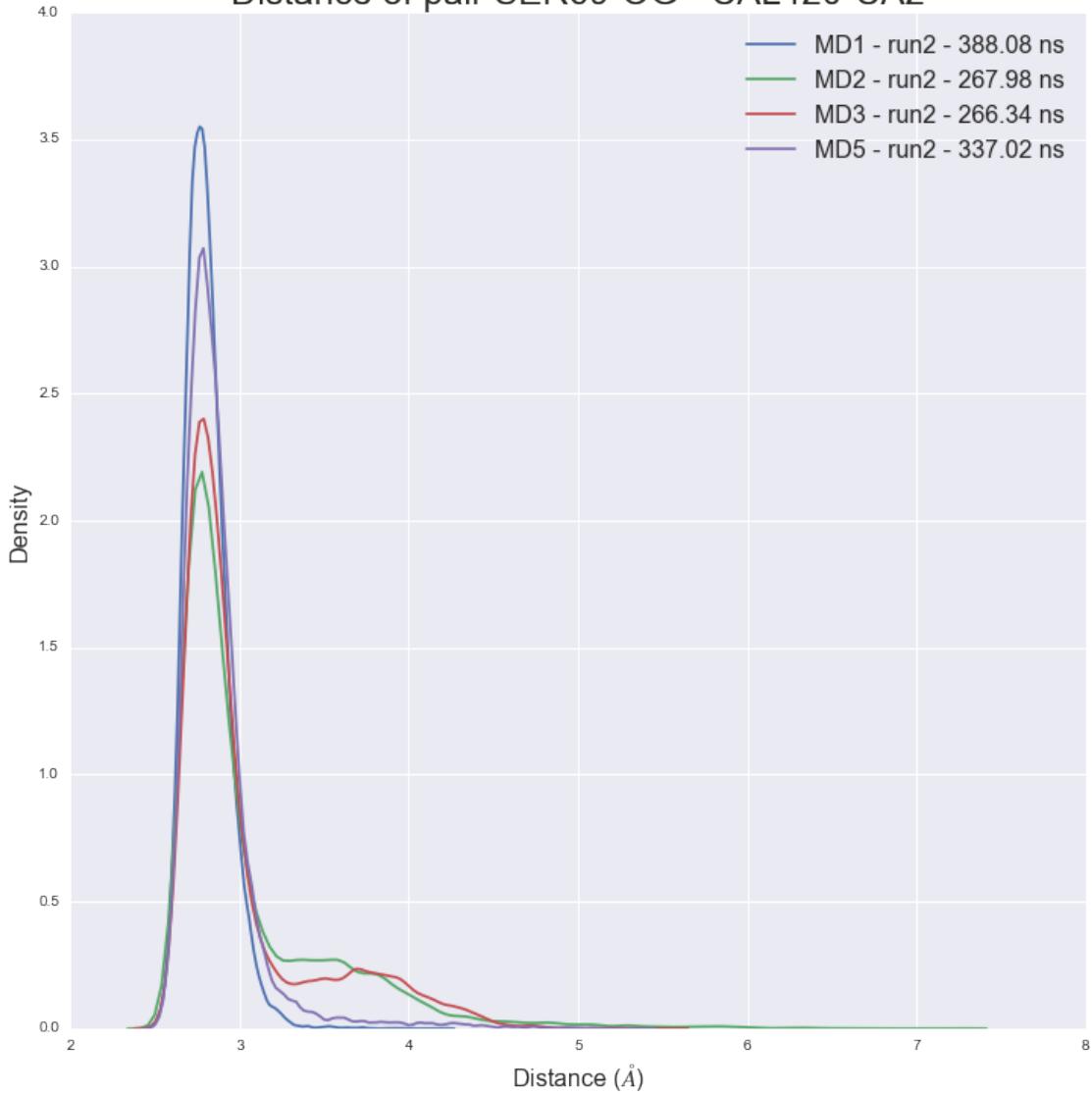
Distance of pair ASP67-OD1 - CAL420-CA2

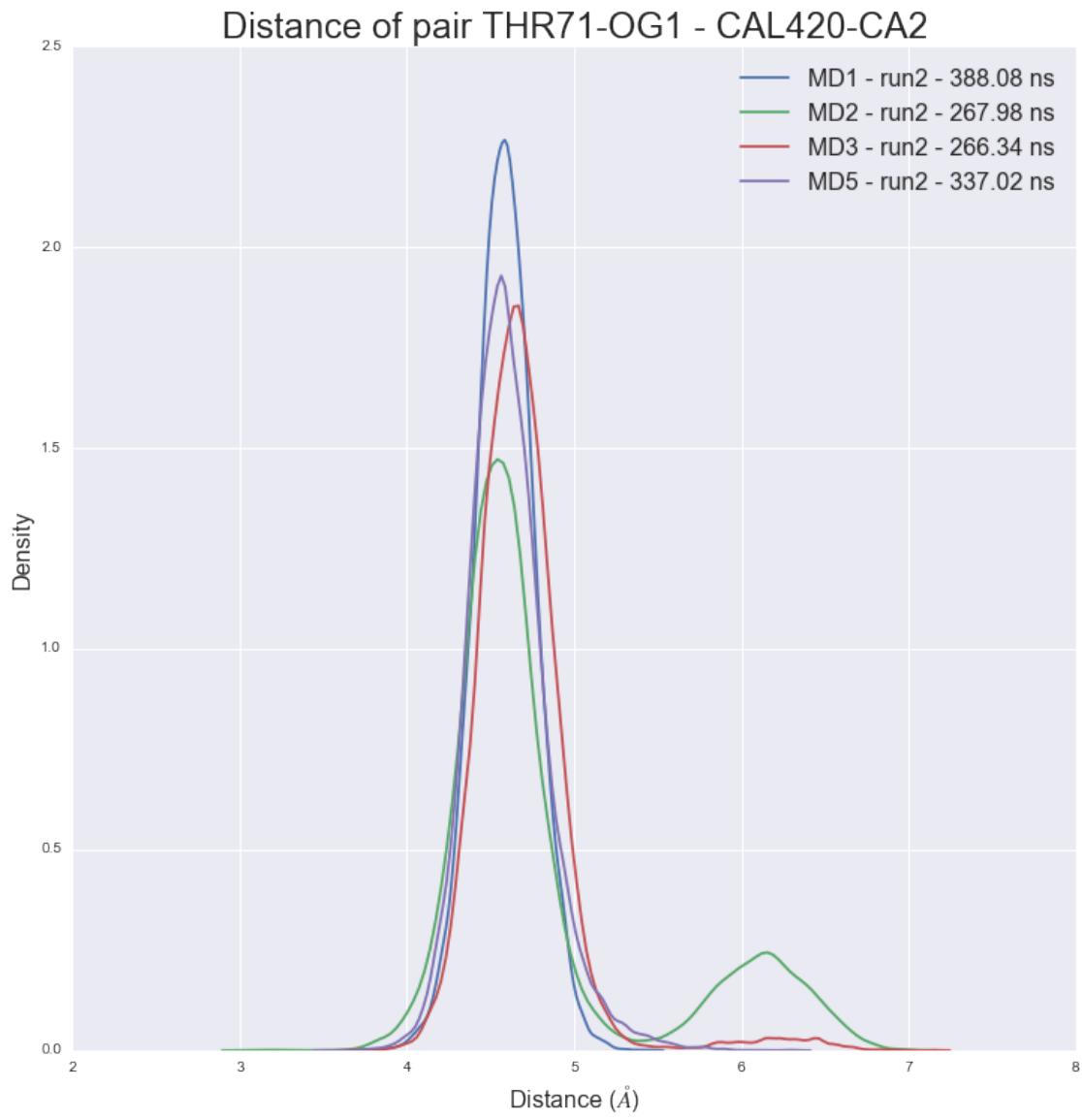


Distance of pair ASP67-OD2 - CAL420-CA2

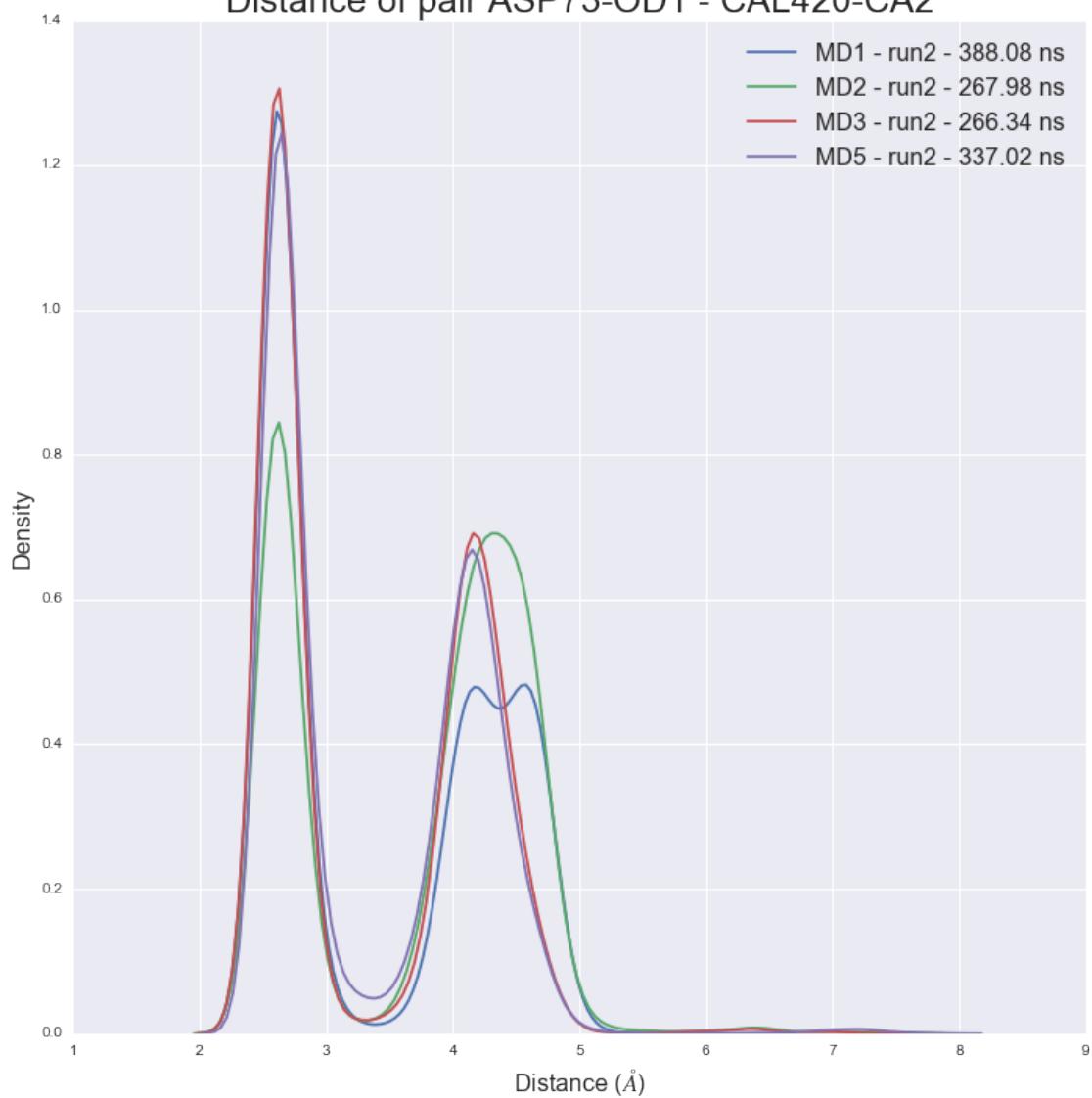


Distance of pair SER69-OG - CAL420-CA2

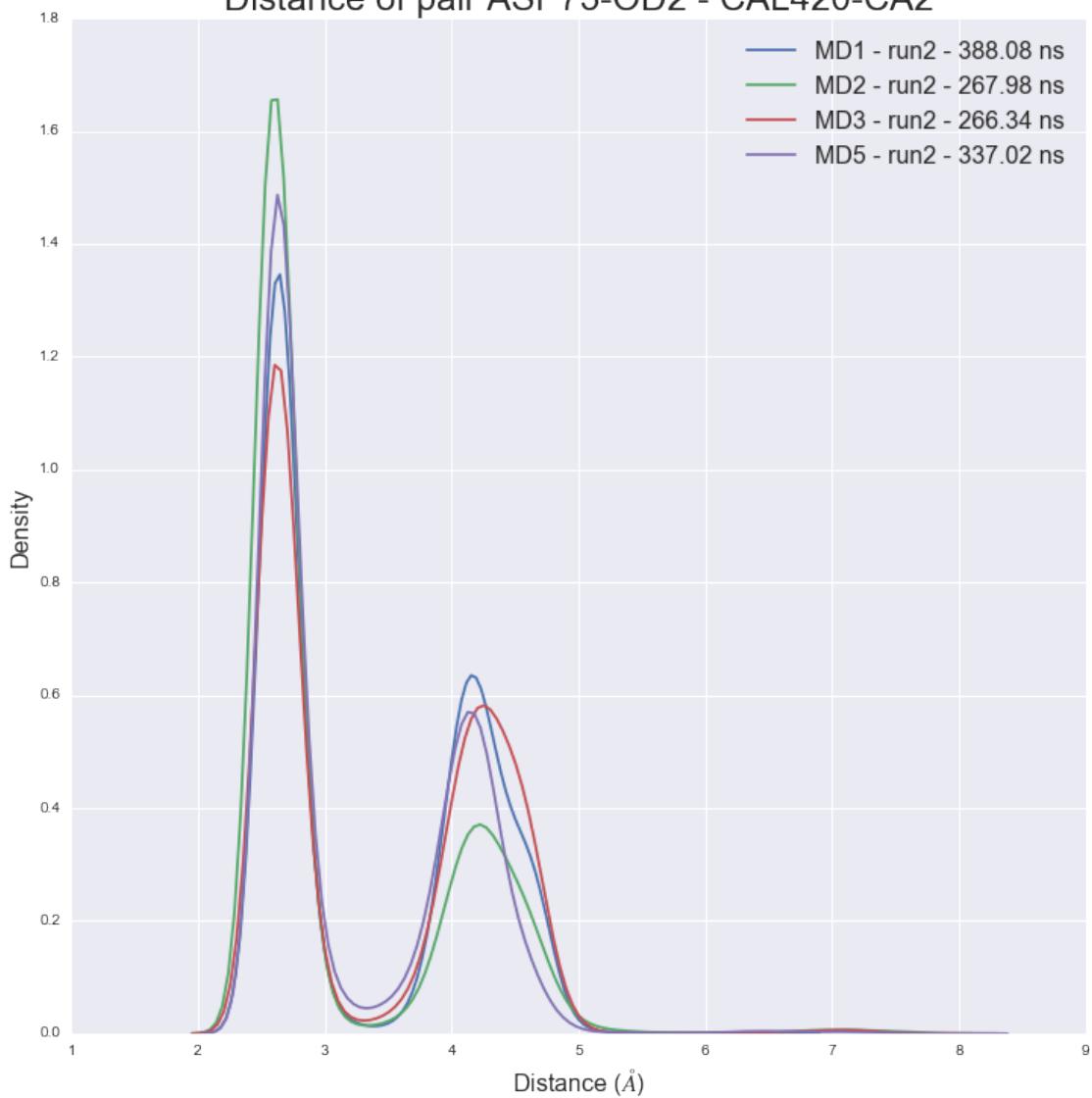


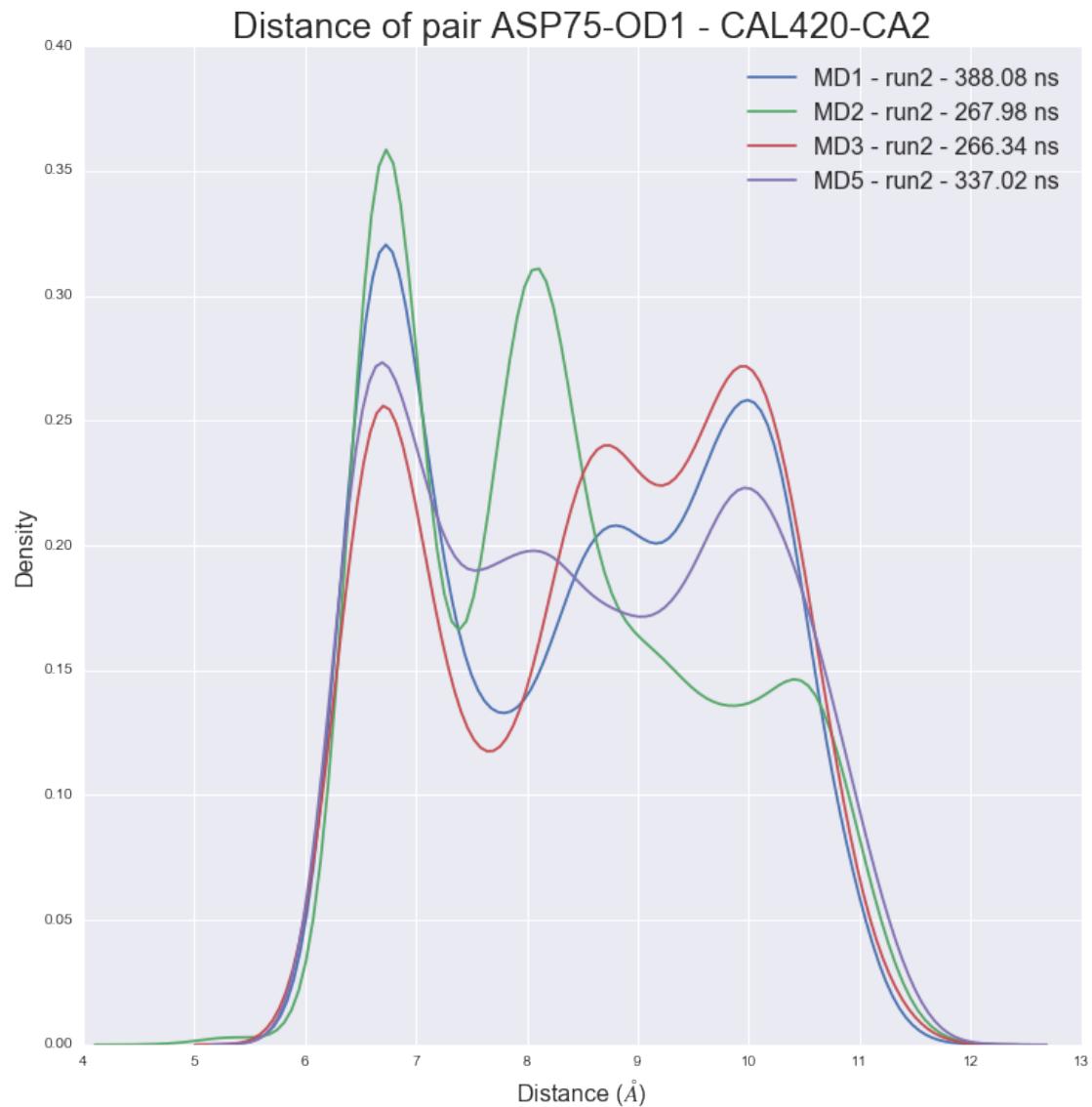


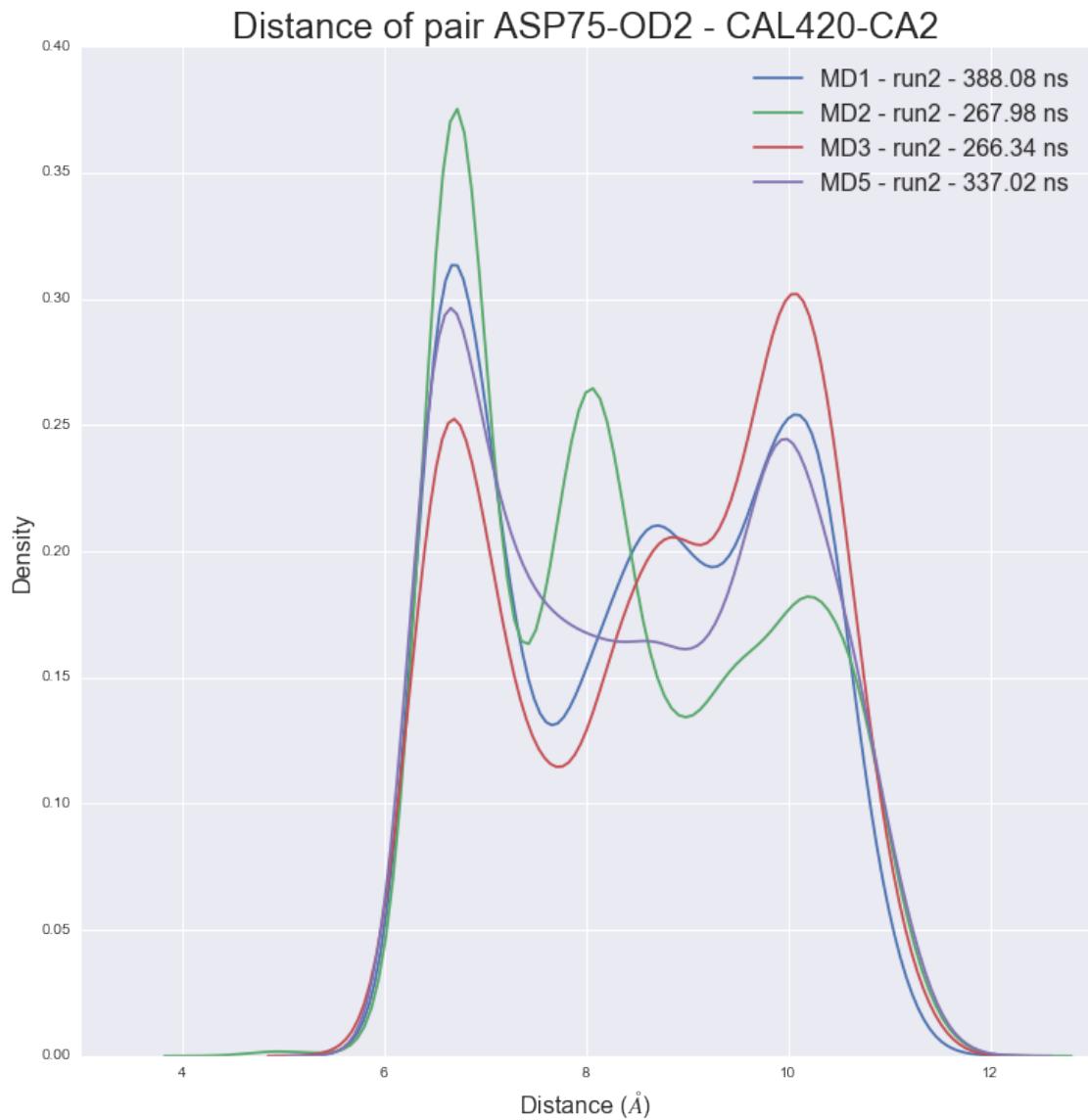
Distance of pair ASP73-OD1 - CAL420-CA2



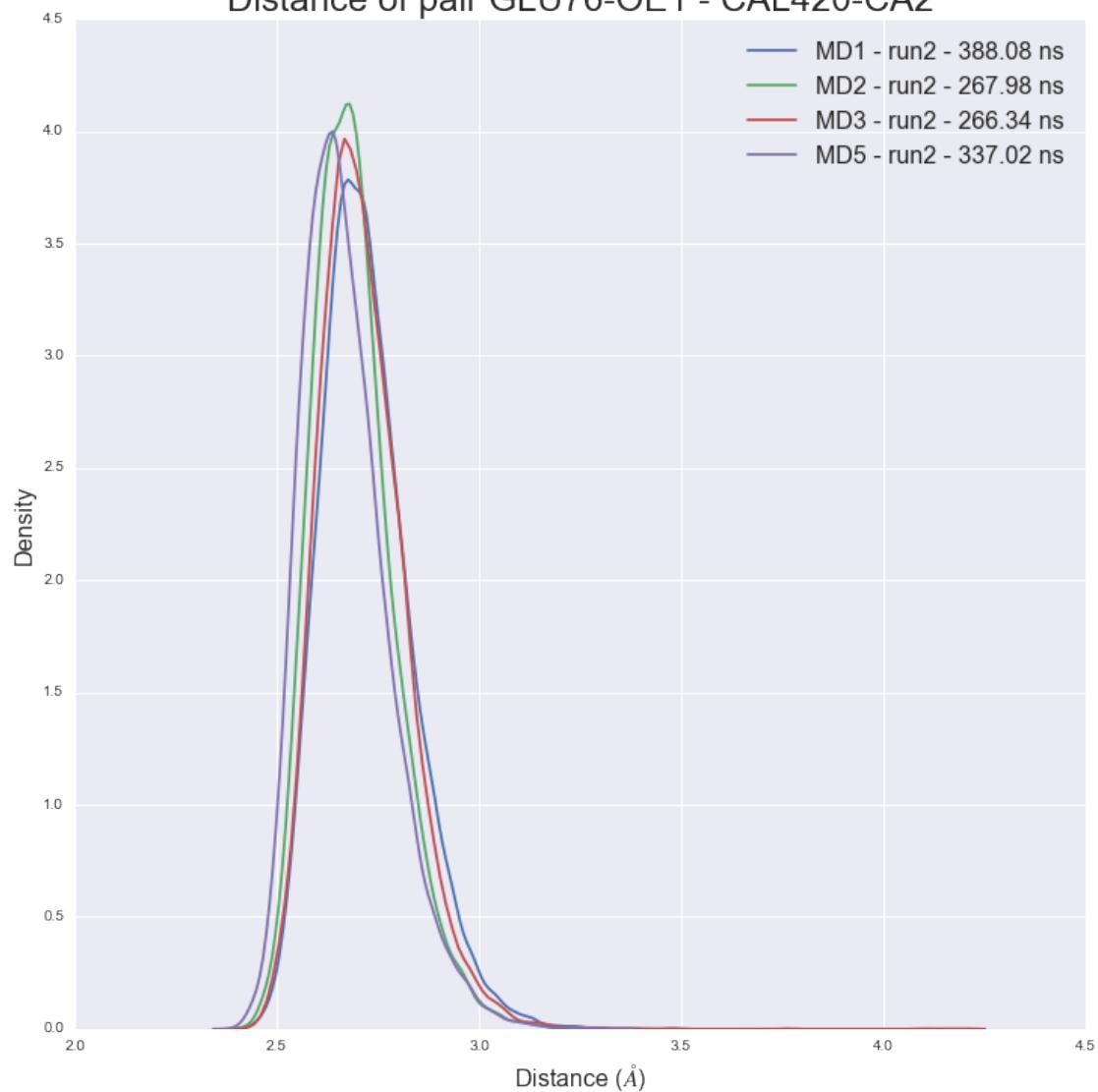
Distance of pair ASP73-OD2 - CAL420-CA2

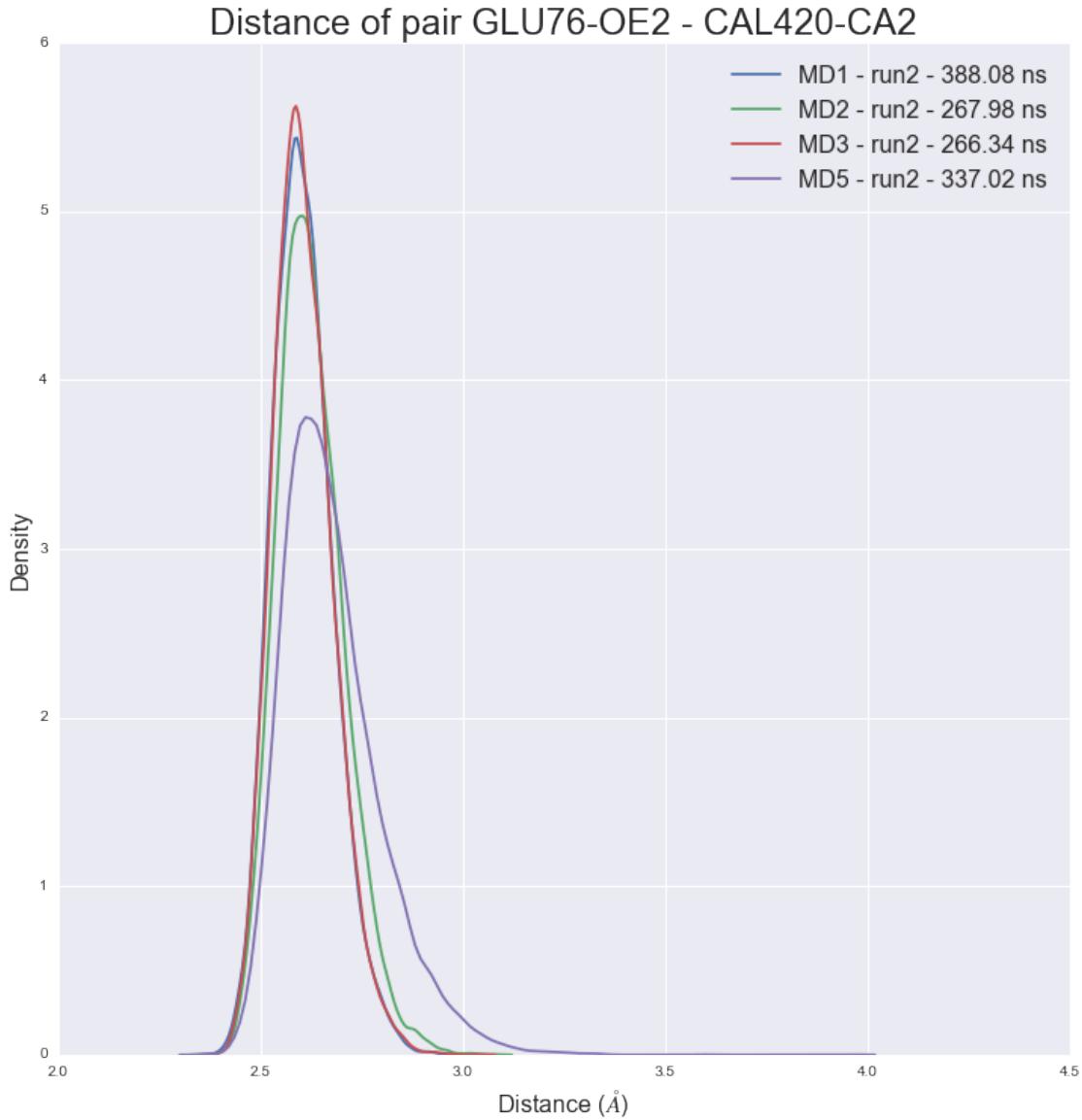






Distance of pair GLU76-OE1 - CAL420-CA2





0.1 MD1

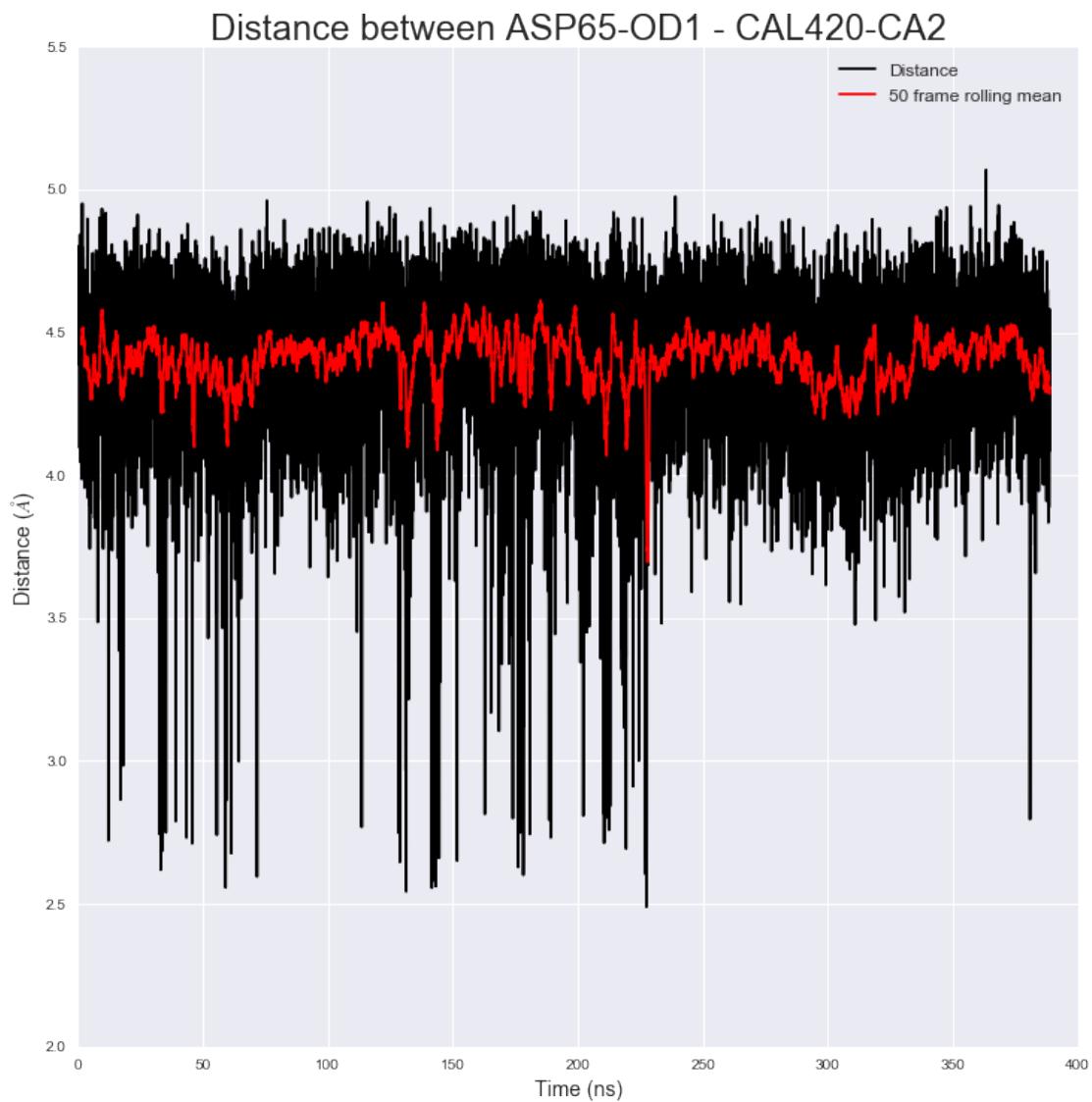
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In [15]: topology_MD1 = '/Users/gil_f.hoben/Troponin_md_processed/MD1/run2/troponin_egcg_MD1_nowater.pr
trajectory_MD1 = '/Users/gil_f.hoben/Troponin_md_processed/MD1/run2/Trajectories/'
atom1_list = ['name OD1 and resid 64', 'name OD2 and resid 64', 'name OE1 and resid 65',
              'name OE2 and resid 65', 'name OD1 and resid 66',
              'name OD2 and resid 66', 'name OG and resid 68', 'name OG1 and resid 70',
              'name OD1 and resid 72', 'name OD2 and resid 72', 'name OD1 and resid 74',
              'name OD2 and resid 74', 'name OE1 and resid 75', 'name OE2 and resid 75']
atom2 = 'resid 419'

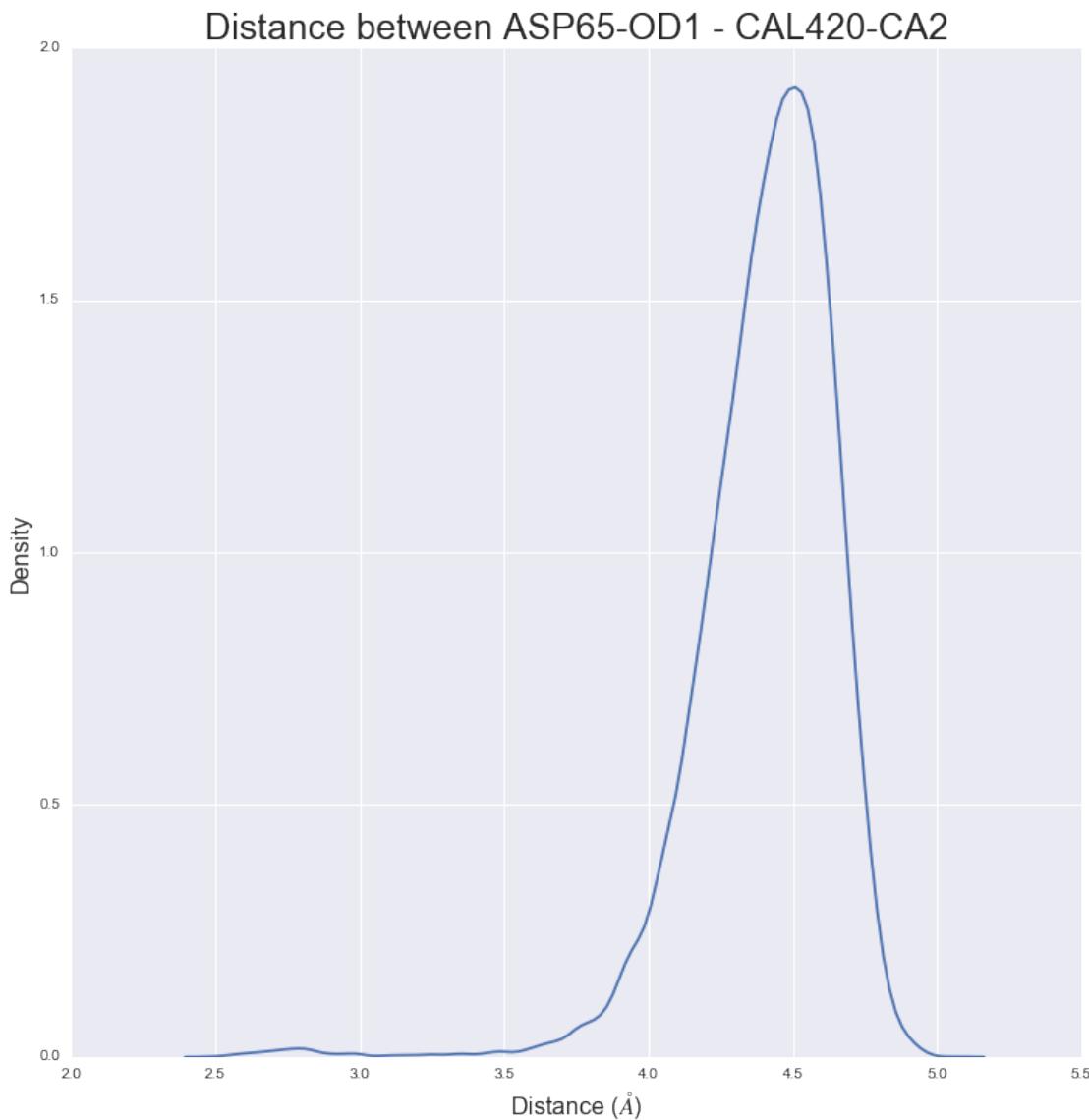
In [16]: for atom1 in atom1_list:
            main(topology_MD1, trajectory_MD1, atom1, atom2, verbose = 1)
```

The following topology file was successfully loaded:
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:
05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 5.58 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

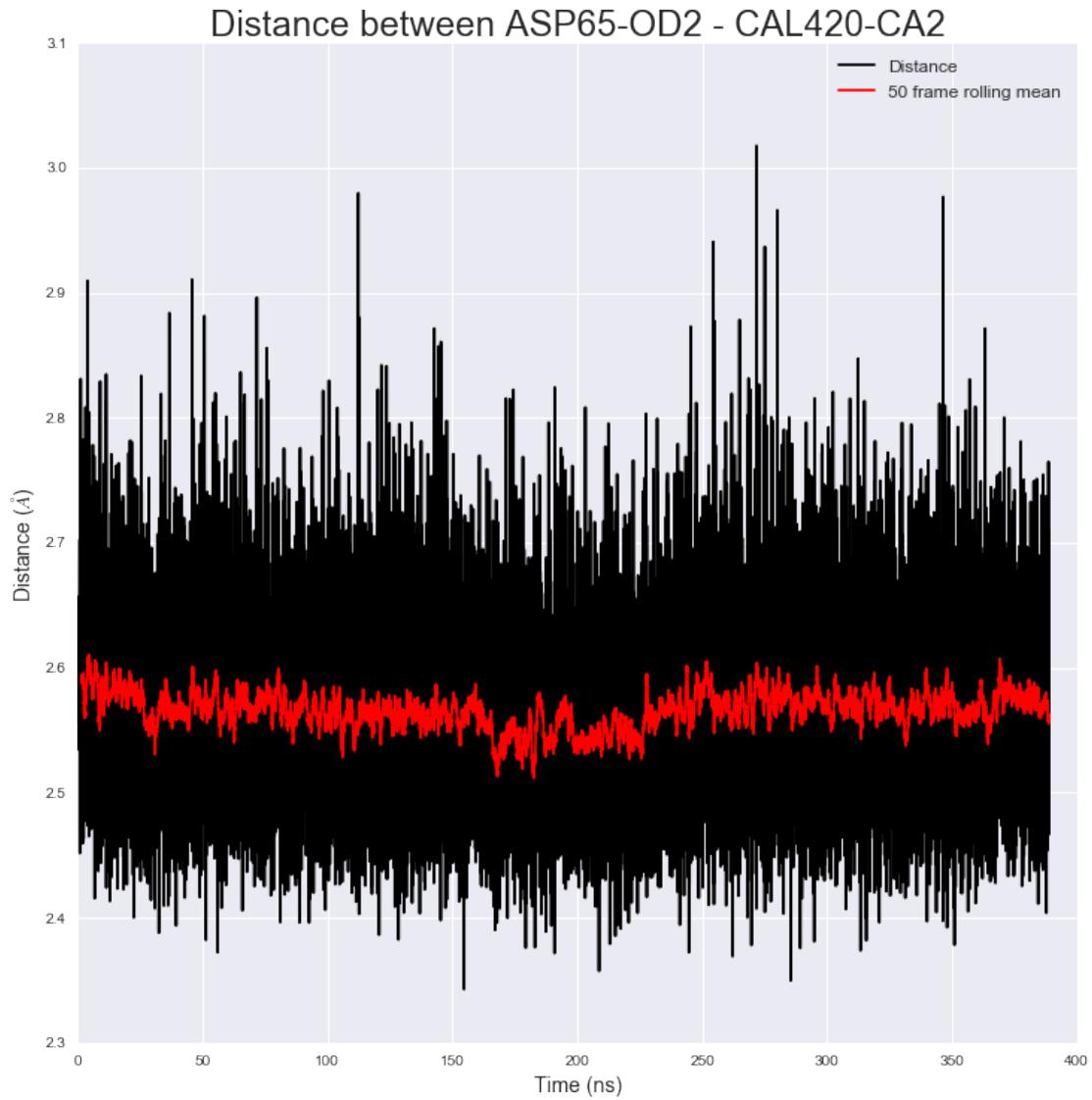
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

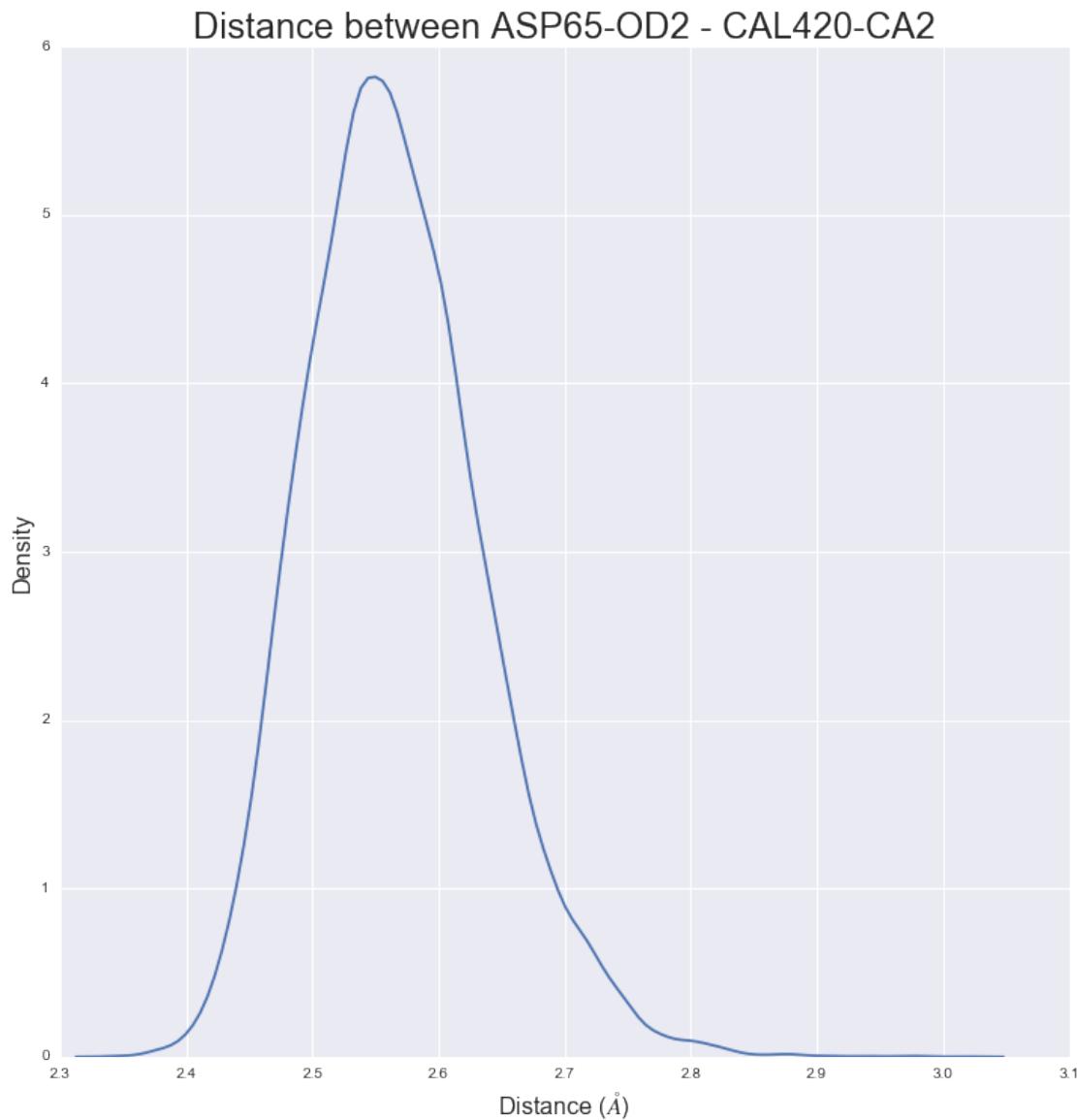
Calculating distance between following atoms: ASP65-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.30 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

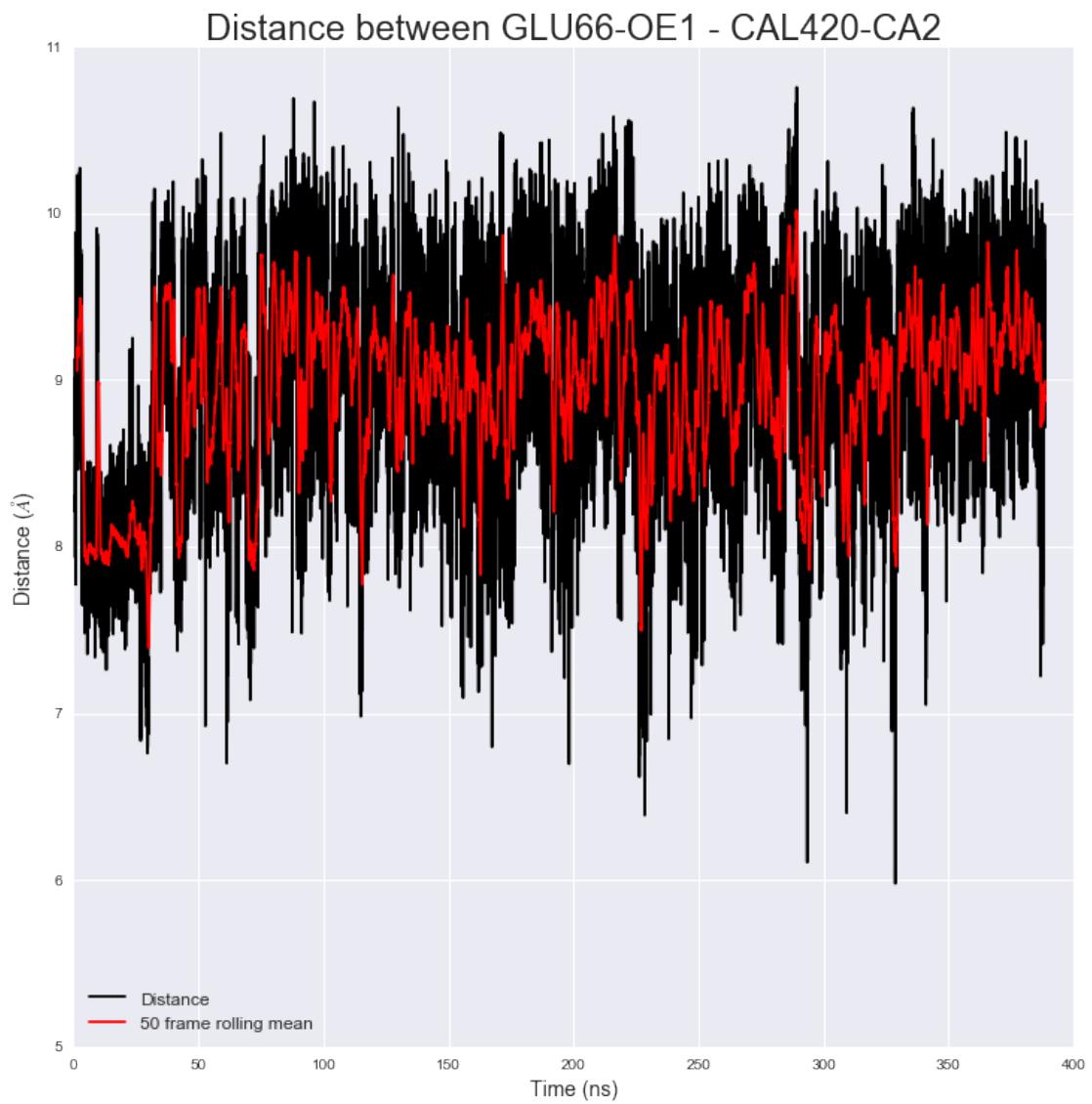
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

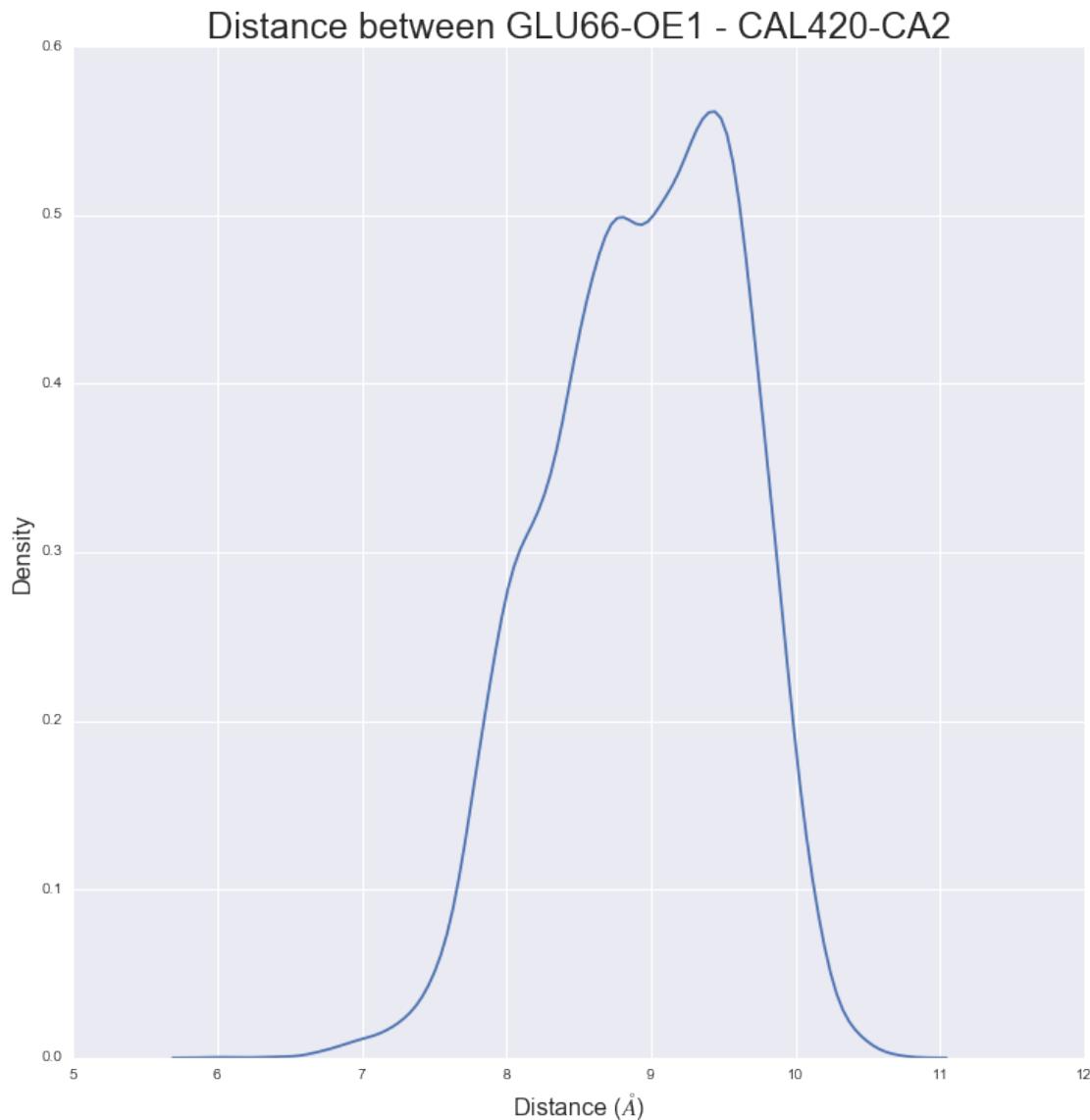
Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.38 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc

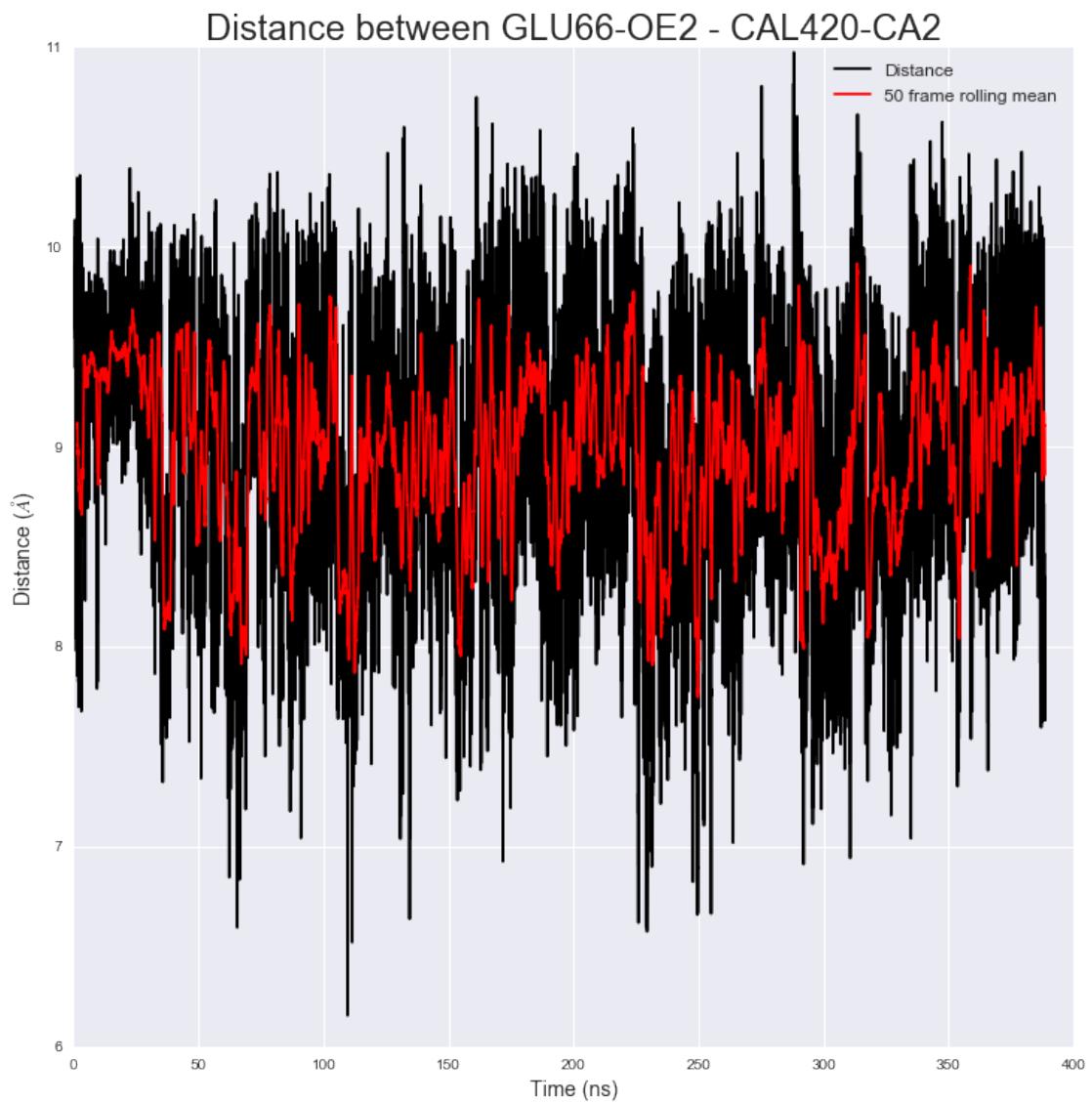
05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc

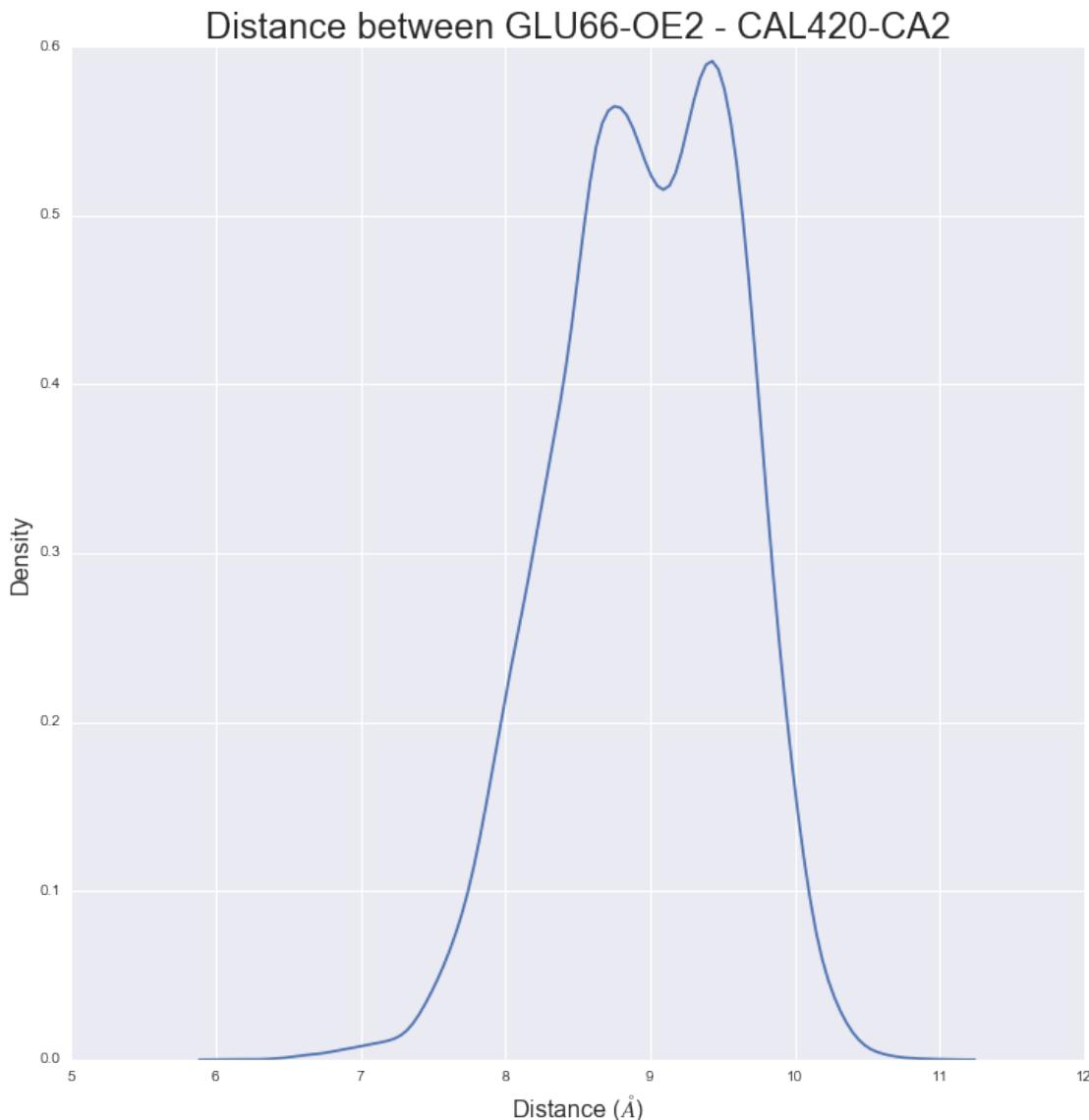
05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc

05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc

05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.34 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

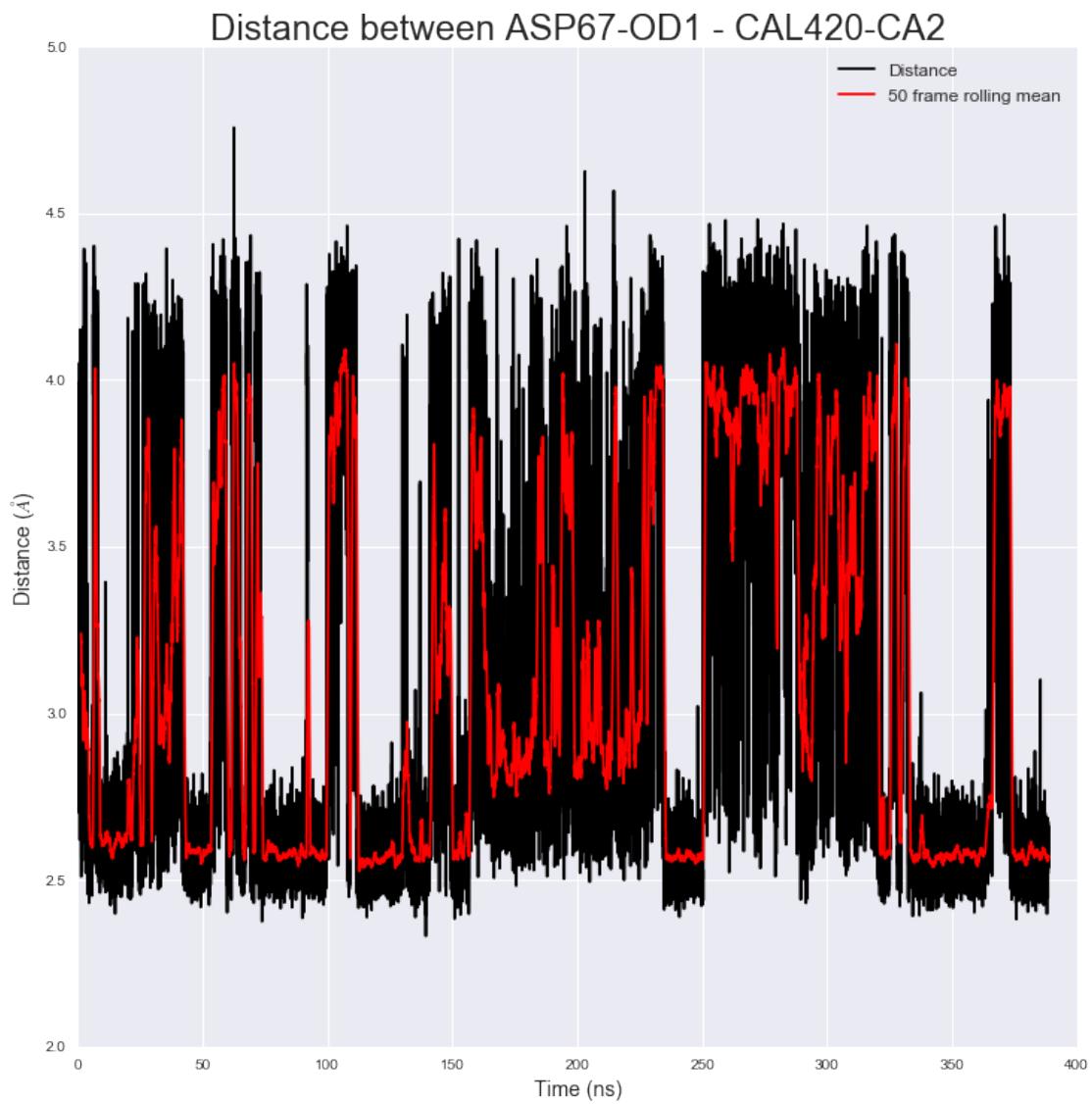
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

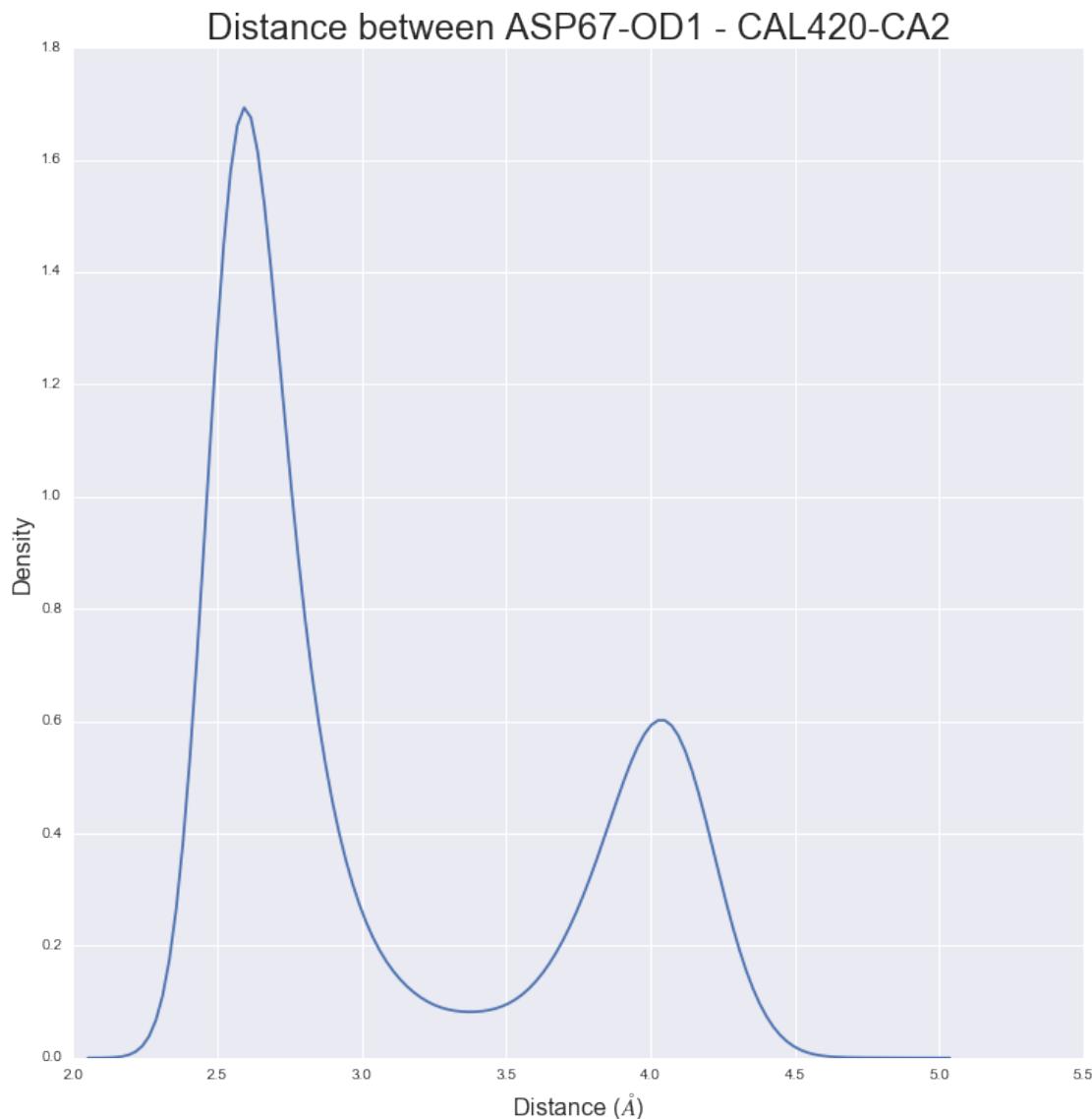
Calculating distance between following atoms: ASP67-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.32 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

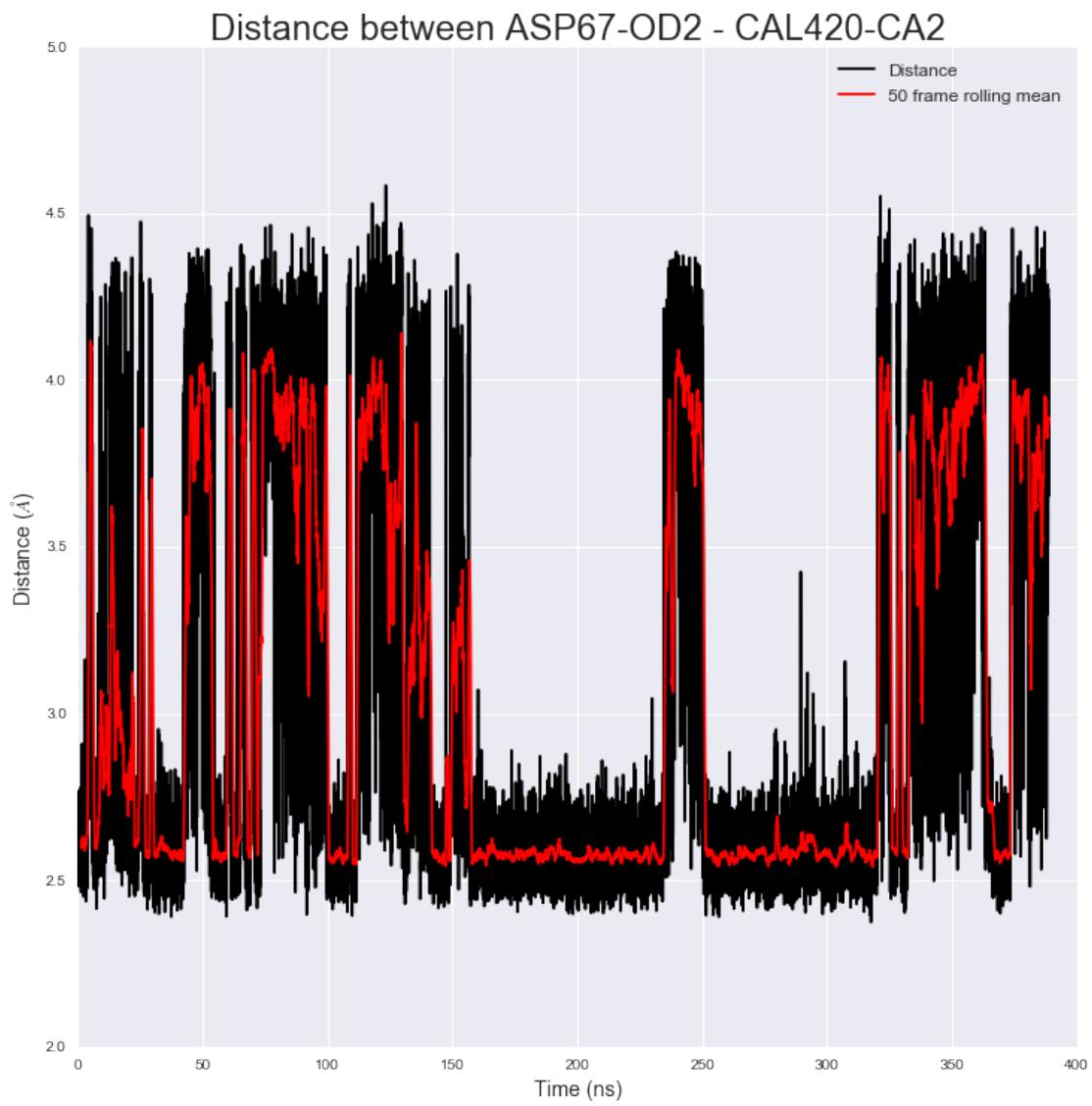
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

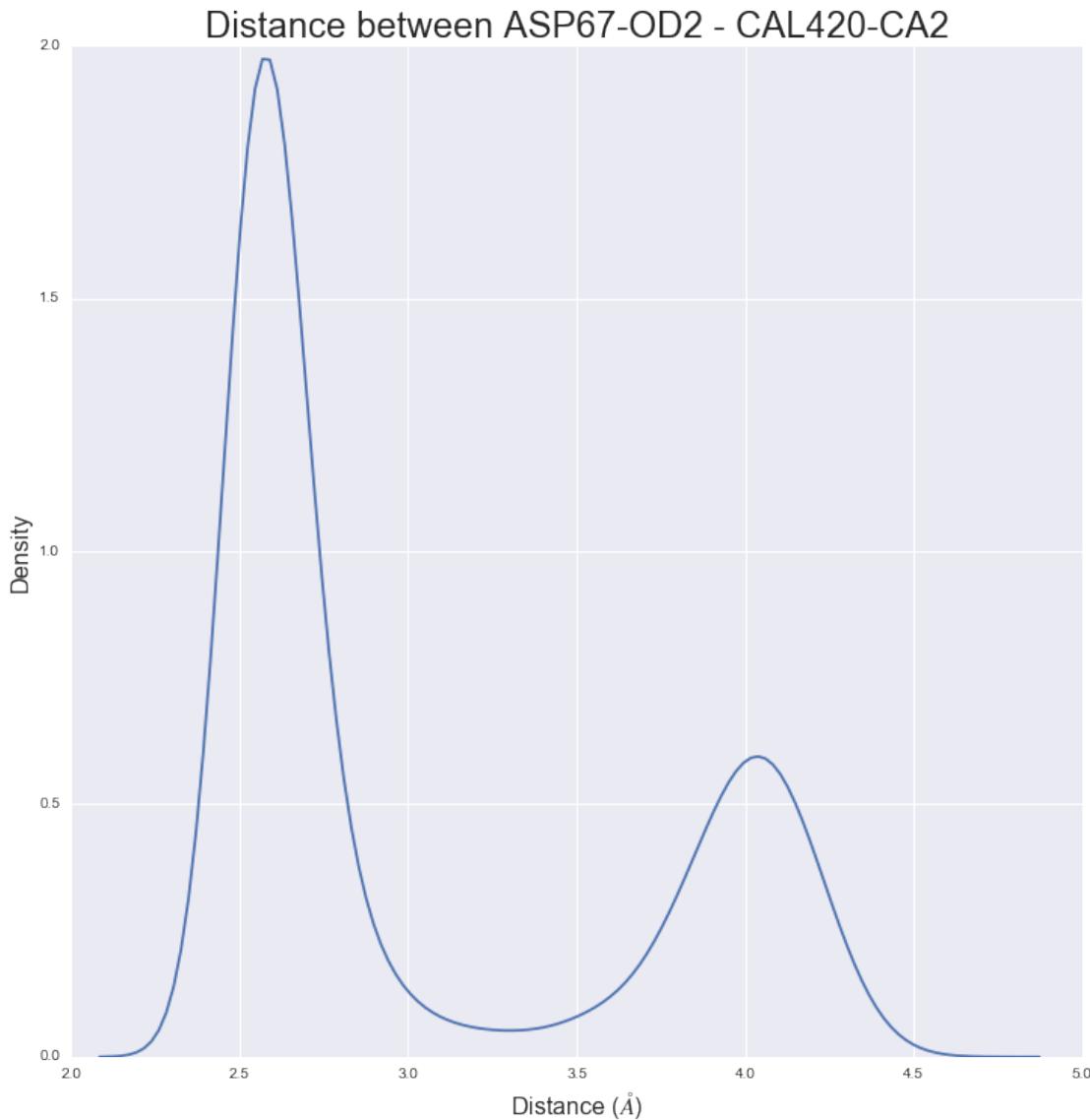
Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.29 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

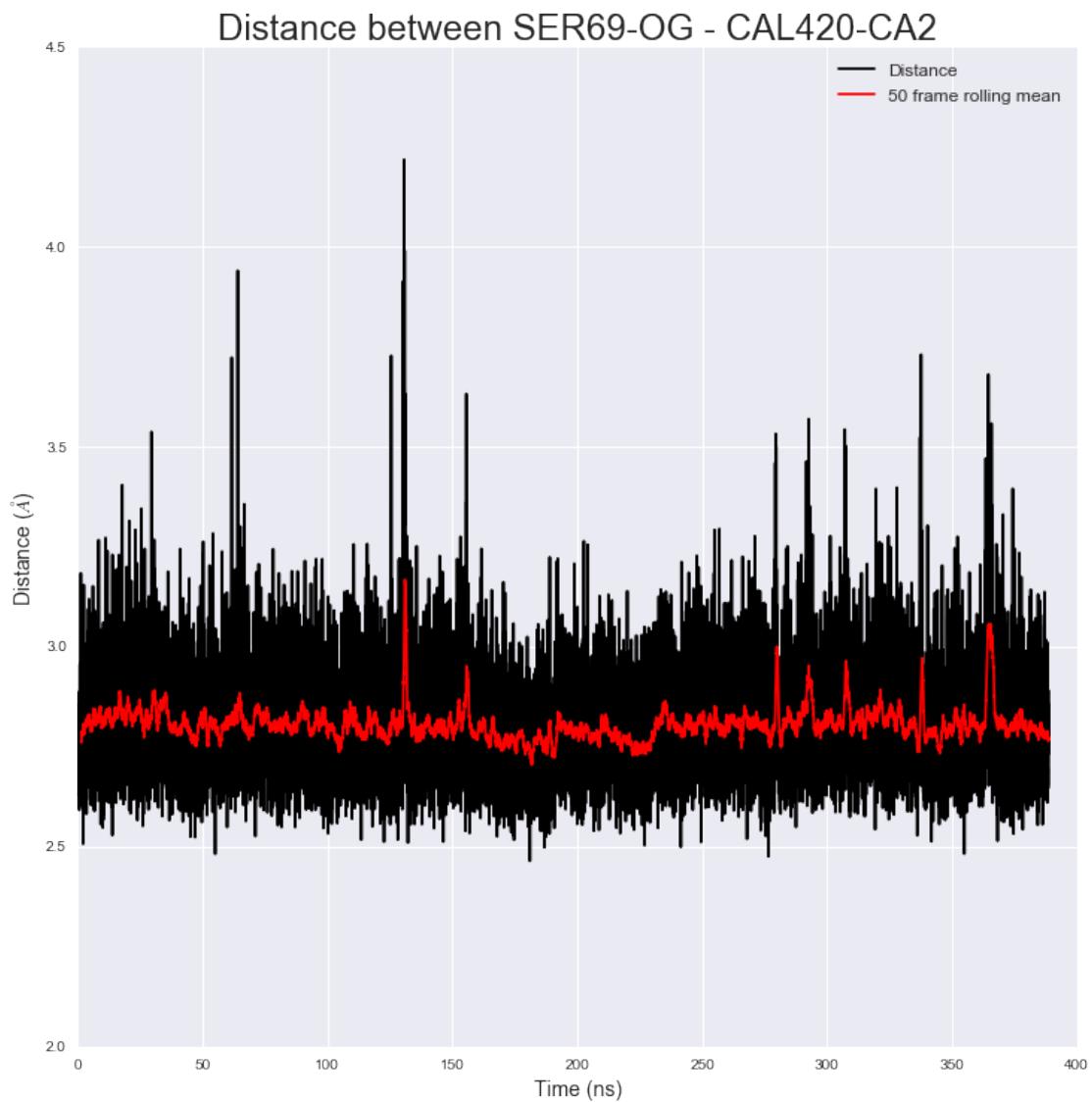
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

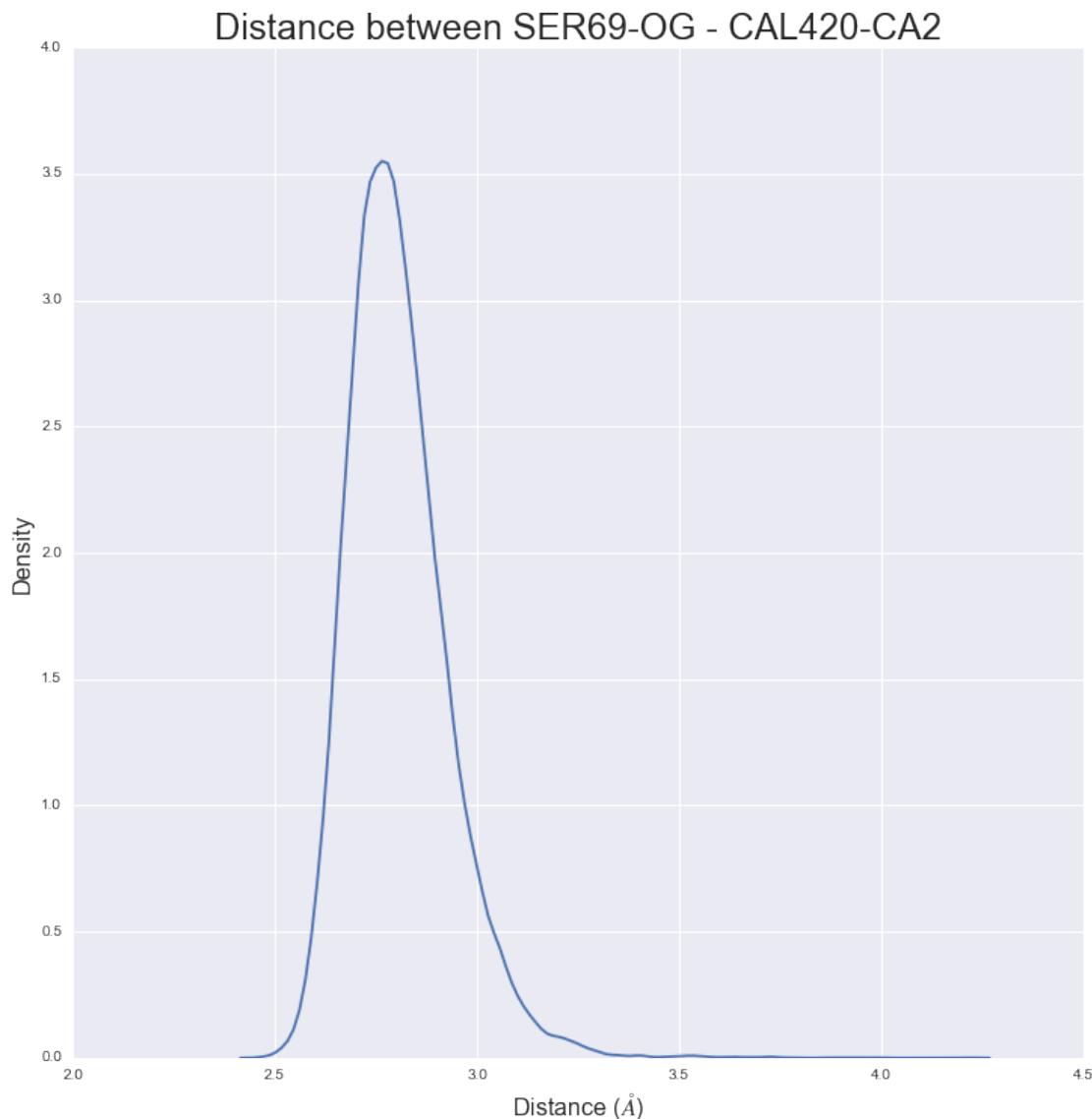
Calculating distance between following atoms: SER69-OG - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.15 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

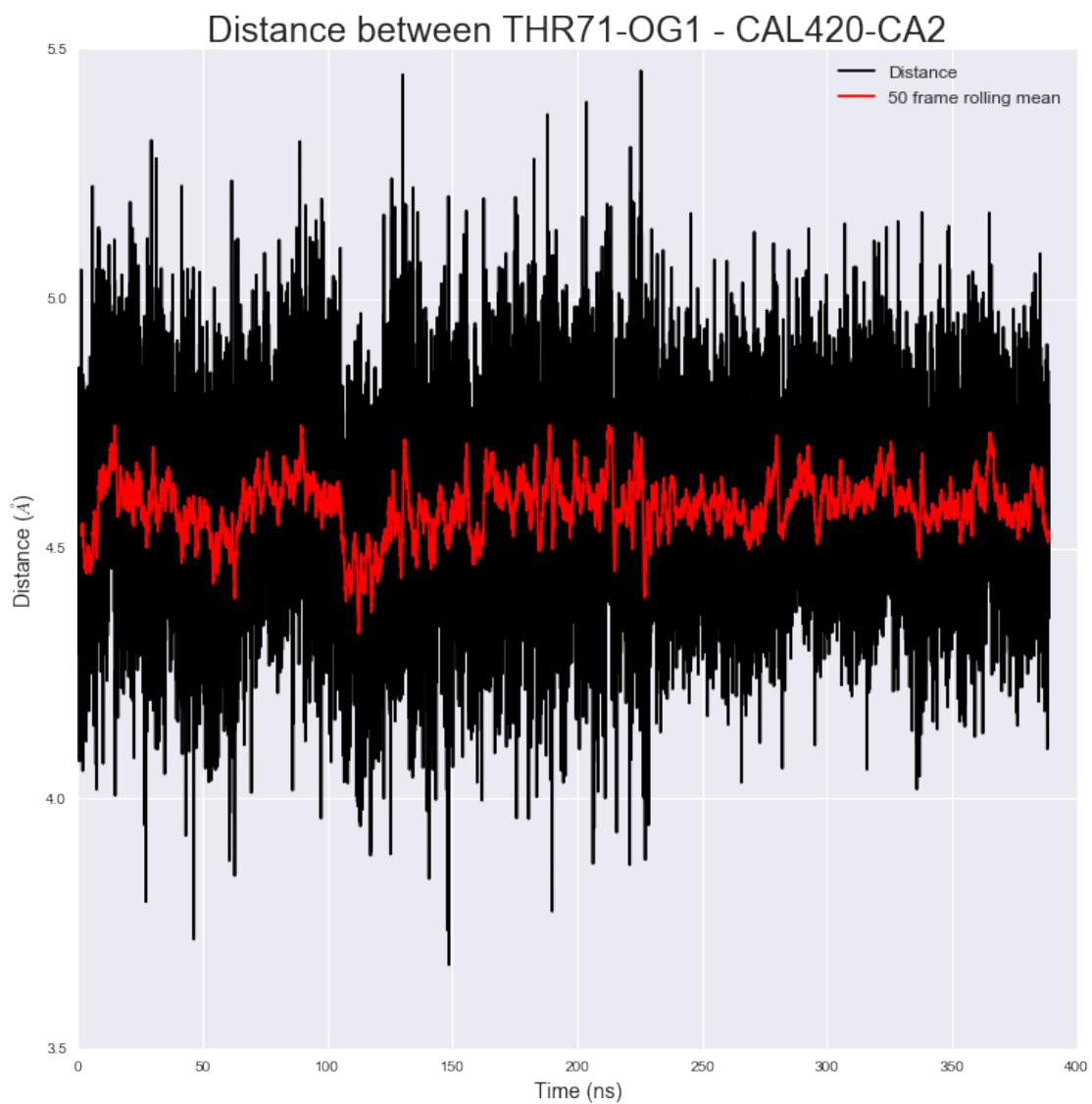
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

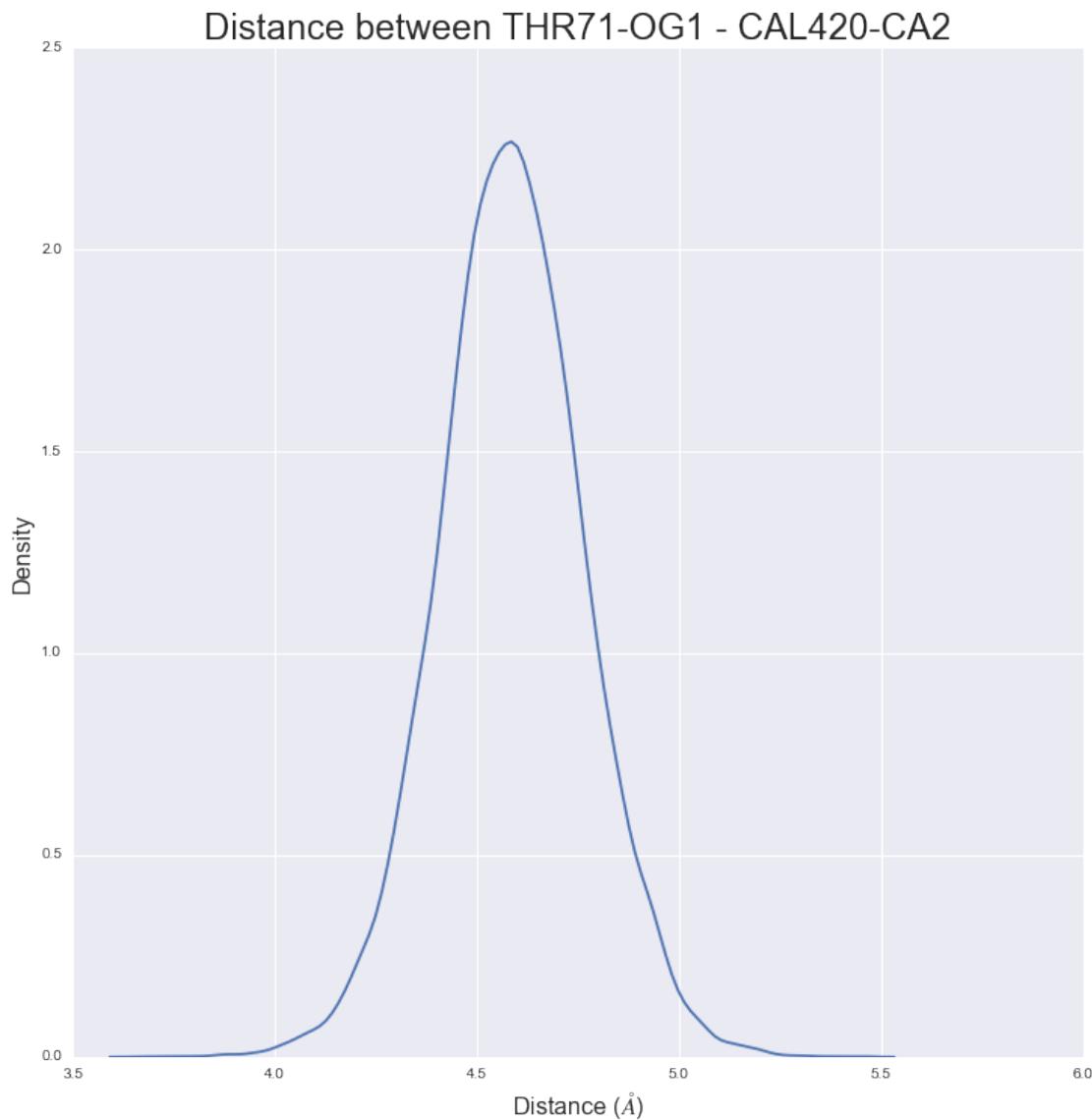
Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.27 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

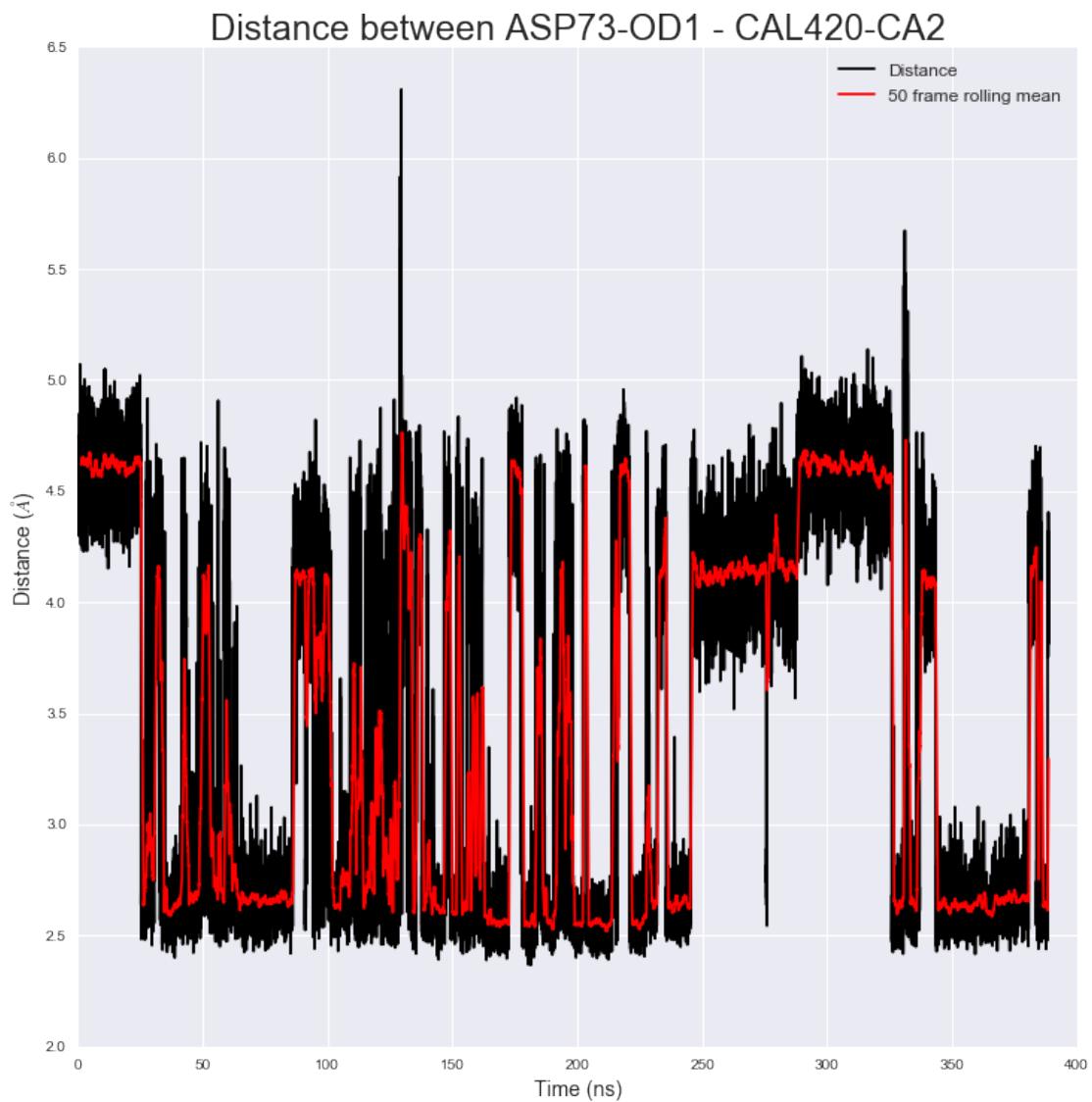
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

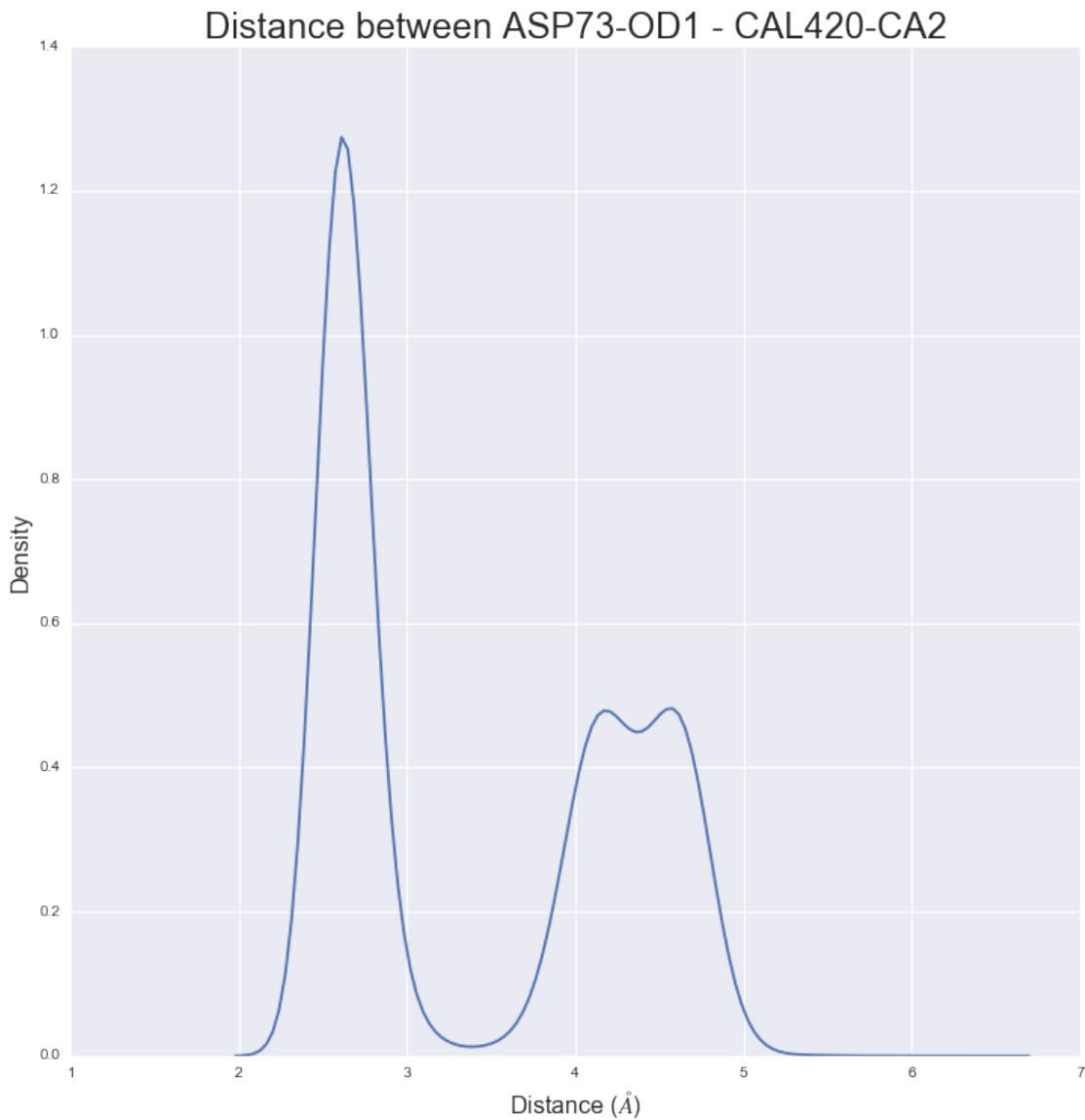
Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.10 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

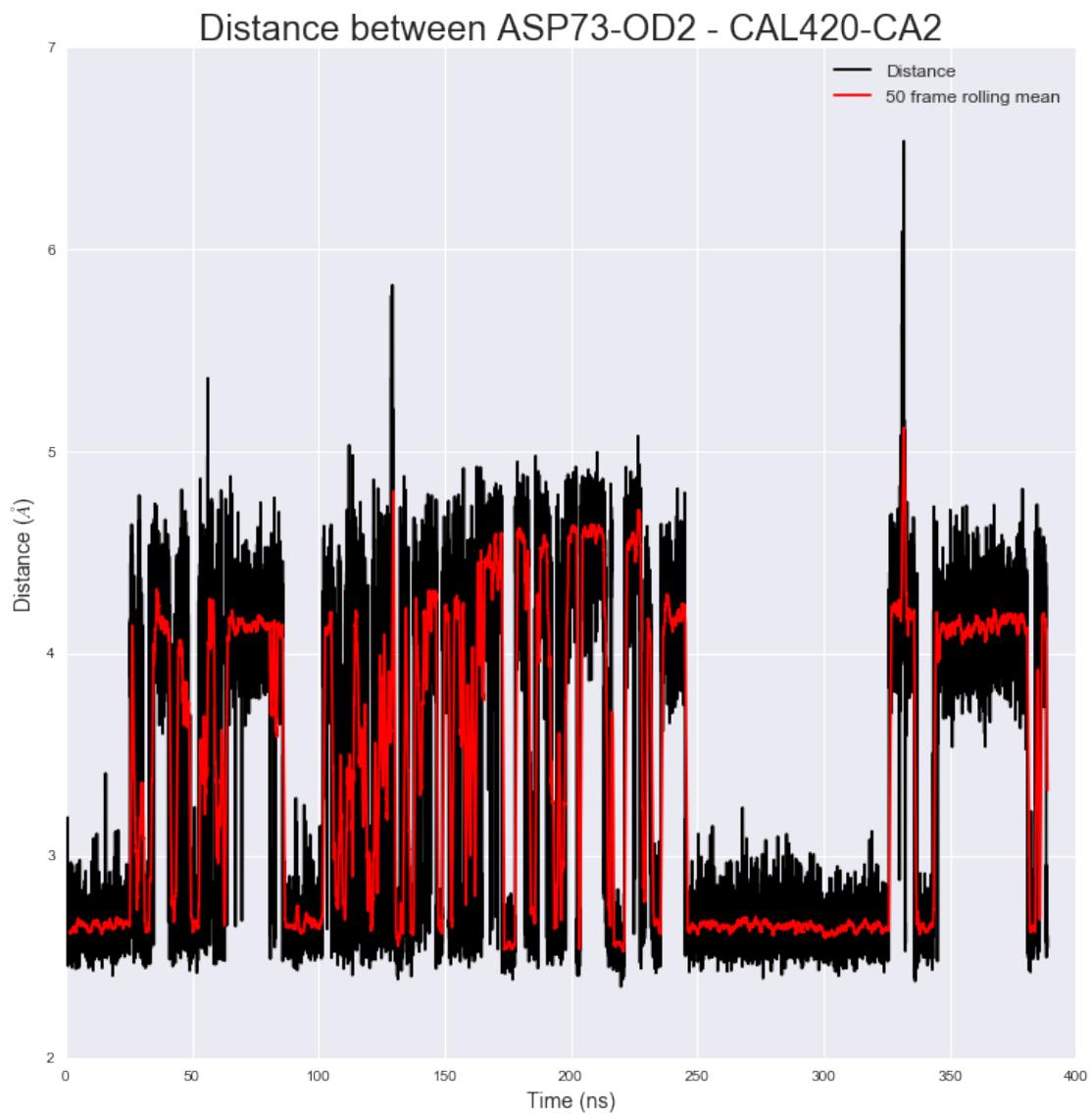
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

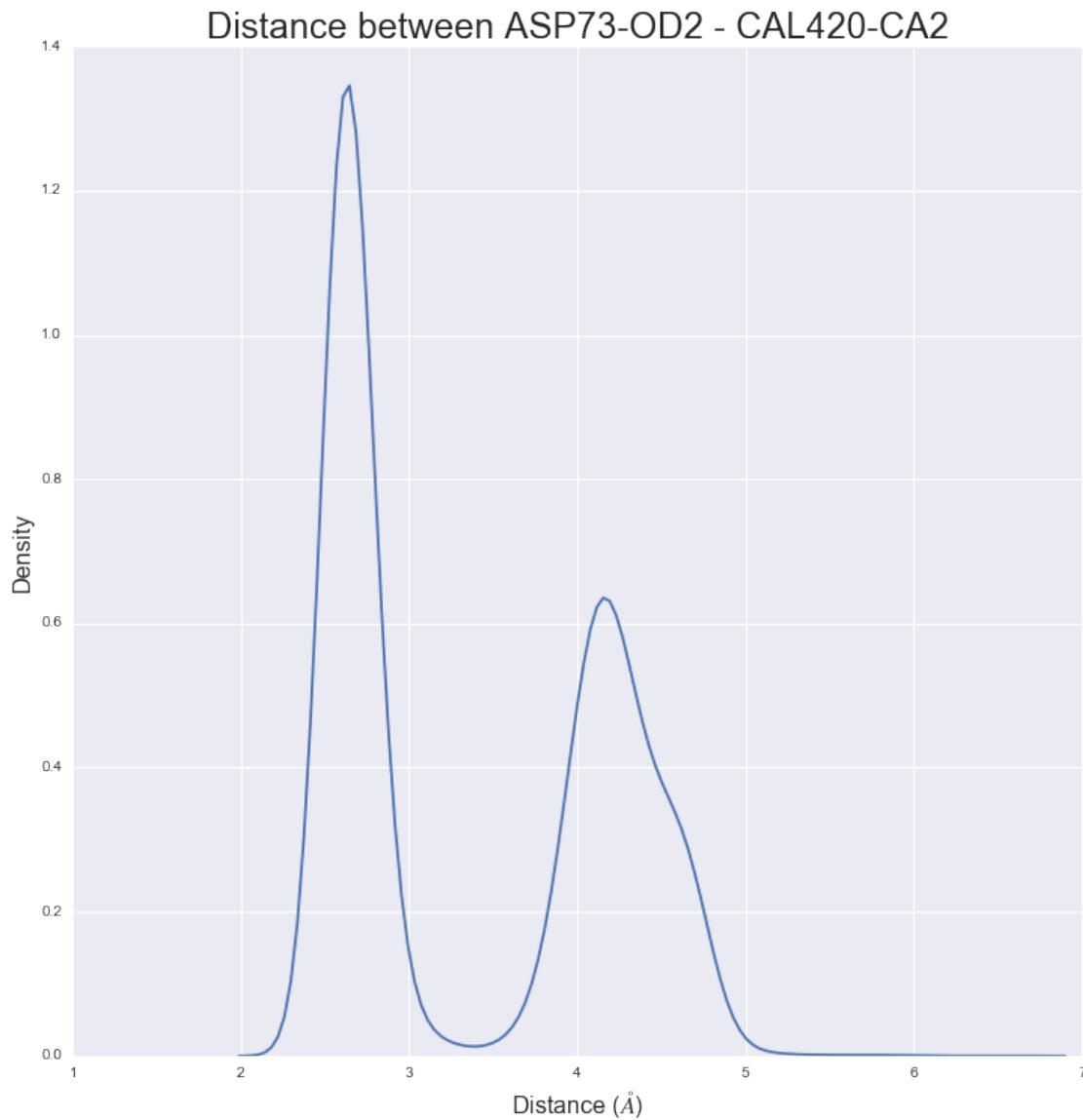
Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.11 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

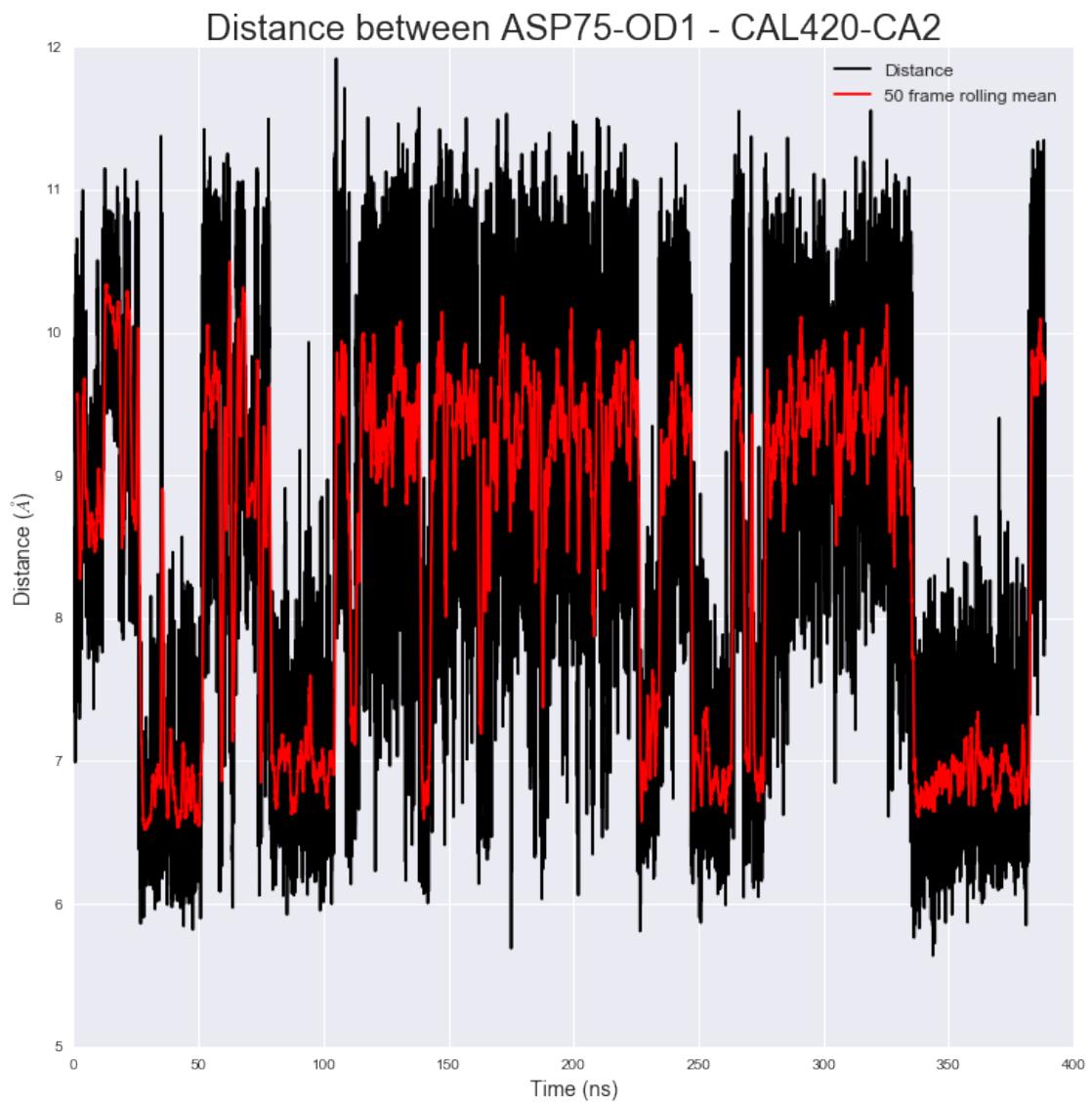
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

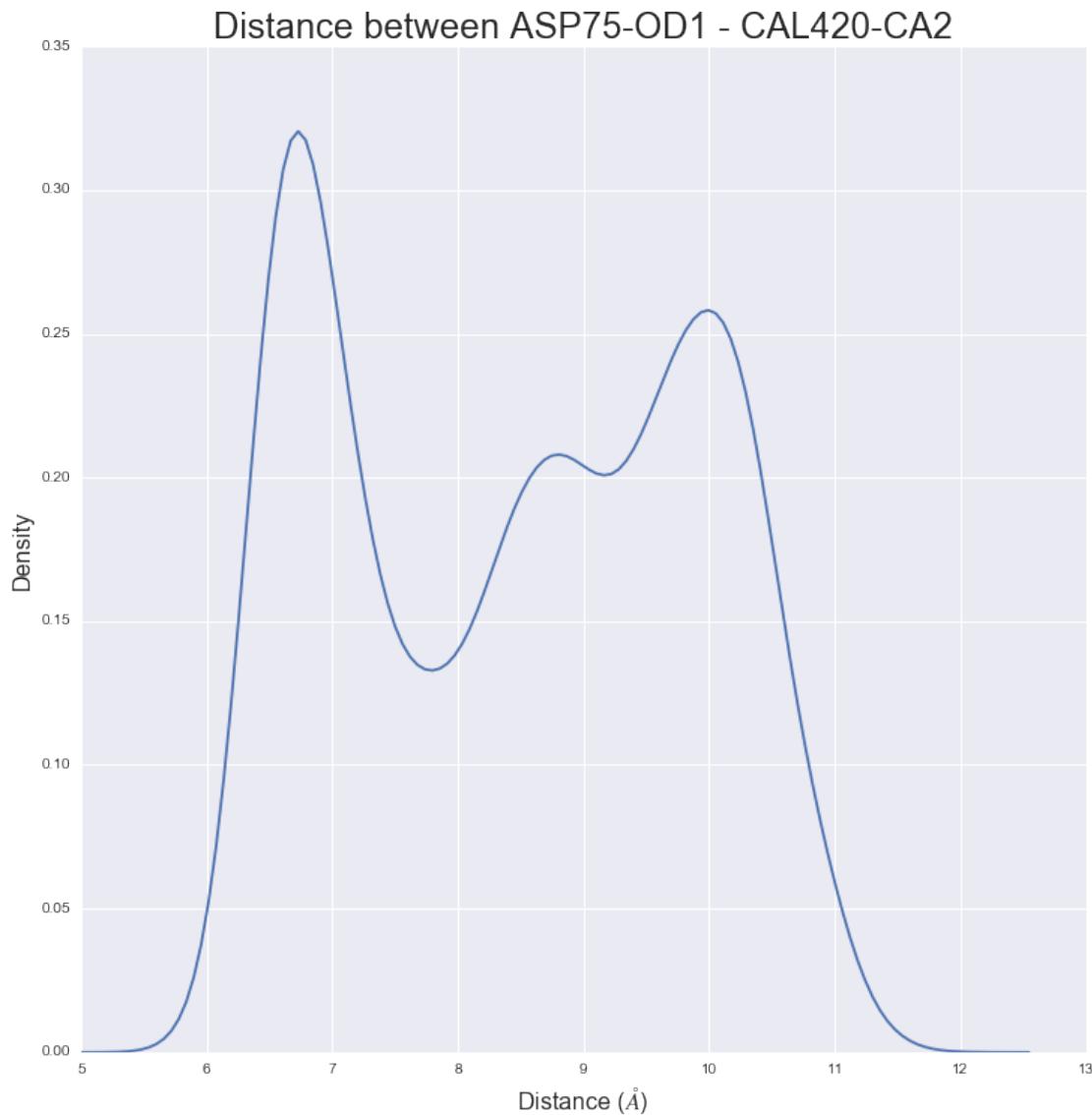
Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_tropomin_egcg_MD1_000-050_run2_nowater.nc
 05_Prod_tropomin_egcg_MD1_050-100_run2_nowater.nc
 05_Prod_tropomin_egcg_MD1_100-150_run2_nowater.nc
 05_Prod_tropomin_egcg_MD1_150-200_run2_nowater.nc
 05_Prod_tropomin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.27 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

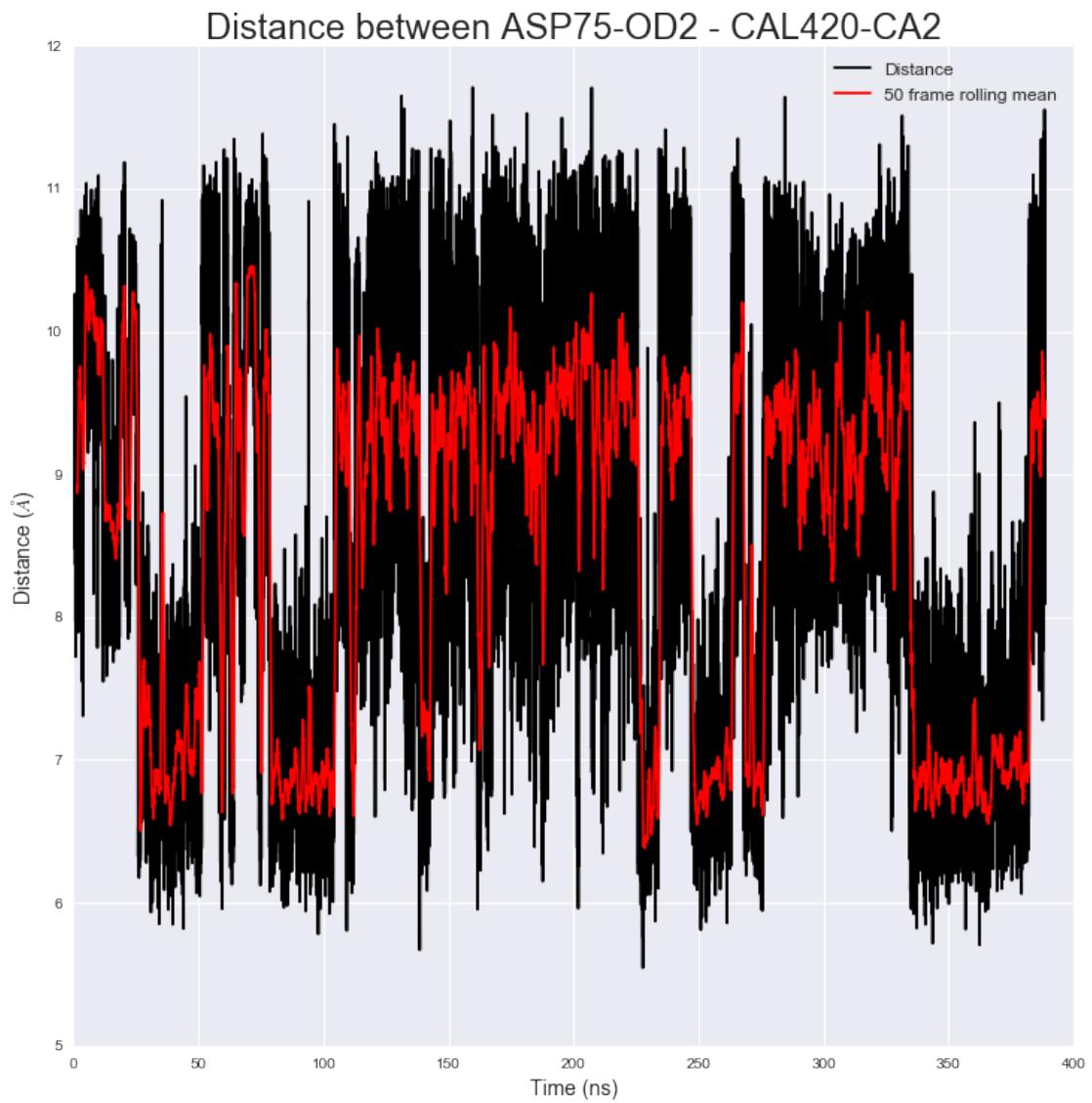
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

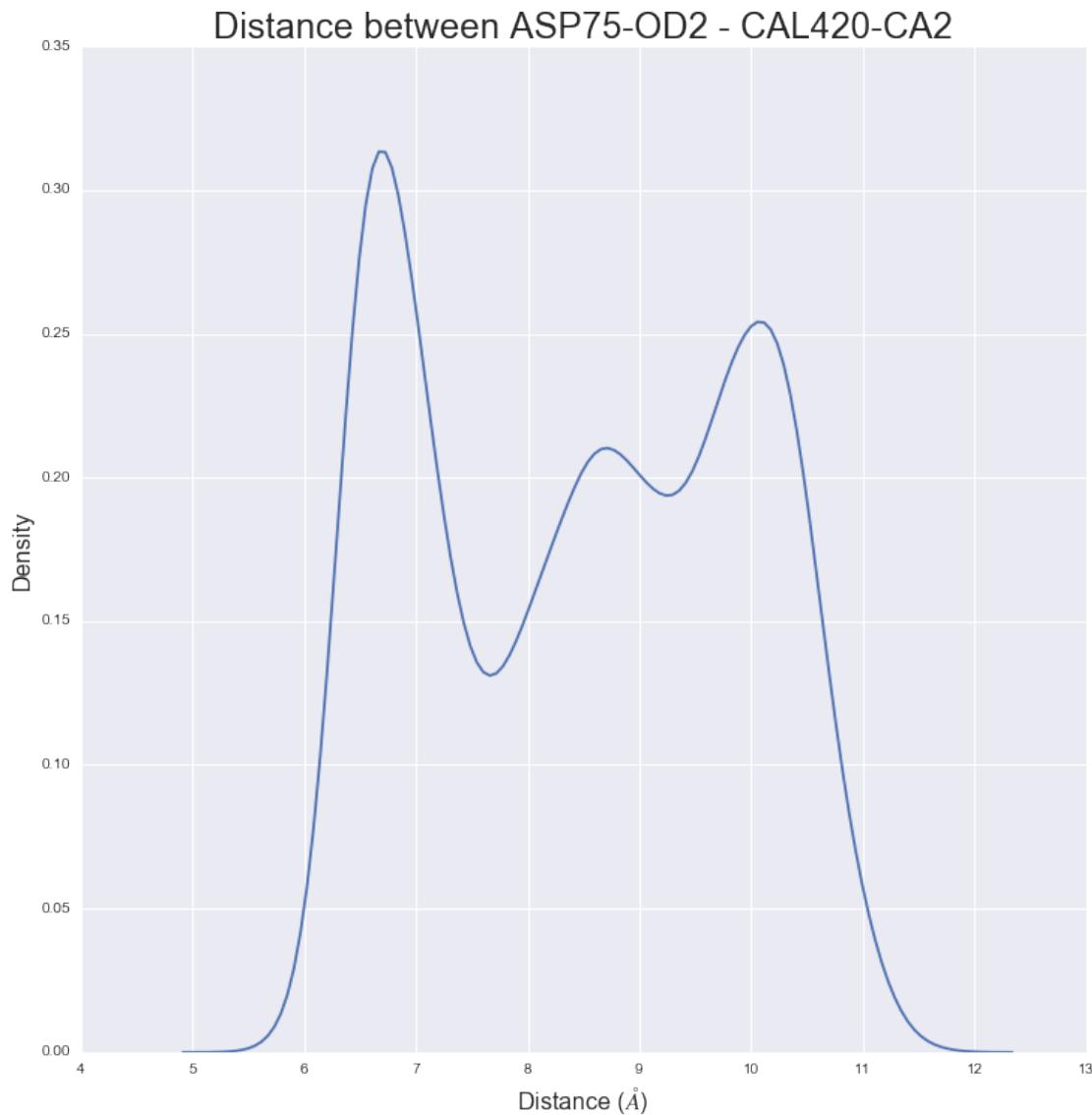
Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc

05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.37 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

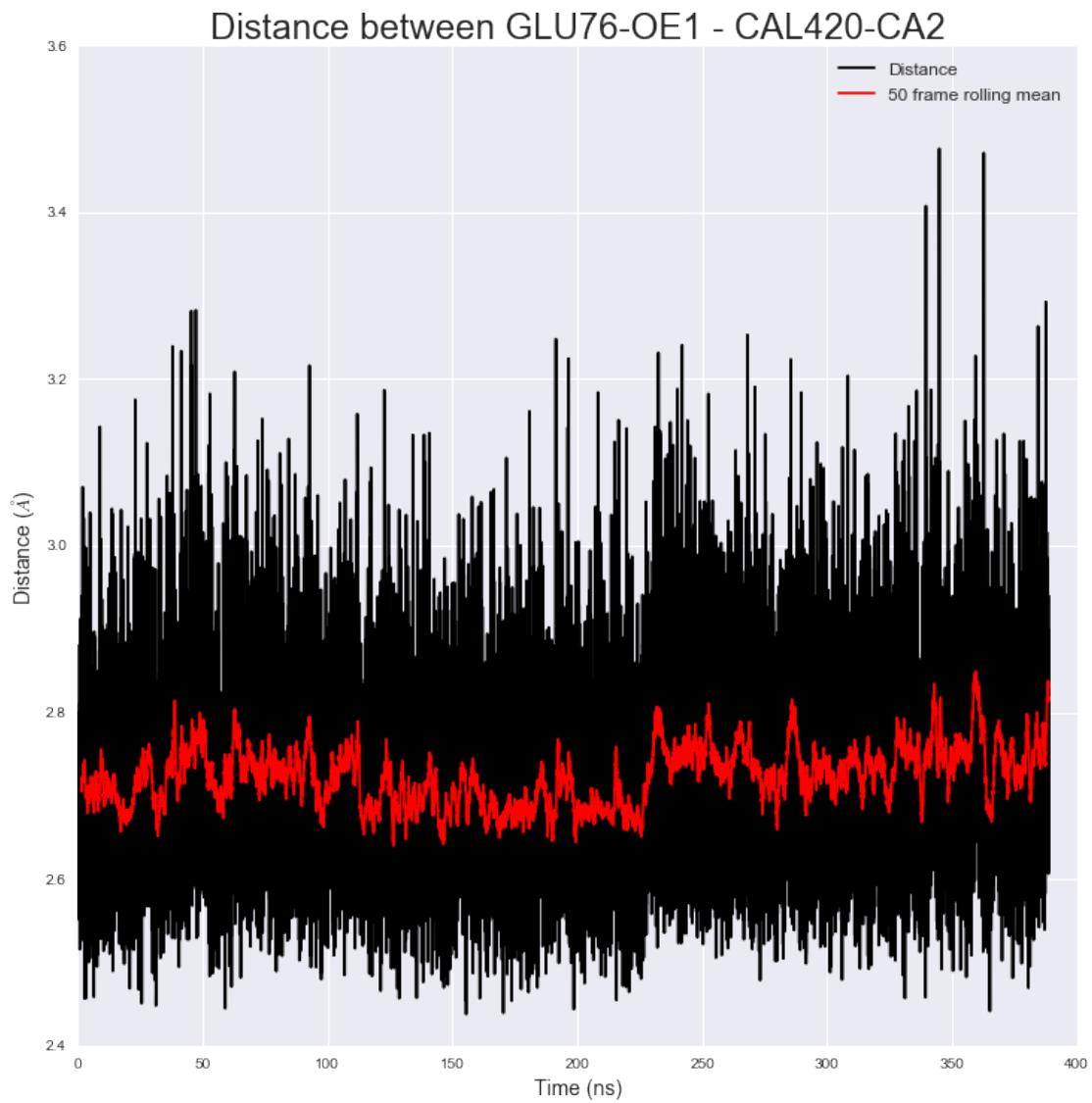
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

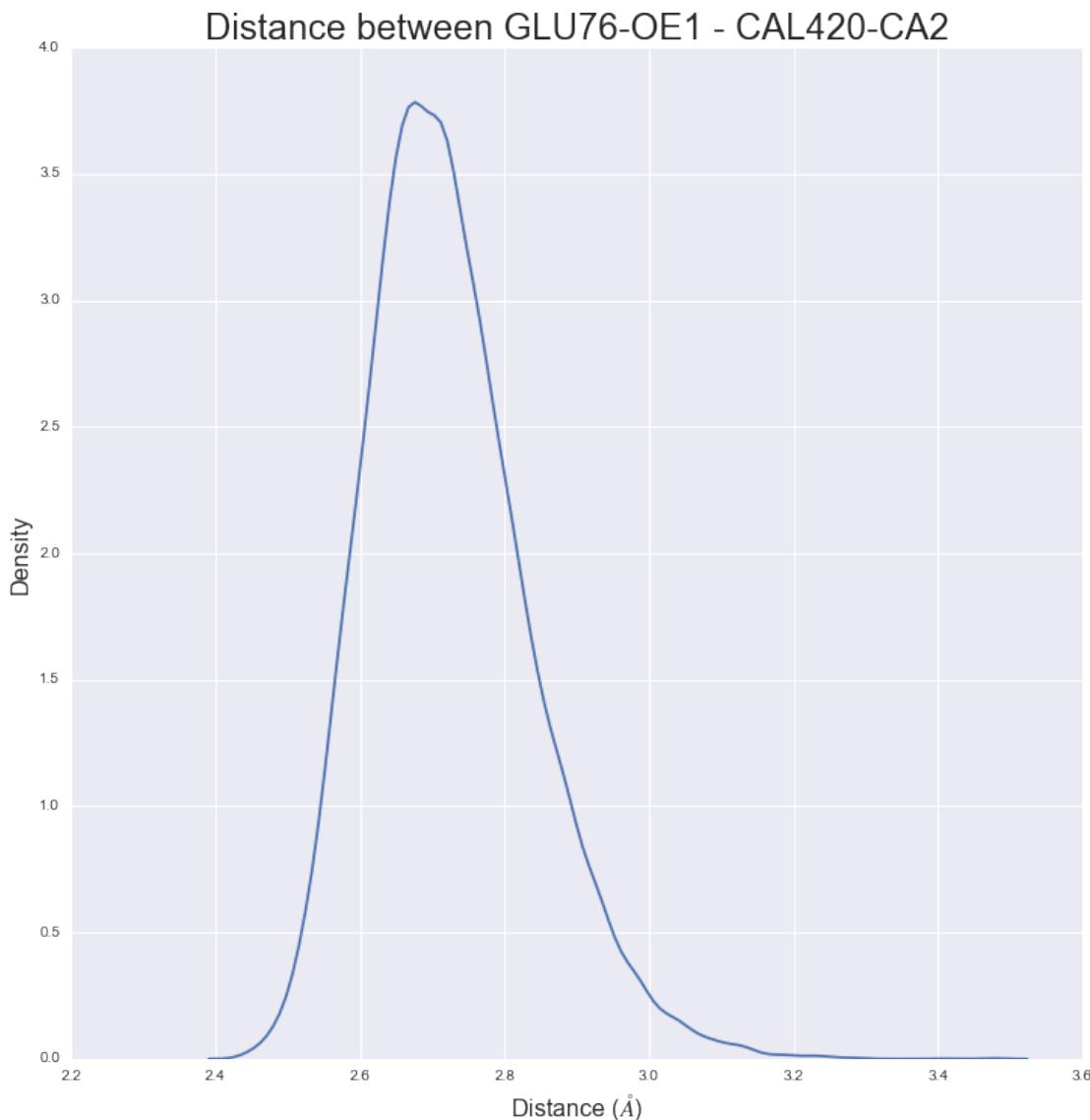
Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc

05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.41 seconds

Total simulation time of all frames: 388.08 nanoseconds

The following topology file was successfully loaded:

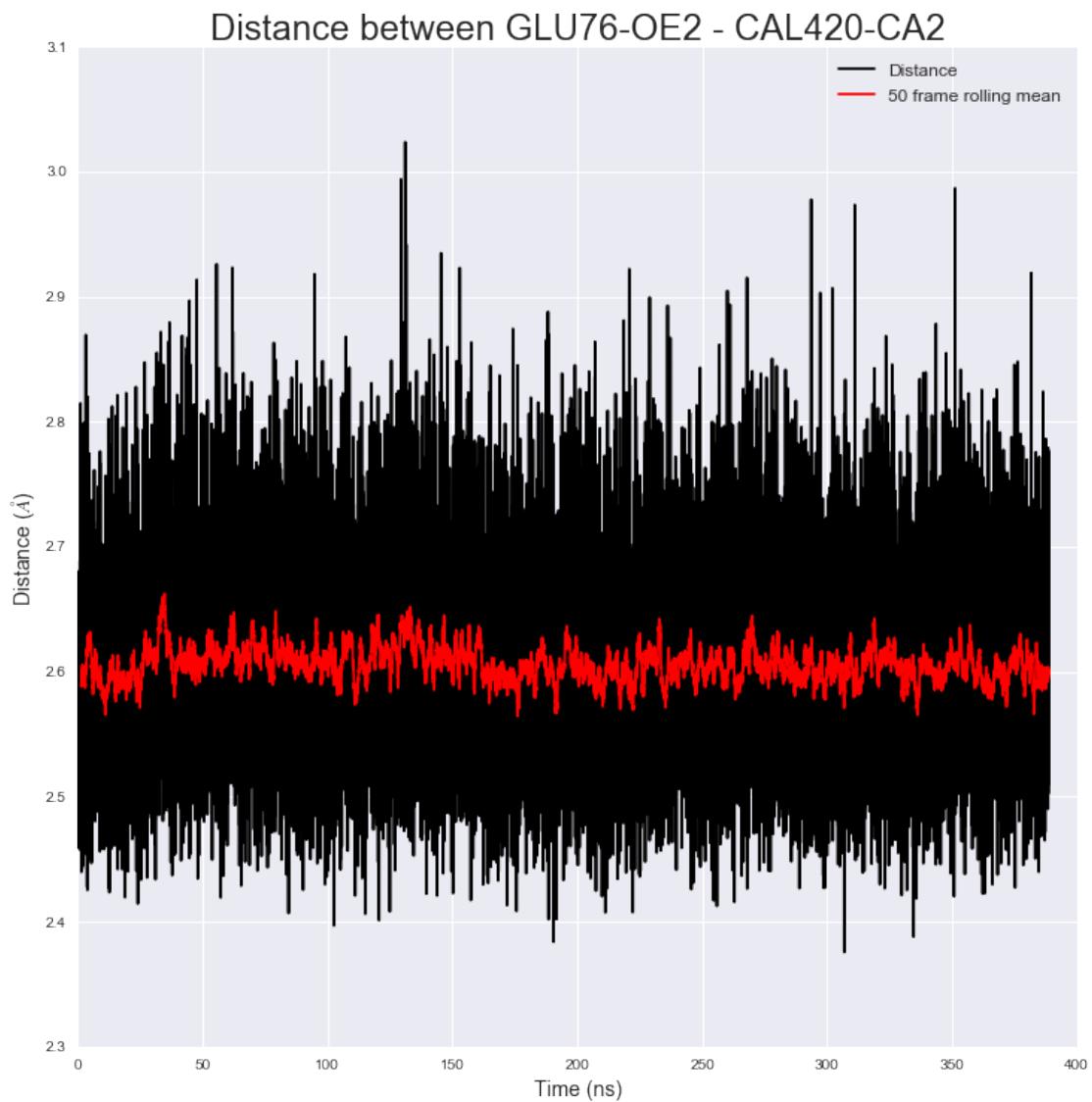
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

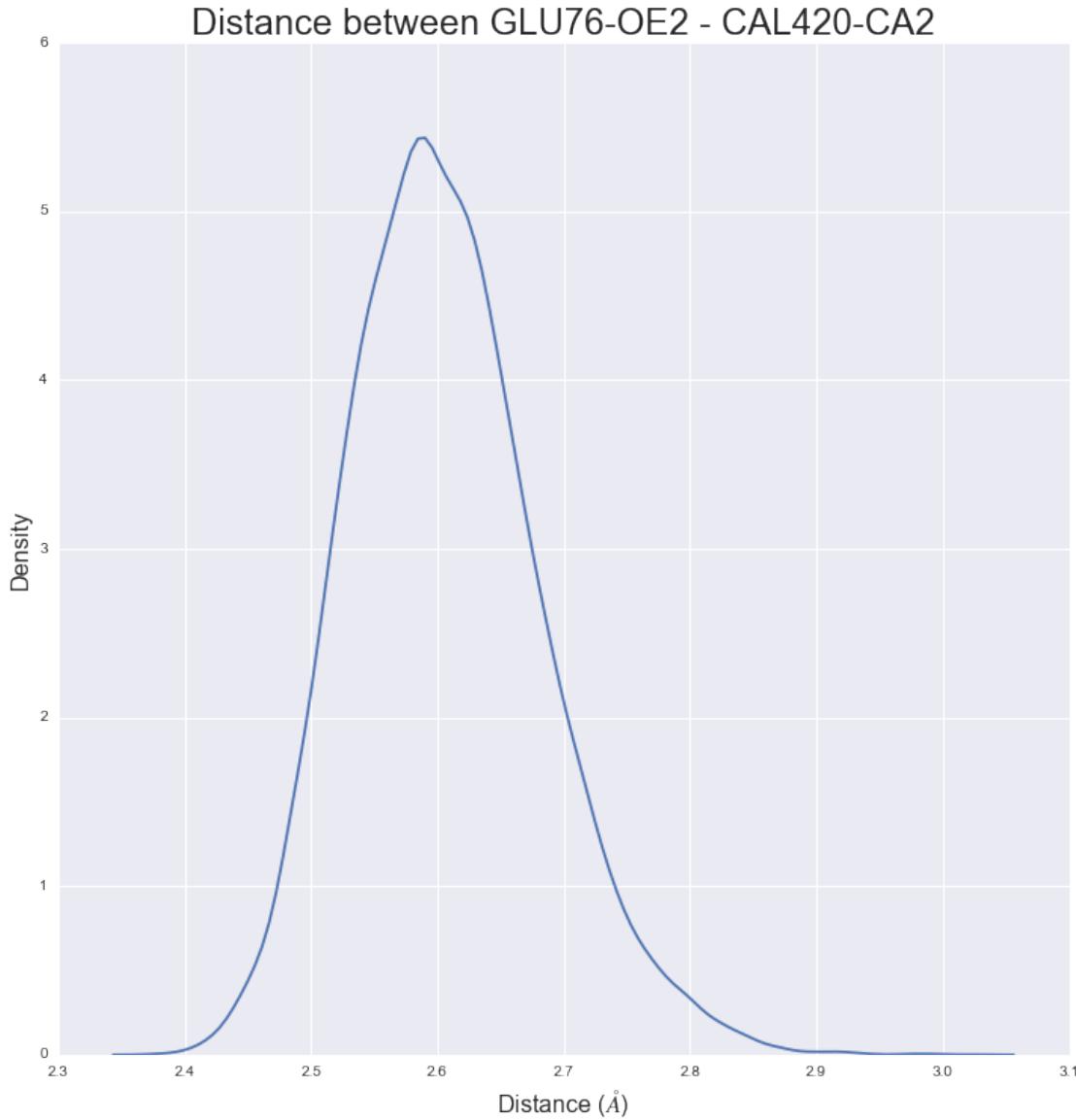
Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD1_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD1_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD1_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD1_300-350_run2_nowater.nc
05_Prod_troponin_egcg_MD1_350-400_run2_nowater.nc





Total execution time: 3.47 seconds

Total simulation time of all frames: 388.08 nanoseconds

0.2 MD2

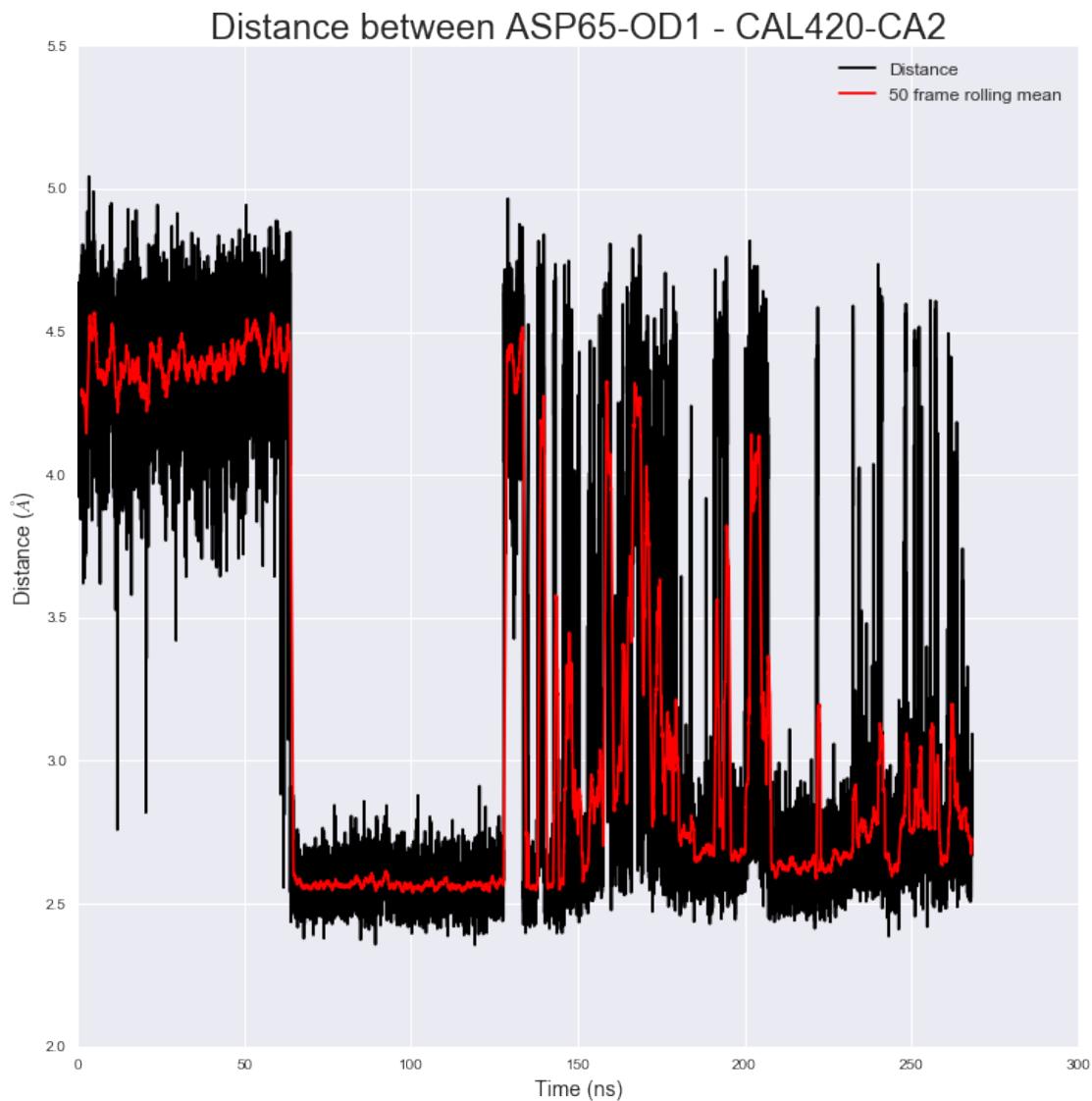
```
In [17]: topology_MD2 = '/Users/gil_f.hoben/Troponin_md_processed/MD2/run2/troponin_egcg_MD2_nowater.pr
trajectory_MD2 = '/Users/gil_f.hoben/Troponin_md_processed/MD2/run2/Trajectories/'
atom1_list = ['name OD1 and resid 64', 'name OD1 and resid 64', 'name OE1 and resid 65',
              'name OE2 and resid 65', 'name OD2 and resid 66',
              'name OD2 and resid 66', 'name OG and resid 68', 'name OG1 and resid 70',
              'name OD1 and resid 72', 'name OD2 and resid 72', 'name OD1 and resid 74',
              'name OD2 and resid 74', 'name OE1 and resid 75', 'name OE2 and resid 75']
atom2 = 'resid 419'
```

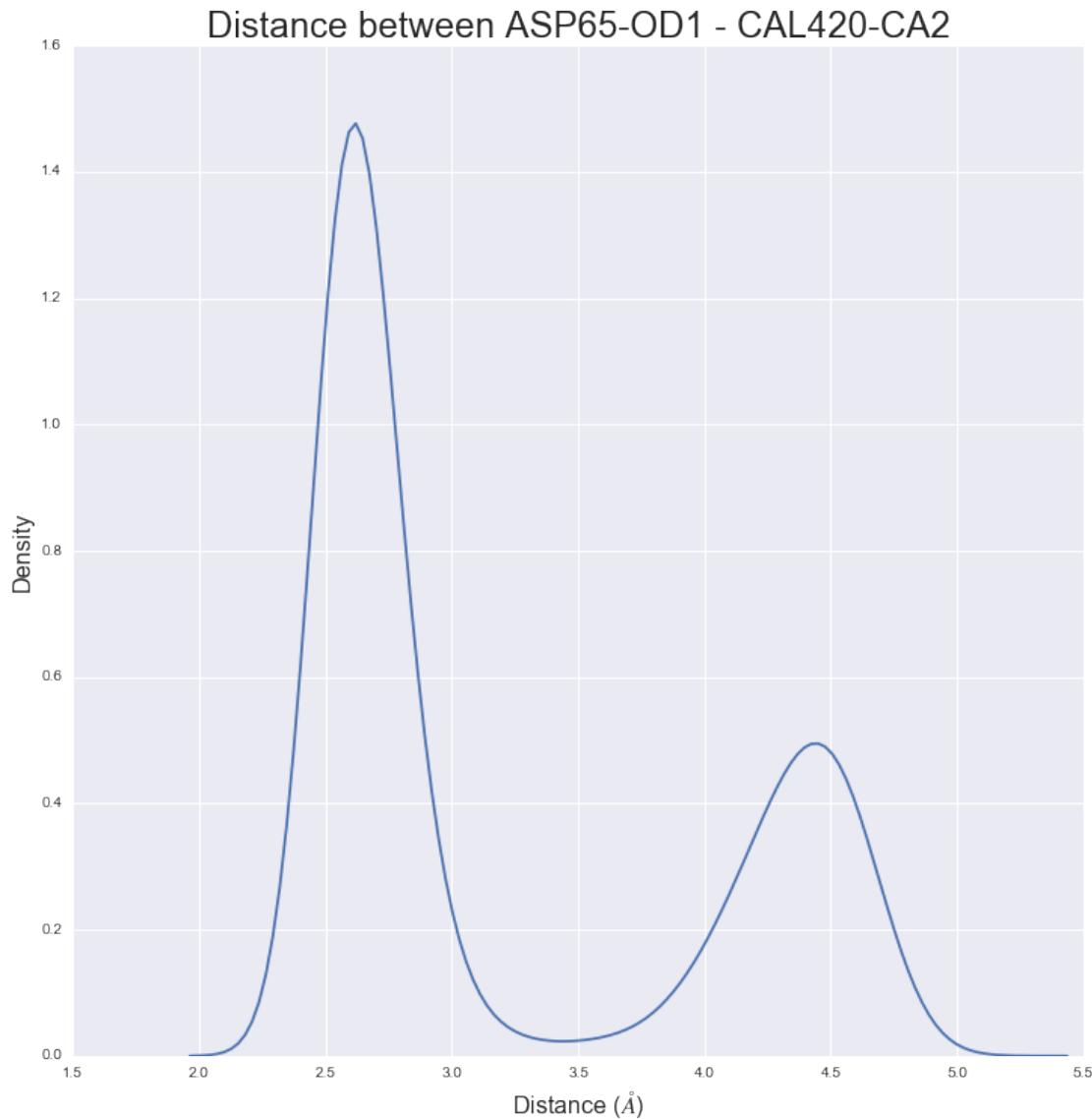
```
In [18]: for atom1 in atom1_list:  
    main(topology_MD2, trajectory_MD2, atom1, atom2, verbose = 1)
```

The following topology file was successfully loaded:
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:
05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc





Total execution time: 4.69 seconds

Total simulation time of all frames: 267.98 nanoseconds

The following topology file was successfully loaded:

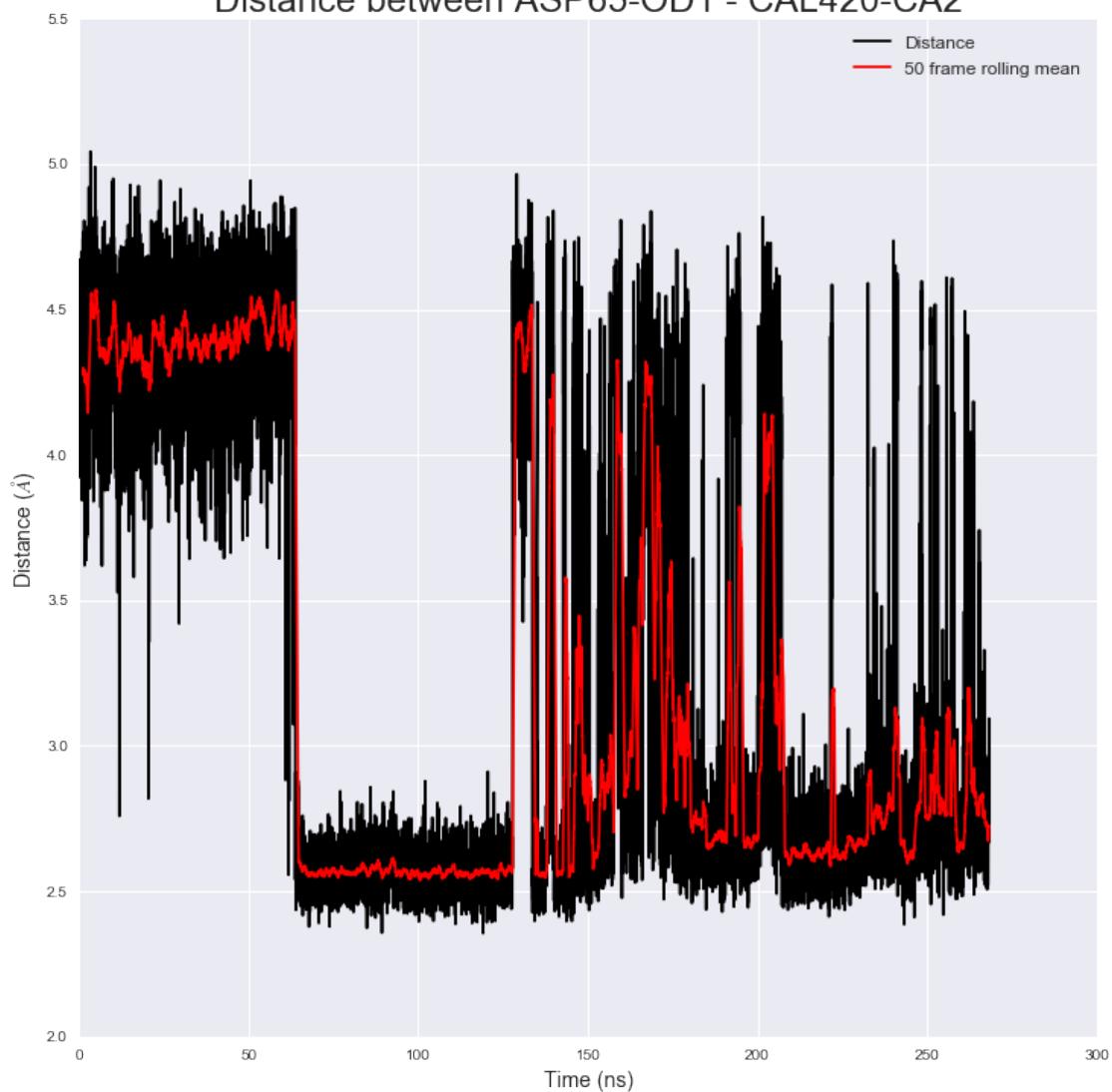
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

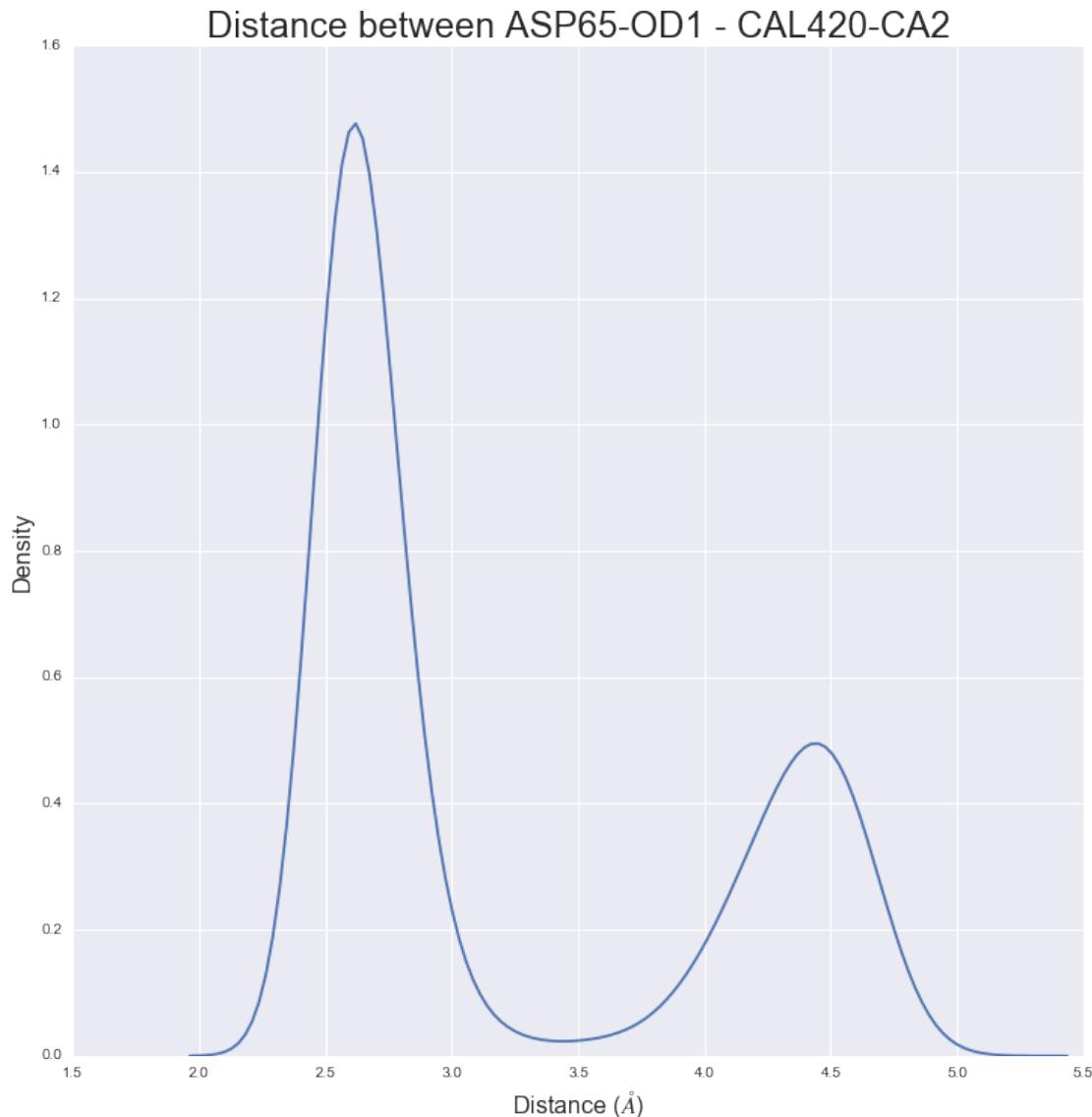
Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc

Distance between ASP65-OD1 - CAL420-CA2





Total execution time: 2.49 seconds

Total simulation time of all frames: 267.98 nanoseconds

The following topology file was successfully loaded:

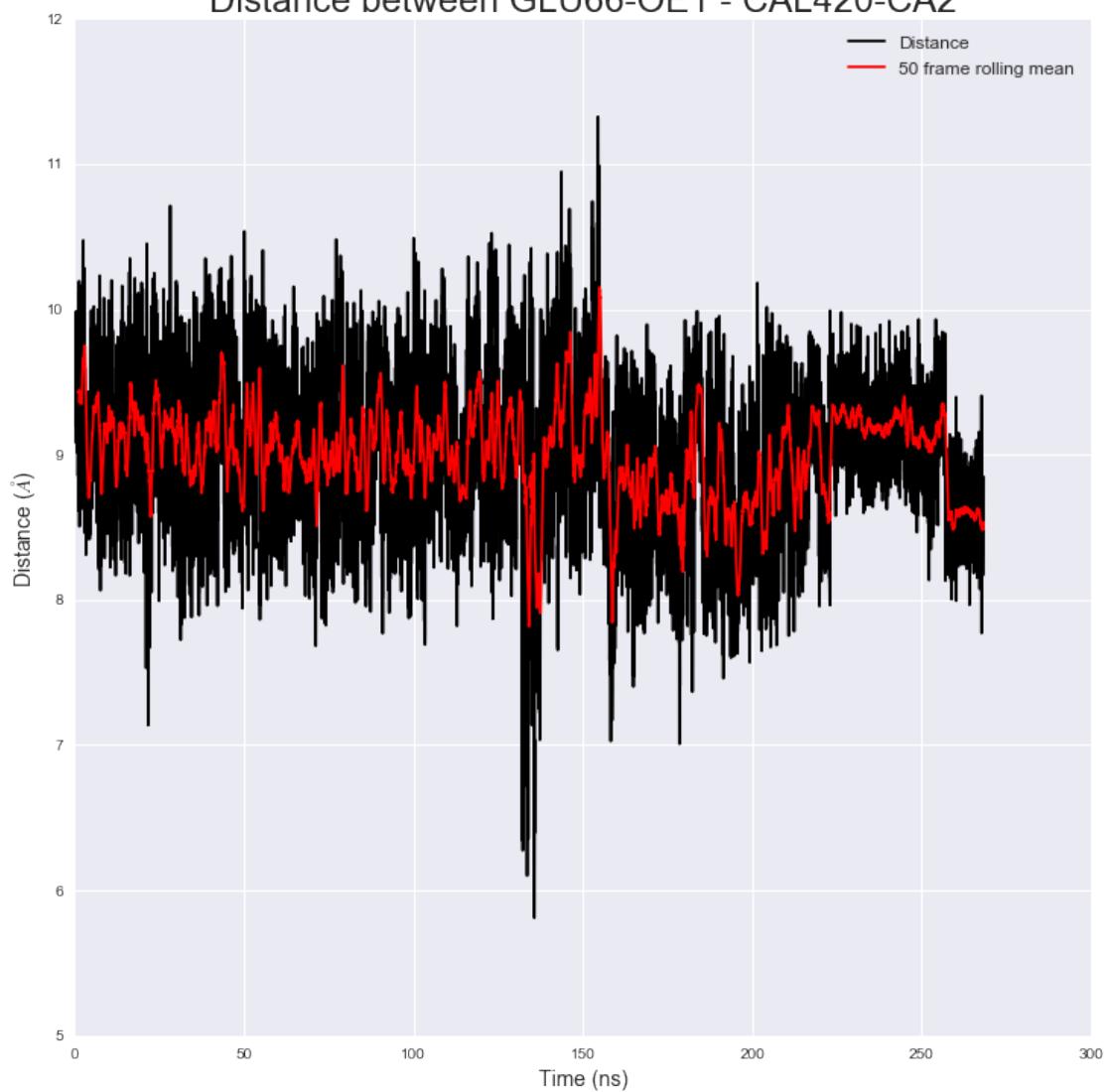
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

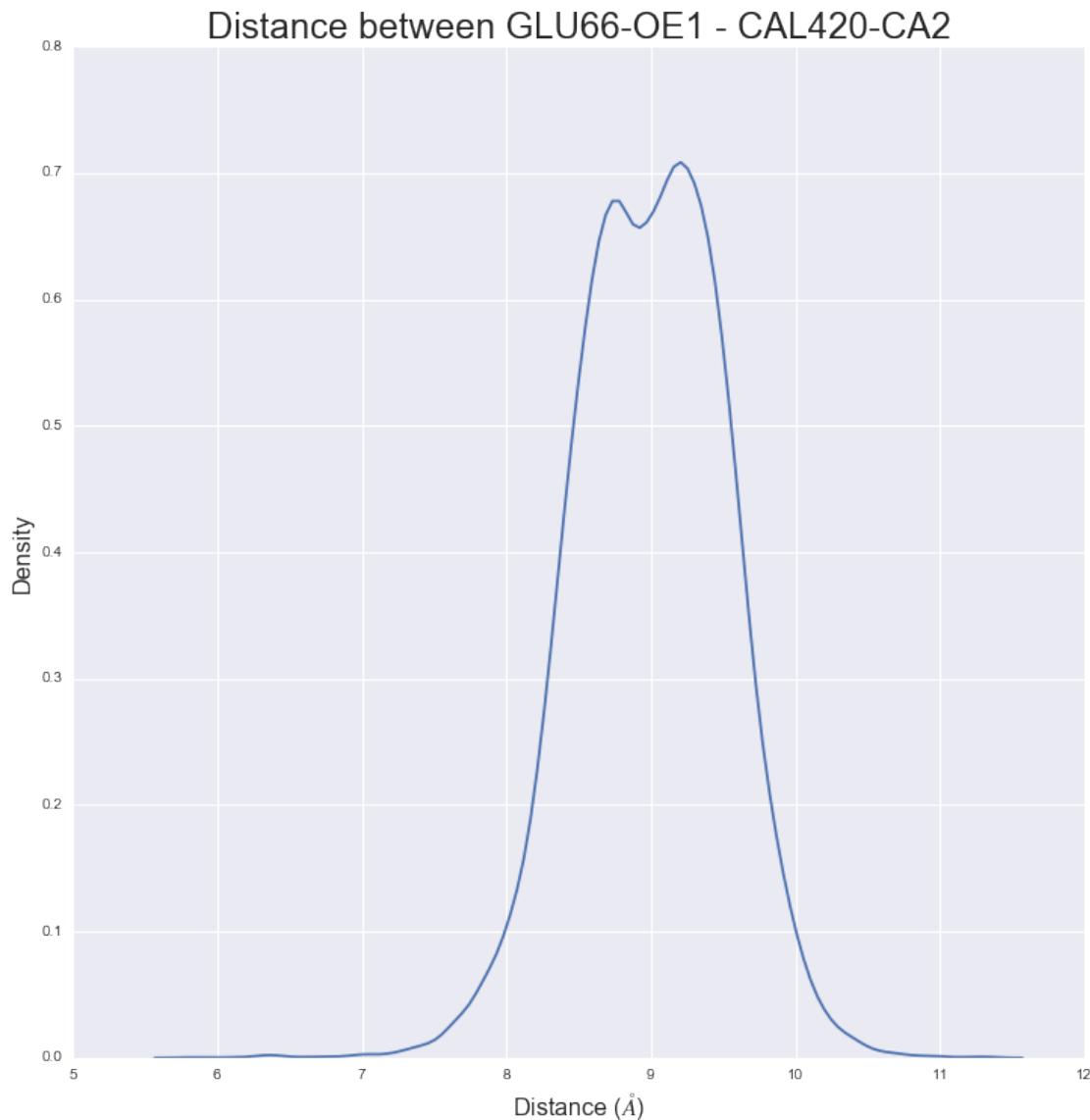
Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc

Distance between GLU66-OE1 - CAL420-CA2





Total execution time: 2.55 seconds

Total simulation time of all frames: 267.98 nanoseconds

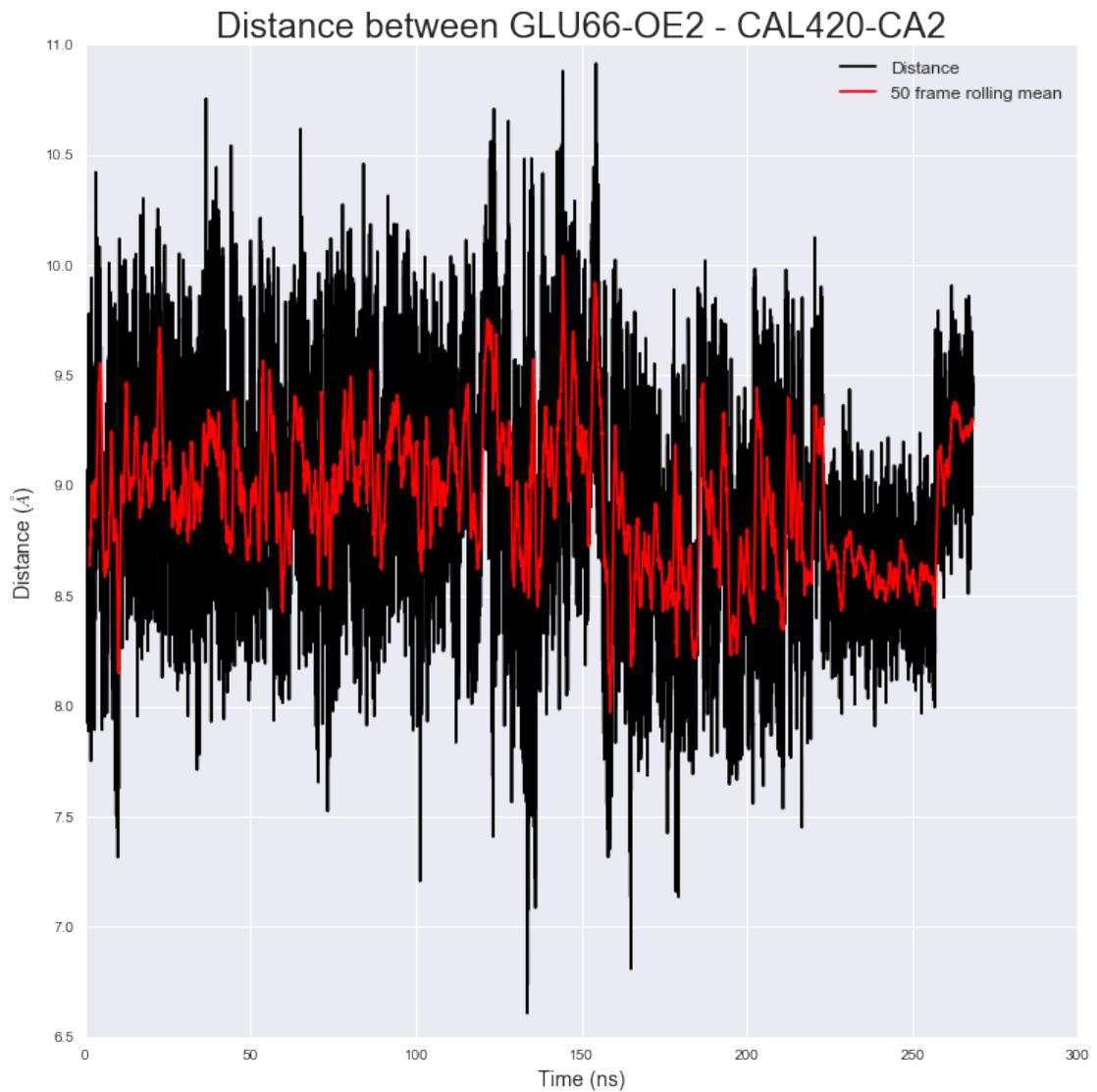
The following topology file was successfully loaded:

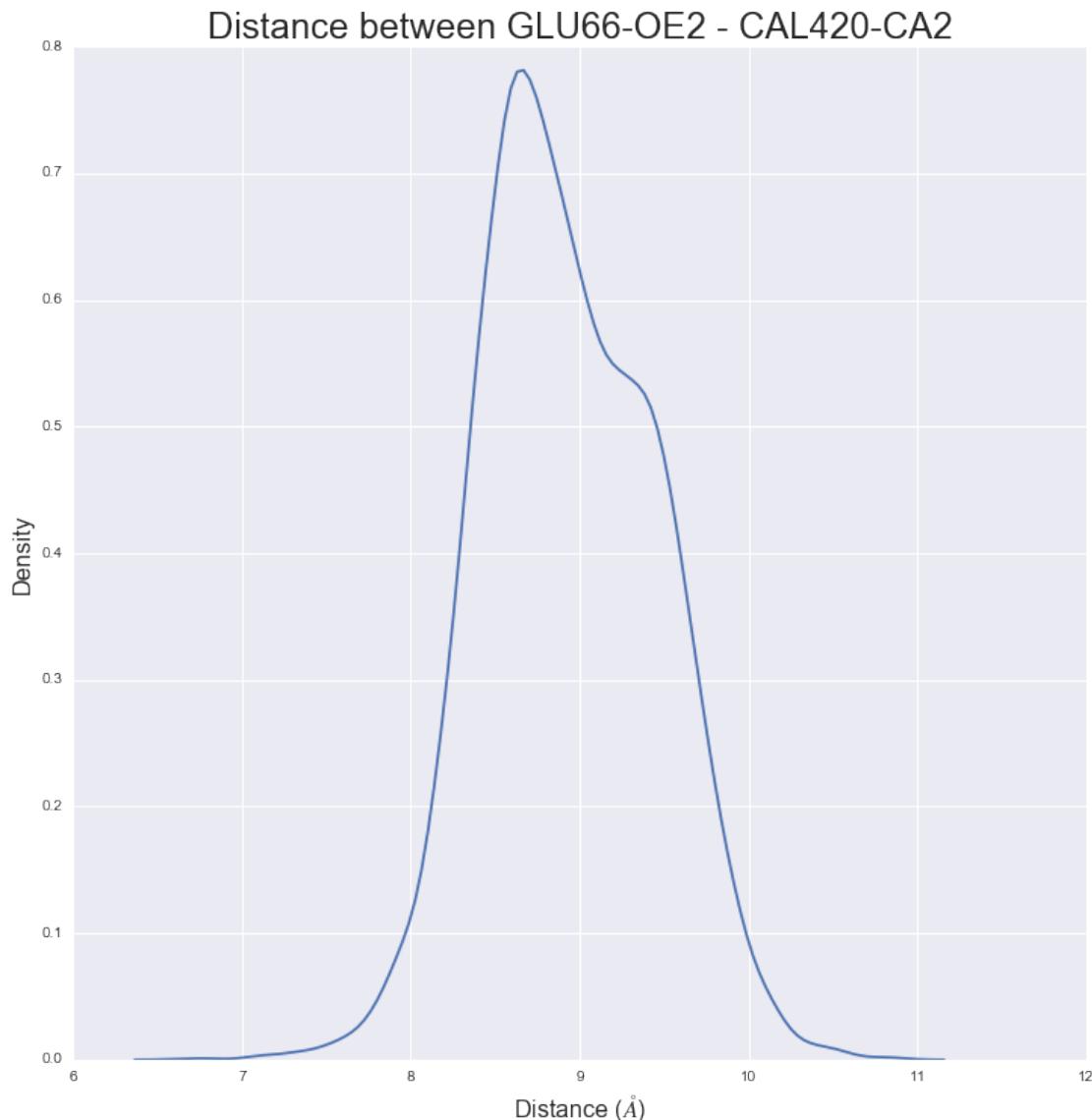
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc





Total execution time: 2.46 seconds

Total simulation time of all frames: 267.98 nanoseconds

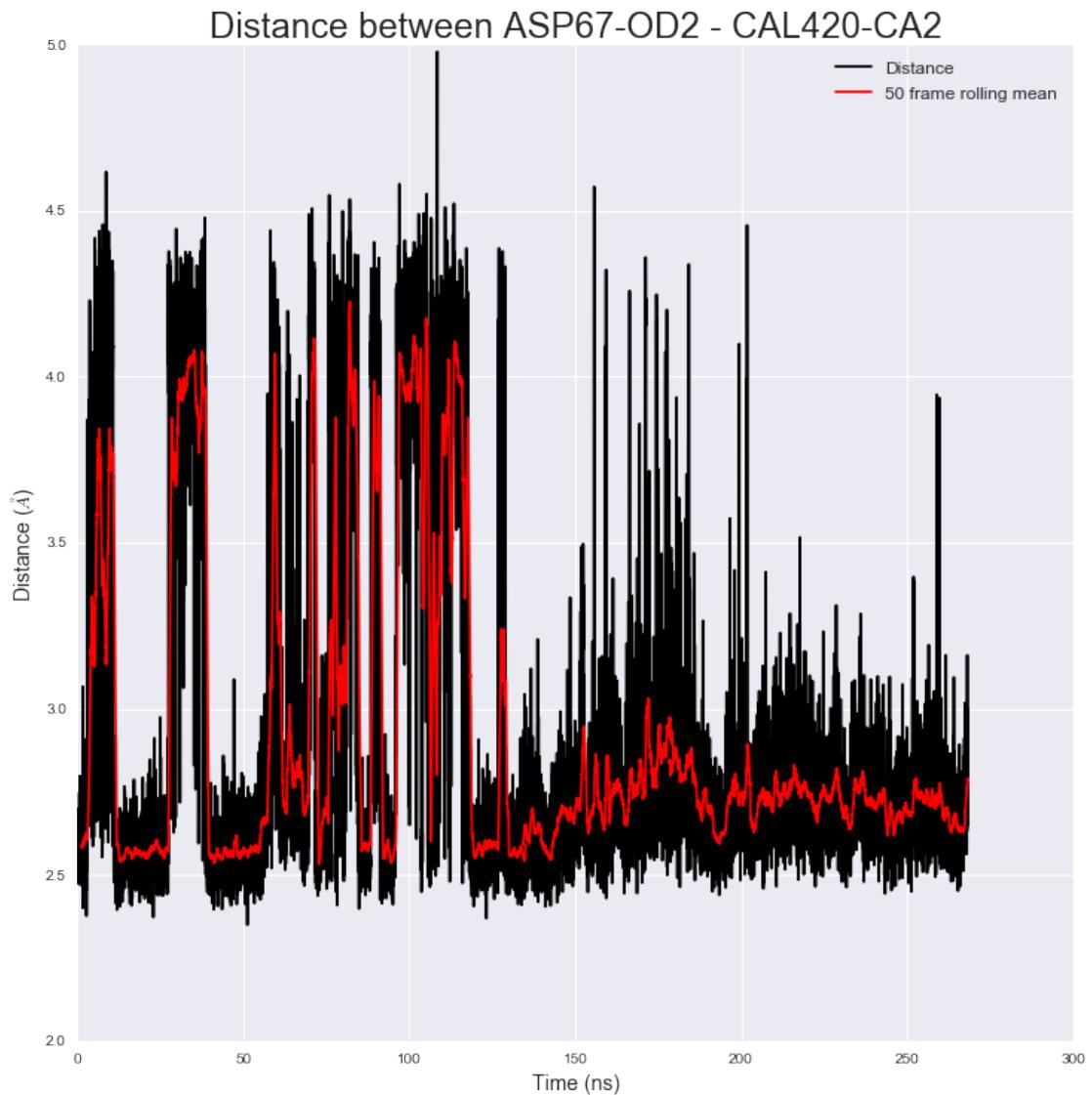
The following topology file was successfully loaded:

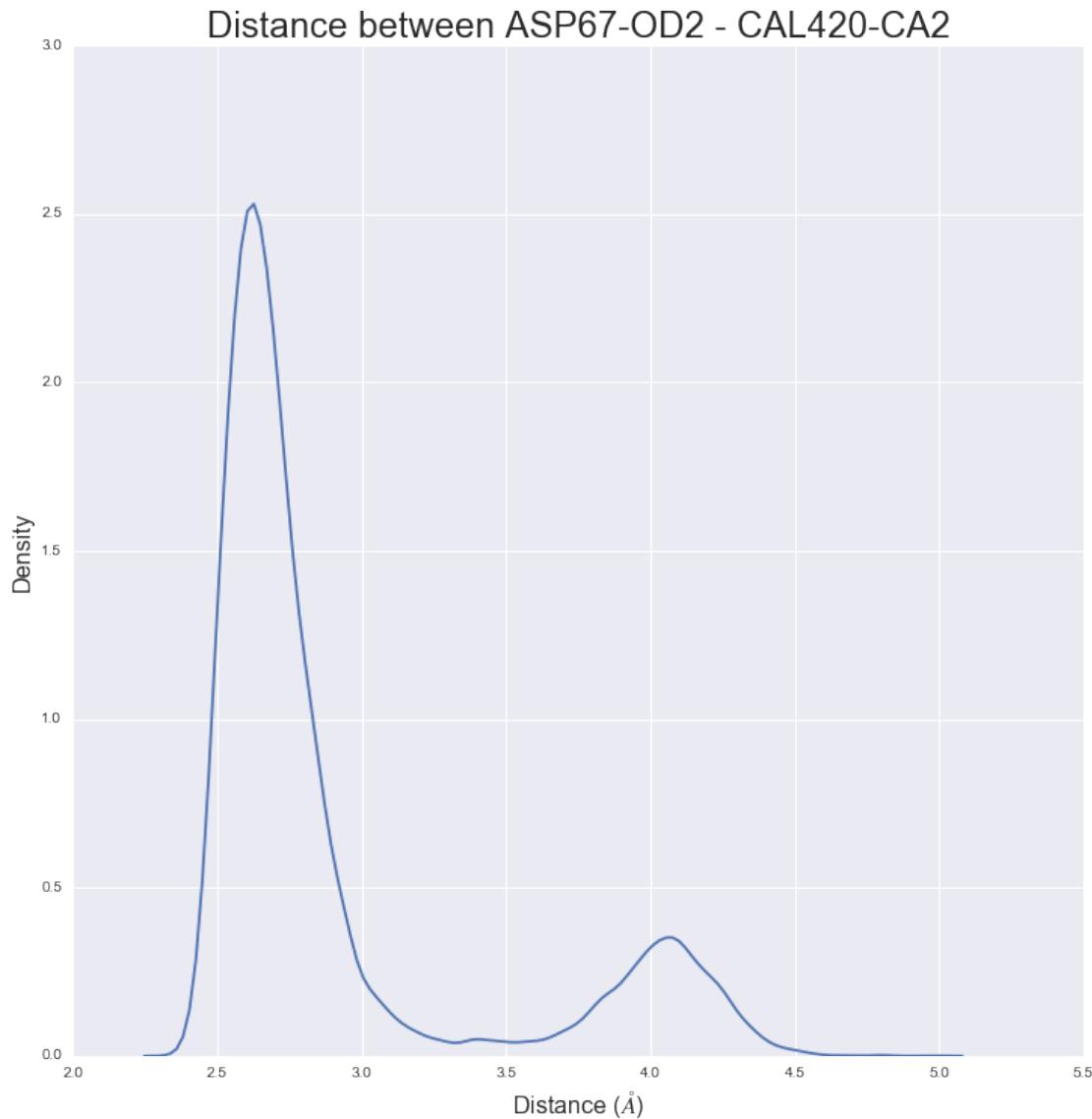
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc





Total execution time: 2.39 seconds

Total simulation time of all frames: 267.98 nanoseconds

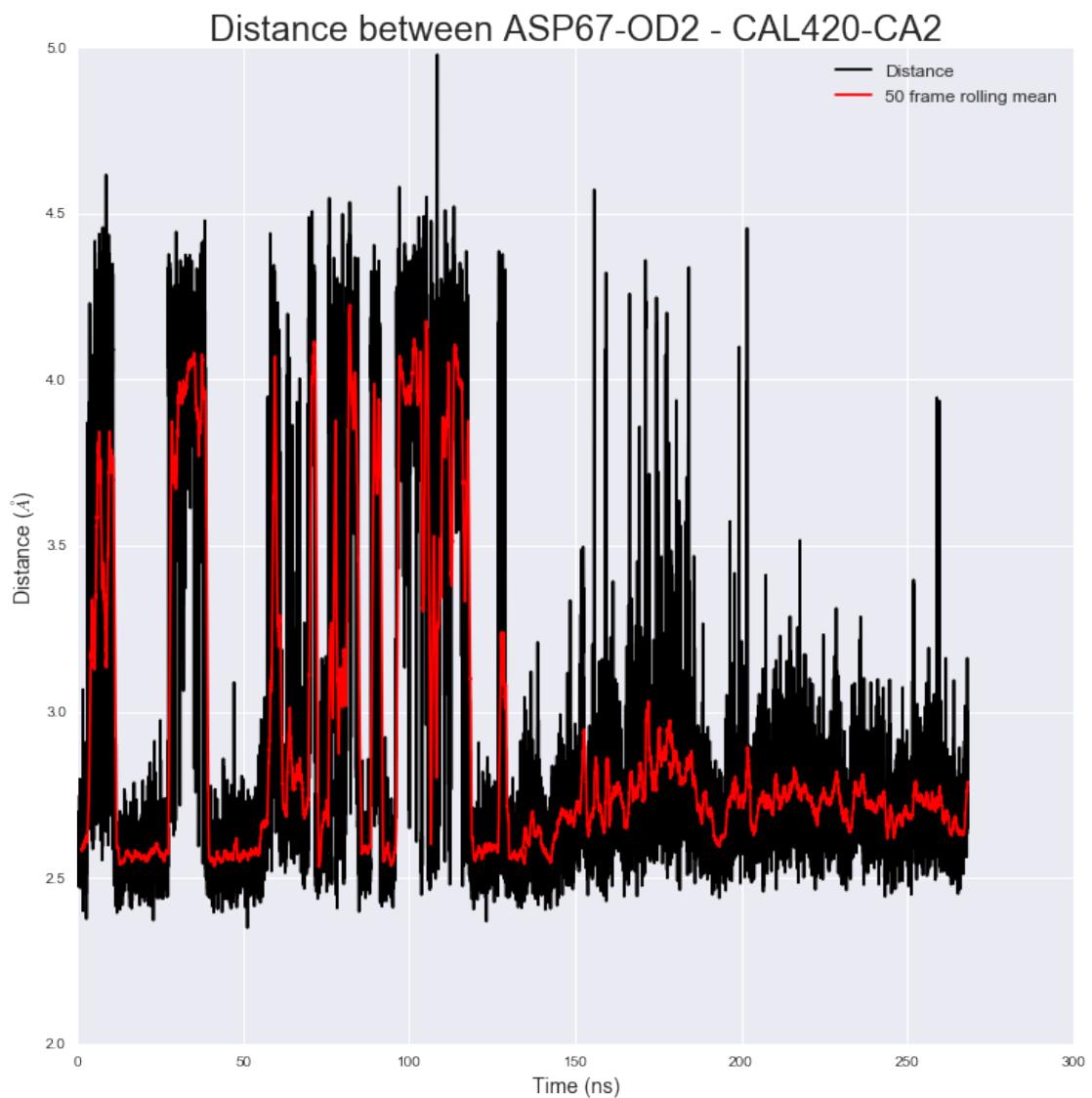
The following topology file was successfully loaded:

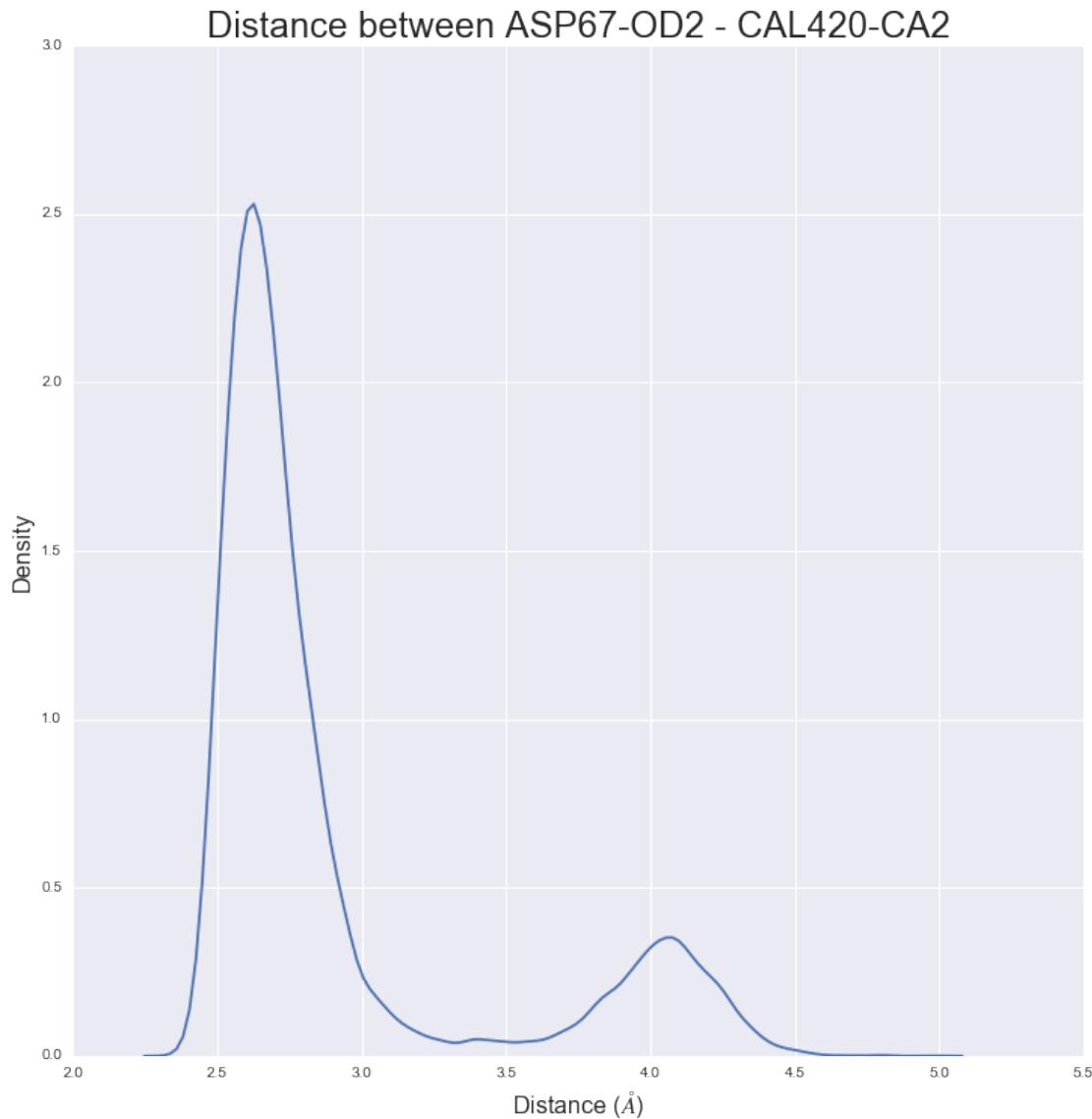
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc





Total execution time: 2.54 seconds

Total simulation time of all frames: 267.98 nanoseconds

The following topology file was successfully loaded:

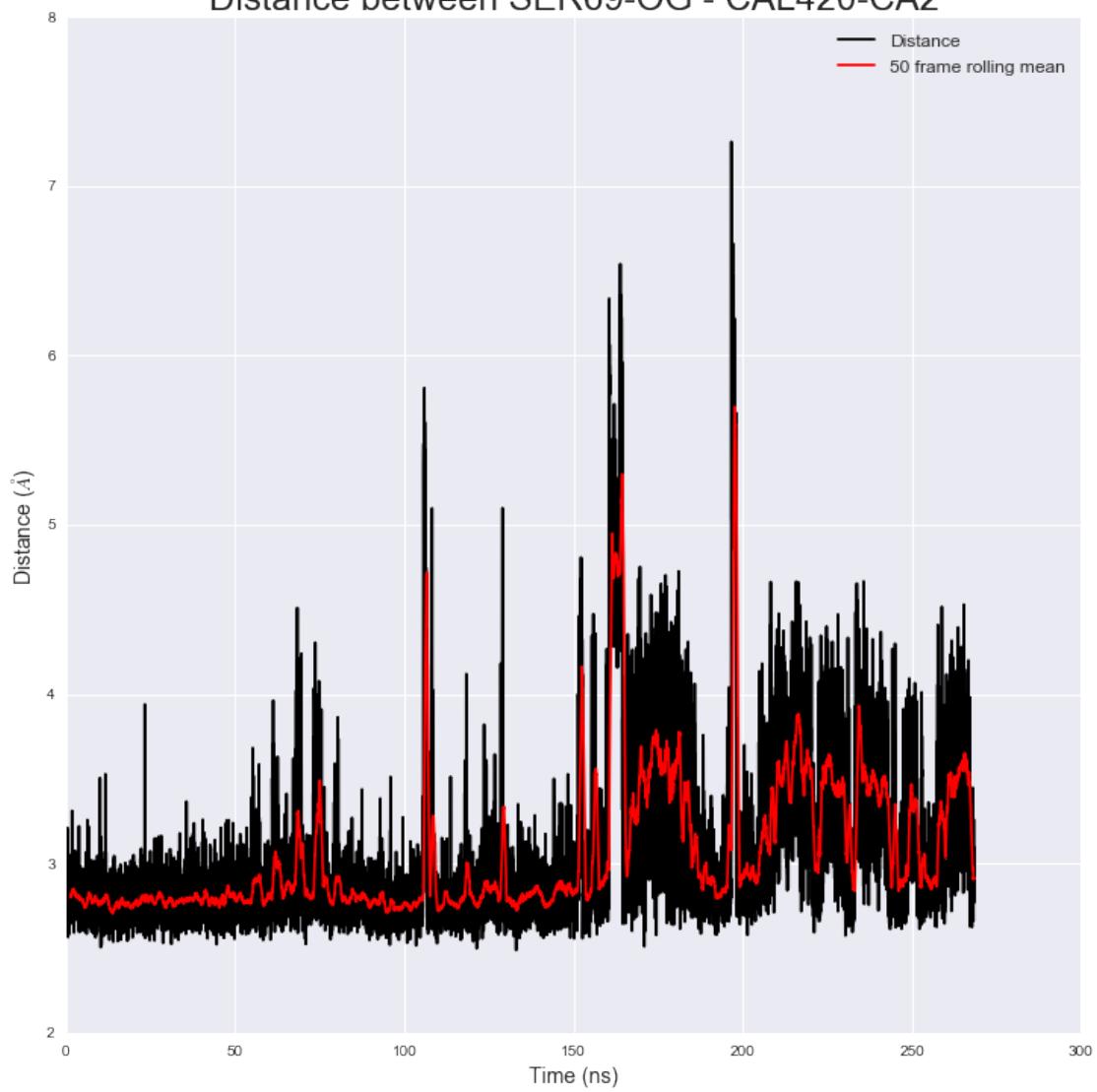
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

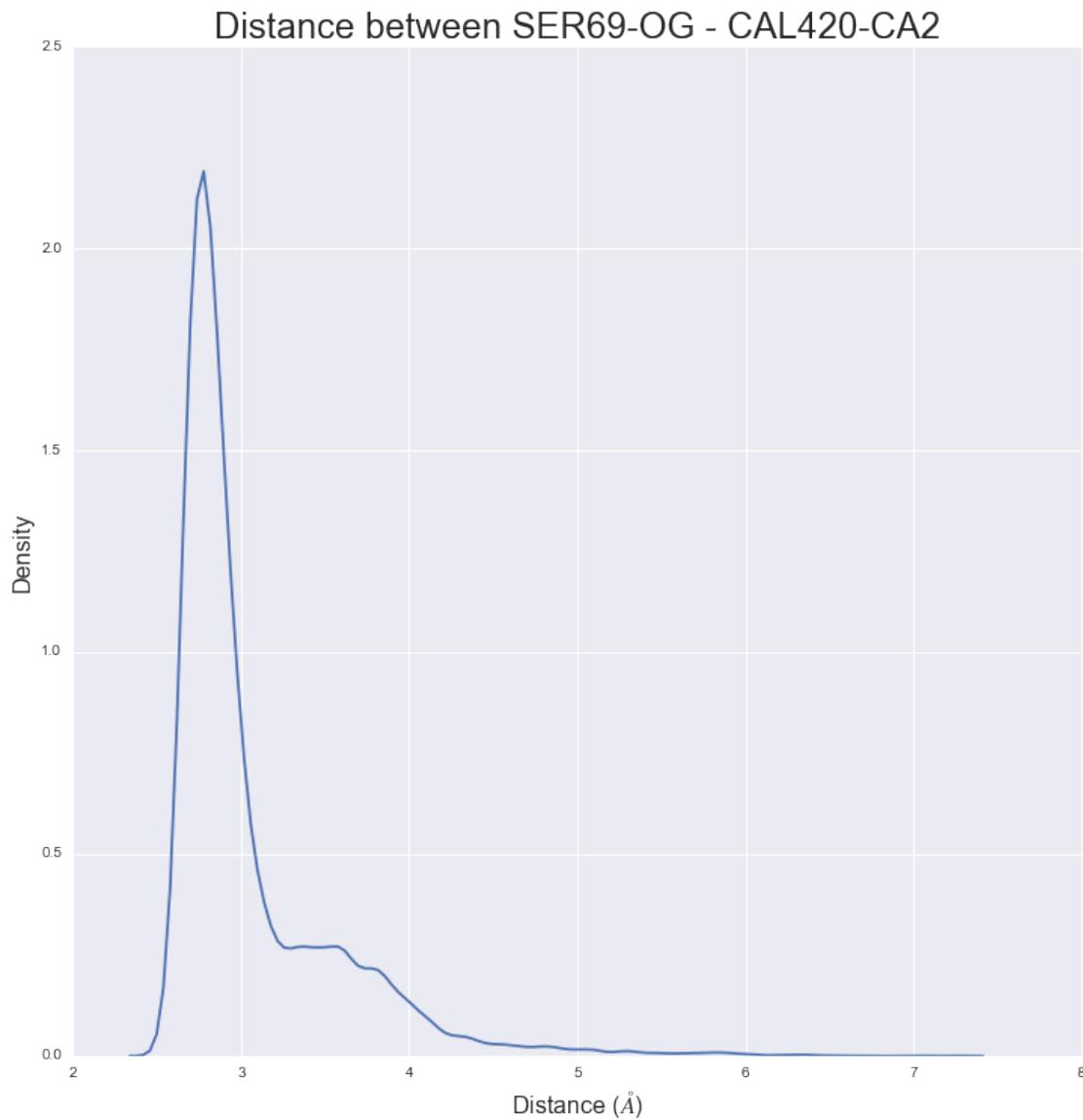
Calculating distance between following atoms: SER69-OG - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc

Distance between SER69-OG - CAL420-CA2





Total execution time: 2.39 seconds

Total simulation time of all frames: 267.98 nanoseconds

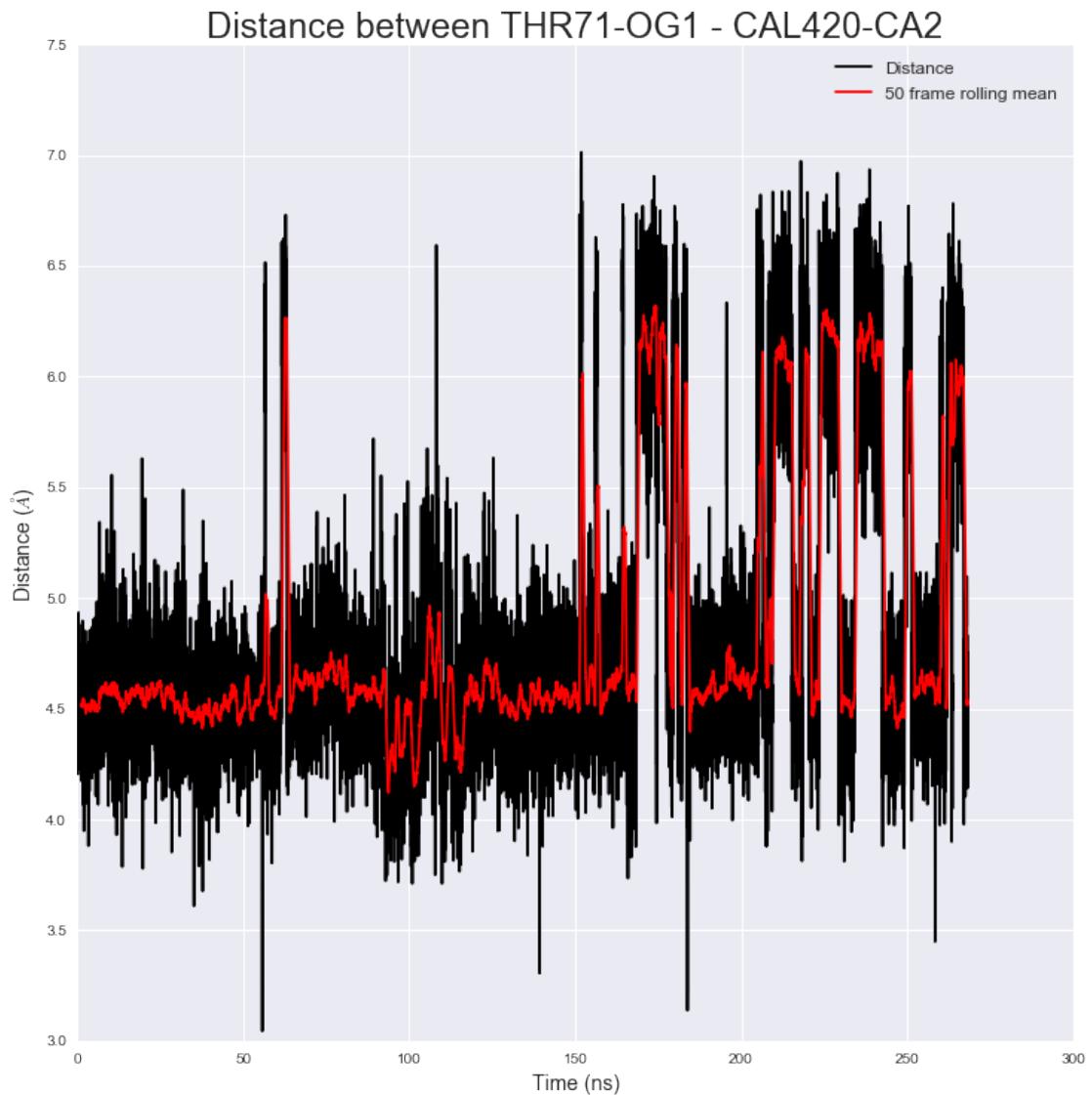
The following topology file was successfully loaded:

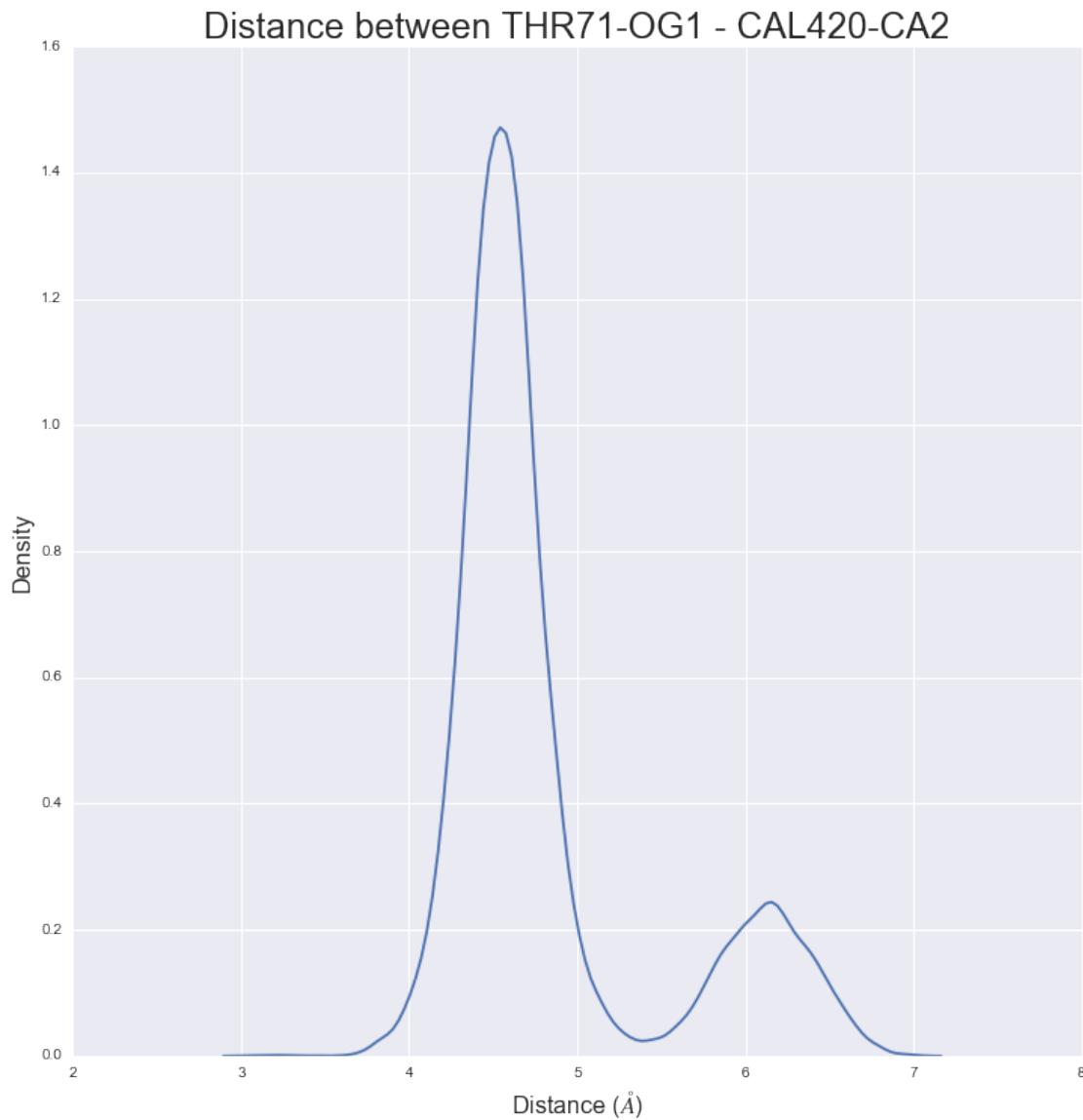
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc





Total execution time: 2.42 seconds

Total simulation time of all frames: 267.98 nanoseconds

The following topology file was successfully loaded:

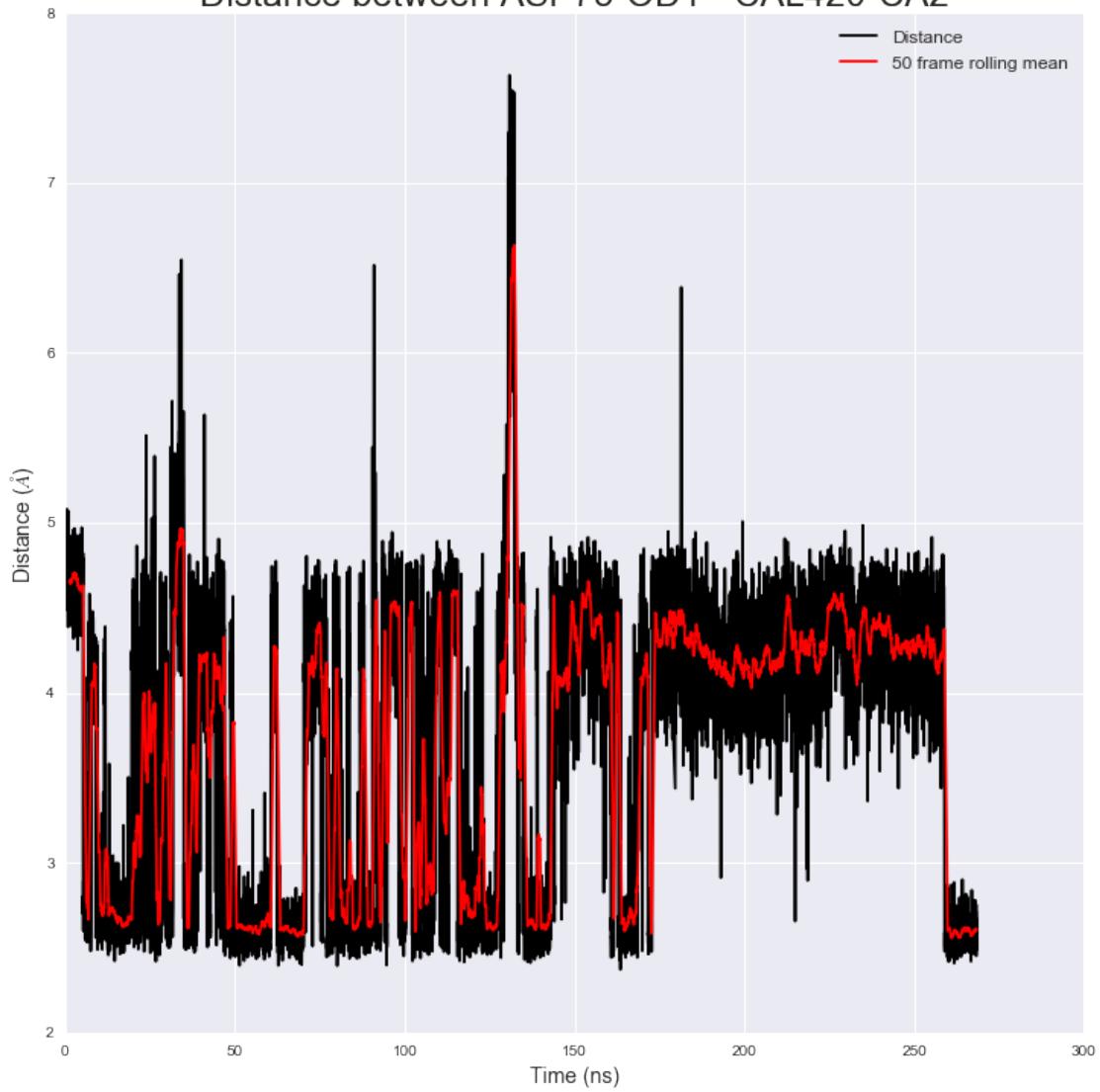
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

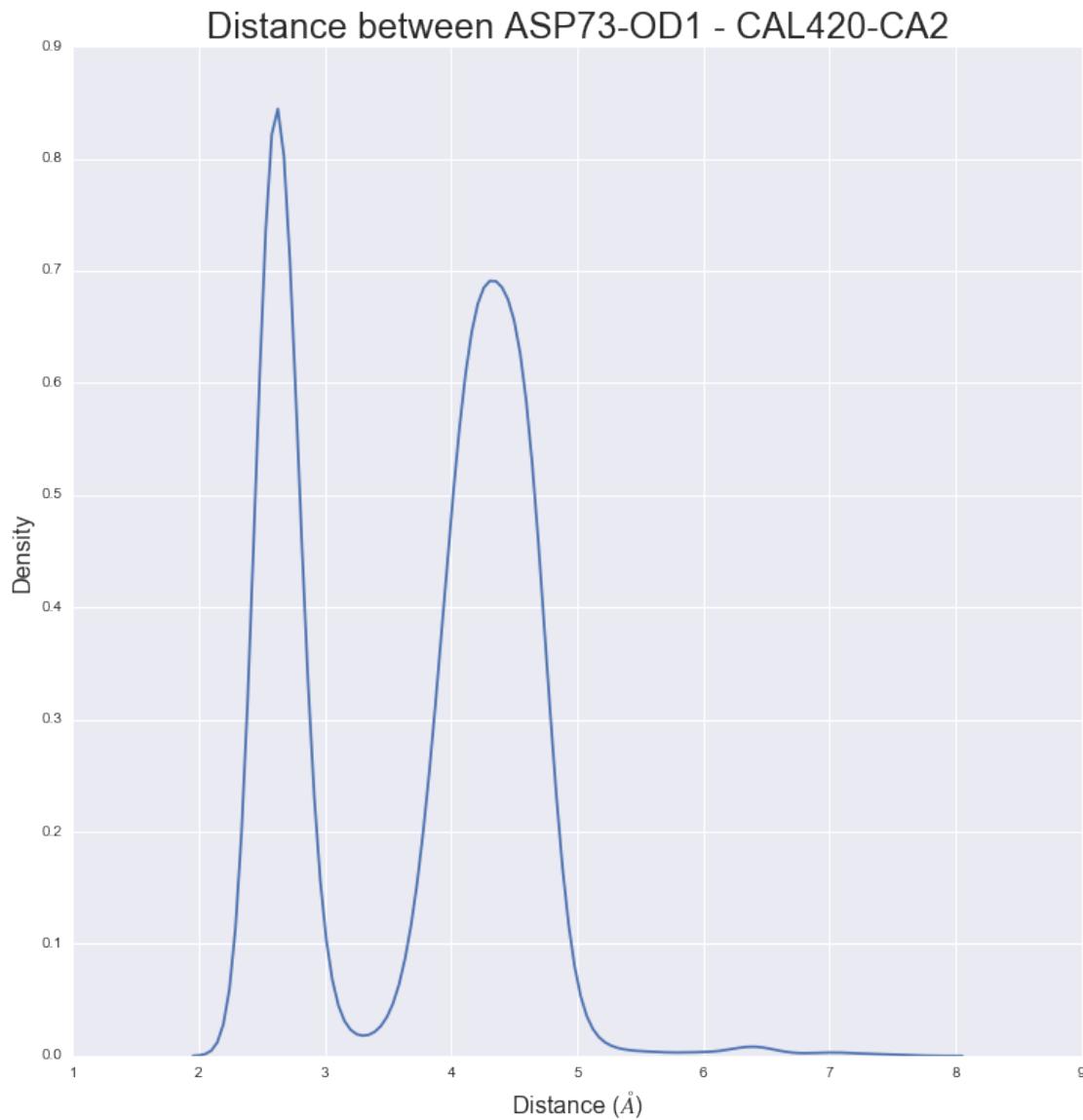
Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc

Distance between ASP73-OD1 - CAL420-CA2





Total execution time: 2.57 seconds

Total simulation time of all frames: 267.98 nanoseconds

The following topology file was successfully loaded:

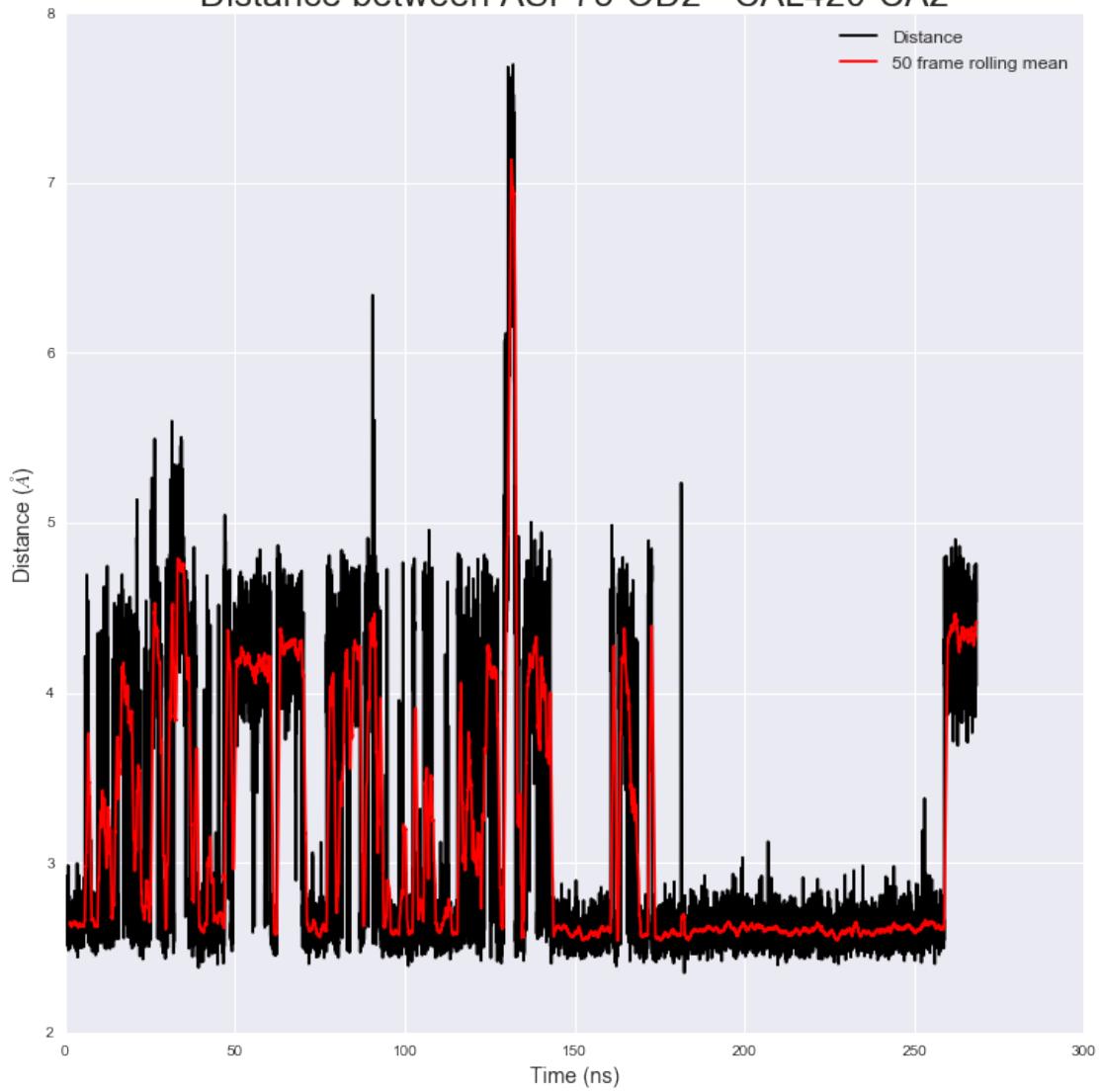
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

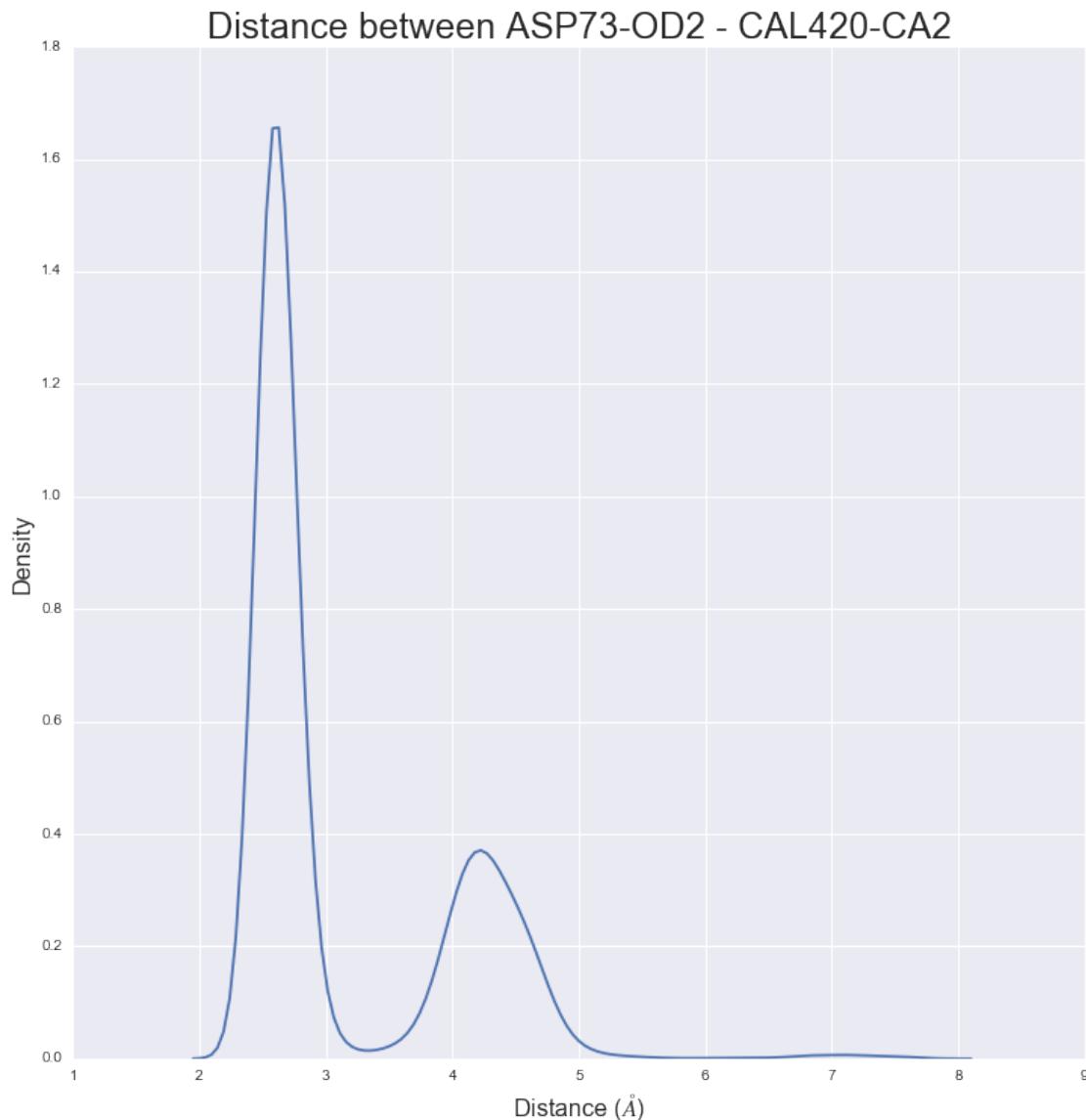
Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc

Distance between ASP73-OD2 - CAL420-CA2





Total execution time: 2.41 seconds

Total simulation time of all frames: 267.98 nanoseconds

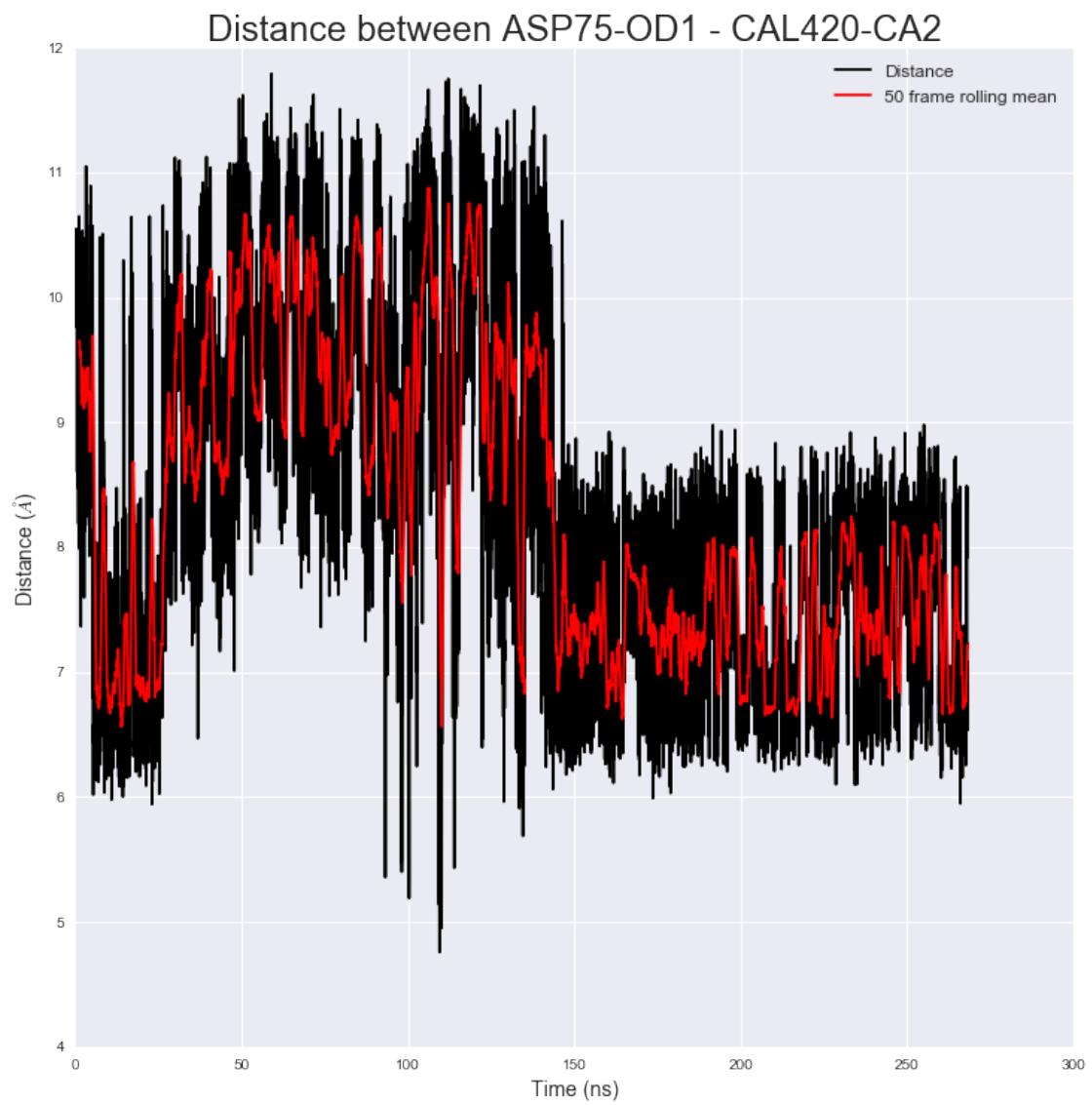
The following topology file was successfully loaded:

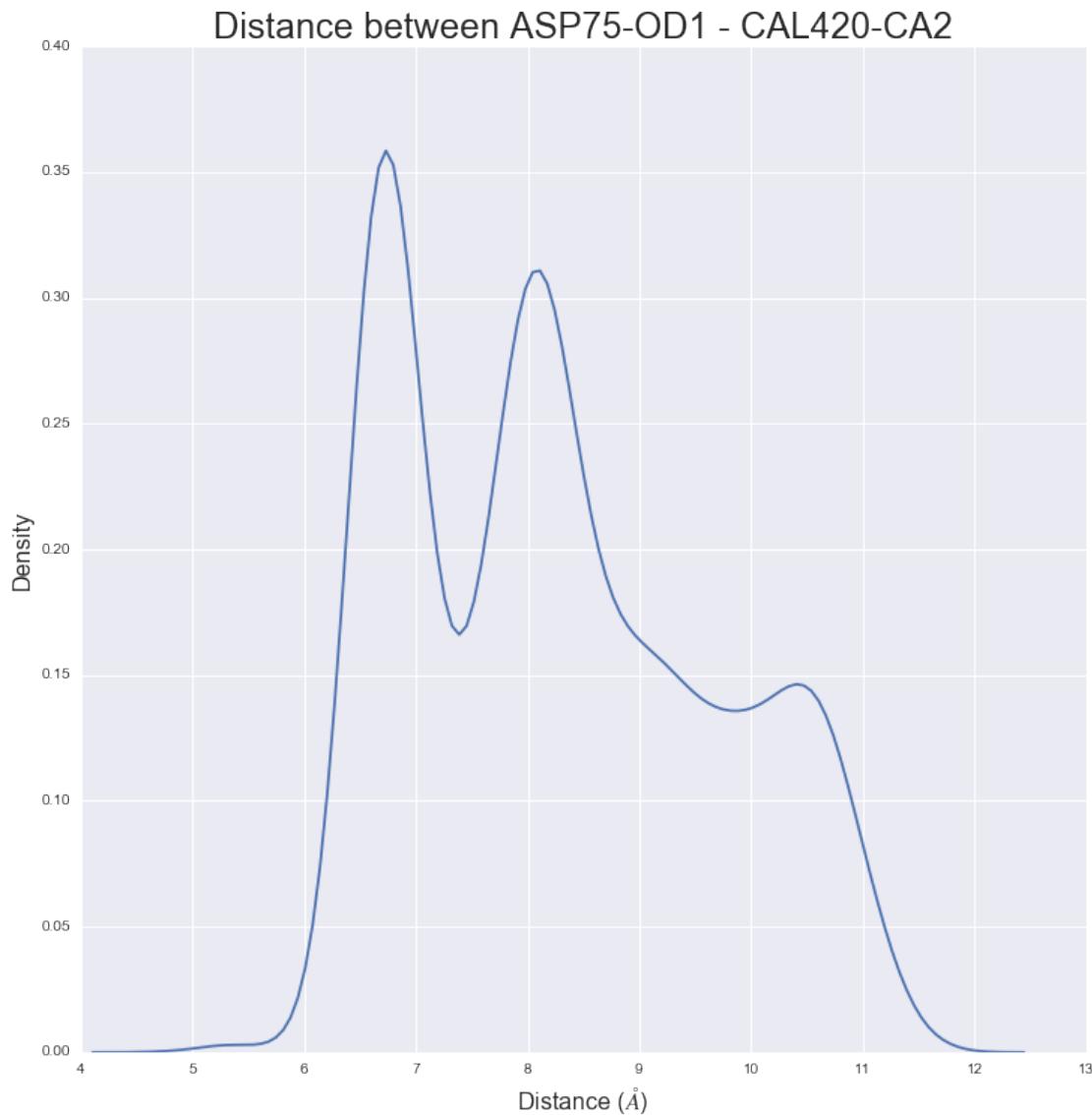
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc





Total execution time: 2.63 seconds

Total simulation time of all frames: 267.98 nanoseconds

The following topology file was successfully loaded:

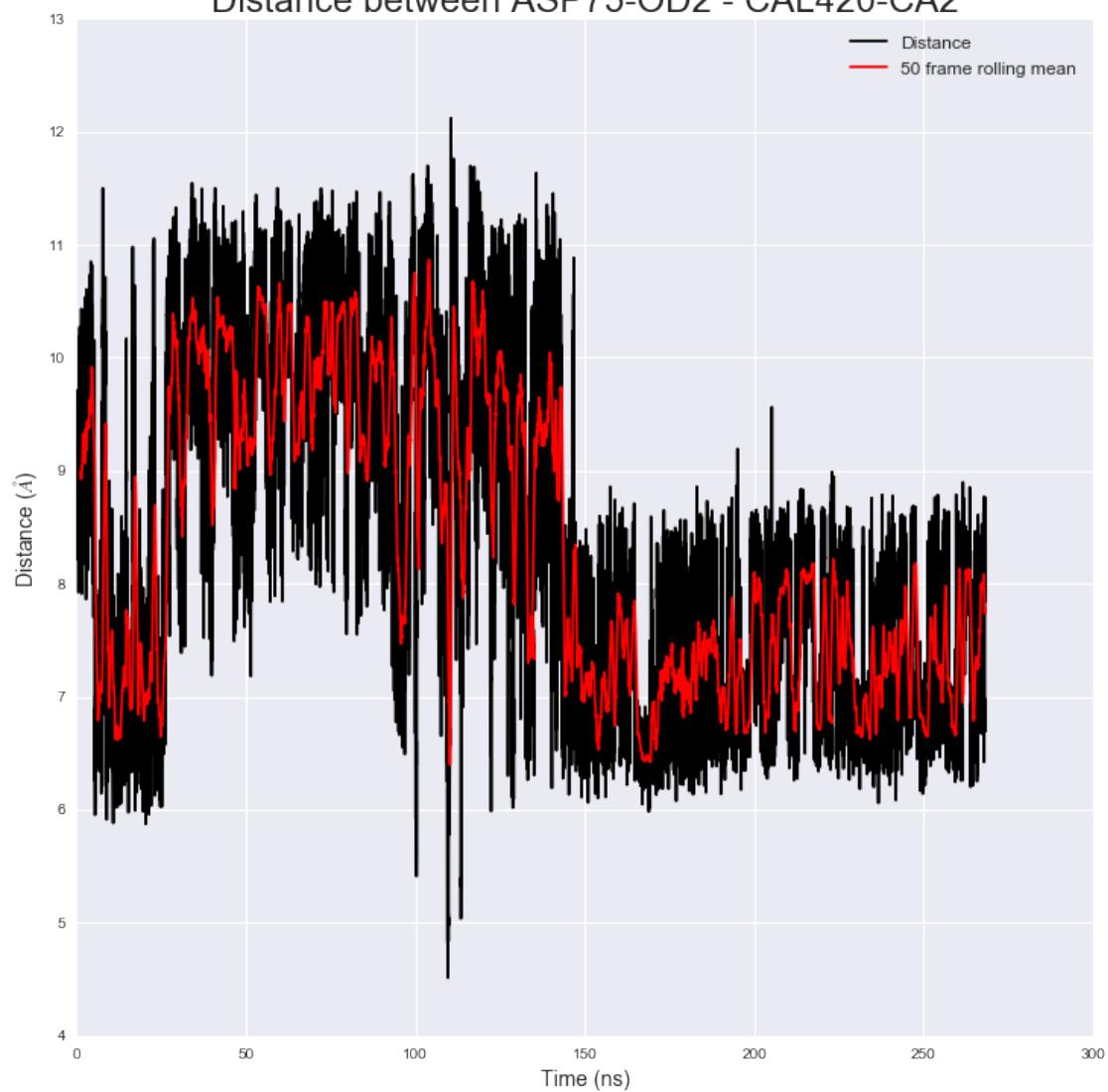
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

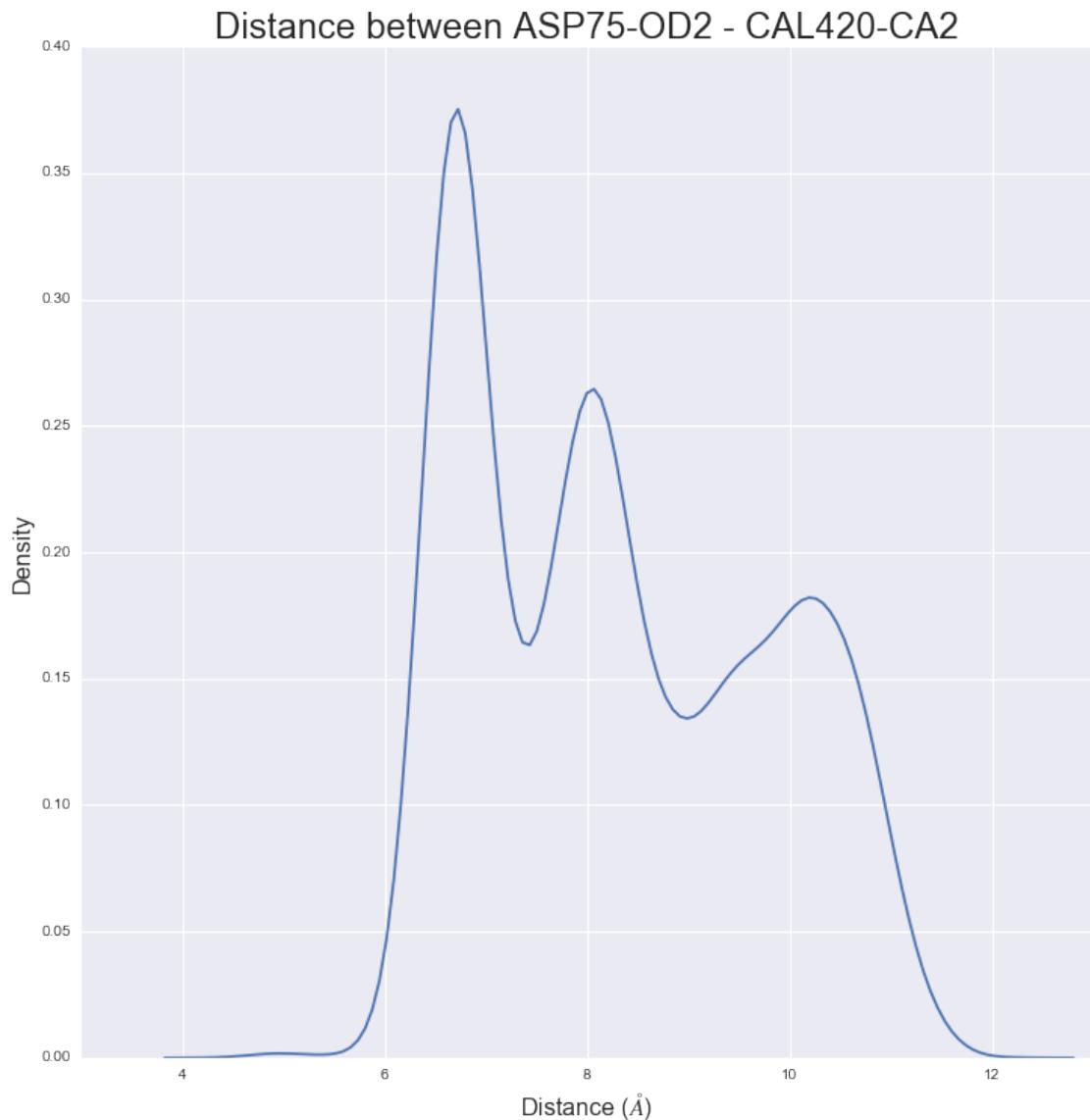
Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc

Distance between ASP75-OD2 - CAL420-CA2





Total execution time: 2.60 seconds

Total simulation time of all frames: 267.98 nanoseconds

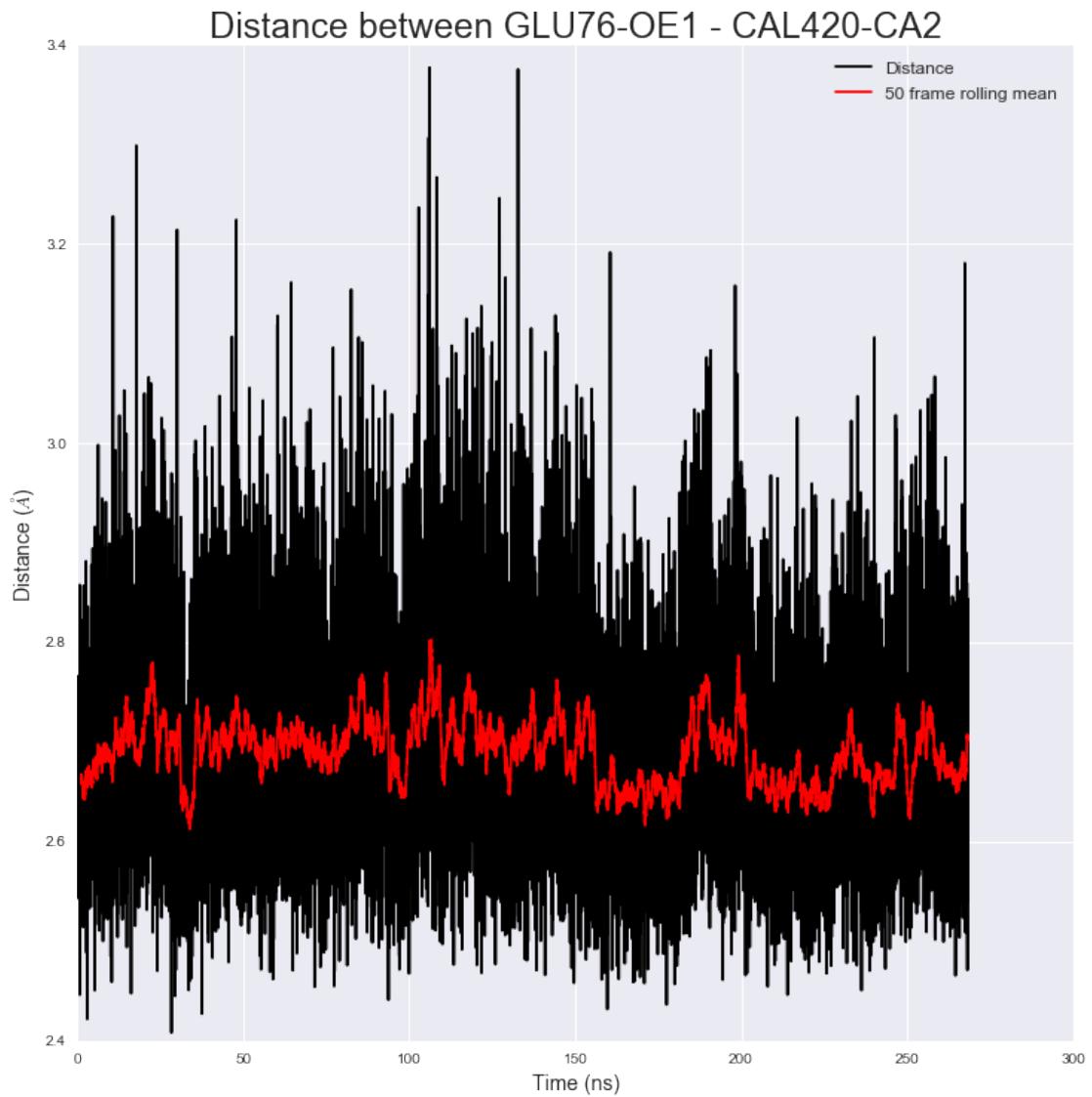
The following topology file was successfully loaded:

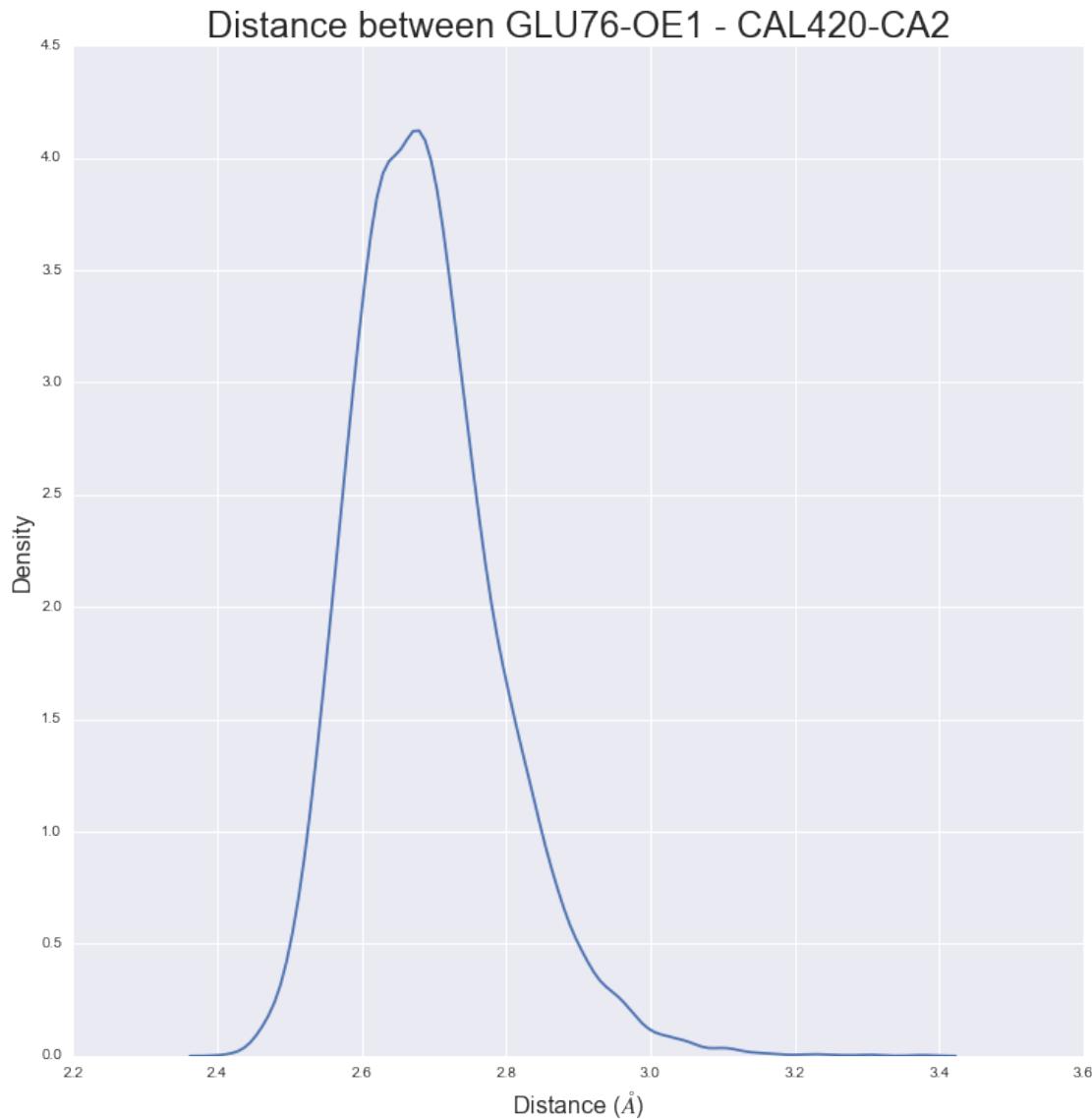
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc





Total execution time: 3.20 seconds

Total simulation time of all frames: 267.98 nanoseconds

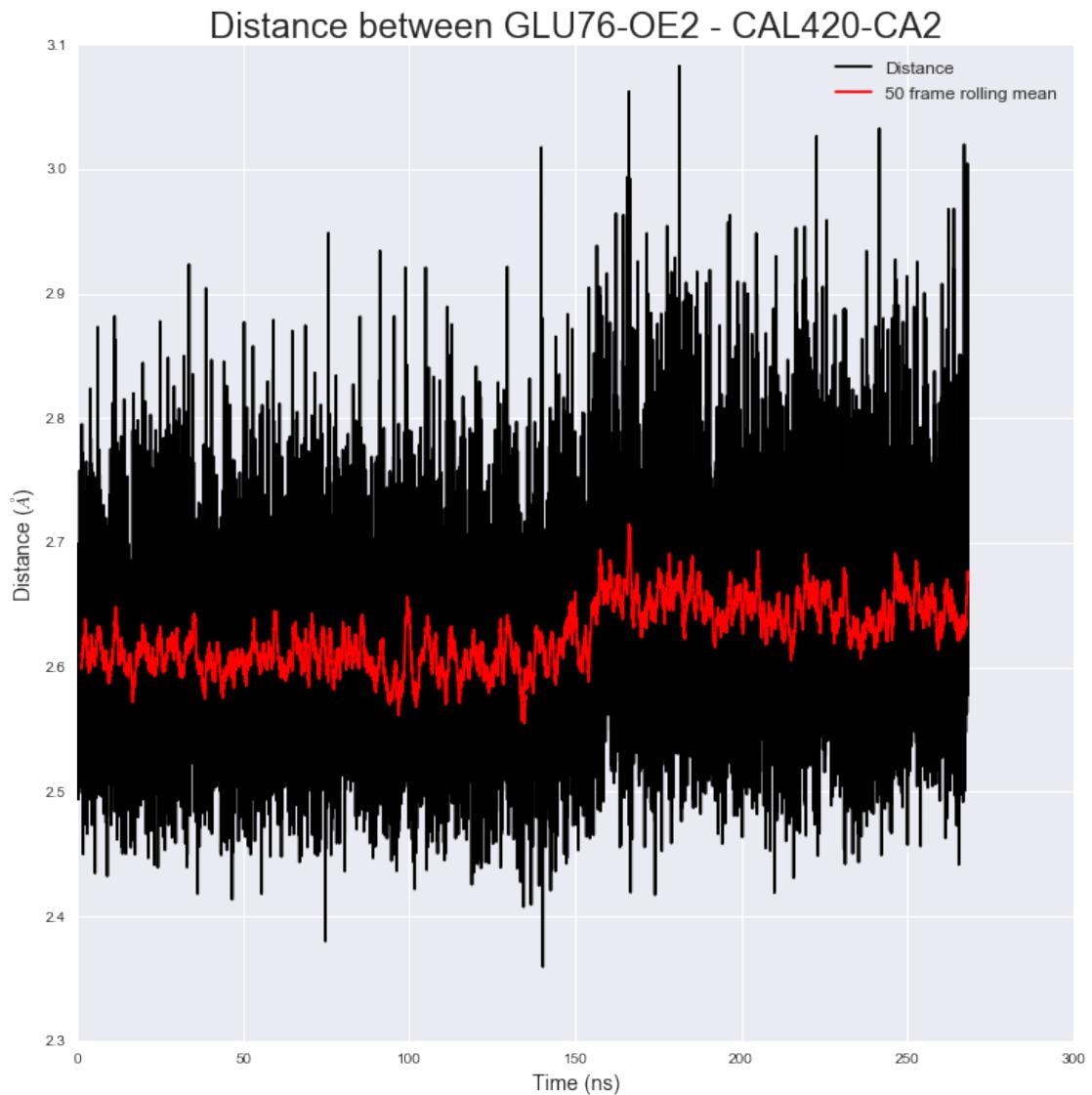
The following topology file was successfully loaded:

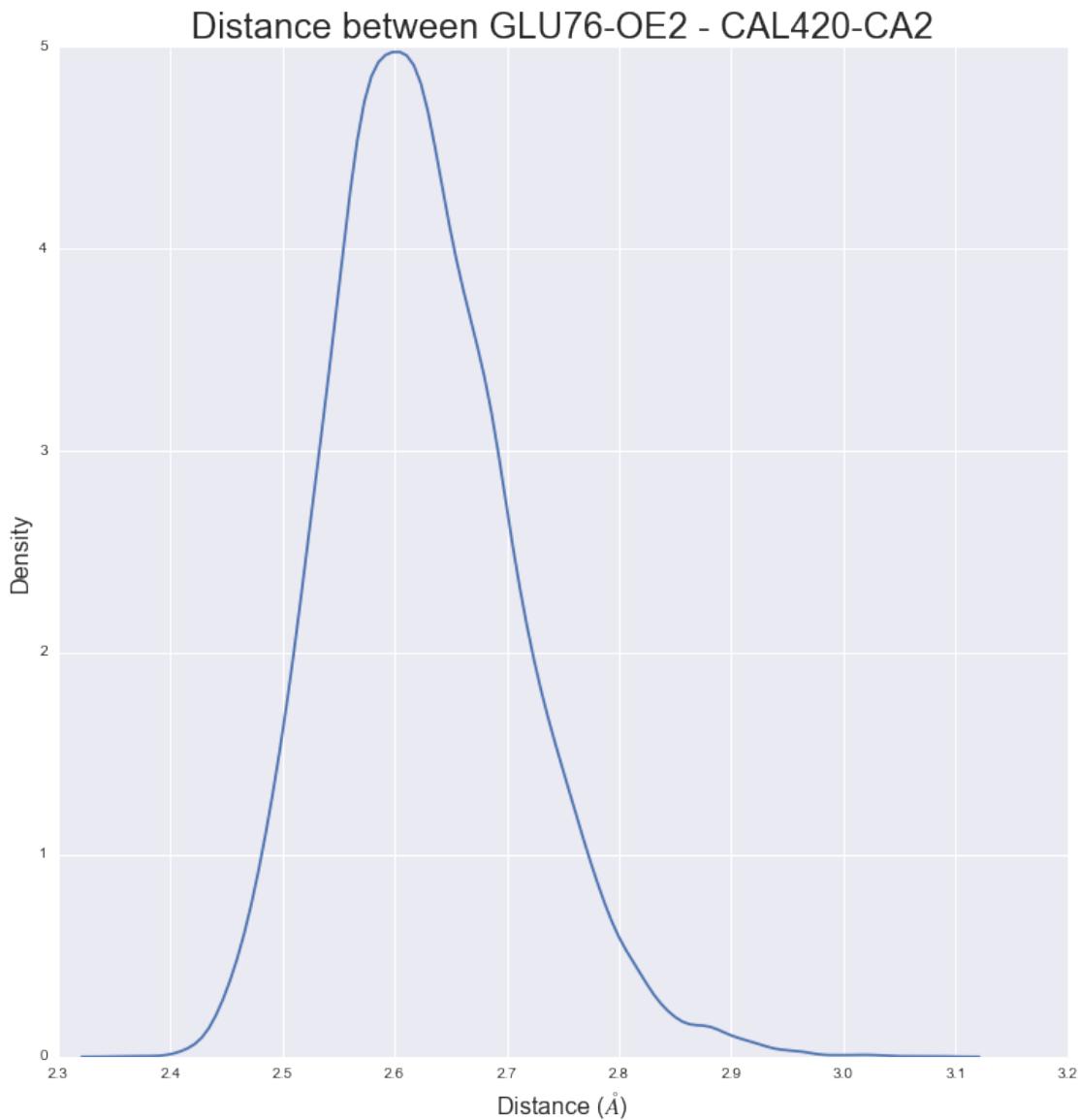
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD2_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD2_250-300_run2_nowater.nc





Total execution time: 2.82 seconds

Total simulation time of all frames: 267.98 nanoseconds

0.3 MD3

```
In [19]: topology_MD3 = '/Users/gil_f.hoben/Troponin_md_processed/MD3/run2/troponin_egcg_MD3_nowater.pr
trajectory_MD3 = '/Users/gil_f.hoben/Troponin_md_processed/MD3/run2/Trajectories/'
for atom1 in atom1_list:
    main(topology_MD3, trajectory_MD3, atom1, atom2, verbose = 1)
```

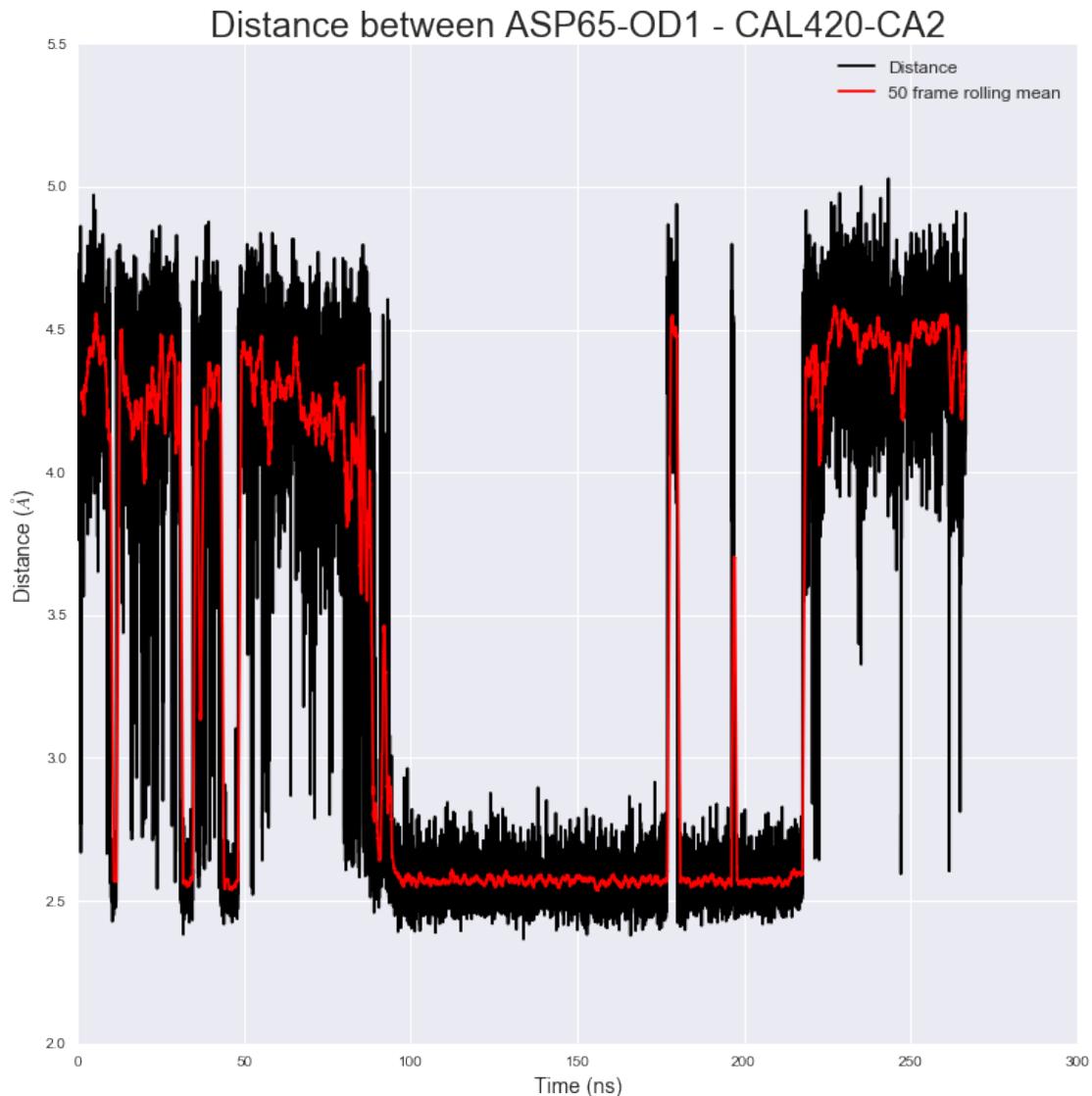
The following topology file was successfully loaded:

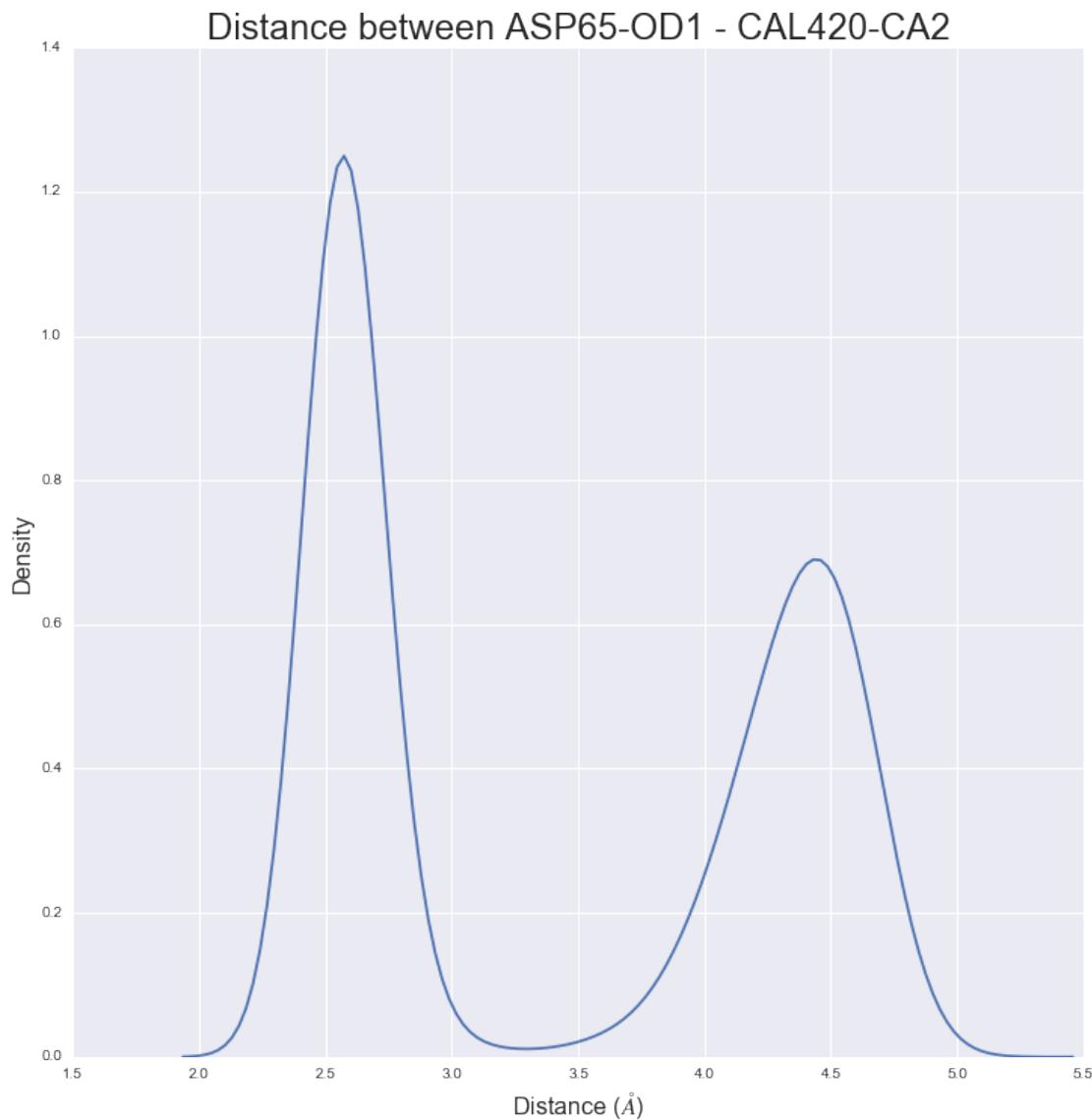
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc





Total execution time: 4.94 seconds

Total simulation time of all frames: 266.34 nanoseconds

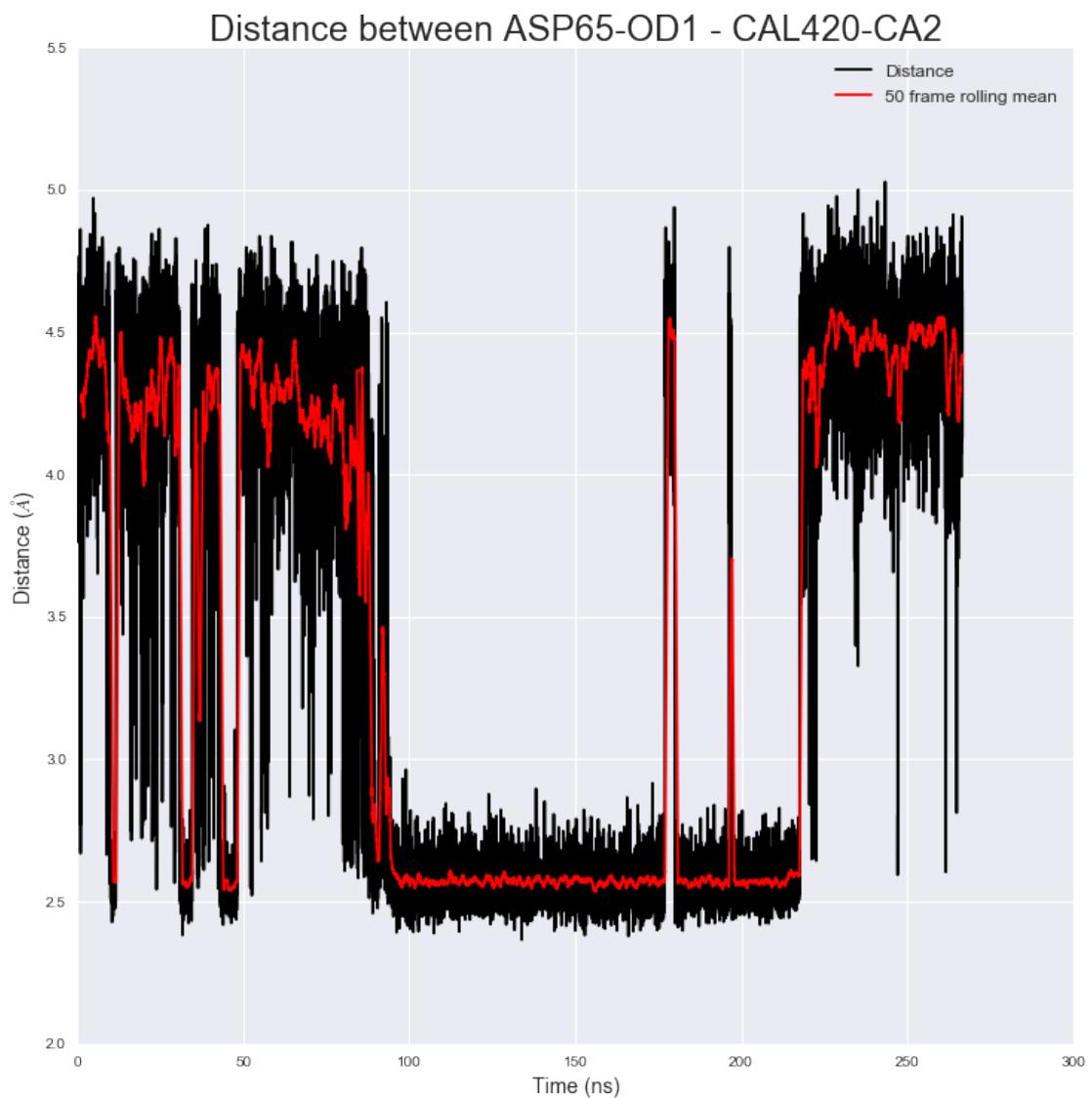
The following topology file was successfully loaded:

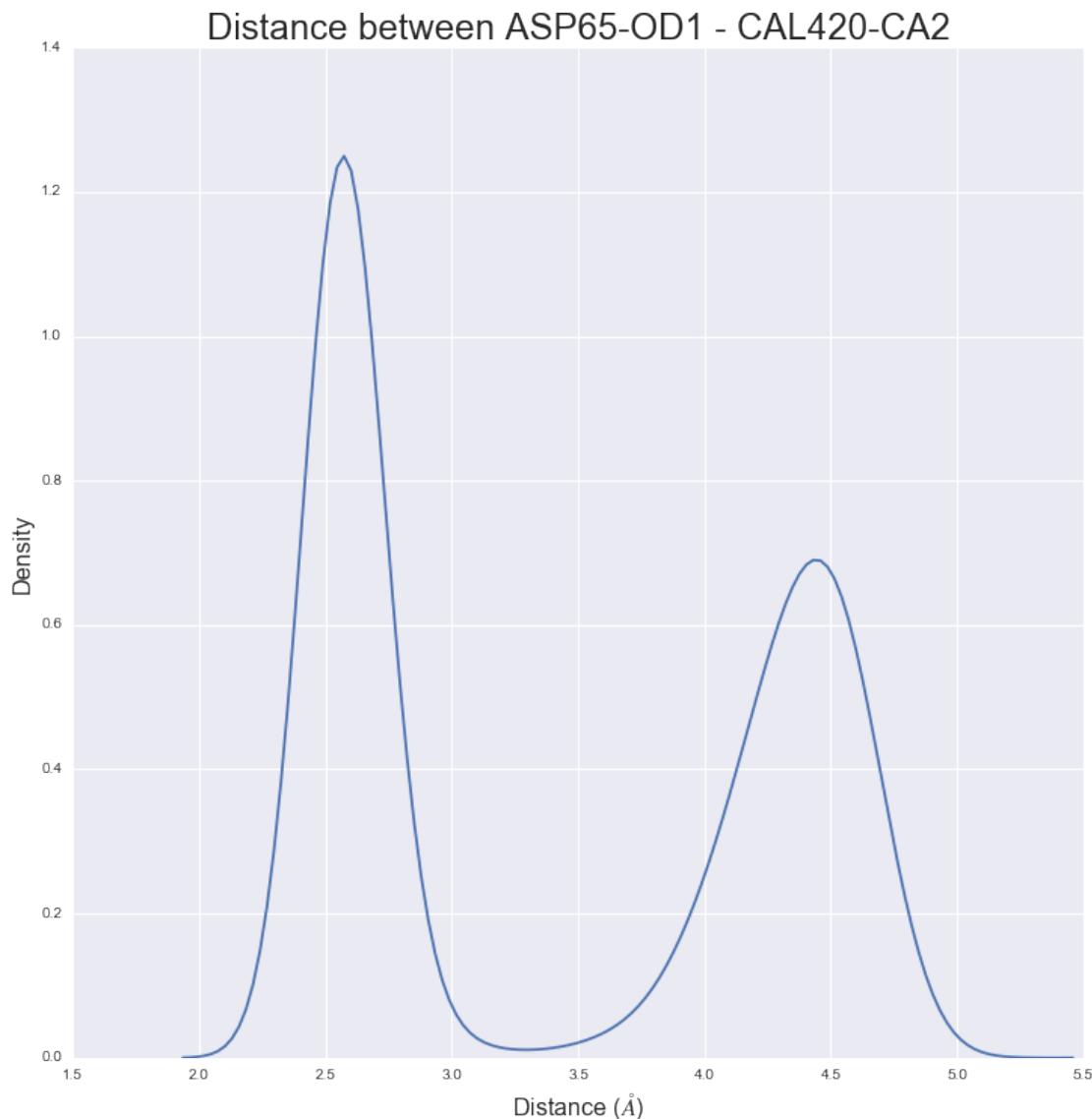
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc





Total execution time: 2.56 seconds

Total simulation time of all frames: 266.34 nanoseconds

The following topology file was successfully loaded:

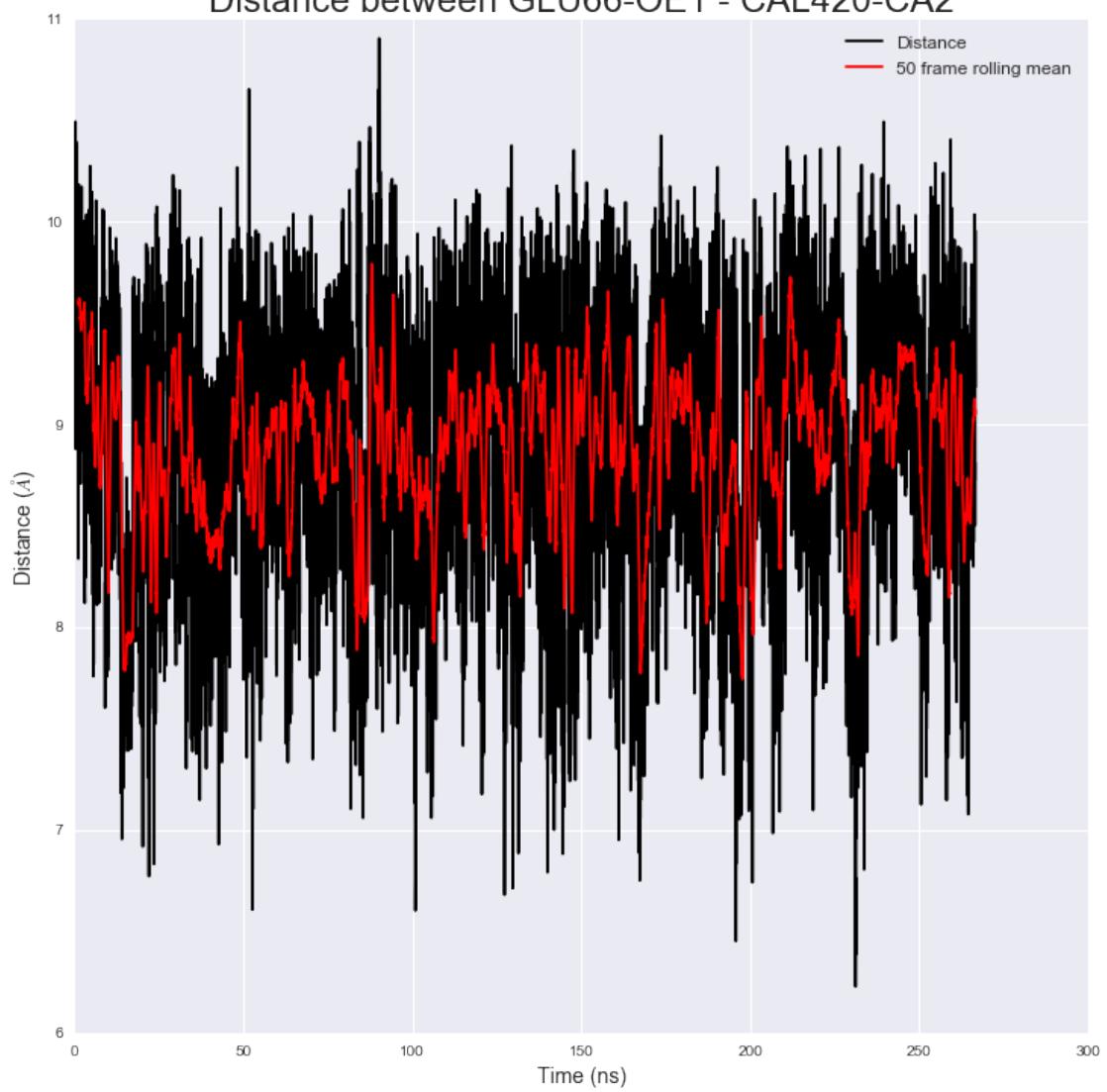
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

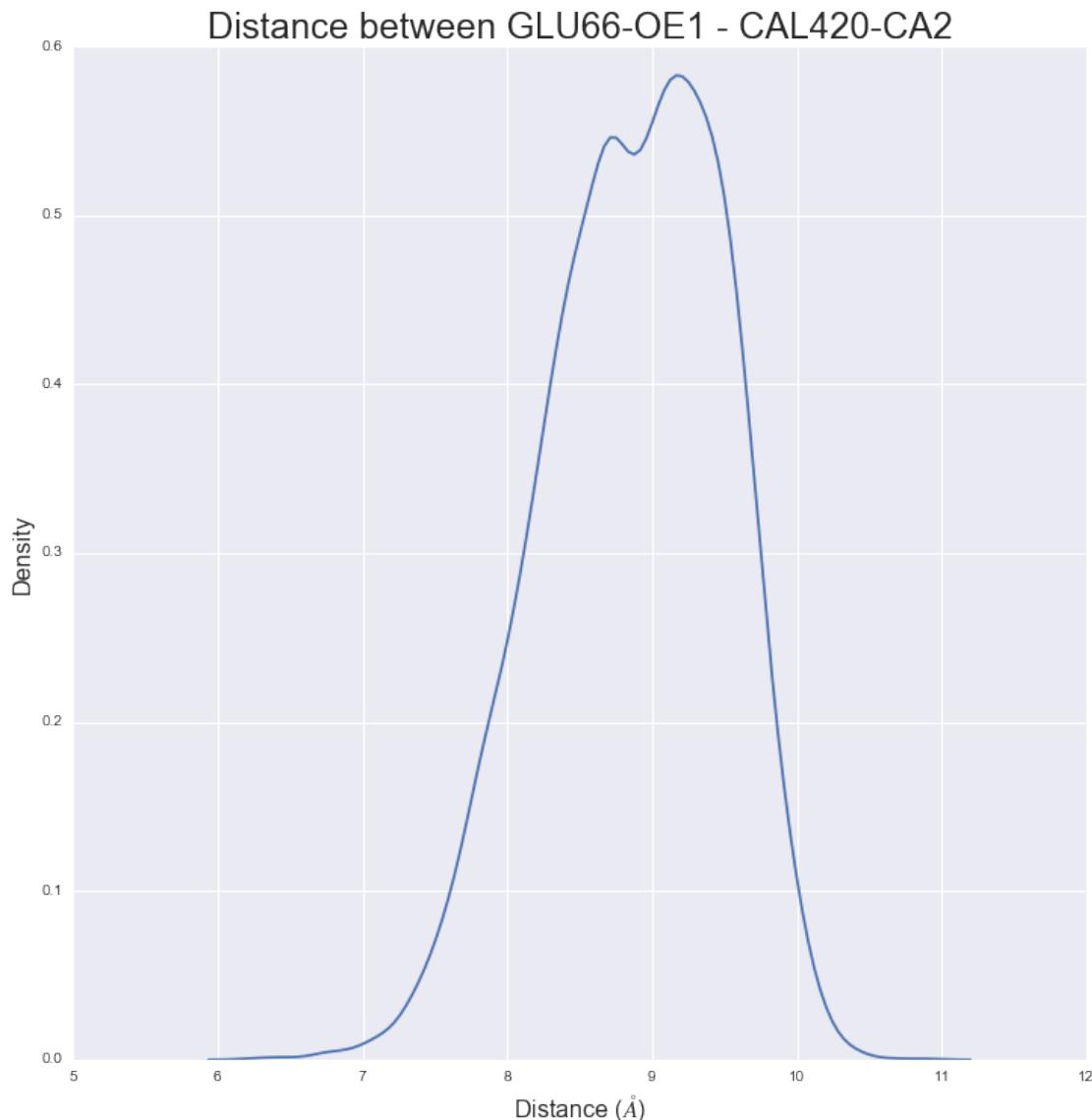
Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc

Distance between GLU66-OE1 - CAL420-CA2





Total execution time: 2.51 seconds

Total simulation time of all frames: 266.34 nanoseconds

The following topology file was successfully loaded:

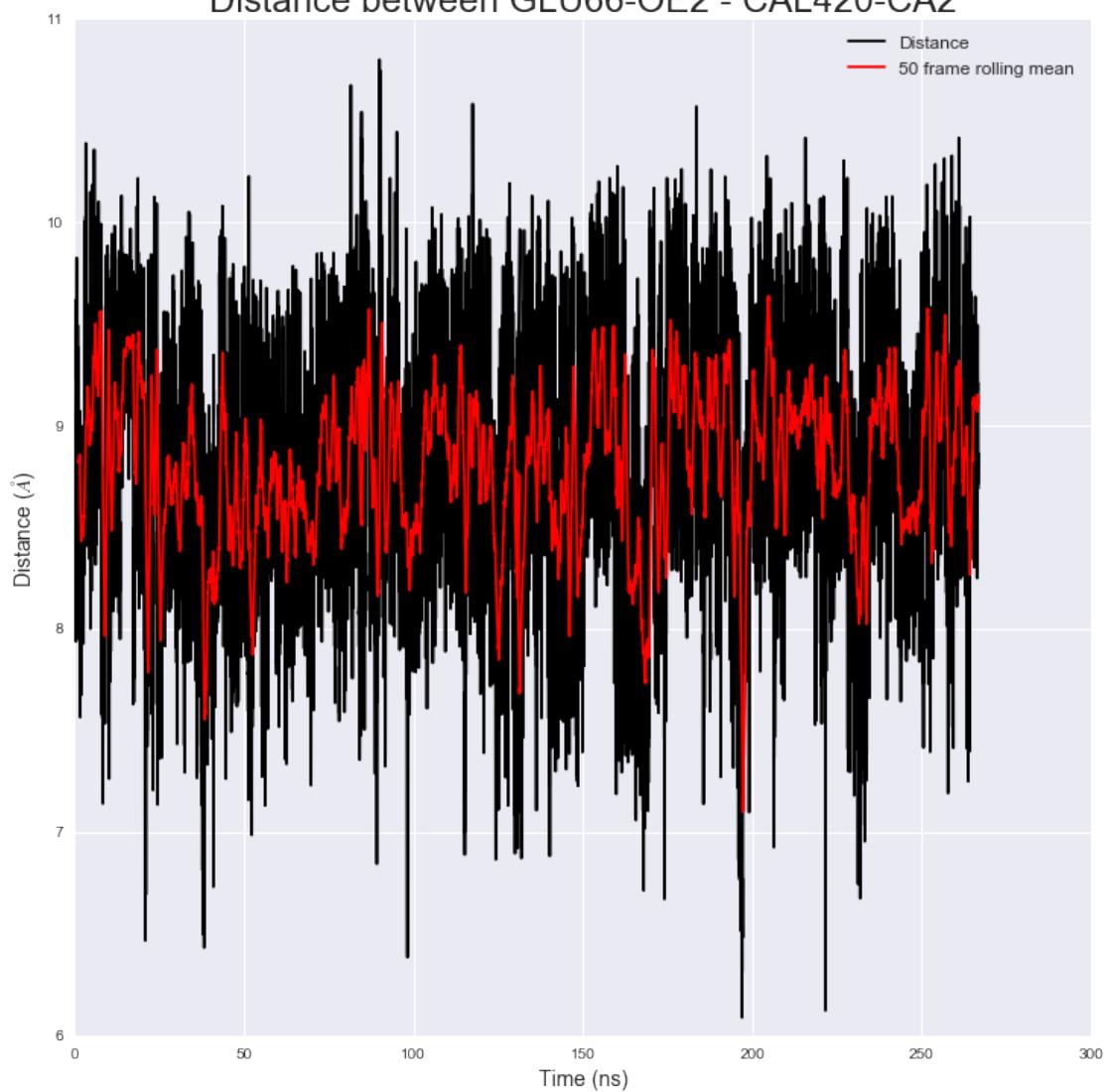
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

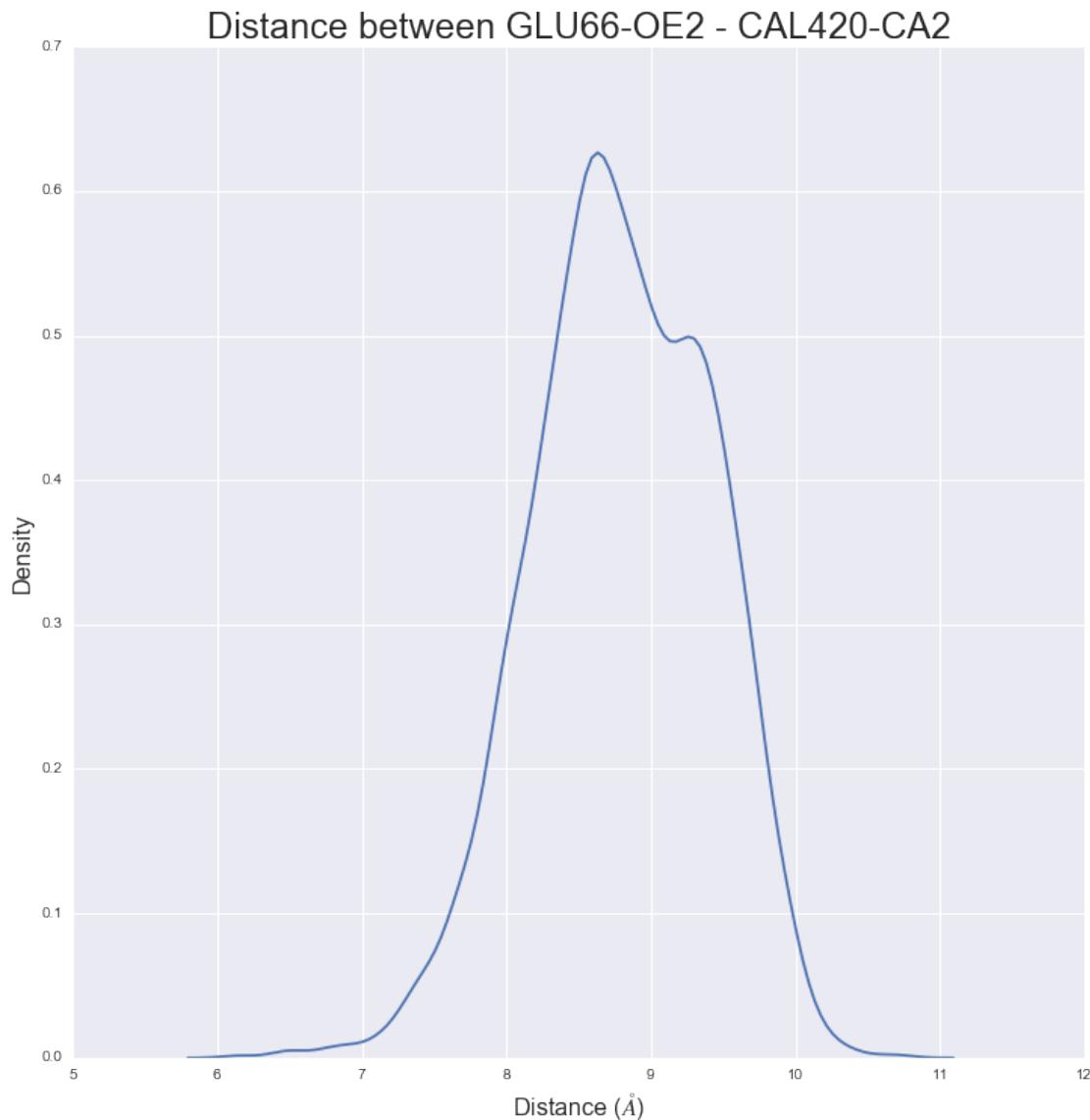
Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc

Distance between GLU66-OE2 - CAL420-CA2





Total execution time: 2.48 seconds

Total simulation time of all frames: 266.34 nanoseconds

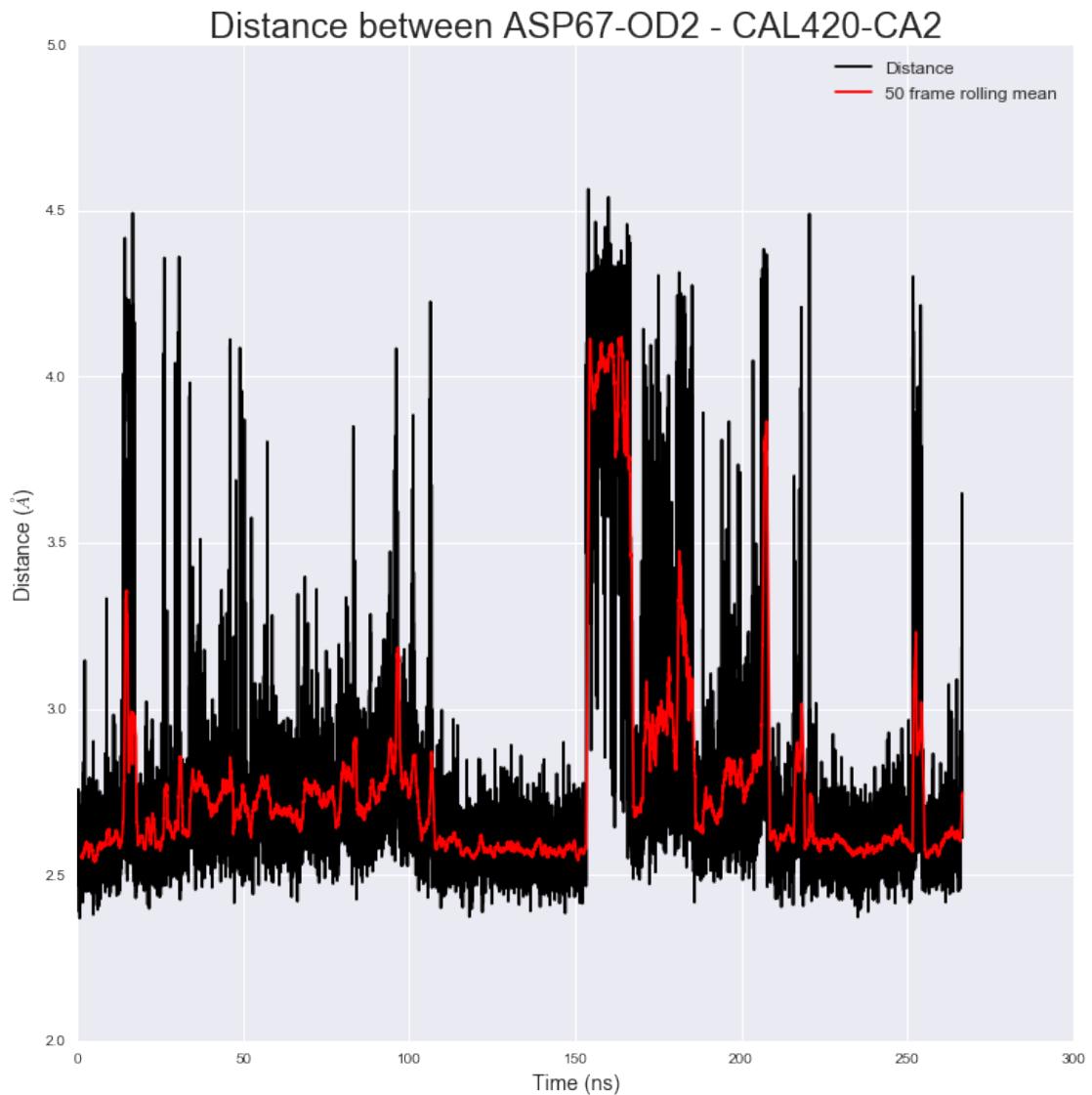
The following topology file was successfully loaded:

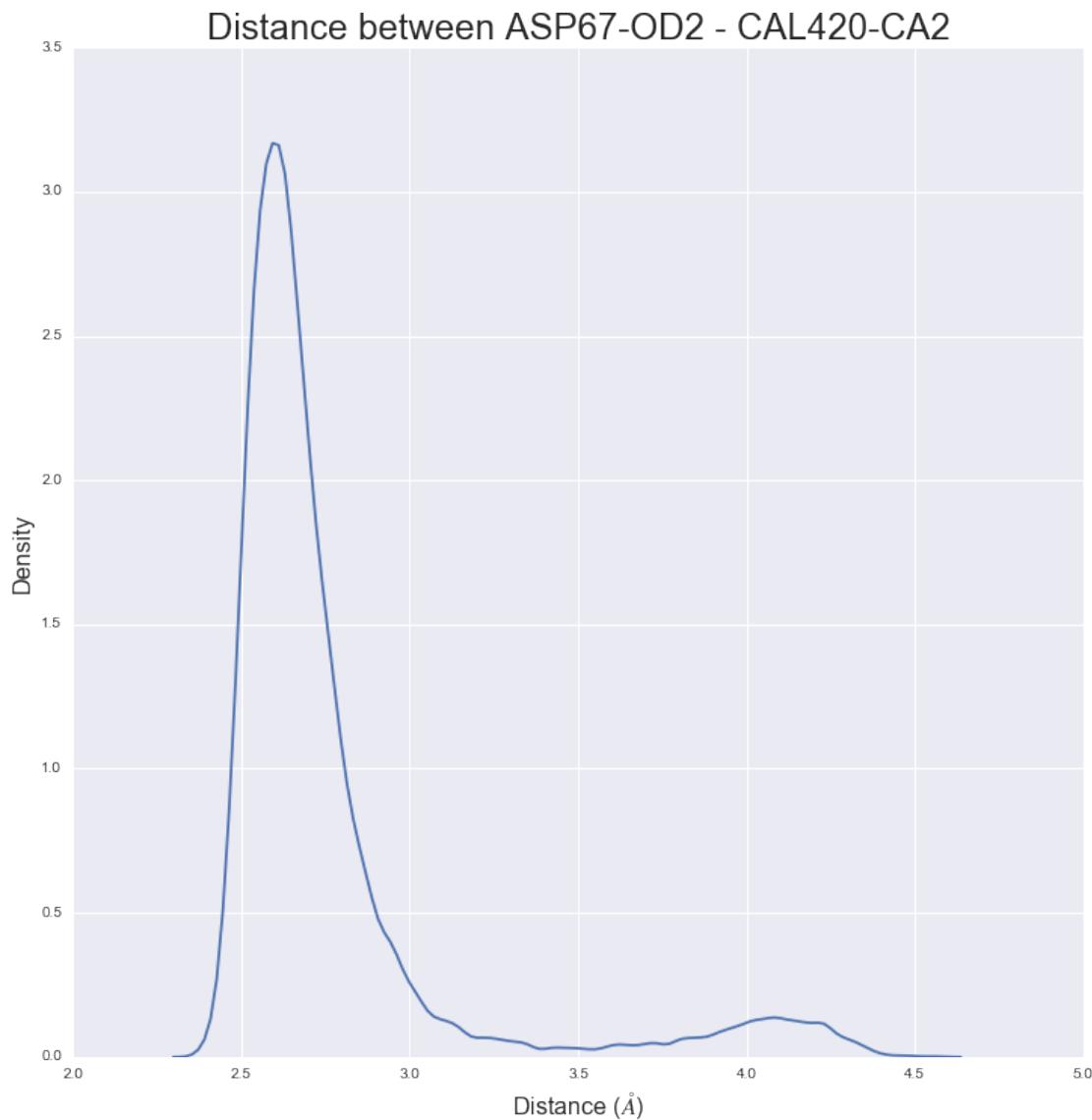
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc





Total execution time: 2.37 seconds

Total simulation time of all frames: 266.34 nanoseconds

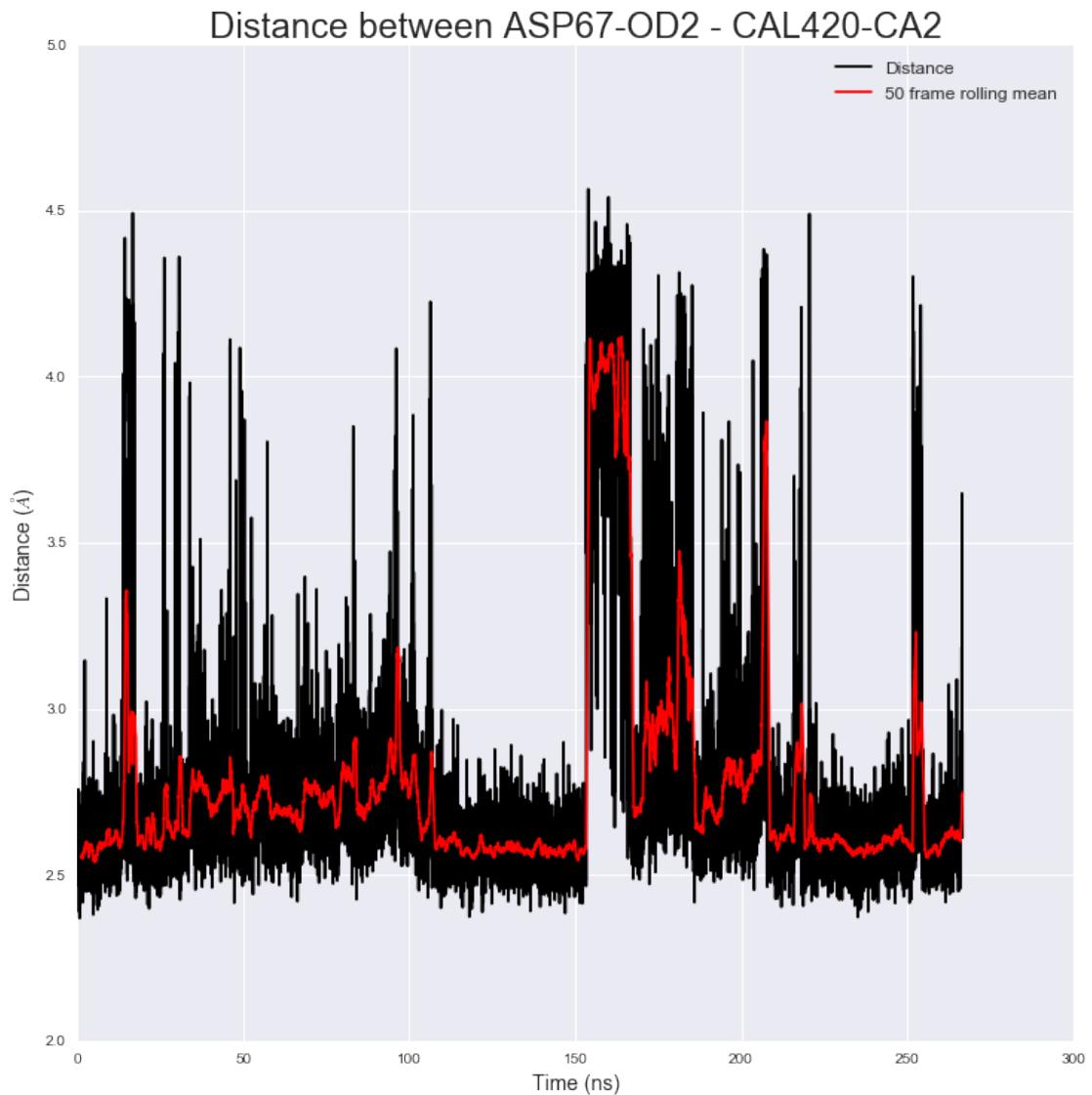
The following topology file was successfully loaded:

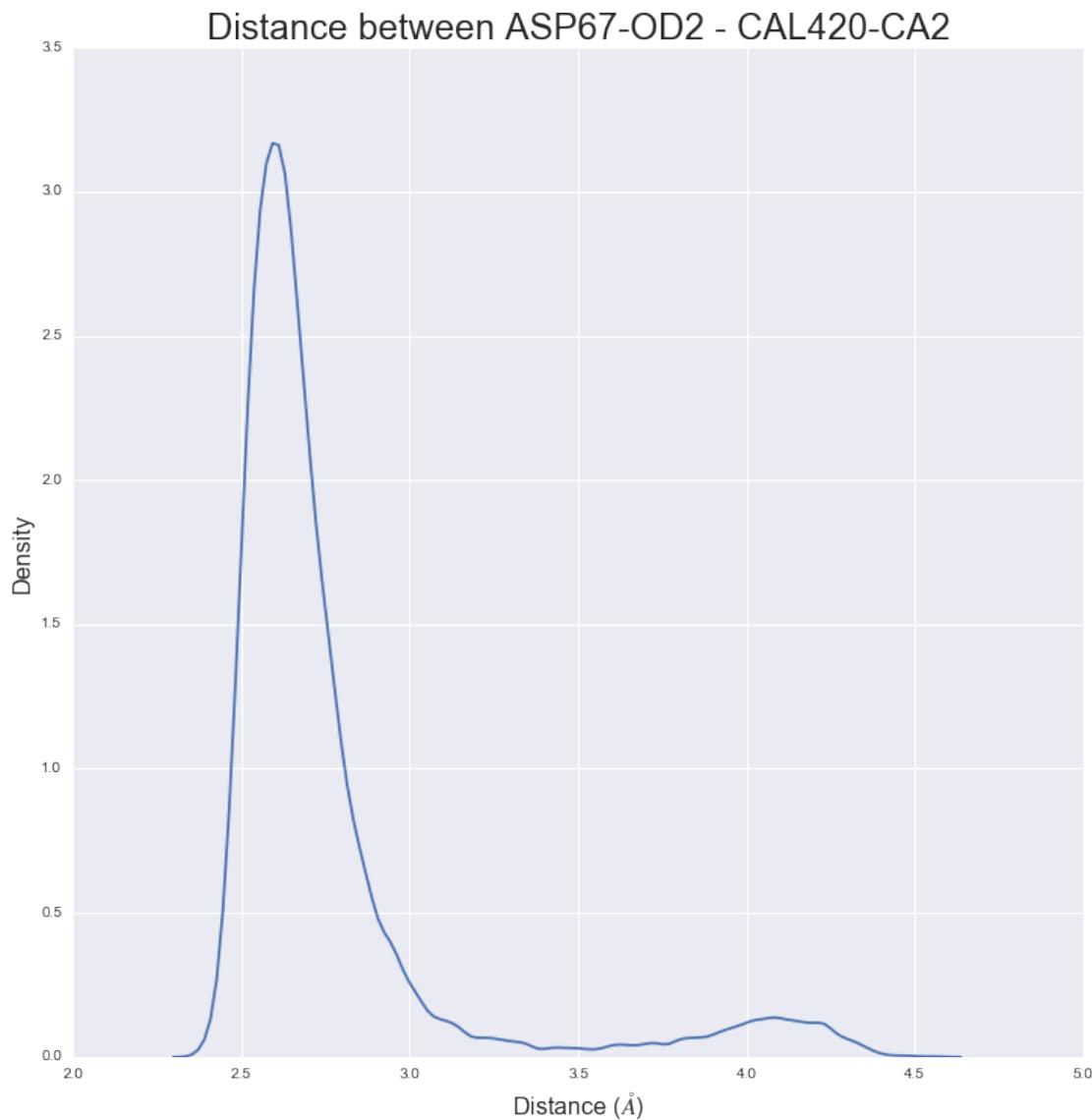
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc





Total execution time: 2.39 seconds

Total simulation time of all frames: 266.34 nanoseconds

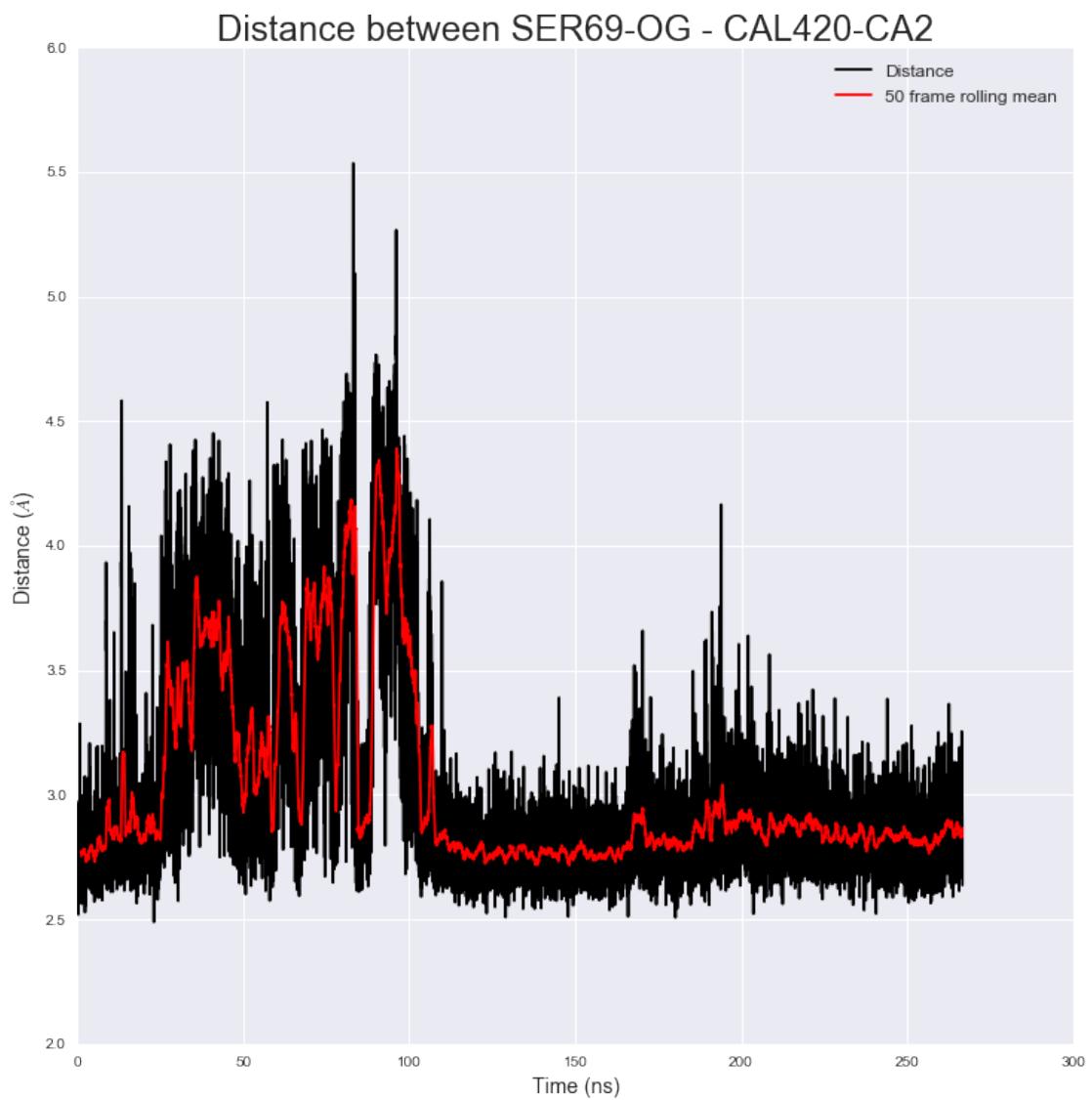
The following topology file was successfully loaded:

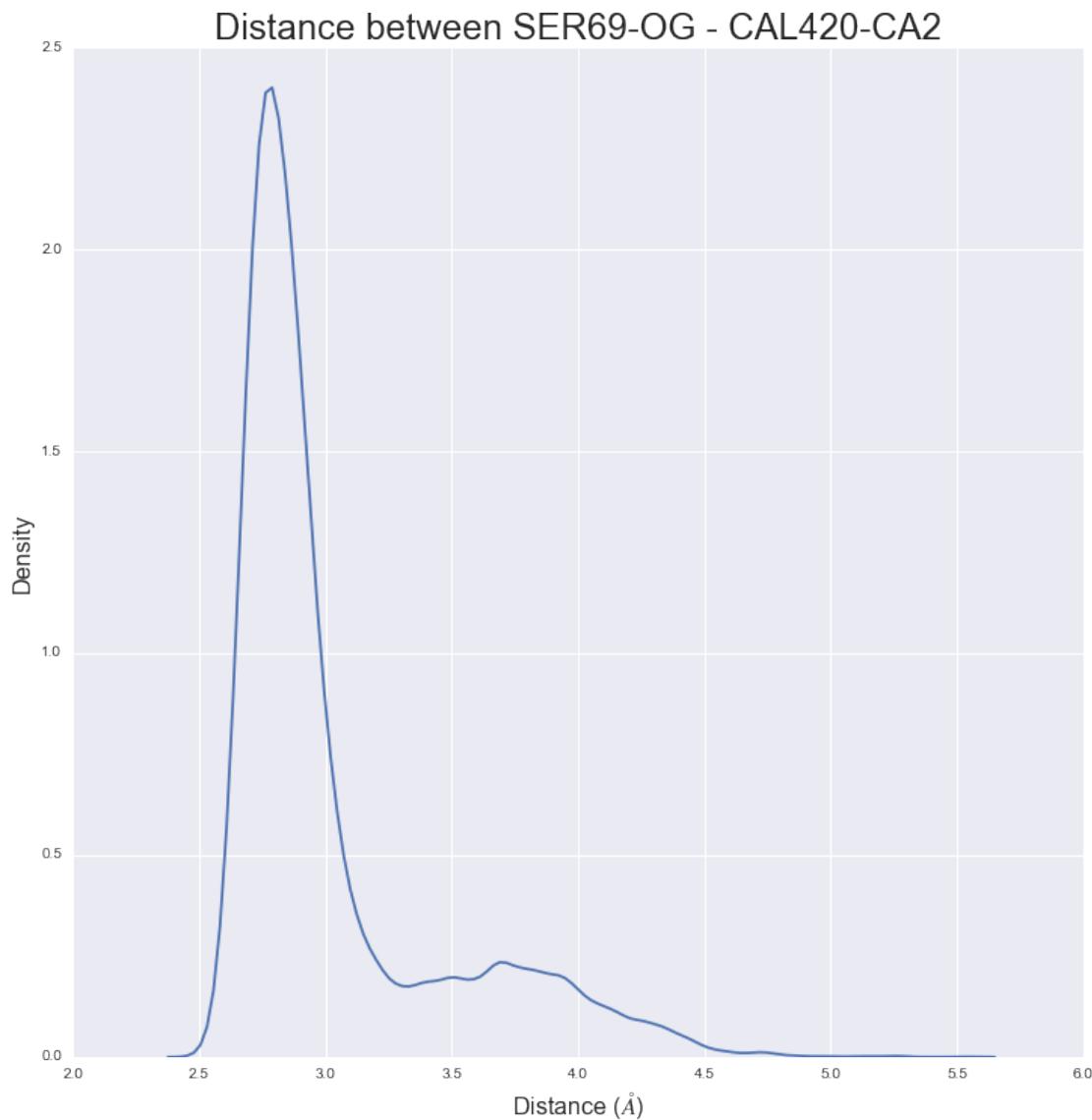
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: SER69-OG - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc





Total execution time: 2.39 seconds

Total simulation time of all frames: 266.34 nanoseconds

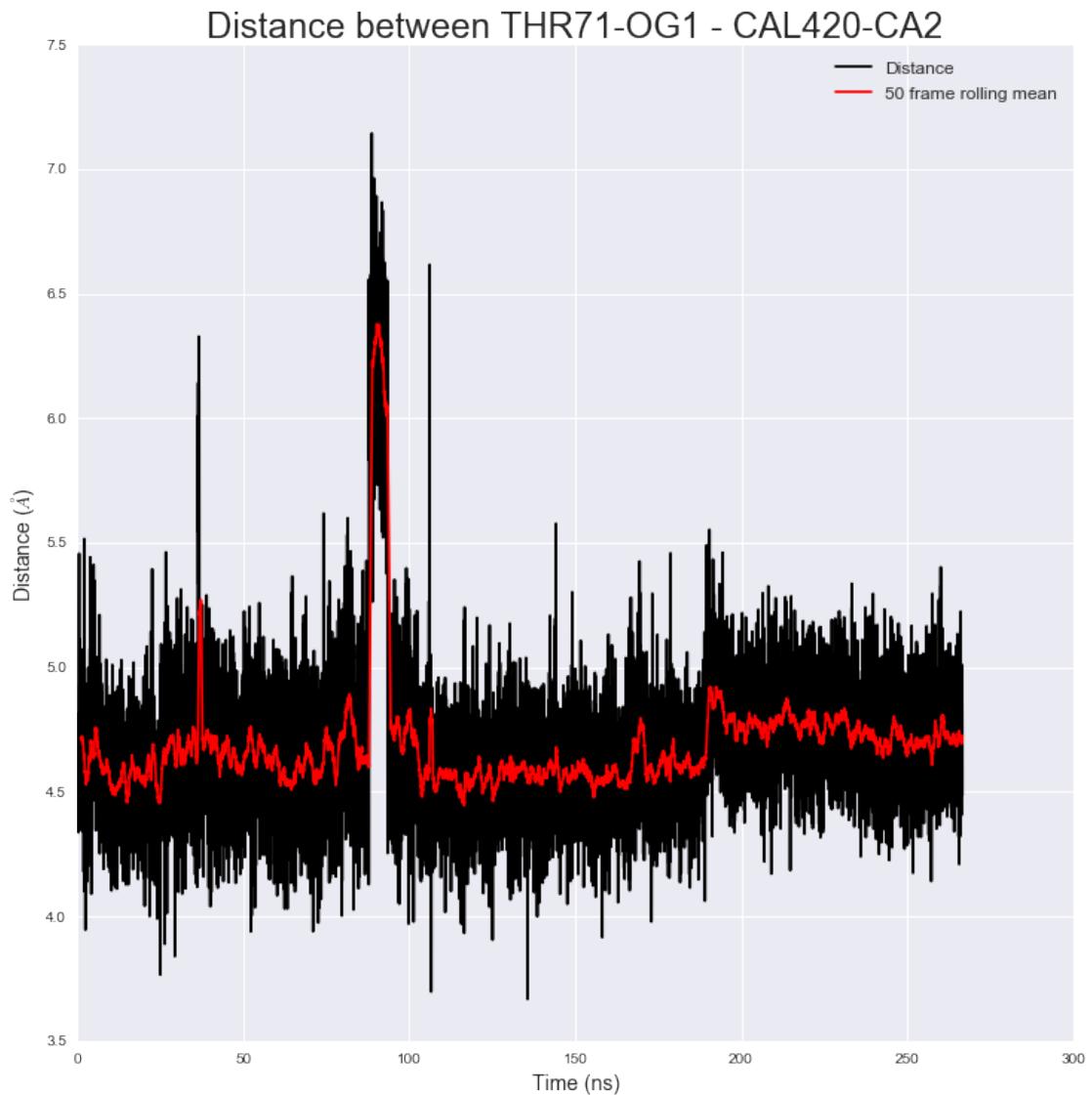
The following topology file was successfully loaded:

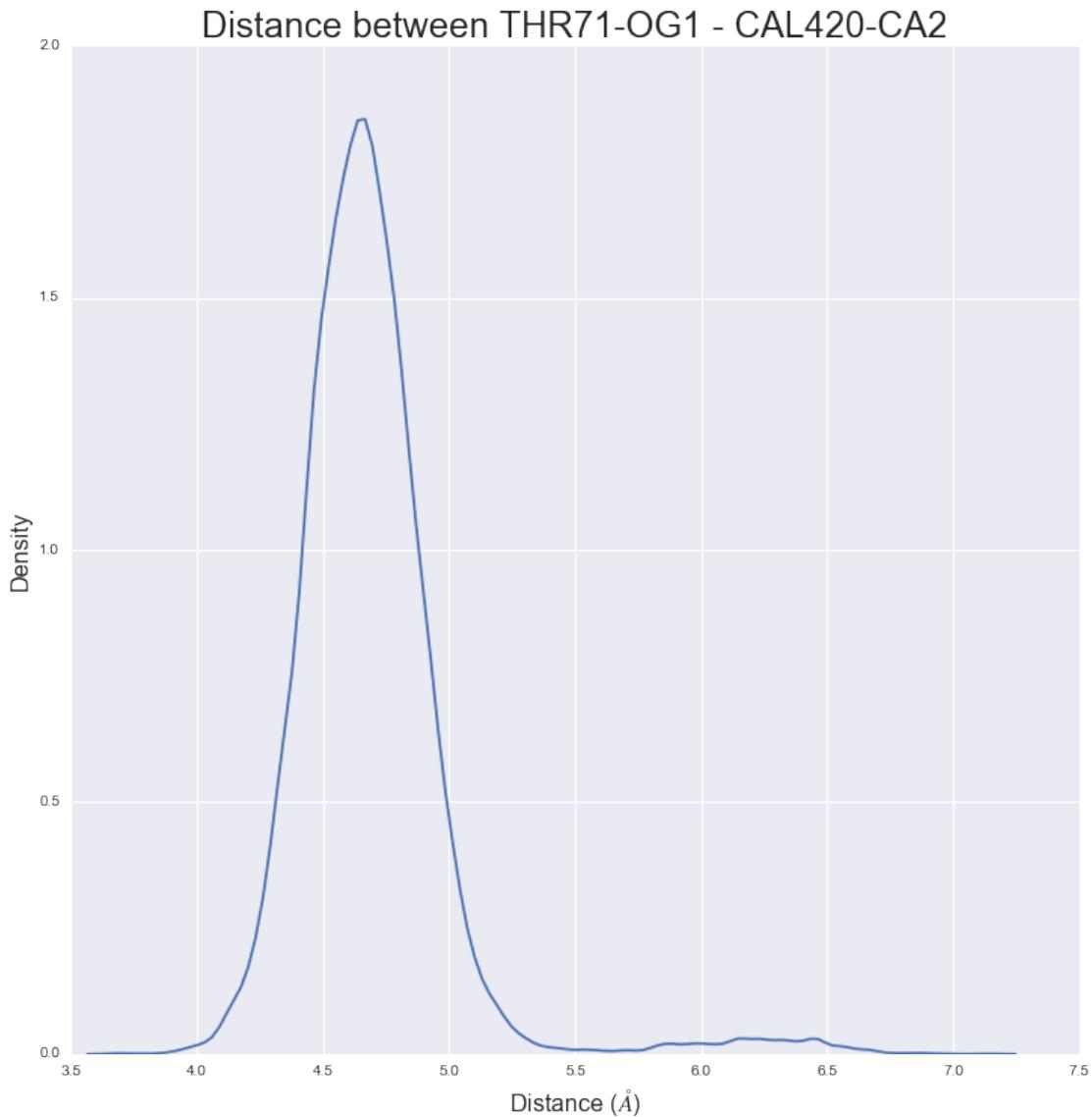
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc





Total execution time: 2.41 seconds

Total simulation time of all frames: 266.34 nanoseconds

The following topology file was successfully loaded:

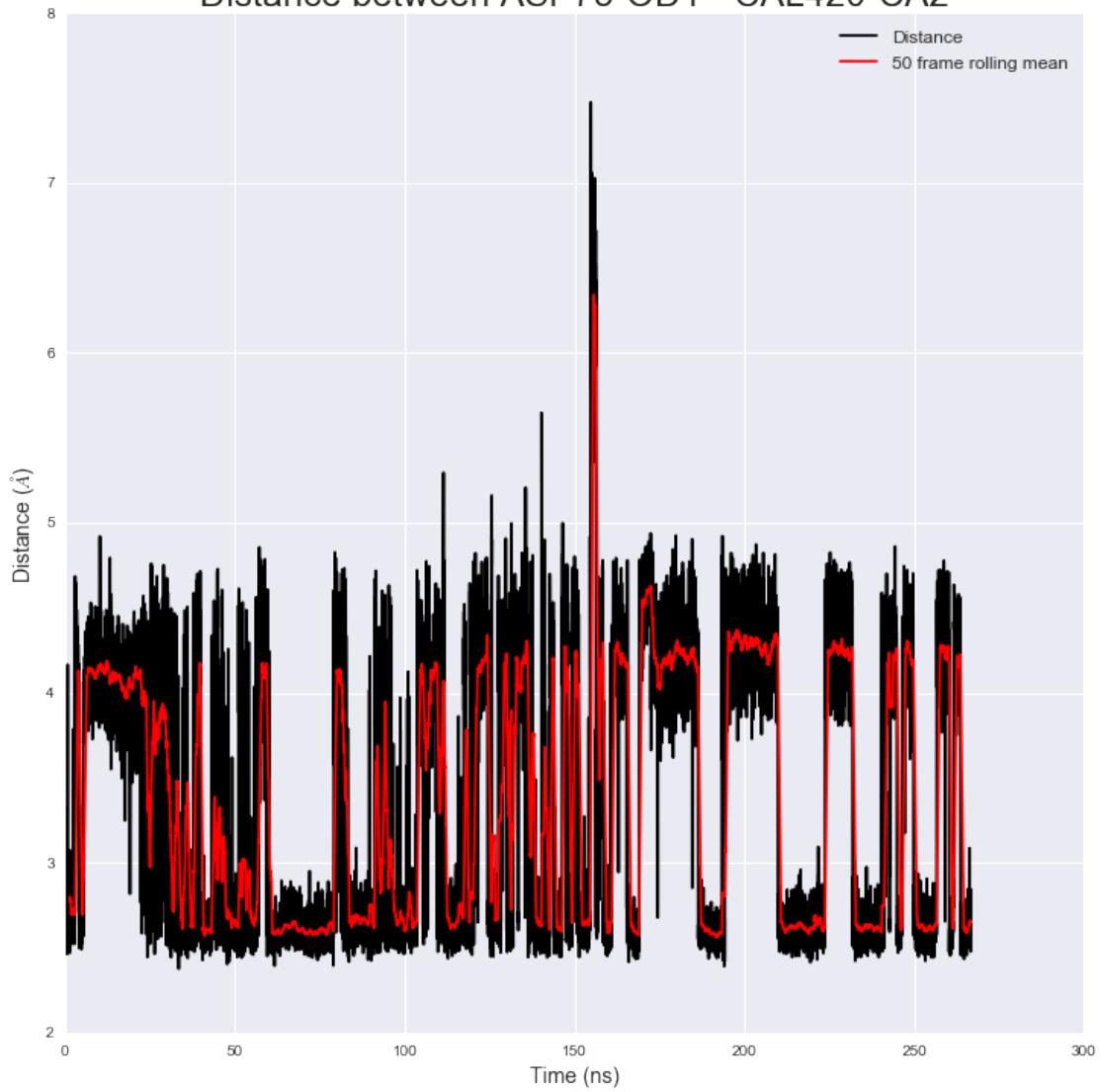
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

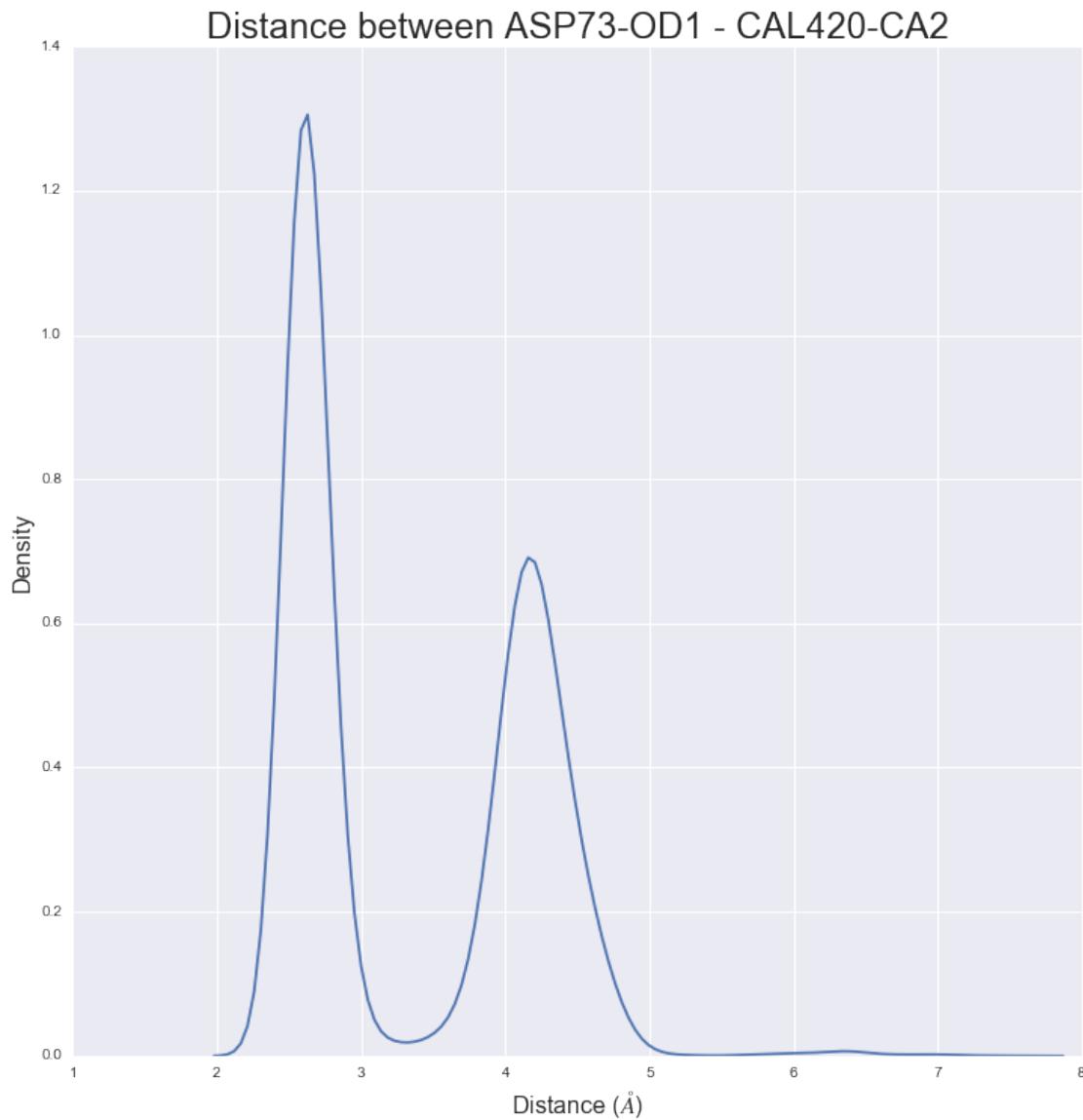
Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc

Distance between ASP73-OD1 - CAL420-CA2





Total execution time: 2.39 seconds

Total simulation time of all frames: 266.34 nanoseconds

The following topology file was successfully loaded:

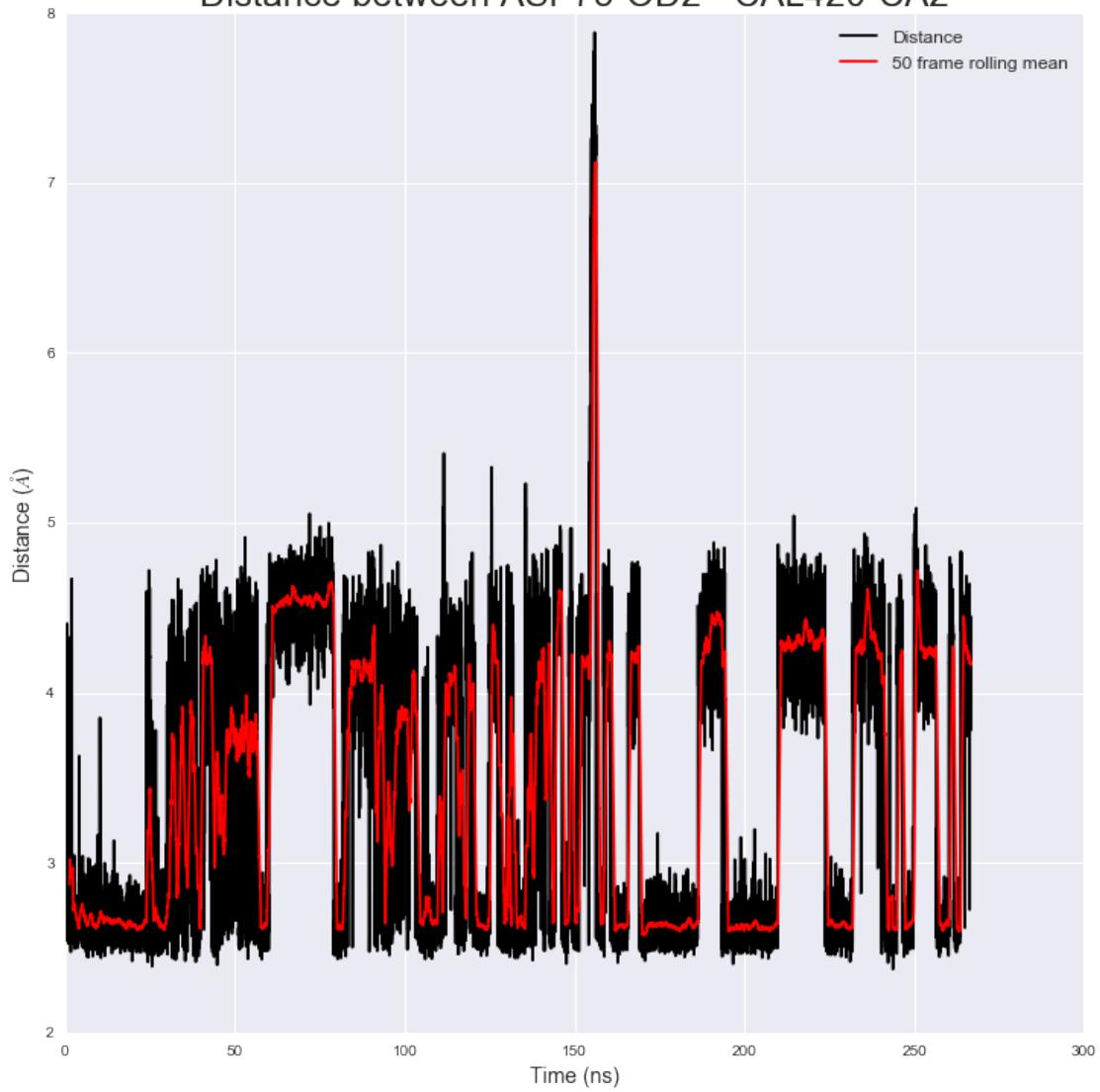
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

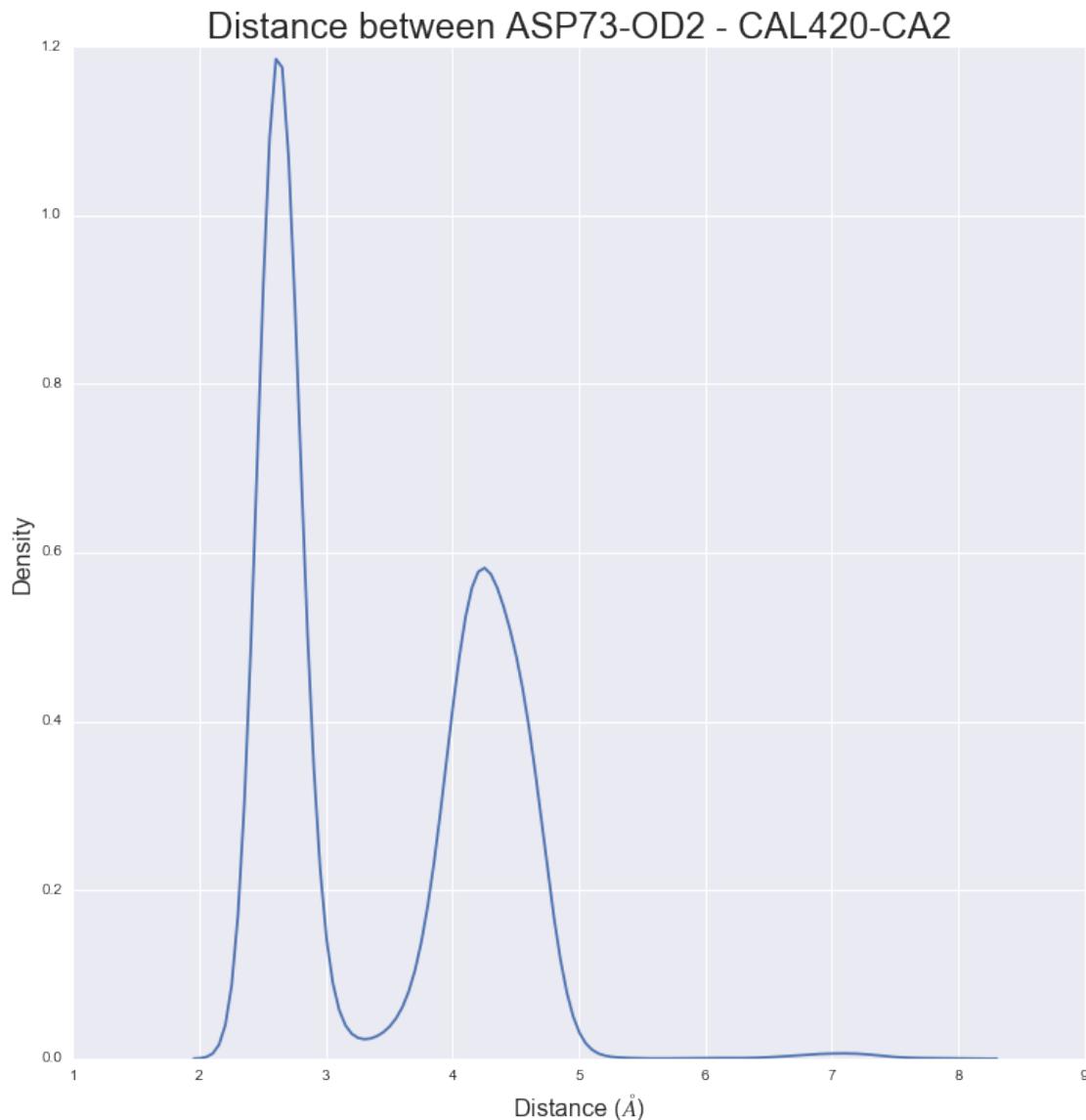
Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc

Distance between ASP73-OD2 - CAL420-CA2





Total execution time: 2.40 seconds

Total simulation time of all frames: 266.34 nanoseconds

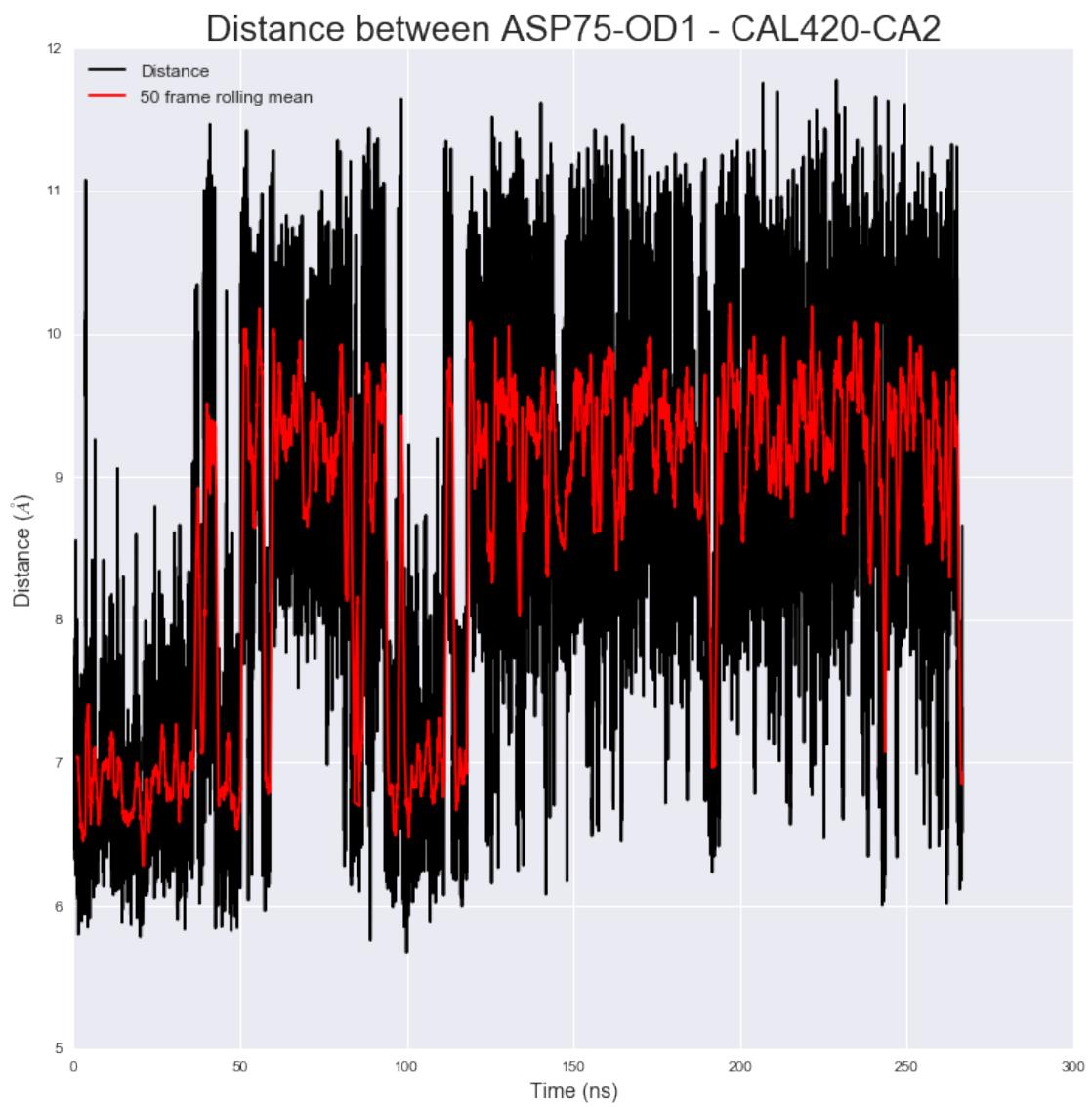
The following topology file was successfully loaded:

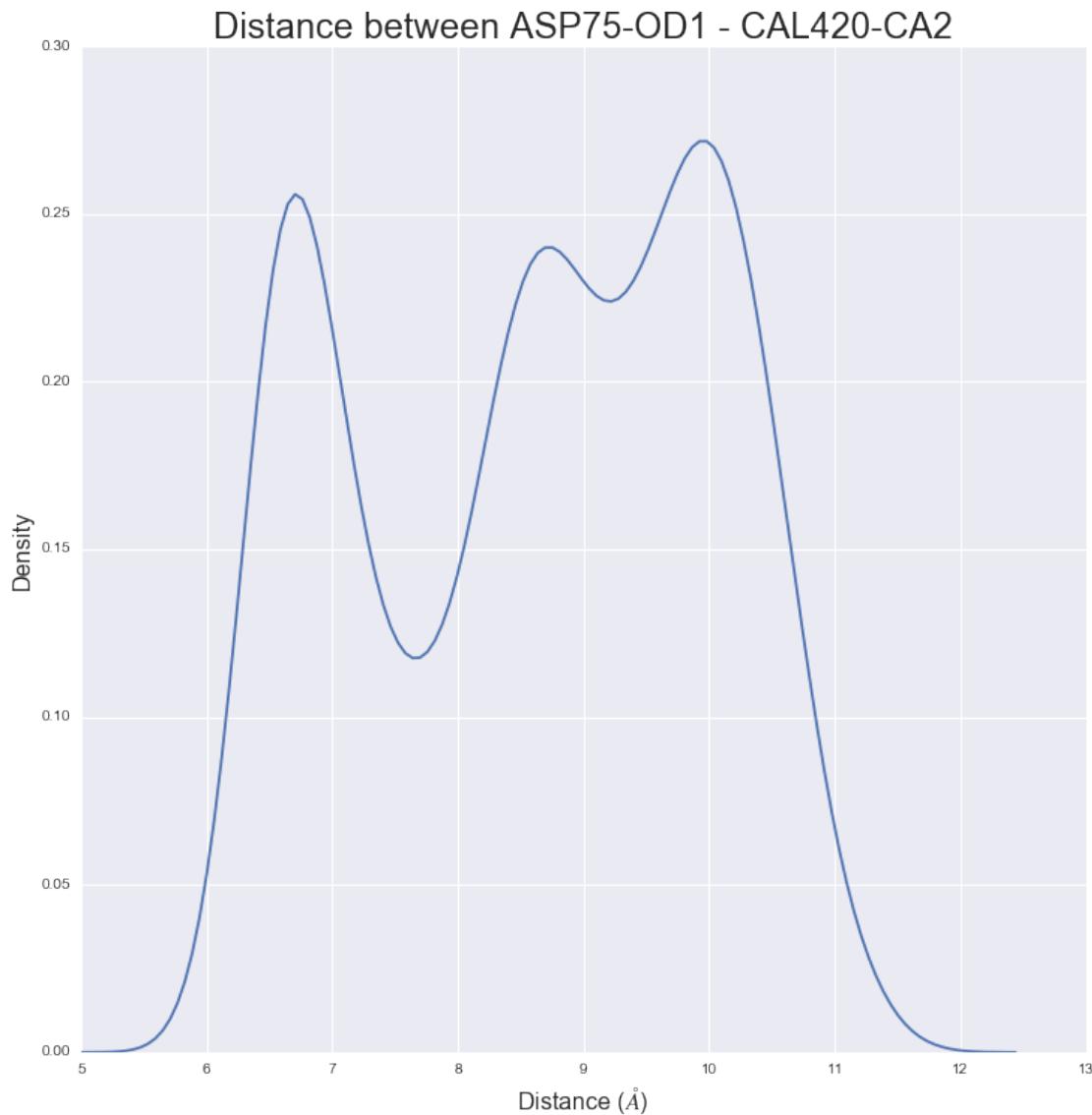
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc





Total execution time: 2.76 seconds

Total simulation time of all frames: 266.34 nanoseconds

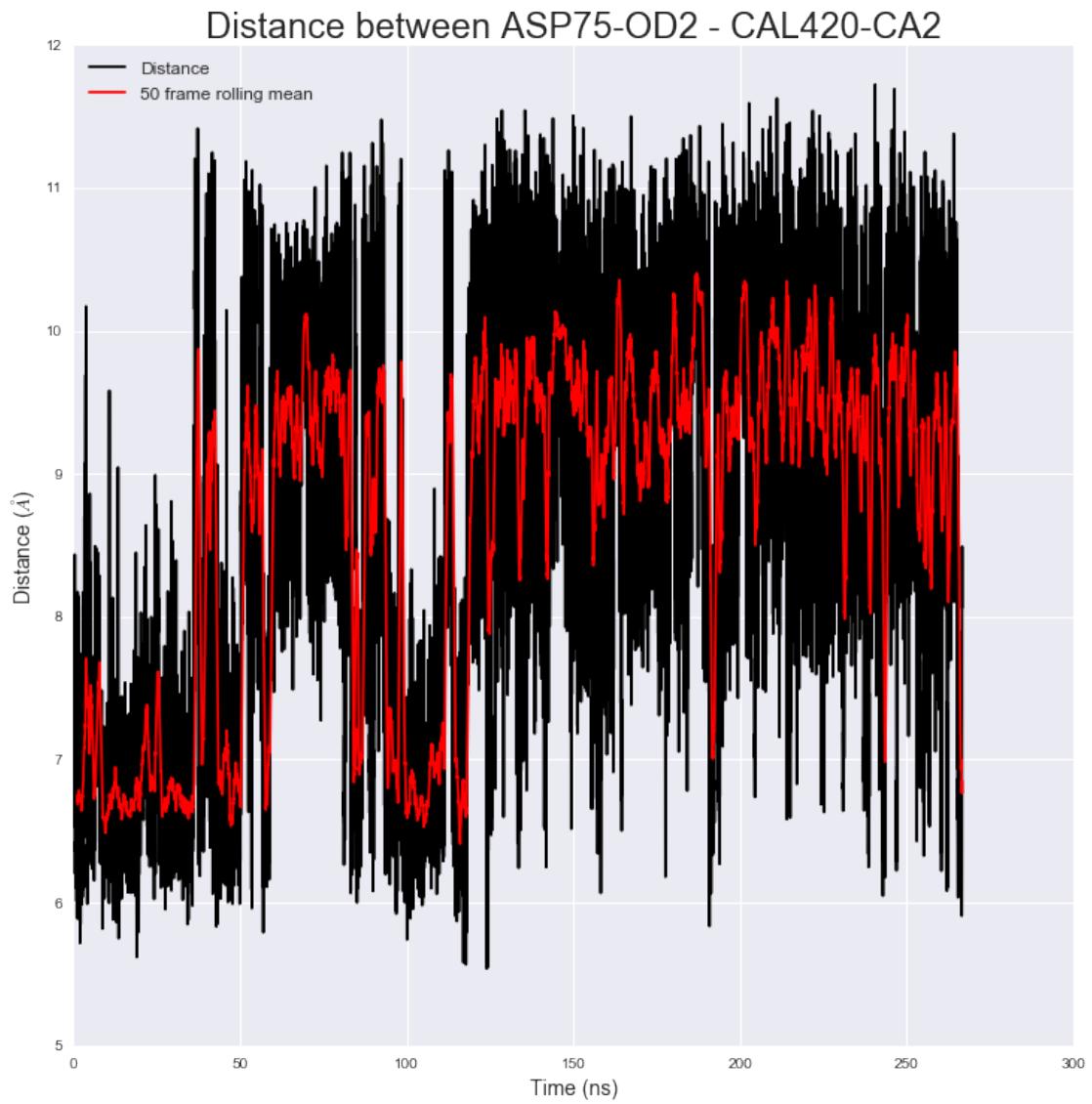
The following topology file was successfully loaded:

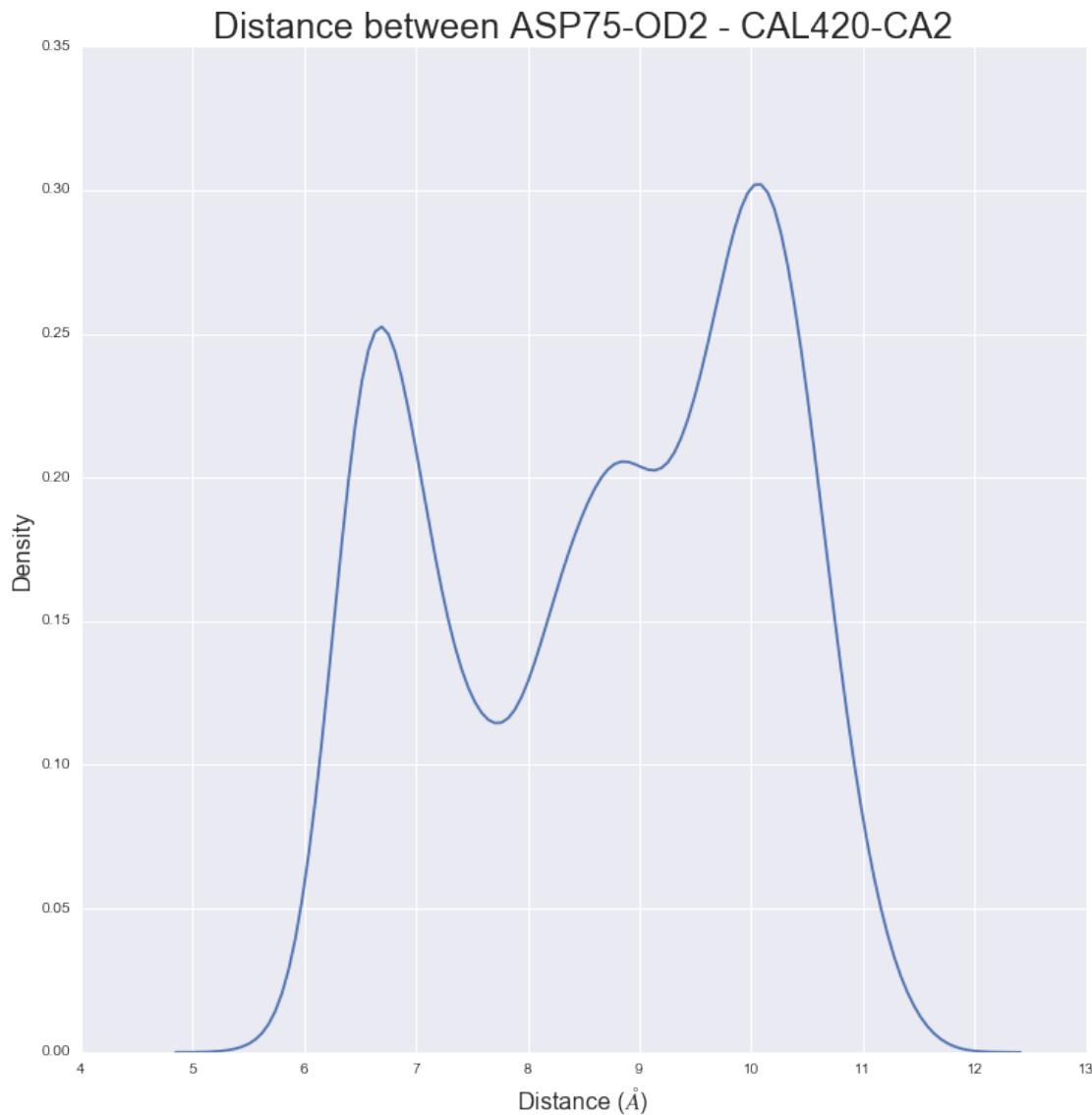
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc





Total execution time: 2.58 seconds

Total simulation time of all frames: 266.34 nanoseconds

The following topology file was successfully loaded:

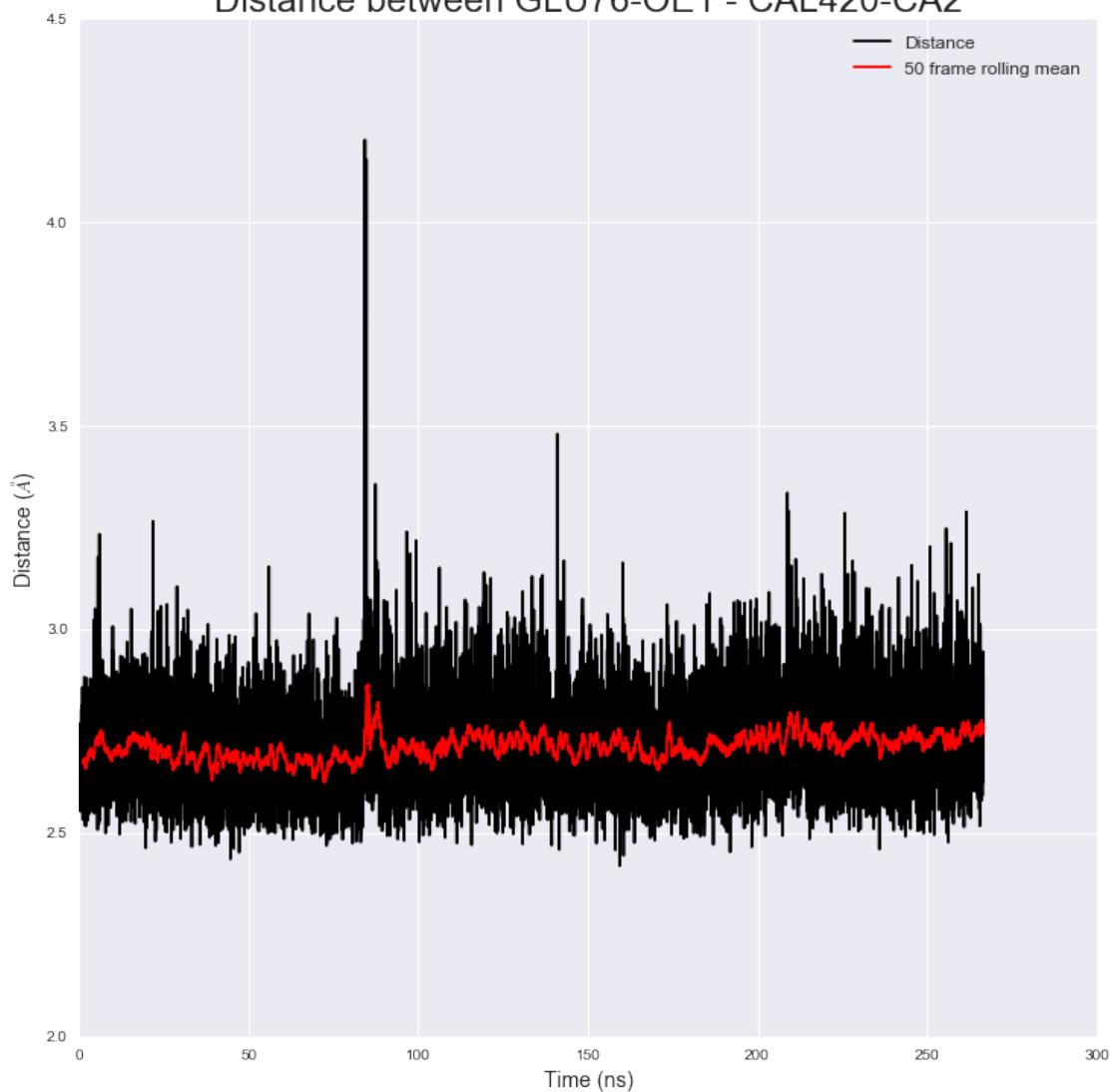
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

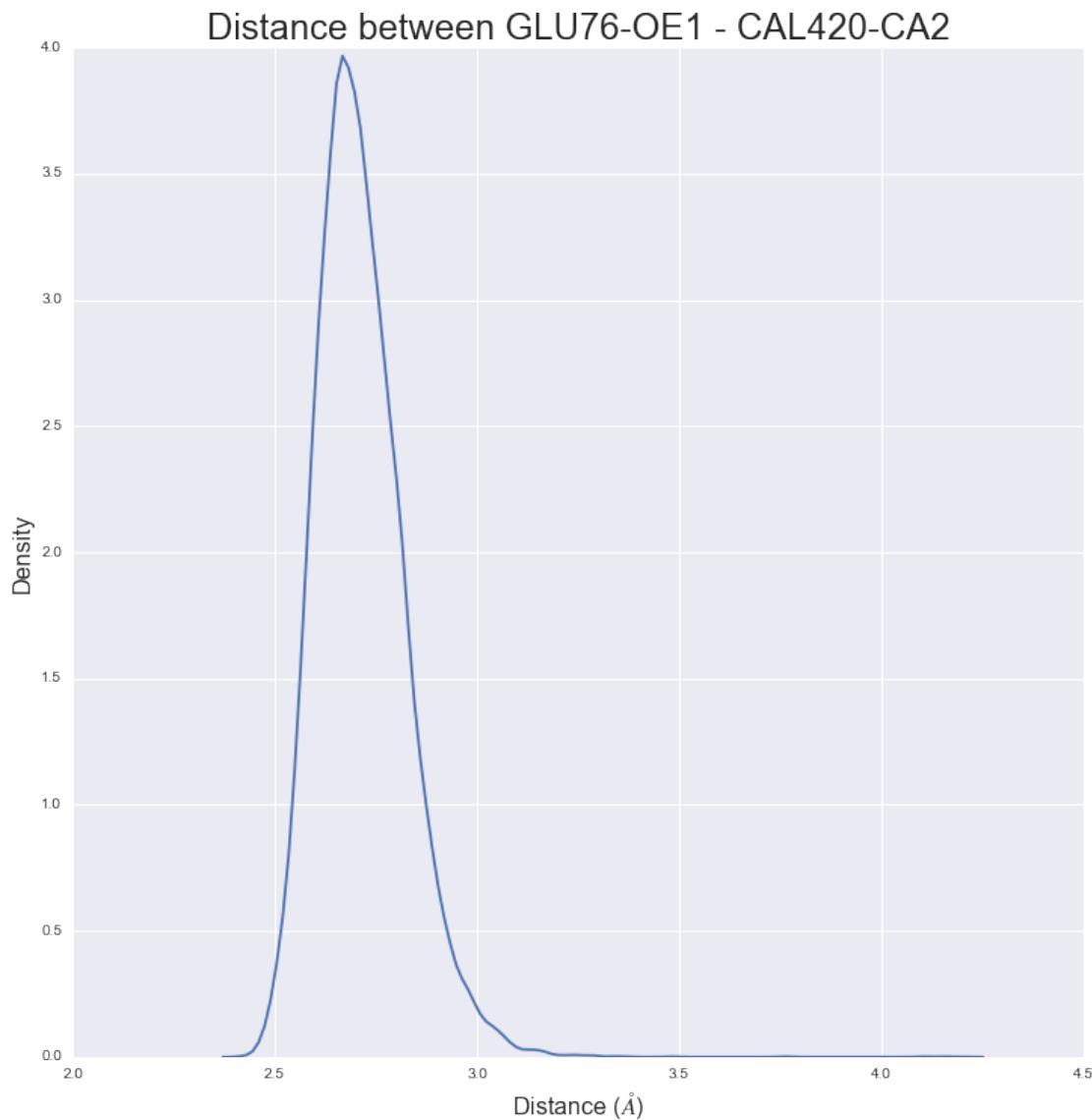
Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
 05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc

Distance between GLU76-OE1 - CAL420-CA2





Total execution time: 2.55 seconds

Total simulation time of all frames: 266.34 nanoseconds

The following topology file was successfully loaded:

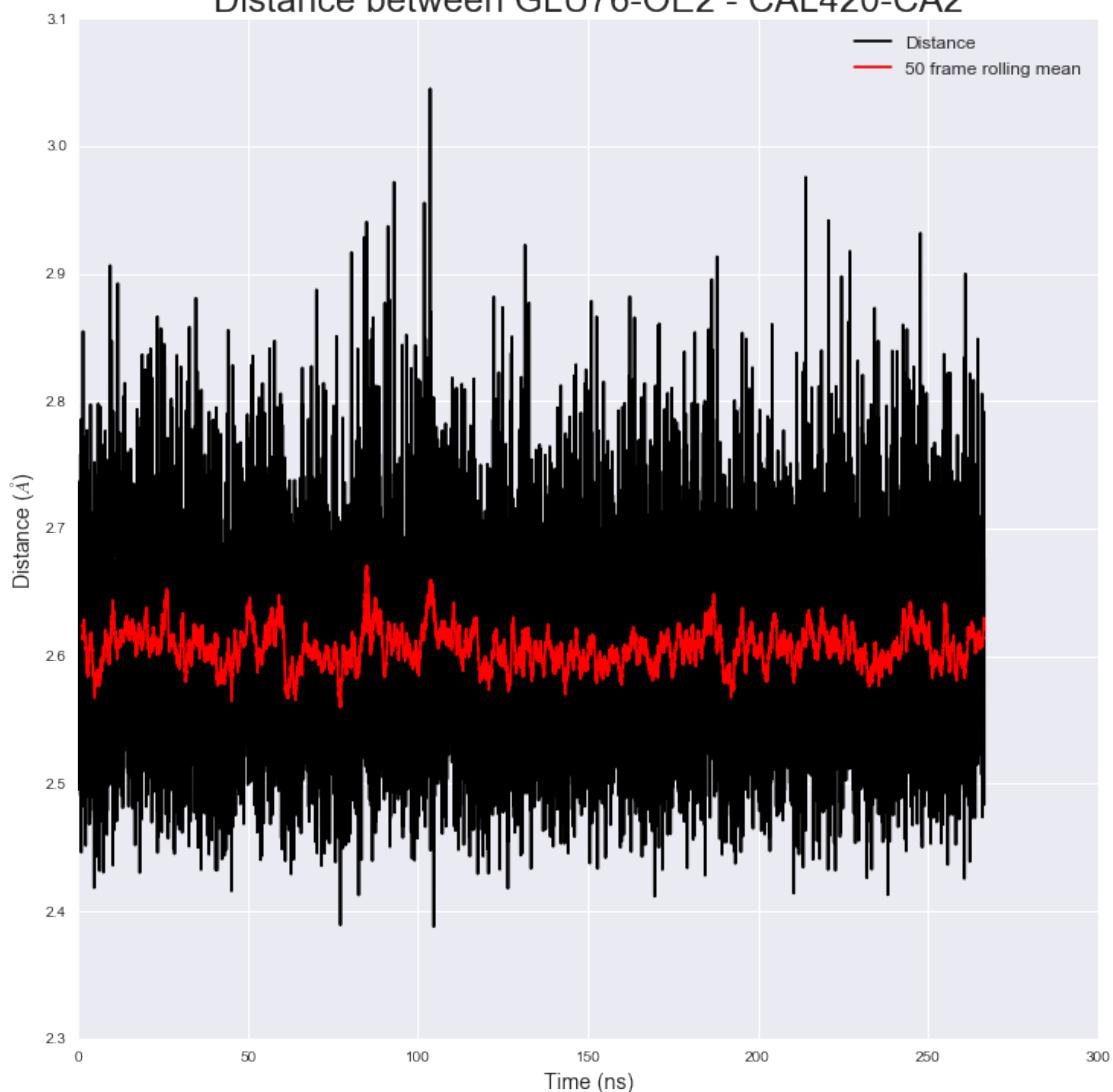
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

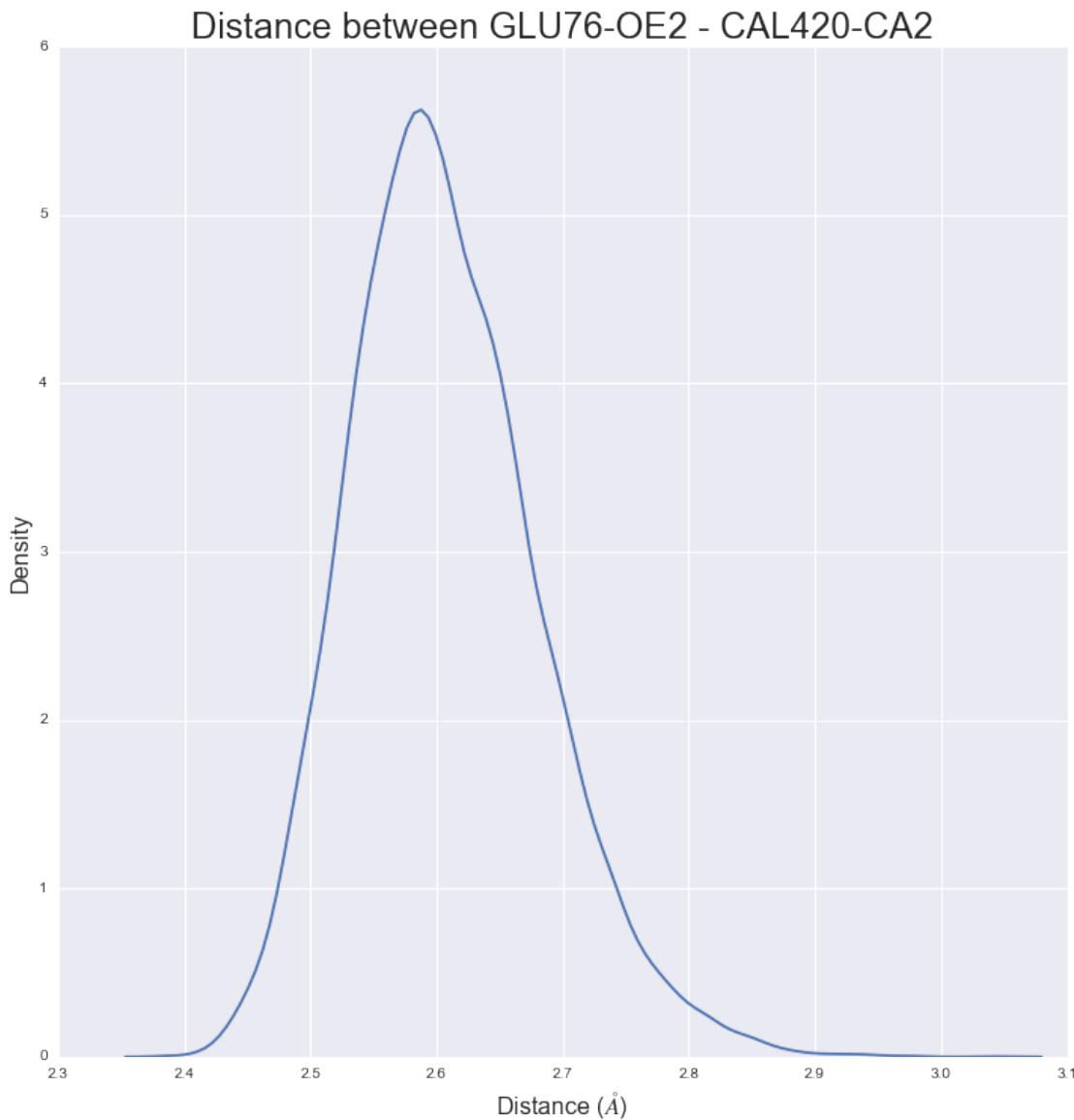
Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD3_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD3_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD3_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD3_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD3_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD3_250-300_run2_nowater.nc

Distance between GLU76-OE2 - CAL420-CA2





Total execution time: 2.69 seconds

Total simulation time of all frames: 266.34 nanoseconds

0.4 MD5

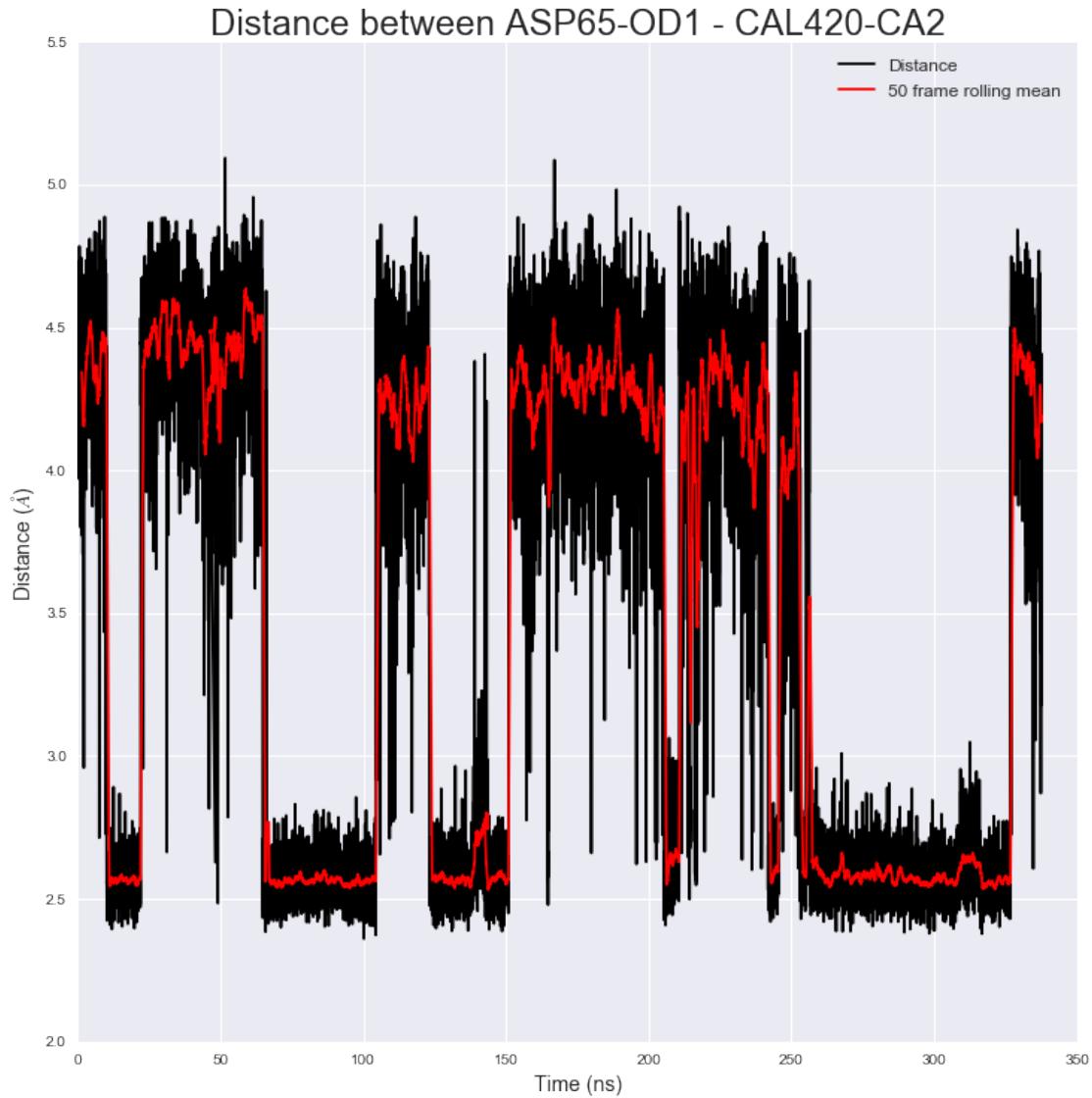
```
In [20]: topology_MD5 = '/Users/gil_f.hoben/Troponin_md_processed/MD5/run2/troponin_egcg_MD5_nowater.pr
          trajectory_MD5 = '/Users/gil_f.hoben/Troponin_md_processed/MD5/run2/Trajectories/'
          for atom1 in atom1_list:
              main(topology_MD5, trajectory_MD5, atom1, atom2, verbose = 1)
```

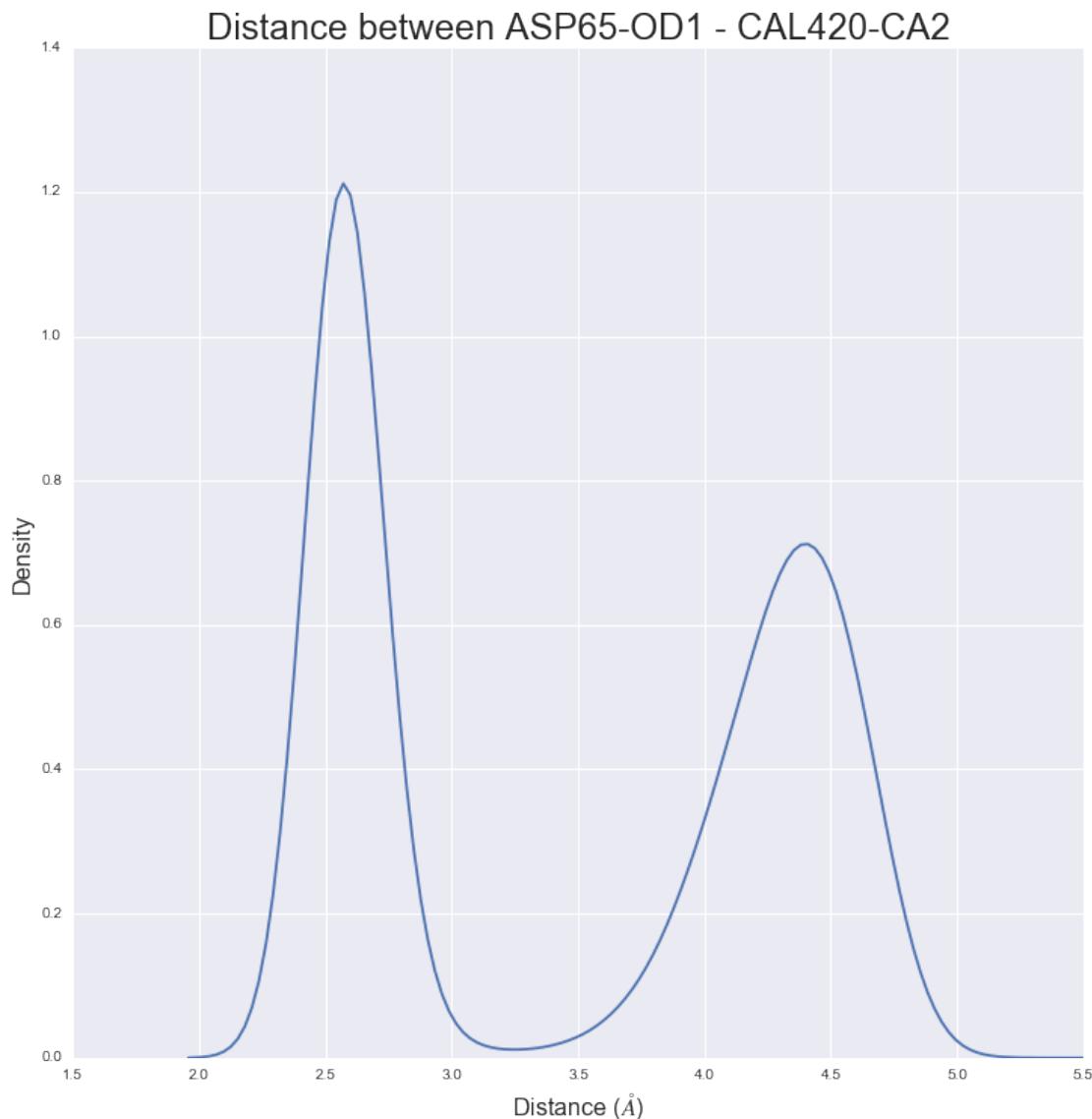
The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:
05_Prod_troponin_egcg_MD5_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD5_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD5_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc
05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 4.93 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

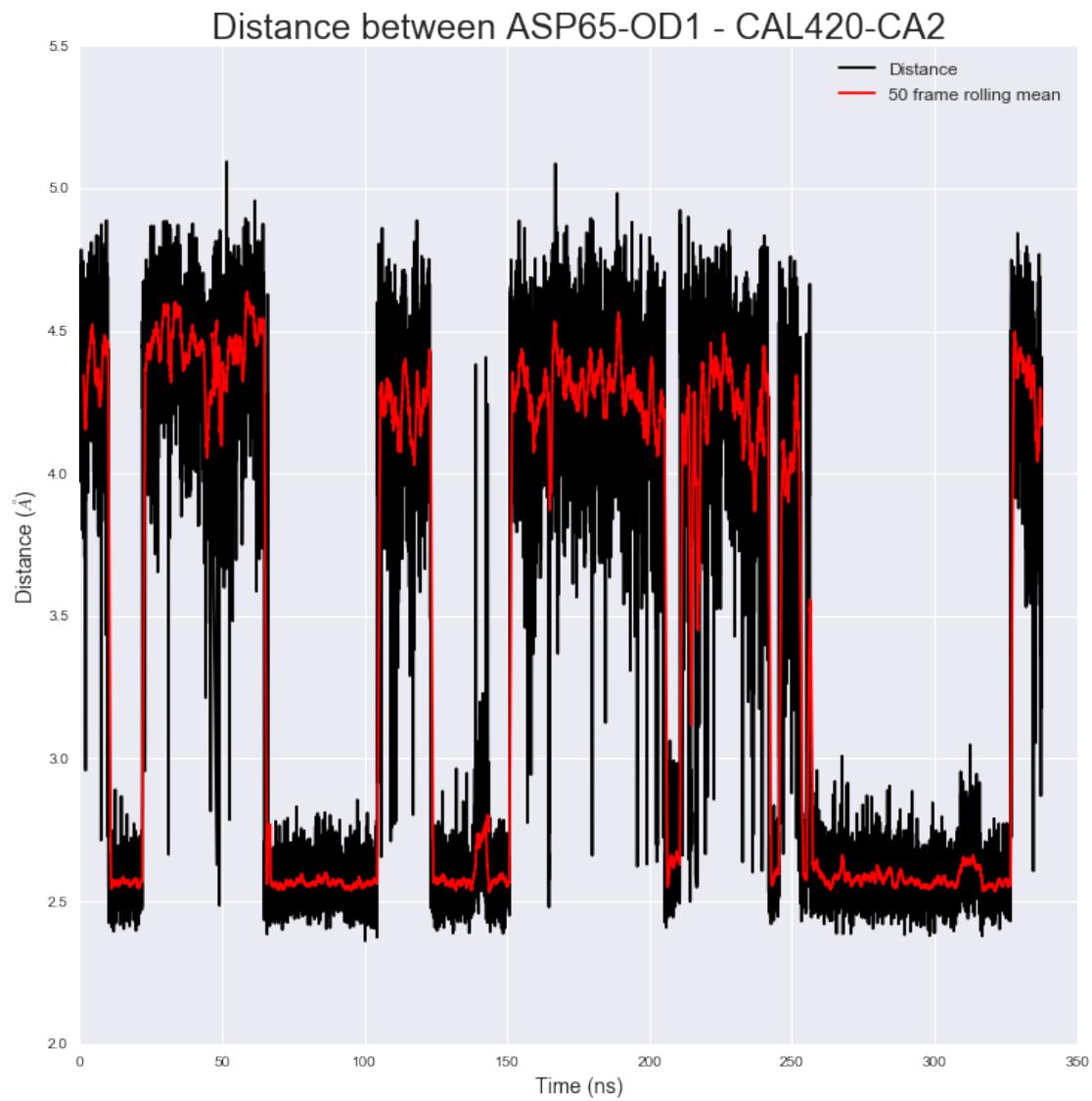
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

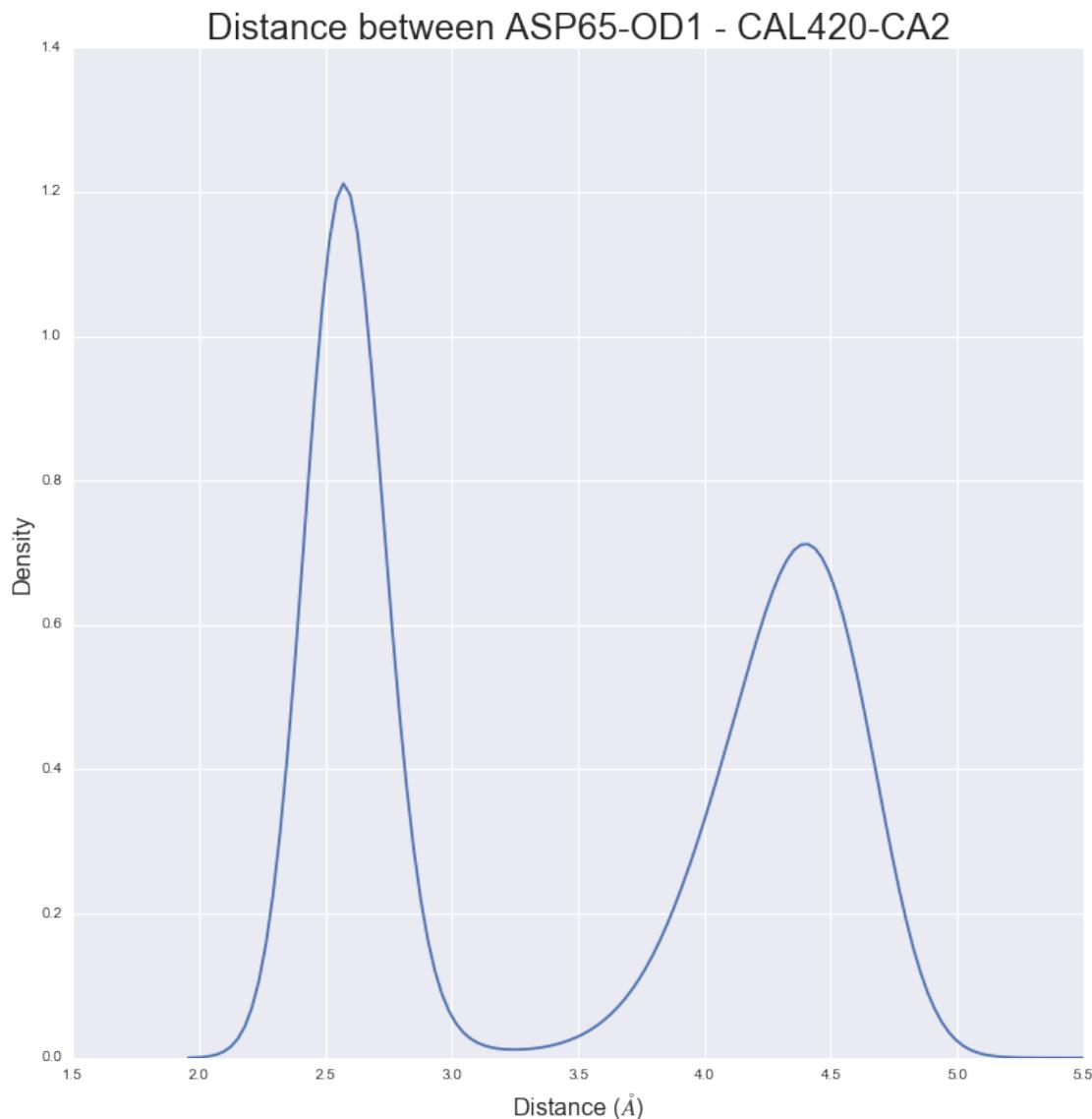
Calculating distance between following atoms: ASP65-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD5_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD5_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD5_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.07 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

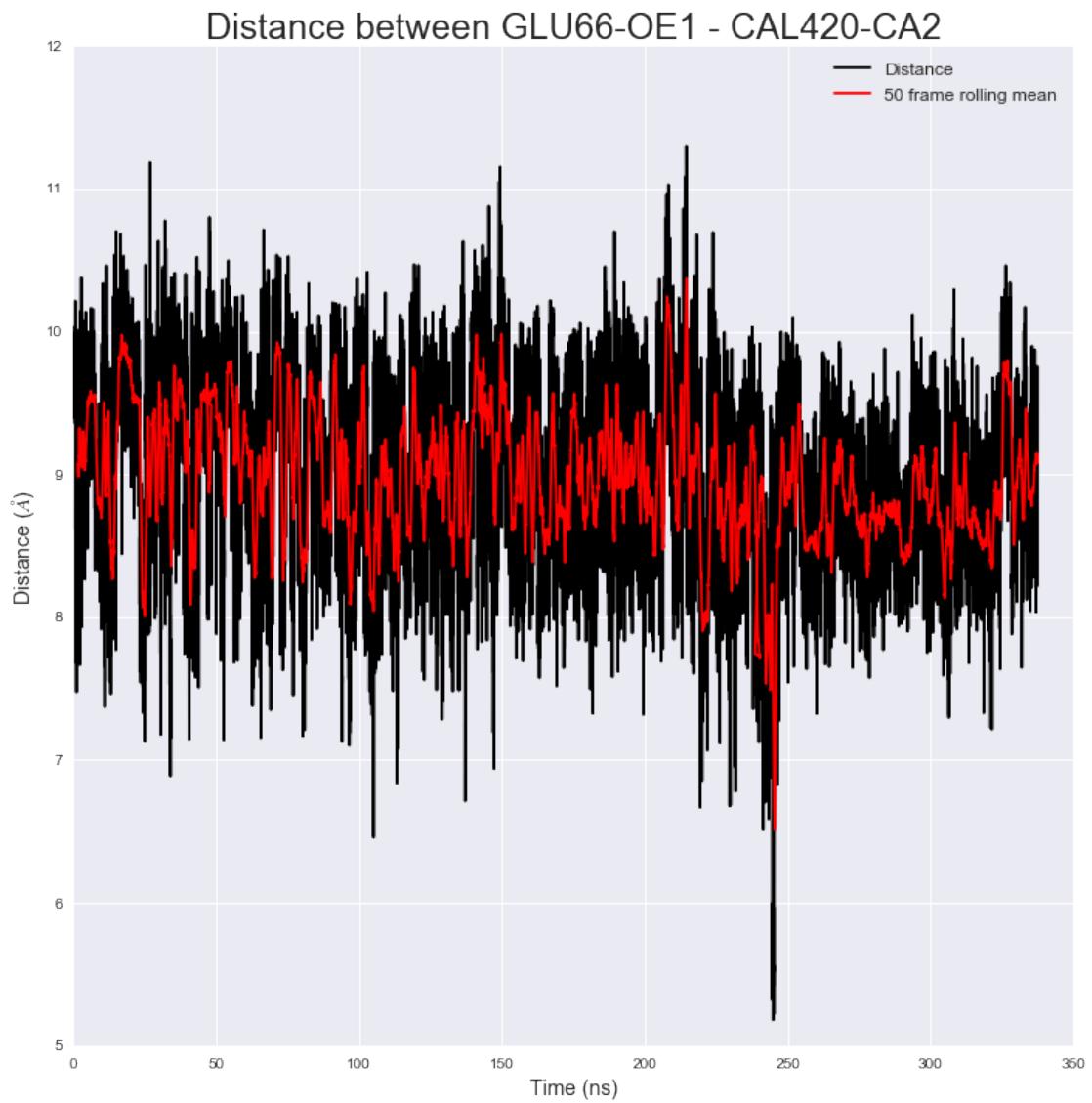
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

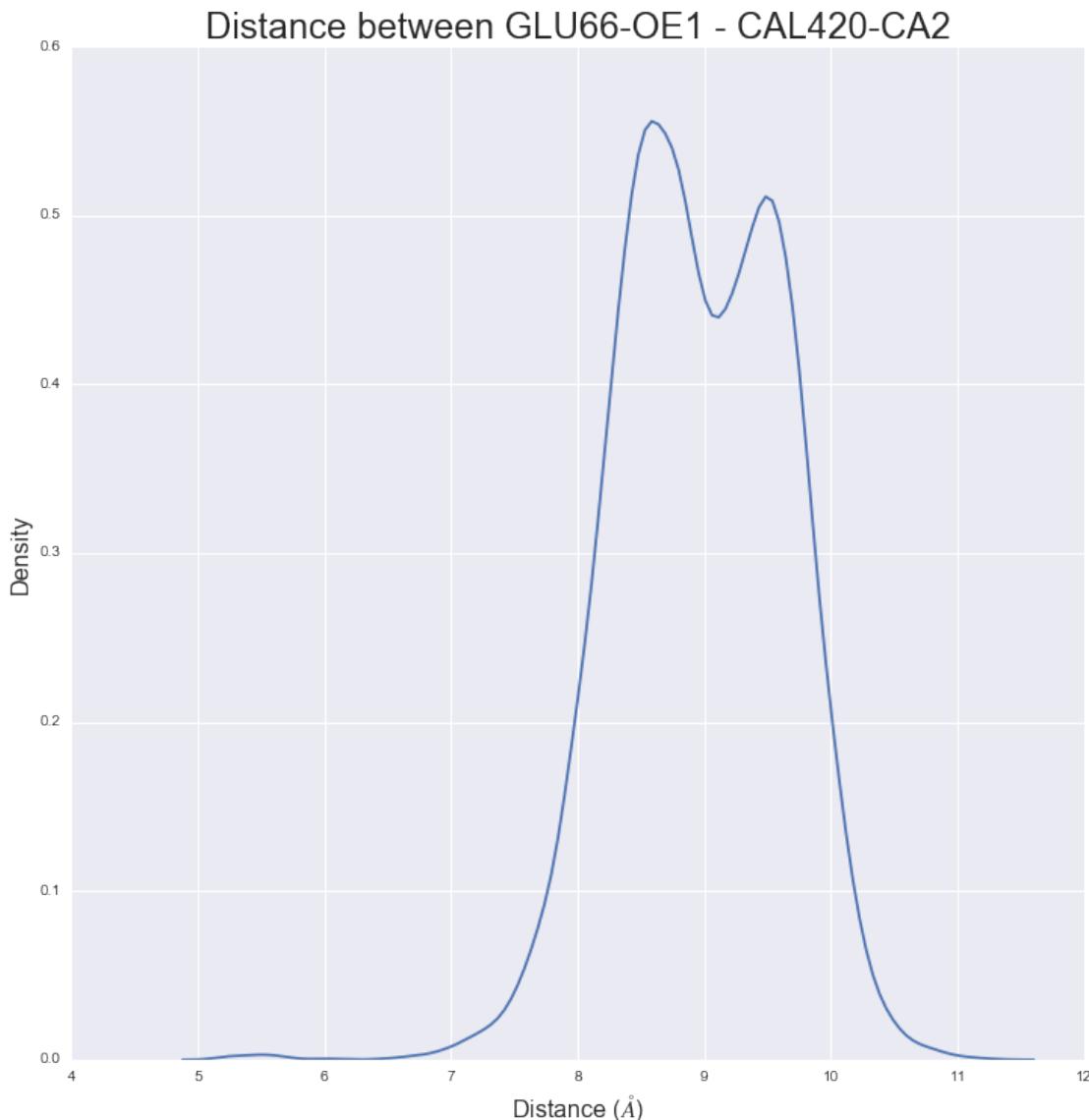
Calculating distance between following atoms: GLU66-OE1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD5_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD5_100-150_run2_nowater.nc
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 05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.07 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

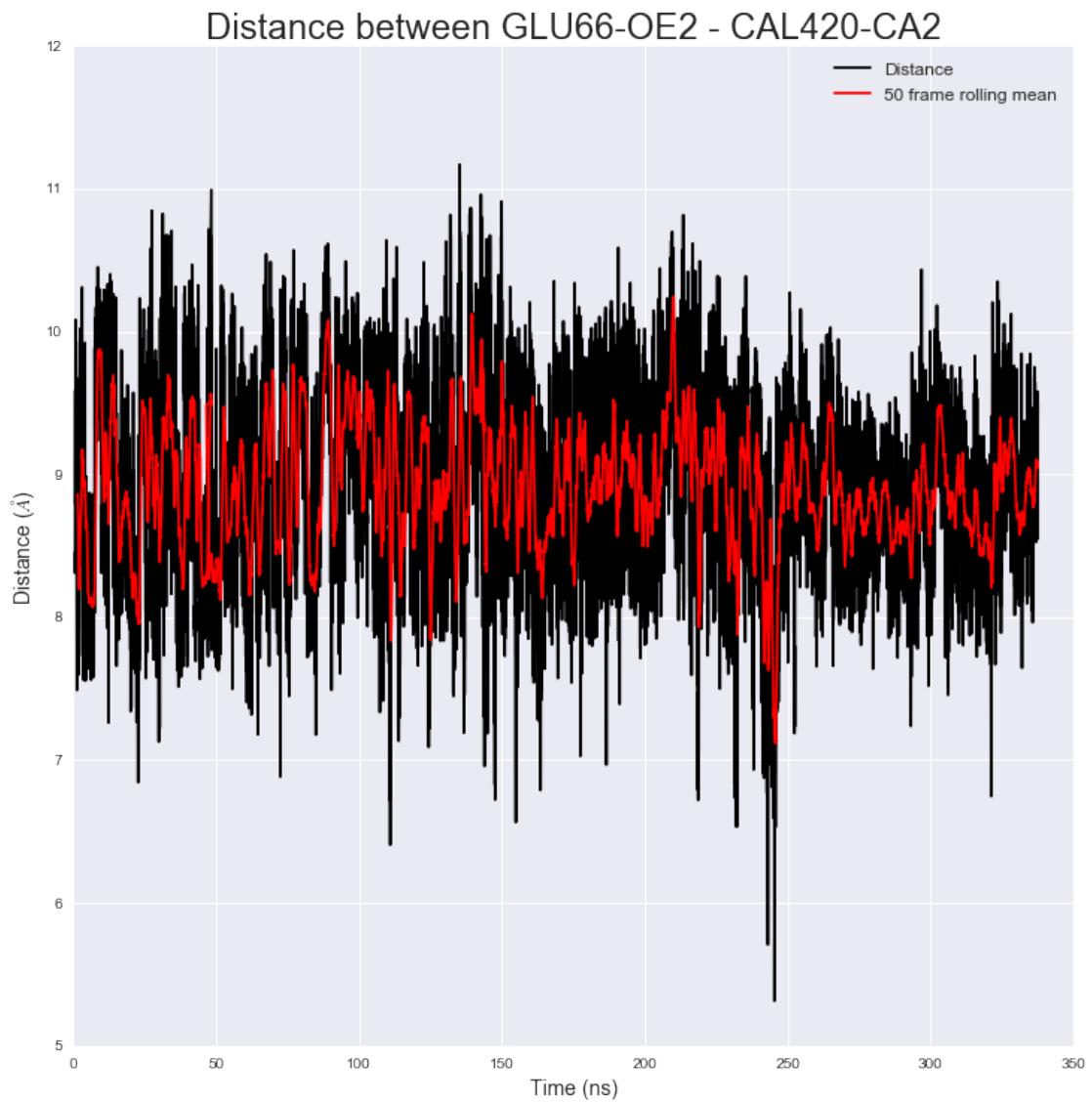
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

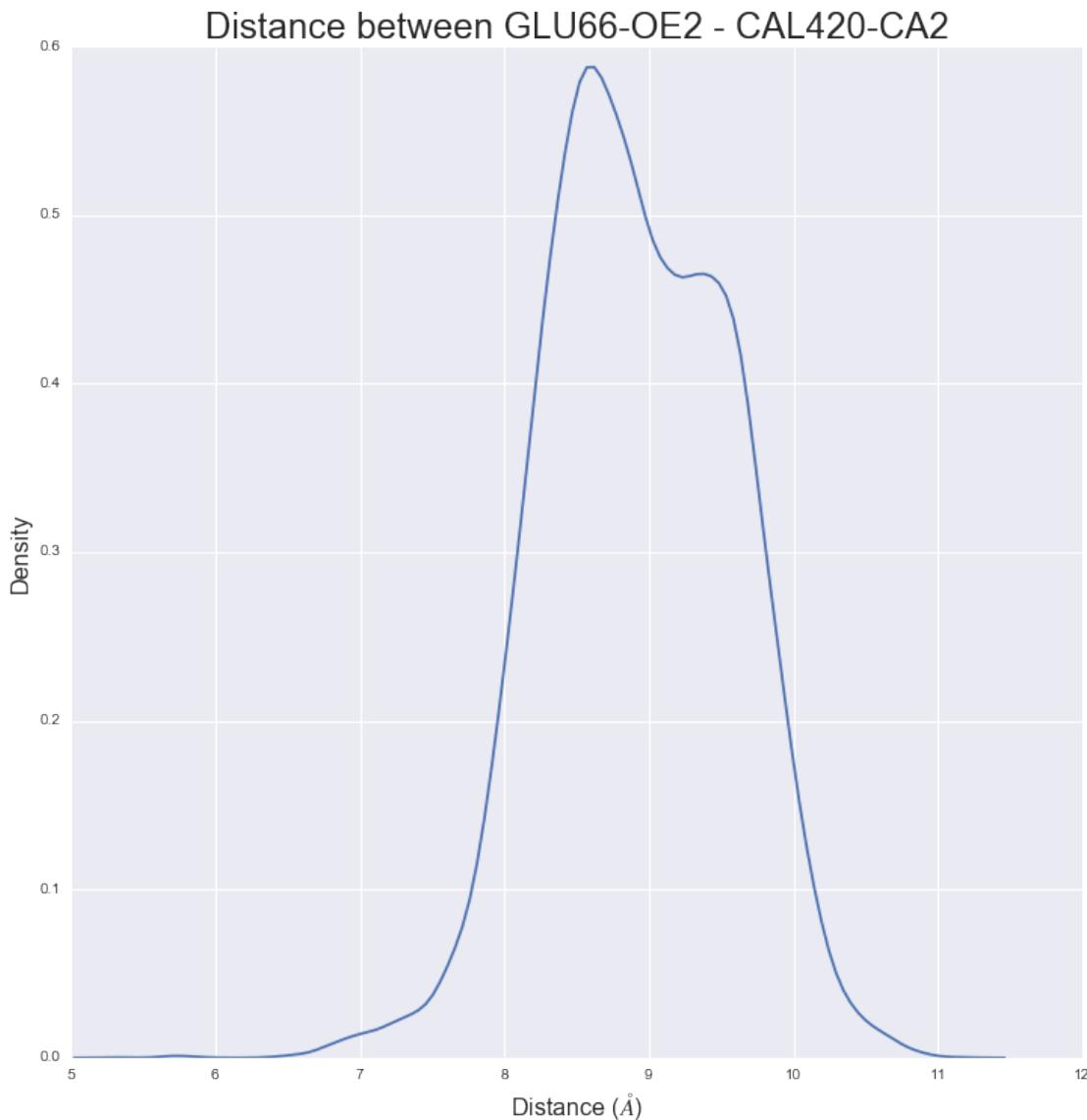
Calculating distance between following atoms: GLU66-OE2 - CAL420-CA2

Loading trajectories from the following files:

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05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.22 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

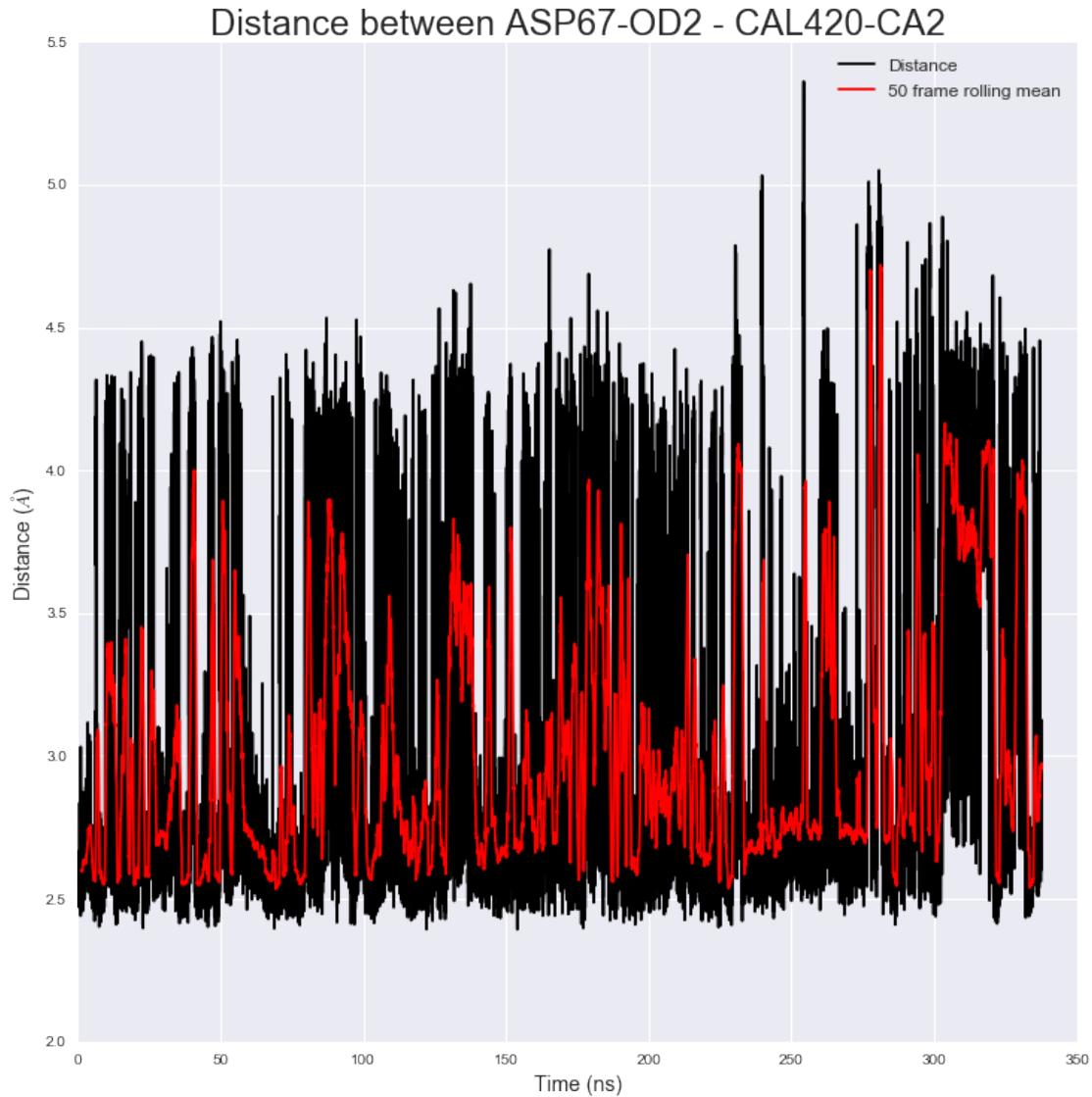
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

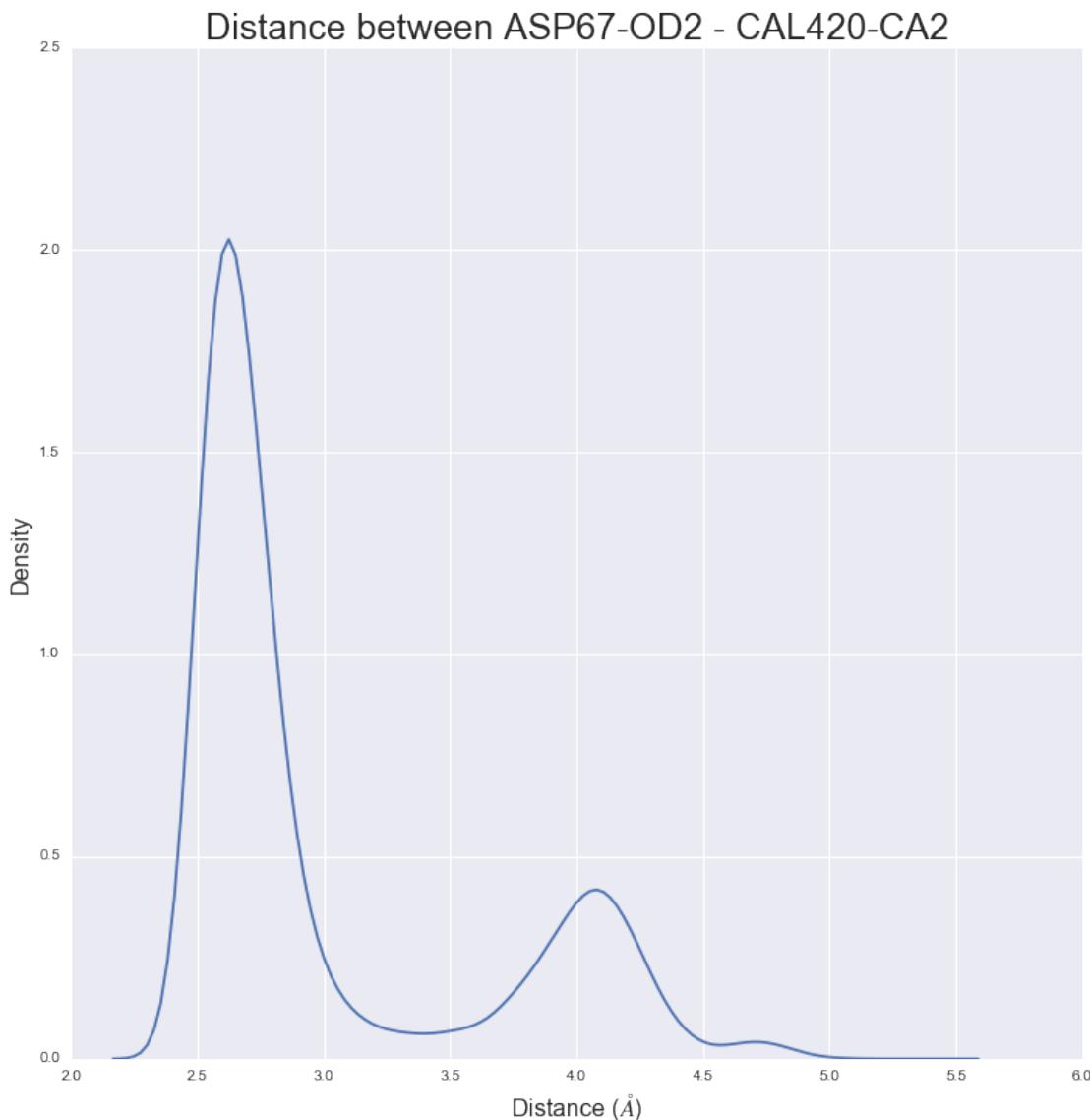
Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD5_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD5_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD5_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 2.98 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

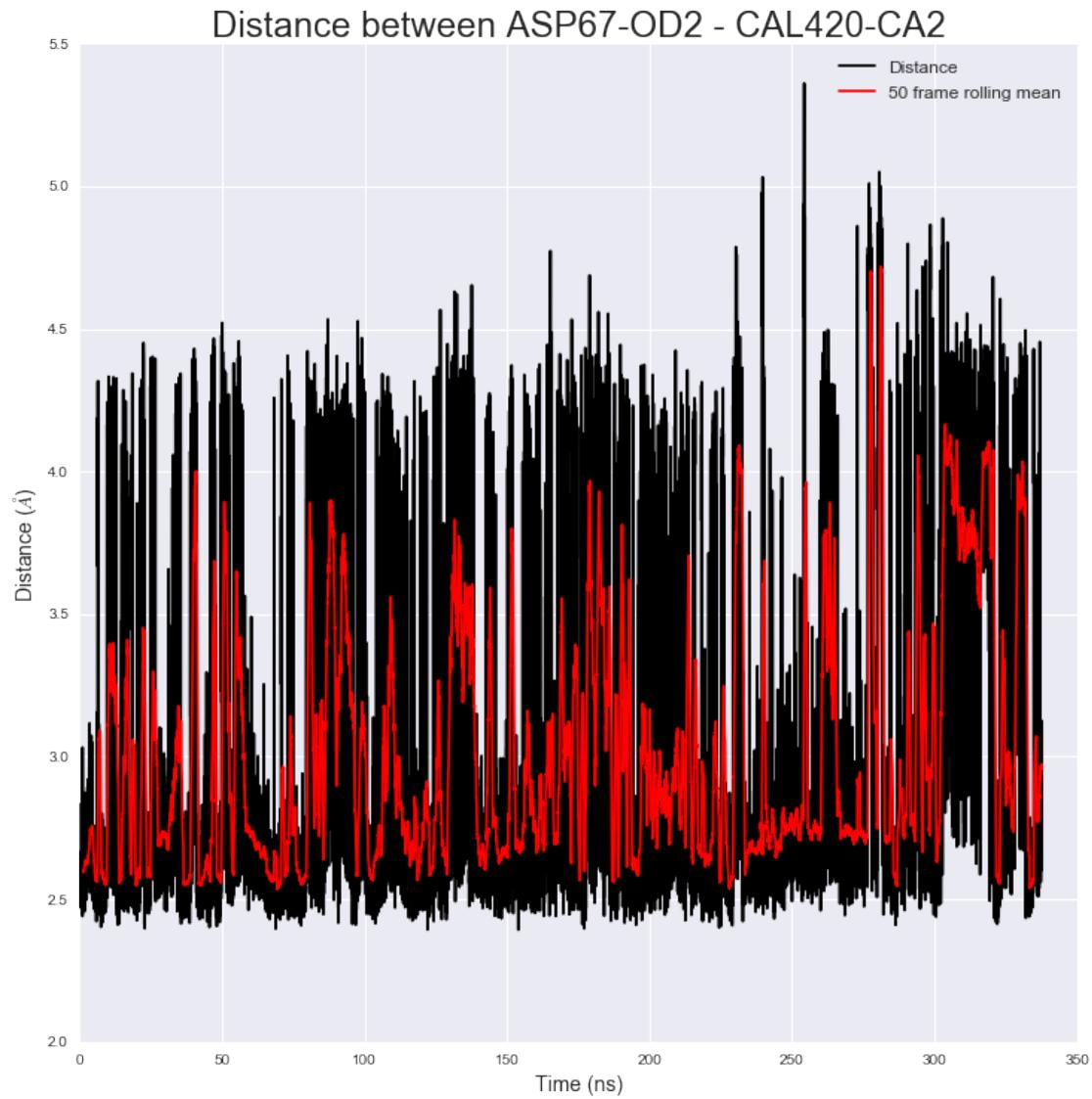
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

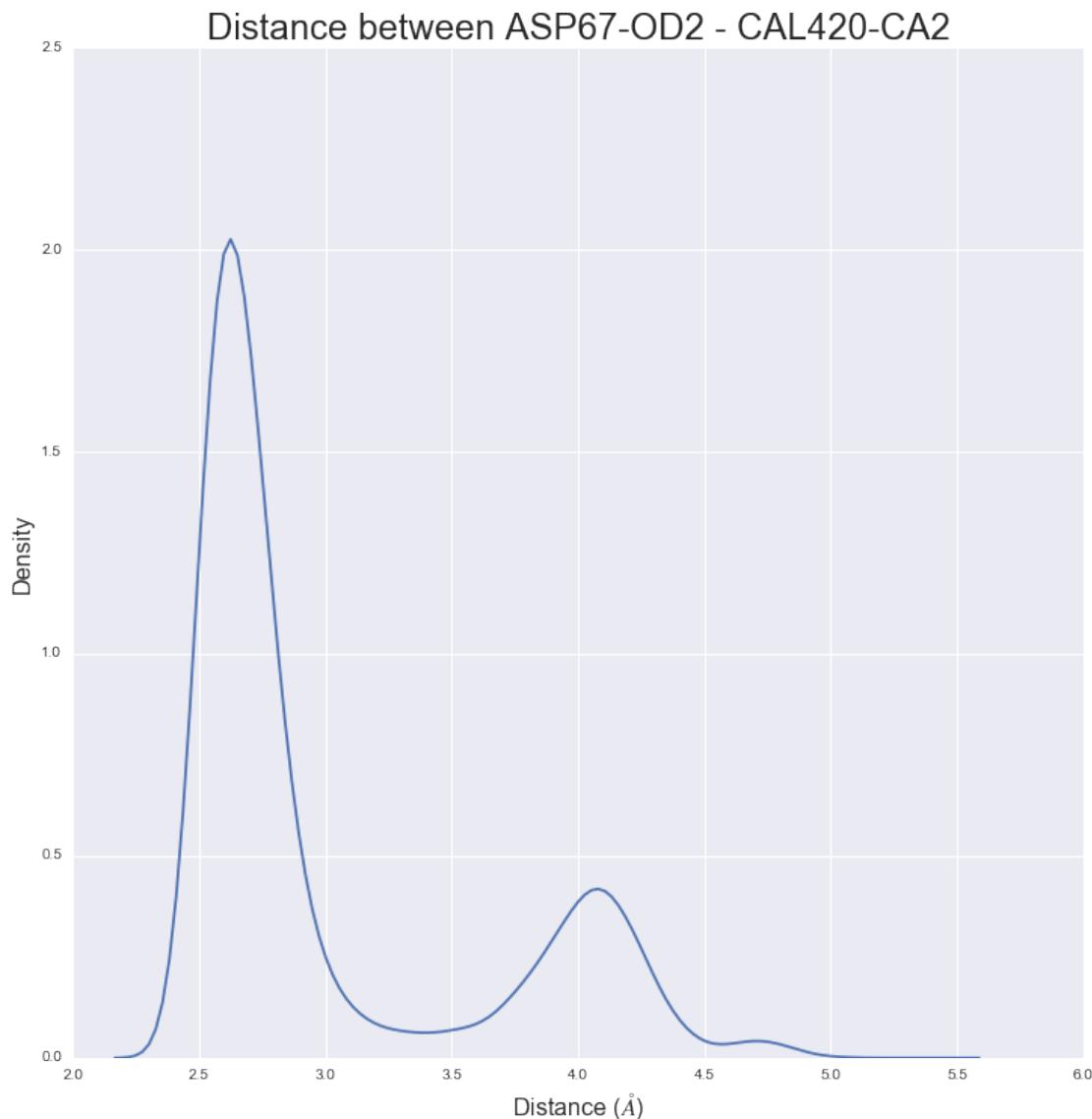
Calculating distance between following atoms: ASP67-OD2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD5_000-050_run2_nowater.nc
 05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
 05_Prod_troponin_egcg_MD5_100-150_run2_nowater.nc
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 05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.20 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

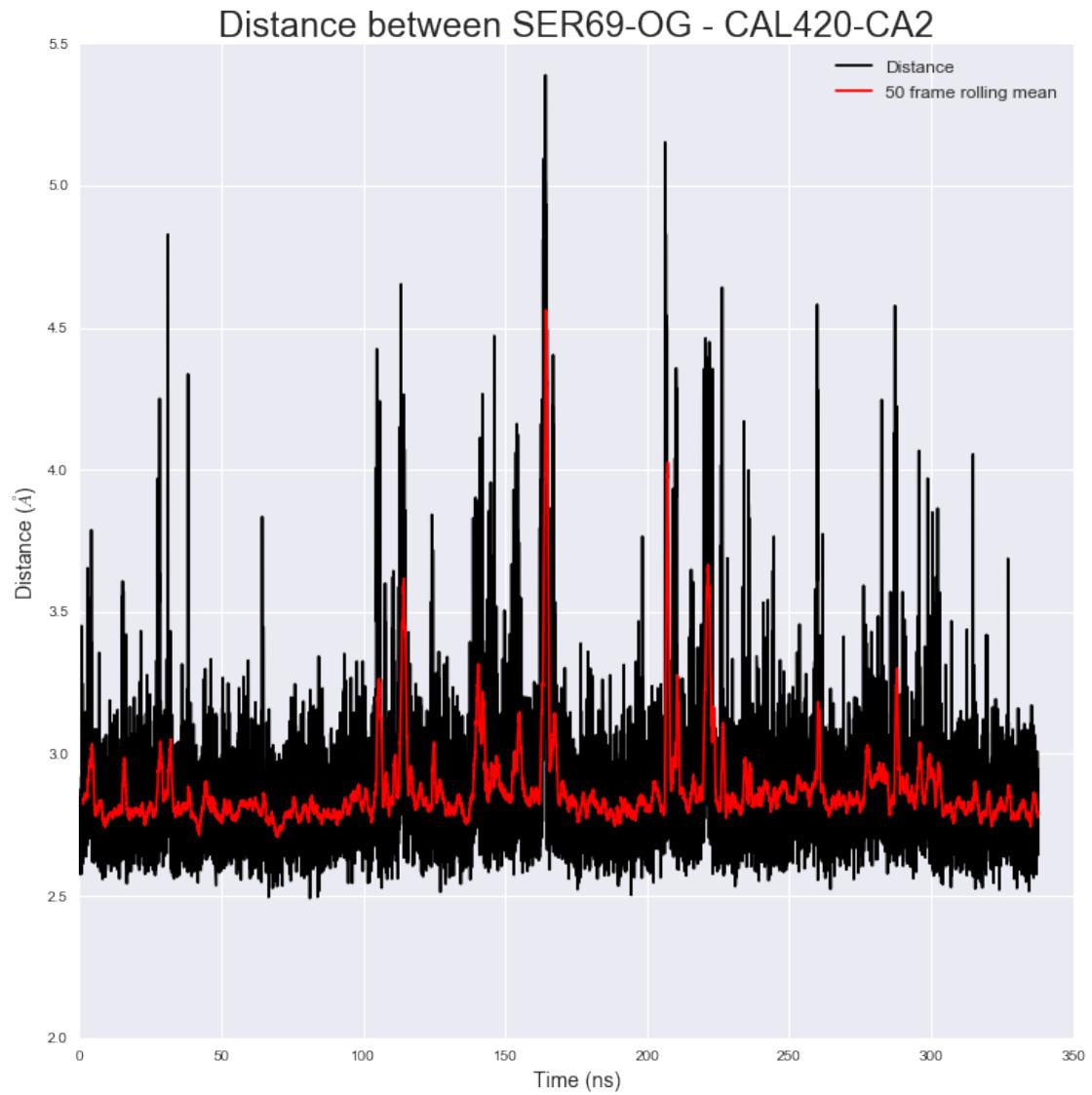
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

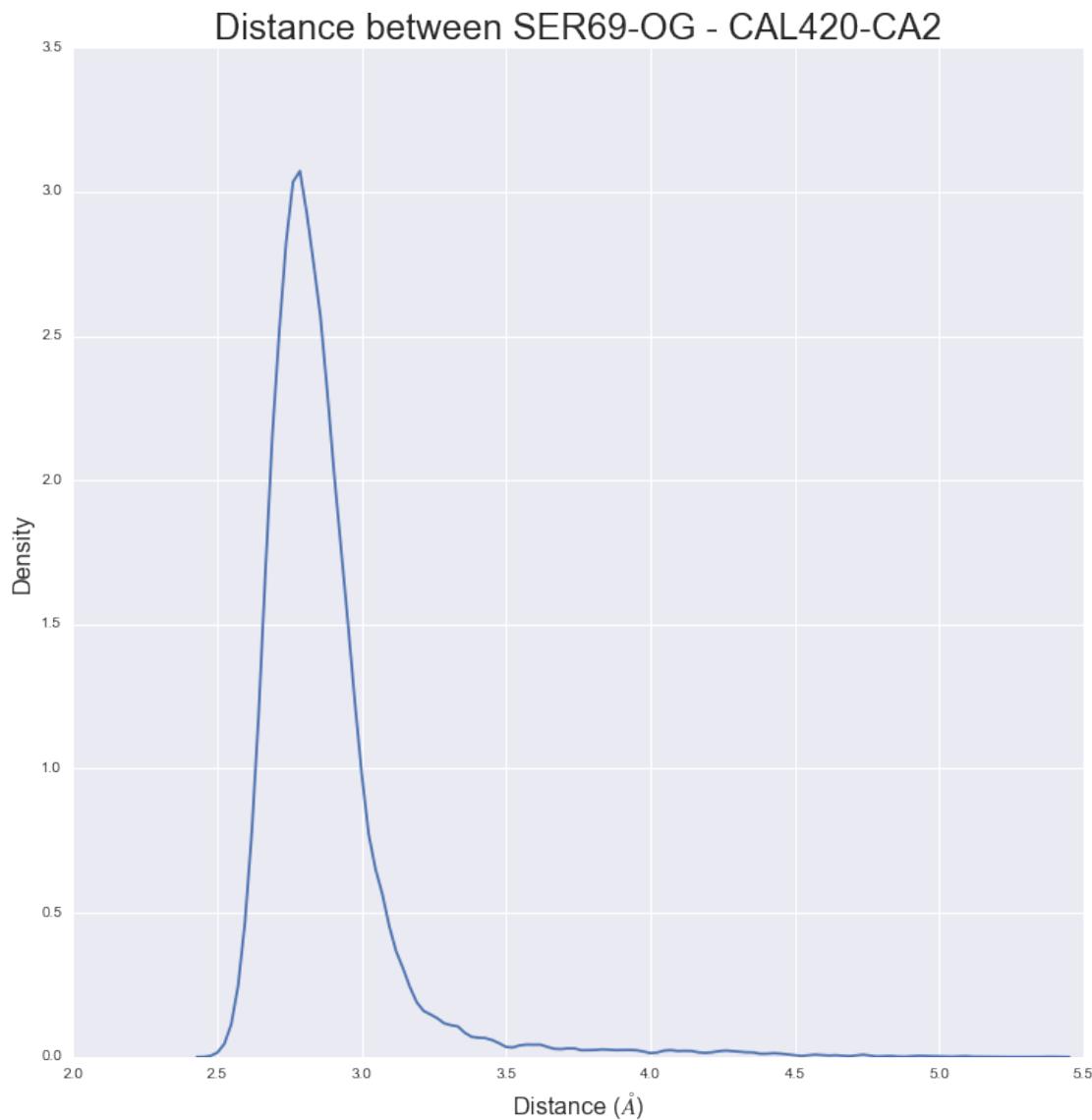
Calculating distance between following atoms: SER69-OG - CAL420-CA2

Loading trajectories from the following files:

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05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.13 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

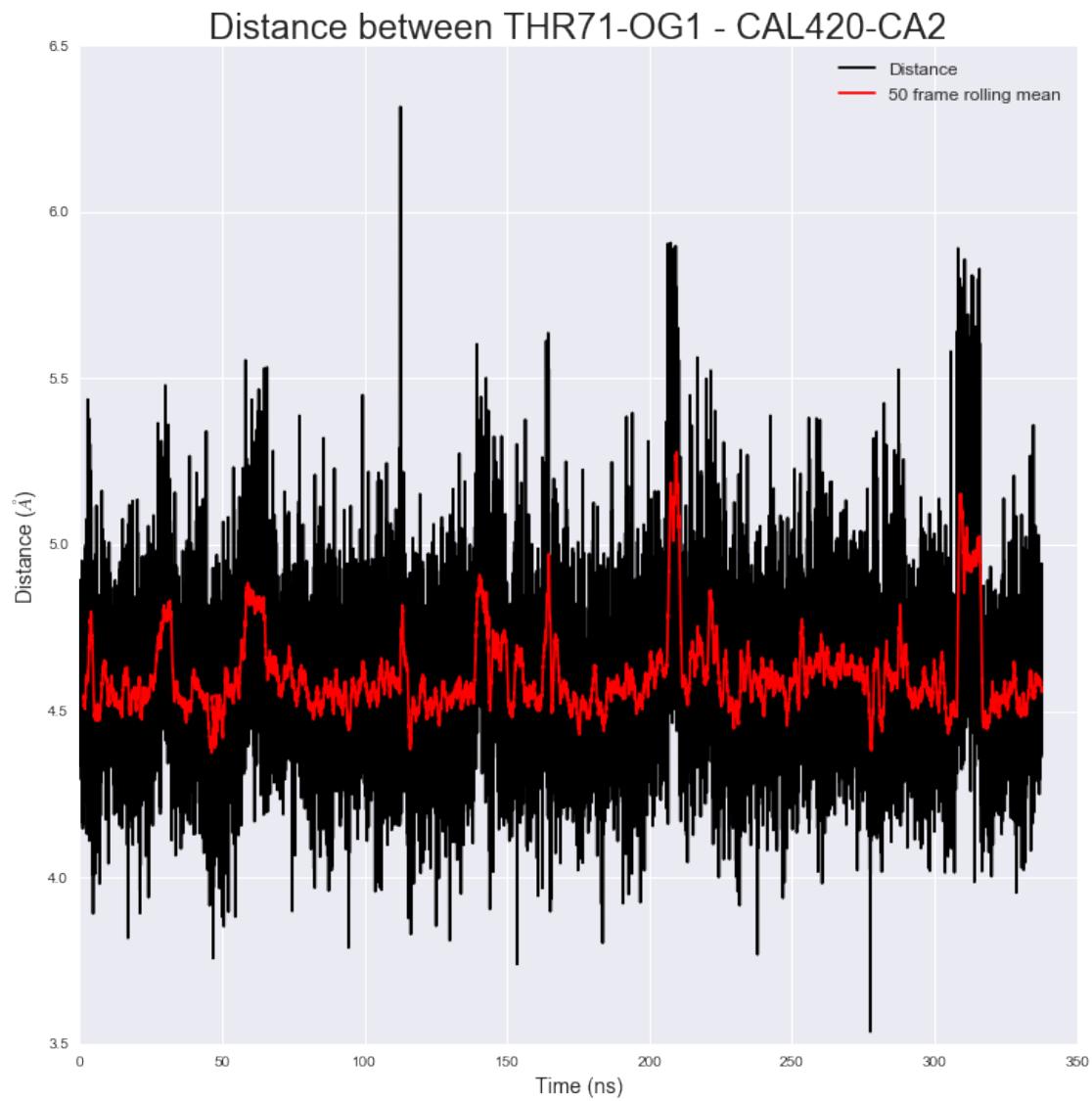
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

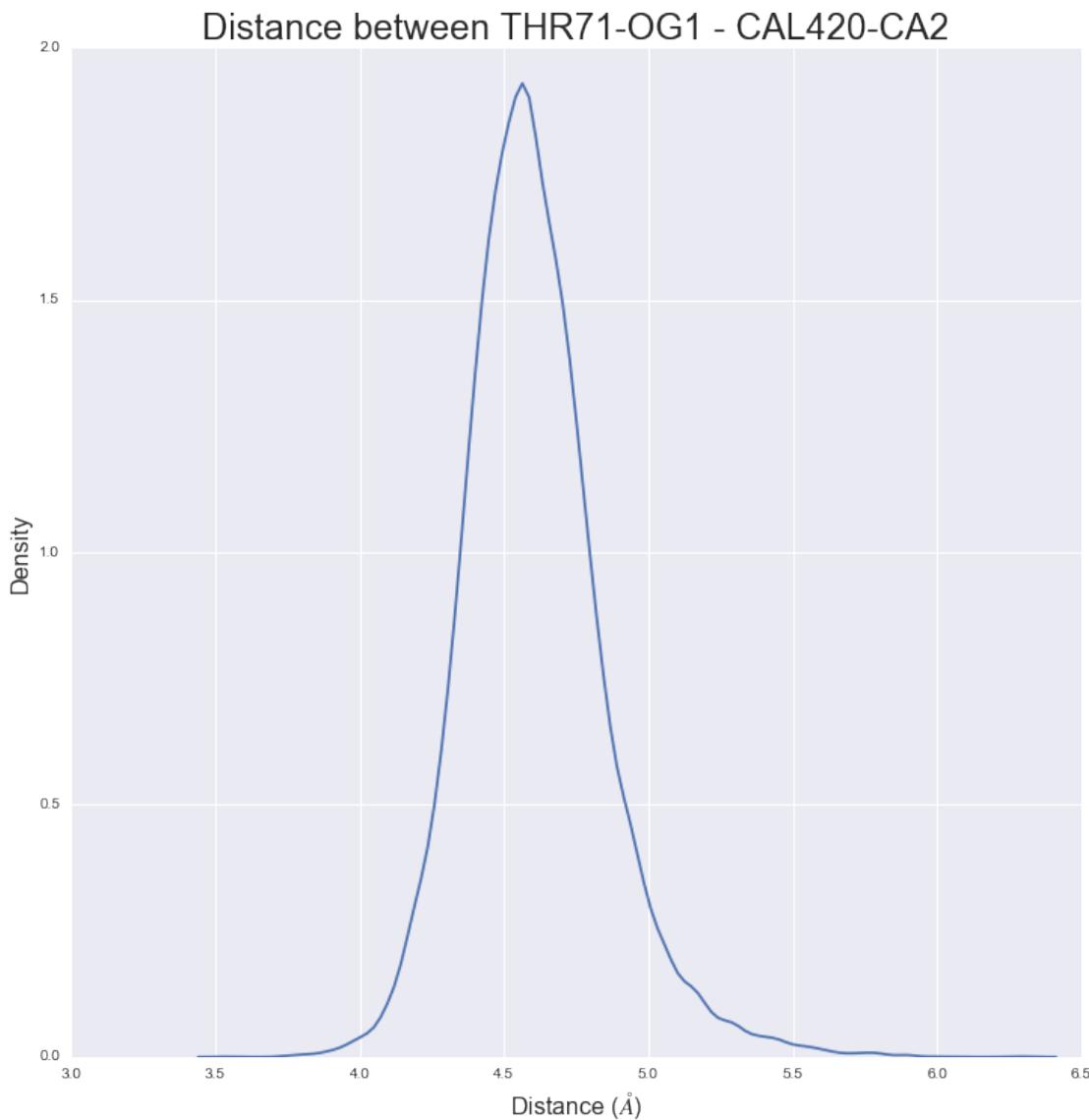
Calculating distance between following atoms: THR71-OG1 - CAL420-CA2

Loading trajectories from the following files:

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 05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
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 05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 2.97 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

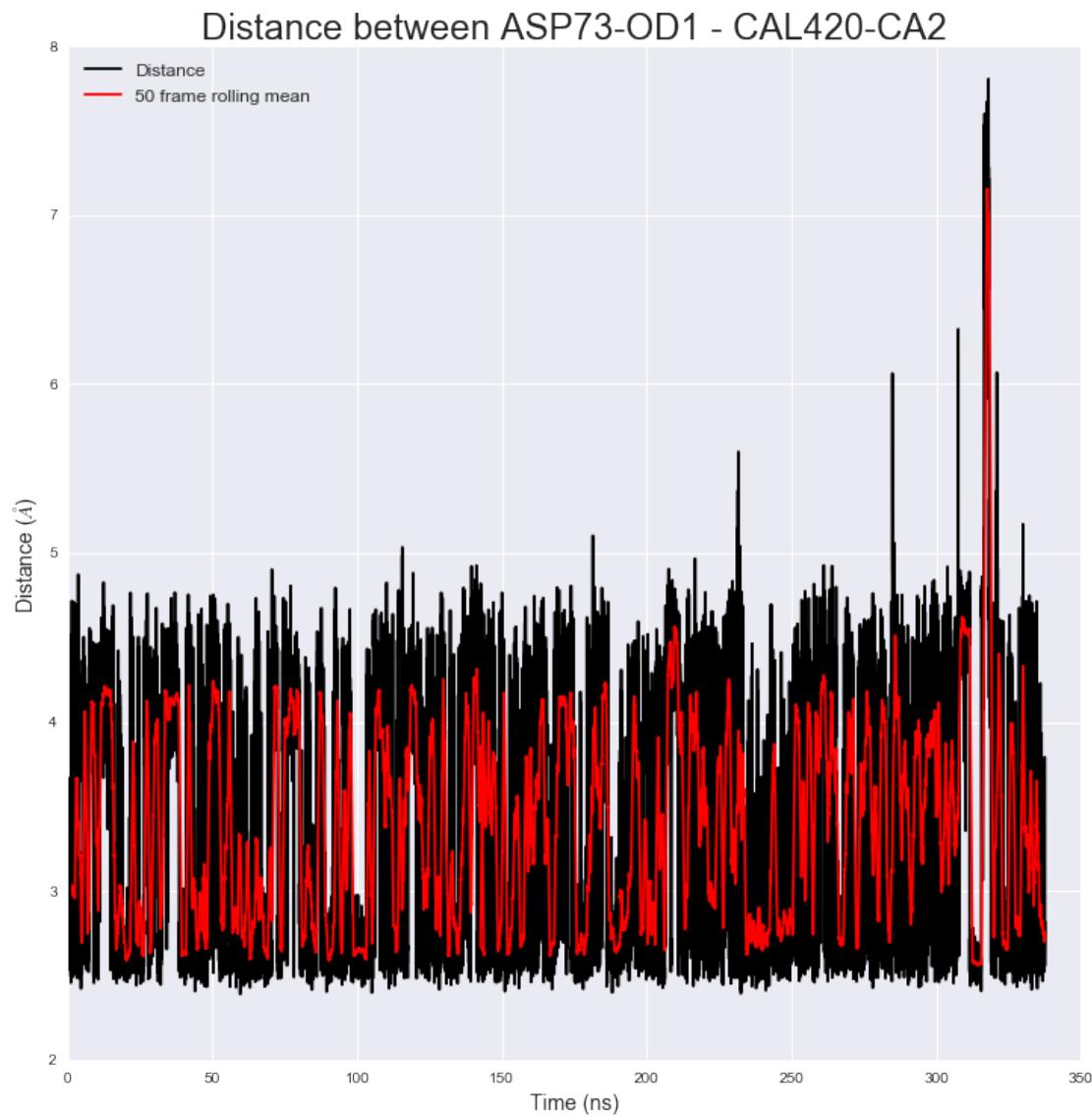
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

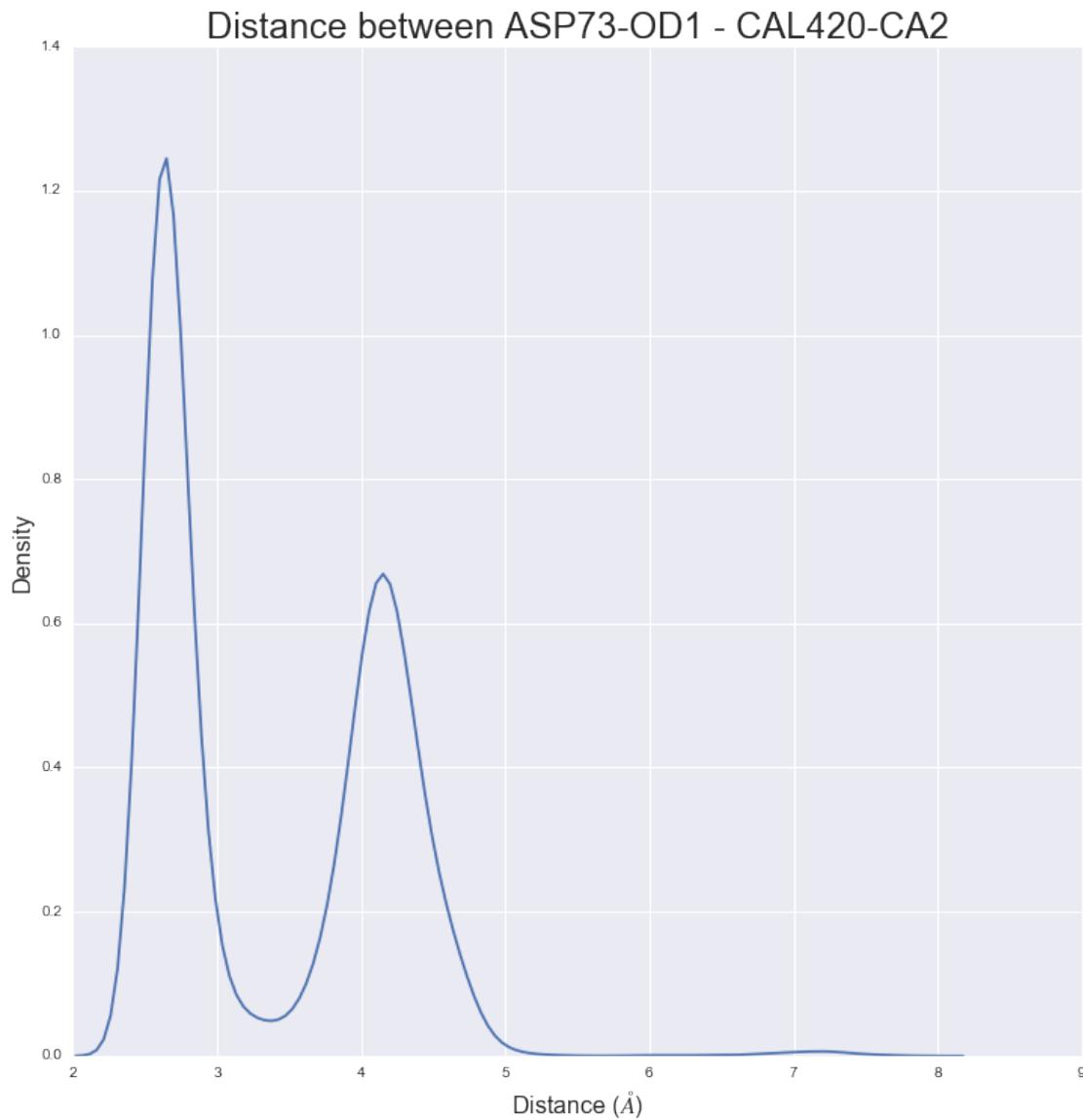
Calculating distance between following atoms: ASP73-OD1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD5_000-050_run2_nowater.nc
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05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 2.97 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

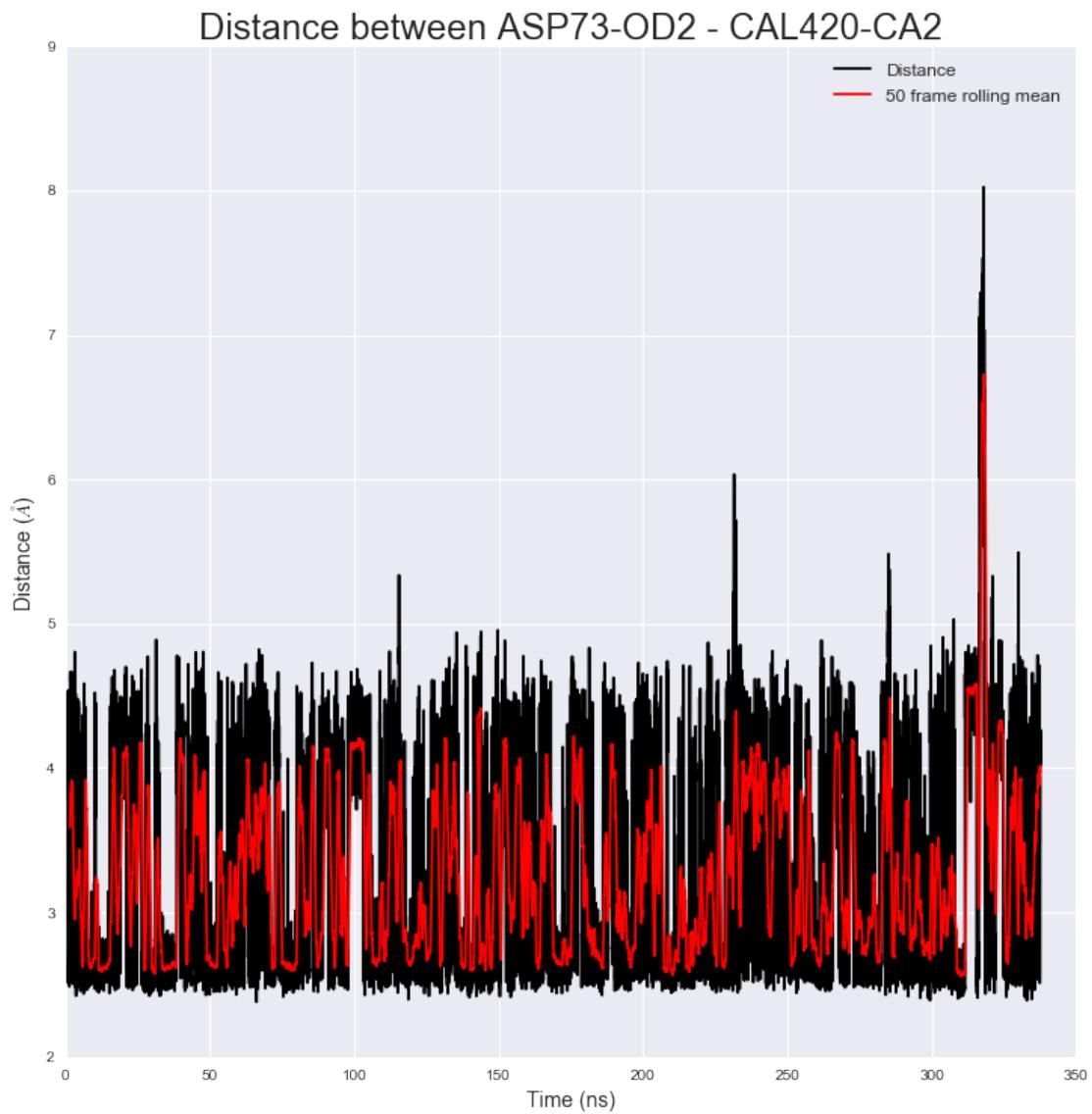
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

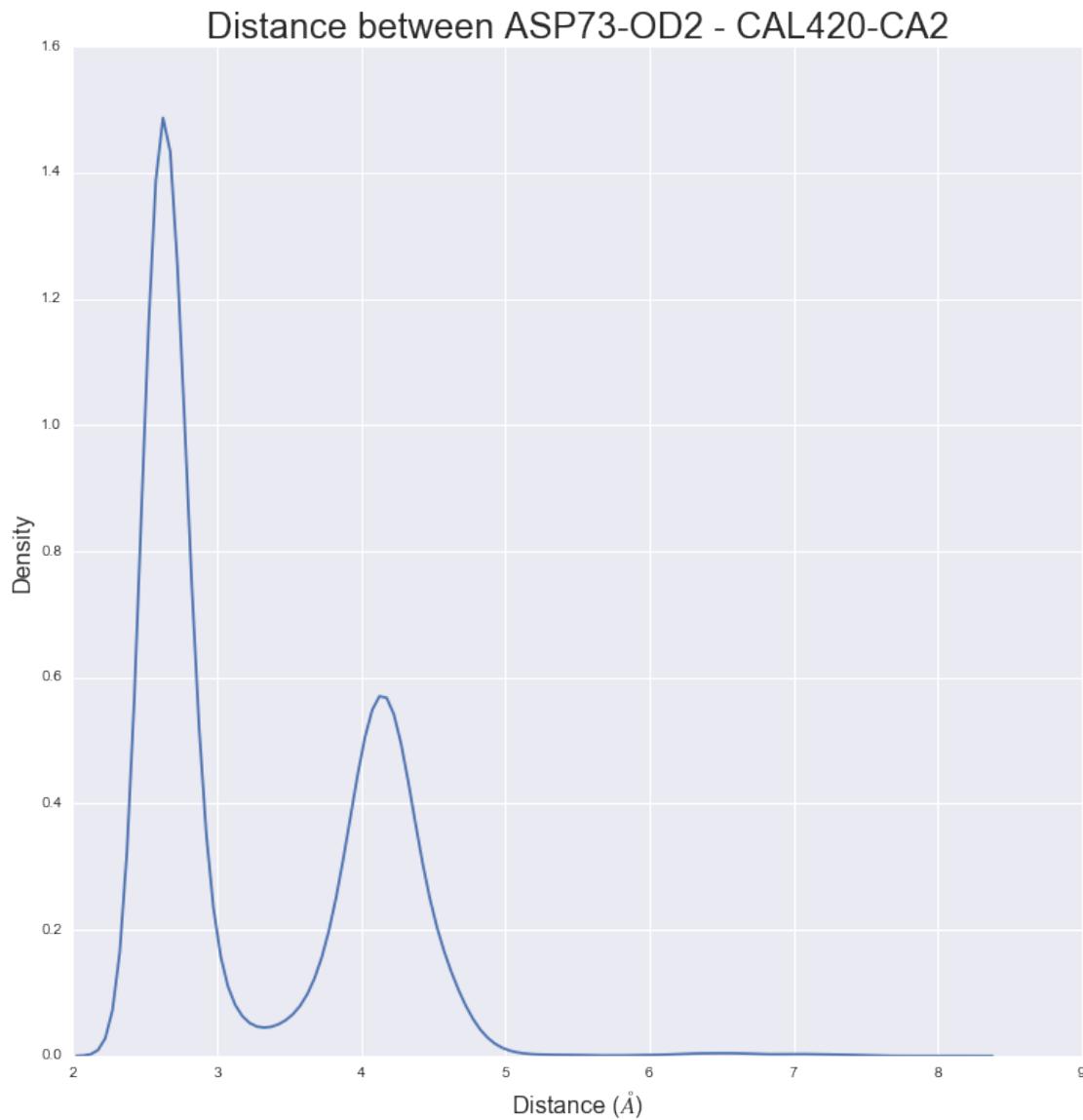
Calculating distance between following atoms: ASP73-OD2 - CAL420-CA2

Loading trajectories from the following files:

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 05_Prod_tropomin_egcg_MD5_100-150_run2_nowater.nc
 05_Prod_tropomin_egcg_MD5_150-200_run2_nowater.nc
 05_Prod_tropomin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.04 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

Calculating distance between following atoms: ASP75-OD1 - CAL420-CA2

Loading trajectories from the following files:

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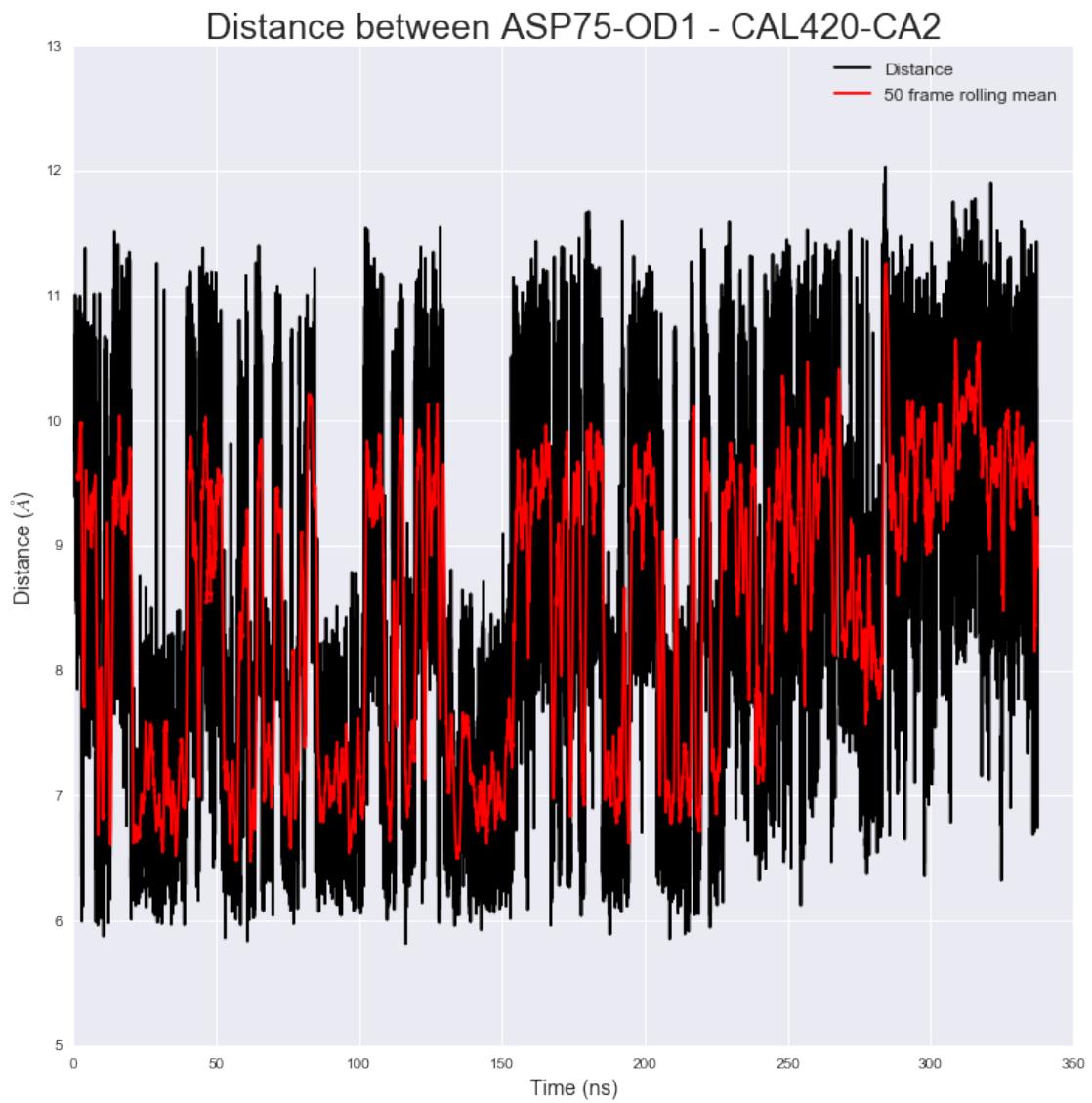
05_Prod_tropomin_egcg_MD5_050-100_run2_nowater.nc

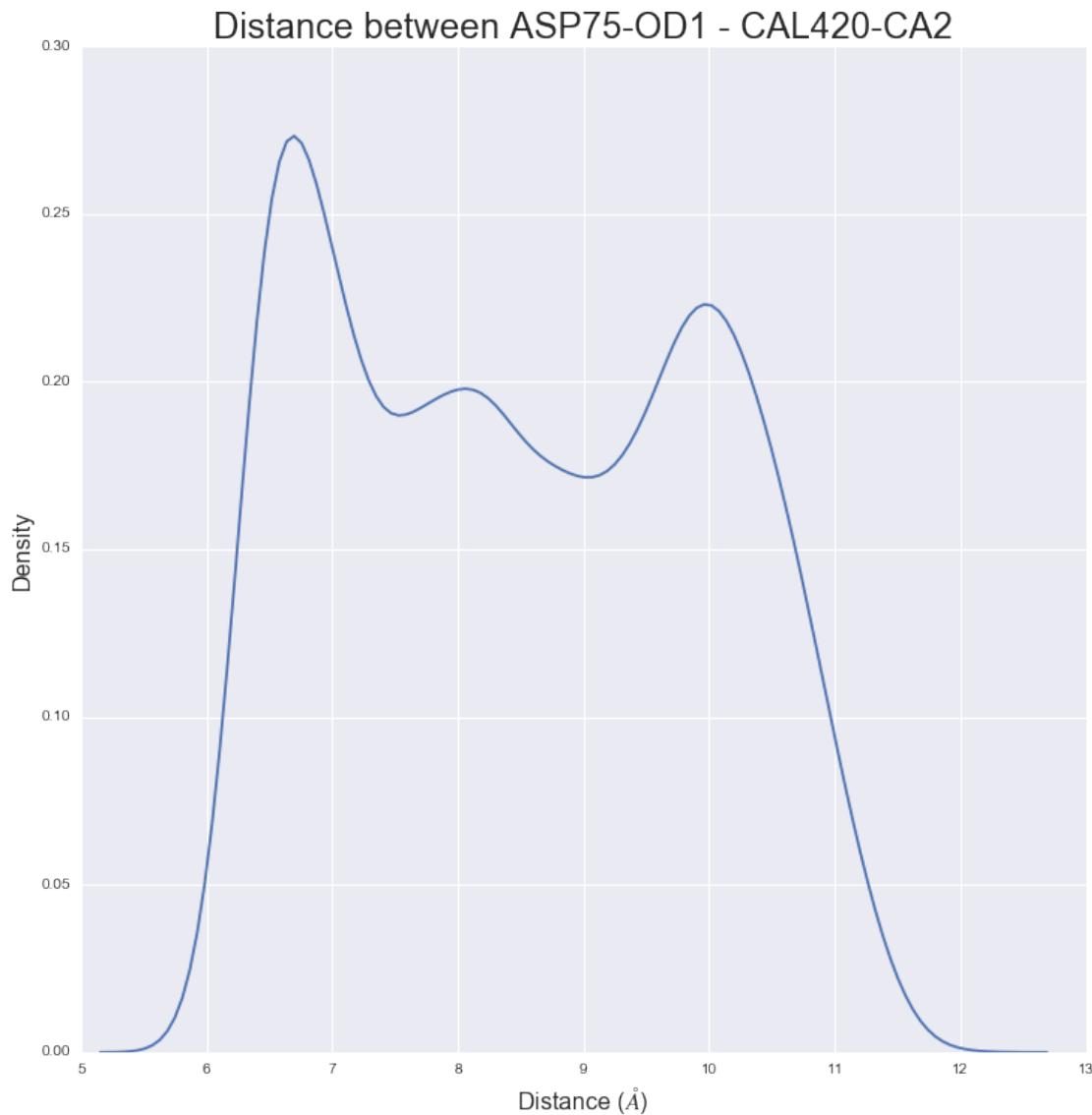
05_Prod_tropomin_egcg_MD5_100-150_run2_nowater.nc

05_Prod_tropomin_egcg_MD5_150-200_run2_nowater.nc

05_Prod_tropomin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.18 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

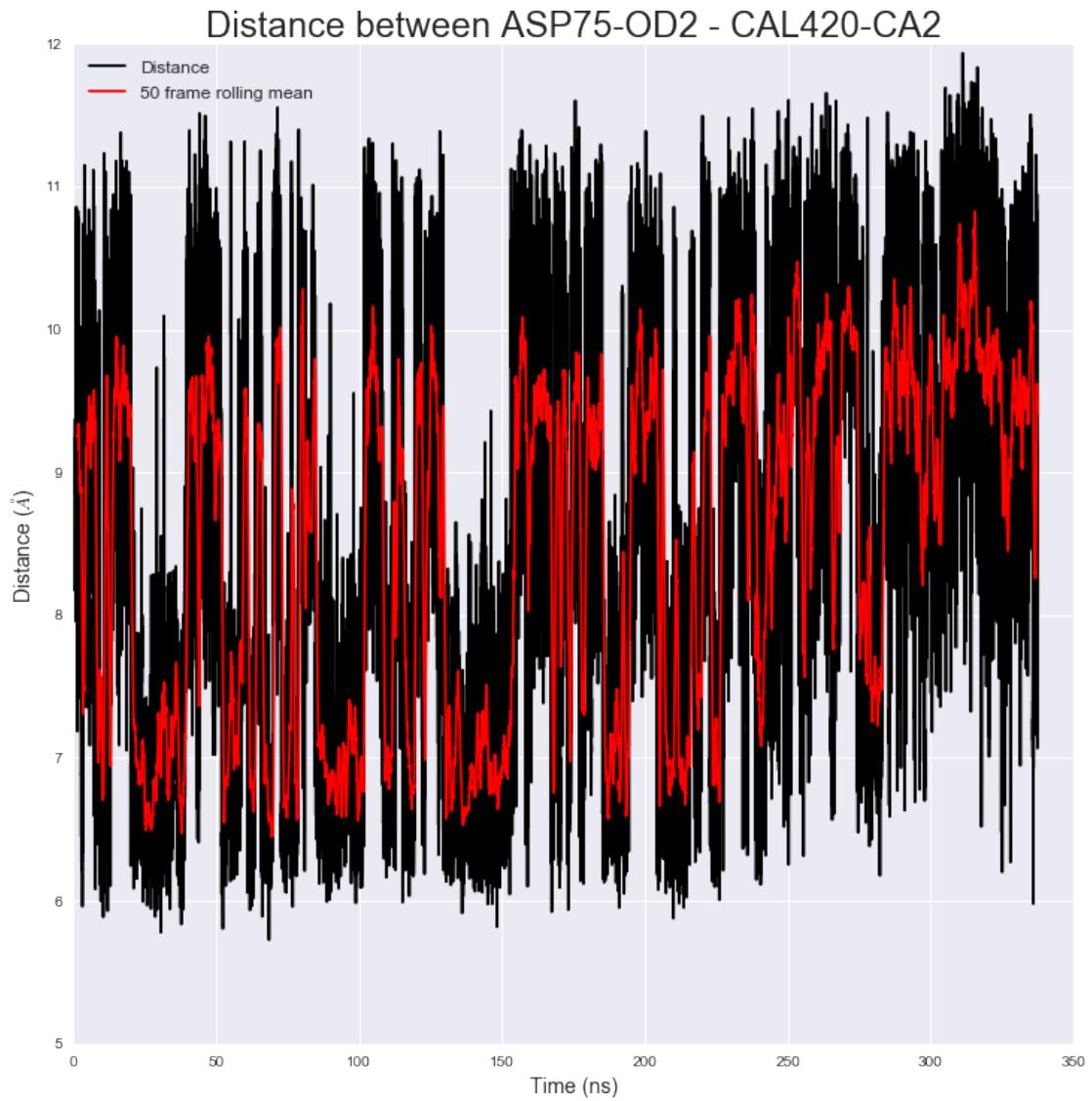
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

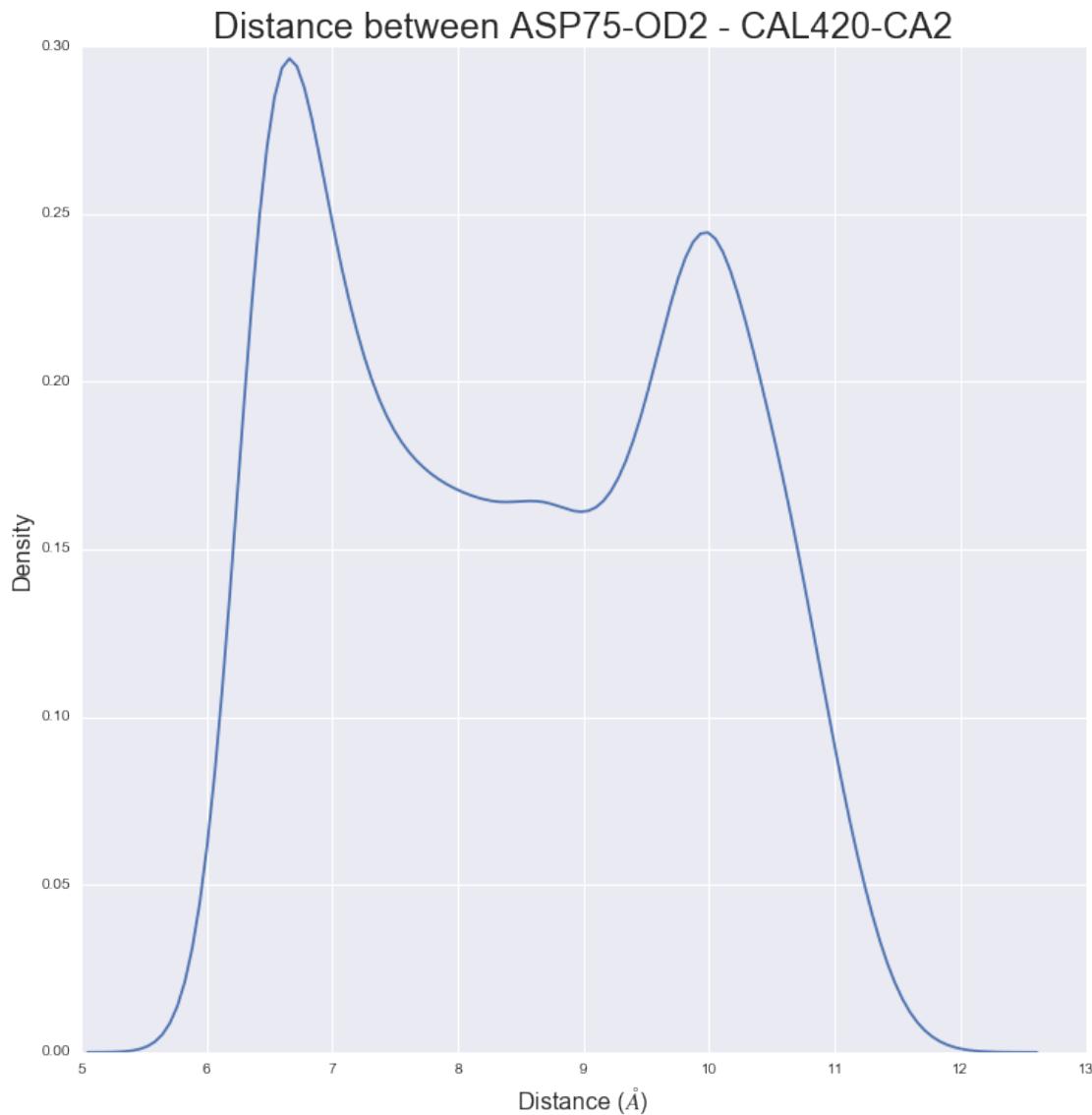
Calculating distance between following atoms: ASP75-OD2 - CAL420-CA2

Loading trajectories from the following files:

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 05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
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 05_Prod_troponin_egcg_MD5_150-200_run2_nowater.nc
 05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.18 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

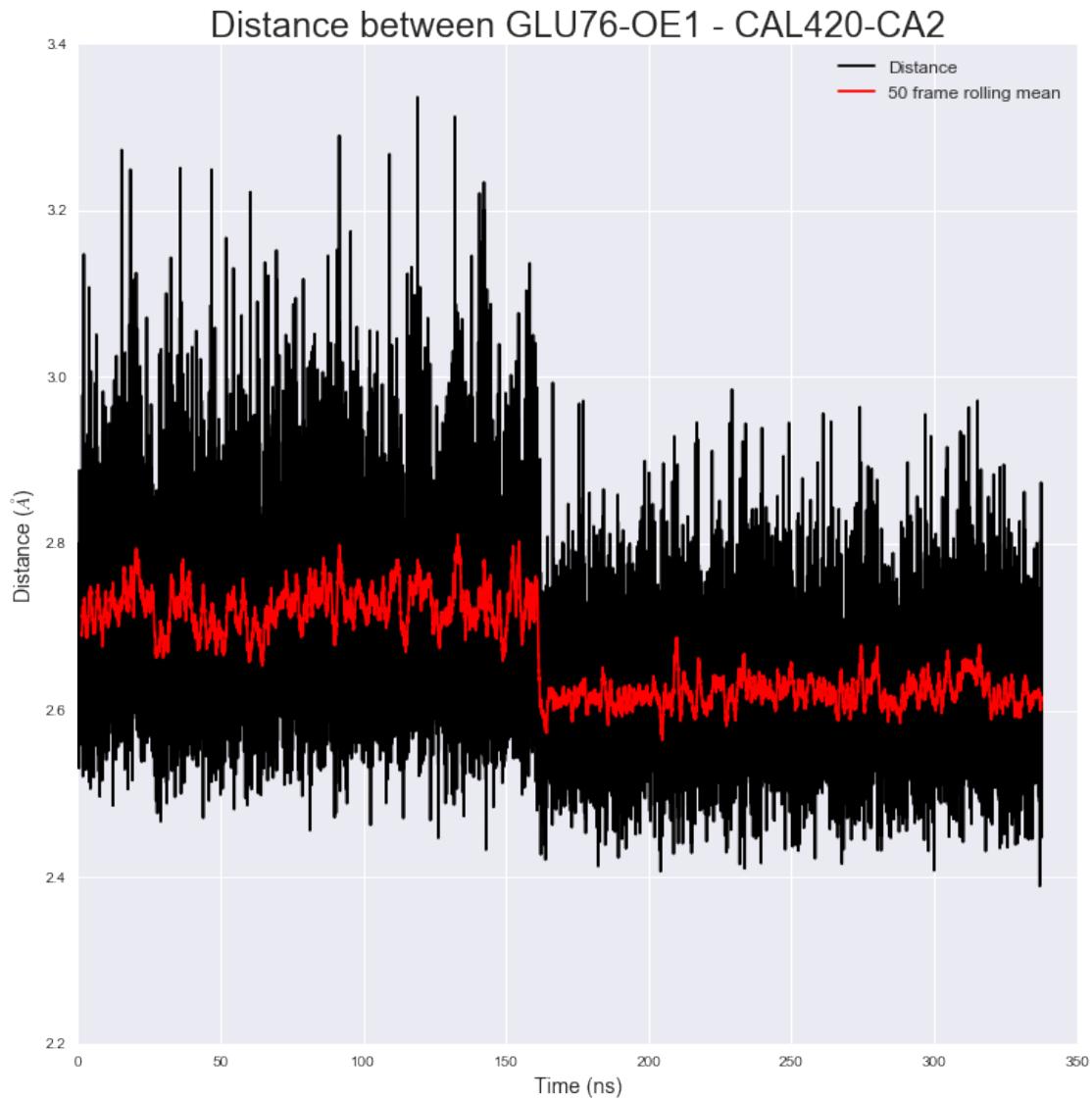
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

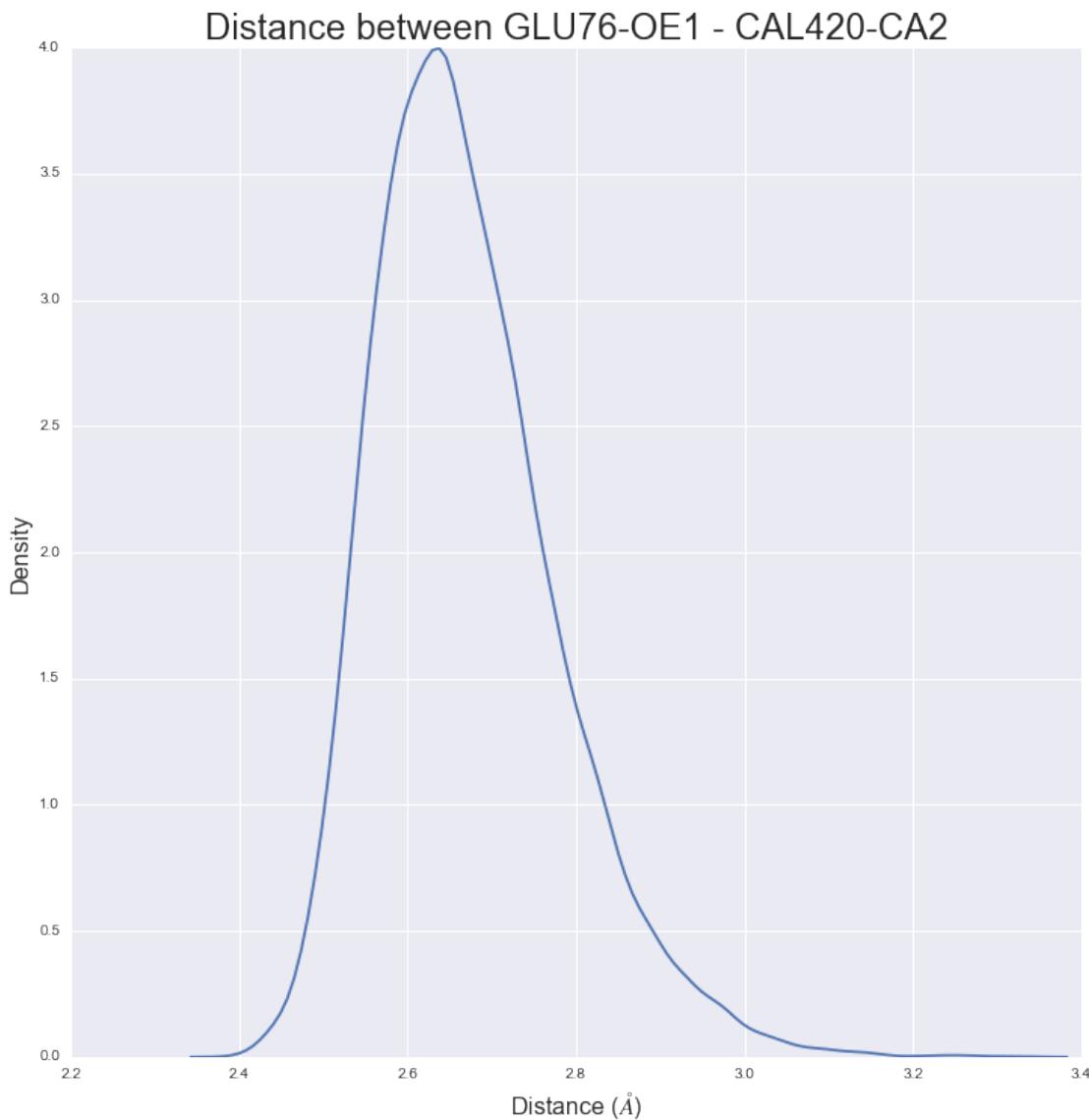
Calculating distance between following atoms: GLU76-OE1 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD5_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD5_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD5_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 3.04 seconds

Total simulation time of all frames: 337.02 nanoseconds

The following topology file was successfully loaded:

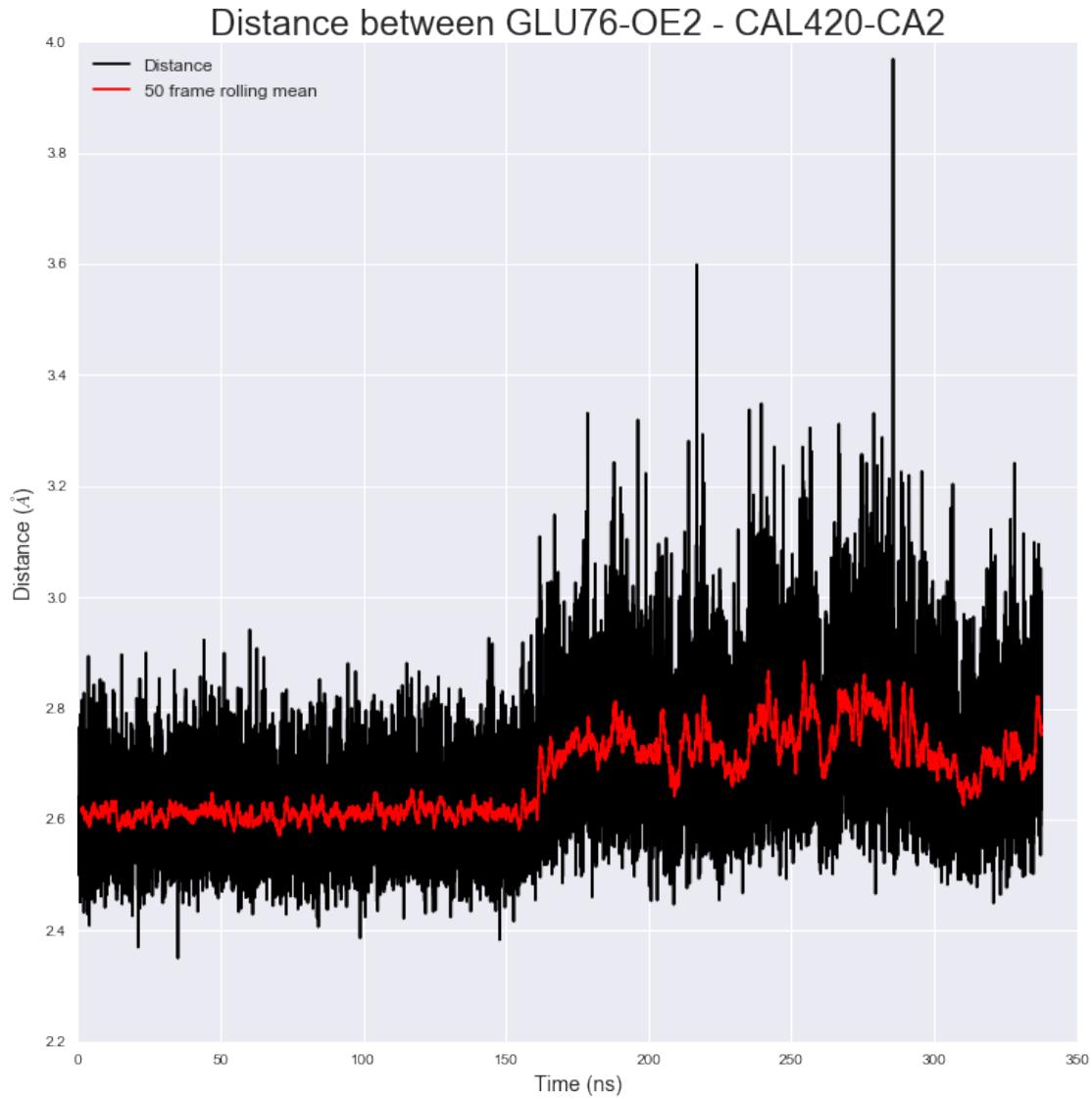
<mdtraj.Topology with 1 chains, 960 residues, 7400 atoms, 6898 bonds>

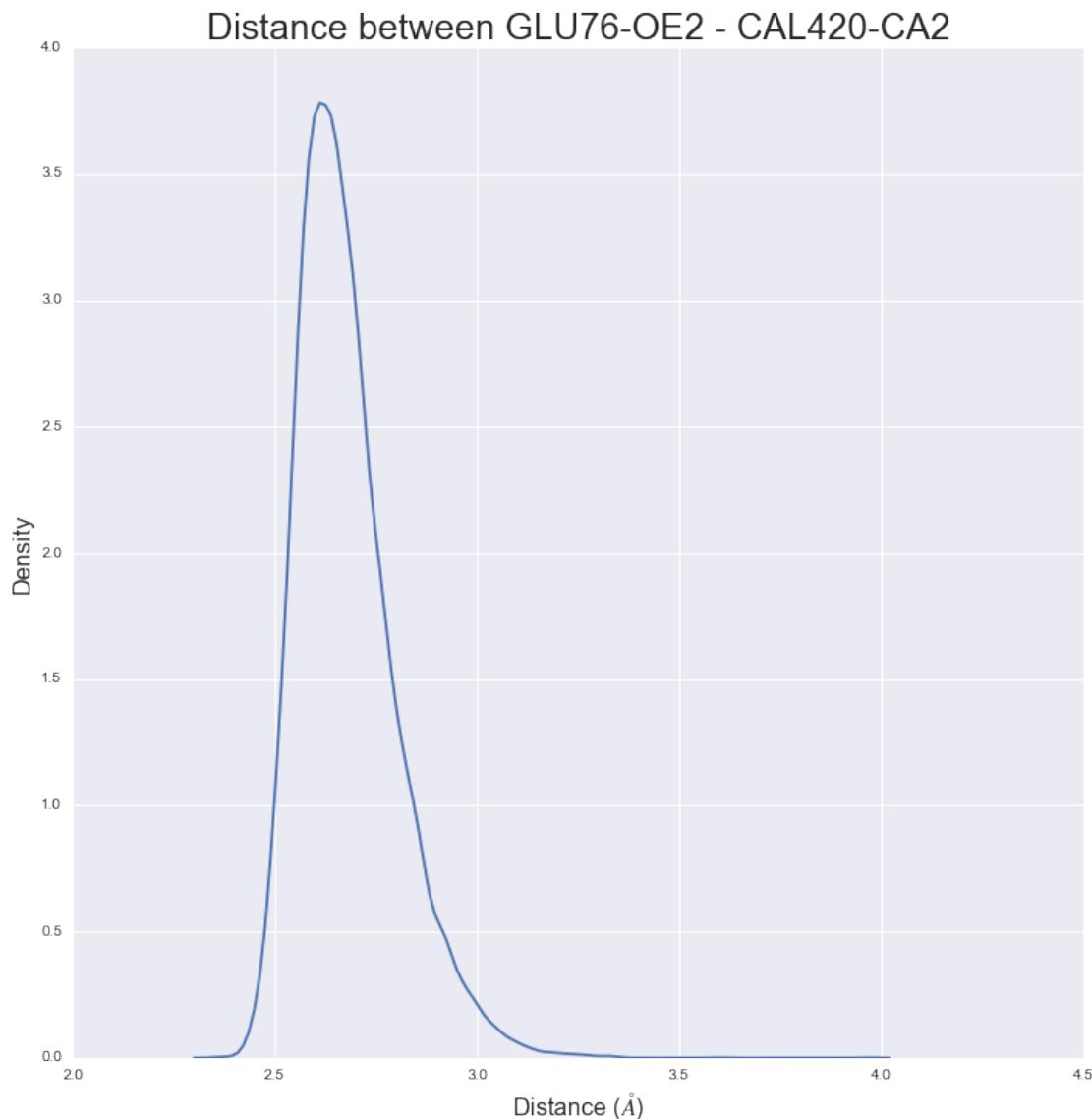
Calculating distance between following atoms: GLU76-OE2 - CAL420-CA2

Loading trajectories from the following files:

05_Prod_troponin_egcg_MD5_000-050_run2_nowater.nc
05_Prod_troponin_egcg_MD5_050-100_run2_nowater.nc
05_Prod_troponin_egcg_MD5_100-150_run2_nowater.nc
05_Prod_troponin_egcg_MD5_150-200_run2_nowater.nc
05_Prod_troponin_egcg_MD5_200-250_run2_nowater.nc

05_Prod_troponin_egcg_MD5_250-300_run2_nowater.nc
05_Prod_troponin_egcg_MD5_300-350_run2_nowater.nc





Total execution time: 2.93 seconds

Total simulation time of all frames: 337.02 nanoseconds

In []:

In []: