In [1]:
```
pip install mdtraj
```

```
Defaulting to user installation because normal site-packages is not w
riteable
Requirement already satisfied: mdtraj in /home/ac7407/.local/lib/pyth
on3.8/site-packages (1.9.7)
Requirement already satisfied: numpy>=1.6 in /share/apps/python/3.8.6
/intel/lib/python3.8/site-packages/numpy-1.19.2-py3.8-linux-x86_64.eg
g (from mdtraj) (1.19.2)
Requirement already satisfied: pyparsing in /share/apps/python/3.8.6/
intel/lib/python3.8/site-packages (from mdtraj) (2.4.7)
Requirement already satisfied: astunparse in /home/ac7407/.local/lib/
python3.8/site-packages (from mdtraj) (1.6.3)
Requirement already satisfied: scipy in /share/apps/python/3.8.6/inte
l/lib/python3.8/site-packages/scipy-1.5.2-py3.8-linux-x86_64.egg (fro
m mdtraj) (1.5.2)
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)
Requirement already satisfied: wheel<1.0,>=0.23.0 in /share/apps/pyth
on/3.8.6/intel/lib/python3.8/site-packages (from astunparse->mdtraj)
(0.35.1)
WARNING: You are using pip version 20.2.3; however, version 22.2.2 is
available.
You should consider upgrading via the '/share/apps/python/3.8.6/intel
/bin/python -m pip install --upgrade pip' command.
Note: you may need to restart the kernel to use updated packages.
```

In [4]:
```
# import mdtraj as md
import mdtraj as md
import mdtraj.testing

# open .pdb file and load into mdtraj
pdb = md.load_pdb('1UBQ_processed.pdb')

# read structure of ubiquitin
print(pdb)

# print total number of hydrogen bonds
hbonds = md.baker_hubbard(pdb, periodic=False)
label = lambda hbond : '%s -- %s' % (pdb.topology.atom(hbond[0]), pdb.
counter = 0
for hbond in hbonds:
    counter = counter + 1

print('Total number of hydrogen bonds: ', counter)

# compute the number of residues (helical amino acids) in ubiquitin
# find secondary structure of ubiquitin
ss = md.compute_dssp(pdb)

# count number of helical amino acid in secondary structure
helix = 0
for i in range(len(ss[0])):
    if ss[0][i] == 'H':
        helix = helix + 1

# print number of helical amino acids
print('Number of helical amino acids: ', helix)
```

```
<mdtraj.Trajectory with 1 frames, 1405 atoms, 134 residues, and unitc
ells>
Total number of hydrogen bonds:  57
Number of helical amino acids:  18
```

In [ ]: