

DNA force field including e/z OL1 - chi OL4

Example on how to use the epsilon/zeta OL1 and chi OL4 modifications to run a DNA simulation.

The file with the modifications is available here: [DNA-99bsc0-ezOL1-chiOL4.tar.gz](https://wiki.chpc.utah.edu/download/attachments/539591372/DNA-99bsc0-ezOL1-chiOL4.tar.gz)

Step-by-step guide

1. Download the tar.gz file that has the actual force field modifications. In linux, you can just type:

```
wget https://wiki.chpc.utah.edu/download/attachments/539591372/DNA-99bsc0-ezOL1-chiOL4.tar.gz
```

2. After downloading, uncompress the file with:
`tar xvfz DNA-99bsc0-ezOL1-chiOL4.tar.gz`

3. Create a text file that will hold the tleap commands to generate the topology file and coordinate files formatted to run an AMBER simulation.

This is an example of the tleap file:

```
-----  
source leaprc.ff14SB  
  
addPath Param-99bsc0-ez1-ol4-for-DNA  
  
addAtomTypes {  
  { "C7" "C" "sp3" }  
  { "C1" "C" "sp2" }  
  { "C2" "C" "sp2" }  
}  
  
loadoff dna-chiOL4-ezOL1.lib  
ez = loadamberparams frcmod-ez1-bsc0.dat  
chi = loadamberparams frcmod.OL4.chi  
  
dna = loadpdb dna.pdb  
-----
```

This tleap file will load the most recent force field for proteins/DNA/RNA which is called ff14SB.

Then, it will set as a path the location of the modified files. In this case, it is just the name of the directory where we downloaded the file. Make sure you set the full path.

The addatomtypes is very important because the modifications requires new atom types so add the section precisely.

The loadoff command loads the library files of the nucleotides with the new atom types and then the command loadamberparams loads the individual modifications, one for the epsilon/zeta dihedral angle and another for a revised version of the chi torsion. In the above example, a PDB file called dna.pdb is loaded to check that the parameters are loaded and everything works correctly.

After this, it is ready, you can just load a PDB with a double stranded DNA and when you generate the AMBER topology and coordinate file, it will be including the e/z OL1 and chi OL4 modifications.

The tleap file can be run using:

```
tleap -s -f <file name>
```

Page:DNA force field including e/z OL1 - chi OL4

Page:CPPTRAJ one-liners