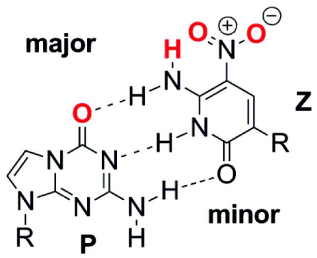
The following summarizes how to deal with non-natural nucleic acids to be analyzed via 3DNA. As an example, we will demonstrate this in terms of P and Z nucleic acids. The structures of these nucleic acids are available below.




It is important that your PDB structure have the proper atom naming. The atom naming convention must be the same in your PDB as is done for natural nucleic acids (see a standard biochemistry text for details). 3DNA interprets the atom labels as the beginning and end of the nucleic acid (i.e., the linkage points between the nucleic acid and the sugar and the nucleic acid and the phosphate). As long as atom labels exist in the PDB that analogously match to the natural nucleic acids, 3DNA can recognize the helical properties. The C1 must connect to the sugar, for example.

The execution command for 3DNA is, for a PDB file named 1.pdb, is

find_pair 1.pdb stdout | analyze

It is important to note that the distinction between error messages vs. diagnostic messages. In running 3DNA, you may get messages such as

```
missing ' P  ' atom : residue name ' DC', chain A, number [   1 ]
```

These are diagnostic messages. In the process of identifying the non-natural nucleic acids, they may occur. It does not necessarily imply failure in analysis. If you have an output file produced (in 1.out, for the above example) that has the standard 3DNA output, it worked fine.